

THE UNIVERSITY OF CHICAGO

INSIDE THE LAB AND OUT: STUDIES TOWARD THE TOTAL SYNTHESIS OF
STRAINED, STEREOCHEMICALLY-RICH POLYCYCLIC SKELETONS AND
ANALYSES OF SYSTEMS FOR THE LEARNING AND DOING OF CHEMISTRY

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Abbreviations

Ac	acetate
ACS	American Chemical Society
ANOVA	Analysis of Variance
aq	aqueous
AR	augmented reality
atmo	atmosphere
BDSB	$\text{Et}_2\text{SBr}\cdot\text{SbCl}_5\text{Br}$
Bn	benzyl
Boc	<i>tert</i> -butoxycarbonyl
BOM	benzyloxymethyl acetal
Box's M	Box's M Test of Equality of Covariance Matrices
br	broad
BSL 3 / BSL 4	Biosafety Level 3 / Biosafety Level 4
Bz	benzoyl
cat	catalytic
CBS	Corey-Bakshi-Shibata oxazaborolidine catalyst
CER	chemistry education research
CHAS	chemical health and safety
CHED	ACS Division of Chemical Education
CLASS	Colorado Learning Attitudes about Science Survey
Cp	cyclopentyl
CSA	camphorsulfonic acid
CURE	course-based undergraduate research experience
d	doublet
DBER	discipline-based education research
DCC	<i>N,N'</i> -dicyclohexylcarbodiimide

DMAP	4-dimethylaminopyridine
DMF	dimethylformamide
DMSO	dimethylsulfoxide
<i>dr</i>	diastereomeric ratio
EC₅₀	median effective concentration
EDC	1-ethyl-3-(3-dimethylaminopropyl)carbodiimide
EDTA	ethylenediaminetetraacetic acid
ee	enantiomeric excess
EFA	exploratory factor analysis
ELL	English Language Learner
eq / equiv	equivalents
ERL	emergency remote learning
ETP	Equipment, Technique, Procedure
F#	factor number (e.g., factor 1)
f2f	face-to-face
h	heptet
HBpin	pinacolborane
hex	hexanes
HLAB	Hybrid Laboratory Action-Based
HOBt	hydroxybenzotriazole
IBX	2-iodoxybenzoic acid
IRB	Institutional Review Board
JCE	Journal of Chemical Education
KI	key informant
KMO	Kaiser-Meyer-Olkin's Measure of Sampling Adequacy
LAB	Laboratory Action-Based
LAH	lithium aluminum hydride
LD₅₀	median lethal dose

LDA	lithium diisopropylamide
LiHMDS	lithium bis(trimethylsilyl)amide
LMX7 / LMX	Leader-Member Exchange scale
m	multiplet
M.S.	molecular sieves
MA	Meaningful Action
MANOVA	Multivariate Analysis of the Variance
<i>m</i>-CPBA	<i>meta</i> -chloroperoxybenzoic acid
MLLI	Meaningful Learning in the Laboratory Instrument
NaHMDS	sodium bis(trimethylsilyl)amide
NBS	<i>N</i> -bromosuccinimide
NGLS	Next-Generation Laboratory Standard
NMM	<i>N</i> -methylmorpholine
NMR	Nuclear Magnetic Spectroscopy
NOESY	Nuclear Overhauser Effect Spectroscopy
p	pentet
PCC	pyridinium chlorochromate
pent	pentanes
PI	Principal Investigator
PIDA	(diacetoxyiodo)benzene
PMB	<i>para</i> -methoxybenzyl
P-P	Predicted-Probability plot
PPE	Personal Protective Equipment
PrIMAS	Prioritization in Mentorship Attributes Survey
PUI	Primarily Undergraduate Institution
q	quartet
Q&A	Question & Answer session
Q-Q	Quartile-Quartile plots

quant	quantitative (i.e., 100 %)
R1	Doctoral University - Very High Research Activity
R2	Doctoral University - High Research Activity
rt	room temperature
RCT	randomized control trial
s	singlet
sat	saturated
SL	sesquiterpenoid lactone
SP	safety professional
std dev	standard deviation
sx	sextet
t	triplet
TA	teaching assistant
TBAI	tetrabutylammonium iodide
TBCO	2,4,4,6-tetrabromocyclohexa-2,5-dienone
TBDPS	<i>tert</i> -butyldiphenylsilyl
TBS / TBDMS	<i>tert</i> -butyldimethylsilyl
TEMPO	2,2,6,6-tetramethylpiperidine oxide
Tf	triflate
TFA	trifluoroacetic acid
THF	tetrahydrofuran
TIPS	triisopropylsilyl
TLC	thin-layer chromatography
TMDSO	tetramethyldisiloxane
TMS	trimethylsilyl
tol	toluene
VIF	variance inflation factors
VR	virtual reality

ZPD

Zone of Proximal Development

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Preface

As the central science, chemistry boasts numerous cross-cutting connections with other fields and high-profile everyday applications. One such connection is discipline-based education research (DBER) which combines rigorously developed methodologies from multiple fields (e.g., psychology, statistics) to provide evidence-based recommendations for improving STEM outcomes at all grain sizes, ranging from national governmental policies to individual classroom teaching tactics. When practiced in chemistry, DBER is referred to as chemistry education research (CER). CER aims to support the teaching, learning, and doing of chemistry for chemistry students, teachers, supporting institutions, and professional chemists. Chemistry research, the “doing” of chemistry, and the “teaching and learning” of chemistry are intimately linked (**Figure 0.1**). Whereas CER is sometimes pursued separately from traditional chemistry research, this dissertation presents side-by-side research into synthetic organic chemistry and CER via 4 discreet arenas, lending contextual strength to a system-oriented investigation of the chemistry education ecology.

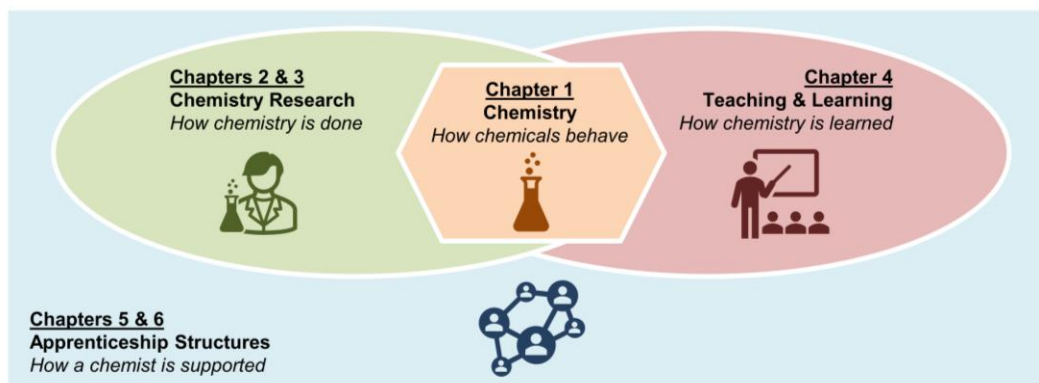


Figure 0.1. This dissertation investigates synthetic organic chemistry and CER through 4 arenas.

In **Chapter 1**, natural product synthesis is pursued toward strained, stereochemically-rich polycyclic skeletons in the dankasterone and illisimonin families. Key motifs targeted include contiguous 4° stereocenters and multiple *trans*-cyclopentaid units within a strained polycyclic core. High yields and diastereoselectivity are accomplished in the ultimate convergent strategy toward dankasterones A and B. Meanwhile, methodological efforts are described toward both the common 2,6-disubstituted piperidine motif via a Mannich-type reaction and the enormous organobromine family via bromonium-induced cyclization.

The described efforts seek to expand the available options for access to synthetically desirable bioactive motifs.

Zooming out from **Chapter 1**'s focus on the outcome of individual chemical reactions, **Chapters 2 – 3** characterize the environment in which this chemistry occurs, revealing commonalities and challenges associated with the oft-obscured details of conducting successful benchwork. In **Chapter 2**, the chemistry research environment itself is examined, first through phenomenological observational case studies characterizing the nature of benchwork followed by psychometric measurement of chemistry safety behavior in **Chapter 3**. These qualitative and quantitative methodologies respectively provide novel benchmarks for the chemistry community in understanding how chemistry research itself is conducted. Such detailed portraits then enable evidence-based discussions on how to more efficiently and effectively support successful chemistry research.

In **Chapter 4**, the process of learning how to do bench chemistry is explored through an exhaustive scoping literature review on lab-based learning during the COVID-19 pandemic. When considered in conjunction with the findings from the preceding chapters, the review exposes areas of misalignment regarding current paradigms for lab-based learning versus the intellectual and physical demands of the chemistry research environment. Taken together, these chapters reveal the complexity of lab-based learning and prompt re-consideration of a one-size-fits-all modality of laboratory instruction.

Finally, **Chapters 5 – 6** address the network nature of chemistry research, the doing of chemistry, and the teaching and learning of chemistry by analyzing the apprenticeship backdrop of laboratory research training. A survey instrument is constructed and validated to evaluate the core tenants of chemistry research mentorship across trainee levels (i.e., undergraduate students → postdoctoral researchers) in **Chapter 5**. Meanwhile, departmental structures for supporting continuing professional development via seminars are subjected to comparative value-added analysis in **Chapter 6**. Considering that the current model of chemistry research training has remained mostly unchanged for over a century, evaluating the strengths and weaknesses of these training models may enable timely adjustments for the next generation of trainees.

Chapter 1

Studies Toward the Asymmetric Total Syntheses of Dankasterone A and B, Illisimonin A, Obtusenol, and Substituted Piperidines

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Collaborators: Scott A. Snyder (PI), Vladislav Lisnyak (project lead), Tessa Lynch-Colameta

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1.1 Abstract

Natural product total synthesis has an illustrious history of contributing to the advancement of science and society, such as by unlocking useful molecular scaffolds and inspiring the development of purpose-built methodologies (**Figure 1.1**). In that vein, the following report details synthetic studies my collaborators and I engaged in to (a) access natural product families with challenging bioactive scaffolds and (b) develop methodologies for asymmetric transformations of common structural motifs. The report begins with a discussion of our successful synthesis of dankasterone and follows with brief descriptions of additional endeavors toward other motifs, which will hopefully enable access to interesting structures by future researchers.

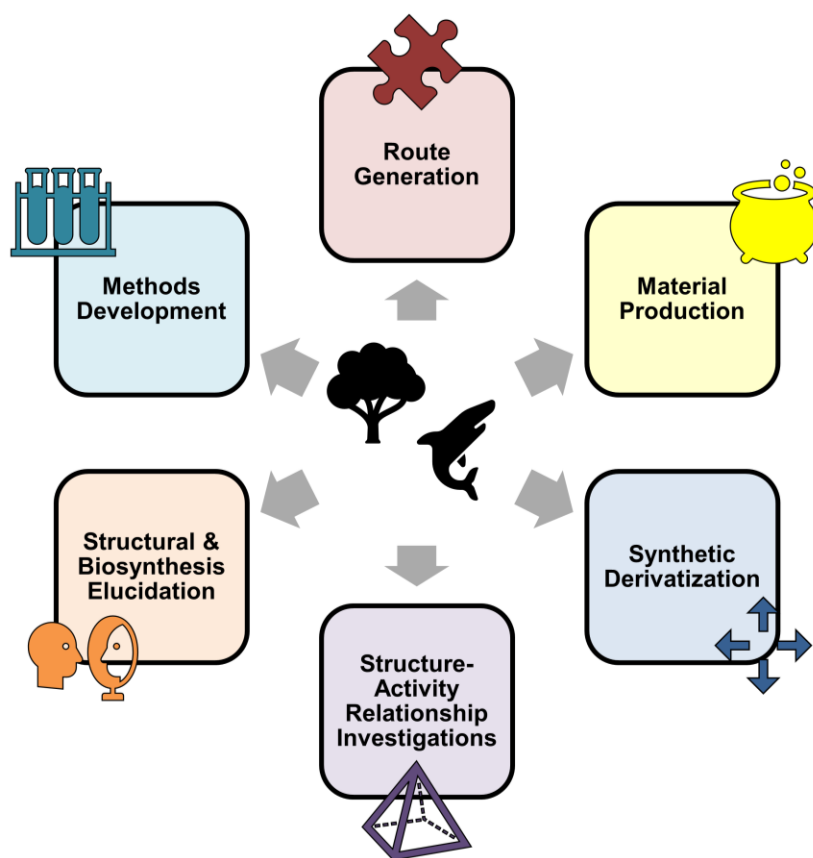


Figure 1.1. Natural product total synthesis offers multiple avenues for scientific advances.

1.2 Introduction

By pushing the limits of synthetic methods to pursue highly functionalized complex molecules (and thus discovering the unexpected *en route*), natural product total synthesis (i.e., the synthetic generation of a naturally occurring chemical within a laboratory) is the premier testing ground for developing new chemistry, accessing complex structures with broad societal implications, and confirming ambiguous structural assignments. Natural products and total synthesis have both been at the heart of the field of organic chemistry since its genesis, and recent reviews of these historied areas affirm their centrality to the advancement of science and society.^{1,2} Key foci for researchers in recent years include (1) the improvement of step-wise efficiency and synthetic discrimination by discovering increasingly selective transformations, (2) the attainment of progressively more complex bioactive polycyclic scaffolds of therapeutic interest, and (3) the improvement in synthetic efficiency overall by identifying routes which broadly unlock entire families, rather than delivering individual members through separate specialized routes.^{1,2}

In consideration of those key foci, the following report details synthetic studies I engaged in across multiple teams to (a) unlock natural product families with challenging bioactive scaffolds and (b) develop methodologies for asymmetric transformations of common structural motifs. The report begins with a discussion of our successful entrance into the dankasterone natural product family and then follows with brief descriptions of additional projects which attempted to access the illisimonin natural product scaffold as well as expand bromonium-induced cyclization methods and nitron-based Mannich-type methods in pursuit of 2,6-disubstituted piperidines (**Figure 1.2**). These synthetic studies and methodological investigations will hopefully enable more expedient, flexible access to synthetically and biologically important substances.

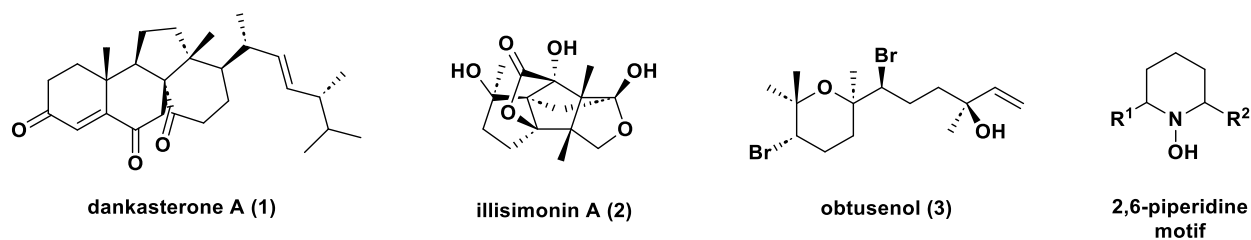
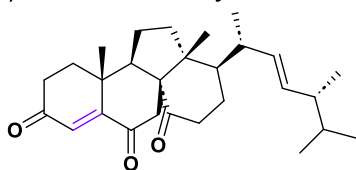


Figure 1.2. Synthetic efforts were made toward multiple complex natural product families and methodologies for common motifs.

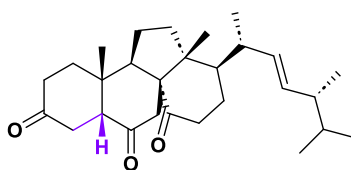
1.3 Dankasterone A and B

Dankasterone A (**1**) was first isolated in 1999 from the *Gimnascella dankaliensis* fungus on the marine sponge *Halichondria japonica* (**Figure 1.3**).³ Isolation of dankasterone B (**4**) followed in 2007.⁴ Both steroids display potent activity in murine cancer models and differ structurally from each other by only a single point of unsaturation. Moreover, the 13(14→8)*abeo* skeleton displayed by the dankasterone family presents an attractive target synthetically due to its multiple challenging structural motifs, most notably a dodecahydrobenzoindene core featuring a *trans*-1,3 substitution pattern and contiguous stereochemistry. Of the 7 stereocenters, 6 are directly adjoined and penetrate the heart of the dodecahydrobenzoindene core, encompassing the *trans*-1,3 pattern at the center. Notably, 3 of the stereocenters are 4°; such crowded motifs have previously been highlighted as especially difficult to install.^{5,6} With an increasing number of bioactive natural products being isolated with similar 13(14→8)*abeo* cores (such as abeohyousterone, **7**, and periconiastone A, **8**),^{7,8} we attempted to unlock access to this challenging shared core by pursuing a total synthesis of dankasterone A (**1**).

(a) Dankasterone family



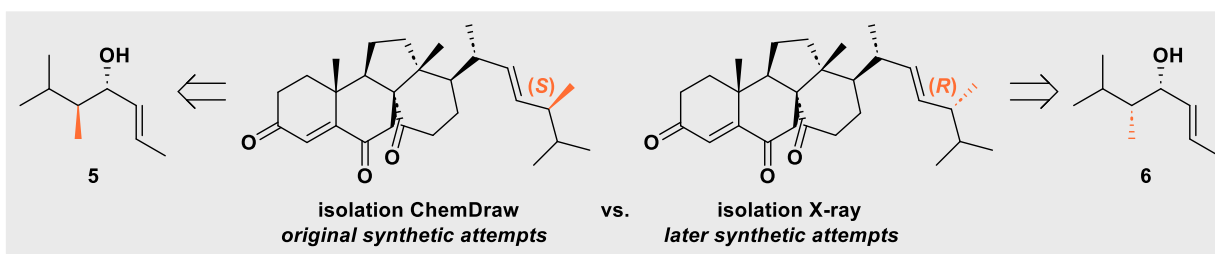
dankasterone A (1)
 $EC_{50} = 2.2 \mu\text{g/mL}$ (murine cancer)



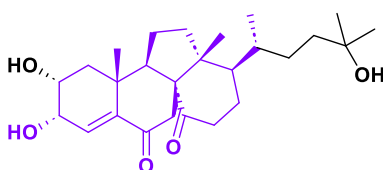
dankasterone B (4)
 $EC_{50} = 2.8 \mu\text{g/mL}$ (murine cancer)



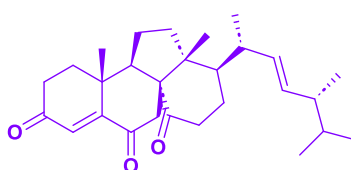
Halichondria japonica



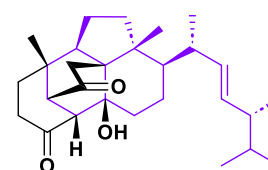
(b) Similarities between dankasterones and other natural products



abeohysterone (7)

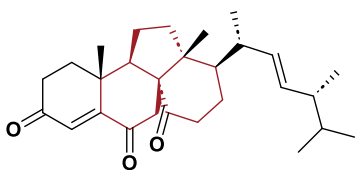


dankasterone A (1)

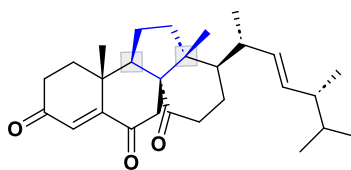


periconiastone A (8)

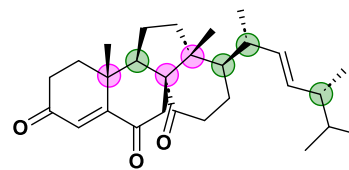
(c) Challenging features of the dankasterone skeleton



dodecahydrobenzoindene core



trans-1,3



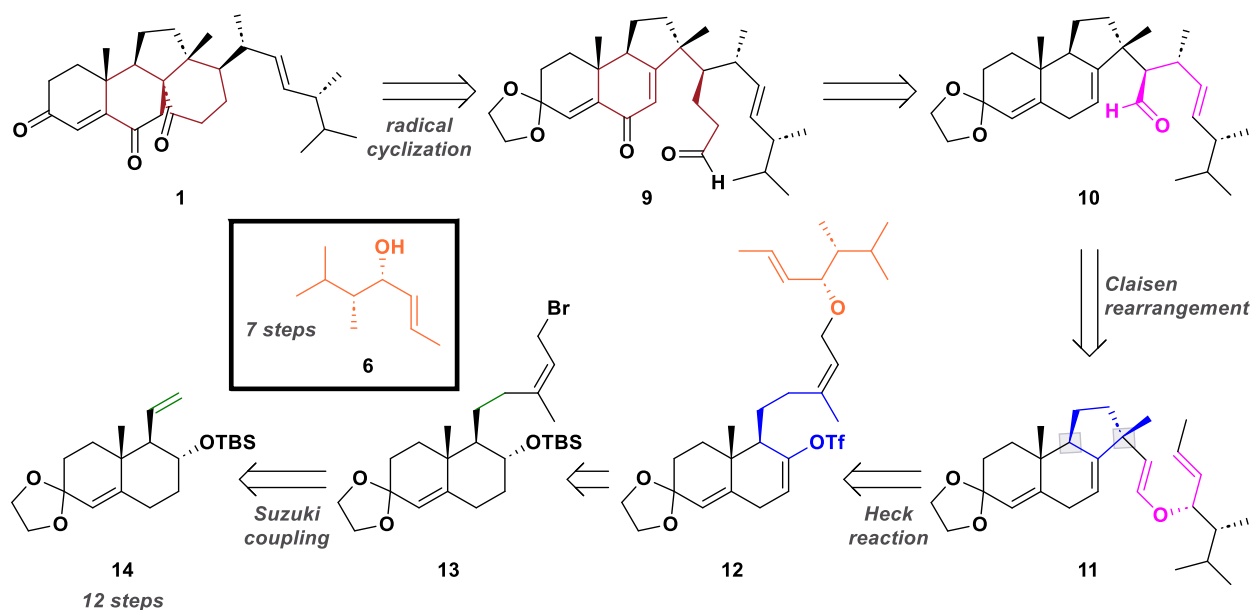
three 4° stereocenters
four 3° stereocenters

Figure 1.3. Dankasterone A (1) and B (4) share multiple challenging structural motifs.

Note: Surprisingly, it was discovered after beginning our synthetic efforts that the isolation structure incorrectly represented the relative configuration of one stereocenter. Whereas the isolation team's X-ray indicated *R* chirality on the hexenyl side chain, their publication assigned the stereocenter as *S*. Fortunately, our synthetic pathway was robust to this revelation due to its convergent nature, and we were able to quickly produce large-scale material in the appropriate configuration. In this chapter, the corrected assignment is displayed in all dankasterone structures for clarity.

1.4 Dankasterone A Retrosynthesis

The retrosynthesis hinged on accessing the dodecahydrobenzoindene core via 6-*exo-trig* radical cyclization with the other stereochemical constituents pre-installed in **9** (Scheme 1.1). We envisioned attaining this cyclization after using a thermal Claisen rearrangement on **11** to prepare the sidechain configuration from **10** onward and relying on the fixed pentanoid's *trans* pattern to force a bottom-face attack during radical cyclization of **9**. That pentanoid could be established beforehand using a diastereoselective intramolecular Heck reaction with **12**.⁹ With our stereochemical preferences depending on the known reliability of the Claisen rearrangement and Heck reaction, our main foci at the beginning of the project were therefore to construct the Heck precursor **12** via a Suzuki coupling and to test model compounds to affirm the feasibility of the later-stage reactions.

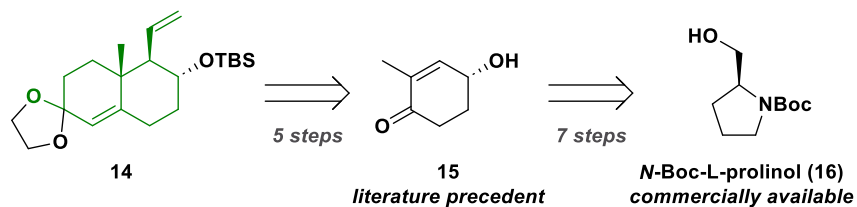


Scheme 1.1. Original retrosynthetic analysis of dankasterone A (**1**).

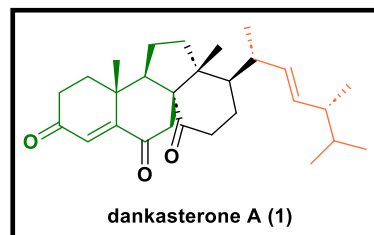
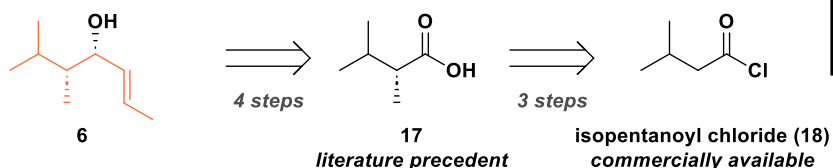
Fortunately, step efficiency on the way to Heck precursor **12** was predicted to be achievable via a convergent strategy to build the bulk of the structure's mass. We would utilize a decalin motif for the left hand of the natural product and construct an alkenol for the right. After generating protected decalin **14** from known cyclohexenone **15** (Scheme 1.2a), previously described by Schultz and co-workers¹⁰, decalin **13** could then be joined with alkenol **6** following Suzuki coupling. The alkenol **6** would arise from known

carboxylic acid **17** (**Scheme 1.2b**), previously described by Klebe and co-workers¹¹, and then displace the halogen in **13** to produce **12** in advance of the intramolecular Heck reaction.

(a) Retrosynthetic analysis for decalin fragment



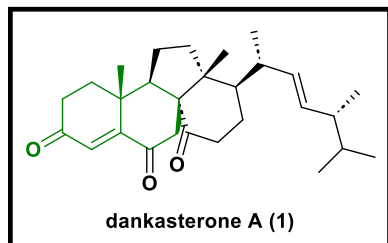
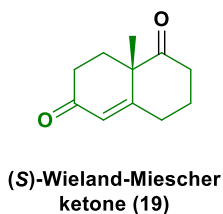
(b) Retrosynthetic analysis for alkenol fragment



Scheme 1.2. The convergent strategy joined together decalin and alkenol units.

This retrosynthetic analysis and initial synthetic forays were completed by my collaborator Jeremy Boilevin. My primary responsibility for this project, therefore, was to generate substantial quantities of precursors **6** and **14** (which were needed to test the later-stage transformations) while also exploring ways to improve yields and step counts for this first half of the synthesis. Additionally, earlier attempts by our team to access haloalkenyl **13** had revealed challenges surrounding the initial coupling stage. Surprising issues in handling the ketalization product **14**, an important step for long-term protection of dankasterone's leftmost ketone, also necessitated further innovation to sidestep a costly material cliff. I therefore engaged first in large-scale material campaigns and optimizations for **6** and **14** before investigating route-shortening options (e.g., starting from the Wieland-Miescher ketone, **19**) and probing conditions for improving retention of labile protecting groups (**Figure 1.4**).

(a) Possible lefthand alternative



(b) Remaining challenges for lefthand fragment

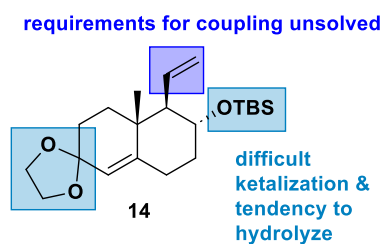
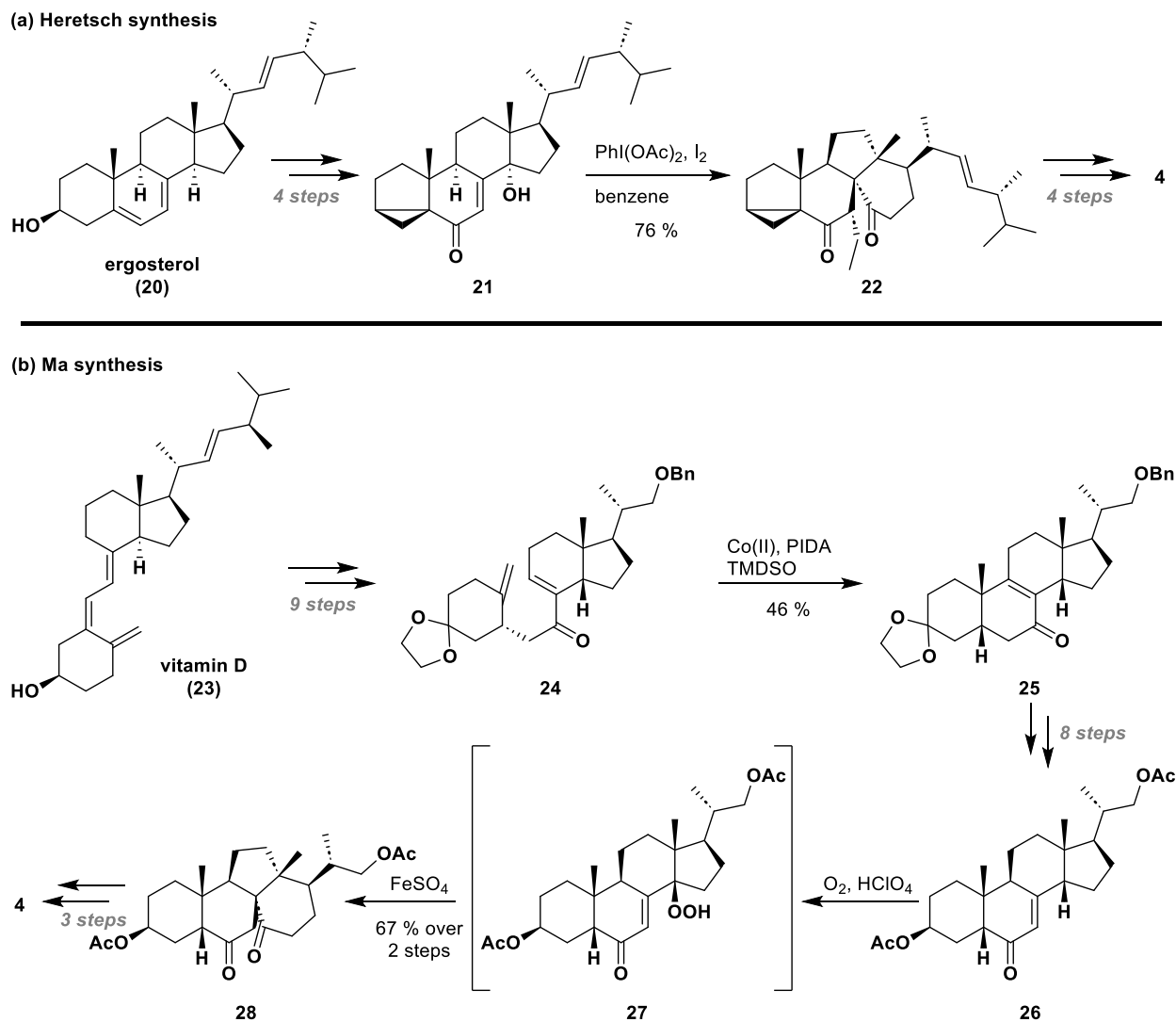


Figure 1.4. Challenges with the final steps before convergence would ultimately precipitate further route explorations.

1.5 Other Dankasterone Syntheses

At the genesis of our strategy toward **1**, no studies of either dankasterone A (**1**) or B (**4**) existed outside of the isolation literature. However, during our work, 2 total syntheses were independently published of **4** by the Herestch group and the Ma group.^{12,13} The Herestch group's synthesis is the shortest with only 9 steps starting from ergosterol (**20**).¹² The Herestch route (**Scheme 1.3a**) employs a key radical cascade utilizing $\text{PhI}(\text{OAc})_2$ and I_2 to transform **21** into **22** early on and thence access **4** 4 steps later. From there, the team demonstrated the ability to attain both **1** and related periconiastone A (**8**) in 1 step each from **4**. The Ma group (**Scheme 1.3b**) similarly employed radical chemistry in their 23-step synthesis of **4**.¹³ Starting from vitamin D (**23**), the Ma route proceeded to a Co(II)-catalyzed cycloisomerization of **24** to establish the *cis*-decalin core in **25**. After a series of functional group interconversions, the Ma group subsequently completed the skeletal backbone with C-H oxygenation of **26**, generating hydroperoxide intermediate **27** for same-pot radical rearrangement utilizing FeSO_4 . From the resulting **28**, 3 more steps yielded **4**.

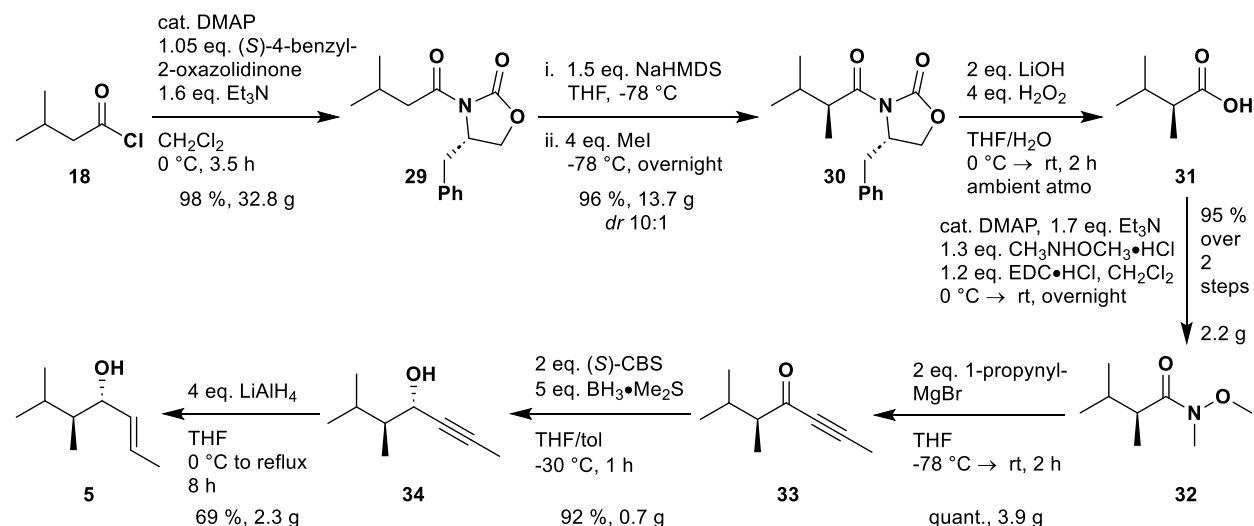


Scheme 1.3. Key steps in the prior syntheses of dankasterone B (**4**).

These excellent syntheses demonstrate the utility of using complex, naturally occurring steroids as starting points for accessing the 13(14 $\rightarrow$ 8)abeo skeleton. The release of 2 competing syntheses during our project tenure also implicitly affirms the desirability of this family as a synthetic challenge to target in the first place. In comparison to the Heretsch and Ma routes, however, our synthesis remains unique in its convergent, bottom-up approach. Our modular route may lend greater flexibility to future researchers wishing to alter the skeleton for purposes outside of total synthesis (e.g., structure-activity relationship assays). Therefore, in science as in art, beauty lies in the eye of the beholder.

1.6 Alkenol Material Campaign

Synthesis of the alkenol moiety began with amide bond formation via the condensation of (*S*)-4-benzyl-2-oxazolidinone with isopentanoyl chloride (**18**) to form enantiopure **29** (Scheme 1.4).¹¹ The speed of reagent addition was crucial for maximizing the yield: earlier iterations generated yields around 85 % instead of the 98 % yield attained with slow cannula addition, minimizing gas evolution and local temperature fluctuations. With the chiral auxiliary secured, oxazolidinone **29** was then subjected to methylation which proceeded with 10 : 1 diastereoselectivity at scale. Ratios up to 20 : 1 *dr* were also observed in prior iterations of the reaction, albeit with lower yields hovering around 90 %. Again, reagent addition speed was a key factor in maximizing yield while the temperature required continued maintenance at -78 °C overnight to avoid loss of product. Prior attempts at direct formation of the Weinreb amide from **30** were suboptimal, so the oxazolidinone was first hydrolyzed¹¹, conveniently under ambient atmosphere, to known carboxylic acid **31** before formation of the novel Weinreb amide **32**. Due to the highly volatile nature of carboxylic acid **31** and that of the subsequent substrates *en route* to intermediate **5**, rotatory evaporation and vacuum drying consistently endangered product yields and therefore were undertaken with great care at lowered temperatures. Highly volatile **31** was itself carried onward to the next step as a concentrated solution in THF to avoid notable loss of product.



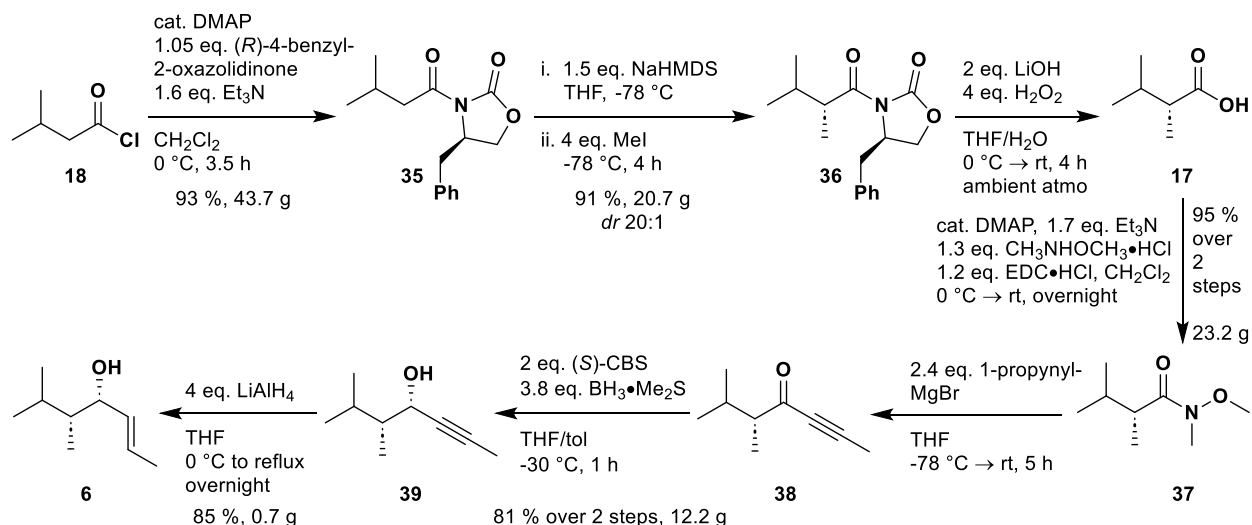
Scheme 1.4. Alkenol **5** was produced with the originally assigned stereochemistry in 57 % net yield over 7 steps.

After forming Weinreb amide **32**, the subsequent Grignard reaction to form ketone **33** proceeded quantitatively followed by enantiospecific Corey-Bakshi-Shibata reduction mediated by CBS and BH_3 . A final

LAH alkyne reduction of alcohol **34** produced the desired *trans* unsaturation in alkenol **5**. Frustratingly, the LAH reduction also afforded dramatically fluctuating yields both in my collaborator's and my hands, ranging from yields below 50 % to above 90 %. Close monitoring of the reaction via repeated NMR aliquots was necessary to determine the soonest advisable quench time based on the prevalence of competing decomposition. Isolated yields in the 60 – 70 % range were most common.

Ultimately, alkenol **5** was obtainable with a net percent yield of 57 % over 7 steps from the commercially available acid chloride **18** after reaction optimizations. Arguably the greatest remaining challenge from the hydrolysis and onward was the notable volatility of the substrates. However, careful execution of each step and painstaking attention to the conditions used during concentration under reduced atmosphere enabled the attainment of almost universally high yields and selectivities on multi-gram scales, such as the 32.8 g obtained of **29** with 98 % yield and the quantitative Grignard reaction at the 3.9 g scale several steps into the synthesis.

Later, upon discovery of the structural misassignment for the dankasterone side chain, the alkenol moiety had to be regenerated with the corrected stereochemistry (**Scheme 1.5**). As expected, yields were again high, albeit with some variations, to afford a net percent yield of 55 % over 7 steps. Discrepancies between the percent yields for individual reactions between the two syntheses were either within acceptable margins and / or accompanied by plausible rationales for the discrepancies. For example, the scale of the condensation reaction to create the amide bond in **35** was approximately 40 % larger, reaching a yield of 43.7 g. Since issues of scale and localized temperature fluctuations in large solutions can impact percent yields and since the larger scale necessitated use of a gradient column for purification instead of a shorter plug (see **Appendix A**), these are presumably the causes of the lower 93 % yield of **35** vs. the original 98 % yield in the corresponding synthesis of its enantiomer **29**. Likewise, higher scales made careful concentration under reduced atmosphere less feasible for the highly volatile intermediates **17** through **39**. However, continued experimentation with conditions and purification procedures did enable some improvements in the route, such as improved consistency and yield for the LAH reduction.

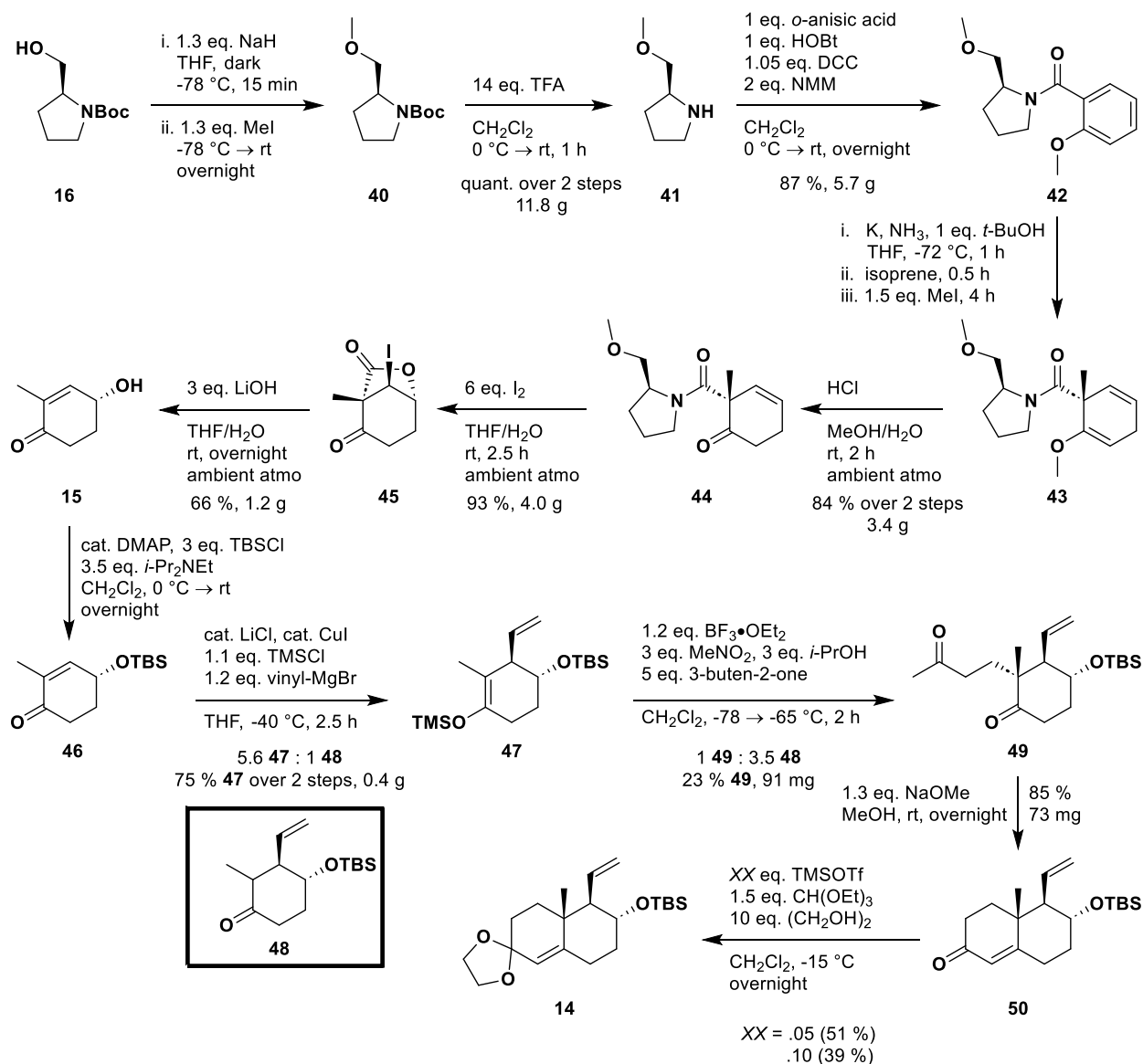


Scheme 1.5. Alkenol **6** was produced with the corrected stereochemistry in 55 % net yield over 7 steps.

Regardless of the increased scaling challenges, the final alkenol **6** was obtained in similar net percent yield to its diastereomeric cousin **5**. With ample quantities of diastereomers **5** and **6** in hand, my collaborator Boilevin was well-positioned to explore possible conditions for the Suzuki coupling, intramolecular Heck reaction, and Claisen rearrangement with model compounds while I undertook a material campaign and route shortening probes for the decalin moiety.

1.7 Decalin Material Campaign

Synthesis of the leftmost decalin fragment began with base-mediated methylation¹⁴ of light-sensitive *N*-Boc-L-prolinol, followed by acidic deprotection¹⁵ of methoxy **40** to afford volatile amine **41** in quantitative yield over 2 steps (**Scheme 1.6**). Although my collaborator's 2-step yields for this reaction were in the 70 – 80 % range, I was serendipitously able to raise the yield to quantitative with careful execution and procedural adjustments, such as basifying the aqueous phase to pH 13 instead of the original procedure's pH 8 for the work-up following deprotection, thus achieving more efficacious extraction. Conversion of the amine **41** to amide **42** was accomplished via traditional DCC coupling with *o*-anisic acid in good yield.



Scheme 1.6. Decalin **14** was produced in 3 % net yield over 12 steps.

Subsequent subjection to the Birch reduction in tandem with a methylating agent happily afforded the reductive alkylation product on a multi-gram scale in the desired isomeric form of methoxy **43**.^{10,16} Again, seemingly trivial adjustments to the procedure unlocked greater yields than originally assumed, such as by maintaining the Birch reaction bath at -72 °C rather than our original choice of -65 °C. Crucially, I observed an apparent emerging relationship between quantity of reducing metal and loss of yield in earlier iterations of this reaction, so I took care to use as little K as possible to induce the diagnostic blue color in solution. While Birch reductions do not, in practice, employ stoichiometric control over metal addition, limiting

unnecessary reducing metal could reasonably explain the resulting ~ 10 percentage point improvement in yield for this step from its prior best yield (not shown). Next, acid-catalyzed deprotection of the methyl vinyl ether generated a transient enol ether which tautomerized into isolated ketone **44** while the other functionalities present remained intact. Further experimentation revealed that the crude Birch mixture could be subjected directly to the acidic solution under ambient atmosphere without compromising yield, thus avoiding laborious column chromatography after reductive alkylation and achieving 84 % yield over 2 steps.

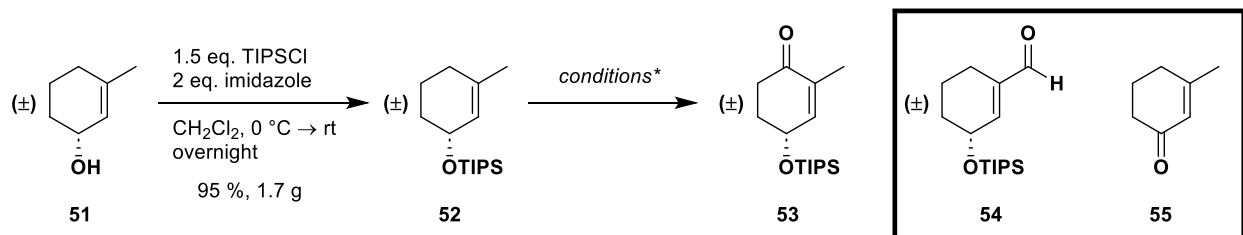
With the prolinol auxiliary's mission of ensuring selective methylation complete, it was allowed to depart upon iodolactonization to **45**. Subjecting iodolactone **45** to hydroxide addition precipitated ring-opening and intramolecular decarboxylation to yield known cyclohexenone **15** with the desired stereochemical objective achieved.¹⁰ TBS protection of the alcohol then set the stage for 1,4-addition to novel product **46** to establish the vinyl fragment necessary for later-stage Suzuki coupling. With the ring's stereochemical preferences set by the bulky OTBS group, **47** manifested with the vinyl fragment in the desired *anti* configuration, thus establishing the first part of the ultimate *trans*-1,3 pattern in dankasterone's core.

A Lewis acid-catalyzed Mukaiyama-Michael addition then afforded **49** as a single diastereomer ready for ring closure in a Robinson annulation to generate decalin **50**. Unfortunately, persistent issues with hydrolysis of the labile TMS protecting group caused suboptimal yields in these ultimate (albeit unoptimized) steps. Challenges were also encountered regarding the following ketalization to yield **14** in that the reaction appeared highly sensitive to equivalents of TMSOTf. The reaction's sensitivity was further complicated by accompanying desilylation of the OTBS group. Additionally, the later coupling reactions tested by my collaborator Boilevin to join the righthand and lefthand fragments of dankasterone also presented challenges (not shown), reinforcing the desirability of exploring alternate strategies to either sidestep these issues or at least shorten step counts to compensate for lower yields later in the synthesis.

1.8 Explorations Toward Alternate Dankasterone Routes

After multiple iterations of the syntheses described above, the material campaigns concluded with ample stockpiles for feeding the remainder of the strategy's later-stage explorations. Therefore, my attention then turned to exploring possibilities for shortening step counts and circumventing challenges associated with the subsequent decalin coupling and ketalization.

One possibility for accomplishing the former was to enact allylic oxidation directly on a silyl-protected version of commercially available 3-methyl-2-cyclohexenol (**51** to **52**), thus shortening the 8-step route to **46** substantially. Due to the lability observed previously with TBS as the alcohol's protecting group, TIPS was utilized instead. Note that, while all route explorations described herein began with racemic reagents, the tested conditions were intended to be amenable to an ultimate transition toward an asymmetric synthesis following an anticipated conversion to using known chiral starting materials after selection of the final route.^{17,18} In that spirit, several conditions were explored using a variety of Mn, ROOH, Cr, and Se oxidants (**Scheme 1.7**). While entry 7 ultimately afforded the desired ketone **53** as the major product, slow conversion and desilylation to 3-methyl-2-cyclohexenone (**55**) were persistent issues across the (unoptimized) conditions.

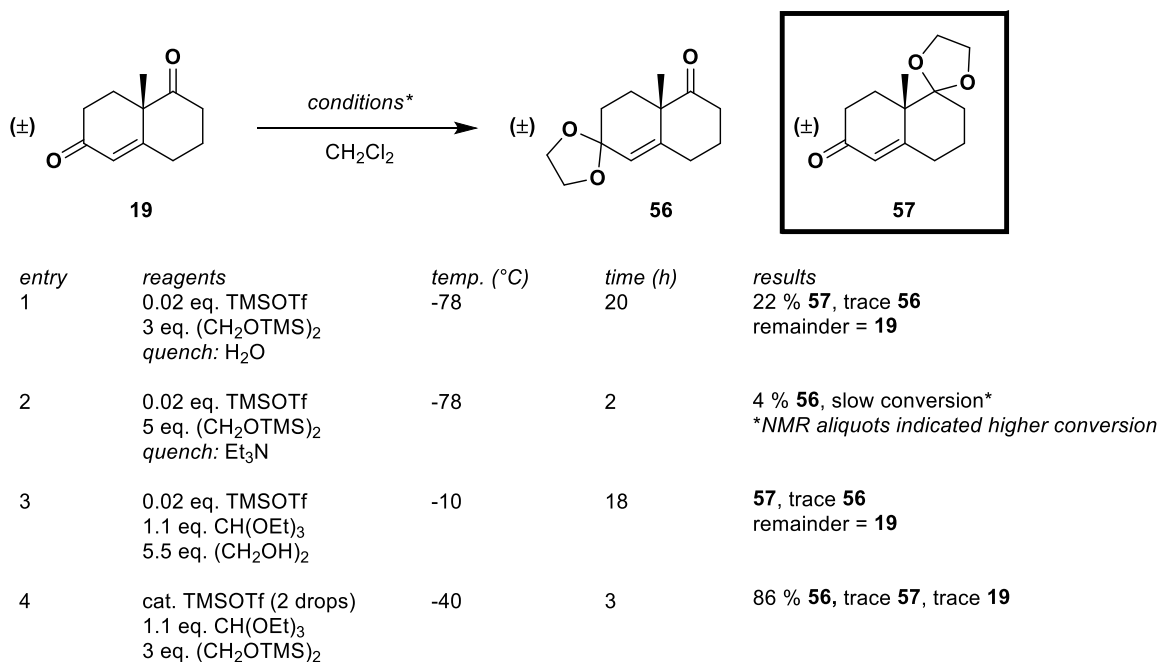


entry	reagents	solvent	temp. (°C)	time (h)	results
1	9 eq. MnO ₂	CH ₂ Cl ₂	rt	24	no conversion
2	0.1 eq. Mn(OAc) ₃ •2H ₂ O 5 eq. <i>t</i> -BuOOH 1:10 3A M.S. w/w	EtOAc	rt	22	slight conversion
3	0.05 eq. Pd/C 0.25 eq. K ₂ CO ₃ 5 eq. <i>t</i> -BuOOH	CH ₂ Cl ₂	0 → rt	23	trace 53 trace 55
4	0.5 eq. Pd/C 1.25 eq. K ₂ CO ₃ 5 eq. <i>t</i> -BuOOH	CH ₂ Cl ₂	0 → rt	31	trace 53 trace 55
5	0.05 eq. Pd(OH) ₂ /C 0.25 eq. K ₂ CO ₃ 2.5 eq. aq. <i>t</i> -BuOOH	CH ₂ Cl ₂	rt	31	trace 53 trace 55
6	30 eq. PCC 30 eq. NaOAc 1:10 celite w/w	benzene	80	2	42 % 55
7	cat. AcOH (2 drops) 1 eq. SeO ₂ 10.5 eq. H ₂ O	1,4-dioxane	40 → 80 stepwise	18	27 % 53 (1.6 53 : 1 54)

*Reactions were terminated and unreacted starting material recovered once conditions appeared unsatisfactory by TLC or NMR

Scheme 1.7. Allylic oxidation to ketone **53** was achieved with suboptimal selectivity.

With the specter raised of potentially systematic issues associated with the allylic oxidation, another alternative explored was to directly ketalize the Wieland-Miescher ketone (**19**) and then effect diastereoselective oxidation to install an oxygen-based handle on the righthand cyclohexyl unit (**Scheme 1.8**). While the ketalization again proved finicky as suggested in existing literature,^{19,20} entry 4 was successful in finding appropriate conditions which, in our hands, tilted the equilibrium in favor of the desired kinetic product **56** and away from undesired thermodynamic product **57**. With a reliable ketalization method established, heteroatom installation could commence.

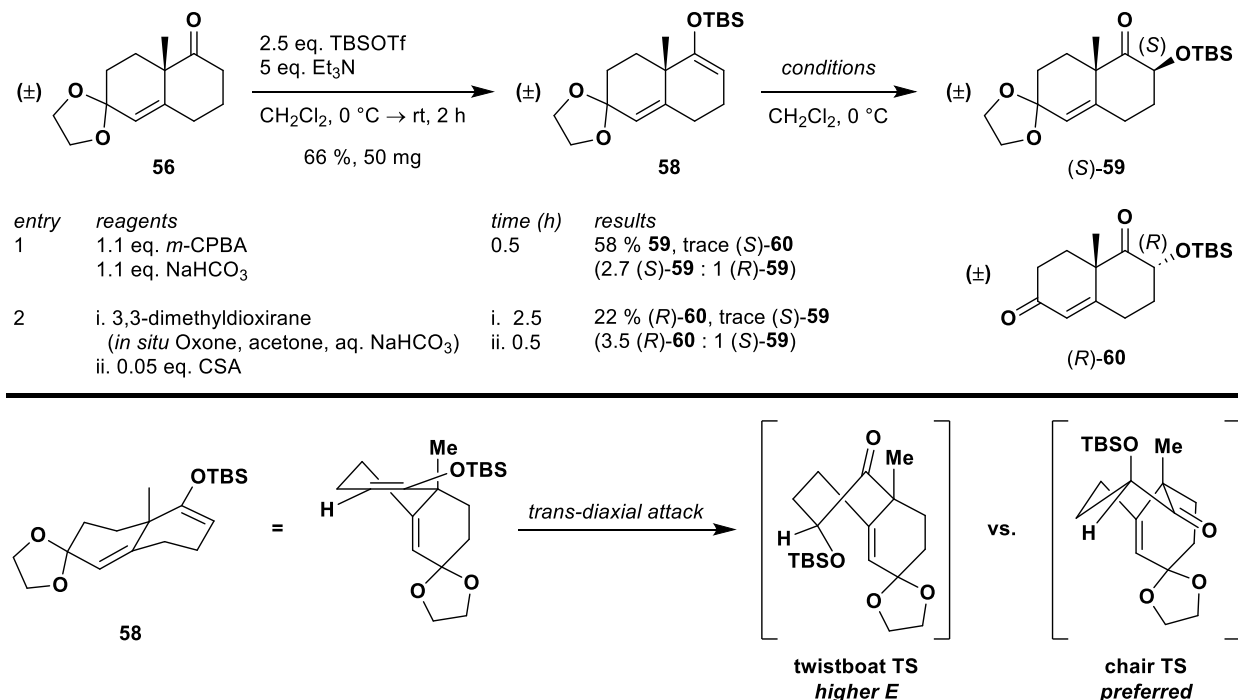


*Reactions were terminated and unreacted starting material recovered once conditions appeared unsatisfactory by TLC or NMR

Scheme 1.8. Ketalization conditions walked a fine line between thermodynamic and kinetic products.

The first answer to the need for α -oxidation was to probe whether silyl enol ether oxidation would produce the desired stereoisomer (**Scheme 1.9**). The α position would ultimately be transformed into a planar triflate handle for the intramolecular Heck reaction downstream. However, since the unprotected ketone would need to be manipulated into an upward-facing vinyl group for coupling before the Heck reaction, the presence of a neighboring 4° *syn* methyl induced concerns about the degree of control we would have over the direction of the vinyl's addition, especially given the preference for axial attack in cyclohexanone systems. Our goal would be to achieve the less desirable up-side equatorial attack. A bulky *anti* OTBS moiety in the down-side position (albeit equatorial) could potentially provide insurance

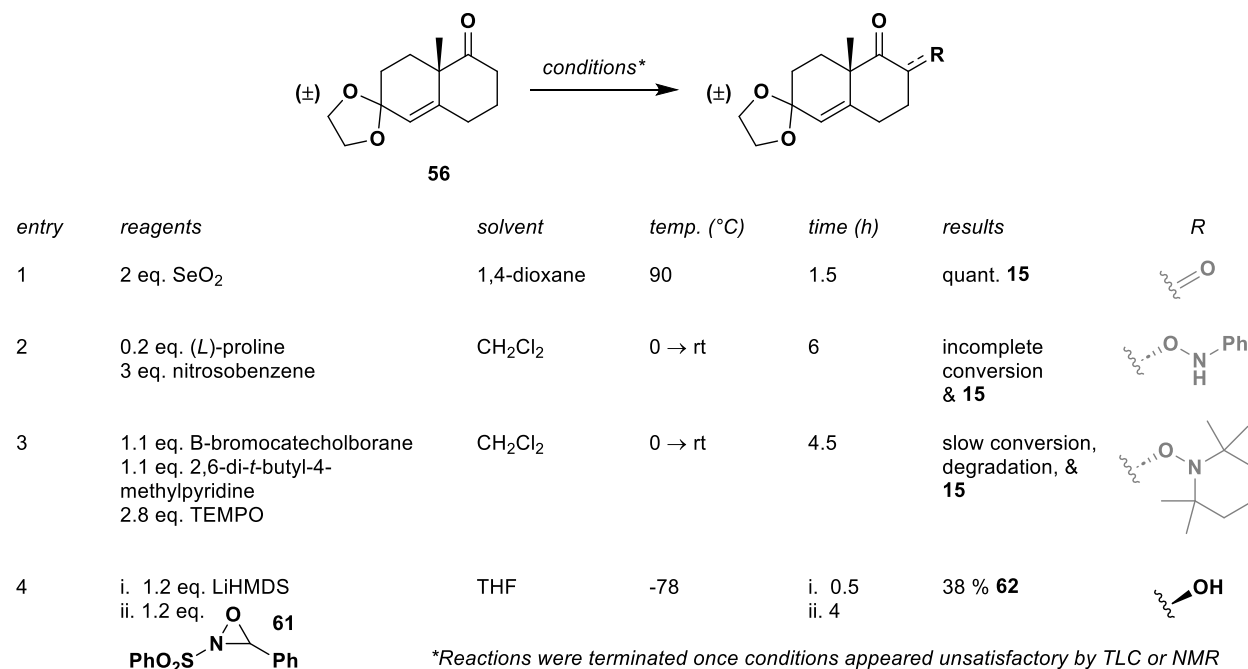
against undesirable diastereoselectivity arising from down-side axial attack at the carbonyl in the subsequent vinyl addition. Oxidative conditions were therefore briefly probed on silyl enol ether **58**, revealing the undesired stereochemical preference for *S* formation (**59**) with *m*-CPBA. This preference for *S* stereochemistry can be explained as a result of *trans*-diaxial transition states giving preference to the most chair-like state (**Scheme 1.9**). Meanwhile, although *R* stereochemistry was isolated in greater proportion than *S* after dioxirane exposure (**60**), it was accompanied by a penchant for deketalization.



Scheme 1.9. *Anti* installation of OTBS was contraindicated due to the preferential transition state for *trans*-diaxial attack.

With *anti* installation of OTBS in **59** contraindicated, the next step was to test whether other potential precursors to the α -triflate group could be installed with *anti* stereochemistry (**Scheme 1.10**). Additionally, it was worth investigating at this point whether the system might serendipitously favor up-side equatorial addition of a vinyl / vinyl-equivalent moiety to the ketone regardless of the presence of a *syn* methyl / absence of an *anti* blocking group. Of the example conditions displayed in **Scheme 1.10**, however, only the Davis oxidation in entry 4 succeeded in effecting a useful transformation, again with the undesired *syn* stereoisomer when R = OH (**62**). Riley oxidation, α -aminoxylation, and TEMPO oxidation unfortunately

effected deketalization. While this alcohol moiety was later able to be utilized as a handle for triflate generation (not shown), the system's stereochemical preference was clearly not as trivial as we had hoped.



Scheme 1.10. Additional attempts at *anti* α-installation were thwarted.

With my explorations demonstrating to us the challenges of using either direct allylic oxidation or **19** to effect the desired route-shortening, an alternative pathway to **15** was eventually developed by my collaborator Vladislav Lisnyak who joined the team in the later stage of the project. The team also ultimately decided to diastereoselectively partially hydrogenate the decalin unit before ketalization. By removing the α,β-unsaturation, the left hand ketal in downstream products would be more robust to the subsequent transformations. Additionally, considering Heretsch's demonstration of the 1-step transformation of **4** to **1** and periconiastone A (**8**) during the course of our project, switching our target from **1** to **4** would automatically result in a formal total synthesis of both **1** and **8** upon accessing **4**.

1.9 Final Strategy for Asymmetric Total Synthesis of Dankasterone B

Therefore, with the departure of collaborator Boilevin from the group after elucidating conditions for the later-stage steps such as the Heck reaction and Claisen rearrangement, Lisnyak brought our synthesis to a close with the final few transformations to achieve **1** in 20 steps from commercially available starting

CC(C)=CC(=O)C1=CC=CC=C1 (63) $\xrightarrow{3 \text{ steps}}$ CC(C)=CC(=O)C1=CC=CC=C1 (64) $\xrightarrow{5 \text{ steps}}$ CC(C)=CC(=O)C1=CC=CC=C1 (15) $\xrightarrow{2 \text{ steps}}$ CC(C)=CC(=O)C1=CC=CC=C1 (65) $\xrightarrow{3 \text{ steps}}$ CC(C)=CC(=O)C1=CC=CC=C1 (66) $\xrightarrow{78 \% \text{ over } 2 \text{ steps}}$ CC(C)=CC(=O)C1=CC=CC=C1 (67) $\xrightarrow{73 \%}$ CC(C)=CC(=O)C1=CC=CC=C1 (68) $\xrightarrow{4 \text{ steps}}$ CC(C)=CC(=O)C1=CC=CC=C1 (69) $\xrightarrow{63 \%}$ CC(C)=CC(=O)C1=CC=CC=C1 (70) $\xrightarrow{2 \text{ steps}}$ CC(C)=CC(=O)C1=CC=CC=C1 (4) $\xrightarrow{\text{Heretsch } 1 \text{ step}}$ CC(C)=CC(=O)C1=CC=CC=C1 (1 or 8)

Starting from (*R*)-carvone (**63**), the thermodynamic enolate of **48** underwent vinylogous *O*-nitroso aldol addition and then oxidative hydrodeisopropelynation over 3 steps, generating intermediate **64** which collapsed into the cyclohexenone **15**. After following the same 4 steps already outlined for transforming **15** into **50** (e.g., conjugate addition of the vinyl group and then annulation), diastereoselective partial hydrogenation produced *cis*-decalin **65**, thus departing from the original route. Ketal protection and

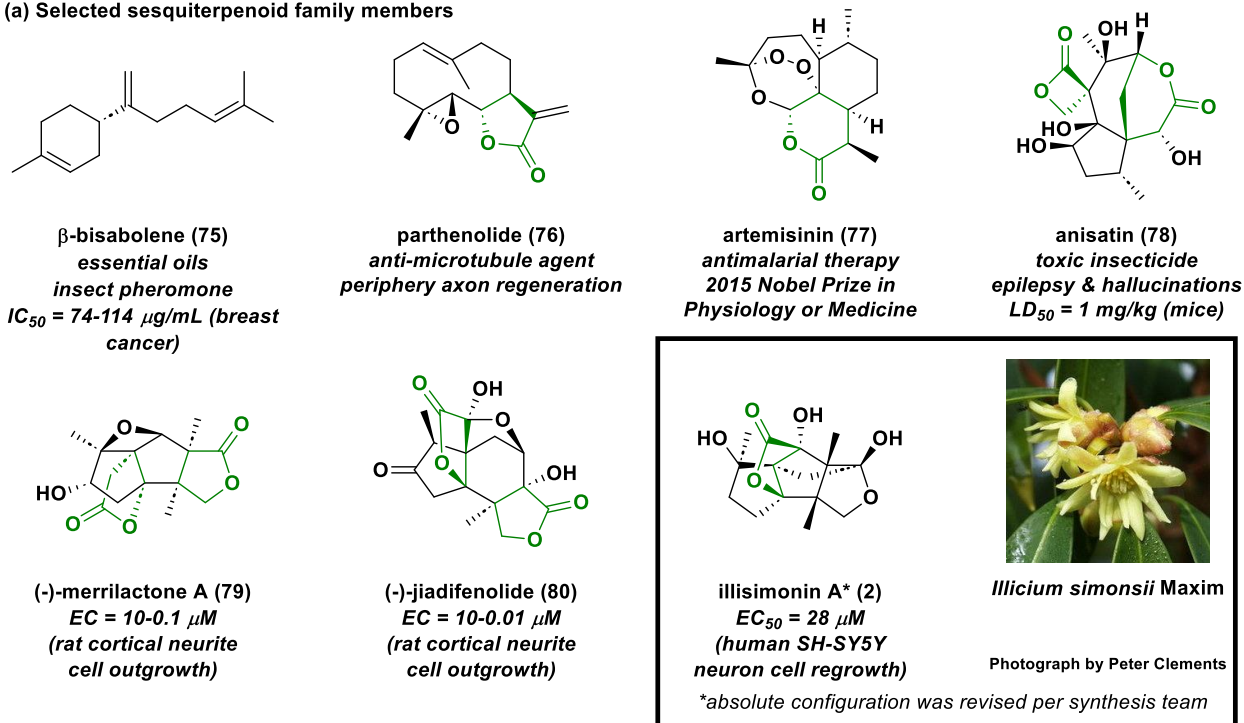
hydroboration generated borane **66** before Zweifel olefination added in vinyl bromide **74**. The vinyl bromide descended directly from alkenol **6** via base-induced S_N2 in 8 steps overall. After Zweifel olefination, functional group interconversions generated triflate **67** for the intramolecular Heck reaction with Pd(OAc)₂ / PPh₃ to yield **68**. Serendipitously, the thermal Claisen rearrangement in toluene and subsequent Horner-Wadsworth-Emmons reaction were amenable to combination in the same pot to afford **69**. After 4 more steps to manipulate the necessary functional groups into place, **70** was ready for 6-*exo-trig* radical cyclization using SmI₂ to close the 13(14→8)*abeo* skeleton. The mixture of isomers observed from the cyclization did not present significant problems since subsequent oxidation resolved them into the same ketal-protected version of **4**. After acidic removal of the ketal, dankasterone B (**4**) was revealed. It is our hope that this synthesis provides a tunable modular pathway for access to dankasterone family members and other 13(14→8)*abeo* analogues as well as enable future derivatizations.

1.10 Illisimonin A

While the dankasterone family sports a select number of relatives within the steroid class, the sesquiterpenoid class is on the extreme end of the spectrum in terms of size and variety. Structurally diverse, naturally abundant, and biologically potent, sesquiterpenoids are one of the most extensively investigated natural product families (**Figure 1.5a**).^{22–24} Elaborations on the defining 15-carbon sesquiterpene motif, derived biologically from the three isoprenoid units of farnesyl pyrophosphate (**103**), yield seemingly infinite structural possibilities. Sesquiterpenoid lactones (SLs) offer possibly the most therapeutic potential with approximately 1,500 publications on SL biological activities between 1990 and 2013.^{25,26} Although over 5,000 SLs are currently known among the plant kingdom, including from historic medicinal plants such as feverfew (parthenolide, **76**) and sweet wormwood (artemisinin, **77**), several SLs from *Illicium* medicinal plants have garnered especial recent interest for their densely oxygenated skeletons, high stereochemical complexity, and potent neurotrophic activities (**2**, **79**, **80**).^{27,28} Illisimonin A (**2**) is an especially attractive target synthetically due to its extremely rare *trans*-bicyclo[3.3.0]octane motif within a unique 5/5/5 all-carbon substructure inside an unprecedented pentacyclic 5/5/5/5/5 sesquiterpenoid skeleton – all fused and bridged together in a mass of complex welding, including a novel C₆-C₁₀ linkage for *Illicium* sesquiterpenoids (**Figure 1.5b**).^{29,30} Indeed, the strain is so high that a 3D molecular model of

2 breaks unless assembled with great care. Enabling access to this unique and intensely challenging skeleton through synthetic means could unlock exciting synthetic pathways and biological studies for future research.

(a) Selected sesquiterpenoid family members



(b) Challenging features of the illisimonin skeleton

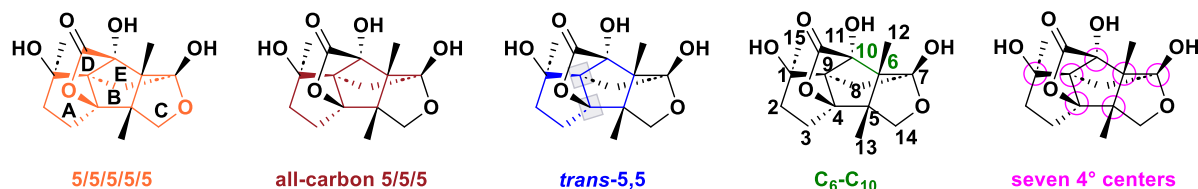
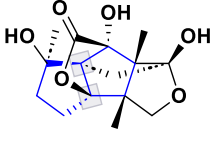
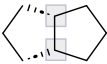


Figure 1.5. Sesquiterpenoids such as illisimonin A (2) are exciting targets synthetically and biologically.

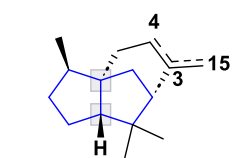
In particular, of the five key challenging features in 2, arguably the most difficult (and most rewarding) to install would be the *trans*-5,5 pattern. At the start of this project, only ten of the 2,000+ known bicyclo[3.3.0]octane structures in the X-ray crystallographic database were *trans*, and only five natural products containing a *trans*-bicyclo[3.3.0]octane had ever been synthesized (**Figure 1.6**), making this area ripe for further development.^{31–39} Moreover, from a biological viewpoint, the approximately +6.4 kcal/mol associated with a *trans*-bicyclo[3.3.0]octane system compared to the normal *cis* posits that perhaps the existence of the *trans* relationship in natural products is important for potency.^{40,41} Thus, to enable further

study of the fascinating illisimonin skeleton and *trans*-bicyclo[3.3.0]octane systems, I engaged in retrosynthetic analysis of **2**.

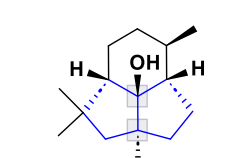
		<u>Strain Energy (kcal/mol)</u>	
		<i>Theoretical*</i>	<i>Experimental</i>
 <i>trans</i> -5,5	 <i>cis</i>	12.2/13.2	12.0
	 <i>trans</i>	24.6/19.6	18.4
		$\Delta = 12.4/6.4$	$\Delta = 6.4$

*First values from Boyd - Second values from Allinger

All-carbon *trans*-bicyclo[3.3.0]octanes

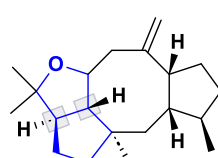


81: α -funebrene ($\Delta^{3,4}$)
82: β -funebrene ($\Delta^{3,15}$)

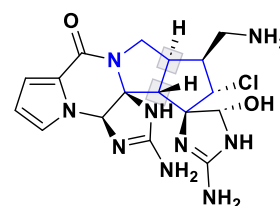


presilphiperfolan-8- β -ol
(83)

Heteroatom *trans*-bicyclo[3.3.0]octanes



(+)-epoxydictymene
(84)



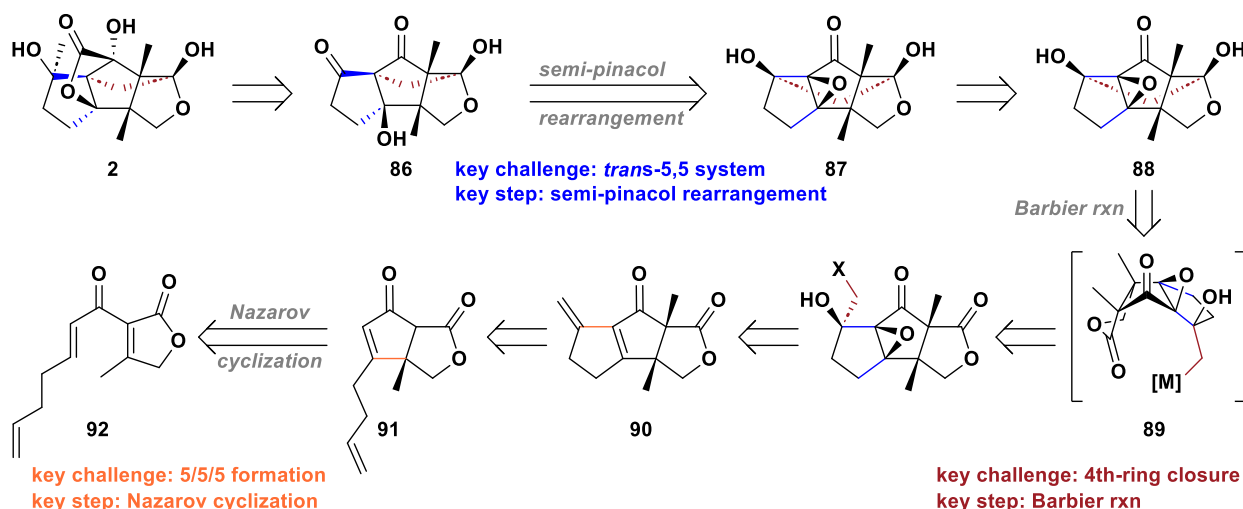
(-)-palau'amine
(85)

Figure 1.6. Previously synthesized natural products with highly strained *trans*-bicyclo[3.3.0]octane systems.

Note: As will be discussed later, it was discovered by another group (while this project was ongoing) that the absolute configuration of **2** may be the opposite of the originally assigned configuration. This discovery reinforces the utility of using total synthesis for structural elucidation of complex molecules. In this chapter, the original assignment⁴² is displayed in all illisimonin structures for consistency.

1.11 Illisimonin A Retrosynthesis

The retrosynthetic plan (**Scheme 1.12**) called for either a Nazarov or radical cyclization of achiral divinyl β -ketoester **92** to form the first bicyclic system which would then be subjected to a Heck reaction on **91** to close the 3rd ring.^{42,43} After stereoselective epoxidations complete molding the curve, the 4th ring would then ideally be installed via a Barbier reaction with **89**, setting the stage for an eventual semi-pinacol rearrangement.^{44–48} This late-stage rearrangement would reveal the ultimate core of illisimonin which, after a few more targeted transformations, would be complete and ready to serve as verification of the isolation team's proposed structure.



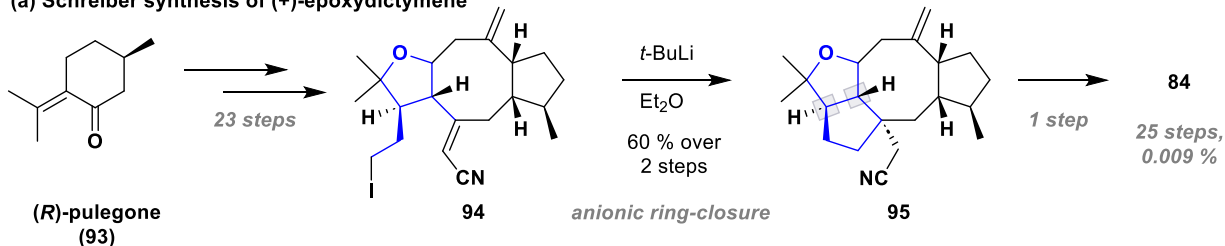
Scheme 1.12. Retrosynthetic analysis of **2**.

Several factors represented key areas of concern in designing this plan:

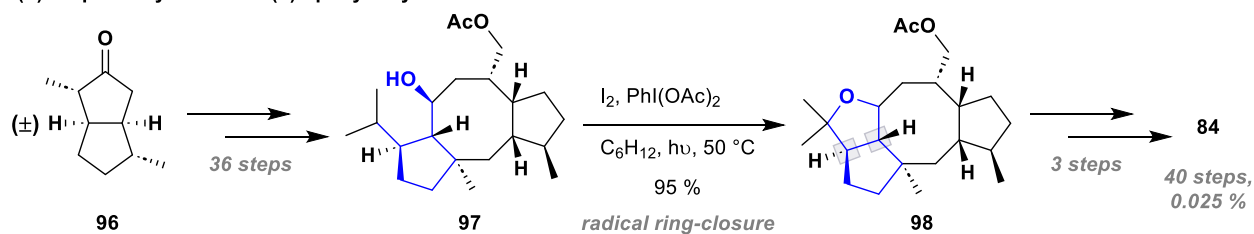
- (1) Forming and retaining the *trans*-5,5 relationship;

Retaining a *trans*-bicyclo[3.3.0]octane system is risky since the molecule might seek any opportunity to relax to a *cis*-5,5 system through either elimination or carbocation formation. Therefore, the establishment of a *trans*-5,5 connection should be as late as possible. Correspondingly, prior examples of synthetic *trans*-5,5 formation (**Scheme 1.13**) utilized late-stage ring closures (anionic and radical), ring contraction, and Wolff rearrangement.^{31,32,34–38} Meanwhile, the proposed biogenetic pathway envisioned a 1,2-alkyl shift accomplishing the key step.³⁰ Due to the uniquely cage-like scaffold of **2**, however, and the all-carbon nature of its *trans*-bicyclo[3.3.0]octane system, the prospect of replicating these precedents was concerning due to the open question of whether there would be sufficient driving force to achieve such an uphill energetic climb.

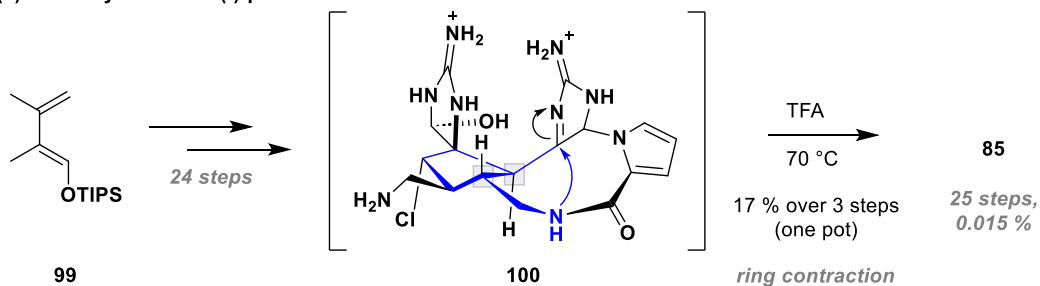
(a) Schreiber synthesis of (+)-epoxydictymene



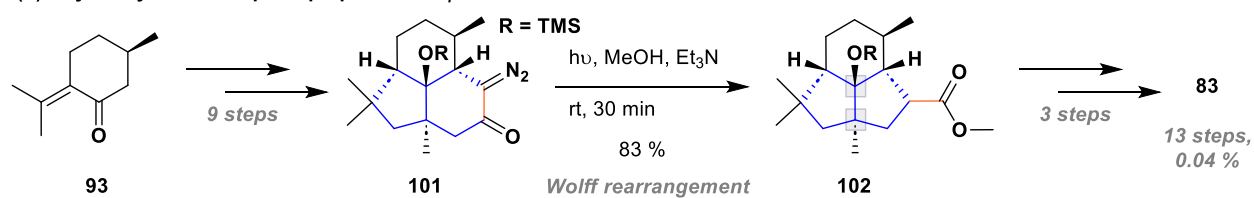
(b) Paquette synthesis of (+)-epoxydictymene



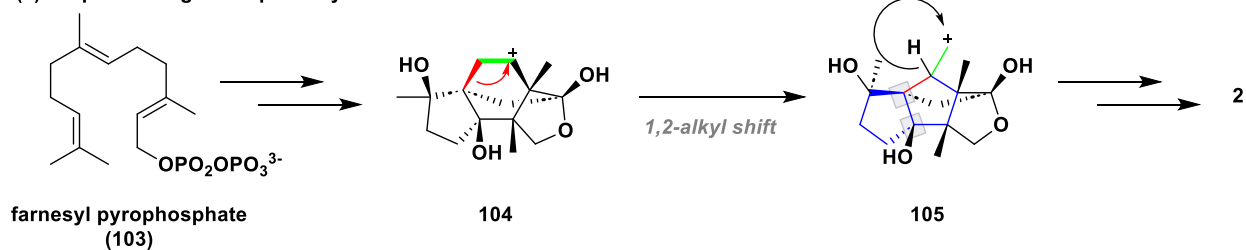
(c) Baran synthesis of (-)-palau'amine



(d) Snyder synthesis of presilphiperfolan-8- β -ol



(e) Proposed biogenetic pathway to illisimonin A

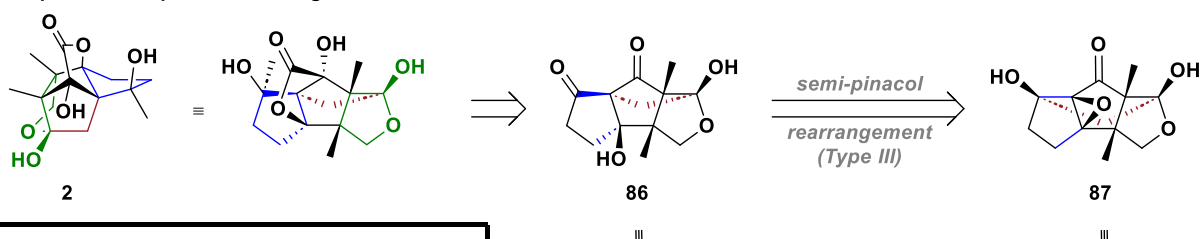


Scheme 1.13. Precedents for accessing *trans*-bicyclo[3.3.0]octane systems.

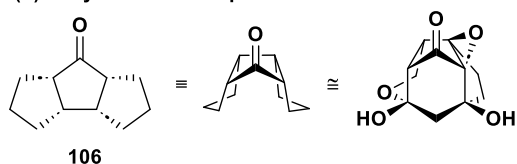
I therefore designed the retrosynthetic strategy principally around this consideration and proposed a late-stage semi-pinacol rearrangement (**Scheme 1.14a**). Type III semi-pinacol rearrangements have been proven

to be effective at forcing increasingly strained polycyclic relationships, such as transforming 6/6 bicyclic (i.e., decalin) systems into 5/7.^{47–49} Driving forces compensating for *trans*-bicyclo[3.3.0]octane strain would include formation of a C=O bond and release of epoxide ring strain. The release of strain energy from the locked boat conformation of **87** (~6.5 kcal/mol relative to chair) should also help to compensate for the strain incurred from cyclohexane ring contraction into a cyclopentane (~6.5 kcal/mol relative to cyclohexane chair). Therefore, while all known constructions of this unit feature a preinstalled *trans* system (not bicyclooctane) which transforms into a bicyclooctane through either ring contraction or closure onto a preexisting polycyclic scaffold, my design (while also a ring contraction) calls for forming the *trans* system directly from a *cis*-bicyclo[3.3.0]octane established by harnessing the inherent geometrical preferences of cyclopentanoids.

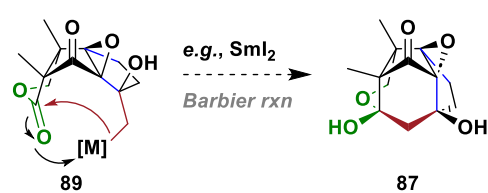
(a) Proposed semi-pinacol rearrangement



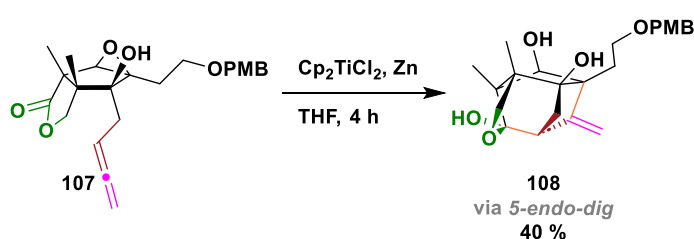
(b) Tricyclic Eaton inspiration



(c) Proposed Barbier step



(d) Liu and Wang's unexpected box-like byproduct



Scheme 1.14. Key details for the proposed semi-pinacol and Barbier steps.

(2) Maintaining the inherent strain of a small cage-like skeleton;

To construct such a strained system, I was inspired by the work of Eaton toward perisylane and dodecahedrane to gradually mold three 5-membered rings into a curve, thereby increasing the system's strain incrementally (**Scheme 1.14b**).⁵⁰ Then, adding a fourth “wall” to make a box-like molecule via a Barbier-like reaction could make the jump to a *trans*-5,5 fused system less dramatic than starting from a more relaxed

system (**Scheme 1.14c**). In addition to building up strain to drive the later semi-pinacol step, the rigid box-like structure would actually be crucial at this point for discouraging 3° hydroxyl departure (according to Bredt's Rule) and establishing the desired $\sigma_{C-C} \rightarrow \sigma^*_{C-O}$ orbital overlap requisite for semi-pinacol. An article by Liu and Wang (serendipitously published after this retrosynthetic analysis was constructed) bodes well for the stability of such a box-like molecule with the report of an accidental curve-to-box by-product **108** (**Scheme 1.14d**).⁵¹

(3) Establishing seven 4° carbon centers, all of which are directly next to at least one other 4° carbon;

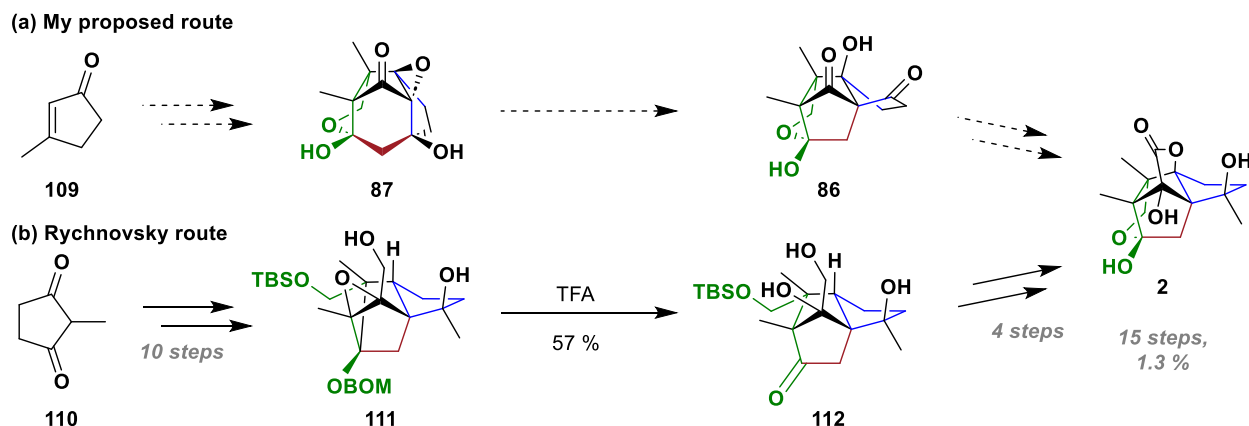
and

(4) Incorporating six oxygen atoms with varying oxidation states in a dense network.

The dense network of oxygen atoms and the contiguous series of seven 4° carbon centers mean that the skeleton needs to be established with particular concern to reactivity and sterics.^{5,6} High oxygen density with different oxidation states is conventionally difficult to establish. Additionally, the 4° centers would likely hamper accessibility to their neighbors if the strategy attempted to install them after the box-like core was assembled. Therefore, by assembling most of the atoms on a flat frame and then folding them into place, concerns about accessing a compact core would hopefully be circumvented.

1.12 Other Illisimonin A Synthesis

With various contingency plans in place for potential route adjustments and with the recognition that even achieving only the pre-pinacol intermediate **87** would be a real achievement, I began synthetic efforts toward illisimonin's synthesis. Unfortunately, before the synthesis could be completed, a competing team published a successful total synthesis (**Scheme 1.15**).⁵² The total synthesis utilized a similar approach as my own retrosynthesis by building up strain and rigidity to effect a Type III semi-pinacol rearrangement for the *trans*-5,5 functionality, albeit on a different part of the molecule.

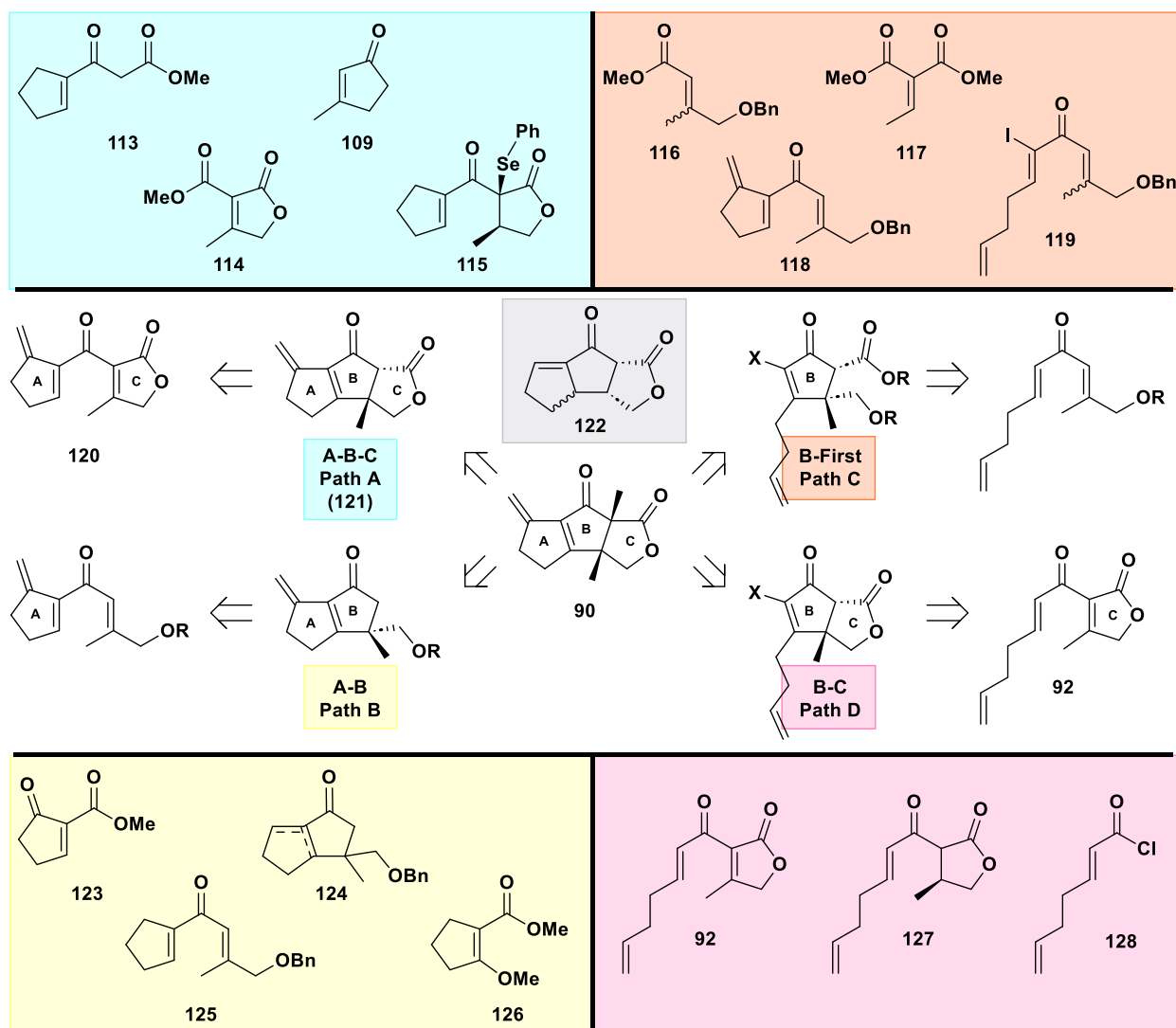


Scheme 1.15. Comparison of key Type III semi-pinacol step in competitor's total synthesis.

As with a double-edged sword, the similarity between the published route and my own felled the project while validating both the feasibility of my design, desirability of target selection, and utility of total synthesis in structure elucidation. In the spirit of the dissertation process, a concise representation of the types of synthetic work that was underway will be briefly discussed in the following section.

1.13 Example Synthetic Efforts Toward Illisimonin A

The selected progress briefly presented herein describes explorations of four possible avenues toward the epoxidation precursor **90** (Scheme 1.16). Displayed are examples of substrates generated either to probe (as a model compound) or to directly advance a pathway. The pathways differ in the sequence and reactions used to assemble the three core rings. A model Nazarov cyclization to create **122** from a divinyl β -ketoester affirmed the reasonableness of the general strategy, so the objective was to replicate the model results with all the requisite atoms for **90** in place.



Scheme 1.16. Four major pathways were probed to assemble the three core rings.

For Path A, Morita-Baylis-Hillman and aldol addition reactions were attempted with furanone **109** to join rings A and C before Nararov cyclization. However, the allylic furanone carbon was found to function as a nucleophile in a roughly 1 : 1 ratio with the α -carbon in the absence of a chelating agent; in the presence of a chelating agent, reactions did not proceed, suggesting the cyclic system was too hindered for such an aldol addition. Attempts to derivatize ester **114** to add ring A into it resulted universally in decomposition or the furanone moiety opening up. Meanwhile, attempts to convert the ester moiety in the divinyl β -ketoester **113** into ring C also resulted in decomposition. With a clear message received that these functionalities could not survive standard basic conditions, selenium oxidation-elimination was pursued as a milder option. However,

while a model compound without the neighboring methyl proceeded smoothly through elimination, the SePh ultimately added into **115** with the unreactive *trans* diastereoselectivity as the major isomer. This result contrasted with literature showing that contrasteric alkylations with cyclic enolates are rare in systems with chains, so the cyclopentene substituent is assumed to have played a role in this outcome.^{53–55} Further attempts to add an alternative α -heteroatom for elimination were unsuccessful downstream, such as when IBX yielded an unusual hydroxylated product rather than a prototypical unsaturation or when dehydration reagents yielded decomposition.^{56,57}

For Path B, the Horner-Wadsworth-Emmons product **125** successfully underwent Nazarov cyclization to create ring B in model compound **124** after condition screening. However, the route's real molecule with a methylene was surprisingly unforthcoming when the Wittig reaction on **123** to make the exocyclic alkene precursor repeatedly yielded decomposition. Literature indicated that Nazarov cyclizations cannot proceed with the lefthand ketone present, and ketone masking motifs such as the enol ether of **126** were not stable to acidic conditions (as expected).^{42,58} This pathway's future was therefore deemed tenuous despite the successful model cyclization.

For Path C, Heck cyclization of **119** was shown to successfully close ring A with the desired methylene in **118**, which remained stable in an acidity stability test. However, **118** did not undergo Nazarov cyclization as desired, likely indicating insufficient polarization. To promote the cyclization, an effort was made to form a 1,3-dicarbonyl variant. Unfortunately, a Knoevenagel condensation screen produced only one 1,3-diester, **117**, which refused to undergo a Horner-Wadsworth-Emmons reaction to prepare the rest of the substrate.

For Path D, the successful results from each of the other three pathways were to be combined in the final attempt to access intermediate **90**. The Horner-Wadsworth-Emmons reaction from Path C constructed the lefthand chain in **128** which was later converted into β -ketoester **127** after acid chloride Claisen condensation. Selenium oxidation-elimination was then attempted on **127** which, with a linear chain instead of a neighboring ring, proceeded without the diastereoselectivity issues previously encountered in Path A. The next steps would have then been to execute the Heck cyclization from Path C and the Nazarov cyclization known to work both in Path B and with the model compound which created **122**. Diastereoselective methylation should have then proceeded easily due to the *cis* preference inherent in cyclopentaoids. However, the project was terminated before progressing beyond this point.

While the project was unfortunately necessarily terminated upon publication of the Rychnovsky synthesis, it should be noted that multiple methodology project possibilities (not shown) arose from unexpected results encountered during these exploratory forays, namely (a) IBX heteroatom transfer, (b) mild tandem halogenation / Friedel-Crafts alkylation with an α,β -unsaturated ketone, and (c) a diastereoselective PhSeCl enolate alkylation contrary to literature precedents. Such results remind us again of the tendency for the total synthesis endeavor to surprise and inspire.

1.14 Example Synthetic Efforts Toward 6-exo Bromonium-Induced Cyclization

While the dankasterone and illisimonin families sport complex strained polycyclic scaffolds discovered in only a handful of biologically potent natural products, more than 5,000 natural products have been identified bearing a far more common, humble motif: the halogen atom.⁵⁹ Organohalogens proliferate across the globe, and almost half are believed to manifest specifically with bromine. Many brominated natural products, especially those arising from marine sources, bear interesting and diverse bioactivities.⁶⁰ From simple variants such as the cytotoxic aplysiapyranoid A (**134**) to the more complex anticancerous thysiferol (**129**), the prevalence of and structural breadth in this multitudinous class underscores a clear need to be able to selectively install bromines on stereocenters of all types (**Figure 1.7**), such as via halogenation reactions which rank as one of the most useful types of transformations in synthetic chemistry.

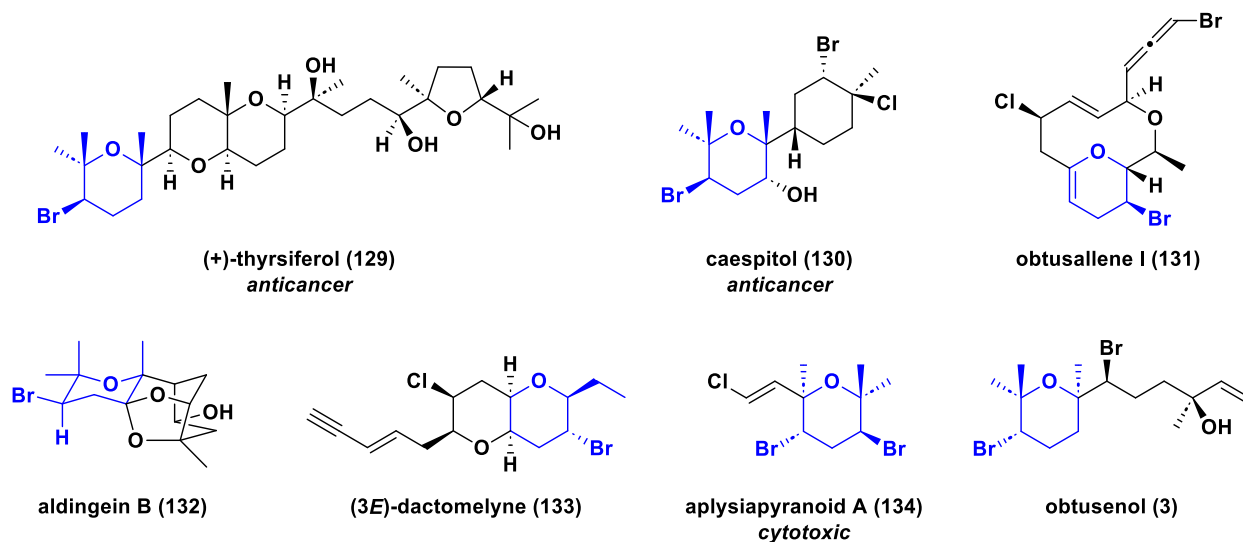
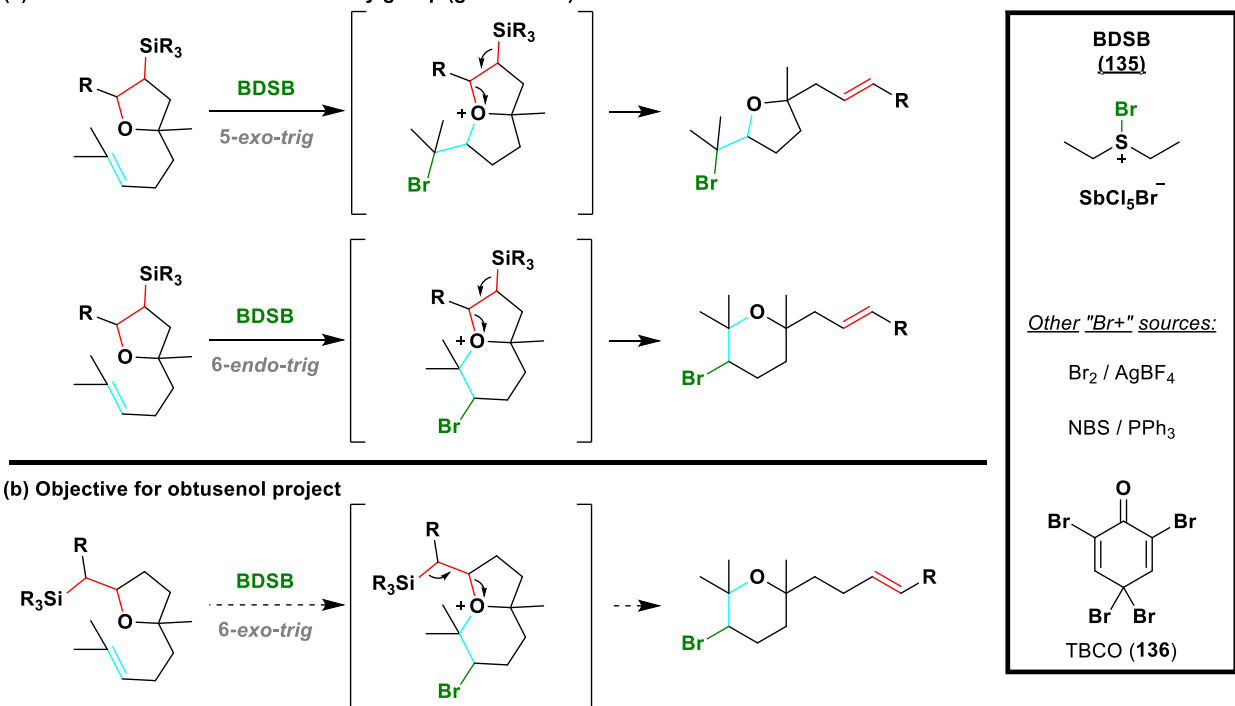


Figure 1.7. Brominated oxanes are extremely common in nature.

In particular, brominated stereocenters in oxanes make frequent appearances in natural products. Therefore, members of our research group previously developed a novel reagent $\text{Et}_2\text{SBr}\cdot\text{SbCl}_5\text{Br}$ (BDSB, **135**) which, among other transformations, can enantioselectively induce bromonium-driven polyene cyclization and ring-expanding bromoetherification. As a highly electrophilic brominating reagent, BDSB offered key advantages over other existing electrophilic bromine sources at the time, such as enantioselectivity and its ability to react with electron-deficient species without undesired side pathways such as elimination.⁶¹ For example, the Snyder group and others have demonstrated BDSB's ability to enact ring-expanding bromoetherifications by precipitating intramolecular bromonium-induced cyclization, such as via 5-*exo* or 6-*endo* (**Scheme 1.17a**) as well as (not shown) ring-expansions with medium-sized 7-9-membered systems. BDSB's broad utility for both this and other transformations has been previously reviewed, and BDSB was commercialized by Sigma-Aldrich after its debut by our group in 2009.^{61–64}

(a) Previous mechanisms achieved by group (generalized)

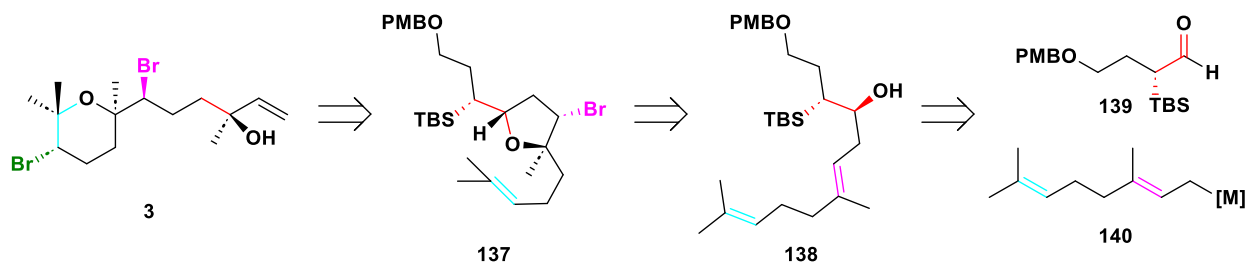


Scheme 1.17. Synthesis of obtusenol (**3**) was envisioned as a case study for exploring the potential to elicit 6-*exo-trig* with BDSB (**135**).

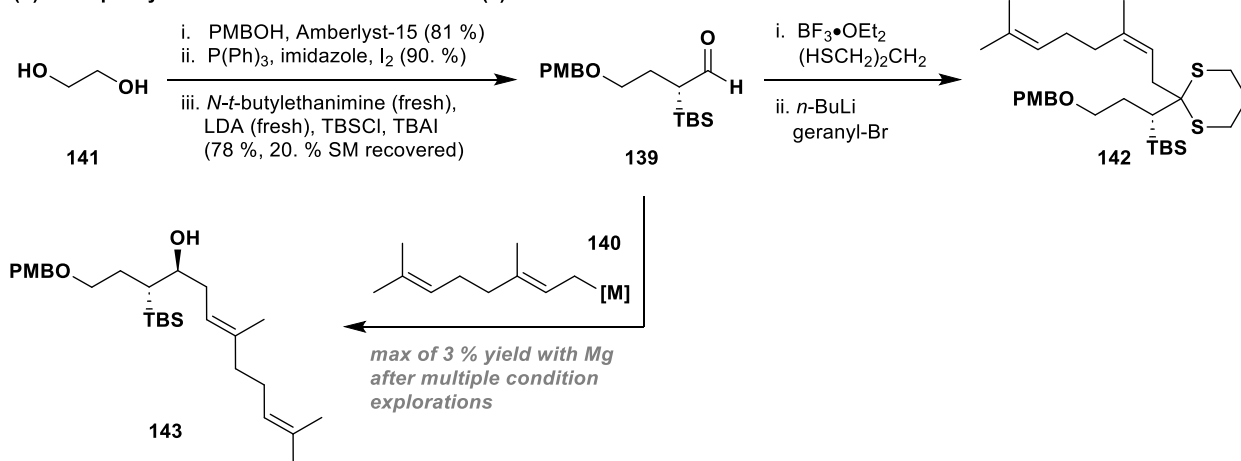
Cheered by this positive reception, our group wished to further explore potential applications of BDSB. Our group had previously demonstrated the ability to induce the challenging 6-*endo* ring-expansion, which is normally outcompeted by 5-*exo* in such systems.⁶⁵ We now wished to investigate whether it was possible

for BDSB to coax a reaction to follow a 6-exo pathway (**Scheme 1.17b**). Therefore, we decided to pursue a total synthesis of obtusenol (**3**) as a case study for 6-exo cyclization (**Scheme 1.18a**).⁶⁶ My responsibility for this project was to complete the first half of the synthesis, which was reached after multiple optimization attempts. For example, despite the penchant for geranyl units to autocyclize in basic conditions, I was ultimately able to push the synthesis to the halfway point. Transmetalation attempts with aldehyde **139** using In, Sn, Zn, Ti, Rieke Mg,⁶⁷ and other variants yielded only 3 % yield at max, but this finicky addition was achievable using thioether **142**, a variant of our originally-envisioned aldehyde (**Scheme 1.18b**). However, the team's efforts were later redirected toward broadening access to 8-membered ring cyclizations instead, successfully producing a generalizable synthetic pathway toward multiple 8-membered cyclic ethers in the *Laurencia* family in the hands of my collaborators Yu-An Zhang and Natalie Yaw.^{64,68} These successes happily broaden the known utility of BDSB as an option for accessing a variety of brominated cyclic ethers.

(a) Original retrosynthetic plan



(b) Example synthetic efforts toward obtusenol (**3**)



Scheme 1.18. Synthetic efforts yielded a pre-cyclization precursor.

1.15 Example Methodological Efforts Toward a Nitrone-Based Mannich-Type Reaction

Another common functionality seen across the natural product landscape is that of the amine. Specifically, piperidines are common motifs observed in bioactive alkaloids (**Figure 1.8**), such as lobeline (**144**) and (-)-3-O-acetylspectraline (**145**), and are highly desirable pharmacological targets for investigation.^{69,70} In piperidines where stereocenters exist on both sides of the amine (i.e., 2,6-disubstitution), pathways for achieving the two-sided chirality are highly desirable.^{69,70} Unfortunately, while several reaction types exist for such access to 2,6-disubstituted piperidines, they tend to involve preinstallation of the substituents and the requisite stereochemistry in complex linear starting materials which then ring-close, such as via nucleophilic displacement or an intramolecular aza-Michael addition.⁶⁹ As a result, methods which could discriminately install functionality on either side directly from commercially available piperidine itself would be particularly advantageous, enabling both convergent strategies for a variety of total syntheses and flexible modular assembly of synthetic derivatives for structure-activity tests.

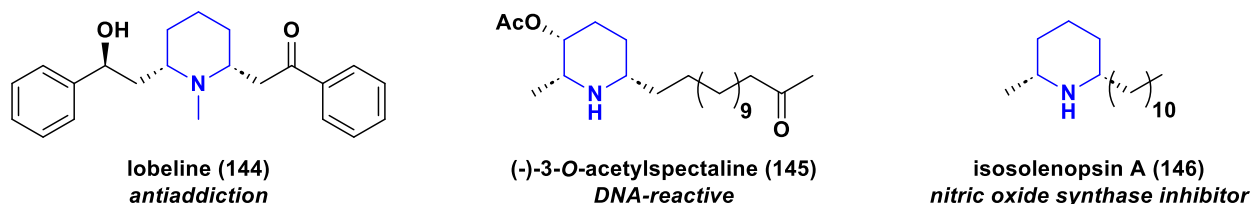
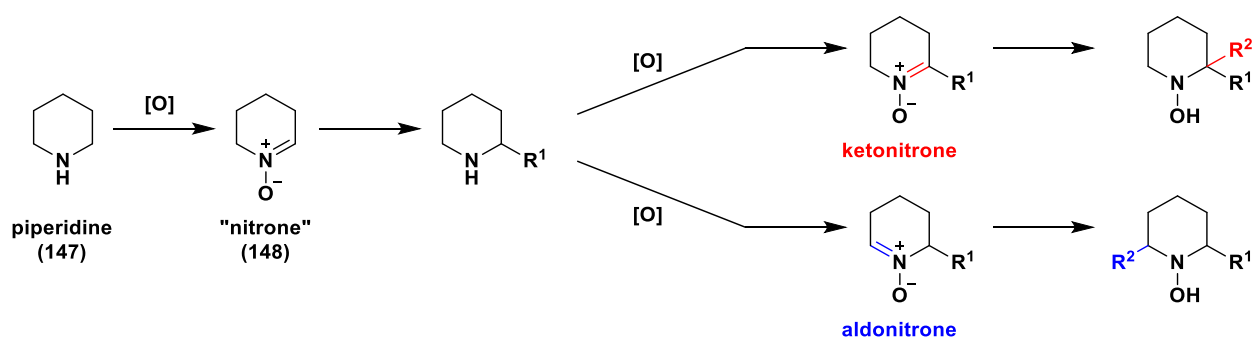


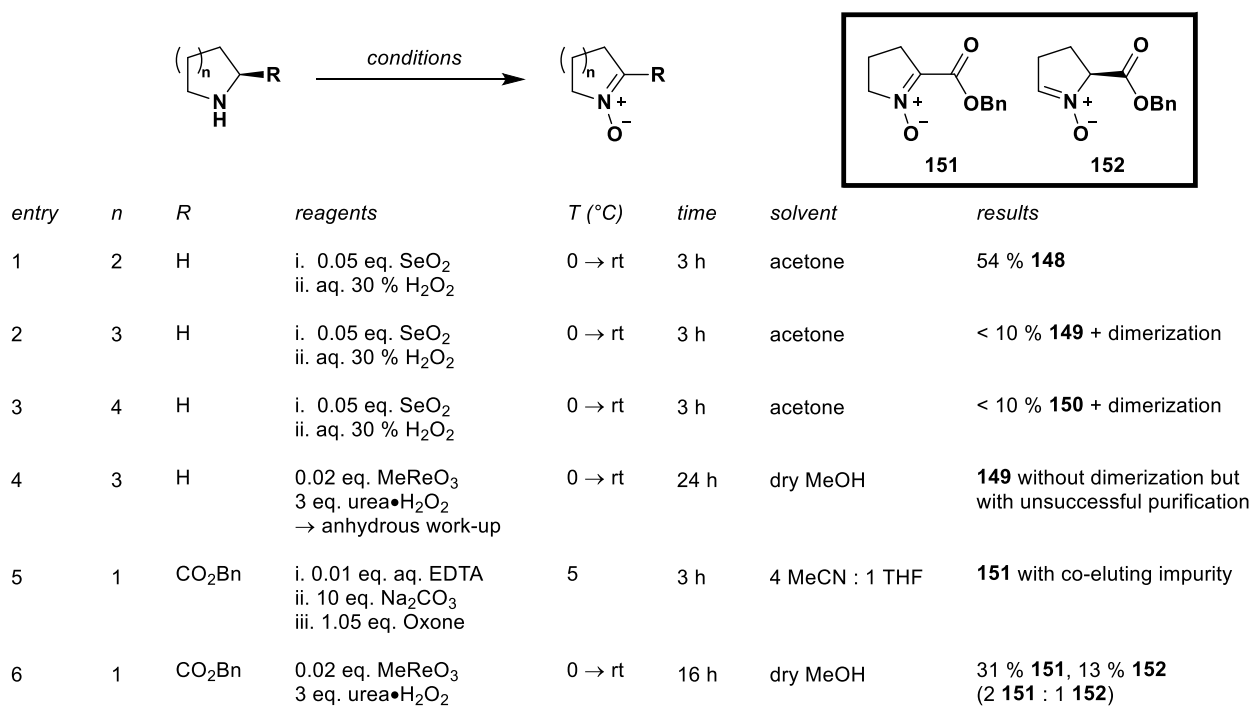
Figure 1.8. 2,6-disubstituted piperidines are common in biologically potent natural products.

Therefore, in pursuit of efficient methods for achieving chiral 2,6-disubstituted piperidines, my collaborator Vladislav Lisnyak envisioned developing a Mannich-type reaction capable of such differentiation, starting from a nitrone. Nitrones were already known to engage in Mannich-type reactions at the time, but regiocontrol remained a key issue (**Scheme 1.19**).⁶⁹ While the ketonitrone is generally favored over the aldonitrone, the ability to selectively induce the latter would greatly facilitate easy access to a variety of connectivities. Our objective was consequently to elucidate conditions which would allow preferential regioformation of either keto- or aldonitrone and, if possible, to do so enantioselectively.



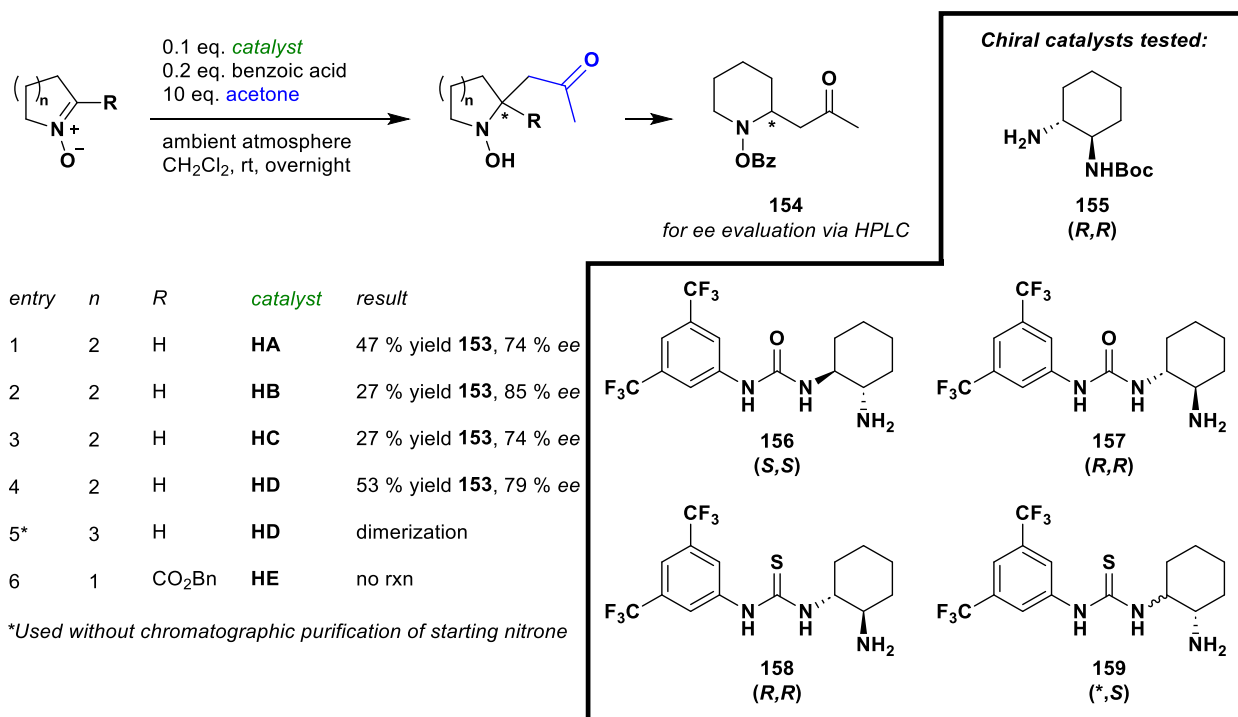
Scheme 1.19. Regiocontrol is a key issue for nitron formation.

My responsibility was to populate initial methodological results by scoping out potential opportunities for achieving such reactivity. I first quickly probed conditions for formation of medium-sized cyclic nitrones (**Scheme 1.20**), which are known to be problematic due to their tendency to dimerize.⁷¹ Fortunately, I was able to generate a 3° hexacyclic nitron (entry 1, **148**) and 4° pentacyclic nitron (entry 6, **151**) for substrate testing in acceptable (unoptimized) yields.^{72,73} Dimerization of the heptacyclic and octacyclic nitrones was not surprising in the presence of water (entries 2 and 3). While maintaining strictly anhydrous conditions in entry 4 indicated formation of the desired monomeric cycloheptanitron **149**, the monomer did not survive chromatographic purification and so was maintained crude after work-up.



Scheme 1.20. Cyclic nitrones were generated for testing.

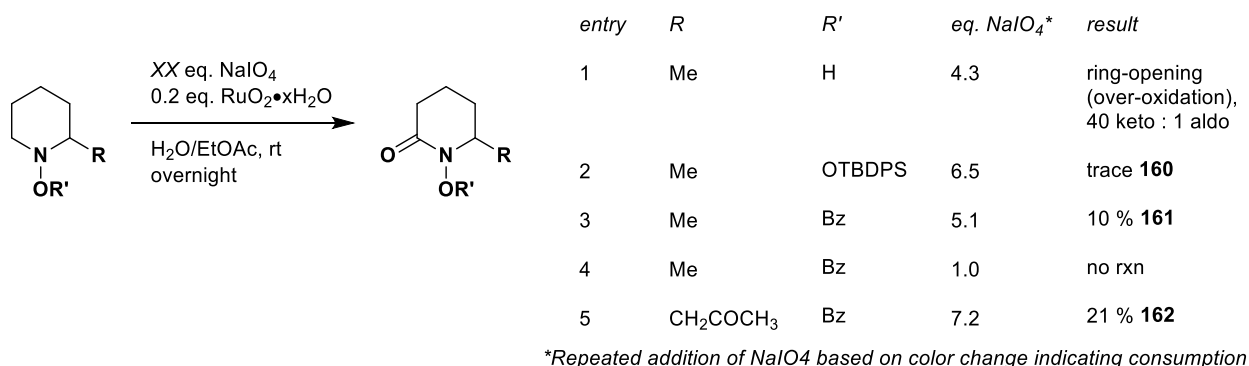
With isolated **148** and **151** as well as unpurified **149** in hand, these nitrones were pushed forward for proof-of-concept screening to confirm their ability to undergo Mannich-type reactions with chiral catalysts (**Scheme 1.21**). The popular urea-derived family of chiral catalysts was selected for these initial screens and prepared as previously described in the literature.^{74–77} While the Jacobsen urea catalysts **156** and **157** produced low yields of hydroxylamine **153** (albeit with good ee), the Wang thiourea catalyst **158** reassured us that yields could likely be improved later on to acceptable levels with strong enantioselectivity. The (unoptimized) yield of 53 % in entry 4 therefore gave the green-light for the project to proceed further by indicating the ability of 6-membered cyclic nitrones to engage in such Mannich-type reactions with enantioselectivity. The next phase was therefore to scope out the potential for preferentially forming aldonitrones over ketonitrones with monosubstituted hydroxylamines, a known challenge. Unfortunately, neither the 4° 5-membered ring nor the 7-membered ring produced encouraging results during catalyst testing, and so only the 6-membered ring was utilized in subsequent screens.



Scheme 1.21. Chiral catalysts were capable of installing a substituent on the 6-membered ring.

Based on prior precedents where ruthenium complexes enabled oxidations adjacent to piperidine-like molecules and other metal complexes formed nitrones from hydroxylamines,^{78–83} I first screened conditions

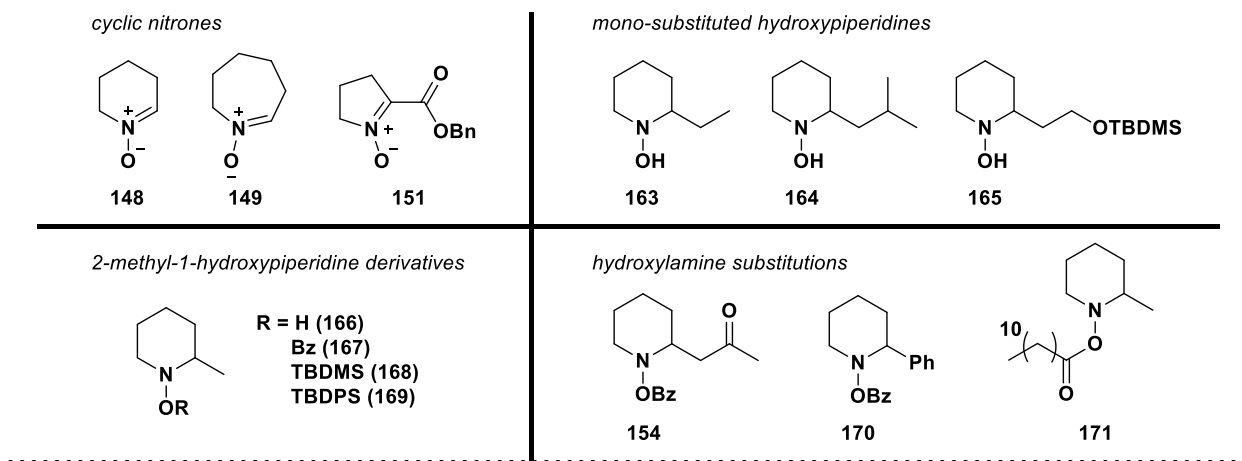
for α -oxidation (**Scheme 1.22**) in the hopes that hydroxamate formation may yield the desired regiocontrol directly for the second substitution pattern. The hydroxamate could theoretically later be used as a functional group handle. Results were not sufficiently encouraging, however, to continue pursuing this pathway for long.



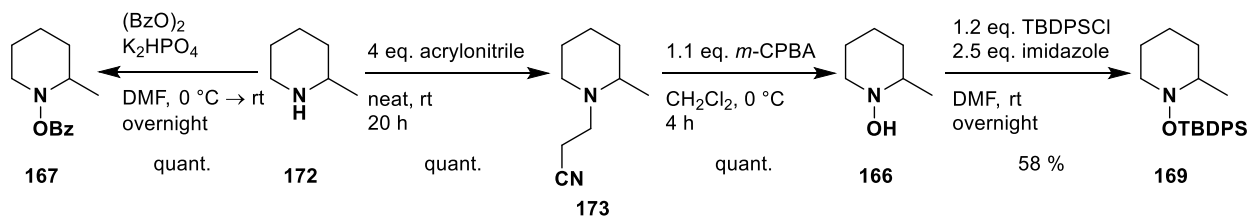
Scheme 1.22. Oxidative screening did not yield encouraging results for a hydroxamate pathway.

My attention was instead turned toward aldonitrone formation using 2-iodoxybenzoic acid (IBX, **174**). IBX is well-known as an excellent oxidizer of nitrogen-based functional groups.^{56,57,84} Therefore, I synthesized a couple IBX variants and conducted a screening campaign to sniff out potential tunability for regiocontrol in nitrone formation. In addition to the substrates previously described, the screening campaign focused mostly on simple aliphatic hydroxypiperidines and their derivatives (**Scheme 1.23a**) which were conveniently accessible, often in a few steps from a series of commercially available amines (**Scheme 1.23b**).

(a) Example selection of substrates prepared for testing



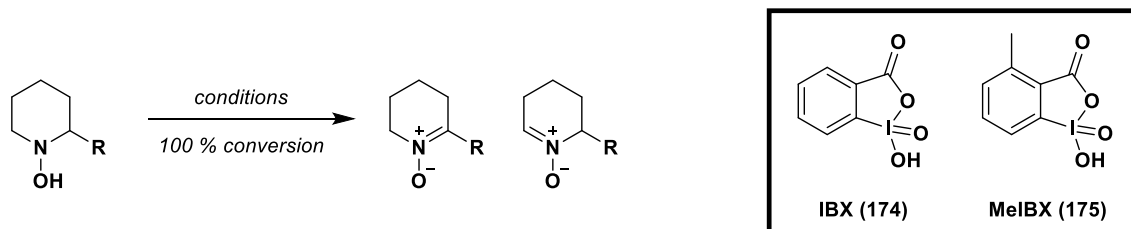
(b) Example synthetic preparation of hydroxylamines & derivatives



Scheme 1.23. Examples of screened substrates.

Of the approximately 40 conditions tested in this final screen, 15 illustrative examples are displayed below for conciseness to demonstrate 4 key themes which emerged (**Scheme 1.24**). Firstly, the sidechain on the hydroxylamine played an important role in regioselectivity whereby the larger aliphatic chains increasingly favored aldonitrone formation (entries 5, 10, 14 and 15). An aromatic side chain (entry 16) was less favorable than aliphatic. Secondly, while MeIBX (**175**) is known for having a lower activation energy barrier than IBX in the rate-determining hypervalent “twisting” step of IBX reactions,⁸⁴ it did not appear to significantly impact the reaction outcome other than to cut down on the required timescale (entries 10 vs. 12 and 11 vs. 13). Thirdly, temperature played a nuanced role in that lower temperatures favored ketonitrone formation while higher temperatures led to complex mixtures; temperatures around 0 °C appeared to be a sweet spot for aldonitrone formation (entries 8, 5, and 9). Finally, the choice of solvent was crucial. Highly polar and moderately polar solvents gave less desirable results than lower polarity, and it seemed possible that H-bond donors / acceptors should also be avoided (entries 1 – 7). Of the solvents displayed here, for example, benzene and dichloromethane were the best performers. Notably, hexanes

appeared too nonpolar; IBX adhered strongly to the reaction flask rather than enter suspension. Additionally, note that the aldonitrone did not necessarily maintain their integrity after formation, with some degradation into an aldehyde noticed for each condition. Aldehyde presence after purification was, however, taken as evidence of aldonitrone formation.



entry	R	oxidant	eq. [O]	T (°C)	time*	solvent**	keto : aldo formation	aldonitrone : aldehyde
1	Me	IBX	1.0	rt	1.5 h	d ₆ -DMSO	100 : 0	---
2	Me	IBX	1.0	0	2 h	H ₂ O	50 : 1	1 : 0
3	Me	IBX	1.0	0	2 h	EtOAc	7.7 : 1	1 : 5.5
4	Me	IBX	1.0	0	2 h	THF	5.0 : 1	1 : 1.5
5	Me	IBX	1.0	0	1 h	CH ₂ Cl ₂	2.2 : 1	1 : 0.1
6	Me	IBX	1.0	5	2 h	benzene	2.4 : 1	1 : 0.5
7	Me	IBX	1.0	0	24 h	hexanes	100 : 0	---
8	Me	IBX	1.5	-40 → -15	2.5 h	CH ₂ Cl ₂	4.8 : 1	1 : 0.2
9	Me	IBX	1.5	rt	2 h	CH ₂ Cl ₂	complex mix	---
10	Et	IBX	1.0	0	2 h	CH ₂ Cl ₂	1.0 : 1	1 : 2.1
11	Et	IBX	1.0	5	1 h	benzene	0.8 : 1	1 : 2.2
12	Et	MeIBX	1.0	0	10 min	CH ₂ Cl ₂	1.0 : 1	1 : 4.6
13	Et	MeIBX	1.0	5	10 min	benzene	1.1 : 1	1 : 1.9
14	<i>i</i> -Bu	IBX	1.0	0	30 min	CH ₂ Cl ₂	0.6 : 1	1 : 0.3
15	Ph	IBX	1.0	0	22 h	CH ₂ Cl ₂	4.0 : 1 in complex mix	1 : 1.8

*Reactions were allowed to run until starting material was consumed

**IBX was insoluble in hexanes, requiring long reaction times

Scheme 1.24. 15 examples of the screened conditions with IBX reveal 4 key patterns.

Ultimately, these initial methodological investigations revealed both that Mannich-type reactions could be conducted enantioselectively with nitrones and that there is potential for preferring aldonitrone formation (entries 11 and 14), albeit with only modest discrimination obtained here. Overall, these results demonstrated the viability of this project which was carried forward to completion by my collaborators Lisnyak and Tessa Lynch-Colameta: they successfully generated a robust set of Mannich-type reaction

conditions for enantioselective synthesis of diverse piperidine motifs.^{21,85} Gratifyingly, the utility of such a convenient entry into enantioselective piperidine substitution was speedily recognized in a following review about stereoselective piperidine syntheses.⁶⁹ We look forward to seeing widespread adoption of these methods in alkaloid synthesis moving forward.

1.16 Conclusion

The discipline of natural product total synthesis has been and remains one of the most ambitious endeavors in the field of organic chemistry – and, concurrently, one of the most challenging with high failure rates and dogged research teams. In this chapter, four separate projects were outlined in the pursuit of natural product synthesis toward the dankasterone, illisimonin, organobromine, and piperidine families. Fortunately, my collaborators and I were ultimately able to together achieve an enantioselective modular total synthesis of the dankasterones in spite of the complex, stereochemically rich skeleton. Conversely, while synthesis of illisimonin was not achieved before a competitor, the other team's success delivered validation of the key approach in my retrosynthetic analysis. Meanwhile, I am gratified that my early investigative efforts toward bromonium-induced cyclization and asymmetric Mannich-type nitron reactions assisted other teams in ultimately achieving methodological breakthroughs toward common structural motifs. By heralding new structural paradigms and inspiring chemists down new pathways, natural products continue to rein as one of nature's greatest gifts.

Chapter 2

A Day in the Life: Characterization of Doctoral Bench Research in Synthetic Chemistry Using Phenomenological Case Studies

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2.1 Abstract

Despite decades of reform efforts, STEM education continues to face calls for improvement, especially regarding the teaching laboratory. Establishing an empirical understanding of the types of hands-on, psychomotor skills that students need to learn to succeed in downstream careers could help ensure laboratory courses are promoting authentic learning. Therefore, this paper reports phenomenological grounded theory case studies characterizing the nature of benchwork in synthetic organic chemistry graduate research. Through first-person video data and retrospective interviews, the results illustrate how organic chemistry students use psychomotor skills to conduct doctoral research and where they acquired those skills (**Figure 2.1**). By understanding the role that psychomotor skills play in authentic benchwork and the role that teaching laboratories play in the development of those skills, chemical educators could revolutionize undergraduate laboratory experiences by enabling evidence-based incorporation of the psychomotor component into laboratory learning objectives.

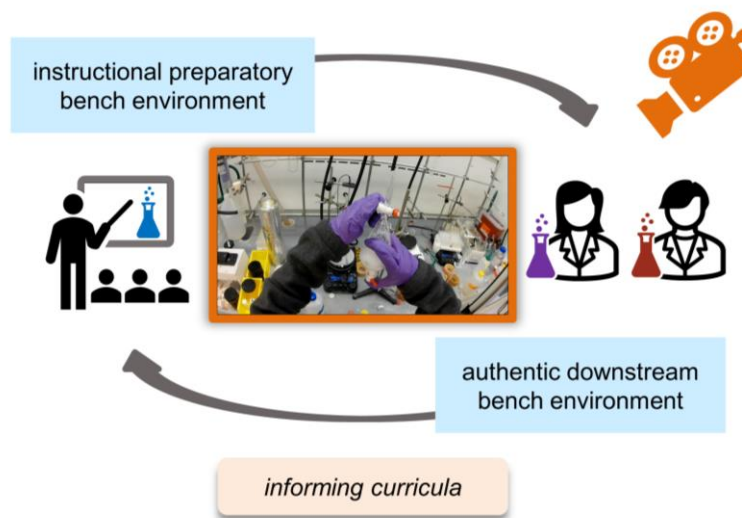


Figure 2.1. Phenomenological case studies of chemists at the bench will inform laboratory curricula.

2.2 Introduction

The purpose, role, and effectiveness of laboratory education are currently subjects of renewed debate.^{86–93} Evidence is building that current practices in undergraduate laboratory courses may not promote desired learning outcomes as effectively as hoped. As a result, curriculum reform efforts in the laboratory sciences are increasingly popular, such as replacing oft-disparaged replicative cookbook experiments with inquiry-based experiments and course-based undergraduate research experiences (CUREs).^{94–99} Concurrently, doubts have also been raised as to whether hands-on laboratories themselves are a worthwhile investment or as pedagogically unique as previously assumed.^{100–115} In the wake of widespread precedents for virtual learning set by the COVID-19 pandemic, some educators are exploring the possibilities afforded by the adoption of increasingly sophisticated virtual laboratories whereas others eagerly return to classrooms with renewed conviction in the value of hands-on laboratories. As a result of the enthusiasm for this topic, publications about the laboratory are proliferating in discipline-based education research (DBER) journals across STEM fields.^{88,100,116,117}

Regardless of the ultimate design elements, content, or modality that future curricula adopt, laboratory education is clearly on the cusp of a revolution. However, while the DBER community's understanding of the landscape of effective laboratory practices is accelerating, the frontier is far from conquered. Many unknowns persist. One glaring black hole compromising educators' abilities to effectively design what are here dubbed as next-generation laboratory standards (NGLSS) is the lack of a shared, empirical understanding for what the product should look like: what do students need to know and be able to do to be successful bench scientists downstream, after they complete their formal education? While many students in chemistry courses do not ultimately become chemists, one rationale for offering such experiences is to prepare students for laboratory careers. Prior research has revealed important aspects of affective and cognitive domains to cultivate in STEM education as well as general traits that support good scientific practices.^{118–121} However, while there have been prior research efforts regarding the cultivation of psychomotor skills (e.g., developing rubrics to assess execution of specific experimental techniques),^{122–125} there is not yet a literature basis for characterizing the specific types of psychomotor skills that students need to learn for future chemistry careers. Likewise, the “neglected materiality” component of chemistry teaching laboratories has recently been highlighted,¹²⁶ suggesting that chemistry education research has

focused less on the physical domain of laboratory science experiences than the non-physical in recent years. Since laboratories are fundamentally physical environments requiring practitioner expertise with a variety of specialized tools and techniques, further deliberate investigation into the development of chemists' psychomotor skills is warranted.

A systematic characterization of requisite psychomotor skills would therefore assist curriculum reform efforts to develop NGLSs for psychomotor skills relevant to laboratory-based careers. While many chemistry laboratory courses include classical techniques shared in common across institutions and decades (e.g., gas chromatography, distillation), each course designer exercises agency over the experiments students will conduct. With this agency comes diversity in the tools and techniques which students are exposed to, trained in, and assessed on, based on the course designer's prior experiences, personal skills, and beliefs about the importance of various skills. Additionally, it is also important to recognize that most existing evidence about laboratory learning (and learning in general) revolves around introductory undergraduate students.^{88,120} The dearth of attention to professional chemists adds uncertainty to the development of NGLSs without knowledge of how laboratory learning sets a foundation for downstream careers. For example, do graduate students rely on cookbook techniques they learned in traditional undergraduate labs, and are those techniques effectively fostered in inquiry classrooms? What types of skills do industrial bench chemists need mastered to meet employer expectations, and does that differ from what academic chemists learn? How do introductory students later build on foundational experimental skills to master complex techniques? Although "the bench" is not the only destination for chemistry students, the bench is nonetheless an integral part of experimental science in downstream careers.

Therefore, to maximize the likelihood that future laboratory course reform endeavors will lead to substantive improvements in the competencies of the STEM workforce, there is a pressing need for evidence regarding what laboratory skills students need for downstream career success and how to most effectively build those skills. Empirically elucidating the nature of the skills that laboratory-based chemists use could generate a shared, empirical understanding of NGLSs that supports educators in their quest to improve STEM education. This paper therefore reports on the validation and implementation of a method used to characterize psychomotor skills executed by practicing chemists (here, PhD chemistry student

workers) in an authentic laboratory workplace environment. Understanding the skills practicing chemists use could then inform subsequent undergraduate laboratory reforms.

2.3 Research Questions

This study sought to characterize the nature of chemical benchwork in an authentic laboratory workplace by asking two driving questions:

1. How do chemists use their psychomotor skills when conducting bench research?
2. Where did those chemists learn the psychomotor skills?

2.4 Frameworks

Due to the dearth of information about professional chemists' experiences in laboratory workplaces, a phenomenological grounded theory case study framework with naturalistic and retrospective data was adopted to capture a set of participating chemists' first-person experiences, thus fueling an emergent understanding of such environments.¹²⁷ Phenomenology is the study of an individual's experience of phenomena through their own perspective, enabling the researcher to accept their reports as true interpretations of their experiences.^{128,129} Phenomenology is distinct from many other frameworks in that it focuses around the individual's experience of phenomena rather than the researchers' outsider perceptions of the experience. Phenomenology also often focuses on illuminating the individual's intentionality in engaging with the world in conjunction with understanding their lived experiences. This phenomenology was pursued using a highly authentic naturalistic observation protocol coupled with retrospective interviews which involved the participants in contextualizing and validating the observations.^{130,131} Due to the inherently physical nature of psychomotor skills, participants were outfitted with action cameras on their heads to capture their first-person perspectives as organically and accurately as possible; the phenomenology was almost literally "through their eyes". Through retrospective interviews, the participants later provided contextualization of those observed experiences.

These naturalistic observations and participant perspectives were analyzed via grounded theory in tandem with data collection. Grounded theory is a methodological framework that relies on emerging themes to concurrently guide data collection and analysis, enabling the researcher to begin a study with

minimal preconceived assumptions about the prospective data.^{132–134} Following where the data leads then results in a tailored framework based authentically on the data. Grounded theory was pursued using case studies to enable a deep dive into the psychomotor skills used by individual chemists and the origins of those skills for each individual.

Together, these frameworks and reflective memoing during the study led to the development of a novel, emergent framework (here dubbed the MA–ETP framework, **Figure 2.2**) through which the final data was analyzed. Inductive open basic coding of the psychomotor actions that participants engaged in during naturalistic observation yielded descriptions of those actions both in terms of the physical action itself and the underlying rationale for engaging in it. These “meaningful actions” were connected to each other in terms of the equipment used, techniques they were a part of, and the real-world purposes that they were meant to achieve (ETP). The MA–ETP framework formed the backbone of the data analysis.

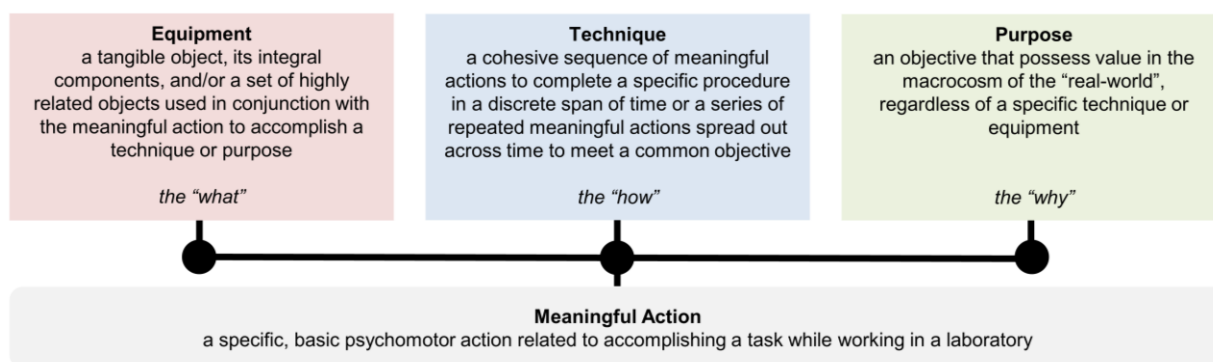


Figure 2.2. Phenomenological grounded theory led to the development of the MA–ETP framework to characterize psychomotor actions in a graduate synthetic chemistry research laboratory. Psychomotor actions were coded with inductive open basic codes (Meaningful Actions) which were later assigned one each of an Equipment, Technique, and Purpose code during axial coding.

2.5 Methodology Overview

Purposeful convenience sampling led to the recruitment of two synthetic chemistry PhD candidates and their research group in an academic laboratory.¹³⁵ Over the course of a few months with 6 recording sessions and 8 interviews, the study activities led to in-depth coding and cluster analyses that yielded rich data about the role of psychomotor actions at “the bench”.

2.6 Recruitment

Academic research laboratories were targeted as sources of potential participants by convenience sampling. Purposeful sampling was then utilized to specifically target wet synthetic chemists due to (1) the bench-intensive nature of synthetic chemistry research and (2) the author's personal background in PhD-level synthetic chemistry (thus enabling accurate identification of psychomotor skills and materials used). Therefore, R1 Principal Investigators (PIs) with synthetic chemistry research laboratories in the United States were approached for consent to recruit their group members and conduct recording activities in the group's laboratory spaces. Participation was limited to PhD students/candidates to ensure that participants (1) were engaged in benchwork as the primary component of their jobs and (2) were recent college graduates who could make informed reflections about their undergraduate education's relationship to their current psychomotor laboratory skills. Additionally, all group members were recruited to give consent to enable the recording to continue uninterrupted regardless of who might enter the camera's range. A laboratory in the recruitment process yielded consent from all group members as well as two participant volunteers. Therefore, that laboratory was selected to proceed with the study. Both participants were 2nd-year organic methodology PhD candidates working on separate projects. Participants received nominal financial compensation for their time. Neither the participants nor their work were previously known to the author.

2.7 Ethics

IRB approval was issued by the author's institution. Due to the placement of the author and recording equipment within a live workplace, special steps were taken to protect privacy rights and comply with laboratory safety mandates. Workplace actions were not adjusted as a result of the recording, as affirmed by the participants. The video stream from the camera was projected live onto a second screen with remote control capabilities and monitored by the author. If a participant left the designated rooms (e.g., to visit the NMR facility), the camera was temporarily removed, and recording was paused. The participants, participating group, and institution are not named. The PI of the participating group reviewed all images in this article to prevent identifiable visual data from appearing in publication, such as images which might identify the group or the status of their unpublished work. Finally, although grounded theory usually follows

a data saturation model to determine when to stop collection, the length of recording was fixed at 2 hours / session over 3 sessions / participant with the assumption that 12 hours of recording would likely provide sufficient data for a thorough analysis.

2.8 Study Activities and MA Coding

1) Pre-Recording: Participants provided contextual information about their projects, current academic position, and prior laboratory experiences when they volunteered.

2) Recording: Visual data only (no audio) was collected using an action camera attached to a hat on the participant's head, angled slightly down to capture what their hands were doing (**Figure 2.3**). A secondary camera was positioned to film the participant if the action camera was not providing sufficient detail, but this precaution proved superfluous. Each participant underwent three 2-hour recording sessions over a few months (**Figure 2.4**). Participants proposed time slots for each recording session a few days prior for when they expected to be actively conducting benchwork.



Figure 2.3. Naturalistic observation was conducted using a first-person action camera worn on a flipped hat.

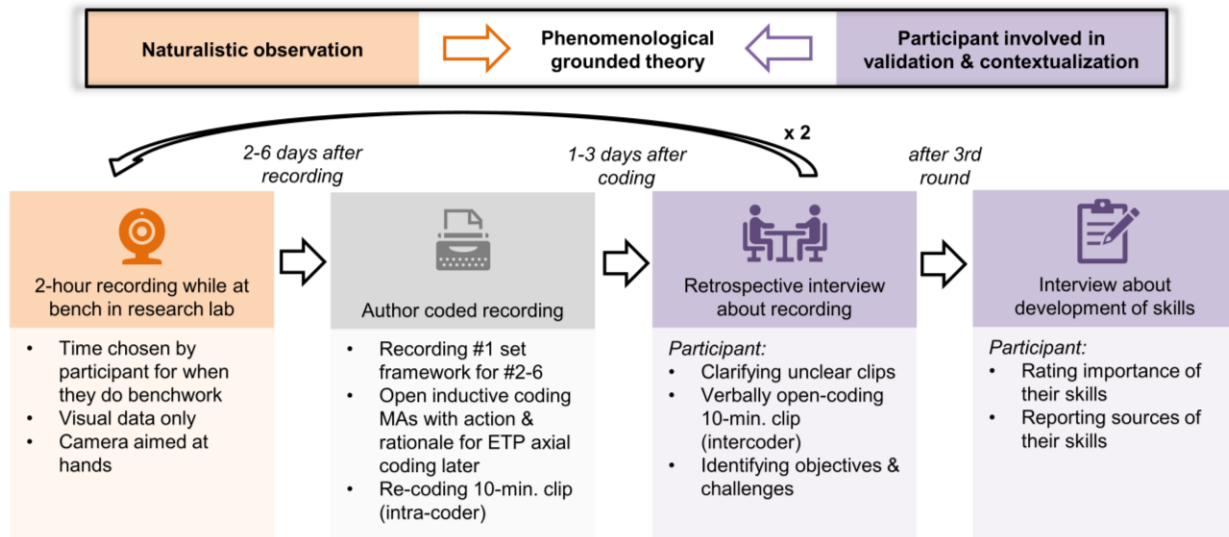


Figure 2.4. Study activities began with a recording session, followed by coding the recording and conducting a retrospective interview. Naturalistic observation and participant-derived contextualization enabled analysis via phenomenological grounded theory.

3) Between Recording and Retrospective Interview: Every recording was coded using inductive open basic coding to identify “Meaningful Actions” (MAs, **Box 2.1**). The author was surprisingly able to deduce not only the psychomotor skills the participants used but also the underlying rationale for the actions, possibly as a result of personal experience with synthetic research and apparent similarity in synthetic methods between groups and institutions. Therefore, MA codes articulated both the action and the apparent rationale for the participants’ psychomotor actions in sentence-like descriptive text. Video clips had to clear three criteria in order to be eligible for coding (**Box 2.1**). Codes could overlap other codes (i.e., the participant could be engaged in more than one MA at a time) and were of varying duration depending on the action. Clips where the action or rationale were ambiguous to the author were marked for later review with the participant. A random 10-minute segment of each recording session was coded again to gauge intra-coder reliability. Reflective memoing for the first recording of the study was used to develop the MA-ETP framework (**Figure 2.2**) for axial analysis based on the emergent themes of “Equipment”, “Technique”, and “Purpose” (ETP) which characterized the ways that participants used their psychomotor skills. Continued reflective memoing and a living codebook were used throughout with new MA codes continuously added to the codebook, and a list of draft ETPs was updated as necessary. The list of ETP codes was finalized and formally assigned to MA codes after completion of all data collection.

Box 2.1. Criteria for coding Meaningful Actions.

1. The MA code must encapsulate a physical action explicitly seen on camera and conducted by the participant themselves.
 - *Example exclusions:* eye movements, mental processes, actions from other people
2. The MA code must encapsulate an apparent underlying rationale for the action.
 - *Example exclusions:* apparently random or idle movements
3. The MA code must appear to contain some form of meaning for the participant's ability to execute laboratory work, either in terms of the action or the rationale.
 - *Example exclusions:* throwing away paper towels after washing hands, physical manifestations of emotion

Example Meaningful Actions:

- Placing a spatula down carefully so as to avoid contaminating the tip
- Closing the fume hood sash to reduce noise level so labmates don't get annoyed

Example Nonmeaningful Actions:

- Placing a spatula down because there is no reason to hold it anymore
- Fiddling with a knob while waiting for a procedure to finish

4) Post-Recording Interview: A semi-structured retrospective interview of up to one hour was conducted within a week after each recording. Audio was recorded. The semi-structured format was selected in order to enable the interviewer to seek clarification on video clips that confused them and to provide a structure in which to elicit the participant's understanding of the recorded actions. First, the participant was shown a sped-up version of the entire recording via a large projection on the wall to prompt recall. Then, the interviewer highlighted the ambiguous clips, and the participant identified the action and/or explained the underlying rationale. Next, the participant verbally coded a random 10-minute sequence to enable analysis of inter-coder reliability. The participant was instructed to articulate each MA they felt they noticed, with their attention drawn specifically to focusing on psychomotor skills; the concepts of affective, cognitive, and psychomotor domains was defined to the participant beforehand. They were not provided with a codebook so that their verbal coding could serve as a validation check for the author's MA coding. The author actively transcribed each MA the participant articulated in their own words and then displayed the list immediately afterward. The participant was asked if they wanted to provide additional context for any MA. Next, the participant was asked contextualizing questions about their overall actions during the recording time slot, such as what the goal of the experiment was. Finally, the participant was asked whether

they did anything differently as a result of the recording, both to continually ensure that the study was not intruding on workplace processes and to check for potential Hawthorne effects. Participants affirmed that they did not adjust their actions.

5) Repeat: The coding and retrospective interview process was completed three times for each participant.

6) Between 3rd and 4th Interviews: The participant compiled a chronological list of their prior laboratory experiences in preparation for the final interview.

7) Final Interview: The participant was presented with 50 randomly selected MAs coded by the author, and they identified which prior laboratory experience resulted in them learning how to conduct each MA. Then, the participant rated how important they felt it was for incoming organic chemistry graduate students to be able to conduct a selection of 100 random MAs and the ETP items. Finally, they discussed their reasoning for determining the importance of a student knowing those skills.

2.9 Data Processing

Initial background information on the participants and their type of research was collected using either Qualtrics or a paper questionnaire during the recruitment process. After recording, the high-resolution videos were converted to lower resolutions using Xmedia Recode 3.5.4.5. 64bit (<https://www.xmedia-recode.de/en/>) to reduce the large file sizes, thereby enabling analysis in MAXQDA. All videos were coded with MA inductive open basic coding in MAXQDA 20.4.1. All interview audio was recorded and then transcribed using intelligent verbatim transcription in MAXQDA. The participants' verbal coding during the interviews was transcribed verbatim into a spreadsheet and then transported into MAXQDA as MA codes described in their own words. At the final interview, participants filled out paper worksheets (which listed out the sample codes) to rate their perception of the importance of being able to execute their MA and ETP skills and handed in a chronological list of their prior laboratory experiences. After all MA coding was complete in MAXQDA, codes were transferred to Microsoft Excel 365 for ETP axial coding and subsequent analysis. Nominal nonhierarchical two-step cluster analysis with Gower's dissimilarity measure was executed using SPSS 28.0.1.1.^{136,137} All other data processing was conducted using Excel.

2.10 Data Analysis

Together, the two participants yielded 11.1 hours of cumulative recorded time, 6.5 hours of which was covered by 2,447 MA codes (**Table 2.1**). Third-person naturalistic observation by the author was more effective at identifying MA codes than expected with only 5.5 % of coded time requiring review by participants to confirm or provide the action/rationale.

Table 2.1. Descriptive statistics of recordings.

Recording Sessions

- Six 2-hour sessions were recorded over three months (three morning & three afternoon sessions) with two participants (three sessions / participant).
- 11.1 h was recorded and analyzed total.
- 0.5 h was not recorded during sessions due to participants' temporary departure from the site.

Coded Time

- 6.5 h of recorded time (58.4 %) was coded.^a
- 0.6 h of coded time (9.4 %) featured overlapping MA codes.
- 100 clips (0.4 h total = 5.5 % of coded time) needed to be reviewed by participants to clarify their action or rationale.

Codes

- 2,447 MA codes were assigned (average 408 codes / recording session).
- 303 incidences of MA code overlaps occurred (24.8 % of MA codes overlapped with another code).
- MA codes were sorted into one each of 32 Equipment, 30 Technique, and 20 Purpose codes.

^aThe recorded time without codes often consisted of nonmeaningful actions such as walking around the lab, pausing to think, visually observing changes, or waiting for a procedure to finish.

Unfortunately, calculating inter-rater and intra-rater reliability (or, more properly termed for this type of nominal data, inter-coder / intra-coder reliability)¹³⁸ is highly challenging for complex naturalistic observational video data featuring overlapping open codes and an evolving, living codebook. Attempts to quantify such comparisons present problematic implications and oversimplification due both to the nature of grounded theory research and the statistical issues arising from a large, complex codebook with multiple rare codes (e.g., prevalence discrepancies).^{130,138–142} However, visual analysis of the coding (see **Appendix B**) illustrated an apparently high degree of agreement between the participants and author in assigning MA codes, especially after accounting for restrictions that the author operated under in assigning codes which the participants did not (**Box 2.1**). The participants sometimes provided more MA codes during their verbal open

coding because they could recall cognitive decisions they were making or report on what their eyes were doing behind the camera. They also sometimes mentioned actions that did not appear meaningful (e.g., walking around the lab) seemingly when there was a long gap between MA codes; they appeared to feel a need to fill the silence rather than believing that the actions were truly meaningful. Since the participants were not trained qualitative coders, these discrepancies were not surprising. The author did not correct or interrupt the participants during their coding in order to avoid cuing and to preserve the authenticity of participants' responses. Accounting for these discrepancies between author and participant coding, the apparent agreement in the visual analysis is encouraging. Since phenomenology is rooted in the acceptance of the participant's observations as true interpretations of their experiences, the strong agreement also validates the author's MA coding.

The emerging ETP axial codebook was then finalized with 32 types of equipment, 30 types of technique, and 20 types of purpose that the MA codes were employed in service of (see **Appendix B** for detailed ETP code descriptions and examples). Each Equipment, Technique, and Purpose code was assigned individually to the MA codes to accurately reflect what the action was, how it was being conducted, and why it was used (**Table 2.2**). This careful coding process enabled differentiation for codes that might share one ETP code but not another (e.g., having different purposes despite both being part of a column chromatography technique). Due to the complexity of authentic benchwork, some ETP codes presented the possibility for overlap with other ETP codes. Therefore, some codes were designated as "secondary" to clarify and streamline the coding process whenever a potential conflict was uncovered during ETP coding. An MA code could only be assigned to a secondary ETP code if no other primary code could reasonably be applied (**Box 2.2**). Purpose codes were assigned using a "film negative" rationale (drawing upon photography film terminology): the purpose was deduced by considering what the consequences would have been if the action was not undertaken. Six types of Purpose codes presented substantial subcategories referred to here as "optimization", whereby the participants engaged in actions meant to save them time, effort, or otherwise proactively act to avert a potential issue that would cost them either.

Table 2.2. Examples of ETP codes.

Meaningful Action	Equipment, Technique, Purpose	“Film Negative” Rationale for Purpose
<i>Example of how Purpose codes can vary with the same Equipment and Technique</i>		
Labeling column name in automated column's computer to keep track of conditions	Equipment: automated column Technique: column chromatography Purpose: enable repetition via records	Without this step, the record of the column conditions would be lost. Future researchers would be challenged to replicate the same purification procedure.
Programming pause to fix leaky connection	Equipment: automated column Technique: column chromatography Purpose: optimization – maximize product yield	Without this step, product would have been lost through the leak as it came off the column. The obtained yield would have been diminished.
<i>Examples of the difference between standard Purpose codes and optimization Purpose codes</i>		
Programming automated column conditions for column	Purpose: purify product	Programming the conditions is a necessary step for automatic chromatographic purification. Purification would not have happened without this step.
Adjusting column conditions to finish up faster	Purpose: optimization – purify product	Adjusting the conditions saves the researcher time. Purification would still have happened without the step, but it would have taken longer.

Box 2.2. Examples of Primary vs. Secondary codes.

Primary Equipment Code: Even though a bump trap is glassware, manipulating a bump trap falls under the primary “rotatory evaporator” Equipment code.

Secondary Equipment Code: Manipulating a separatory funnel did not fall under any primary Equipment codes and so was assigned to “standard glassware”.

2.11 Results Overview

The MA coding documented how the participants were using specific psychomotor skills in the research laboratory environment. The large number of actions and time spent executing them suggest that the participants were effective at using a diverse skillset productively and continuously in the laboratory in pursuit of a variety of goals. Considering that nonmeaningful actions (e.g., walking around, observing changes, consulting with labmates) were not coded, the 6.5 hours of coded time out of 11.1 hours of recorded time implies that the participants moved quickly from one MA to another with a high level of sustained activity at the bench. Diving deeper into specifics regarding what they were doing and how those actions relate to one another offers interesting insights into how they used their skills to meet the demands of their jobs.

2.12 ETP Code Frequencies

Evaluating the code frequencies illustrates which equipment and techniques were most commonly employed. The most commonly used types of equipment were directly involved in the transfer of chemicals (**Table 2.3**). 30.7 % of participants' coded time was spent manipulating solid and liquid transfer tools (e.g., spatulas, weigh paper, syringes, capillary tubes) during 684 distinct incidents. The human body was also frequently employed as a tool itself and often involved in transfer, such as by hitting containers to encourage chemicals to dislodge. Other uses of the body as a tool included warming vials with body heat and applying vigorous force to swirl heterogeneous solutions to encourage dissolution. While the use of records (e.g., personal lab notebook, communal group logs), rotatory evaporators, sundry items (e.g., caps, clips, septa), and standard synthetic glassware (e.g., separatory funnels, Erlenmeyer flasks) featured in another 25.8 % of the participants' coded time, most of the remaining equipment used were interacted with for fleeting time periods. While all the equipment used served vital roles in the participants' work, this frequency analysis demonstrates an uneven distribution in the materials with which participants most frequently interacted. At the same time, in order to execute their work, participants needed to harness a diverse set of materials for discrete needs, such as the use of a static gun to stabilize a balance's fluctuating mass measurement or a propane torch to dry glassware for immediate use.

Table 2.3. Frequency of Equipment codes.

Equipment (N = 32)	1° / 2° ^a	Count ^b	Duration (%) ^c
Transfer tools – liquid	1°	470	18.7
Transfer tools – solid	1°	214	12.0
Human body	2°	301	9.6
Records	1°	117	7.6
Rotatory evaporator	1°	198	6.3
Sundry items	2°	127	6.1
Standard glassware	2°	164	5.8
Computer	1°	118	4.5
Balance	1°	71	3.5
Schlenk line	1°	45	3.3
Fume hood	1°	162	3.2
PPE	1°	81	2.0
Calculator	1°	35	2.0
Monkey bars & clamps	1°	48	1.9
Automated column	1°	35	1.8
UV lamp	1°	25	1.6
Heat gun	1°	12	1.5
Glovebox	1°	27	1.3
Sonicator	1°	12	1.2
Phone	1°	16	1.0
Waste collector	1°	41	0.8
In-house utilities	1°	33	0.8
Stir plate & bar magnet	1°	11	0.8
Temperature bath	1°	11	0.6
Column	1°	19	0.5
Transfer tools – gas	1°	14	0.5
TLC chamber & stain	1°	18	0.3
Propane torch	1°	3	0.3
Static gun	1°	9	0.2
Oven	1°	6	0.2
Solvent system	1°	3	0.1
Fridge	1°	1	0.02

^aCodes are “primary” or “secondary” to account for potential overlap.

^b2,447 Meaningful Actions coded across all recordings

^cPercentage of the cumulative 6.5 hours coded, not the 11.1 h recorded

Concurrently, a frequency analysis of the techniques that these equipment were used to execute illustrates the most common techniques participants employed (**Table 2.4**). Rotatory evaporation, cleaning and waste disposal, and thin-layer chromatography featured prominently, accounting for 31.1 % of coded time. Management of personal lab notebooks, liquid-liquid extraction, column chromatography, and transfer of solids represented another 32.3 %. The allocation of time to these techniques reflects patterns seen in the

equipment frequency analysis, where transfer tools, rotatory evaporators, records, and glassware featured notably. Similarly to the equipment frequency analysis, the technique analysis indicates that participants' time is not divided evenly among techniques but, rather, is weighted toward specific techniques. At the same time, a larger collection of less frequently utilized techniques continue to fulfill distinct roles. The participants were able to move seamlessly between these equipment and techniques, displaying familiarity with their operation.

Table 2.4. Frequency of Technique codes.

Technique (N = 30)	1° / 2° ^a	Count ^b	Duration (%) ^c
Rotatory evaporation	1°	305	10.9
Cleaning & waste disposal	1°	292	10.4
Thin-layer chromatography	1°	252	9.8
Notebook management	1°	96	8.1
Liquid-liquid extraction	1°	263	7.4
Schlenk line operation	1°	103	6.0
Column chromatography	1°	118	5.5
Mass transfer – solid	2°	127	5.3
Laboratory & workspace management	2°	195	4.3
Mass measurement – solid	1°	92	3.9
NMR analysis	1°	113	3.9
Inventory management	2°	46	3.6
Glovebox operation	1°	48	2.6
Mass transfer – liquid	2°	64	2.1
PPE management	1°	83	2.1
Air-free mass transfer	1°	39	1.8
Vacuum filtration	1°	23	1.6
Dissolution	2°	49	1.6
NMR sample preparation	1°	28	1.4
Mass transfer - phase change	2°	8	1.4
Mass measurement – liquid	1°	29	1.4
Sonication	1°	12	1.2
Solution drying & gravity filtration	1°	11	0.9
Glassware drying	1°	15	0.7
Temperature bath manipulation	2°	15	0.6
Literature searching	1°	3	0.4
Airstream evaporation	1°	7	0.4
Light-sensitive reaction management	1°	3	0.3
Solvent system operation	1°	7	0.2
Chemical drawing software usage	1°	1	0.1

^aCodes are “primary” or “secondary” to account for potential overlap.

^b2,447 Meaningful Actions coded across all recordings

^cPercentage of the cumulative 6.5 hours coded, not the 11.1 h recorded

These equipment and techniques were together employed in pursuit of a set of ultimate objectives that the participants valued (**Table 2.5** – see **Appendix B** for detailed definitions and examples). The purposes for much of the participants' efforts were oriented toward avoiding contamination, purifying desired products out of mixtures, analyzing results, and synthesizing products. However, the participants' actions also sometimes intersected with the non-experimental realm (albeit less frequently), such as working to address situations that were causing them personal annoyance without respect to the chemical research itself as well as maintaining good working relationships with their labmates. Participants also spent a quarter of their time engaged in optimization actions, illustrating the degree to which the pursuit of proactive efficiency featured in their efforts. These optimization tactics were especially on display while attempting to avoid contamination, purify a product, and maximize product yield.

Table 2.5. Frequency of Purpose codes.

Purpose (N = 20)	1° / 2° ^a	Count ^b	Duration (%) ^c	+ Opt. Count	+ Opt. Duration (%)
Avoid contamination	1°	365	13.7	437	17.3
Purify product	1°	249	11.0	475	20
Analyze results	1°	258	10.6	339	12.6
<i>Optimization - purify product</i>	1°	226	9.0		
Synthesize product	1°	155	8.1	221	11.6
Enable repetition via records	1°	79	6.3		
<i>Optimization - maximize product yield</i>	1°	187	5.7		
Maximize product yield	1°	159	4.9	346	10.6
Enable repetition via measurements	1°	87	4.3	117	5.8
Protect equipment	1°	94	4.0		
<i>Optimization - avoid contamination</i>	1°	72	3.6		
Protect people	1°	125	3.5		
<i>Optimization - synthesize product</i>	1°	66	3.5		
Enable next step only	2°	38	2.8		
Reduce personal annoyance	1°	98	2.3		
<i>Optimization - analyze results</i>	1°	81	2.0		
Maintain work relationships	1°	45	1.8		
<i>Optimization - enable repetition via measurements</i>	1°	30	1.5		
Preserve amount of supply	1°	21	1.0		
Preserve product integrity	1°	12	0.3		
All <i>Optimization</i> codes together	---	662	25.3		

^aCodes are “primary” or “secondary” to account for potential overlap.

^b2,447 Meaningful Actions coded across all recordings

^cPercentage of the cumulative 6.5 h coded, not the 11.1 h recorded

2.13 ETP Code Relationships

The frequency analyses provide insight into the types of psychomotor skills the participants employed and the materials they interacted with in pursuit of macroscopic purposes. These purposes can be mapped broadly in terms of their relationships to experimental goals or even to social domains (**Figure 2.5**). Synthesis, purification, and analysis of experimental results formed the core of participants' psychomotor actions in the laboratory, but the need to maximize yield and avoid contamination were common cross-cutting concerns among experiments. The participants also operated under the awareness that their work needed to be reproducible by both themselves and other individuals in the future, leading to a prerequisite to both maintain accurate records of their plans and accurately execute those plans as detailed. The centrality of these experimental purposes to the participants' time in the laboratory helps explain why the participants focused on optimizing their efforts in these areas. Optimization tactics can be viewed as a form of defensive behavior to guard against wasting precious physical resources (e.g., loss of material), time, and affective resources (e.g., patience to wait for a process to finish). The other purposes which were not tied as directly to the execution of the experiment themselves can also be viewed as defensive in nature: the defense of social (e.g., relationships with labmates) or other affective resources (e.g., emotional state) and the defense of physical resources (e.g., a chemical prone to degradation, personnel who could be injured, specialized equipment that would be expensive to replace).

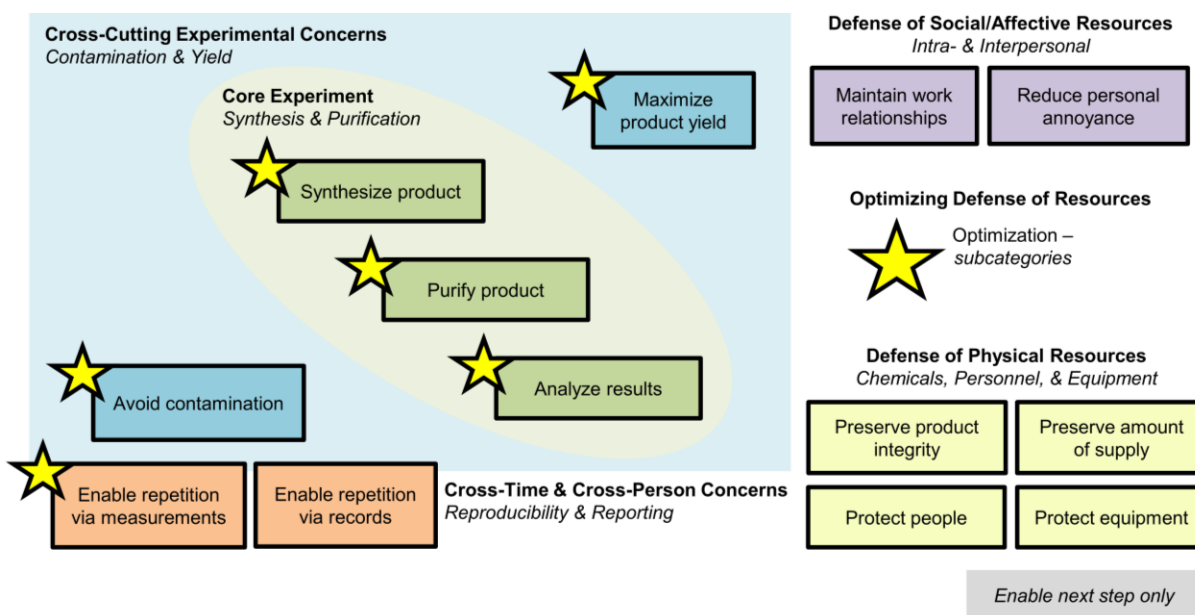


Figure 2.5. Conceptual map of Purpose codes.

The concept mapping helps to illustrate why participants did what they did but does not, by itself, explain *how* the techniques and equipment highlighted earlier were used to this effect. As seen in temporal analyses of selected ETP codes (**Figure 2.6**), the participants deployed their skills in complex ways. In the sample temporal analyses displayed, some ETP codes are concentrated in time (e.g., liquid mass transfer) whereas others (e.g., the use of solid transfer tools) are distributed widely. The use of flagship equipment such as the rotatory evaporator does not fully account for all the equipment used during its namesake technique, rotatory evaporation. Steps taken to optimize purification often immediately followed the pursuit of purification but not always. These temporal analyses demonstrate the complexity of the laboratory work and lack of surface-level discernable patterns in the interplay between equipment, techniques, and purposes.

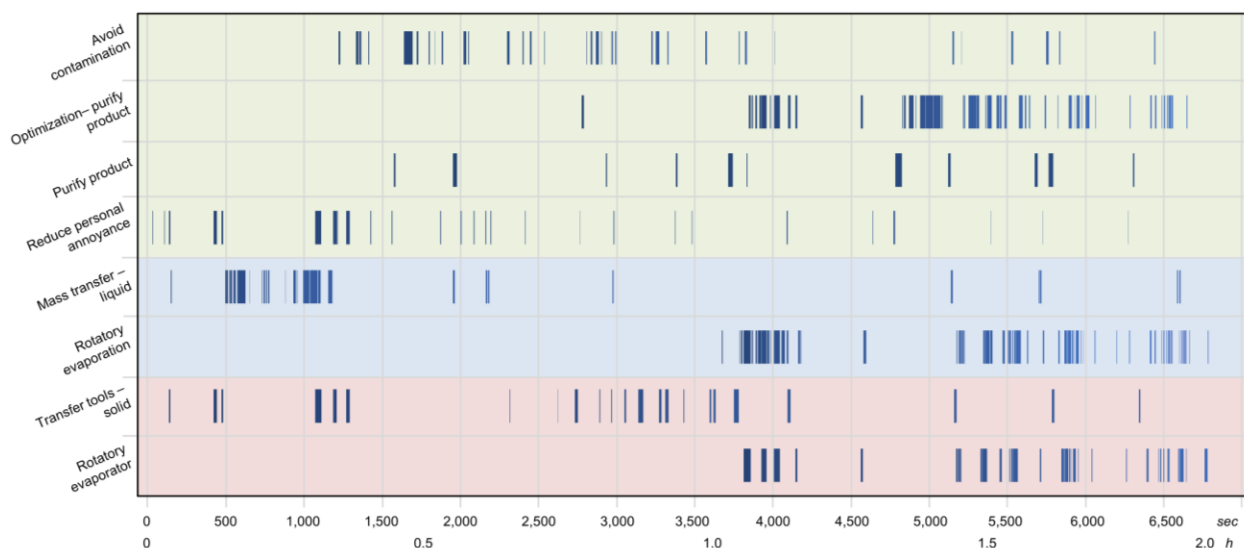


Figure 2.6. Example temporal analyses of selected Equipment (red, bottom), Technique (blue, middle), and Purpose (green, top) codes in one full recording session.

Cluster analysis, however, helps illuminate the interactions on a deeper level (**Figure 2.7** – see also supplemental figures in **Appendix B**). Cluster analyses were modeled between ETP codes until a maximum average silhouette value was reached at $k = .2670$ with eight clusters (see **Appendix B**). Due to the descriptive nature of cluster analyses, there is no formal cut-off for determining the “significance” of an exploratory, descriptive cluster analysis.^{136,137} Instead, uniformity in items’ silhouette values, a high average silhouette value, and perceived reasonableness of the resulting clusters are a set of approaches often considered in evaluating a cluster analysis. Since the presence of overlapping codes between

clusters was expected based on the complex nature of laboratory work, some overlap in the clusters is not necessarily seen as an indicator of poor clustering for this data.



Figure 2.7. Distribution of Equipment, Technique, and Purpose codes by cluster (legend top right corner).

The resulting 8 clusters can be described via the following themes (**Figure 2.8**):

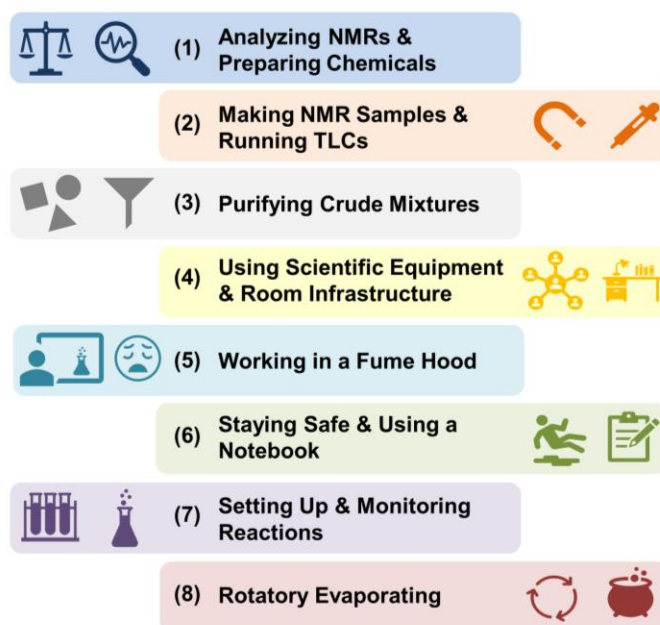


Figure 2.8. Summary characteristics of clusters.

- 1. Analyzing NMRs and Preparing Chemicals:** Cluster 1 demonstrates that using a balance, computer, static gun, and solid transfer tools are often associated with chemical drawing software usage, literature searching, solid mass measurement, solid mass transfer, and NMR analysis techniques. These equipment and techniques are employed when working to analyze results, measure accurately while employing optimization tactics, and synthesize a product. **In sum, cluster 1 describes both how participants carefully prepared the chemicals for their upcoming reactions and later analyzed the final spectroscopic results.**
- 2. Making NMR Samples and Running TLCs:** Cluster 2 demonstrates that using a fridge, heat gun, the human body, phone, records, sundry items, a TLC chamber and stain solution, liquid and solid transfer tools, and a UV lamp are often associated with inventory management, liquid mass measurement, NMR sample preparation, and thin-layer chromatography techniques. These equipment and techniques are employed when working to analyze results while employing optimization tactics, enable necessary next steps in a procedure, employ optimization tactics while

avoiding contamination, and preserve a desired product's integrity. **Cluster 2, therefore, describes how participants efficiently analyzed results using TLC and prepared NMR samples, all while keeping accurate records of this work and handling related chemical storage.**

3. **Purifying Crude Mixtures:** Cluster 3 demonstrates that using an automated column machine and its associated column, a heat gun, the human body, a Schlenk line, sonicator, and standard glassware are often associated with air-free Schlenk line operation, column chromatography, liquid-liquid extraction, solution drying and gravity filtration, sonication, and vacuum filtration techniques. These equipment and techniques are employed when working to avoid contamination, employ optimization tactics while maximizing yield, and purify a product while employing optimization tactics. **Cluster 3 describes how participants purified desired products out of crude mixtures while trying hard to be efficient throughout.**
4. **Using Scientific Equipment and Room Infrastructure:** Cluster 4 demonstrates that using a heat gun, fume hood, glovebox, the human body, in-house utilities (e.g., sink water line, ventilated cabinets), oven, propane torch, solvent system, sundry items, stir plate and bar magnet, gas/liquid/solid transfer tools, and waste collector are often associated with air-free mass transfer, airstream evaporation, cleaning and waste disposal, solvent system operation, glassware drying, glovebox operation, inventory management, light-sensitive reaction management, and rotatory evaporation techniques. These equipment and techniques are employed when working to avoid contamination, enable the next procedural step, maintain work relationships, preserve materials, and protect people and equipment. **Cluster 4 describes how participants used a variety of scientific equipment and specialized infrastructure to maintain social and physical resources (e.g., chemical stock supplies, equipment, personnel safety) in prime operating condition and ready for experimental use.**

5. **Working in a Fume Hood:** Cluster 5 demonstrates that using a fume hood, monkey bars and clamps, and sundry items are often associated with airstream evaporation and laboratory and workspace management techniques. These equipment and techniques are employed when working to protect equipment, reduce personal annoyances, and synthesize a product. **Cluster 5 describes how participants worked within the confines of a fume hood to optimize the set-up of their workspace and to deal with recurring annoyances associated with fume hoods (e.g., sash alarms).**
6. **Staying Safe and Using a Notebook:** Cluster 6 demonstrates that using a calculator, phone, personal protective equipment (PPE), and records are often associated with notebook and PPE management techniques. These equipment and techniques are employed when working to enable procedure repetition and protect people. **Cluster 6 describes how participants utilized PPE for their own personal safety and kept appropriate records of their work to enable future reproducibility.**
7. **Setting Up and Monitoring Reactions:** Cluster 7 demonstrates that using the human body, monkey bars and clamps, solvent system, stir plate and bar magnet, temperature bath, and liquid transfer tools are often associated with air-free mass transfer, dissolution, solvent system operation, glassware drying, liquid mass measurement and mass transfer, phase change transfer manipulations (e.g., manipulating the phase of a chemical to move it as a liquid instead of as a solid or vice versa), solid mass transfer, temperature bath manipulation for reactions, and vacuum filtration techniques. These equipment and techniques are employed when working to maximize yield and synthesize a product while employing optimization tactics. **Cluster 7 describes how participants efficiently assembled the materials for reaction set-ups, started reactions, and made necessary adjustments to maintain desired conditions throughout the reaction.**
8. **Rotatory Evaporating:** Cluster 8 demonstrates that using a rotatory evaporator is often associated with rotatory evaporation techniques. These equipment and techniques are employed when

working to employ optimization tactics while maximizing yield and purifying a product. **Cluster 8 describes how participants' interactions with a rotatory evaporator were primarily intended to optimize the expenditure of their time and effort during the overall purification process.**

2.14 Perceptions of Values of Skills

Together, the eight clusters describe the complex ways in which the participants employed their equipment and techniques in pursuit of their overall purposes. To probe how the participants themselves perceived these skills and the role that the skills played in their ability to conduct their doctoral research, the participants were asked to rate how important it would be for an incoming organic chemistry graduate student to be able to use each equipment item, execute each technique, and accomplish each purpose. Participants were shown the overall list of ETP codes and a list of 100 randomly selected MA codes (without the corresponding ETP codes shown). They marked items as being either essential (score = 1), very helpful but not essential (2), good to know (3), or not important (4) for an incoming organic chemistry student to be able to do to be successful in graduate research.

Participants' averaged responses indicate that the participants overwhelmingly held these skills in high regard (**Table 2.6**). Approximately half of the items in each ETP category received unanimous "essential" scores. One participant tended to rate the remaining codes lower than the other participant as a reflection of their belief that "these are things that really help you if you can come in and be independent on them and understand what's happening, but they are pretty easy to pick up along the way" (*Participant B*). Only two ETP codes received an average face value score of 3 or lower: "phone" (Equipment) and "airstream evaporation" (Technique). The phone was mostly used to take pictures of results or the notebook for reference later, and airstream evaporation was utilized on a few occasions to reduce the solvent volume in a vial by applying nitrogen gas flow. Otherwise, participants agreed on the important role that most of their demonstrated skills play in achieving research success.

Table 2.6. Perceived value of lab skills.^a

Equipment	Face Value Score _b	Avg. Item Score	Technique	Face Value Score	Avg. Item Score	Purpose	Face Value Score	Avg. Item Score
Calculator	1.0	1.0	Mass measurement - liquid	1.0	1.0	Analyze results	1.0	1.0
Computer	1.0	1.0	NMR analysis	1.0	1.0	Enable repetition via records	1.0	1.0
Temperature bath	1.0	1.0	NMR sample preparation	1.0	1.0	Protect equipment	1.0	1.0
Transfer tools - liquid	1.0	1.3	Notebook management	1.0	1.0	Enable repetition via measurements	1.0	1.3
Balance	1.0	1.5	Solution drying & gravity filtration	1.0	1.0	Avoid contamination	1.0	1.5
Records	1.0	1.5	Mass transfer - solid	1.0	1.4	Protect people	1.0	2.4
Fume hood	1.0	1.7	Mass transfer - liquid	1.0	1.4	Purify product	1.5	1.3
Transfer tools - solid	1.0	1.7	Thin-layer chromatography	1.0	1.4	Synthesize product	1.5	1.4
Standard glassware	1.0	2.0	Cleaning & waste disposal	1.0	1.5	Maximize product yield	1.5	1.7
Stir plate & bar magnet	1.0	2.0	Mass measurement - solid	1.0	1.7	Maintain work relationships	1.5	2.0
Column	1.0	2.5	Column chromatography	1.0	1.9	Preserve amount of supply	1.5	2.5
PPE	1.0	2.5	PPE management	1.0	2.3	Preserve product integrity	1.5	---
Fridge	1.0	--- ^c	Glassware drying	1.0	3.0	Reduce personal annoyance	2.5	2.8
Monkey bars & clamps	1.0	---	Liquid-liquid extraction	1.0	---	Optimization – avoid contamination	---	1.0
TLC chamber & stain	1.0	---	Literature searching	1.0	---	Optimization – analyze results	---	1.5
Waste collector	1.0	---	Rotatory evaporation	1.5	1.1	Optimization – maximize product yield	---	1.5
Rotatory evaporator	1.5	1.0	Vacuum filtration	1.5	1.7	Enable next step only	---	1.7
Human body	1.5	2.0	Dissolution	1.5	1.8	Optimization – purify product	---	1.9

Table 2.6. Perceived value of lab skills.^a [continued]

Schlenk line	1.5	2.0	Mass transfer - phase change	1.5	2.0	Optimization – enable repetition via measurements	---	2.0
UV lamp	1.5	2.0	Laboratory & workspace management	1.5	3.0	Optimization - synthesize product	---	2.0
Sundry items	1.5	2.2	Air-free mass transfer	1.5	---			
Heat gun	1.5	---	Chemical drawing software usage	1.5	---	“Optimization” presented to participants as one category ^d	1.5	1.8
Oven	1.5	---	Solvent system operation	1.5	---			
Sonicator	1.5	---	Light-sensitive reaction management	2.0	1.0			
Glovebox	2.0	1.0	Temperature bath manipulation	2.0	1.0			
Transfer tools - gas	2.0	1.0	Glovebox operation	2.0	1.6			
In-house utilities	2.0	1.5	Schlenk line operation	2.0	2.1			
Solvent system	2.0	---	Sonication	2.0	---			
Static gun	2.0	---	Inventory management	2.5	2.2			
Automated column	2.5	1.0	Airstream evaporation	3.0	2.0			
Propane torch	2.5	---						
Phone	4.0	---						

^aThe participants' scores for each item were averaged. Participants rated items by importance for an incoming synthetic graduate student to be able to do (1 = essential; 2 = very helpful but not essential; 3 = good to know; 4 = not at all important).

^bParticipants were asked about each item's importance explicitly (“face value score”) and about random MA codes representing a sample variety of categories, later averaged together per category (“avg. item score”).

^cDue to the large number of codes and realistic constraints on participants' time, participants were not able to rate the importance of MA codes for every ETP code. Participants were given 100 randomly selected MA codes to rate, and those sample items enabled composite scores for the ETP codes shown here.

^dIt was thought that participants might struggle to meaningfully distinguish between optimization categories without in-depth training with the codebook, and so they were presented with “optimization” as one single category.

Of note, however, is the trend where some individual MA codes received lower composite scores than their ETP codes did at face value (bolded). Both participants explained that, while they may highly value the skill represented by an overall ETP code, there can be different ways of executing an ETP skill:

Participant B: There, it was more things that everyone has their own way of doing this. You'll figure out a way to do this. The destination is more important than the journey, so it doesn't matter if you're doing it the same way that I'm doing it.

Therefore, participants tended to give lower scores for the essentiality of certain specific MA codes because they perceived potential flexibility in how another person might execute an equivalent skill. However, there were multiple instances where the MA codes were rated higher than the ETP codes they represented, possibly reflecting the expressed belief that sometimes there is only one right way to execute a skill and that proper execution is essential in such cases:

Participant A: Like, maybe using a glovebox is very helpful for students to do if they enter, but not every reaction needs a glovebox. But for the specific [meaningful action item], if they don't purge the glovebox, that could harm the glovebox irreparably.

2.15 Perceptions of Originations of Skills

Participants' beliefs that most of their skills are essential or very helpful for incoming graduate students also reflects on their own educational histories and preparations for PhD-level research. Both individuals participated in chemical research during college, took a set of introductory and upper-level laboratory courses, and engaged in research experiences outside of academic labs (**Table 2.7**). Both specialized in organic synthesis as undergraduates and in organic methodology as PhD students, but they also pursued additional experiences in other subfields of chemistry before entering their PhD program. When participants were asked to identify when they learned how to do a random selection of 50 MA codes (**Table 2.8**), they overwhelmingly reported learning the skills before entering the PhD program. Their PhD experiences sometimes served to refine certain skills, but the participants reflected that they were using equipment and conducting techniques without substantial differences from their undergraduate training via formal laboratory coursework and undergraduate research experiences. Both participants, however, commented

that they have encountered situations where they themselves created a solution to a psychomotor challenge they were encountering, rather than having learned the solution somewhere else:

Participant B: I think there is a lot of MacGyvering that goes into labwork or arts and crafts. Making different contraptions to accomplish what you need to get done. And that's been really helpful for me and I guess the fun part of research. Oh, I need to evaporate solvent from these two small vials, but I don't have an adaptor directly for my line. And then figuring out what kind of things you can put together to make the contraption you need.

Table 2.7. Participants' prior laboratory experiences.

Participant's Context	Participant A	Participant B
<i>Year in PhD program</i>	2 nd	2 nd
<i>Pathway from undergrad</i>	NIH postbaccalaureate for 2 years	Immediate transition to PhD program
<i>Degree before PhD program</i>	Master's	Bachelor's
<i>Type of undergrad institution</i>	R1, USA	R1, USA
<i>Types of lab experiences before PhD program</i>	• Cookbook lab • Inquiry lab • Research lab	• Cookbook lab • Inquiry lab • Course-based research • Research lab
<i>Overview of STEM laboratory experiences before PhD program</i>	• Intro undergrad biology, honors physics, & majors organic chemistry lab courses • Upper-level lab courses in organic, inorganic, analytical, & physical chemistry • Research in organic synthesis, inorganic synthesis, & radiochemistry in academia & NIH	• Intro undergrad physics, biology, & honors general chemistry lab courses • Upper-level lab courses in analytical & physical chemistry • Research in organic synthesis & medicinal chemistry in academia & industry
<i>Focus of PhD research</i>	Organic methodology (mostly solo projects)	Organic methodology (mostly solo projects)

Table 2.8. Perceived sources of lab skills.

Experience Resulting in Lab Skill ^a	Initially Learned ^b	Improved / Adjusted	Improved / Adjusted (again)
Participant A			
High school	1		
Organic chemistry I laboratory course	8		
Synthetic organic/inorganic chemistry research lab (undergraduate)	10	5	
Advanced organic chemistry laboratory course	3		
Synthesis & radiochemistry research laboratory (NIH postbaccalaureate)	10	5	
Synthetic organic chemistry research lab (doctoral)	7	7	1
Participant B			
“Common sense”		1	
General chemistry I laboratory course	6		
Biology I laboratory course		1	
Synthetic organic chemistry research lab (undergraduate)	31	2	
Medicinal chemistry research laboratory (industry internship)	4		
Synthetic organic chemistry research laboratory (doctoral)	8	1	

^aOrganized in descending chronological order for when the participant started the experience

^bFor 50 random Meaningful Actions each from a list of actions that each individual participant demonstrated

2.16 Role of Automaticity

Finally, it is worthwhile to note a theme about automaticity which emerged over the course of the eight interviews. When participants were asked to discuss the rationale for their specific actions or their overall experimental goals, they often mentioned either challenges they encountered or their observation that the session “went smoothly”. On several occasions, participants noted that, after encountering a challenge to their psychomotor actions in the laboratory, they made a decision to either redo the sequence of previous actions (e.g., recollect bumped material and attempt rotatory evaporation again), adjust their standard operating protocol moving forward (e.g., add in a different solvent to the liquid-liquid extraction to try to improve solubility), or add in a supplemental technique to address the challenge (e.g., try to sonicate a silica gel mixture to achieve dissolution before attempting rotatory evaporation in preparation for dry loading

a column). In the absence of an unexpected challenge, participants appeared to view most of their psychomotor actions as routine which, coupled with the high level of physical productivity displayed over the 11.1 hours of recorded time, suggests that the participants had achieved psychomotor automaticity regarding the use of their equipment, execution of techniques, and pursuit of purposes. Skills which were perceived as requiring a certain degree of familiarity and automaticity also tended to be rated as essential skills:

Participant B: [The essential skills are] mostly the skills that we use everyday that typically we maybe don't think exactly about all of the reasoning behind.

When they encountered a disruption to their automatic processes, however, they were forced to reevaluate and engage deliberately in determining the best next steps:

Participant A: There is a lot of muscle memory with certain lab techniques, so good researchers will be able to complete these techniques quickly without hesitation. However, they must also be able to change course and re-assess if something goes wrong, such as an unexpected heat, color change, precipitation.

Automaticity with cognitive skills such as arithmetic have previously been shown to be helpful with general chemistry performance.¹⁴³ The interplay of psychomotor automaticity with chemical research competencies likely deserves additional attention in future studies.

2.17 Discussion

This paper sought to illuminate how chemists use their psychomotor skills when conducting bench research and how they learned those skills. Through phenomenological grounded theory case studies with naturalistic first-person recordings and retrospective interviews, a MA–ETP framework was established through which to characterize psychomotor actions in laboratories and enable future development of NGLSS.

2.18 Implications

From a methods standpoint, third-person naturalistic observation was more effective than expected in a complex workplace. The discovery of the MA-ETP framework lent effective and much-needed structure to the coding process. Future laboratory-based research could employ this framework when dealing with similarly large volumes of complex data about the physical realm. Additionally, the high degree of agreement in coding could indicate that synthetic chemical methods are similar between groups and institutions. If so, such commonalities could perhaps empower undergraduate laboratory experiences to expose students to many of the equipment and techniques in use in graduate-level synthetic laboratories.

Interviews with faculty have already shown that learning practical techniques is a key focus of some laboratory courses, especially in organic chemistry.^{106,144} The chemist participants had learned a range of relevant psychomotor skills before entering their PhD program, mostly as a result of prior research experiences as well as laboratory courses. Descriptive statistics and temporal analyses of the recordings indicate that participants engaged frequently with their psychomotor skills, maintaining a high level of sustained activity. The participants' comments about automaticity and essentiality scores highlight the value they placed on entering their PhD program with a suite of familiar skills as well as being able to adjust their actions when necessary. They displayed their own abilities to deploy skills seamlessly, as evidenced by their high degree of psychomotor activity and ability to weave diverse skills together throughout time and clusters. Their activity level and educational chronologies indicate that their prior laboratory experiences provided relevant training opportunities and that psychomotor automaticity played an important role in their current work. They reported positively on the need for students to attain similar skills before entering graduate school with the caveats that specific skills may differ in whether there is flexibility in the exact methods used. While some of their equipment and techniques were employed often (e.g., transfer tools, rotatory evaporation) in pursuit of their ultimate purposes (e.g., avoiding contamination), many of the ETP codes appeared infrequently (e.g., static gun, reduce personal annoyances). However, the objects of these infrequent ETP codes still played crucial roles.

These observations imply that undergraduate synthetic chemistry students would be well-served by being exposed to a variety of equipment and techniques and being given opportunities to practice and refine their physical execution. Students could also benefit from being coached on how to engage in practical problem-

solving (or “MacGyvering”) to generate solutions to physical challenges. Moreover, the role of proactive efficiency-seeking featured positively and prominently. This focus on efficiency provides a contrast to common anecdotal complaints among undergraduate educators that a major focus of students in laboratory courses is how quickly they can manage to finish an experiment (and undergraduates’ stress about finishing in time¹⁴⁵). The majority of the participants’ recorded time was occupied by coded psychomotor activity of which most was in service of the experimental domain but also featured defensive concerns about social, affective, and physical resources. The quests for purity (both in terms of achieving purity and maintaining it) and efficiency constituted the largest demands on their time. Time is, after all, a limited, nonrenewable resource, and the participants displayed an awareness of many ways they could work to safeguard their time. The parallels between the participants’ and undergraduate chemistry students’ attention to time may indicate that efficiency is ultimately a valuable learning objective itself (albeit not the only learning objective). This observation dovetails with the theme of automaticity: automatic skills can be deployed efficiently. Undergraduate educators may find themselves working in the future to balance how to train students such that they achieve automaticity with psychomotor skills but also possess practical problem-solving skills and understand the conceptual underpinnings well enough to adjust to unexpected circumstances.

2.19 Limitations

A study involving two participants as case studies provides strength in depth but not in breadth. Especially since the participants were in the same research group, the equipment, techniques, and purposes shown here may not reflect the average experience in other synthetic chemistry research laboratories. Since the participants were in their second year of their PhD program, the participants’ psychomotor competencies may have substantially improved since they entered the program, despite their recollections of learning a greater proportion of their skills beforehand. Additionally, academic graduate research laboratories represent only one type of laboratory workplace. In general, more research needs to be done with industrial, governmental, and other types of chemists to elucidate their experiences and how those experiences relate to their earlier formal educational training.

The participants reported (when explicitly asked at the end of each interview) that they did not change their actions in the laboratory as a result of the recordings. The participants were aware from the explicit study

recruitment information that the study was not evaluating them or their experimental results but instead was an exploration of how bench research happens inside synthetic chemistry labs. Presumably, if the participants felt pressure to behave in a specific way (e.g., due to a Hawthorne effect), they would have wanted to increase their productivity and/or avoid mistakes while being recorded. However, they were told that it was completely ok to make mistakes (e.g., spills, breakages), take down time, or struggle with their experiments because seeing them go through the process of stopping to think or address challenges was important, authentic data for the observer. They were told that the purpose of filming them was to help improve undergraduate laboratory experiences and to understand how advanced researchers like themselves actually do their work. The participants' repeated affirmations that they did not change their actions as a result of the recording and their readiness to self-identify (during the interviews) challenges they experienced subsequently lends support to the authentic representativeness of the data for the benchwork-intensive parts of their workday. The interviewer adopted a casual, conversational attitude during these discussions to normalize challenges and mistakes. However, it is also possible that the presence of recording equipment adjusted how other people in the laboratory behaved: the prevalence of social interactions may have been lower as a result of the visible camera on the participants' heads. While investigating social interactions was not a purpose of this study, it is relevant to keep in mind.

Of course, there are other activities that participants engaged in to conduct their doctoral research; this study did not purport to focus on the cognitive or affective domains of their jobs. The recording time slots were ultimately chosen by the participant in anticipation of when they would be working at the bench, so the high degree of physical action illustrated in the data should not be construed as comprising their overall workday. Some of the ETP codes may also appear, on the surface, to be underrepresented due to the need to employ a primary-secondary hierarchy for the sake of consistent coding. For example, the participants handled glassware more often than for 5.8 % of the coded time. The bump trap of a rotatory evaporator, the Schlenk line, and other glassware that constituted integral components of primary Equipment codes were not represented in the "standard glassware" secondary code.

Additionally, the nature of the research itself presents limitations in the data analysis process. Besides the participants who engaged in validative open coding, the author was the sole trained coder. Literature generally does not support the use of inter-rater / inter-coder reliability for complex naturalistic observational

video data featuring overlapping open codes and a living codebook, and literature is also hesitant about applying reliability analyses in qualitative grounded theory research due to the importance of the reflective memoing and iterative, cyclical nature of analysis.^{138,140–142} Additionally, calculations of reliability coefficients in situations with large data sets involving many codes with wildly different prevalences can be problematic because they might present artificially low values as a result of mathematical demands. While **Appendix B** provides detailed notes and applied examples of the codebook for precisely these reasons, being able to conduct a reliability analysis would lend greater support to the credibility of the data analysis and subsequent conclusions.

Finally, this data provides an idea for what the product of undergraduate education could look like but does not offer a pathway for achieving it. The participants themselves identified that there can be variability in how skills are executed, and the author noticed during the recordings that they did not always conduct the same technique in the same way as the other participant, despite being in the same group. The questions of how to best teach students psychomotor skills, automaticity, and practical problem-solving remain open. Finally, most students in undergraduate chemistry courses do not proceed to doctoral chemistry programs; their learning objectives in laboratory courses may not necessarily align with that of molding students into future graduate student researchers.

2.20 Conclusion

Psychomotor skills are crucial in the laboratory since it is a physical, hands-on workplace. As the DBER community and educators across the world work to improve STEM education, the psychomotor domain deserves explicit attention in investigating how to promote effective, authentic learning. These case studies offer unique insight into the laboratory as a dynamic, challenging environment that undergraduate education seeks to prepare students to enter. Viewing the psychomotor domain in terms of the *what-how-why* MA-ETP framework discussed herein may guide future research and educational innovations. Sharing a consensus across chemistry education on how to view and evaluate the types and purposes of psychomotor actions in laboratory settings could set the stage for innovations deliberately cultivating students' capabilities in these areas. By elucidating the role that psychomotor skills play in the competencies of laboratory-based chemists, DBER can lead to the development of relevant NGLSs for future generations of chemistry students.

Chapter 3

Structural Predictors of Safety Behavior in Graduate Student Chemical Researchers

Collaborators: Sarah R. Zinn (project co-lead), Nasim Mirzajani, Monica Mame Soma Nyansa

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3.1 Abstract

Academic chemical research laboratories are high-hazard environments, and universities are currently investing sizable resources in attempting to improve their safety outcomes in light of repeated tragedies. While these investments are commendable, insufficient evidence exists as to their effectiveness. Without a means of empirically determining which programs and policies support safety outcomes as intended, institutions are blind as to the next steps they should pursue. Therefore, this report details the development of a validated survey instrument capable of inferring a chemistry student's safety behavior in research laboratories as well as characterizing the types of programs and policies accessible to students. Notably, a 16-item short form of three psychometric scales was developed which can be quickly issued separately from the overall survey and so may find broad utility in the chemical health and safety (CHAS) field. Taken together, data from this survey will enable institutions to assess whether the resources they provide are supporting safety as anticipated – and if not, may enable those institutions to identify ways they can reallocate resources more effectively. Additionally, a national study is underway using this instrument to establish benchmarking data on the status of chemical research safety at R1 and R2 universities.

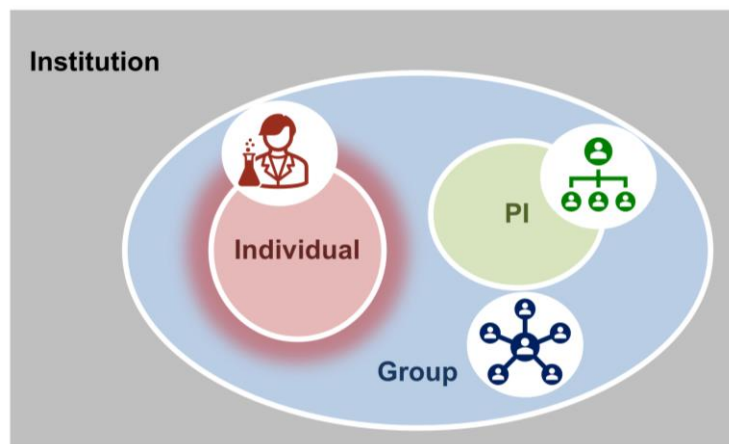


Figure 3.1. Safety behavior is a trait which can be extrapolated using psychometric measurement of relationships and related attitudes.

3.2 Introduction

If you want to become a chemist, you will have to ruin your health.

Justus von Liebig [19th century]¹⁴⁶

Academic chemical research laboratories are high-hazard environments staffed by a young trainee population with continuous turnover, overseen by PIs who often are physically absent due to their other obligations, and funded by limited grant money. It should come as no surprise to anyone that safety knowledge and behaviors can languish in such environments. Over the past decade, however, universities nationwide have increasingly turned their attention toward improving their safety records by funding safety programs / staff (e.g., UCLA's Center for Laboratory Safety founded after the infamous death of Sheri Sangji¹⁴⁷) and instating institutional policies specifically meant to decrease injuries and property damage. These actions likely stem both from prosocial motives to protect individuals and from insurance premium / regulatory standpoints. As a result, chemical safety in academia is experiencing a surge of interest in safety.^{146,148–154}

While fostering good intent is arguable half the battle won, it remains to be determined from an empirical standpoint whether these actions are having the intended effect. Are safety outcomes improving? Which programs / policies are having the desired effect – and which are not? Current practice is typically to count the number of accidents which happen in labs and watch how that statistic develops over years. Frustratingly though, accidents are often underreported. Even when they are reported, they are inherently a lagging indicator. A leading indicator which proactively reports on changes in safety outcomes as a result of contemporaneous behaviors would be of great value.

However, key problems surrounding the use of non-counting data are the joint issues of quantification and contextualization. What makes something “safe” in a chemistry lab? How can safety behavior be parameterized? In order to evaluate safety outcomes in labs such that one can confidently advise universities, funding bodies, and government agencies on their allocation of major (limited) resources, it is essential to develop instruments which are capable of measuring the unseen in a valid and reliable way. In other words, there is a pressing need to be able to measure (1) types of programs and policies being implemented at universities and (2) whether people are behaving safely on a day-to-day basis in the

chemistry labs. With the ability to measure these aspects, researchers could then make direct claims about the efficacy of institutions' investments and provide evidence-based recommendations about next steps. Therefore, this report details the development of an instrument which can execute both charges.

3.3 Research Question

The primary objective of this study was to first generate an instrument capable of answering the question "What types of institutional practices and interactions promote a safe chemical research lab environment?". The secondary objective was to then field this instrument nationally to answer that question. Considering the general dearth of such instruments in the CHAS space, the instrument needed to be designed in such a way that it would be (1) contextualized to the demands and needs of the academic chemistry laboratory research community and (2) adaptable for other CHAS researchers to continue utilizing it for related programmatic assessment purposes.

3.4 Methodology

The academic chemistry research laboratory is a unique setting, and therefore the instrument needed to be well-contextualized and carefully constructed. This manifested in six key aspects:

- (1) Chemistry students work long, odd hours in locations requiring keyed access. The instrument needed to be easy to administer remotely and flexible to interruptions at any time of day. *An online survey with an average length of 20 min maximum was therefore established as the mode.*
- (2) Chemistry students are not necessarily exposed to safety evaluative processes or even how other labs conduct experiments. The instrument needed to be designed with careful attention to the problems of self-report data amid the specter of students not being able to normalize their behavior or their environment accurately.¹⁵⁵ *Therefore, literature scales which have been shown to objectively predict safety behavior in similar environments to chemistry benchwork were adapted for use.*
- (3) Specific types of programs, policies, and jargon are utilized in chemistry research laboratories. *Key informant interviews and cognitive testing were utilized to navigate these idiosyncrasies.*

- (4) International students are estimated to populate up to half of chemistry graduate programs on average. *While international populations are often excluded from survey designs, this instrument needed to be designed to be accessible throughout for non-native English-speaking adults from other cultures.*
- (5) Graduate students are dependent trainees in a highly polarized power dynamic with PIs. *The instrument needed to encapsulate that relationship and its impact on student behavior.*
- (6) While improving safety has been embraced by many, safety programs also often draw ire from individuals who feel, for example, that they decrease productivity.¹⁵⁶ Similarly, individuals frustrated by a lack of safety improvement also may be inclined to give exaggerated responses on a survey, and so the potential for measurement interference needed to be guarded against from both sides. *The instrument therefore needed to be resistant to potential sabotage by both minimizing the presence of opinion-dependent questions and detecting effects to introduce bias deliberately.*

In light of these considerations, the methodological approach was to design a survey grounded in statistically inferable psychometrics. Psychometrics is the field of psychological measurement using objective assessment tools. By rooting the survey design in psychometrics (rather than, for example, observing subjects or conducting exclusively interviews), we could generate an instrument that...

- (1) conforms to the required modality,
- (2) draws statistically correlations based on literature precedent rather than participants' self-reports,
- (3) is systematically validated for the community's idiosyncratic jargon and context,
- (4) is systematically validated and statistically testable for demographic performance (e.g., English Language Learners),
- (5) deliberately measures important variables such as supervisor relationships across all participants, and
- (6) shields results from intentional manipulation by obfuscating the measurement process (i.e., participants cannot necessarily guess how items such as "How well does your PI recognize your potential?" would factor into a predictive model and so are limited in being able to induce specific outcomes deliberately).

3.5 Survey Development, Frameworks, and Validation

Instrument development followed best practices in survey design (**Figure 3.3**).^{157,158} To address the research question, we first needed to be able to parameterize both “safety behavior” and “lab environments”. Fortunately, a literature review of safety behaviors in other environments yielded suitable scales and frameworks for evaluating safety behavior in chemistry research laboratories.

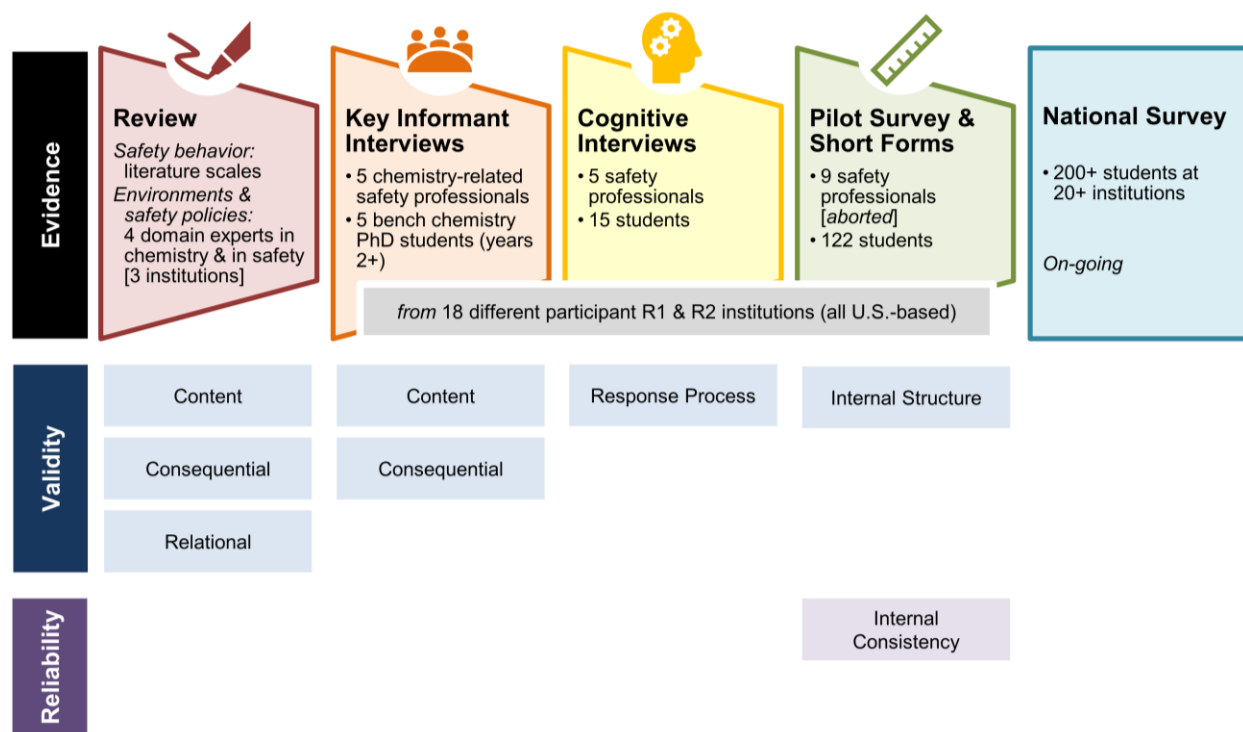


Figure 3.2. Survey development addressed content, consequential, relational, response process, and internal structure validity and internal consistency reliability before proceeding to national survey distribution.

In particular, research with United States military engineering crews (who work in small teams in high-hazard environments which include explosives and machinery) established relational validity between the team members’ actual safety behaviors in the field (as rated by a knowledgeable supervisor in the team) and the members’ responses to a set of psychometric survey items aka “scales”.^{159,160} Those items, referred to here as the “Leader-Member Exchange (LMX7)”, “Safety Climate”, and “Safety Citizenship” scales, serve as the methodological and framework anchors for this survey by providing a correlational pathway to extrapolate actual safety behavior of chemists from their scale responses. The scales were developed based on the theoretical frameworks of role theory, social exchange, and group climate. The

LMX7 scale reports on the quality of relationship between the respondent and their supervisor. The Safety Climate scale accounts for how members of the entire team signal their feelings about safety via a variety of actions. The Safety Citizenship scale collects data on how a respondent themselves internalizes safety as being a part of their professional identity. We envisioned them interacting through a bespoke conceptual framework¹⁶¹ here dubbed “Ecologically-Mediated Safety Behavior” (**Figure 3.2**) to influence safety behavior in chemistry labs. And all three of the scales can be used via only pen and paper to predict the respondent’s actual safety behavior when on the job.

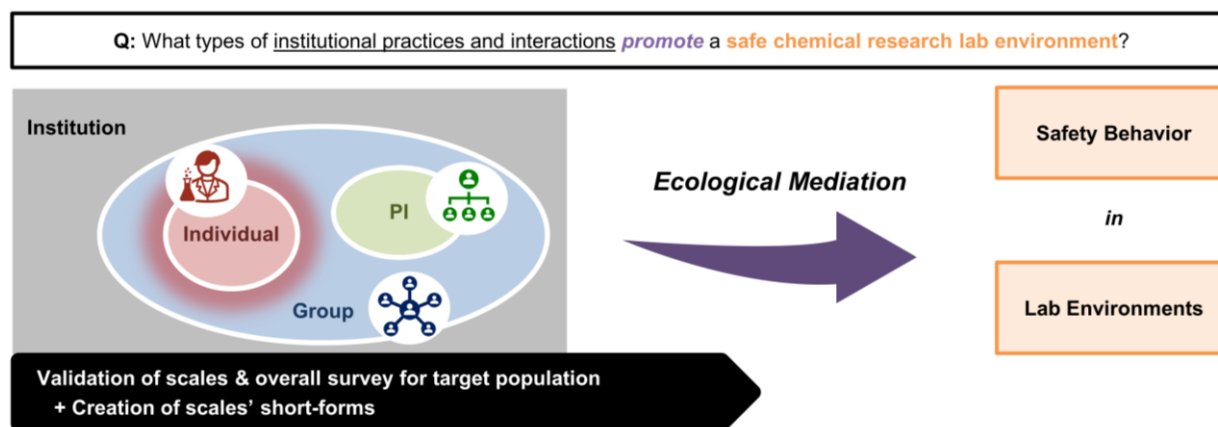


Figure 3.3. The Ecologically-Mediated Safety Behavior conceptual framework viewed safety behavior / outcomes in lab environments as a product of how interactions with peers in the research group and the PI supervisor impact an individual’s internalization of safety behaviors.

Next, to contextualize the scales specifically for chemistry, the wording of the scales was revised slightly by our team to address jargon differences (e.g., “crew members” → “group members”, see **Appendix C**). Meanwhile, our team’s own domain knowledge in bench chemistry and CHAS informed a preliminary list of programs, policies, and types of environments to be assessed in addition to the scales, thus addressing the issues of content and consequential validity. Key informant (KI) interviews were then conducted with students and safety professionals (SPs) to evaluate the draft survey’s content and consequential validity outside of our own team’s expertise, followed by the appropriate survey revisions to incorporate the nuances learned from the KIs. Cognitive interviews were then conducted both on our constructed questions and on the literature-based scales (after the aforementioned preemptive phrasing revisions).^{162,163}

Fortunately, cognitive testing strongly supported the response process validity of the survey questions, including the adapted scale items. After incorporating additional revisions recommended by the cognitive

testing (e.g., removal of idioms which were confusing to international students), the pilot survey was issued at several universities. Survey items which did not appear to perform properly or provide discriminant utility (e.g., high skip rates, lack of response distributions) were removed. Additionally, the long literature scales (57 items total) were analyzed using factor analysis both to evaluate internal structure and to create “short forms” (i.e., trimmed scales). Short forms prevent a survey from exceeding its time constraint or inducing survey fatigue by identifying the minimum number of items needed to measure the intended construct. The three scales were ultimately trimmed down to 16 items total. With the primary objective of instrument creation met, the validated survey was then distributed nationally, in line with the secondary objective.

3.6 Ethics

The research team spanned three institutions: the University of California – Los Angeles and the University of Chicago Institutional Review Boards (IRBs) both separately determined this study to be exempt, and the Michigan Technological University IRB accepted these determinations. For each participating university, either the department chair and / or an executive administrator in the department approved email recruitment of students via institutional listservs for cognitive interviews, the pilot survey, and / or the national survey. KI student candidates and all SP candidates were approached directly via email.

Due to the reach of the study and the closeness of academic circles, conflicts of interest were of particular ethical concern. In cases where a potential conflict of interest may be perceived for a team member engaged in recruiting or interviewing, another member of the team was tagged to take their place. For example, for one of the schools in the sampling frame, the department chair had worked with a team member on a grant application recently; that team member was blacklisted from engaging in any recruiting activities with that school to avoid the perception of pressuring the chair to agree to recruitment. However, mutual connections were not necessarily avoided in cases where the connection was perceived to be beneficial to the study activities without applying undue pressure on a participant (e.g., snowball recruitment).

Due to the potentially sensitive nature of laboratory safety, interviewees were asked to affirm that they were in a space where they felt comfortable expressing their full opinions, with the option to reschedule if

not. Audio was recorded for all interviews and destroyed after transcription by the respective interviewer. Any personally identifiable information found in the data was removed. Data was stored in the UCLA Google Drive only after anonymization was complete. Participants gave verbal consent at the start of each interview or completed an online consent form before viewing either survey. Interviewees were each offered a \$20 Amazon gift card, and survey-takers were entered into a randomized lottery for the chance to win one of a selection of Amazon gift cards from \$15 to \$75 in value. Neither institutions nor participants are identified by name.

3.7 Sampling Methodology

There were four distinct phases of sampling for the KI interviews, cognitive interviews, pilot survey, and national survey.

For the KI interviews, 10 participants were recruited via convenience and snowball sampling until data saturation was reached.^{135,164} A list of the research team's relevant professional contacts was assembled (both primary contacts and secondary contacts), and selected candidates were sent a recruitment email. Both SPs connected to chemistry operations (e.g., Environmental Health & Safety staff, chemistry department lab safety managers) and PhD chemistry students were recruited with the aim of collecting data from both the students' and the institutional safety teams' perspectives. As is recommended for KI interviews, priority was given to contacting individuals perceived to have deep experience or interest in the topic area, such as students involved in safety clubs or serving as safety officers for their research groups. In some cases, a participant recommended another person for the research team to contact; those recommended individuals were subsequently sent recruitment information.

For the cognitive interviews and the pilot survey, students were recruited via department listserv emails if the university agreed for their students to be recruited. Schools with doctoral-granting chemistry programs were recruited using convenience sampling (typically the existence of a professional contact at said schools) until data saturation was reached with 20 cognitive interviews and 122 retained pilot survey responses. The schools which were recruited in these testing stages were later blacklisted from the national survey sampling frame to avoid contaminating the national dataset. For the cognitive interviews, eligible interested individuals provided their contact information on a private form, and a selection of volunteers

were chosen to interview. For the pilot survey, anyone meeting the eligibility criteria was able to take the survey directly from the recruitment email.

While SPs were always contacted directly via email using publicly listed contact info on institutional websites, the students for the cognitive interviews and pilot survey were sent recruitment information via student listservs operated by chemistry department administration. To encourage sufficient and diverse participation, the help of additional people at the schools was sometimes enlisted where necessary to spread recruitment awareness, such as by asking a student-run chemistry club to endorse the study.

Between the interviews and pilot surveys, the participants represented 18 different universities. For the national survey, a list of universities in the United States offering doctoral degrees in chemistry was assembled using the Carnegie Classifications database.¹⁶⁵ A randomized assortment of institutions was drawn from that list to form the sampling frame. The sampling frame was comprised of 15 institutions of each of four types: private R1, public R1, private R2, and public R2. Recruitment of institutions continued until at least six schools in each category consented to participate or until the sampling frame was exhausted. Additionally, individuals at some additional schools volunteered their schools for participation after attending an American Chemical Society (ACS) presentation about this ongoing work; those institutions were also contacted. Overall, recruitment of private R2 institutions was challenging due to a lack of responsiveness from school officials, but the quotas were successfully reached for the other three categories. Very few institutions directly denied consent. In total, students from 24 institutions have participated so far in the national survey (8 private R1, 7 public R1, 3 private R2, and 6 public R2). Data collection is still ongoing.

3.8 Participant Screening

Since this study sought to understand laboratory safety behavior in academic chemistry research environments, individuals had to meet multiple eligibility criteria. For safety professionals (SPs), they were required to (1) have some familiarity with the chemistry department at their institution and (2) have been at their current institution for at least one year. For students, participants had to be (1) a current PhD student, (2) in their current research group for at least one year, and (3) currently practicing in a bench-centric chemical research area (e.g., computational chemists and chemical education research chemists were excluded).

These criteria helped ensure that respondents would have recent, informed perspectives about the current state of affairs in a specific bench chemistry group (for students) or the institution's overall chemistry environment (for SPs).

PhD students were particularly attractive to us over other types of students and postdoctoral scholars because of the length of time that a PhD student spends at an institution and because of the high proportion of their time that they spend physically in their research laboratory, meaning that they are typically deeply embedded in their institution's and group's cultures for several years. Research trainees who tend to spend less time in a specific group (e.g., Master's students, postdoctoral scholars) were therefore excluded.

Additionally, within the surveys / interviews, some questions were meant only for individuals with specific experiences (e.g., Laboratory Safety Contacts). The questions asked were therefore controlled carefully with detailed interview guides / survey display logic (**Appendix C**). These individuals were not specifically recruited separately except for the KI interviews.

3.9 Data Collection

Interviews were conducted during August 2022 – January 2023, and the pilot survey was administered March – May 2023. The national survey was distributed from June – August 2023. Each member of the research team was responsible for recruiting and interviewing one category of participant each (e.g., my collaborator Nasim Mirzajani handled the student cognitive interviews for the scales). Responsibility for recruiting institutions for the pilot and national surveys were likewise subdivided.

All interviews occurred via Zoom (<https://www.zoom.us/>) and were conducted in English following convenience scheduling using Calendly (<https://www.calendly.com/>). All surveys were administered online in English via Qualtrics (<https://www.qualtrics.com/>). KI interviews and cognitive interviews each took 1 h except in some cases where a KI knowingly wanted to continue talking past the 1-h mark. The pilot survey took an average of 20 min to complete as did the national survey.

KI interviews followed a semi-structured interview guide (**Appendix C**) and were highly fluid based on participant responses. The primary focus was on investigating the participants' most relevant experiences rather than on asking all the questions in the interview guide.

Cognitive interviews followed a more rigid interview guide (albeit still semi-structured) to test items according to Tourangeau's 4-stage response process theory: *Understanding, Retrieval, Judgement, and Response* (**Appendix C**).^{163,166} Half of the interviewees tested "*Survey*" items while the other half tested "*Scale*" items. *Survey* questions were all the questions in the survey except the *Scale* items (i.e., LMX7, Safety Climate, and Safety Citizenship). *Scale* testers were always students since only students would receive those questions in the national survey. Half of the *Survey* testers were SPs and the other half students. The items presented in the cognitive interviews were randomized ahead of time from a carefully considered selection of items which were most anticipated by the team to merit testing. Both questions and survey instructions themselves were tested. For each interview, the interviewer first explained the concept of cognitive testing and then walked the participant through a mock question to simulate the unusual-to-them discussion style before presenting the experimental items. All items were presented on a PowerPoint slide via a shared screen one at a time (**Appendix C**).

Student participants in the pilot survey likewise received either *Survey* or *Scale* questions. SP participants in the pilot survey received only *Survey* questions. The *Survey* testers saw all questions except for standardized demographic questions (e.g., race), the *Scale* items, and the hazard / research classification questions. The *Scale* participants, meanwhile, saw the scale items as well as the hazard / research classification questions but not the other survey questions. These participants received *all* the scale items (with the chemistry-specific revisions as tested in the cognitive interviews), thus enabling Exploratory Factor Analysis (EFA) afterward to create short forms of the scales for the national survey. At first, the type of survey presented to participants was randomized until sufficient responses were received for *Survey*. At that point, all future participants were routed to *Scale* to boost sample size for EFA.

3.10 Data Processing

Consent was obtained for all interview participants. Interviews were transcribed via intelligent verbatim transcription using assistive technology (e.g., Zoom automated transcription). Each interviewer manually edited their own automated transcriptions to ensure accuracy.

N.,b: For one PhD student's cognitive interview, their English was so challenging to understand that the automated transcription was unintelligible and the interviewer was also forced to abandon manual

transcription, instead writing a summary document. Note that the research team hailed from America, Israel, and Jamaica. Fortunately, while a few other interviews with international students had moments of unintelligibility, most of their interview content was amenable to transcription. The large presence of international researchers in chemistry in the United States and the challenges we sometimes encountered with understanding them underscore the importance of this validation process. Significantly, there were multiple problems flagged by the international students with several items (both those constructed by us and those from the literature), such as the use of American idioms. Without interviewing individuals who we sometimes struggled to fully understand, it would not have been possible to learn the ways in which they did not understand us.

Consent was logged for 191 eligible responses for the pilot survey, and 122 proceeded to take the survey (26 *Survey* and 96 *Scale*). Of the *Scale* recipients, those who failed an attention check item were removed as were any highly incomplete submissions. Respondents who skipped only a few items were retained. The vast majority of responses retained provided complete data; items were rarely skipped. Notably, scale items for the *Scale* pilot could not be skipped, a restriction imposed due to the potential impact on EFA analysis. Otherwise, few questions were required. Straightlining was rarely observed despite the prevalence of multiple large matrices nor were bots. In total, 87 *Scale* responses were retained with apparently high survey quality.

3.11 Data Analysis

Quantitative data was analyzed using Microsoft Excel 365 or IBM SPSS 28.0.1.1. A critical value of $p = .05$ was used for significance tests except where noted. Qualitative data was analyzed using MAXQDA 2022 Analytics Pro.

KI interviews underwent both (1) deductive coding with content analysis according to the interview guide and (2) inductive coding with thematic analysis for additional emergent codes beyond the existing survey structure. This exhaustive analysis was completed by my collaborator Sarah Zinn to evaluate content and consequential validity. Cognitive interviews underwent exclusively deductive coding with content analysis by me to evaluate validity according to Tourangeau's 4-stage response process theory.¹⁶³ The results of these analyses were incorporated into the pilot survey to ensure optimal content, consequential, and response process validity for the target population.

The students' pilot survey underwent two general types of analysis. Firstly, the *Survey* items were evaluated for item-level response rates and discriminant performance (i.e., Were people skipping specific items? Were items eliciting the intended distribution spreads, or were they failing to offer distinctions between respondents?). Secondly, the *Scale* items were evaluated for (1) ways to characterize lab environments and (2) ways to decrease scale length without compromising internal structure. Since the *Survey* item evaluation was overwhelmingly positive with only minor adjustments prescribed, the remainder of this chapter will focus on the analysis of the *Scale* respondents' data.

Notably, recruitment for the SP pilot survey was halted after it became apparent that SPs were giving systematically different responses about institutional policies than their colleagues *at the same institution*. Since KIs and cognitive testing had strongly supported the validity of the survey, it was concluded that this variability arose from fragmented knowledge-sharing among SPs, the convoluted nature of institutional policies, and the individuality / obscured nature of research groups' behaviors. Therefore, SPs at the same institutions did not share the same understanding of their own institutions' policies, programs, and processes. KI data and our team's domain knowledge supported this rationale as well, although we were surprised by the severity of the problem. SP data had been intended to serve as an authoritative source of information about the institutional resources and policies available to student. SP data thereby would ideally have served serve as a check to the student data by indicating whether students were well-informed about and using all the resources available to them. However, since SP data could not be verified as accurate, SPs were removed from the national survey recruitment plan, and their pilot data is herein discussed no more.

3.12 Chapter Scope

Analysis of the national survey data is ongoing. Therefore, that dataset will not be discussed further. Similarly, the KI interview data analyzed by Zinn, the cognitive interview data analyzed by myself, and our *Survey* pilot data will also be omitted for the remainder of this chapter other than to say that (1) the survey was revised to incorporate our interview findings before piloting the survey, (2) both sets of interviews strongly supported their respective validity claims, and (3) the *Survey* pilot data revealed no major problems with item performance.

Instead, from here on out, the focus will be on the pilot survey *Scale* data. The sample will first be described followed by cluster analysis to yield generalizable characterizations of the types of lab environments that chemistry graduate students work in. Then, the scales will be validated using EFA and reduced to novel short forms. Together, these two types of analyses will enable the national survey to make correlational claims about safety outcomes in lab environments by both parameterizing what those environments are and providing short scales.

3.13 Pilot Survey Sample

The pilot survey sample represented a variety of institutions, research types, programmatic years, and English language skills. All of the retained *Scale* responses happened to come from 7 of the 8 institutions involved in the pilot survey. Five institutions were R1s and two R2s. 75.9 % of the respondents came specifically from three prestigious R1s.

In terms of students' programmatic years in their PhD (e.g., 2nd-year student), the distribution was remarkably even across years 2 – 5 with an average of 23.8 % in each of the 4 major program years. The outstanding 4.5 % of respondents were in years 6 and 7 but not beyond. This distribution was largely reflected in students' length of tenure in their research group as well, minus one year (with some variation). These variations (data not shown) are easily explainable by institutions' different policies for when PhD students can / must join a research group and by the reality that sometimes students switch groups during their program.

Respondents also came from a decent variety of research subfields, with concentration seen in disciplines typically thought of as bench-intensive and focused on “wet” chemistry (**Table 3.1**). The types of hazards they reported encountering in their labs supported this generalization, as seen by the high prevalence of hazards such as flammables and sharps and low prevalence of lasers and high voltages (**Table 3.2**). Since the intention was to evaluate safety in bench chemistry laboratories, this distribution indicates that respondents should indeed have a plethora of experiences with hazardous environs to reflect on. A method for reducing these research types and hazard types to more generalizable classes will be discussed later.

Table 3.1. Respondents' research fields.

Research Type ^a	% ^b
Biochemistry	25.3
Materials chemistry	21.8
Inorganic chemistry	17.2
Organic chemistry	17.2
Physical chemistry	12.6
Analytical chemistry	3.4
Polymer chemistry	2.3

^aList composed based on ACS & RSC classifications^{167,168}

^bMultiple choice – no one selected “Nuclear chemistry” or “Chemical engineering”

Table 3.2. Types of hazards in respondents' research labs.

Hazard Type ^a	% ^b
Flammables or Combustibles	87.4
Needles or Sharps	87.4
Corrosives	85.1
Environmental Hazards	70.1
Cryogenics	65.5
Toxins	65.5
Compressed Gases	63.2
Reactives	60.9
Irritants	56.3
Sensitizers	39.1
Asphyxiants (Non-Cryogenics)	25.3
Biosafety Level 2	23.0
High Voltages	21.8
Class 3B or 4 Lasers	17.2
Biosafety Level 1	17.2
Radioactives	12.6
Potentially Infectious Materials	11.5
Controlled Substances	10.3
Live Animals	4.6
Non-Airborne Pathogens	2.3
Airborne Pathogens	1.1
Biosafety Level 3	1.1

^aList composed based on multi-expert domain knowledge in chemistry and safety – terms were accompanied by definitions & examples in survey

^bIndividuals reported an average of 8.3 types of hazards in their lab – no one selected “Biosafety Level 4” or “None of these”

Additionally, 24.1 % of respondents were English Language Learners (ELLs) while 66.7 % were native English speakers (9.2 % did not identify). The ELLs boasted a diverse range of native and non-native languages (data not shown). The average age at which they started acquiring English was 7.8-years-old, and the ELLs rated their own English-speaking skills highly (mean of 8.1 on a 10-point scale aka “Very Good”). Strong literature precedent relevant to the graduate academic environment happily indicates that strong inferences can be made about ELLs’ actual English-reading proficiency based on their self-reported English-speaking proficiency.^{169–171} Therefore, our ELLs should have good proficiency in reading colloquial English.

3.14 Saboteur Monitoring

Due to the previously discussed potential for sabotage of a safety evaluation instrument, participants were screened for potential biases. In particular, each participant was presented with items dubbed here as “anti-saboteur” items which were intended to expose strong or manipulated opinions (see **Table 3.3** for a selection of the items and **Appendix C** for the complete list). The rationale was that if a participant wanted to sabotage survey results (as discussed above in the Methodology section) due to anti-safety sentiments, they would say that lab rules slow down work, do not help keep people safe, and do protect the university from litigation. Meanwhile, saboteurs on the other end of the spectrum would theoretically say that their labs are very hazardous and that their lab does a bad job mitigating hazards. And both types of saboteurs would likely exhibit an us-versus-them mentality by expressing an opinion that either SPs or their peers / PI see the hazards and risks in their labs differently than they themselves do.

Table 3.3. Descriptive statistics for a selection of example anti-saboteur items.

#	Item ^a	Mean ^b	Std. Dev.	Skew	Kurtosis
1	I think that overall, safety in my lab could be improved.	4.37	1.139	-0.457	0.208
2	My lab does a good job of mitigating the hazards associated with our lab work.	4.62	1.151	-1.253	1.987
3	I personally feel that lab safety rules and regulations prevent experiments from being done.	2.35	1.382	0.974	0.165
4	I personally feel that lab safety rules and regulations make my lab a safe place to work.	5.20	1.048	-1.857	4.165
5	I personally feel that lab safety rules and regulations are to protect the university from litigation.	5.34	0.971	-1.982	5.119
6	If [Safety Professionals] watched me work in the lab, they would probably evaluate my lab behavior as being...	4.38	1.183	-1.101	1.072
7	How hazardous do you think [You] view your research lab as?	3.58	1.257	-0.067	-0.551
8	How hazardous do you think [Your Fellow Group Members] view your research lab as?	3.21	1.243	-0.149	-0.719
9	How risky do you think [You] view your research lab as?	2.92	1.187	0.381	-0.180
10	How risky do you think [Safety Professionals] view your research lab as?	3.19	1.207	0.381	-0.720

^aAll item responses on a 1 to 6 ordinal positive agreement response format (i.e., “; “Strongly disagree” → “Strongly agree”; “Very unsafe” → “Very safe”; “Not at all hazardous” → “Extremely hazardous”; “Not at all risky” → “Extremely risky”)

^bTotal 87 cases; missing data excluded pairwise; 79 cases contained complete data for all items

Fortunately, evidence was lacking for either type of saboteur on a systematic level, with participants expressing fairly balanced opinions overall. All the items in **Table 3.3** (and **Appendix C**) displayed unimodal distributions, albeit with some skewing toward safety-positive individuals. The participants believed that their labs were somewhat to moderately hazardous (entries 7 – 8, **Table 3.3**) but only slightly to somewhat risky (entries 9 – 10) – and, notably, with space to improve. Safety rules are unequivocally partly intended to protect a university from litigation, so the high mean for entry 5, for example, helped reassure us that the participants held reasonable opinions on this front without malicious intent to sabotage.

Meanwhile, EFA of the risk and hazard magnitude items failed to reveal evidence for an us-versus-them mentality. First, in order to evaluate the suitability of the data for factor analysis, a Pearson *r* correlation matrix was generated (not shown). Significant correlations among the items ranged from low to high which indicated that the data could be factorable and appropriate for EFA. Kaiser-Meyer-Olkin's Measure of Sampling adequacy was executed to verify sampling adequacy ($KMO = .592$) while Bartlett's Test of Sphericity ($\chi^2(28) = 635.539, p < .001$) indicated that correlations between items were sufficiently large for factor analysis. Since the risk and hazard magnitude items were expected to represent unobservable latent constructs of individuals' opinions about the safety environments of their labs, Principal Axis Factoring was selected as the most appropriate EFA method per the common factor model theory.¹⁷² Since factors were expected to be correlated (i.e., perceptions about risks and hazards seem related at face value), oblique rotation was executed using Direct Oblimin rotation.

The eigenvalues-of-one condition and scree plot (not shown) were used to discover factors. A 2-factor model was natively generated (**Table 3.4**) with clean, strong factor loadings. A high cumulative variance of 66.6 % also manifested alongside strong face validity. Therefore, the model was accepted without further modification. The factors were named based on perceived item relationships.

Table 3.4. Factor loadings^a for Exploratory Factor Analysis^b concerning perceived safety level of lab environments.

Item Code ^c	Hazard Magnitude	Risk Magnitude
Hazard_PI	.986	
Hazard_Peers	.802	
Hazard_SPs ^d	.763	
Hazard_Self	.725	
Risk_Self		.922
Risk_Peers		.777
Risk_SPs*		.763
Risk_PI	.237	.562
% of Variance ^e	50.9	15.7

^aPattern matrix from Principal Axis Factoring and Direct Oblimin rotation ($\delta = 0$) with Kaiser normalization converged in 6 iterations; missing data excluded pairwise

^bKMO = .592; Bartlett's Test of Sphericity $\chi^2(28) = 635.539$, $p < .001$

^cFor clarity, pattern coefficients less than $\pm .2$ not shown; items organized by descending factor loading value; no items were removed

^dSP = Safety Professionals

^e66.6 % cumulative variance accounted for

These EFA results indicate that respondents felt that they, their peers, their PI, and SPs were on the same page regarding the hazard and risk levels of their respective labs (**Figure 3.4**). This level of agreement rejects the presence of the us-versus-them mentality expected in potential saboteurs. However, this data should not be construed to imply that respondents were accurately predicting either the relative magnitudes of the hazards and risks in their labs or the actual opinions of the people around them.

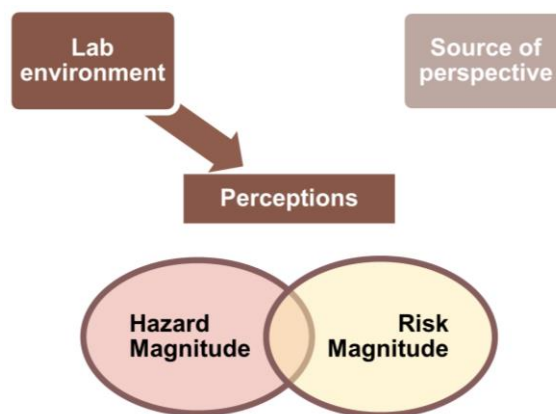


Figure 3.4. Perceptions of the Hazard and Risk Magnitude of a lab were driven by the lab environment itself rather than the perspective source (e.g., SPs vs. peers).

Additionally, the two factors were moderately positively correlated (correlation coefficient = .488), indicating that the higher the perceived Hazard Magnitude, the higher the perceived Risk Magnitude and vice versa. Indeed, labs were rated more hazardous than risky on average, as should be the case. With both theoretical and statistical soundness established, the raw scores of each retained item passing the cut-off condition were multiplied by the corresponding absolute loading value and summed with the factor's other items to generate a weighted sum score for each factor. This type of "non-refined / coarse method" for estimating factor scores is considered appropriate with (1) simpler factor structures, (2) data that, when on the same response format range, produce similar standard deviations (**Appendix C**), and (3) factors which are not highly correlated.¹⁷³ The weighted sum factor scores were then averaged according to their respective total weights (e.g., Hazard Magnitude weights = 0.986 + 0.802 + 0.763 + 0.725 = 3.276) to scale each factor according to its respective summed weight (**Table 3.5**). This scaling enables the reader to intuitively compare the factor scores while ensuring that the stronger loading items contribute more to the scores than the weaker.

Table 3.5. Descriptive statistics and internal consistency of factor scores for perceived safety levels of lab environments.

Factor ^a	# of Items	Scaling Weight ^b	N ^c	Mean	Std. Dev.	Skew	Kurtosis	Cronbach's α^d
Hazard Magnitude	4	3.276	84	3.41	1.116	-0.103	-0.391	.902
Risk Magnitude	4	3.024	84	2.81	0.945	0.299	-0.247	.858

^aAll factor scores are scaled weighted sums of the items' raw Likert scores (1, "Strongly Disagree" → 6, "Strongly Agree" response format without a Neutral option)^{174,175}

^bScaled per sum of the factor loadings

^cTotal 87 cases; missing data excluded pairwise; 84 cases had complete data

^dMissing data excluded pairwise; reliability analyses are for the items' raw Likert scores

Notably, although self-report data about safety behavior is not reliable, we did ask them to report their own beliefs about their safety behavior (**Table 3.3** and **Appendix C**). The low deviation and high average informed us that the participants *wanted* to believe that they are good actors, even if they are not able to self-normalize; we find the lack of distribution dubious. Overall, this self-report data informs us that the sample was generally lacking in saboteurs but was still skewed toward people who want to think well of their own

behavior and who want to work in safe environments. Although we will leave the actual evaluation of safety behavior to the psychometric scales, this data reinforces that (1) we likely cannot trust self-reported behavior data (as discussed in the Methodology section), (2) participants *want* to believe that they are personally safe actors and *want* to be in safe labs, (3) participants have a hard time normalizing their behavior to others, and (4) participants recognize the potential for improvement in their own labs. Such indications reinforce the survey design decisions we made in anticipation of such issues while also boding well for ultimately effecting change in such a receptive population.

N.b., although these anti-saboteur items helped to characterize the sample population in the pilot survey, the items were discontinued for the national survey since larger sample sizes usually display the regression-toward-the-mean phenomenon. In other words, since the national survey was unlikely to skew further from the opinions seen here, there were only marginal returns to including the items. Therefore, they were removed to maintain the 20-min maximum administration time for the national survey.

3.15 Characterization of Lab Environments

With an understanding of the students' perceptions of the risk and hazard levels of their lab (**Table 3.5**), the types of research conducted (**Table 3.1**), and the types of hazards present (**Table 3.2**), cluster analysis could now be conducted to build a generalizable model for the types of lab environments these students operated in. In **Figure 3.5**, the five input variables are displayed. Since fewer than 10 % of respondents identified airborne / non-airborne pathogens, live animals, or BSL3 / BSL4 as hazards present in their labs, those hazards were excluded to protect cluster quality. Similarly, polymer chemistry (N = 2) and analytical chemistry (N = 3) were excluded. Since the data was both categorical and continuous, nominal nonhierarchical two-step cluster analysis was executed with Schwarz's Bayesian clustering criterion and log-likelihood distance measures.¹³⁷ Due to the descriptive nature of cluster analyses, there is no formal cut-off for determining the "significance" of a descriptive cluster analysis. Instead, uniformity in items' silhouette values, a high average silhouette value, and perceived reasonableness of the resulting clusters are a set of approaches often considered in evaluating a cluster analysis.

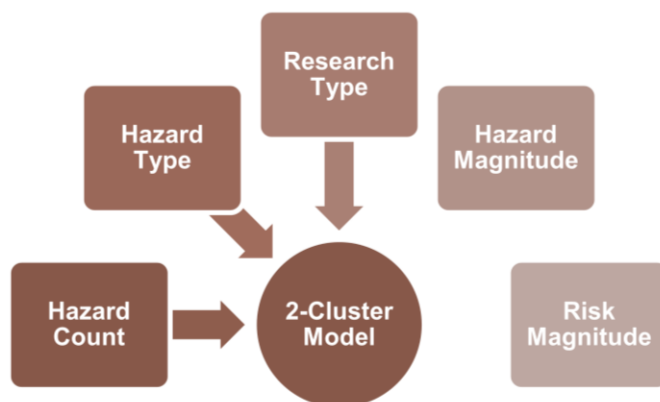


Figure 3.5. Three components clustered meaningfully in a 2-cluster model whereas two did not.

The first clustering result produced was a 2-cluster model. However, not all of the inputs contributed in a meaningful way toward the cluster. Risk Magnitude provided almost no contribution to the cluster outcome (predictor importance = .07). This appears to indicate that perceptions of the magnitude of risks had no discernible relationship to the actual research and hazards present. Therefore, the factor was removed and the analysis rerun. The resulting 3-cluster model reported Hazard Magnitude with an importance of .13, so it too was removed. Clusters of size 2 – 6 were then modeled with the remaining variable types (**Figure 3.5**), reaching a maximum average silhouette value occurring at $k = .280$ with a 2-cluster model (**Appendix C**). The silhouette value method utilized Gower’s dissimilarity measure to evaluate cluster fit.

With all the input variables now playing a meaningful role in the outcome, **Figure 3.6** illuminates the nature of the clusters. Apparently, the types of laboratory environments the students work in can be simplified down to that of “Many Hazards” (blue) or “Few Hazards” (yellow). Hazard Count itself was the most important contributor (predictor importance = 1.00) while Research Type offered a predictor importance of .53. The different hazards themselves within the overall Hazard Type category had predictor importances ranging from .69 – .02. Note that clusters were defined both by the hazards *present* as well as the hazards *absent* (e.g., while ~50 % of labs with corrosives were in cluster 2, 100 % of labs *without* corrosives were also in cluster 2). Considering the enormous diversity in types of research and hazards encountered in chemistry, this 2-cluster model provides a much-needed simplification for later assessing the relationship between lab environment, safety behaviors, and safety programs / policies.

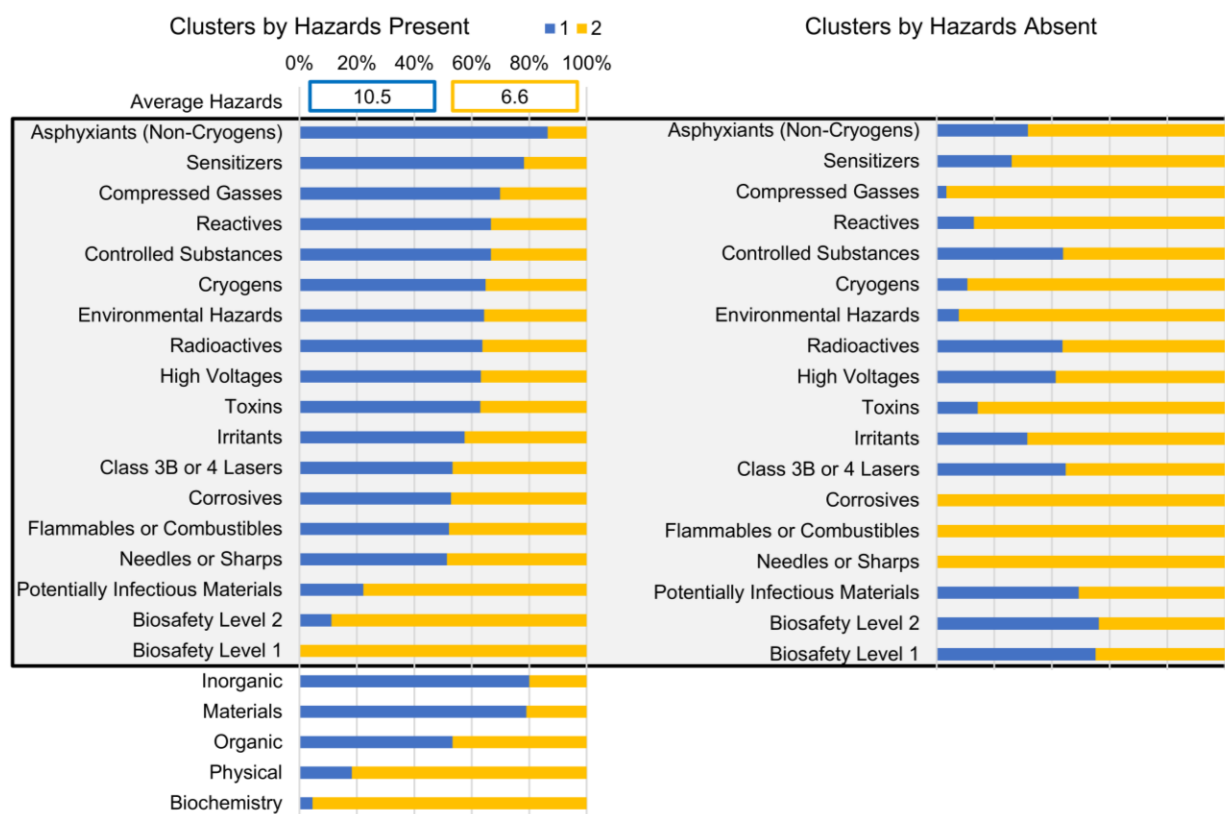


Figure 3.6. Hazard count, hazard types, and research type clustered to describe the types of lab environments chemistry graduate students work in. Rare items were excluded from the analysis.

3.16 Characterization of Safety Behavior

With the lab environments characterized, behavior itself remained to be addressed. EFA was utilized to first assess the internal structure of the full-length scales in this novel context with the chemistry-specific revisions before shortening them. The same process utilized for the earlier EFA was replicated. At first, the eigenvalues-of-one condition natively returned a 13-factor model which, upon evaluation of item distribution, possessed questionable face validity. The scree plot, however, suggested a 3-factor model would be appropriate, which was supported by the original literature that the scales derived from. Therefore, the analysis was rerun with a 3-factor model imposed upon it ($KMO = .666$, Bartlett's Test of Sphericity $\chi^2(596) = 4025.851$, $p < .001$). The loading of the climate-derived and citizenship-derived items encouragingly reflected literature precedent (**Appendix C**). However, the LMX7 items engaged in substantial cross-loading with the climate items. Multiple items also loaded $< .5$. Overall, the internal structure for the

scales in this study's context was not ideal and signifies the need for adjustments should future researchers attempt to use the full-length versions.

Next, in pursuit of the short forms, the model was iteratively purged of low-performing items. Since the number of respondents was fewer than 100, a factor loading value of .4 was set as a removal condition for the first round of trimming, followed by .5 and then .6 for subsequent iterations, constituting a much stricter cut-off value than often used.^{172,176,177} After the first few iterations, all the items loaded cleanly onto one factor each with all loading values > .6. However, the number of items retained was still too large considering the purpose of this exercise was fundamentally to create short forms. Yet, if the trimming was pursued further according to the typical practice of removing the lowest loading values, the resulting factors were of questionable utility: the retained items were almost identical. Since an overly homogenous scale can backfire by pigeonholing responses, an alternative method was employed for the final shortening steps: for the fifth and sixth models, every other item was selected for deletion after organizing them in order of loading value (e.g., the lowest item was deleted – the second lowest item was retained – the third lowest was deleted – etc).

Therefore, after these six total rounds of trimming, the seventh model was accepted as the final version with factor loadings ranging from |.637| – |.922| and 64.6 % cumulative variance explained (**Table 3.6**, color-coded to match **Figure 3.2**). The factors appeared reasonable according both to factor loading values and face validity. The factors were then named based on the perceived similarities between their items and using the original scale names as inspiration. The 16 items represent roughly a quarter of the original scales' combined lengths.

Table 3.6. Factor loadings^a for Exploratory Factor Analysis^b to make scales' short forms.

#	Item ^c	F1 Safety Climate ₂	F2 Safety Citizenship ₂	F3 LMX ₂
1	My PI seems to care about my safety.	.922		
2	Lab safety practices are important to my PI.	.863		
3	My PI would act quickly to correct safety issues.	.729		
4	My PI views safety regulation violations very seriously even if they don't result in apparent damage.	.686		
5	My PI is willing to implement new ideas for improving safety.	.657		
6	Members in my group comply with safety regulations.	.637		
7	Telling other group members to follow safe working procedures		.811	.208
8	Encouraging others to get involved in safety issues		.791	-.220
9	Voicing safety-related recommendations concerning work activities		.780	
10	Trying to improve safety procedures		.743	
11	Helping other group members learn about safe work practices	.243	.684	
12	Getting involved in safety activities to help my group work more safely		.659	
13	How well does your PI recognize your potential?			.786
14	Do you usually know how satisfied / unsatisfied your PI is with what you do?			.747
15	How would you characterize your working relationship with your PI?	.283		.673
16	How well does your PI understand your job problems and needs?	.220		.657
% of Variance ^d		40.0	18.3	6.3

^aPattern matrix from Principal Axis Factoring and Direct Oblimin rotation ($\delta = 0$) with Kaiser normalization converged in 6 iterations; missing data excluded pairwise

^bKMO = .884; Bartlett's Test of Sphericity $\chi^2(120) = 870.110, p < .001$

^cFor clarity, pattern coefficients less than $\pm .2$ not shown; items organized by descending factor loading value; factor loading cut-off value of .6 for factor inclusion, then randomized deletion to reduce factor size

^d64.6 % cumulative variance accounted for

Notably, each factor strongly reflected the character of the corresponding literature scales at this point with minimal cross-loading. However, while neither Safety Citizenship₂ – LMX₂ nor Safety Citizenship₂ – Safety Climate₂ were appreciably correlated (**Table 3.7**), Safety Climate₂ – LMX₂ were moderately positively correlated, reinforcing the advisability of oblique rotation. This correlation implies that the safety climate

within a research group is strongly linked with individuals' relationships with their PIs. The better the relationship, the stronger the safety climate.

Table 3.7. Factor correlation matrix for scales' short forms.

Factor	F1 Safety Climate ₂	F2 Safety Citizenship ₂	F3 LMX ₂
F1 Safety Climate ₂	---		
F2 Safety Citizenship ₂	.252		
F3 LMX ₂	.516	.091	---

Next, with both theoretical and statistical soundness established, scaled weighted sum factor scores were calculated as previously described (**Table 3.8**), revealing that respondents on average reported slightly to moderately positive feedback in terms of their relationships with their PIs, their group's attitude toward safety, and their own internalization of safety as a component of their job. The three factors displayed acceptable skews, kurtoses, and unimodal histograms (not shown) for claiming normality. Internal consistencies were Good – Excellent according to Cronbach's α .¹⁷⁸ The scaled scores were used throughout the remaining analyses and treated as continuous interval data.

Table 3.8. Descriptive statistics and internal consistency of factor scores for the scales' short forms.

Factor ^a	# of Items	Scaling Weight ^b	N ^c	Mean	Std. Dev.	Skew	Kurtosis	Cronbach's α ^d
F1 Safety Climate ₂	6	4.494	79	4.71	1.095	-1.073	0.726	.914
F2 Safety Citizenship ₂	6	4.468	79	4.61	0.969	-0.614	-0.375	.874
F3 LMX ₂	4	2.863	81	4.29	1.027	-0.829	-0.385	.873

^aAll factor scores are scaled weighted sums of the items' raw Likert scores (1, "Strongly Disagree" → 6, "Strongly Agree" response format without a Neutral option)

^bScaled per sum of the factor loadings

^cTotal 87 cases; missing data excluded pairwise; 79 cases had complete data

^dMissing data excluded pairwise; reliability analyses are for the items' raw Likert scores

3.17 Scale Validity Assessment Between Groups

With the scale validated for the overall population, the last step in the piloting process was to search for potential discrepancies in response patterns. Since the goal was to develop short forms for use with PhD chemistry research students, we needed to evaluate whether scale performance varied between key groups within the PhD cohort. The group comparisons of concern were (1) native English speakers vs. ELLs, (2) participants from the three overrepresented, prestigious R1s vs. the four other schools, (3) program years (excluding years > 5 due to small sample size), and (4) length of tenure in current research groups (excluding years > 4 due to small sample size). Therefore, Two-Way Multivariate Analysis of the Variance (MANOVA) was executed for between-group comparisons for the three factor scores and four group types. The excluded values were treated as missing data.

MANOVA assumptions were first checked in preparation for the procedure. The factor scores were already known to be variably correlated from EFA testing (**Appendix C**), and univariate normality was previously described with skews and kurtoses in **Table 3.8** and histograms (not shown). Independence of observations was inherently protected. Scatterplots suggested the presence of linear relationships between the factor scores. Quartile-Quartile (Q-Q) plots were visually determined to be linear (not shown) for the scores, suggesting multivariate normality. No multivariate outliers were found per Mahalanobis distances with the commonly-accepted critical value of $\alpha = .001$ for this highly sensitive test ($p > .001$ for $N = 71$ complete entries).¹⁷²

Since subsample sizes between the groups were unequal, Levene's and Box's M tests were both executed. Box's M Test of Equality of Covariance Matrices failed to find unequal covariance matrices between the variables across groups, Box's $M = 54.622$, $F(30, 1142.541) = 1.300$, $p = .130$, indicating homogeneity of variance-covariance matrices. Using the trimmed mean due to the low kurtoses, Levene's Test of Homogeneity of Variance (**Appendix C**) did reveal significant differences in variance for Safety Citizenship. Therefore, Pillai's trace was selected for MANOVA interpretation, an additionally appropriate decision given the uneven cell sizes and small sizes of some of the subsamples.¹⁷²

Two-Way MANOVA proceeded to reveal only nonsignificant interactions (not shown) between the respondents' groups (i.e., program year, research group year, native status, and institutional group). Simple main effects also happily failed to find significance for any of the groups and their factor scores (**Appendix**

C). In other words, there were nonsignificant mean differences for ELLs and native English speakers, $F(3, 42.000) = 2.548$, $p = .069$; Pillai's trace = .154; nonsignificant mean differences for the three prestigious R1s and the other four schools, $F(3, 42.000) = 1.020$, $p = .393$; Pillai's trace = .068; nonsignificant mean differences for program years 2, 3, 4, and 5, $F(9, 132.000) = 1.606$, $p = .120$; Pillai's trace = .296; and nonsignificant mean differences for research group years 1, 2, 3, and 4, $F(9, 132.000) = .2254$, $p = .985$; Pillai's trace = .051.

In other words, the respondents' scores on the LMX, Safety Citizenship, and Safety Climate short forms were not significantly affected by these pertinent demographics except that there was greater variance for the Safety Citizenship short form. Visual analysis of histograms for the split groups' Safety Citizenship₂ scores indicated similar distribution shapes, so follow-up Kruskal-Wallis H tests were conducted to confirm the MANOVA results out of an abundance of caution. None of the H tests were significant (**Appendix C**), thereby reiterating the Two-Way MANOVA results.

3.18 Discussion

The primary focus of this report was to detail the systematic development of a validated survey instrument that can be used for measuring the safety behavior of PhD graduate students in academic chemical research laboratories. Overall, this survey development process was successful in generating a validated instrument that should be applicable to US-based PhD student populations in chemistry and likely other related populations such as Master's students. Implications, limitations, and recommendations both for the use of this instrument and for similar research are discussed.

3.19 Implications

In order to address the question "What types of institutional practices and interactions promote a safe chemical research laboratory?", it is necessary to be able to parameterize and contextualize both behavior and environments (**Figure 3.7**). Therefore, a crucial discovery from this work is that the scale short forms (and the overall survey, although minimally discussed here) are valid for the target population according to multiple validity metrics. Conveniently, it was found that the types of lab environments can be reduced down to a manageable set of classifications (i.e., clusters) to better enable comparison later on during inferential testing (e.g., as to whether behaviors or resources vary for different types of lab environments).

Unsurprisingly, it was found that the quality of the individual relationship between a student and their PI is well-correlated with the overall group's safety climate, reinforcing the important roles that the PI and personal relationship dynamics play in safety outcomes. Fortunately, there were no significant differences found regarding scale scores and either the type of institution, ELL status, program year, or group tenure. Respondents overall felt somewhat positively about the hazards and risks of their labs on average but with room still definitely needed for improvement. Unfortunately, however, SPs were found to be part of a fragmented institutional knowledge base with SP survey-takers giving different answers than other SP colleagues about the safety resources and policies at their schools. This may make institutional improvements challenging, so school officials are encouraged to consider ways to strength communication channels and consistency between their constituents.

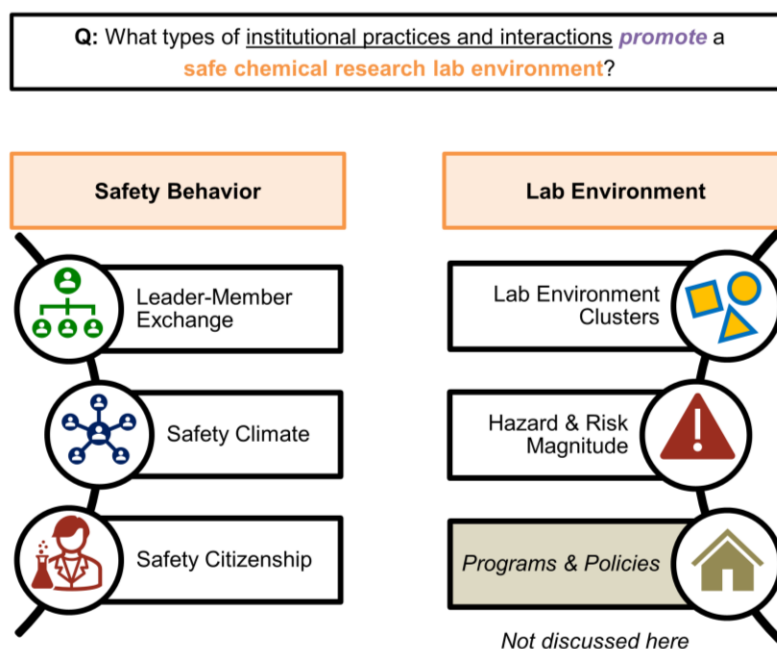


Figure 3.7. Parameters were established in this instrument for “safety behavior” and “lab environment”.

3.20 Limitations

This study employed gold standard psychometric survey design protocols widely accepted in the field. However, key limitations remain. Firstly, the methodological anchor of the research was the previous work done to establish relational validity between the three scales and safety behavior in military engineering crews. Ideally, the scales would also have been similarly validated in chemistry research groups as well. Additionally,

larger sample sizes for the EFA, MANOVA, and clustering analyses would have been beneficial. For example, certain types of hazards and research fields unfortunately had to be excluded from the clustering analysis due to their rarity, leaving the final model a reflection of the more prevalent data entries. Similarly, the descriptive statistics indicate that the sample respondents likely skewed toward a safety-positive mindset, which may have introduced some bias into the results (n.b, this theoretically should not affect EFA though). Social desirability bias also was not formally evaluated. Some of the international interviewees were difficult to understand during cognitive testing, raising the possibility that miscommunications may have occurred.

Finally, there were limits to the extent of contexts that the developed instrument could be applied: the SP pilot survey was abandoned upon realizing that (despite validation of the instrument) the SPs did not share the same understanding of their universities' resources and policies. It should also be noted that, due to the cultural nature of group dynamics and relationships, this instrument may not be valid outside of American academic cultures due to the scales' heavy dependence on relationship measurement. However, within the United States and similar Western nations, this instrument appears to offer strong performance with a variety of validity evidence types gathered, clean EFA metrics, and inferential evidence that performance was consistent across demographic groups.

3.21 Recommendations

This instrument was deliberately designed to be used by other research groups, and we encourage its adoption in the CHAS field. The final survey sequence (**Figure 3.8**) collects evidence about safety behavior, training, communication, inspections, reporting practices, laboratory safety contacts, and pertinent demographics (**Appendix C**). Since validity evidence does not necessarily translate across survey versions, we caution other researchers to carefully weigh the pros and cons of adjusting the final survey items, especially the scales. The scales are appropriate to detach from the overall survey and administer separately, potentially in conjunction with other surveys. However, the scale short forms themselves should remain intact in lieu of additional validity testing for any revisions.



Figure 3.8. Sequence of the validated nation survey after revisions from the pilot survey.

3.22 Conclusion

The primary objective of this study was to generate a purpose-built psychometric instrument capable of inferring a chemistry student's safety behavior in research laboratories *and* capable of being used by future researchers for related purposes. Happily, the data presented herein supports the appropriate contextualization and structure of this survey with content, consequential, relational, response process, and internal structure validity data in hand. In particular, short forms of statistically inferable literature scales were developed which can be quickly issued separately from the overall survey and so may find broad utility in the CHAS field. Moving forward, a national benchmarking study is underway to apply this instrument in generating baseline data for the status of chemical safety in universities across the United States. It is our hope that a wide variety of institutions and individuals will find the data and this instrument useful in supporting the safe work of chemists everywhere.

Chapter 4

LAB Theory, HLAB Pedagogy, and Review of Laboratory Learning in Chemistry during the COVID-19 Pandemic

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4.1 Abstract

The role and efficacy of the laboratory in chemical education have recently been a subject of renewed discussion as researchers are called upon to address the question of whether laboratory education lives up to expectations. The COVID-19 pandemic, which forced most of the global student population to temporarily adopt remote learning, offers an unparalleled case study to investigate types of outcomes resulting from a variety of adjustments made to laboratory education. This scoping review article focuses on the reports of laboratory learning in chemistry and closely related disciplines during COVID-19 to analyze the types of adjustments made to laboratory curricula and the immediate effect of these adjustments on students (**Figure 4.1**). The aggregated findings suggest that a lack of hands-on laboratory experience was detrimental to certain types of learning and engagement but that other types of learning were successfully achieved remotely. For researchers, departments, and university administrators, the differentiation in these findings could help inform the ongoing discussion about the future of laboratory education. For instructors and student support staff, the findings indicate potential areas of deficiency and strength for the COVID-19 student cohort going forward. Finally, a laboratory learning theory and pedagogy are proposed to guide use of the laboratory in chemical education and potentially in other laboratory-based sciences as well.

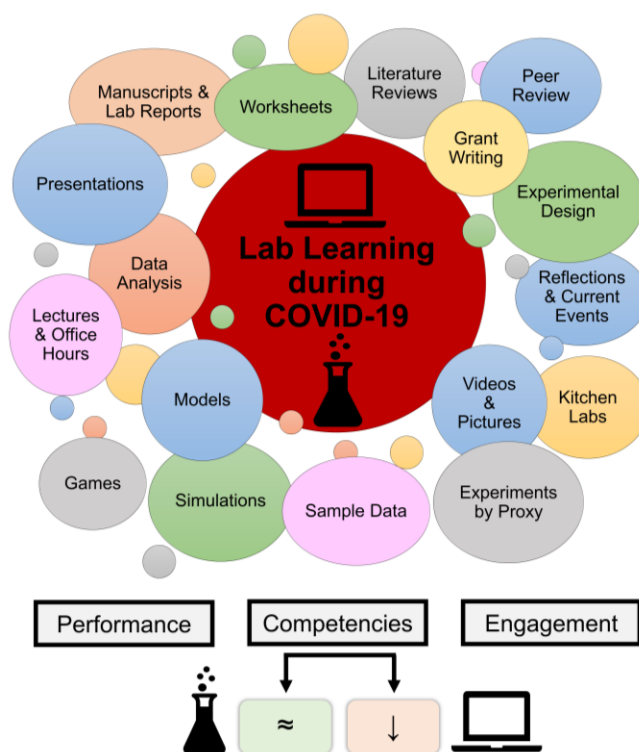


Figure 4.1. A scoping review reveals the initial effects of COVID-19 remote learning on laboratory learning.

4.2 Introduction

The laboratory is central to both the popular image of chemistry and the professional self-identity for many chemists. It is the day-to-day workplace for professional bench chemists, a site of discovery and innovation, and a training ground for future chemists. However, the role and efficacy of the laboratory in chemical education have been a subject of debate for decades and have recently come under renewed scrutiny,^{86,89,90,102–105,120,179,180} especially amid discussions about the soaring costs of higher education, an increased awareness of hazards, concern over the environmental footprint of bench chemistry, and continued issues with the STEM career pipeline. Such discussions fuel the need for research-based evidence to inform future decisions: Should universities build up-to-date teaching labs with expensive fume hoods or provide students with digital simulations of experiments? Should instructors use tried-and-true “cookbook” procedures or develop Course-based Undergraduate Research Experiences (CUREs)? Should funding agencies prioritize proposals that place students physically in labs for hands-on experience or that link students with professionals for mentoring through virtual events? The list of questions goes on for which stakeholders need evidence to make informed decisions. While most chemists will likely reflexively rally around the lab in defense of its irreplaceability (and perhaps be surprised that the lab is even under fire), administrators and other stakeholders involved in financial decisions are likely to increasingly request proof that the chemistry department merits its lofty budget for outfitting teaching laboratories in the face of institutional budget cuts and the examples of virtual lab-based learning set by this pandemic. Bretz’s recent editorial call to action⁸⁹ (coincidentally issued right before the pandemic) exemplifies the stakes at play for departments in this debate (**ref 89**, p. 194):

What evidence does your department have that the significant investment of space, time, personnel, and resources is essential for your students to learn chemistry? What arguments and data would your department amass to defend laboratory instruction if your university administration decided that virtual laboratories and simulations would be a far less expensive pedagogy that does not compromise student learning? Chemists can no longer afford to believe that the importance of teaching laboratories is a truth we hold to be self-evident. As scientists we must support our research claims with evidence. Our claims about student learning require this same standard.

The gauntlet has therefore been thrown by various stakeholders to demand that contemporary education researchers either (1) determine whether the traditionally heavy investment in wet labs and research laboratory experiences is worthwhile or (2) generate appropriate alternatives that better meet the needs of developing chemists and the constraints of the modern age. In this vein, the literature surrounding undergraduate research experiences (such as the NSF REU program or the increasingly prevalent CURE curricular reforms) has already shown how early and prolonged exposure to research substantially increases student interest, retention, and research skills in chemistry.^{97,181} Similarly, student experiences in physics laboratories have been shown to result in improved expert-like experimentation practices, attitudes, and beliefs about experimentation but with no significant impact on exam scores in the associated lecture course.^{114,115,182} On the other end of the spectrum, the literature also features many examples of how technology can be used to prime students for learning in the laboratory. For example, virtual laboratory simulations and technique videos utilized in conjunction with hands-on experiments can improve both cognitive and affective learning compared to hands-on experiments alone.^{109,183,184} Several publications have even indicated that augmented reality (AR) and virtual reality (VR) can match or outperform the laboratory in certain areas (either pedagogically or logistically),^{109,185,186} although one should always take care to acknowledge the confounding role of phenomena such as the Hawthorne effect, novelty bias, halo effect, confirmation bias, etc. when implementing new technologies.^{111,187,188} However, as a whole, the literature appears to indicate that although hands-on work in the laboratory promotes certain types of learning and engagement, not all types of knowledge traditionally taught in the laboratory *require* the laboratory to learn – or are best learned in the laboratory.

These are just a couple examples of progress in generating evidence regarding laboratory-based learning, but questions still remain regarding which modalities are best suited for certain types of learning and how to deliver those learning experiences in the most cost-effective, environmentally-friendly, safe, and authentic manner while promoting the most effective, evidence-based techniques for teaching and learning. For example, the Meaningful Learning in the Laboratory Instrument (MLLI) has been used to show that general and organic chemistry undergraduates' cognitive and affective expectations for their laboratory learning go unfulfilled, an alarming finding considering the significant resources invested in undergraduate laboratory courses.¹⁸⁹ Meanwhile, a comparison of a virtual vs. hands-on electrochemistry experiment

showed that students trained in the virtual and hands-on groups demonstrated very similar learning outcomes but with a couple key differences: the hands-on students were statistically significantly more likely to correctly use the electrochemical apparatus but were also more likely to repeat a poor procedural decision seen in the instructional lab due to a supply shortage.¹⁹⁰ Therefore, as Seery recently concisely articulated, research needs to address the following questions: “Why do we have laboratory work in the curriculum? What is distinctive about laboratory work that cannot be met elsewhere in the curriculum?”¹⁰⁴ This work will address such questions by using the COVID-19 pandemic as a case study for evaluating the role of laboratory-based learning in chemical education.

4.3 COVID-19 Cohort as a Case Study

COVID-19 originated in China in the winter of 2019 and swept across the world in a matter of a couple months, rapidly becoming the most significant pandemic and cause of death in recent global memory.¹⁹¹ By March 2020, much of the world was in lockdown due to the novel coronavirus. Schools at all levels were almost universally obliged to suddenly transition to emergency remote learning (ERL) for the foreseeable future, a modality that was new and unwelcome to most people. As societies confronted the stark reality of living amongst a highly contagious virus with no vaccine in sight, the world worried about the education of its students. The *Journal of Chemical Education (JCE)* issued a call for papers at the end of the 2019-2020 academic year to report on “lessons learned” about teaching chemistry during the COVID-19 pandemic with the hopes of informing preparations for 2020-2021 and providing a historical record for secondary analysis.¹⁹² Among the many changes that the COVID-19 student cohort underwent were the cessation of hands-on laboratory experiences at school. Although no one would have wished this situation to occur, the sudden disruption and *en masse* shift to ERL provides a rare case study on a scale with few comparable precedents. In a time when the role and efficacy of laboratory learning are under investigation, the impact of this transition on students provides an unexpected angle to inform future discussions surrounding the future of teaching labs.

4.4 A Note on Timing and Validity for a Non-Pandemic Society

Due to the need for instructors to act swiftly in the coming couple years to address any deficiencies in learning or engagement endured by the COVID-19 cohort, this review was published in 2021 rather than waiting for another year or two. Although this rapid turn-around meant that additional subsequent reports later in the pandemic would be missed, it seemed important to produce a timely review to inform the community about any available consensus regarding the COVID-19 cohort's laboratory learning. Especially considering the suddenness of the pandemic and suboptimal preparation for instructors and students to transition to ERL, it should be presumed that instructors' reports from pandemic times do not represent the ideal for how well the laboratory curricular adjustments *could* be implemented if done with sufficient planning and resources; ERL is not the same as well-planned online learning.¹⁹³ Therefore, this review, albeit a collection of many data points, is not at all a final say in discussions about the advisability of these adjustments in the future, especially as technology and technological familiarity improve.

Despite this inherent limitation, the opportunity to learn more about what happens when students' laboratory experiences are suddenly altered and shifted away from hands-on, wet lab experiments for an extended period of time is valuable and informative. The value of this amalgam of imperfect results is additionally underscored by its contrast to the research community's usual tendency (in all disciplines) to publish positive implementation results and not negative or null results. Additionally, unsurprisingly, researchers rarely conduct studies where they deliberately give students what are expected to be *worse* educational experiences than the status quo! Yet such information is useful in planning for contingencies; perhaps reviewing reports from this pandemic could inform what might happen if a department suddenly shifted to solely virtual laboratories (for example, if their budget was cut dramatically) or if students no longer had social support systems for processing labs (e.g., lab partners, TAs). Most studies which compare hands-on laboratory learning to other formats (such as virtual labs) do so only for a single experiment and not for an entire semester. Additionally, analyzing the reports from the COVID-19 pandemic presents a different angle than a standard randomized control trial (RTC) would for comparing scenarios. Although RTCs are often considered the "gold standard" for many types of investigations, they can be problematic for certain scenarios within educational research; additionally, studies embedded in "messy" real-life educational settings often unearth invaluable contextual data which RTCs do not.^{194–197} Therefore, distilling

these lessons learned from the pandemic should be helpful not only in future disasters or low-resource situations but also in charting the path forward for whatever the post-COVID educational modality may be.

4.5 Research Questions

This review focuses on the reports of laboratory learning in chemistry and closely related disciplines during COVID-19 to determine what consensus there is (if any) about the types of adjustments made to laboratory curricula and the immediate effect of these adjustments on students. The research questions are:

1. What types of adjustments did instructors make to laboratory-based learning due to the COVID-19 pandemic?
2. What were the immediate effects of those adjustments on students?
3. How do the outcomes inform discussions about the laboratory as a learning environment?

4.6 Scoping Review Framework

This review was approached under the framework of a descriptive scoping literature review focusing on almost a hundred first-hand accounts from instructors/researchers who were working with laboratory students when the lockdowns hit. Due to the recentness of the situation, a scoping review is most appropriate to provide a general map of the results stemming from the diversity of actions taken and modality of results reported during the COVID-19 pandemic.¹⁹⁸ In a sense, the entire COVID-19 cohort is being treated as a case study overall for this scoping review to build an impression of the aggregated lived experiences rather than attempting to quantify the instructors' provided thick descriptions or to focus on specific institutions separately. Frameworks to consider specifically for laboratory learning are discussed with the results at the end of the review.

4.7 Positionality Statement

Although scoping reviews are considered to generally be less vulnerable to author biases than systematic reviews,¹⁹⁸ it is important to explicitly communicate author positioning within works like this which deal with topics strongly bound up in professional self-identity, in order that others may weigh potential

confounding factors like confirmation biases. Therefore, the following description is provided for the sake of transparency to illustrate my approach to this work and position within the overarching discussion of the chemical teaching laboratory.

I consider myself to have received a strong holistic education in the liberal arts, but my higher education academic background is most heavily centered around organic chemistry and education. In the context of laboratory education, I believe in the value of hands-on, experiential learning (probably because of my synthetic organic chemistry background), but I recognize that there are flaws and limitations to such approaches and that a poorly designed or poorly implemented hands-on experience does not possess inherent value just because it is “hands-on”. I value virtual experiences such as videos and simulations, especially when they compensate for the limitations of the real world and especially as technological capabilities improve; however, I am always cognizant that simulations are made by human designers and therefore do not perfectly mirror the natural world’s complexity. I am increasingly doubtful about whether the laboratory is the best place to foster conceptual knowledge, and I make a distinction between a person’s conceptual skills and their technical skills. In both the teaching laboratory and the research laboratory, I have noticed differences in whether a chemist excels in conceptual thinking or in technical experimentation capabilities; skills in one area do not appear necessarily contingent upon skills in the other.

During the summer of 2020, I read the *Journal's* special issue to analyze the main takeaways from other instructors’ experiences with laboratory instruction during COVID-19 ERL. After contributing one of the laboratory-focused action research papers to the COVID-19 special issue¹⁹⁹ and personally believing that hands-on labs are indispensable for a complete chemical education (due to my experiences as a student, my research background, and a teaching background in higher ed and K-12 settings), my goal was to determine if other people had had similar experiences which suggested that a lack of hands-on labs had been detrimental to student learning and engagement – and, if so, how. With a small school grant (pre-COVID) in hand to develop a laboratory curriculum for an upcoming high school organic chemistry course starting Fall 2020, I also needed to determine whether adjusting the original curricular development plan for at-home laboratory work was worth investing the effort. The course was scheduled to start in a remote format with no certainty of in-person, face-to-face (f2f) resumption later on (indeed, the course ultimately concluded while still remote). Reading the special issue presented a good case that the adjustment was

indeed advisable, and the process of developing the subsequent at-home, hands-on organic chemistry laboratory curriculum has since been published in *JCE*.²⁰⁰

As part of my original manuscript on the at-home organic chemistry laboratory curriculum, I wrote about my findings from the summer reading process. At the request of the anonymous peer reviewers, I expanded that review section until it reached a length that the editor requested it be detached from the manuscript as it then more closely resembled a stand-alone article than an introduction. This review is the matured version of that earlier work, disseminating the net findings of the summer review process and buttressed by additional reports published since the summer. The review process has supported some of my pre-existing stances that (1) laboratory learning is not easily replaced by other modalities without hindering development of technical skills, (2) simulations and videos can be useful laboratory supplements broadly speaking but have limitations, and (3) most students want to engage with wet labs. However, other stances were challenged by the findings that (4) a lack of hands-on labs does not necessarily translate to poorer performance on assessments, (5) students can still have an engaging, differentiated education in a remote format, and (6) videos of experiments and lectures on data analysis can be surprisingly difficult for students to grasp remotely.

4.8 Method Boundaries

While this review builds on prior literature to help inform the discussion about the role and efficacy of laboratory learning, it is neither a comprehensive review of all literature on laboratory learning^{86,89–91,103–105,120,179,180,201}, virtual laboratories^{111–113,188,202}, nor distance, online, remote, or emergency remote education in general^{193,203}. This review focuses primarily on articles about ERL in the laboratory published in *JCE*'s special issue "Insights Gained While Teaching Chemistry in the Time of COVID-19" which was published at the end of summer 2020. The special issue deliberately solicited reports globally from instructors, researchers, or anyone who had something to report about their experiences with chemical education during the first wave of COVID-19.¹⁹² As such, it is a behemoth compendium (over 180 papers) of first-hand accounts of various types from different countries, institutions, courses, and student populations.²⁰⁴ Additionally, articles published in other journals and in later issues from *JCE* during the 2020-2021 academic year are also incorporated in this review where relevant to the subject of laboratory

learning in chemistry. Discussions of other STEM laboratory courses are only selectively included here in order to focus the review on chemistry and closely related disciplines and to make data analysis more manageable, although past work has pointed to the advisability of pedagogical exchange between disciplines and rightly so.²⁰⁵ Indeed, disciplinary lines become murky and even arbitrary at intersections such as biochemistry vs. molecular biology, quantum physics vs. physical chemistry, and even organic chemistry vs. inorganic chemistry. Therefore, some articles from physics, biology, and even forensic science education journals are included.

4.9 Data Collection and Analysis

In reviewing *JCE*'s special issue, the titles, keywords, and, if necessary, abstracts of every contribution were briefly evaluated as to whether the article likely addressed the laboratory in significant detail. Any article that seemed likely to discuss laboratory instruction or for which it was not readily apparent that the paper was *not* discussing the laboratory was opened for further evaluation. Many of the articles sported highly generic titles and abstracts. Due to this vagueness, it was sometimes difficult to ascertain whether or not the laboratory was part of the article at first glance or by keyword searches. The indeterminate articles were therefore skimmed to gauge if there was enough discussion of the laboratory to determine (1) what adjustments were made and/or (2) the impact upon students. Without engaging in this extra, time-consuming step, several articles would have been missed for this review, even after searching for keywords. The articles which made the relevancy cut were put aside for later reading.

After finalizing the collection of articles with perceived relevance, each article was then read through at least twice. The first exploratory read-through featured taking general notes to inform an initial frame of mind for coding. This first pass led to the generation of initial themes for (1) laboratory adjustments that instructors utilized in addressing the transition to ERL, (2) types of evidence cited for presenting results, and (3) types of results commonly discussed. Then, the articles were read through again more carefully specifically to sort them into categories of laboratory adjustments and to note which articles presented some form of evidence (beyond just instructor reflections) regarding student outcomes related to laboratory work. The articles which presented relevant evidence were set aside to read through a third time and generate a summary table (see **Appendix D** for an overview of the relevant articles). Although the special issue editor

identified that 44 papers dealt primarily with the laboratory and 3 dealt primarily with undergraduate research,²⁰⁴ this review process identified 57 articles that addressed to some extent how laboratory instruction and undergraduate research experiences were altered due to COVID-19, although the level of detail and quantity of evidence provided about the student / instructor experiences varied greatly. Papers which briefly mentioned that the laboratory was affected by COVID-19 but did not elaborate *how* instruction was altered are not included in this tally. Articles which propose laboratory adjustments for remote learning but did not discuss implementing those adjustments with real students during COVID-19 were discarded as were articles which replaced one type of remote activity for another (such as making a new simulation to replace an existing simulation).

Additionally, other relevant articles were subsequently published later in *JCE* and in other journals. Therefore, after forming the bulk of this review around the special issue articles, articles from subsequent issues of *JCE* and from additional sources were then evaluated for potential inclusion (**Table 4.1**). The ACS Division of Chemical Education (CHED) list of common publication venues for CHED members helped guide the selection of sources.²⁰⁶ The utilized search terms were “covid” OR “covid-19” OR “pandemic” OR “remote” OR “laboratory” as keywords or in the title. The search encompassed the date range January 1, 2020 – June 11, 2021 except for *JCE* which was constricted to September instead of January to avoid sifting through the special issue articles again. Articles were then selected to evaluate based on perceived relevance of the titles to laboratory-based learning *during* COVID-19 ERL in chemistry or a closely related discipline. Again, articles which did not meet the specifications for adequate laboratory description and use with real students as an adjustment to COVID-19 ERL were subsequently discarded. Please note that the journals listed in **Table 4.1** published more articles about learning during COVID-19 and laboratory experiments than listed in the table, but only articles which provided meaningful data for this review and fit within the specified boundaries are tabulated here.

Table 4.1. Number of articles deemed relevant to this review.

Journal	# Articles
Journal of Chemical Education	57 ^a + 14 ^b
Chemistry Education Research and Practice	0
The Chemical Educator	0
CBE – Life Sciences Education	0
Biochemistry and Molecular Biology Education	12
Physical Review Physics Education Research	1
Physics Education	1
The Physics Teacher	1
American Journal of Physics	0
Journal of Forensics Science Education	5
Journal of Science Education and Technology	0
Journal of College Science Teaching	0
Journal of Research in Science Teaching	0
Science Education	0
International Journal of Science Education	0
Total	91

^afrom the *JCE* special issue about COVID-19

^bnot from the *JCE* special issue about COVID-19

Surprisingly, few articles relevant for this review were found outside of *JCE*. The source which provided the most additional relevant articles after *JCE* was *Biochemistry and Molecular Biology Education* which also solicited communications for a COVID-19 special issue in the spring of 2020: “Teaching in the Time of COVID-19”. Perhaps potential authors for the other journals listed were simply overwhelmed with the situation and so did not have the energy to publish or did not realize (in the absence of a call for papers) that their reports would be considered valuable to a scholarly audience. Maybe chemistry teachers were more concerned about or more interested than physics or biology teachers in providing laboratory work during the pandemic (doubtful but theoretically possible), or maybe instructors from other disciplines published in outlets not listed in **Table 4.1**. Alternatively, a reasonable explanation could be that, since *JCE* issued its call for papers early in the pandemic (April 2020) and made it clear that almost-raw or nonexistent data about student learning was acceptable¹⁹², instructors may have (1) felt comfortable with submitting reports about imperfect implementations, (2) deliberately collected data during the spring semester with the expectation to publish, and / or (3) prioritized submitting specifically to *JCE* over others. Many of the course subject areas featured in the special issue would have also appropriately fit under the jurisdiction of other

journals as well. Later in the pandemic, the *Journal of College Science Teaching* issued a call for COVID-19 papers for July 2021 and so may yield additional relevant reports from after the 2021-2022 academic year. In any case, reports from chemistry instructors overwhelmingly form the foundation of this review.

4.10 Curricular Adjustments for ERL

All in all, every instructor should be commended for their rapid response to an unexpected, challenging situation. Although some authors noted that they and their students were well-positioned to adjust to ERL due to their individual circumstances and pre-existing curricular development initiatives, more authors reported the opposite and had to instigate curricular innovations in a short timeframe while learning a new-to-them modality of education, struggling with technological and other practical issues, and coping with a world plunged into chaos. Additionally, authors (and *Journal* staff and reviewers) managed a tight submission deadline for *JCE*'s special issue which, in order to publish with time to inform preparations for the upcoming Fall 2020 instruction, required a very quick turnaround time at the end of the academic year. Everybody's efforts on behalf of the COVID-19 cohort's education, as well as the efforts of the COVID-19 cohort students themselves, should be commended.

4.11 Types of Laboratory Adjustments

Authors reported various ERL curricular adjustments adopted to substitute for f2f laboratory instruction, which was suddenly incompatible with the widespread pandemic lockdowns. Those adjustments are here broken down into several major categories, with most instructors implementing approaches from multiple categories (**Table 4.2**). The overwhelming majority of these reports were from Spring 2020, the beginning of the pandemic for much of the world, but several supplemental reports were from the subsequent summer and fall academic sessions. Citations are provided for the categories according to each paper's main talking points, but there was significant bleed-over into multiple categories for each paper, whether noted in the table or not. The table is therefore guaranteed to underrepresent the diversity of actions undertaken but is provided for approximate comparative purposes. Some types of work also inherently belonged to multiple categories simultaneously; categories are not mutually exclusive. The most popular types of adjustments specified appeared to be using second-hand experiments (an approach used by 50.5 % of the articles

reviewed) and simulated experiments (45.1 %). Many instructors also provided sample data to analyze (36.3 %), had students plan or communicate about experiments (35.2 %), or enabled students to conduct first-hand experiments (29.7 %). Additionally, one report detailed that COVID-19 restrictions eased enough in their region before the semester ended to enable some students to return to the laboratory.²⁰⁷

Table 4.2. Major types of laboratory curricular adjustments during COVID-19.

Type	Description	Count ^b
First-Hand Experiments	Adapting experiments to be hands-on, at-home activities (either wet or dry) with household/school/commercial kit supplies, followed by some form of analysis ^{199,200,208–232}	27 (29.7 %)
Experiments by Proxy	Conducting student-planned experiments in the school laboratory on the students' behalf and sharing videos/pictures/data from the experiments back to the students or enabling students to conduct data collection live themselves through remote control means ^{228,233–235}	4 (4.4 %)
Second-Hand Experiments	Distributing procedures and non-interactive videos/pictures of experiments, from which students might or might not collect data themselves ^{199,208–213,225,227,228,236–271}	46 (50.5 %)
Simulated Experiments	Using digital simulations, models, AR/VR, games, or interactive videos, from which students might or might not collect simulated/real data themselves ^{200,207,208,212–215,228,230,232,234,239,240,245,247,250,253–257,259,261,262,264,265,267,269,271–283}	41 (45.1 %)
Sample Data Analysis	Distributing pre-collected sample data (real/mock, processed/raw, quantitative/qualitative) for student analysis ^{207,216,227–229,240–242,244,248,250–260,262,263,265–270,274,284–286}	33 (36.3 %)
Extensions	Assigning extensions based heavily on students' past experimental work done before remote learning began ^{199,251,254,287,288}	5 (5.5 %)
Planning or Communicating Experiments	Assigning experimental design planning, formal lab reports, or poster/oral presentations ^{212,214,215,219,221,222,226,232,233,238–240,243,244,248,251–256,263,265,266,269,274,277,287,289–292}	32 (35.2 %)
Conceptual Exercises or Practice Problems ^a	Assigning conceptual questions, practice problems, or other worksheets (in addition to or separate from a lab report or other formal write-up/presentation)	NA
Other Endeavors	Assigning reflections, journal readings, literature reviews, mock funding proposals, community outreach projects, or other creative/review work ^{212,213,232,233,238,247,250,251,259,265,272,274,289–293}	17 (18.7 %)

^aIndividual citations are not provided because many instructors appeared to imply to use this approach within other approaches but did not explicitly specify.

^b91 articles total – many articles contributed a count to multiple categories.

Some of the laboratory curricula changed as ERL proceeded whereas others were set from the beginning of the transition. For example, undergraduate organic chemistry instructors at the Autonomous University of Nuevo Leon (Mexico) initially provided students with pre-recorded videos of experiments but, due to perceived inadequacy of the videos in achieving the desired learning outcomes and student interaction, later devised a column chromatography purification for students to conduct at home with household supplies.²⁰⁹ High school general chemistry students at the University of Chicago Laboratory Schools (USA) first completed a follow-up worksheet analysis of a f2f wet lab; the students later conducted two additional hands-on labs at home or video-based alternative assignments and completed follow-up worksheets.¹⁹⁹ At the University of Connecticut (USA), analytical students focused on data analysis for the remainder of the semester, and the class sessions were devoted to addressing analysis mistakes and confusions.²³⁶ Organic chemistry instructors at Wesleyan University (USA) provided students with pre-recorded videos, and then students presented a COVID-19 journal article to their classmates in a final project mimicking a symposium.²³⁸ A biochemistry course at the University of Oxford (UK) used an enzyme simulation to enable students to plan and collect data on a simulated Michaelis-Menten enzyme kinetics experiment, where each student had their own unique theoretical enzyme to characterize.²⁷⁷ A University of California–Irvine (USA) general and organic chemistry team provided students with videos and sample data to analyze but then suddenly had to pivot the large end-of-semester organic exam to offer a choice of lower-stakes creative reflection assignments in response to national social upheaval.²⁴⁸ These variations in curricular adjustments serve as reminders of the diversity of contexts in which education occurs.

Additionally, many authors also mentioned providing virtual office hours, changing the schedule or purpose of virtual meeting times, making work and meetings synchronous vs. asynchronous, offering new problem-solving/tutorial sessions, and even conducting personal tutoring for students in need. Some authors kept grading and the syllabus the same (either to provide constancy or to meet institutional requirements) whereas others redesigned the remainder of their course, sometimes more than once. Instructors from across many papers tended to express similar concerns about their students (for example, mental health, quality of education, academic integrity, access to resources) but did not necessarily converge regarding the best way to address those concerns, partially as a result of the variable situations each instructor found themselves in.

4.12 Student Outcomes

Discussions of the laboratory within chemical education are difficult to separate from professional affinity, years of inherited belief surrounding the irreplaceable importance of laboratory-based learning, and expectations from all stakeholders regarding what constitutes a proper chemical education. At times, analyzing the curricular adjustments and their outcomes felt ambiguous due to the superficiality of the reported data which often appeared intertwined with authors' predisposed expectations. Many authors provided either very limited or no evidence to support claims about student learning or engagement, presumably due to the difficulty of planning and conducting such data collection during the on-going crisis, lack of familiarity with chemical education research methods, and / or a tight timeline (spoken from personal experience – I barely managed to submit 5 hours past the deadline for *JCE*'s COVID-19 special issue). If I am still dissatisfied with the manuscript I submitted and thinking of data I should have collected, other authors are also surely in a similar position. While instructors had more time to prepare for Fall 2020 remote learning than Spring 2020, time and energy were still scarce, thereby limiting the ability to pre-plan carefully designed studies (again, spoken from personal experience – the at-home chemistry kit I developed for a fall course was finished right before the school year, thereby curtailing any rigorous effort to investigate my students' learning).

Therefore, due to the limitations imposed by the situation, it is difficult to evaluate the outcomes of many of the adjustments. Some authors offered feedback from the occasional student (or class feedback without identifying methods or response rates) and their own reflections / intuition as instructors which, although circumstantial and not reflective of the rich, rigorous methodologies and methods developed for education research, are definitely still invaluable insights as “boots on the ground” perspectives. The decision by editors to publish such reflections with either limited or nonexistent data on student learning has enabled the collection of diverse reports for posterity and future secondary analysis. However, admittedly, not all the articles were equally useful in analyzing outcomes.

Fortuitously, multiple authors were also able to supplement their work with quantitative and / or qualitative data from a variety of sources such as surveys, pre / post-tests, grade comparisons, submission rates, attendance, and computer logs. Therefore, from here on out, this review gives greater preference to the conclusions from the 51 articles reporting some form of data (either quantitative or qualitative) which

appeared to go beyond solely instructor opinions; brief descriptions of these articles' findings as related to laboratory-based learning are provided in **Appendix D** in case readers would like a quick overview of the pertinent data. These analyzed articles represent a variety of courses (**Figure 4.2**) and institutions (**Figure 4.3**). In analyzing the aggregated outcomes, three major categories emerged regarding how the instructors contrasted the COVID-19 cohort's learning to other cohorts. These main categories were the students' differences in (1) performance, (2) competencies, and (3) engagement (**Figure 4.4**). The overarching themes of how students reacted to the ERL transition in these three areas are now covered descriptively in order to elicit a general message about how the interruption to their laboratory learning was received by the students.

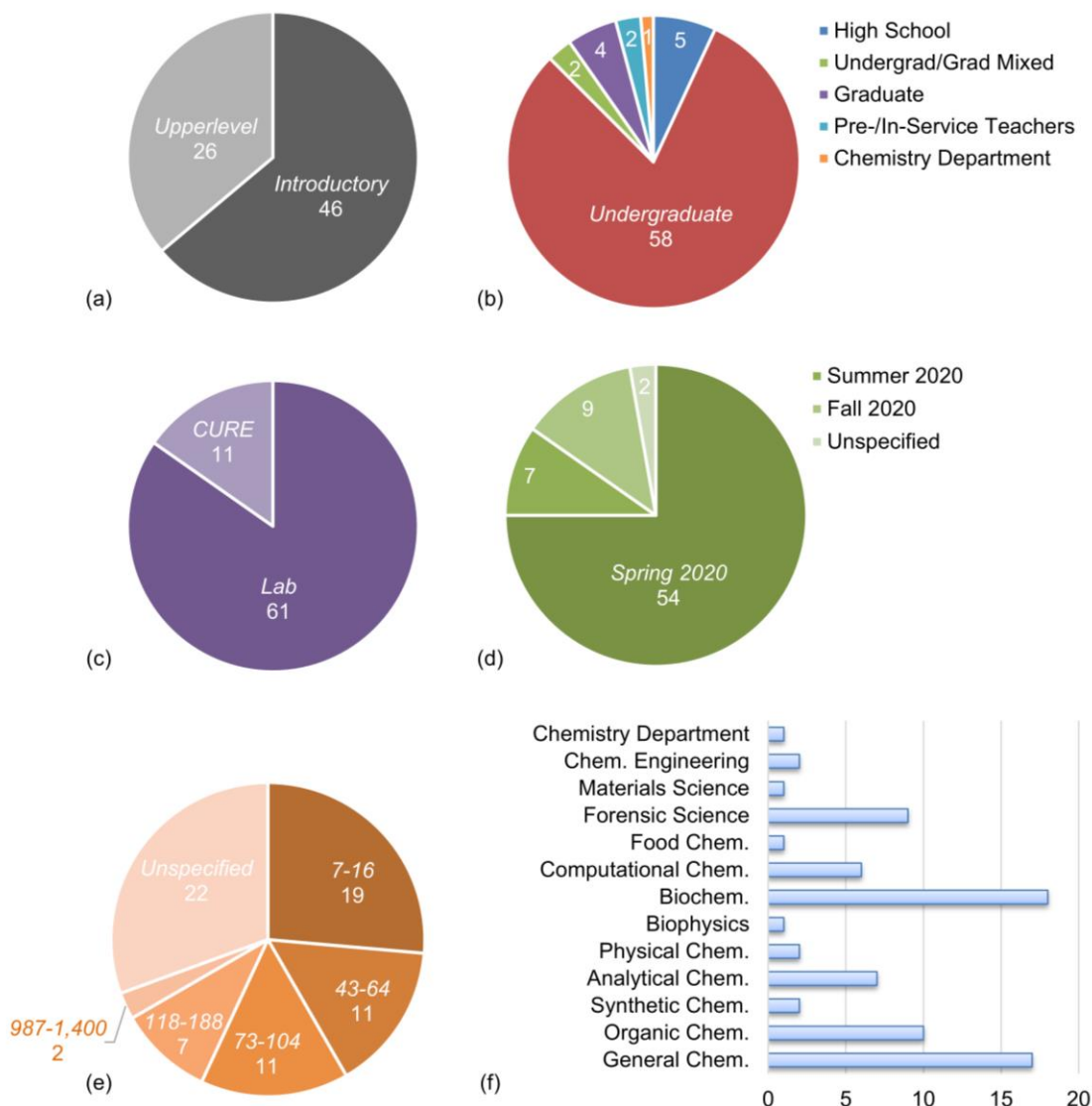


Figure 4.2. Characteristics of the courses analyzed. Some authors reported on multiple courses within one institution. (a) Introductory vs. upper-level, depending on the intended level of the course but not the student (for example a junior biochemistry course would be “intro” if it’s introductory biochemistry, but a junior organic course would be “upper” if it’s the second year of organic). (b) Type of student population meant for the course. (c) Traditionally-styled lab, guided inquiry lab, or lecture/lab courses vs. Course-based Undergraduate Research Experience lab courses. (d) Semester. (e) Number of students in course. Numbers were not specified for 18 courses. (f) Subject areas. Some courses listed multiple subject areas (for example, biochemistry and computational chemistry) and therefore contributed more than one count to the graph.

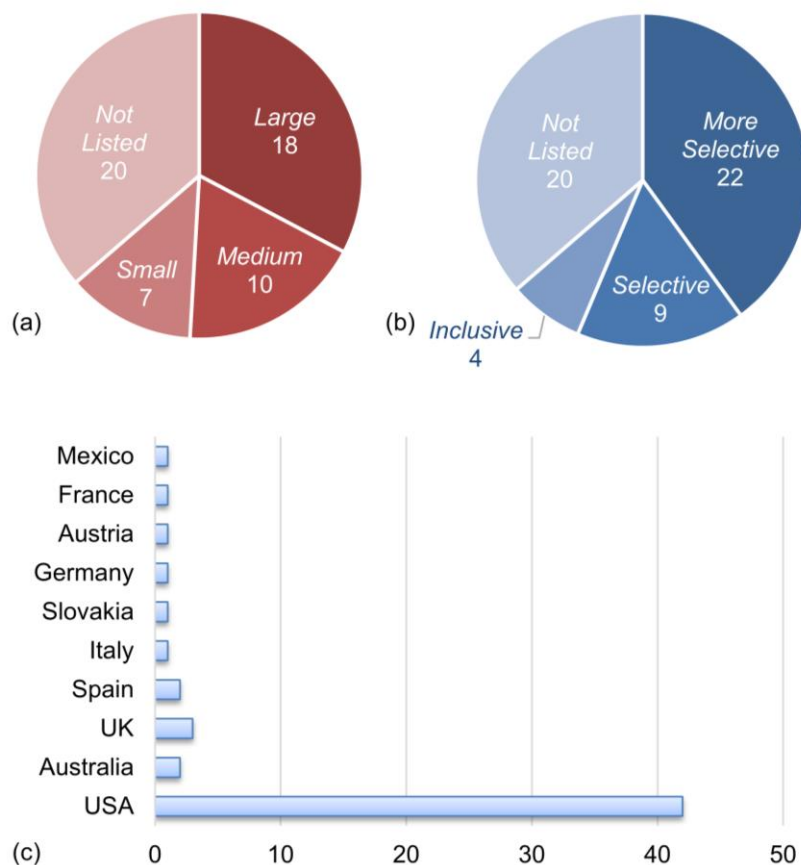


Figure 4.3. Characteristics of the institutions analyzed, based on the Carnegie Classifications database.¹⁶⁵ Institutions outside of the USA or which are not in higher ed were not listed in the database. A few reports featured multiple institutions. (a) Size. (b) Admissions selectivity. (c) Country.

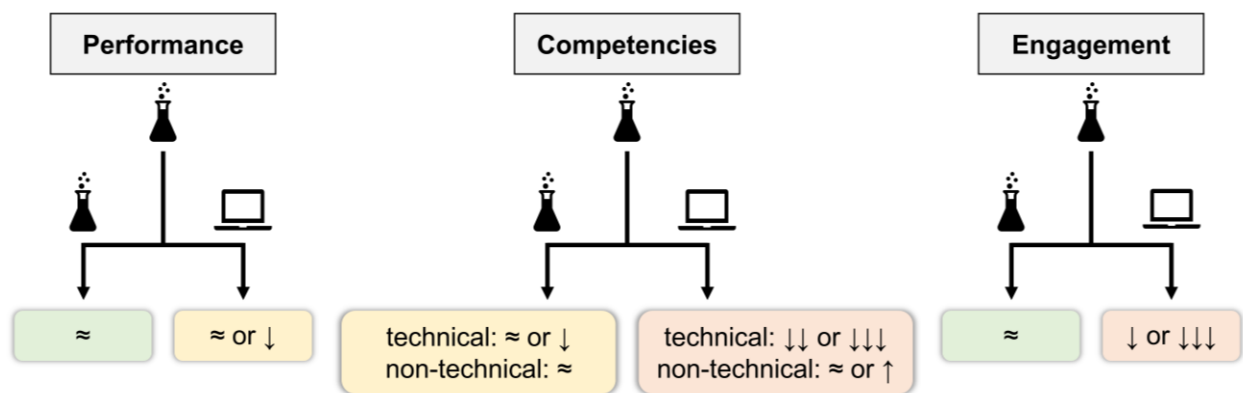


Figure 4.4. The major types of comparisons that authors noted between students were differences in performance, competencies, and engagement, especially in the context of whether hands-on labs were conducted (denoted by an Erlenmeyer flask icon) or not (laptop icon). $\uparrow$ = better; $\approx$ = roughly equivalent; $\downarrow$ = worse.

4.13 Performance Metrics

The major categories of performance metrics (i.e., grades) are articulated according to the type of comparison (**Table 4.3**). For example, “Same Cohort” refers to situations where instructors compared performance within the same student cohort (for example, before ERL vs. during ERL). Likewise, “Different Cohort” might refer to a comparison of the COVID-19 cohort to a different cohort from an earlier semester. Performance metrics were infrequently specified in the special issue, but the picture that the presented data paints is suggestive that there could be a difference between the performance on *experimental-based* assignments for students who completed hands-on labs vs. those who did not (**Figure 4.5**).

Table 4.3. Major types of performance comparisons for laboratory work during COVID-19.

Cohort Comparison	Activity Type	Results
Same Cohort	At-Home Hands-On vs. At-Home Non-Hands-On	For a few scenarios where performance metrics were compared between students within the <i>same</i> cohort who completed an <i>at-home hands-on lab</i> during ERL vs. those who completed an <i>at-home non-hands-on</i> alternative (for example, watching a video of the lab instead of doing the lab at home), instructors tended to indicate that the hands-on students performed better than the non-hands-on, although this wasn’t unanimous. ^{199,207,211}
Same Cohort	At-School Hands-On ↓ At-Home Hands-On	For a couple scenarios where performance metrics were compared for students within the <i>same</i> cohort who completed <i>hands-on labs at school and then later at home</i> , instructors indicated a lack of significant difference for performance between the labs. ^{199,217}
Same Cohort	At-School Hands-On ↓ At-Home Non-Hands-On	For several scenarios where performance metrics were compared for students within the <i>same</i> cohort who completed <i>hands-on labs in school and then later watched videos and analyzed data at home</i> , instructors reported either that the students performed better when hands-on or that there was no significant difference. ^{199,211,244,250}
Different Cohort	Both Hands-On	For a few scenarios where performance metrics were compared between <i>different</i> cohorts who <i>both completed a hands-on lab</i> (e.g., 2019 spring semester students in f2f school labs vs. 2020 at-home labs), the instructor indicated a lack of a significant difference between the cohorts. ^{211,216,226}
Different Cohort	At-School Hands-On vs. Non-Hands-On	For several scenarios where performance metrics were compared between <i>different</i> cohorts who completed a <i>hands-on lab at school vs. those who did not</i> (e.g., 2019 spring semester students vs. 2020), instructors also varied as to whether there was a noticeable difference in performance, either for better or for worse. However, three of four cases where instructors reported comparable or better performance for the non-hands-on students (Spring 2020) were accompanied by a discussion of either the assignments being easier or concerns about academic integrity (sometimes truly flagrant cheating). ^{211,212,215,228,236,242}

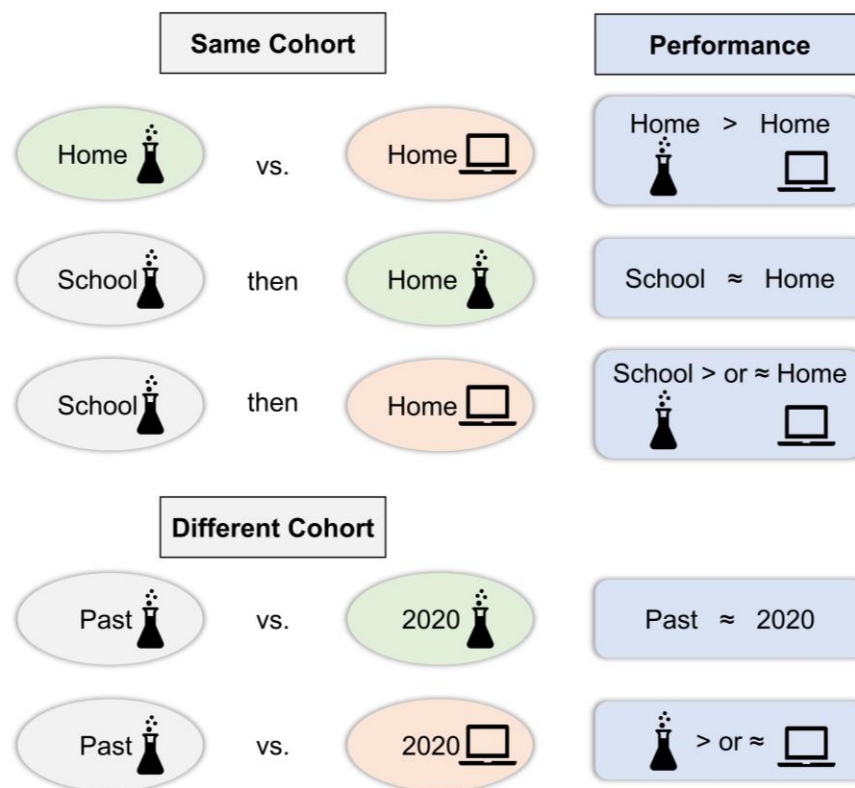


Figure 4.5. Historical and contemporary comparisons of performance metrics appear to indicate that students who completed hands-on labs (Erlenmeyer flask icon) tended to perform better on experimental-based assignments than students who did not (laptop icon).

There appear to be multiple possible reasons for the conflicting reports about performance. One likely explanation is that much of the conflict encountered when trying to build consensus across these reports could be due to whether the grade reflects a student's ability to write a formal lab report, answer conceptual questions, or answer questions about data analysis / procedural reasoning, for example. On the one hand, Deakin University (Australia) transitioned to remote learning after only 21.5 % of general chemistry students had completed a f2f lab experiment.²¹¹ The lab was filmed for the remaining students who filled out a worksheet after viewing the video. Grades for the first lab were significantly lower for the video group when compared to both the f2f students within that course and to a prior cohort. On the other hand, organic chemistry students at the University of Michigan – Dearborn (USA) earned lab report grades comparable to prior cohorts after watching videos, interacting with simulations, analyzing sample data, writing lab reports, and analyzing a procedure and techniques.²¹² However, the instructors noted the students evidenced significant difficulty with building on knowledge, connecting topics, using relevant data to

generate conclusions, knowing how to execute physical techniques, and incorrectly assuming that a simulated experiment was done. Interestingly, a report comparing the performance on the final (remote) exam between general chemistry students in a traditional lab vs. in a general chemistry CURE (students self-selected into either group during course registration – both groups followed the same lab manual during remote learning) at the University of Nebraska at Omaha (USA) showed no statistically significant difference between their grades, despite the difference in their laboratory work before ERL.²⁹⁴ A student's demonstrated abilities to handle data and understand the experiment therefore appeared to be independent of their grade-based performance in several examples. Since many authors explicitly made a distinction between lab assignment grades vs. the student's struggles to complete the assignment (for example, a student might have earned a good grade but required more TA support than normal in the process), this seems like a likely explanation for the variation in reported performance comparisons. This is unsurprising considering the oft-noticed issue of misalignment between a student's work in the lab and the assessment metrics. A lack of alignment between course activities and assessment metrics are a well-established problem in education in general, and assessments will likely be a major topic of research in the near future. A recent article in *Chemical & Engineering News* features JCE's editor identifying some anticipated big trends for research in 2021: "While laboratory activities represent a clear challenge, the place where chemistry education is going to need to make advances is in testing and assessment."²⁹⁵

Additionally, some authors attributed the improvement in performance to concerns about academic integrity, the use of easier assignments, or a more lenient grading structure than for past cohorts. For example, a high school general chemistry instructor (me) who reported lower performance in non-hands-on students than their contemporary hands-on peers was able to continue issuing the same type of lab assignment questions as earlier in the semester due to the online homework portal's features,¹⁹⁹ but an undergraduate general chemistry instructional team which reported better performance in non-hands-on students than prior cohorts attributed the students' higher lab grades to the simpler, easier assignment questions that ERL necessitated for their grading situation.²¹⁵ Some authors also did not report relevant grade-related data to support claims or contextualize the situation enough to enable analysis. Overall, the emerging consensus tentatively suggests that (1) assessment misalignment and the poor validity of laboratory grades in measuring certain competencies are still as problematic now as they have been for

decades¹⁷⁹ and (2) hands-on experience may improve performance *when the performance metrics are analyzing abilities closely related to technical work* (e.g., analyzing data, proposing a procedural step) but does not necessarily impact performance *when performance metrics are not analyzing abilities closely related to technical work* (e.g., writing a lab report, answering conceptual questions).

4.14 Technical vs. Non-Technical Competencies

Although few authors reported performance metrics, many discussed various types of competencies. Many authors noted discrepancies between cohorts' performance on conceptual questions, writing, presenting, and other non-experimental skills vs. knowledge of how to physically conduct experiments, plan procedures, troubleshoot real-world problems, process raw data, and interpret results (**Figure 4.6**). The former are here dubbed "non-technical competencies", and the latter are dubbed "technical competencies". The phrase "practical work" is also often used in the literature to refer to hands-on wet laboratory skills. I use the term "technical" here instead because of its close relationship to the words "technique" and "technician" (words commonly used in the research laboratory) and to encompass activities such as data analysis which could be seen as subsidiary to but not the same as hands-on "practical work". In chemistry, a lab technician is often responsible for maintaining equipment, helping design and conduct experiments, analyzing data, and other tasks meant to be included under the umbrella of "technical competencies".

A convincing number of authors who assigned videos / worksheets / simulations to students remotely, distributed sample data, or required some form of data / procedural analysis reported that the students evidenced lower comprehension of data and procedures, greater discomfort, or poorer quality of interpretation than prior cohorts (**Box 4.1**).^{199,209,211,212,226,233,236,239,242,244,248,250,252–254,259,268,273,287–289} For example, physical chemistry students at Pennsylvania State University (USA) who watched videos and analyzed data were noticed by the instructor to copy out mistakes from the lab manual into their reports, despite the experimental video showing a different procedure.²⁴⁴ Analytical chemistry students who watched videos and analyzed sample data for two labs and then did simulations and recorded simulated data for two more labs at Lander University (USA) appeared confused about the data, where it came from, what it meant, and how to analyze it, although the students did not appear as confused for the simulated data they recorded themselves.²⁵³ At Alfred University (USA), organic chemistry students did a series of

“Choose Your Own Adventure”-styled digital labs where students made decisions to progress the reaction game along to the simulated experiment’s conclusion; despite having conducted standard experiments before the ERL transition, students repeatedly made the same mistakes within and across “labventures”, struggled with making proper experimental decisions (such as deciding in what order to do steps and which analytical techniques to use), and did not properly interpret provided data.²⁷³



Figure 4.6. Students evidenced different types of competencies based on their ERL experiences. For example, student development in technical and non-technical competencies were commonly contrasted between those who conducted hands-on labs (fume hood icon) vs. those who used videos / simulations / sample data (laptop icons) or did non-laboratory work (presentation icon).

Box 4.1. Examples of problematic competencies frequently mentioned by instructors and students.

1. Understanding and analyzing procedures
2. Noticing relevant details in procedures, experimental recordings, or data
3. Evaluating and analyzing data, especially if nonideal
4. Recognizing sources of error and evaluating data trustworthiness
5. Troubleshooting and recognizing problems
6. Generating evidence-supported conclusions
7. Writing lab reports and other experimental write-ups
8. Proposing experiments or procedural steps
9. Predicting experimental outcomes

Additionally, authors who surveyed/discussed the experience with their students reported that the students often self-identified similar problems themselves, making comments to the effect that they struggled with understanding where the data “came from”, what the data “really meant”, how to design an experiment, predicting future experimental outcomes, etc. and that doing hands-on work was more helpful for learning than the remote alternative activities.^{208,211,212,233,236,239,240,242,254,259,268,283,288} The connection between comprehension and involvement in the data collection process is also supported by the results of

a large-scale survey of physics students at five European universities. At the end of the spring / start of summer, 220 physics students who reported that their labs transitioned to an online format (videos, simulations, sample data) for Spring 2020 self-reported higher gains in experimental skills and reinforcement of content knowledge if they gathered their own, real data over video vs. the students who either were given data or collected simulated data.²⁹⁶ However, several authors did not appear to encounter such issues to such an extent. Perhaps their students did not encounter such problems, these struggles were seen as typical, student struggles weren't visible to instructors in the remote setting, or it didn't occur to anyone to mention. On the other hand, several authors who pivoted to a fully virtual laboratory modality also sometimes implied that performance on conceptual questions and non-technical skill development appeared roughly comparable (especially for skills such as presenting and non-experimental writing) and that their students had now received valuable experiences with activities they would not normally have engaged in in the original course format (for example, community outreach or presenting at a course symposium).

Notably, technical deficiencies did not appear to be as much of an issue for students who continued some form of hands-on experimental work at home, either via lab kits or "kitchen chemistry" (here distinguished between a student using school laboratory supplies at home vs. using home supplies).^{200,209,210,217,221,225,226,229} Students undergoing preservice teacher training in general chemistry at the California State Polytechnic University – Pomona (USA) did not display difficulties interpreting data from their at-home, hands-on experiments,²¹⁷ and food chemistry students at the College of the Ozarks (USA) successfully proposed, troubleshooted, and executed their own experiments at home, impressing the instructor with their creativity.²²¹ Even my high school organic chemistry students in Fall 2020 at the University of Chicago Laboratory Schools (USA) met my expectations for skill and knowledge development while conducting labs at home from a rudimentary lab kit, despite several of the students having only about half a year's worth of high school general chemistry lab experience to draw on from before transitioning to ERL the year prior.²⁰⁰ Interestingly, for the report comparing general chemistry students in a traditional lab vs. a CURE at the University of Nebraska at Omaha (USA), where the students in both groups did the same lab work while remote, there was no statistically significant differences between their pre/post-test scores (either when compared between the two groups or when compared between the start of the semester to

the end) on the CLASS-Chem survey which assesses “expert-like thinking” in chemistry students. Perhaps this suggests that early hands-on experiences are not sufficient in enacting enduring change if the experiences are not continued.²⁹⁴

It is conceivable that these discrepancies in competency development could be partly due to student affective attitudes; perhaps students who were provided hands-on experiments were more invested in their work and so displayed greater growth than students who were obliged to stare at a computer screen. As will be discussed in the following section, there was considerable difference in engagement based on the course activities during ERL. However, this seems to be an inadequate explanation for the widely noted differences in technical vs. non-technical development in this situation, especially considering the diversity of student populations and institutions as well as data indicating that many of these students were trying hard to learn and maintain a positive attitude. On a similar note, perhaps changes in social support structures also influenced changes in competencies (and in related grades / performance); perhaps students find tasks such as data analysis more difficult without a lab partner or TA present. However, realizing that, many instructors proactively changed the format of their courses so that laboratory class meetings (online) focused more deliberately on tasks such as talking through a procedure or completing data analysis. Since many authors noted that students attended problem-solving sessions as a class, asked questions in discussion sessions, or worked with peers and instructors in breakout rooms and yet still evidenced these issues, changes to social support structures do not seem to sufficiently explain the discrepancies.

Therefore, it appears that the types of competencies that students develop are linked to the activities that the students themselves engage in first-hand. These results seem to suggest that second-hand or simulated experiences are not as valuable as first-hand experiences in building technical competencies. Of the second-hand / simulated experiences, though, it is inconclusive whether “real” data or simulated data is more valuable. Simulated data can be cleaner and easier to analyze for students, provided it does not reach a level of complexity that cognitive load becomes significant (as has been noted with simulations using virtual reality headsets; liking does not equal learning^{111,297}). However, real data can be more interesting and motivational for students and more closely mirrors what professional chemists would handle in the workplace.

4.15 Engagement

Engagement has previously been defined as “the student’s psychological investment in and effort directed towards learning, understanding, and mastering the knowledge, skills, or crafts that academic work is intended to promote”.²⁹⁸ It has been proposed to be a construct with four pillars: cognitive, emotional, behavioral, and social engagement.^{299,300}

- Cognitive engagement refers to a student’s intellectual endeavors with meaningful learning and concepts.
- Emotional engagement refers to affective attitudes regarding the learning environment, both the living and non-living components.
- Behavioral engagement refers to the student’s specific actions in the learning environment.
- Social engagement refers to the student’s commitment and interaction with their learning community.

The type of engagement referred to in the COVID-19 reports was not uniformly or explicitly defined by authors but can be assumed in this context to consist of instructor-perceived student behavior, attendance and participation in virtual meetings, submission of work, perceived motivation and enthusiasm, and overall interest in the course. That is to say, it appeared that instructors were reflecting on a holistic analysis of their students’ engagement (to the extent that they could observe such in a remote setting) rather than critiquing one specific pillar. Additionally, multiple authors reported that pre-existing relationships before the pandemic often helped foster engagement, community, group work, general positivity, and social safety nets and that their students remained interested in the course despite the challenging situation. One report of a summer course for Indonesian high school students offered through Covenant College (USA) where students were able to collect data themselves remotely (by controlling the instructor’s computer while the instructor was in the lab) showed that students also displayed greater engagement when they were watching their peers collect data rather than the instructor, especially if they knew that peer in real life, demonstrating how peer-peer relationships have a real impact on student investment.²³⁴ Similarly, a summer general chemistry course at Georgia Institute of Technology (USA) described students self-reporting (80 % response rate) that the synchronous lab sessions with simulations, which featured live work

with peers and TA facilitation, were more helpful than asynchronous sessions or non-TA sessions would have been.²⁸²

However, many authors reported that, despite a positive environment, students either appeared less engaged by the end of remote learning or that the students themselves reported a preference for hands-on work over virtual and / or a preference for f2f learning over remote, even if they had positive experiences with ERL (**Figure 4.7**).^{199,207,210,211,215,229,230,233,238–240,242,245,246,248,254,255,259,268,272,283,287,289} For example, the majority of respondents on a survey (38 % response rate) about general chemistry at St. John's University (USA), where students watched videos and did simulations, reported that doing labs via videos and simulations produced greater anxiety whereas f2f labs produced greater emotional satisfaction and educational growth, despite also rating the remote activities as somewhat effective for learning.²⁴⁰ For an honors general chemistry course in the fall at Duke University (USA), responses to a post-lab survey implied that students felt that watching a prerecorded video of a polymer chemistry experiment increased their excitement about doing similar hands-on work in the future.²⁷⁰ In five different courses (at different institutions with different teachers in different countries) where students had to obtain supplies to complete an at-home, hands-on lab but also were offered the option to forego the experiment and / or use sample data, students were more desirous to do the lab than not, despite the additional effort and supplies required.^{199,200,216,217,229} In an end-of-course survey (100 % response rate), high school students in a summer program at the University of Michigan – Ann Arbor (USA) rated the hands-on kitchen chemistry labs higher than the experiment videos live-streamed by instructors in the lab; they also rated the labs which featured at-home hands-on components higher than the previous year's cohort had done for the corresponding at-school experiments.²³² Students in a biochemical CURE in 6 courses distributed across 5 American institutions reported being glad to have sample data from other students to analyze for their projects, in addition to watching videos and completing computational modules, but they were also sad that they could not gather the data themselves. Motivation was perceived to decrease for the students who had to rely on others' data rather than their own.²⁵⁴ 81 % of responding analytical chemistry students in two different courses at Complutense University (Spain) (46 % response rate combined), where they watched videos, analyzed sample data, and presented orally to the class, preferred f2f over remote, although they still rated their instructors and the teaching favorably.²⁴⁶

Unsurprisingly, instructors who focused on hands-on labs, real-life applications, a variety of research options, active collaboration with others, interesting presentations, or interactive videos / simulations appeared to report more favorable engagement from students than instructors who focused predominantly on data analysis, writing lab reports, lecturing, watching non-interactive videos, and doing worksheets, although this fluctuated (for example, some students had negative experiences with trying to do group work remotely) and is inherently a difficult comparison to make due to the many non-academic factors that influence a student's situation. The overarching consensus, though, is clear from the students' own mouths: most like and wanted to do hands-on experiments in a f2f laboratory setting. While this preference does not necessarily mean that the students learn more or are best served with hands-on experiments, their affective reactions are noteworthy.

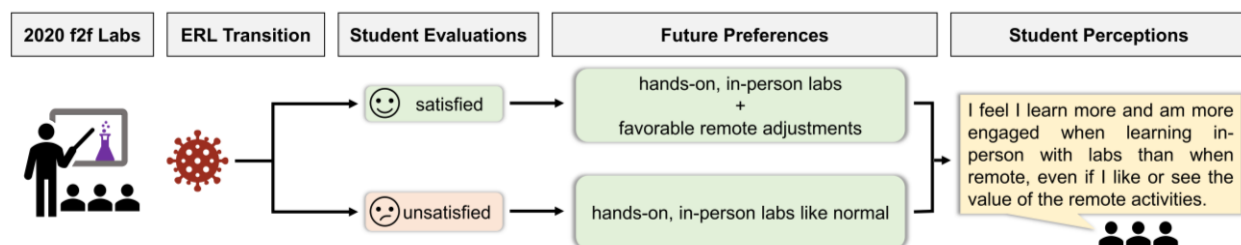


Figure 4.7. Students expressed a desire for hands-on labs, even if they had positive experiences during ERL.

4.16 Considering the Role of Prior F2F Labs

Although some courses were able to meet their revised learning goals and provide students with a valuable education for the situation, it is important to note the role of prior knowledge in enabling successful transitions from f2f to ERL. Additionally, pre-existing social support structures, which are important components to a student's success,³⁰¹ were also mentioned as boons for courses which transitioned to ERL after a classroom community had already been established. For future courses, the role of prior knowledge and the differences in how social communities are established f2f vs. online will be crucial to consider if instructors or administrators faultily assume that successful instances of remote laboratory learning can be picked up and seamlessly transposed onto future courses to replace all wet lab experiences after this pandemic. The role of f2f labs may become even more apparent the longer the pandemic

continues and the more that students progress in their degrees, completing consecutive laboratory courses without any f2f labs at all.

4.17 The Role of Prior Knowledge

Students in most of the courses reviewed benefitted from the prior knowledge acquired before ERL. Several authors noted that the earlier, hands-on experiences and personal relationships that students formed in the laboratory before the course transitioned to ERL were likely crucial in facilitating remote laboratory work, whether hands-on or theoretical. For example, biochemistry students at Gonzaga University (USA) had already completed multiple f2f experiments and so were already exposed to most of the techniques and materials that they later encountered virtually during remote learning.²⁴² 90.7 % of responding students later reported on a survey (44 % response rate) that it was easy to become comfortable with doing labs when f2f vs. 16.3 % who reported so for remote labs. Biochemistry CURE instructors at 5 American institutions also predicted that their students would have been less successful in the remote portion of the course if they had not had their earlier f2f experiences; this prediction is tentatively supported by a comparison to historical data which showed student learning gains in Knowledge-Experience-Confidence were lower than for previous students.²⁵⁴ A survey of physics students at five universities in Europe also found that, of 220 students who reported that their labs transitioned to an online format, the 1st-year students were significantly more likely than second-year students to report that the remote labs did not help them develop experimental skills;²⁹⁶ presumably the second-year students felt they had greater development partly because they were able to use their prior knowledge in laboratories to extract useful information from their remote learning. Tellingly, the type of student did not significantly differ in their perception of their content knowledge development. The role of prior knowledge also translated over to less technical work: organic chemistry students at Wesleyan University (USA) credited prior laboratory-based science courses for teaching them about techniques and concepts that enabled them to successfully complete their symposium-styled presentation projects by helping them to understand the article they were reading.²³⁸ Additionally, in terms of affective learning, incoming 1st-year students in a summer general chemistry course at Georgia Institute of Technology (USA) gave much lower affective scores on a modified version of the Meaningful Laboratory Learning Instrument than returning students.²⁸² When considering

the importance of prior knowledge, the lack of hands-on learning during COVID-19 (especially for inexperienced novice students) may hinder their performance in future courses and workplaces.

4.18 Intentions for Hybridity

Many authors *and their students* also opined that, although the course adjustments produced performance gains for certain learning objectives and were viewed favorably, they were by no means replacements for hands-on, experimental laboratory work. This opinion was expressed even by instructors who planned to revise their future courses to incorporate their curricular innovations from ERL into hybrid approaches to traditionally wet, hands-on, f2f laboratory courses. For example, a biochemistry CURE consortium plans to generate more online modules of traditional experiments.²⁵⁴ These instructors noted that the online modality met the needs of more learning objectives than expected and could enable new types of objectives not yet considered; however, they also noted that some objectives still cannot be met without hands-on experiences. Forensic science instructors at Virginia Commonwealth University (USA) realized that one of their software-based labs no longer needed to occur in a crowded computer room at school but could now be executed more effectively via individual remote access to a school computer with the installed program.²²⁸ Interestingly, some students also indicated a preference for (or lack of opinion against) hybridity, although they were in the minority. For example, 20 % of respondents on a survey (53 % response rate) about general chemistry at SUNY College at Old Westbury (USA) indicated that they would prefer a combination of f2f and remote learning in the future; these students had completed several f2f labs before the transition and then conducted several at-home, hands-on labs and simulations afterward.²¹⁵ However, the majority viewpoint of students and instructors across varied contexts regarding the importance of f2f labs was extremely clear: hands-on labs are seen by many as irreplaceable components of a chemical education, although they might not be as ideal as previously thought.

4.19 Discussion and Limitations

Taken individually, no paper offers a concrete conclusion about student outcomes from the laboratory adjustments made during the pandemic. Certainly, the stresses of handling the pandemic could reasonably help explain students' struggles, both with learning and engagement. Discrepancies in learning and

engagement may depend greatly on pandemic stress, student population, student-instructor relationships, remote learning formats, digital tools used, policies, workload, socioeconomic and familial situations, etc. And just as students were likely not learning at their best, instructors were also likely not teaching at their best. Instructors were scrambling to produce effective resources as they adapted to the situation, forced into a modality of teaching which they did not choose. These issues could highly affect student learning and engagement, instructor perceptions of the situation, and the ability for instructors to validly compare students to previous cohorts. Since students and instructors also expect and usually look forward to doing hands-on experiments, those expectations and general frustrations with the forced transition to ERL may have skewed their perceptions of actual learning. Additionally, some types of learning struggles may have already existed and were merely made more visible by the remote format; for example, students may have required more one-on-one TA support because they were unable to listen in on conversations with peers in the lab room regarding how to process data. ERL does not constitute high-quality online learning, so it is important to not read too far into overly minute comparisons of f2f and ERL.¹⁹³

Despite these limitations, the message presented here regarding the impact of a lack of hands-on experiences on student learning and engagement is difficult to ignore, especially considering the variety of institutions, student populations, curricular adjustments, and types of courses reviewed. While the lessons learned from educating during COVID-19 will certainly not be the final say in the discussion about the role of the laboratory in chemical education, these claims about performance, competencies, and engagement merit serious consideration and future research. Anyone planning to replace wet labs with dry should do so only after careful planning and consideration of both the learning objectives and the context of that course in the students' overall education; the same goes for those planning to replace dry labs with wet or those planning to resist suggestions for reform merely on the specious grounds of instinctive reasoning and personal anecdotes.

4.20 Implications

In reflecting on Bretz's call to action⁸⁹ and on Seery's stated questions "Why do we have laboratory work in the curriculum? What is distinctive about laboratory work that cannot be met elsewhere in the curriculum?"¹⁰⁴, the insights offered about laboratory work during COVID-19 suggest the following:

1. Personal, hands-on experience with conducting experiments and collecting data is important for developing technical competencies and long-term engagement in a way that simulations, videos, or other alternatives can help with but cannot yet comprehensively replace.
2. Conceptual knowledge (e.g., the theories underpinning laboratory experiments), non-technical competencies (e.g., presenting, writing), and short-term engagement can be effectively fostered without a laboratory or a f2f setting.
3. Assessments should be better aligned with what a student is doing and learning during the laboratory activity in order for grades or other performance metrics to accurately reflect their development as a bench scientist (for example, being graded^{122,124,302,303} or badged^{304,305} on experimental execution, data collection, and data analysis rather than writing a lab report unless learning how to write is an explicit and central part of the lab session).
4. Use of hybrid modalities, technology, and non-experimental activities could be useful in preparing for, streamlining, and amplifying the impact of laboratory-related activities on student learning and engagement in many types of courses, student populations, and research experiences.
5. Lack of prior laboratory experience may be a significant hindrance to students' future laboratory learning, technical skills development, workforce preparation, and interest in chemistry, particularly for benchwork-intensive subdisciplines.

Additionally, flagship professional societies such as the American Chemical Society and the National Science Teaching Association unequivocally assert that hands-on laboratories are essential components of chemical education and that simulations, although acceptable during the current crisis, are not appropriate substitutes long-term for chemical education and degree accreditation.^{92,93,306–308} The ACS's aspirational report *Tomorrow: The Report of the Task Force for the Study of Chemical Education in the United States* from 1984 strongly emphasized the need for students to undergo significant laboratory education.³⁰⁹ Today, virtual experiences cannot count toward the 400 hours of laboratory time required for ACS accreditation of Bachelor's degree programs.³¹⁰ More recently, the *Next Generation Science Standards* list a series of important science practices, which prominently feature the formation, testing, and evaluation of experimental ideas.¹²¹ Although it is a common complaint of instructors that students fail to

grasp the reasons behind procedures or merely follow laboratory instructions unthinkingly, such issues are strongly tied to the use of cookbook procedures and have not been shown to be inherent problems with laboratory work itself. Professional and government entities instead suggest reforming laboratories to address these issues, such as the 2012 report from the President's Council of Advisors on Science and Technology recommending to “advocate and provide support for replacing standard laboratory courses with discovery-based research courses”.³¹¹

Notably, instructor expectations for what students should and do learn in a chemistry laboratory have fluctuated with time. Currently, however, the research community appears to be shifting away from the belief by some that the laboratory is an appropriate place for fostering both conceptual knowledge and technical skills. Instead, evidence is building for the advisability of reorienting around a narrower lens: to develop technically skilled scientists, leaving the theory to be developed more thoroughly in the lecture room.^{114,115,124,182,302,303,312} Although deliberately encouraging the compartmentalization of knowledge should be viewed hesitantly, the findings of this review suggest that this reorientation may be somewhat appropriate for ensuring that laboratory resources are devoted *exclusively* to learning objectives which are *uniquely* developed in the laboratory, meaning the learning objectives which *cannot be adequately produced elsewhere*.

4.21 LAB Theory and HLAB Pedagogy

It is therefore incumbent upon researchers to generate a model articulating which learning objectives *require* a laboratory. Multiple generic and chemistry-specific theories already exist which support that the laboratory is the place for learning skills through hands-on experiences. For example, Seery recently suggested that, while instructors should define what the unique learning objectives for laboratory work are which cannot be met through other, less resource-intensive environments, the laboratory is quintessentially a place for *doing* chemistry.^{104,313} Meanwhile, Novak's Theory of Meaningful Learning posits the importance of integrating psychomotor, affective, and cognitive domains to promote learning,³¹⁴ and laboratory work inherently falls into the psychomotor domain when considering how we *do* much of chemistry.³¹⁵ Situated Cognition Theory also proposes a three-category system composed of social, cultural, and physical contexts whereby knowledge is inseparable from *doing*, similar to Embodied Cognition Theory.^{316,317} Kolb's

Experiential Theory Cycle provides another layer by proposing a strong, cyclical relationship between *having* an experience and *learning* from the experience.³¹⁸ Theories surrounding gestures, which have been shown in a variety of situations to promote learning and to serve as a medium to express knowledge, and the Community of Practice Theory³¹⁹ could also be integrated with a psychomotor framework to describe how physical actions and common ground enable effective communication between TAs and students and engender proper acculturation of novice experimentalists into experts, thus contributing to knowledge acquisition about *how to do* chemistry. And although Piaget's sensorimotor stage³²⁰ formally refers to infants and although Gardner's Theory of Multiple Intelligences³²¹ is often overly inflated into the discredited concept that each person learns best through only one modality, it is telling that we have many learning theories which feature physical interactions with the world. Since humans have five core senses (touch, smell, hearing, sight, and taste), it is unsurprising that the use of our senses would play an important role in knowledge acquisition and skill development.

Considering these precedents, it is important to recognize that our experiences with the physical world form a foundation of prior knowledge upon which constructivist approaches can transform the novice experimentalist into an expert. We already know that, when parts of the experimental process are taught as disparate pieces (for example, cookbook procedures not employing inquiry), students struggle to learn meaningfully. Now, this review also suggests how a prolonged lack of first-hand experiences with experimental practices in the real world can also lead to suboptimal learning by resulting in students lacking appropriate laboratory experiences on which to base their thinking. The findings from this review therefore suggest that psychomotor-oriented and communication-oriented learning theories integrate well into a forward-looking approach at *what is special about the laboratory's role in education*, here proposed as the Laboratory Action-Based (LAB) Theory (**Figure 4.8**): that there is a fundamental connection between a person's actions to manipulate the world with the *learning of how to do*, the *doing*, the *making sense of what was done*, the *proposing of what to do*, and the *wanting to do* laboratory science. "Laboratory" is used here on out to exclusively refer to a real-world physical space where authentic experimentation and associated activities occur, not online simulations or other abstractions. In other words, when students engage in action-based work in the laboratory, the laboratory work is playing a crucial role in their (1) exploration of materials and techniques, (2) ability to do lab work, (3) sense-making of what was done in

the lab, (4) ability to propose future lab work, and (5) desire to continue doing lab work – these are the five pillars of the LAB theory. While activities such as sense-making and proposing future work might formally happen during a homework assignment after the lab, the laboratory experience is important for the student to successfully engage in these activities. When students do not engage in action-based laboratory work, the LAB theory suggests that the students will be underdeveloped in those five areas. The laboratory is therefore *special* because it is *essential* for *robustly* achieving learning objectives associated with these five pillars. Combined, the lived experiences from COVID-19, prior theories, and existing literature which this theory are based upon present a compelling argument for the continuance of hands-on experiments as important components of a meaningful, “complete” education for laboratory-based sciences.

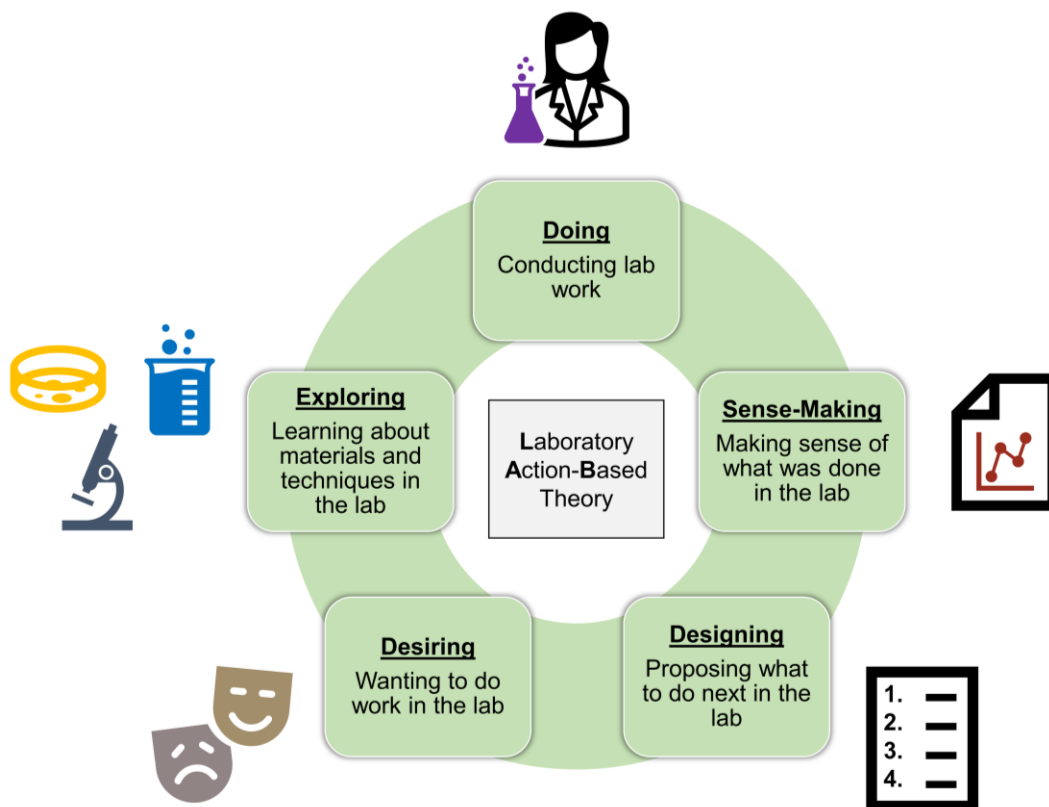


Figure 4.8. Proposed Laboratory Action-Based Theory posits five major pillars of what makes the laboratory a special learning environment for laboratory-based sciences.

However, it is also clear that the laboratory is not wholly *unique* in its ability to foster pillars of the LAB theory. Notably, this theory does not exclude virtual experiences (such as simulations), abstractions (such as drawing chemical structures), or interpersonal interactions (such as verbal discussions) from *contributing*

to laboratory learning but, rather, posits that these experiences alone would be insufficient in achieving a “complete” laboratory education (aka the five pillars of the LAB theory). To bring in a metaphor: watching videos of the indomitable Serena Williams surely matures aspiring tennis players’ strategy and form, but you cannot learn tennis by merely watching others play. At some point, you have to swing the racquet yourself. However, at the same time, playing tennis without any reflection on strategy or analysis of other people’s form would be a missed opportunity to refine your development as a professional tennis player. Therefore, non-psychomotor experiences will also play a role in the tennis player’s development; however, time spent physically on the tennis court is not necessary for such components of the player’s development. In a parallel metaphor: interactions with a simulation for running a distillation would still provide a student with an experience to learn from, but the simulation is more distant from the authentic practice than a first-hand experience with running the real experiment. Although moving a mouse does technically classify as a psychomotor experience, using actual distillation equipment clearly registers further along the spectrum. The simulation certainly has real value in helping the student understand their laboratory work and connect concepts to physical actions and phenomena, especially if the simulation is well designed with high fidelity (or simplified to help with cognitive load) or enables a student to overcome real-world limitations such as time constraints. However, the student should also practice running distillations in order to (1) become thoroughly familiar with the materials and techniques involved (“Exploring”), (2) build competence at running real-life distillations (“Doing”), (3) better make sense of distillation results (“Sense-Making”), (4) design distillation experiments for new situations (“Designing”), and (5) develop an informed desire to continue doing distillations in the future (“Desiring”).

The laboratory is therefore *special pedagogically* and *unique practically* in that its presence is required to meaningfully achieve specific learning objectives in laboratory-based sciences, but it is not *unique pedagogically* in that what is learned in the lab can also be learned somewhat elsewhere to a certain extent. Use of non-laboratory pedagogical techniques can be deployed to foster the partial development of each of these pillars and of related learning objectives, thereby improving the outcomes and resource-effectiveness of laboratory sessions. It is already common for a lecture teacher to promote the desire to conduct laboratory work through discussions of real-life applications. Pre-lab videos are often used to show how a technique is conducted before a laboratory session.¹⁸³ TA discussion sessions frequently guide

students in proper data analysis post-lab. Such use of preparatory / debriefing strategies and technology can help address issues such as laboratory anxiety, a negative instructor effect¹⁰⁸, constraints on time and other resources, etc. However, effectively utilized technology can even overlap directly with activities traditionally confined to a laboratory room. Recently, an AR phone app was developed to use within the laboratory room to show students how to properly conduct titration, thereby avoiding wasting large quantities of caustic solvents.¹⁸⁶ Similarly, a virtual tour of a chemical laboratory helped students get accustomed to the space and materials they would use for their first lab.³²² Computer simulations can walk students through the entire process of an experiment beforehand.¹⁸⁴ Such simulations could theoretically even show students what would happen if they made a dangerous mistake in a wet lab – but without actually causing an explosion or risking a chemical splash to the eyes. Additionally, visualization technologies enable bridging between technical and non-technical competencies; for example, a liquid-liquid extraction mobile app could help students practice mapping the chemical structures of solutes with the phase they partition into, thereby helping students recognize how acidity affects chemical structure and how structure affects solubility.³²³ The list goes on for potential applications of non-laboratory work to laboratory and laboratory-related learning.

Therefore, combining the LAB theory with the literature on technology and other types of learning suggests that the laboratory will be at its most effective as a learning environment when it is part of a hybrid pedagogy. In this way, the laboratory and non-laboratory experiences combined could (1) *compensate* for each other's respective limitations, (2) *complement* each other with different focuses on an overarching topic, (3) *reinforce* learning with similar exercises to cement the same knowledge, and (4) *bridge* between technical and non-technical competencies to efficiently provide a holistic education. Consequently, a Hybrid Laboratory Action-Based (HLAB) Pedagogy (**Figure 4.9**) offers examples for how instructors can think about optimizing their department's laboratory offerings in a post-pandemic society. Many laboratory courses already utilize some form of a prelab video, discussion, or quiz, but the HLAB pedagogy encourages instructors to go beyond what might be surface-level add-ons or one-dimensional assessments aimed at safety compliance or reducing instructor workload. Instead, consider thoroughly integrating effective technological or interpersonal interactions with the core design of laboratory courses.

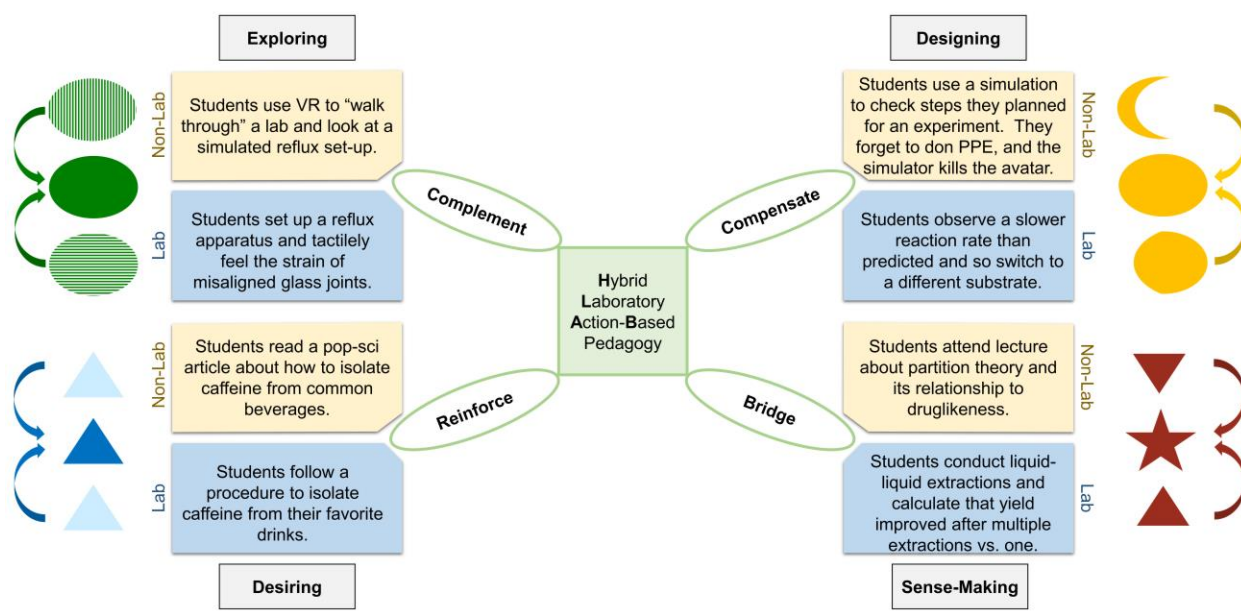


Figure 4.9. Proposed Hybrid Laboratory Action-Based Pedagogy combines strategies in four major ways to optimize effective laboratory learning and a holistic science education. Laboratory experiences must be experienced in order to satisfy a LAB pillar, but non-laboratory experiences can significantly aid in development as well. Scenarios are provided for four of the five LAB pillars to demonstrate examples for the four HLAB components.

Finally, it should be noted that, depending on a student's career aspirations, it is not necessarily crucial for them to attain a complete laboratory education. While instructors may want all their students to choose a chemistry career path or to develop an intrinsic love of chemistry, a student who is enthusiastic about public health policy, for example, might not need to physically practice conducting column chromatography in order to excel in their chosen career path or to experience educational fulfillment. In such situations, there is a good case to be made that the university does not need to invest financial resources on such students to get them into a physical laboratory. Rather, instructors could utilize other experiences without depriving that student of a quality education, especially as the complexity and fidelity of online laboratories are rapidly improving. Additionally, different science disciplines utilize the laboratory to different degrees. For example, synthetic organic chemists conduct almost all their work in a wet laboratory whereas computational chemists conduct almost all their work on a computer. Depending on the student's intended track, the degree to which laboratory experiences are incorporated into their education could reflect the degree to which the laboratory is expected to feature in their career. People should be practical with respect to the law of diminishing returns of how resources are invested.

4.22 Recommendations and Future Areas for Work

Based on this review, the following recommendations are proposed with the caveat that not all recommendations are appropriate depending on the context. Additionally, recommendations about how to conduct laboratories for any future pandemics should not be taken out of context to be used to contest the sound advice of contemporary medical experts; lives trump learning.

Serving the COVID-19 Cohort:

- When teaching students who took a laboratory-based course during COVID-19 ERL, prepare for students' technical competencies to be underdeveloped but, *potentially*, for their non-technical competencies (or “soft skills”, such as presentation skills or self-management habits) to be normal or *perhaps* stronger than usual.
- Recognize that “learning loss” (the phenomenon of forgetting knowledge from an earlier course) from previous laboratory courses will likely be worse than normal.³²⁴
- Feed COVID-19 students' enthusiasm and underdeveloped psychomotor learning by providing some of the lost experimental and f2f opportunities where feasible and reasonable (although, obviously, instructors cannot run two courses within one to rewrite the past!). Recognize that less experienced students likely suffered the most in terms of affective learning in particular.²⁸²
- Acknowledge those positive or useful experiences that students *did* receive during ERL, and encourage students to build on those beneficial experiences.

Future Remote Learning with Labs:

- In future disaster or low-resource situations, recognize that students will likely struggle in technical areas such as data analysis and procedural comprehension, even if provided with videos and procedures of experiments. Explicitly devote time and energy to coach students in areas such as how to make good observations over video and enable them to guide the experiments in real time.
- If students can be at school for part of the time, instructors and institutions should prioritize providing hands-on lab experiences during that time. Additionally, the less experienced students should receive the highest priority for f2f experiences.

- If students cannot be at school, consider sending them a lab kit or designing *relevant* at-home experiments with readily available supplies.
- Do not expect videos, simulations, and sample data to be adequate substitutes for f2f labs in all areas of learning and engagement, but do not shy away from using them. Try to enable student ownership, authentic interest, and multimedia interactivity with the provided resources.
- Proactively address possible complaints against at-home hands-on experiments since students responded negatively in a few instances to perceived inauthenticity or childishness of using household supplies.^{199,210,211} Discuss with students how chemistry and chemists are not confined to a traditional wet laboratory (“chemistry was born in the kitchen”, as the common saying goes).

Future f2f Labs:

- Revisit your lab course’s learning objectives to determine which objectives are best fostered through f2f experiences.
- Prioritize laboratory time for having students physically practicing techniques and learning to use laboratory materials. Conceptual knowledge and non-technical competencies could be shifted to time outside of the laboratory.
- Consider using virtual experiments as make-up labs for students who miss a f2f laboratory session or as opportunities to offer experiments that would not be feasible or safe with your institution’s resources.
- Consider boosting learning and engagement by incorporating supplements such as simulations, videos, asynchronous mini-lectures or group meetings, or other adjustments which worked for your remote teaching into traditional lab courses. In addition to boosting learning, this could potentially have a side benefit of reducing the amount of time students must be physically in the lab, reduce the number of mistakes and therefore resources wasted, and enable a department to place more students in the laboratory per week due to the lower f2f time requirements for each class section.
- If possible, incorporate options for student-selected research, literature reviews, and inquiry-based experimentation into lab courses. Enable students to become invested in a long-term experimental project over which they have legitimate ownership and responsibility.

- Reconsider how you frame laboratory work. Interestingly, multiple reports mentioned that students, although preferring f2f instruction, appreciated aspects to their remote learning, such as the clearer structure of the remote activities compared to traditional labs.^{215,259,272} Although it is important to learn to deal with the “messy”, circuitous, and imprecise side of science which is experimentation, instructors should consider ways to help students structure their laboratory experiences in their heads to build a mental structure to the work. Strong mental frameworks are powerful ways to organize, cement, and retrieve knowledge for researchers and students alike. Perhaps concept maps could be a useful pedagogical tool to implement regularly in laboratory courses.
- Discuss with students how computational work and non-laboratory planning / tasks intersects with hands-on experimentation so that they come to view their virtual work as legitimate contributors to their laboratory education.

Future Research:

- Develop ways to explicitly develop technical competencies without hands-on labs.
- Inventory precisely which modalities best facilitate development of specific skills and knowledge. To start with, categorizing which types of knowledge and skills count as “technical” vs. “non-technical” could be useful since current popular standardized constructs such as the *Next Generation Science Standards* science practices¹²¹ integrate them into a curricular mixture (for example, analyzing data vs. communicating results) which may not be conducive to decision-making for science departments trying to optimize which experiences require a laboratory and which do not.
- Determine the ideal balance between out-of-lab and in-lab activities toward achieving a cohesive learning objective. The ideal balance may differ depending on the student’s intended specialization and the quality of the instructional experiences.
- Investigate the validity of the LAB and HLAB models proposed in this work.

4.23 Conclusion

It is important to note that the role of the laboratory in chemical education is currently the subject of renewed debate. While there is incomplete evidence for how exactly laboratory instruction impacts student

learning, the evidence which is emerging sometimes challenges chemists' professional affinity for and belief in the efficacy of labs. Previous work has pointed to either the lack of evidence for how laboratories influence learning or to research which shows that dry simulations have been as successful, if not more, in teaching certain concepts compared to a wet experiment. Prelab videos, mini-lectures, and simulations have been shown before now to be great assets when used as supplements to boost conceptual learning, prime students for more meaningful experiences, and mitigate issues such as laboratory anxiety, variation in instruction quality, or other inequities. Some instructors may therefore view the pandemic favorably as the catalyst which shifts focus away from hands-on laboratories and toward a greater dependence on simulations and other dry experiences which are also typically cheaper, safer, more environmentally friendly, and logistically easier to arrange.³²⁵

However, just as the traditional chemist may be too fired up about the all-encompassing virtues of wet labs, so too may be the progressive chemist who is surfing the technology wave. Although it takes no great stretch of the mind to imagine effectively learning how to conduct computational techniques in a fully virtual environment, most practicing synthetic organic chemists would balk at the notion. Additionally, it is important to keep in mind that most studies which compare virtual labs to hands-on labs do so for one experiment and not for the entirety of a course. Studies regarding the implementation of virtual labs have also been criticized as too one-dimensional / superficial or compromised by biases such as the novelty bias and confirmation bias.^{111,188} Therefore, while the substitution of one hands-on lab for a virtual lab may have no significant effect on technical competencies, the situation may be different over a prolonged period of time. Indeed, instructors who ran biochemistry CUREs during Spring 2020 noted a difference in the degree of learning gains for computational techniques vs. biochemical techniques during remote learning.²⁵⁴ Research has yet to crack the mystery of "good hands" (a somewhat mystical phrase³²⁶ invoked by chemists to describe why an experiment might work in one person's hands but not another's), but physical, first-hand experiences are likely crucial for building experimental expertise. Disciplinary differences, combined with the aggregated data from learning during the time of COVID-19, attest that the lack of personal, hands-on experience with wet experiments can be a real detriment to student learning and engagement, especially for benchwork-intensive disciplines. Notably, the evidence from many types of courses suggests that several crucial technical competencies may still be best developed through psychomotor experiences,

although improvements in online laboratory software will be important developments to watch in coming years.

Additionally, student excitement and expectations regarding experiments are not trivial affective features to be casually brushed aside. Students do not always recognize which pedagogical initiatives are best for them, but their expectations for laboratory work do frame how they perceive labs and chemistry as a field. Students entering a laboratory course already have specific expectations formed for what their experience will entail, and they may react negatively to changes in those expectations. Socioemotional aspects can drive students' chemical education, career selection, and ultimately retention in a challenging and oft-feared subject area, the desired end goal of many chemistry departments' (and universities') endeavors. If a student enrolled in a f2f course and not an online one, then they might prefer f2f interactions and hands-on experiences.

In the end, it is important to remember that there are multiple types of learning, students, expectations, subdisciplines of chemistry, etc. and that any lopsided approach to education (whether solely wet labs or solely dry labs) is unlikely to yield optimal dividends on its own. There are certainly limitations to development of student learning and engagement via current technology, but not all aspects of learning were negatively affected even in this suboptimal learning environment. However, while technology certainly has an increasingly important place in chemical education, there does not yet appear to be perfect replacements for all types of wet labs and likely will never be until we can download knowledge like in the sci-fi Matrix movies or until virtual technology reaches the point of an open-ended realism that rivals the fictional Star Trek holodeck. Even then, designers will have to contend with the reality that, for as long as humans design and code the simulations, simulations will never perfectly mirror nature's penchant for surprise and inspiration. Therefore, as the 700 BCE Greek poet Hesiod once wrote (and as has been reiterated by many others over time): "moderation is best in all things". Use wise discernment to marry together the wet experiences with the dry; students will benefit from the union.

Chapter 5

Which Attributes Matter Most in the Mentors of Early Career Chemists?: Instrument Development for Assessing Mentorship

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5.1 Abstract

PIs and fellow group members provide key mentorship for chemistry students and postdocs. However, considering that time and emotional bandwidths are often stretched, it is important to recognize that a mentor has limits. Recognizing such constraints, it would be useful to identify the most important types of mentorship for a chemistry mentor to provide. Such knowledge could (1) inform mentors' efforts both to support mentees in the most impactful way and to solicit targeted mentoring training, (2) help third-parties understand where best to invest resources in supporting healthy mentorships and professional development, and (3) better enable clear expectations between mentors and mentees. Therefore, this paper details the development and validation of a survey that can be used to assess which types of mentorship early career chemists feel are most important (**Figure 5.1**). Such information might then be useful in improving training outcomes and retention rates of early career chemists (and their mentors). Moreover, by looking at three mentee cohorts together (i.e., undergraduate students, graduate students, and postdoctoral scholars) with the same instrument, the trajectory of mentorship needs over time could theoretically be illuminated without a longitudinal study.

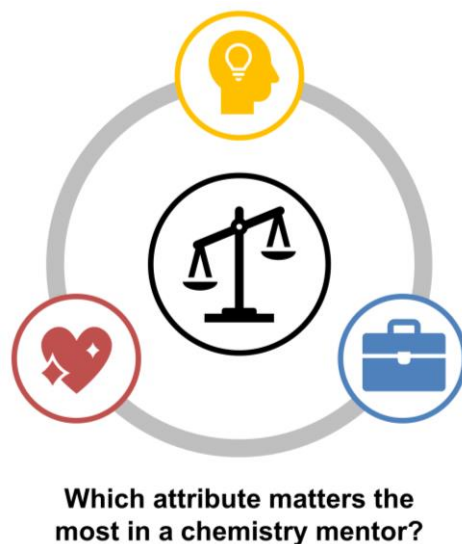


Figure 5.1. A survey was developed to assess which types of mentorship are the most important according to mentees.

5.2 Introduction

Next Mentor rose to speak, a comrade-in-arms of noble Odysseus. To him the king had committed his entire household, when he sailed off to Troy; he had ordered everyone to obey the old man, trusting that he would keep all things steadfast and undisturbed.

*Odyssey, 2.224-27 [translated]*³²⁷

Telemachus: “Mentor, how will I stand before the king, how will I greet him? I am not good at sophisticated conversation; a young man like me might get nervous asking an older man questions.”

*Odyssey, 3.22-24 [translated]*³²⁷

Mentorship is essential for success. Moreover, both the United States President's Council of Advisors on Science and Technology and the National Academies identified mentorship as important for strengthening STEM education programs and increasing graduation rates.^{311,328} In academic chemistry research groups, faculty (aka Principal Investigators, PIs) and research group peers often play key mentorship roles for early career chemists (i.e., students and postdoctoral scholars). While the relationship quality, goals, and efficacy of these mentorships vary, one commonality persists: one mentor cannot be all things at once in all situations to all mentees. Therefore, mentees are often encouraged to foster synergistic relationships with multiple mentors to build holistic support systems. For PIs and peer mentors in chemistry research groups, this situation consequently invites the question of which of their mentees' needs they should focus on. If a mentee receives support from other teachers, peers, family, career advisors, etc., what is the most important support that a chemistry research mentor provides? Viewed from a different lens: since a mentor's resources (e.g., time, emotional bandwidth) can be limited, over-committed, and / or unwillingly conscripted,^{329–332} which mentorship domains should they *prioritize*? What does a mentee *most need* from a PI or peer mentor?

Understanding how chemistry research mentors fit into a support system would enable deliberate differentiation by mentors. Additionally, understanding where a support system is most likely to fail (e.g., if a research mentor does not address these needs) would enable third-parties such as the American

Chemical Society, universities, and affinity groups to step in where they are needed most. However, existing instruments for assessing mentorship do not appear well-suited to illuminate this situation. Instruments do exist which evaluate the perceived quality of mentorship and quantify the outcomes (e.g., by counting the number of publications a mentee produces).^{333–339} These instruments have revealed that highly regarded mentors hold certain behaviors in common (e.g., active listening) but that individual mentees (and mentors) vary in how they view mentorship quality and how they value mentors' attributes.^{333–335} Trained, supportive mentors have been shown to be more effective at boosting mentees' metrics of success (e.g., number of publications).^{335–337} Unfortunately, negative mentor-mentee relationships and untrained mentors are still common, causing mentees to abandon career pathways and lose faith in their abilities.^{330,340–344}

The literature, then, clearly supports the importance of effective, positive mentorship. However, while considerable research has been conducted about mentorship in general, as of yet there is insufficient exploration into the issue of prioritization and a paucity of examples contextualizing mentorship in chemistry research. The closest analogous instruments are (1) rarely contextualized for STEM research environments, (2) cater to discrete age groups / career stages rather than being applicable across multiple cohorts (i.e., undergraduate to postdoctoral), and (3) do not appear valid for addressing the concept of prioritization. Additionally, apparent contradictions between prior mentorship studies attempting to ascertain the most important type of mentorship and literature suggesting interpersonal mismatches are partially responsible for negative mentoring experiences underscore how mentorship needs are contextual for a mentee's position and the surrounding environment.^{330,339,341,342,344–347}

Therefore, this paper details the development and validation of a new instrument (dubbed the "Prioritization in Mentorship Attributes Survey, PRIMAS") that can be used to assess the domains of support that an early career chemist feels they (1) currently receive and (2) need more of from PIs and group mentors. Such information might then be used to improve training outcomes and retention rates of early career chemists (and their mentors) by improving the efficacy and efficiency of mentorship, clarifying expectations between mentees and mentors, and revealing pressure points where professional development for mentors and targeted supplemental supports for mentees may be most useful. Moreover, by looking at three mentee cohorts together (i.e., undergraduate students, graduate students, and

postdoctoral scholars) with the same instrument, a comprehensive portrait of the trajectory of mentorship needs over time could theoretically be painted with a cross-sectional analysis rather than requiring a time-consuming longitudinal study.

5.3 Research Question

This study sought to develop and validate a survey which could answer the question “How do early career researchers prioritize their mentorship needs from chemistry research mentors?”. “Early career researchers” (aka the mentees) are here classified as undergraduate researchers, graduate researchers, and postdoctoral researchers in academic chemistry research groups. “Chemistry research mentors” are here classified as a mentee’s faculty advisor (PI) and primary group mentor (if one exists) within the research group. The group mentor is simply another member of the mentee’s research group who is not the PI (e.g., an upper-level graduate student, a group’s lab technician).

Crucially, throughout this study, the participating mentees are treated as subject area experts of mentorship, meaning that their expressed perspectives about mentorship and its impact on their development are treated as truthful and accurate. The study looks exclusively through the mentee perspective, although the perspectives of mentors are also valuable areas to explore in future work.

5.4 Frameworks

In creating the PRIMAS instrument, it was necessary to develop both a clear set of categories for the types of mentorship a mentor might provide in the chemistry research context and a way for respondents to indicate prioritization of said categories. A bespoke conceptual framework¹⁶¹ of System-Structure-Content (**Figure 5.2**) was articulated using three theoretical frameworks to delineate the pathway toward prioritization for the specific population under study.³⁴⁸

How do early career researchers **prioritize** their **mentorship needs** from *chemistry research mentors*?

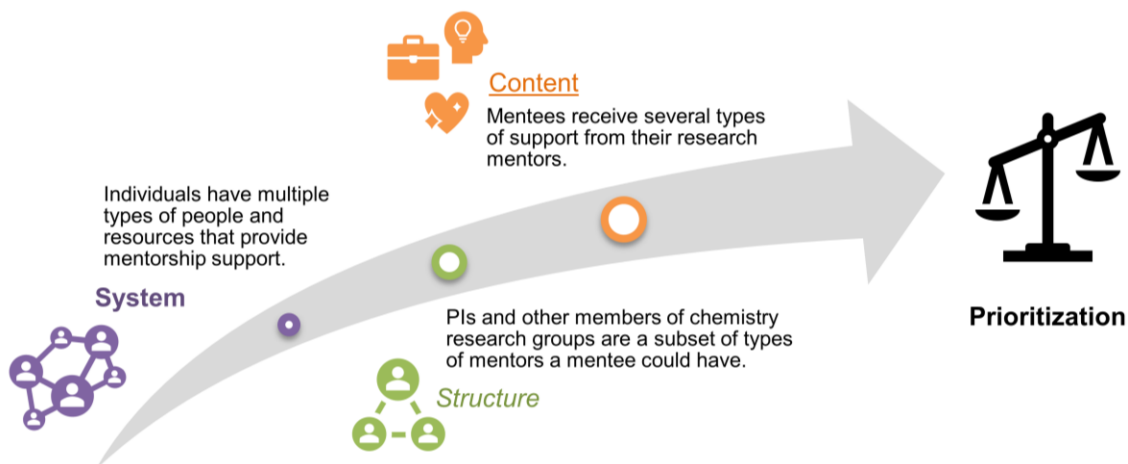


Figure 5.2. The System-Structure-Content conceptual framework unites ecological systems theory, triadic mentoring structures, and Intellectual + Professional + Psychosocial domains in pursuit of an understanding of how mentees prioritize chemistry research mentors' attributes.

System

Mentees engage in mentorship with multiple types of resources in a dynamic environment, and their needs evolve with time as a result of multifarious interactions. Since mentees have multiple resources providing dynamic support, it can be said that there is a *systems* nature to mentorship. Ecological systems theory can therefore be invoked to describe how mentorship happens within an ecology in which both human mentors and nonhuman resources occupy space.

Ecological systems theory was developed by Bronfenbrenner in the 1950s – 1970s, articulating how human development is the result of contextual, variable interactions between an individual, their environment, and their environment's environment (i.e., the classical diagram of concentric rings moving out from the Individual to the Macrosystem).^{349,350} In this theory, although the individual is an active agent, they exist within an ever-changing system where external and internal factors interact to shape the individual, thereby introducing contextual variability to the individual's development. The theory has been useful in dualistically guiding and using policymaking as social science research in contrast to exclusive reliance on controlled laboratory experiments. Such work has fueled greater understanding among both researchers and the general public of the effect of systems on individuals, such as how neighborhood zoning regulations impact childhood loneliness.^{349,350}

For this study, by viewing mentorship through the lens of ecological systems theory, we are empowered to separate out the unique aspects of a mentee's relationship with one individual mentor from the mentee's holistic network – without castigating the mentor for failing to meet all the mentee's needs. A mentor might provide unique (or duplicated) support in one arena but not another. Mentees are presumed cognizant of and at least partially accepting of a mentor's inherent limitations within their ecology as a result of their other sources of mentorship. In other words, mentees are assumed *capable of prioritizing an individual mentor's attributes* as a result of mentorship's systems nature.

Structure

Within the mentorship ecology, there is a common *structure* to mentorship in academic chemistry research groups specifically. Prior work by multiple investigators over the past decade has shown that the highly conserved, traditional mentoring structures in STEM research tend to manifest formally as open or closed triads, although less common variants do exist.^{351–353} In an incomplete, open triadic structure, the mentee is counseled by either a group member or the PI. When a mentee is counseled exclusively by a group member, that group member may also be communicating information to / from the PI without direct mentorship occurring between the PI and mentee. In dyadic cases, a mentee is mentored exclusively by the PI. However, the most advantageous cases feature the mentee being counseled jointly by both a group member *and* the PI directly. In completely “closed” triads, the group member and PI also work together behind-the-scenes to coordinate their mentorship, thus completing the triangle of communication.

The difference between the different triadic structures therefore lies in the communication lines between what is ideally a triangular relationship; correlational research indicates that mentees typically benefit the most from the closed triad.^{351–353} Notably, extended informal mentoring structures which include more members within and without research groups also exist. However, within the overall ecological system of mentorship, this study is *bounded on the formal triadic mentoring structure*.

Content

Within the chemistry mentoring structure, there is a typical *content* paradigm for the types of support mentees tend to receive. That paradigm can consist of up to three major domains: intellectual, professional,

and psychosocial. These three domains have been repeatedly uncovered by multiple mentorship investigators and were recently collated in Hernandez's 2018 review.^{339,340,351} Intellectual support includes mentorship meant to improve content knowledge, develop experimental skills, advance the progress of a project, etc. Professional support includes academic advising, words of wisdom about career decisions, assistance with networking, etc. Psychosocial support includes displays of kindness, offers of sympathy, efforts at inclusion, etc. While not all mentors will cater to all three domains, these categories encapsulate the *expected range of possibilities*.

5.5 Methodology

Using the System-Structure-Content framework, the survey was developed and validated to enable assessment of how early career researchers prioritize their mentorship needs from chemistry research mentors. Survey development began with a literature review and key informant interviews before progressing to cognitive testing and generation of reliability statistics to guide revisions.^{131,157,158,162,348,354}

5.6 Ethics

The author's IRB office determined this study to be exempt. Approval for recruitment was obtained from each of the sample departments. The institutions are not identified by name. Participants completed an online consent form via email before viewing the survey or signing up for an interview. Participants were offered nominal gift cards (for interviewees) or entry into gift card drawings (for survey-takers). Survey-takers were anonymous. Personal identifiers (e.g., email addresses) for interviewees were collected for scheduling purposes and then destroyed. Interviewees were selected based on demographic responses on a sign-up form, but names and email addresses were not viewed until after selection. Interviews were recorded for transcription except in one case where the participant requested summary notes be taken instead due to the sensitive nature of conversations about mentorship. All names provided here are pseudonyms from a list of names common to the United States for the reader's convenience; pseudonyms were randomly generated irrespective of race, ethnicity, or gender to further protect confidentiality using the Random Word Generator (<https://randomwordgenerator.com/name.php>).

5.7 Sample

Undergraduate students, graduate students, and postdocs in academic chemistry research groups at two universities in the United States were recruited by email between Spring 2021 – Summer 2022. Both departments were doctoral-granting chemistry departments at R1 institutions. One institution was more selective with a majority graduate population while the other was selective with a majority undergraduate population.¹⁶⁵ This purposeful sampling was conducted with respect to institutional research status because R1s usually host large numbers of all three mentee cohorts of interest and represent most major subfields of chemistry research.¹³⁵

From the volunteers who signed up to be interviewed, the people ultimately invited were purposefully selected to represent the widest demographic variety available. Due to the intersectionality of mentoring with other factors (e.g., societal barriers / advantages, cultural overlap with mentors),^{328,329,355} a random sample might have resulted in the absence of key perspectives. Therefore, factors under consideration ranged from academic (e.g., year in program) to personal (e.g., gender). Survey-takers, however, remained anonymous in order to reduce survey fatigue by omitting demographic questions.

5.8 Data Collection

In Phase 1 of the study (**Figure 5.3**), a literature review on mentorship enabled the *a priori* creation of survey items, such as about the triadic mentoring Structures, and category descriptions for the mentorship Content domains (i.e., Intellectual, Professional, Psychosocial). Then, in Phase 2, key informant interviews of 20-30 minutes each were conducted. The interview protocol was intended to evaluate the validity of the frameworks and assumptions made in generating the survey by probing...

1. how mentors support mentees (i.e., domains of support in the “Content” framework),
2. the definitions / institutional roles of chemistry research mentors (i.e., “Structure”),
3. the ability of participants to contextualize their chemistry research mentorship in the grand scheme of mentorship (i.e., “System”), and
4. the ability of participants to prioritize when asked about the relative importance of different mentorship activities (i.e., System-Structure-Content → Prioritization).

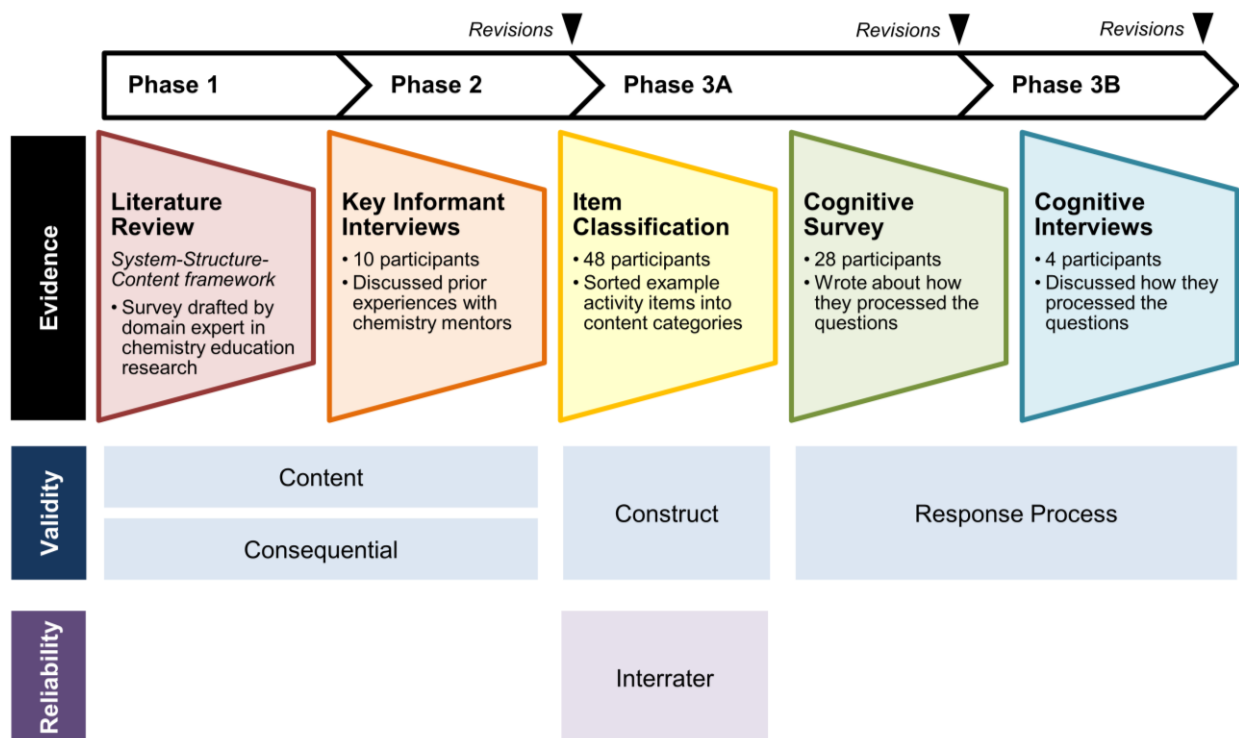


Figure 5.3. Data collection addressed content, consequential, construct, and response process validity as well as interrater reliability.

After conducting revisions to incorporate the key informant data, the third phase tested response process validity and interrater reliability. For this phase, participants took a pilot survey online (Phase 3A) and / or were interviewed for cognitive testing (Phase 3B). The survey-takers were split further into two groups: one which engaged in item classification and one which took the pilot survey.

In the classification group, participants were presented with a 54-item list describing types of support that chemistry research mentors might provide (e.g., “Give advice on a research project”, “Introduce you to other people in chemistry”). The participants chose the subcategory they believed each item belonged to. Each of the three parent categories (e.g., Intellectual) were each broken down here further into three hypothetical constituent subcategories with finer grained boundaries to enable greater differentiation (e.g., Intellectual → Conceptual, Technical, and Project). Participants were provided with definitions of the subcategories and then selected the one they felt an item belonged to, enabling reliability calculations and evaluation of construct validity based directly on the population’s input.³⁵⁴ The best-performing items were retained in the final survey to provide future survey-takers with concrete examples of the mentorship domains the survey evaluates. For

example, rather than vaguely asking a mentee about the intellectual support their mentor provides, items under the Intellectual category (e.g., “Give advice on a research project”) could be offered as concrete examples.

Next, in the pilot survey group, participants were presented with a selection of questions from the survey along with a short-answer text box accompanying each item. Instead of answering the items, participants wrote about *what* they thought the item was asking (an *Understanding* probe, from Tourangeau’s 4-stage response process theory) and *whether* they would be able to answer it (a *Response* probe).^{162,163,166} Using only two probes for a selection of items instead of also requesting item answers or using the full survey kept the administration at approximately 15 – 30 minutes (similar to the classification group) in a bid to allay survey fatigue and attrition. During the key informant interviews, the more experienced respondents (e.g., late-stage graduate students and postdocs) provided lengthier responses, seemingly as a result of having impassioned reflections and longer histories; staying mindful of their time and potential for fatigue was therefore deemed prudent during cognitive testing. This pilot survey informed revisions to the survey before engaging in the oral cognitive interviews.

In the cognitive interview group, participants remotely viewed the researcher’s shared computer screen which displayed the revised survey items. Then, similarly to the pilot survey group, they engaged in response process validation. The 30 – 60-minute interview format in Phase 3B, however, allowed for concurrent follow-up about their responses and deeper discussions than the written response process from Phase 3A allowed. All four stages were investigated (i.e., *Understanding*, *Retrieval*, *Judgement*, and *Response*). Minor revisions were enacted based upon the interviews, but the instrument overall was well-supported by this final stage of data collection.

5.9 Participant Screening

The number of participants was capped in part according to the available funds for incentives. Since some of the interviewees may have also entered the pool of anonymous survey-takers, the total number of unique participants is unknown. A screening survey accompanied the online consent form to check that respondents met the eligibility criteria before signing up for the interview or accessing the survey. If a prospective participant did not report being an undergraduate student, graduate student, or postdoctoral

scholar either currently or previously working in a chemistry research group, they were screened out. Participants were encouraged to use a computer, but modality was not enforced.

For the survey, Qualtrics quota caps based on respondent roles were implemented to ensure sufficient responses were collected from each of the three cohorts. Differentiated quotas ensured that any one cohort would not be locked out of the survey. The graduate student cohort was given a higher cap than the other two in recognition of the wider programmatic time span for PhDs (i.e., typically 5 – 7 years) than for postdocs (i.e., 1 – 2 years) and undergraduates (i.e., 1 – 3 years in research). Increasing the graduate student quota increased the odds of capturing responses from different parts of the degree. The ratio of retained responses from undergraduate survey-takers : graduate : postdoc was 1.5 : 4 : 1.

Survey-takers were not filtered further after screening, but additional purposeful sampling was conducted in selecting interviewees. As described earlier, interviewees were selected to maximize the diversity in their academic and personal backgrounds. In cases where the originally invited key informant / cognitive interviewee was ultimately not interviewed (e.g., they did not appear for their slot), an alternate was selected only after further communication failed to bring the original subject in for the interview. Demographic data is provided in **Table 5.1** to illustrate backgrounds.

Table 5.1. Demographics of all interviewees.^a

Role ^b	Program Year	Chem. Major / Highest Degree ^c	Prior Institutions	Research Experience	National Status	Race & Ethnicity ^d	Sex & Gender ^e	1 st -Gen ^f
U	1	Major		Biochemistry Computational	Domestic	Asian	Male	
U	2	Non-major		Biochemistry	Domestic	White Hisp./Lat.	Female	
U	3	Major		Computational Organic	Internat'l	White ^g Middle Eastern	Male	
U	4+	Non-major		Biochemistry	Domestic	White	Female	
U	4+	Major		Organic	Domestic	White	Female & Male Trans	
G	1	Bachelor	R1	Organic	Domestic	White	Male	
G	1	Master	R1	Physical	Internat'l	Asian	Male	
G	2	Master	R2	Materials Organic	Internat'l	Asian	Female	

Table 5.1. Demographics of all interviewees. [continued]

G	3	Master	PUI	Analytical Inorganic Physical	Domestic	White	Male	G
G	4	Bachelor	PUI	Physical	Internat'l	Asian	Female	G
G	6+	Master	R1	Computational Physical	Internat'l	White	Female	G
G	6+	Master	PUI R2	Biochemistry Physical	Internat'l	Asian	Female	G
P			R1	Computational	Domestic	White	Male	G
P			R2	Biochemistry Inorganic Organic	Internat'l	Asian	Female	G

^aRace, ethnicity, and gender response options were guided by federal data classification standards^{356,357}

^bU = Undergraduate student; G = Graduate student; P = Postdoctoral scholar

^cHighest degree earned before enrolling in current degree program

^dAll except one interviewee were not of Hispanic or Latino ethnicity – for clarity, those responses are excluded

^eAll except one interviewee were cisgender – for clarity, those responses are excluded

^fG = interviewee was the first person in their family to go to graduate school; no one was the first person to go to college

^gOne interviewee wrote in “Middle Eastern” as their race; this was reclassified as “White” according to federal data classification standards^{356,357}

5.10 Data Processing and Analysis

The interviews were conducted via Zoom (<https://www.zoom.us/>) after participant selection from a Qualtrics sign-up form and following convenience scheduling using the researcher's Calendly (<https://www.calendly.com/>). 14 people were interviewed (ten key informant and four cognitive).¹⁶⁴ 13 were recorded; live summary notes were taken for one. Audio was transcribed using intelligent verbatim transcription and analyzed via deductive content analysis in MAXQDA 2021 / 2022 Analytics Pro.³⁵⁸

The two survey groups completed their tasks online via Qualtrics (<https://www.qualtrics.com/>). For the pilot survey, 76 responses for Part I (N = 48) and Part II (N = 28) were retained after removing 15 incompletes. All retained submissions for Part I passed two attention checks (adopted due to the heavy use of matrices in Part I).³⁵⁹ Microsoft Excel 365 was used to process the data before analysis. MAXQDA was used to analyze the written response process data via deductive content analysis.³⁵⁸

For the item classification task, items with the highest agreement were retained for the final survey. A max of 4 items per subcategory was retained with at least 60 % of participants needing to select the same

subcategory for a retained item. Each subcategory therefore received 3 – 4 illustrative items for a total of 29 items. One subcategory (“Psychosocial: Awareness”) was removed due to poor performance; its items often crossed onto the subcategories “Emotion” and “Life”. The KALPHA syntax in SPSS 28 was used to calculate interrater reliability between the participants using Krippendorff’s α for the retained items’ categorical assignments.^{360–362} For the 29 retained items, 30 of the 1,392 selections (29 items x 48 respondents) were “Awareness”; these selections were treated as missing data since that category was removed. Due to the known over-sensitivity of Krippendorff’s α to category rarity,³⁶⁰ the reliability analysis was run using the implicit parent category rather than subcategory (e.g., all Conceptual, Technical, and Project selections were transformed into Intellectual selections).

5.11 Validation Results

The purpose of the key informant interviews was to qualitatively evaluate the content and consequential validities of the conceptual framework for the target population.^{131,354,363} The data ultimately supported the validity but introduced important nuances that could increase performance. Revisions were consequentially incorporated. Subsequent cognitive testing via a pilot survey and then interviews mostly endorsed only minor wording and formatting changes which are reflected in the final version of the survey (**Appendix E**).^{157,158,162}

5.12 Content and Consequential Validity via Key Informants

The key informant data is presented according to the conceptual framework (**Figure 5.4**):

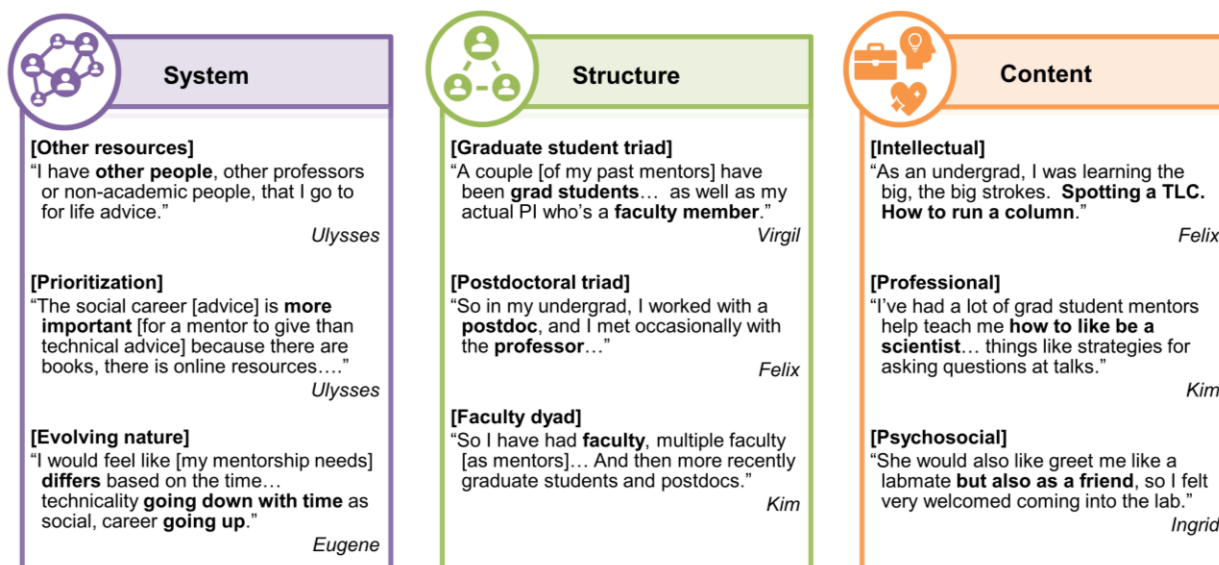


Figure 5.4. Key informant data support the content and consequential validities of the System-Structure-Content framework. Sample transcript excerpts have been edited lightly for improved reader comprehension.

System

The interviewees reported having many mentors over the years, some good and some bad. A common thought articulated was that chemistry mentors do not need to be a holistic "life mentor" because other people (e.g., family, friends, other mentors) also contribute to the interviewees' mentoring landscape. The older interviewees displayed rich, reflective memories about their many prior mentors. However, whereas older mentees were verbose, younger students betrayed their more limited experiences with more succinct responses which typically included information about only a couple mentors.

Crucially, interviewees (unbeknownst to them) disagreed with each other on the relative importance of different types of mentorship supports and whether a "hands-off" or a "hands-on" mentoring style is best, despite agreeing that the best mentors help mentees grow into independent individuals. Interestingly, some interviewees articulated a desire for more distance from their mentors, either because the mentor was abusive...

Adriana: When I say it was bad, it was like logging into my computer and taking my files sort of stuff. Like, I mean bad bad. Like, I don't mean he wasn't good at teaching me things. I mean it was like an adversarial relationship.

... or because they felt distance gave them space for growth. Notably, the latter participants did not dislike their mentor but rather appreciated having freedom to try out new ideas and to make a few educational mistakes before the mentor became more involved.

When combined with interviewees' reflections that excellent mentors are ones who adapt to mentees' needs and idiosyncratic backgrounds by changing their mentoring style over time, this data underscores the ecological aspect of mentorship, mentorship's evolving nature, and the ability of a mentee to contextualize mentorship in the grand scheme of their own trajectory. At the same time, it was apparent that the survey would need to enable participants to indicate not only the type of support they would want more of but also whether they would want less and whether the mentorship was destructive.

Structure

The type of mentor reported ranged the expected gamut from students to postdocs / staff scientists to faculty PIs. Mentors were typically more senior than interviewees except for the oldest interviewees (e.g., postdocs, 6th-year graduate students) who described the peers closest in experience to them as their current mentors, even if technically junior (e.g., an advanced PhD student assigned by the PI to guide a new postdoc). These mentorships aligned well with the anticipated triadic structure. The student / postdoc mentors appeared more likely to provide focused technical mentorship whereas the PIs were frequently described as providing project support by posing the "big questions". PIs were distant figures (perhaps interacted with weekly) whereas student / postdoc mentors existed in a mentee's day-to-day environment, providing more frequent guidance. Interviewees did not, however, necessarily view the differences between PIs and student mentors as undesirable. On the contrary, they often expressed a preference for the separation of roles, believing one type of mentor was best for certain activities (further supporting the concept of prioritization).

However, interestingly, when first asked to describe their "mentors", most interviewees initially spoke only of their *good* mentors and did not count bad mentors as "mentors" until further prompted by the interviewer:

Eugene: Well, now that I think about it, the mentors that I mentioned were the good ones. Because there were also mentors that were bad in my opinion. So now, if I consider bad ones, the number increases.

Additionally, interviewees differed on whether they instinctively interpreted "mentor" to refer to their PI, a student / postdoc mentor, or both; explicit prompting was again required to elicit discussion about both types.

Once these definitions were made explicit, however, interviewees effortlessly discussed their memories, whether about good / bad or about PI / student / postdoc.

Overall, this data supports that the triadic mentoring structure originally discovered with undergraduate research students extends to graduate student and even to postdoc mentees in chemistry. Crucially, it was apparent that future participants would need to be explicitly instructed to consider bad mentors as “mentors” when answering survey items and that a definition of “mentor” would need to be provided which included both PIs and peers for the sake of clarity.

Content

From learning how to run a column to how to be a scientist, interviewees described a wide range of ways that mentors supported them. All of the described activities aligned with the *a priori* categories. Their diversity reinforced the anticipated utility of providing example items for the categories to ground respondents in category definitions for the final survey. The interviewees did not, for example, each list activities from all three categories. Fortunately, when provided with a sample list of the drafted category items as a test question at the end of the key informant interviews, the interviewees almost unanimously agreed upon the importance and comprehensiveness of each item:

Salvatore: ... “Help a mentee make significant contribution to a project”, I think that's pretty important...

Advising also important. I feel like I'm gonna say that about all of these... [finishes reading the remaining items]

Interviewer: Ok. Great. Is there anything that you think should or shouldn't be in the question? Would you add, remove, or modify anything?

Salvatore: No, I think it's quite good. Very comprehensive.

and

Virgil: These are all good categories, dammit... I think they're pretty good actually. It covers pretty much the breadth of research experience.

However, when asked to identify what their *ideal amount* of each support would be, interviewees struggled with the abstract nature of the question. They instead resorted to discussing how much support they *currently* receive and how they would like it to *change* (i.e., increase or decrease). Fortunately, when subsequently

pressed to prioritize the items, the interviewees were able to do so as well as differentiate which mentor would be the best source of each type of support. In other words, the participants could not abstractly identify the ideal amount of mentorship support they would want from a mentor, but they could deftly identify (1) how much support they currently receive, (2) how they would like to see that support change, and (3) which type of support currently matters most to them.

Interestingly, some interviewees were apologetic about their responses when weighing the importance of different domains. They sometimes would say they previously valued certain types of mentorship or how they thought other people would respond instead of themselves. Therefore, while there was strong support for the validity of the domains, it became clear that the survey instructions would need to repeatedly remind participants to answer according to their own, current opinions. Additionally, to determine how much mentorship a participant would want in each category, the survey would need to be designed to first collect baseline data on how much support they believe they currently receive and then investigate how a participant would ideally want that support to change.

5.13 Interrater Reliability and Construct Validity via Item Classification

After validating the frameworks via key informant interviews, an *a priori* 54-item list of example actions was subjected to classification in Phase 3A. Participants chose which of the nine types of mentorship a mentor is acting on when they, for example, “show sympathy” (**Table 5.2**). This task therefore identified concrete ways that chemistry research mentors intellectually, professionally, and psychosocially support a mentee. By having members of the population do the sorting themselves, the validative purpose was achieved while ensuring that the list was contextually appropriate for the population. The items could then be used in the final survey to provide concrete examples of what it means for a mentor to provide, for example, emotional support. Participants then would share a common understanding about category definitions *before* ranking the relative importance of the categories. The key informant interviews had indicated that, without concrete examples, survey-takers might not otherwise share the same understanding for what emotional support is versus, for example, life or advising. Considering the diversity of participants’ backgrounds (e.g., native English speakers and non-native, undergraduates and postdocs), the differences in participants’ assumptions are unsurprising. Example items could therefore correct assumptions efficiently.

Table 5.2. Example items and descriptive statistics for each Content domain.^a

Parent	Subcategory (Definition & Example Item) ^b	Number of Items ^c	Avg % Selection	Avg Parent % Selection
	Conceptual = improving conceptual knowledge and conceptual skills <i>"Explain how techniques work theoretically on the abstract level"</i>	4	79.7	89.0
	Technical = improving technical knowledge and technical skills <i>"Show how to do advanced research techniques"</i>	4	86.5	
	Project = guiding the development and progress of a research project <i>"Give advice on a research project"</i>	3	67.1	
	Advising = providing advice and guidance on academic and career topics <i>"Advise you on careers"</i>	4	75.9	88.7
	Norms = showing professionalism and scientific norms used in the field <i>"Explain field-specific norms for presenting research"</i>	3	72.7	
	Professional Socialization = facilitating professional socialization in the field <i>"Introduce you to other people in chemistry"</i>	3	80.0	
	Emotion = providing emotional support and a sense of belonging <i>"Show sympathy"</i>	4	89.9	91.8
	Life = supporting life goals outside of research and the professional world <i>"Encourage a healthy work-life balance"</i>	4	78.5	

^aKrippendorff's $\alpha = .73$ for all 29 items' implicit parent assignments

^bDisplayed for reader convenience in their final forms after response process revisions

^c29 of 54 items retained after trimming to achieve a maximum of 4 items / subcategory and > 60 % selection

^dPsychosocial subcategory "Awareness" (of backgrounds & knowledge level) was removed due to items crossing substantially with other subcategories

Table 5.2 provides the summary outcome of the classifications (see **Appendix E** for the full list). Considering participants chose from nine subcategories, the averages for their selection decisions are encouragingly high. The items for "Awareness", however, frequently crossed on other subcategories, and so the subcategory was removed. After further trimming to remove the worst-performing items and to decrease the length of the overall list for succinctness, Krippendorff's α for the retained items yielded .73, indicating that

participants did not disagree often on the assignments.^{360,361} When they did disagree, they often selected another subcategory from the same parent category despite not being informed of the parent categories' existence (e.g., selecting "Life" rather than "Emotion" for "Show sympathy"). Note that, when comparing **Table 5.2** to the items in **Appendix E**, the category "Professional Conventions" was changed to "Norms" due to later learning in the response process data that some participants misunderstood the word "conventions" to mean academic conferences. Other items also underwent slight wording changes as a result of the response process data, but they are shown in **Table 5.2** in their final form. The assumption is here made that the revisions would have either improved or at least not changed the interrater reliability.

5.14 Response Process Validity via Written and Oral Cognitive Testing

As a result of the key informant interviews, moderate revisions were made to the draft survey before Phase 3A to adjust the content and wording of items to (1) improve clarity about the types of mentorship being investigated, (2) encompass the potential for adversarial or stifling mentorships, and (3) ground the measurement of mentorship on the respondents' opinions about the value of different Content domains *relative* to what they currently receive. Next, cognitive testing was conducted on purposefully selected items (i.e., the ones anticipated to be most misunderstood) via written response process.^{162,163,166} It became again apparent that respondents would need explicit guidance on *which* mentorships were being explored. For example, older mentees wanted even clearer instructions about reflecting upon the mentorship of either their current mentors or their best prior mentors. Similarly, respondents wanted clearer instructions about time-bounding: should they reflect on the current month or the overall year?

Encouragingly, however, the response process obtained for the remainder of the items seemed mostly well-aligned to produce the intended effect (with the occasional adjustment warranted). Crucially, respondents appeared to address the questions about rating and ranking the relative importance of the categories as intended. Respondents noted a desire to keep the definitions and examples accessible throughout the survey in case they wanted to refer back to them to refresh their memory.

After incorporating the indicated revisions, oral interviews were conducted to probe all the items in the refined survey in greater depth. Happily, the biggest issue revealed through the interviews was that the phrase "professional conventions" was sometimes misinterpreted as referring to academic conferences rather than

norms. Similarly minor wording changes were enacted to a handful of other items. Overall, this data was encouraging that respondents understood most items as intended and were capable of answering the refined survey through the intended cognitive processes.

5.15 Discussion

The purpose of this study was to generate and validate a survey that could be used to answer the question “How do early career researchers prioritize their mentorship needs from chemistry research mentors?”. A bespoke System-Structure-Content conceptual framework and the resulting PrIMAS instrument were subsequently articulated and validated herein using a literature review, key informant interviews, and iterative rounds of cognitive testing.

5.16 Implications

Ultimately, the key outcome from this work was the successful creation and testing of the PrIMAS instrument for content, consequential, construct, and response process validity as well as interrater reliability for the list of example category items. The data indicated both that the System-Structure-Content framework expresses crucial components of how mentees prioritize the attributes of chemistry research mentors and that the PrIMAS instrument is adequately contextualized for the three cohorts of interest. The instrument therefore appears ready for deployment in a statistically relevant sample in order to enable inferential analyses about how mentees value mentors’ attributes.

Interestingly, some of the qualitative data implied that mentees share some commonalities in how they view mentorship but disagree on other points. For example, interviewees tended to express the opinion that peer mentors are better sources of technical support than PIs are, but they differed on whether a hands-on or hands-off approach is best. When taken in conjunction with apparent contradictions between prior studies attempting to identify the most important mentorship domains, this preliminary data underscores the personal nature of mentorship: individuals’ experiences fluctuate between unique and ubiquitous. Ideally, by looking across multiple mentee cohorts, types of environments, and demographics, greater clarity regarding the statistical relationships between these variables could be achieved in the future thanks to the high degree of PrIMAS’s contextual sensitivity.

5.17 Limitations

Although this study followed a standard, systematic process for establishing validity, three key limitations may threaten the results: (1) the limited diversity of participants, (2) the almost-exclusive use of mentees' self-reports, and (3) the lack of quantitative evidence for internal structure validity. Although efforts were made to achieve a diverse interviewee pool, certain identities (e.g., underrepresented racial minorities) were not present. Considering the intersectionality of marginalized identities with experiences in academia,^{328,329,338,346,353} their absence raises the specter that perspectives may have been missed which could have impacted this paper's findings.

Additionally, while using mentees themselves as content area experts in mentorship lends certain strengths and sampling convenience, it also introduces potential for bias, most notably that of self-report bias and the Dunning-Kruger effect. Self-reports often deviate some from reality, and mentees are not omniscient. Mentees are therefore limited in the extent to which they can project which type of mentorship they would most benefit from. Basing the framework off of extensive prior literature and mostly relying on the mentees to validate the frameworks for the target population hopefully helped to address these limitations, but future research supplementing this work with data taken from the mentors' perspectives may help address this design threat further.

Similarly, while drawing the identities of the Content categories from the literature hopefully indicates a certain degree of internal structure validity, quantitative evidence (e.g., factor analysis) was not conducted, partly as a result of limited resources. Interrater reliability supports the consistency of the item classifications, but dimensionality would be best supported by internal structure data.

5.18 Recommendations

Moving forward, other researchers (and perhaps mentee-mentor pairs) are encouraged to utilize the refined survey (**Appendix E**) to investigate relevant issues of mentorship in chemistry research settings. **Figure 5.5** provides a brief outline of the final survey sequence. Time estimates indicate an average administration of 20 – 40 minutes. Note that, during interviews and pilot survey administration, the older mentees frequently took longer than the undergraduate students to finish items, sometimes double the time. Two leading hypotheses for this disparity are the higher incidence of non-native English speakers in graduate

chemistry programs and the richness of the older mentees' memories about mentorship, thereby inducing a higher cognitive load and longer reflections.

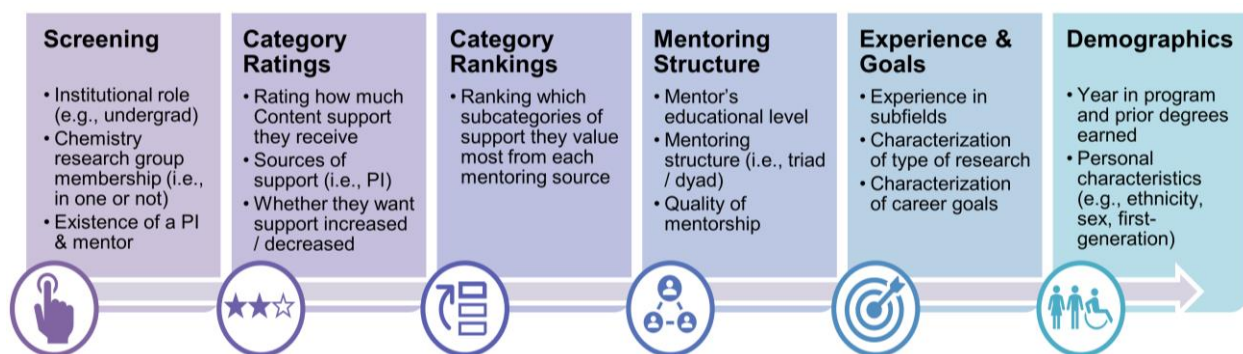


Figure 5.5. Sequence of the validated survey.

While future researchers are of course at liberty to conduct whichever analyses are most pertinent to their agendas, **Figure 5.6** outlines the intended analytical pathway for the data that can be gathered using PRIMAS. Since prioritization is theorized to result from the System-Structure-Content framework, inferential analyses should be conducted to understand the constructs which influence mentees' Content domain priorities. The constructs which appear most likely to control mentees' priorities are the mentee's own position in the ecology ("Self"), the mentorships they engage in ("Mentors"), the domains they are currently supported in ("Current domains"), and the context in which they conduct their research ("Context"). Creating clusters and composite scores may be useful in achieving item reduction before executing these higher-level analyses. Ideally, PRIMAS can be used to improve the training outcomes and retention rates of mentees and mentors in chemistry departments as well as guide the allocation of supportive resources by third-parties. Hypothetically, the survey may also be useful in other STEM disciplines, provided appropriate validation can be conducted to substantiate such a transplantation.

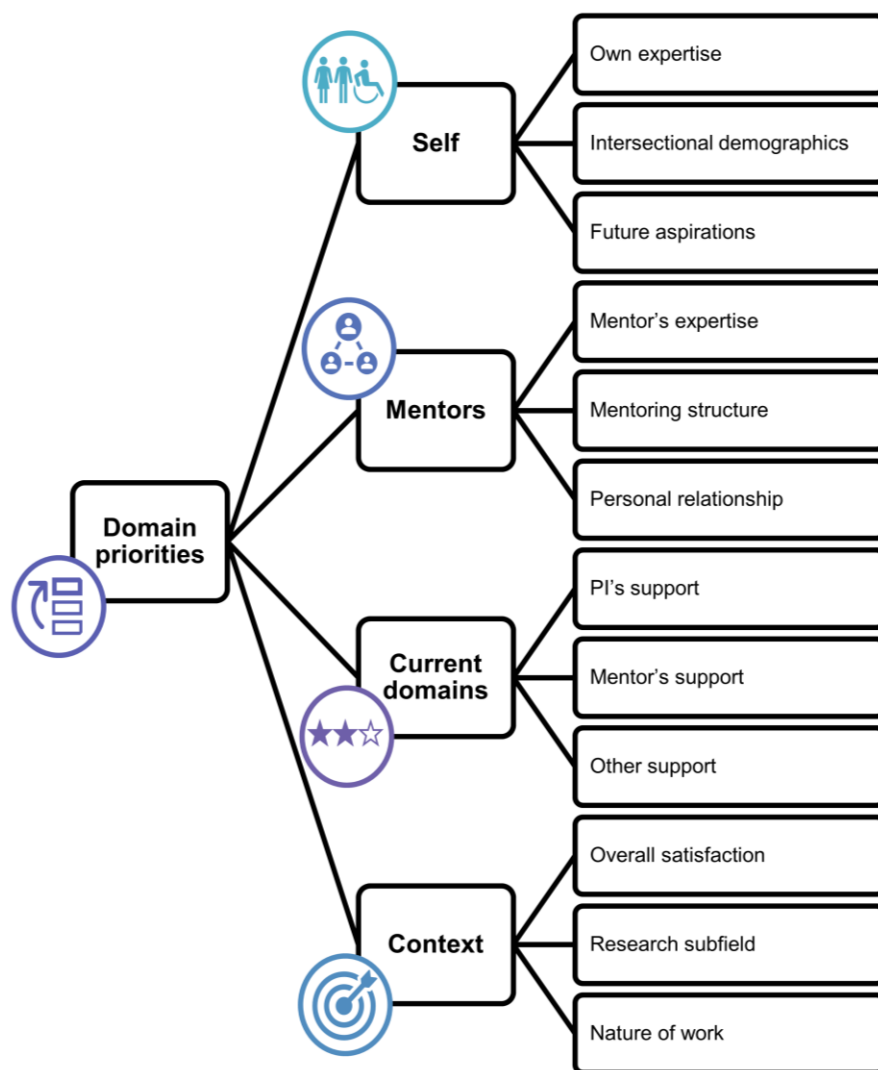


Figure 5.6. Proposed analytical pathway for data that can be gathered with the final survey (icons match those from **Figure 5.5** to indicate the survey provenances of key data for each construct).

5.19 Conclusion

Mentorship is crucial for success, which means institutions, mentors, and the mentees themselves share responsibility for ensuring that the previous commodity of mentorship is allocated wisely. To promote the effective and efficient expenditure of time and effort in mentorships, the validated PRIMAS instrument can be used as a tool for assessing both the current state of a mentoring relationship and the direction it should next pursue to address a mentee's evolving needs. By looking at multiple types of chemistry mentee cohorts together with the same instrument, comparative nuances could be drawn to ensure early career chemists are receiving the support they need most when they most need it.

Chapter 6

Comparative Analysis of a Department's Perceived Value of Seminar Talks

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Part I: Beliefs about and Experiences with Attending Seminars in an R1 Chemistry Department

6.1.1 Abstract

A department seminar is a traditional scientific activity for disseminating discoveries and networking. However, the seminar's role in supporting chemistry students and professionals is underinvestigated. Empirically understanding the role that seminars play in the community could help departments confidently design seminar experiences to maximize benefit for both students and professionals. Therefore, this paper reports the perceived value of and practices surrounding seminars for an R1 chemistry department (**Figure 6.1.1**). The emerging portrait illuminates consensus and disagreement between department members regarding their practices and beliefs about seminars. The results also underscore the benefits of intergenerational research between various educational levels.



Figure 6.1.1. Department seminar talks offer multiple anecdotal benefits, but few of those supposed benefits have been substantiated with empirical evidence.

6.1.2 Introduction

Seminars are an academic staple. Scientific progress depends on not only making discoveries but also disseminating results. In 1971, an author in the *Journal of Chemical Education* declared “Lord Rutherford used to tell his students that a piece of research is not completed until it has been written up in simple and clear language. One might well add a rider to his comment – until, also, a successful seminar has been prepared in which the results and conclusions are clearly described and explained.”³⁶⁴ Today, participation in departmental seminars manifests throughout academia, and most departments offer seminars and/or seminar-like experiences.^{365,366} However, how this long-standing tradition contributes to attendees’ development is an underinvestigated topic. Considering seminars’ prevalence, exploration is warranted to ensure the chemistry community is capitalizing on these learning opportunities.

Traditionally, departmental seminars (also called “colloquia”) are oral presentations by external invited faculty or industry speakers to a departmental audience about recent progress in their group’s research agenda, followed by Q&A and networking. Relatedly, student-centric seminar-like courses / workshops (often also called “seminars”) and capstone projects might have students practice presentation and writing skills, give project updates, learn about careers, or engage in other training exercises. In 1956, a survey of 233 ACS-accredited chemistry departments nationwide (81 % response rate) revealed that 45 % reported some type of seminar or seminar-like experience was available to undergraduates.³⁶⁶ Departments indicated that they believed these experiences improved students’ knowledge, ability to discuss ideas, professional disciplinary skills, interest in research or career options, self-confidence, and camaraderie. Subsequent literature also supports that seminar-like experiences and national conferences offer advantages for undergraduates such as developing communication skills, exploring careers, networking, improving self-confidence and sense of belonging, increasing interest in research, and elevating metrics of degree persistence.^{367–372}

However, despite literature supporting the value of conference attendance and seminar-like experiences, minimal research has investigated the impact of formal, traditional departmental seminars. Additionally, literature on conferences and seminar-like experiences often focuses on undergraduates, limiting generalizability for faculty and graduate students. In one study, attending seminars helped postbaccalaureate students feel academically ready to pursue a biomedical graduate degree.³⁷³

Meanwhile, in a “snapshot” survey of civil engineering departments, graduate students and department heads reported that seminars were valuable for students but less useful for faculty.³⁷⁴ However, the free-response data suggests that respondents may have been mostly reflecting on seminar-like, course-based experiences (e.g., practicing dissertation talks, sharing project updates with peers) rather than departmental seminars.

Therefore, exploration into how chemistry department members engage in this widespread scientific practice is merited, especially since an ACS survey determined in 2008 that approximately 96 % of 139 responding departments who offered PhD programs hosted colloquia.³⁶⁵ The need for such exploration is accentuated by Busby and Harshman’s recently reported interviews with four chemistry doctoral students who reported seminars as boring, overly complex, irrelevant to their own research, and exclusively focused on academia.³⁷⁵ While these students perceived that seminars could also benefit them with exposure to presentation styles and a variety of topics, their frustration with seminars appeared to grow over time. In general, reports from chemistry and physics doctoral students suggest that graduate programs in the United States may provide inappropriate professional development and insufficient support.^{375–377} Understanding how seminars fit into the complex network of learning and research in academia could enable organizations to maximize positive impact on students and professionals. Therefore, to lay the groundwork for further investigations on this topic, this study probed the perceived value of and practices associated with attending seminars in one R1 chemistry department.

6.1.3 Research Question

The goal of this study was to produce a snapshot portrait of how one R1 chemistry department values attending departmental seminars. The research question was “How does an R1 chemistry department perceive the value of attending seminars?”. Subsequent research could use these results to build a generalizable understanding of the value of seminars. Results might then inform who should be encouraged to attend seminars and why, how speakers could tailor their presentations, and what types of associated activities should accompany a seminar to support attendees’ development.

6.1.4 Frameworks

In considering the possible value of seminar attendance, literature about conferences suggests that the goals of attendance could be viewed as improving knowledge / skills and participating in a disciplinary culture. Therefore, the study was guided by a bespoke conceptual framework¹⁶¹ here dubbed as Speaker-as-a-Guide with two theoretical frameworks explaining how the speaker impacts the attendees in this capacity: Vygotsky's Zone of Proximal Development³⁷⁸ (attendees improve knowledge and skills with the assistance of the speaker) and acculturation³⁷⁹ (attendees transition from being a member of the general public into a member of the academic field). These frameworks guided the study design to probe how attendance could improve knowledge / skills and disciplinary belonging (**Figure 6.1.2**). However, without strong evidence that seminars play a similar role as conferences, these frameworks might fail to capture the value of seminar attendance. Therefore, there was also an opportunity for participants to provide phenomenographic descriptions of their opinions about the value of attending seminars through open-ended free-responses. These responses could be analyzed via a grounded theory methodological framework.^{132,380}

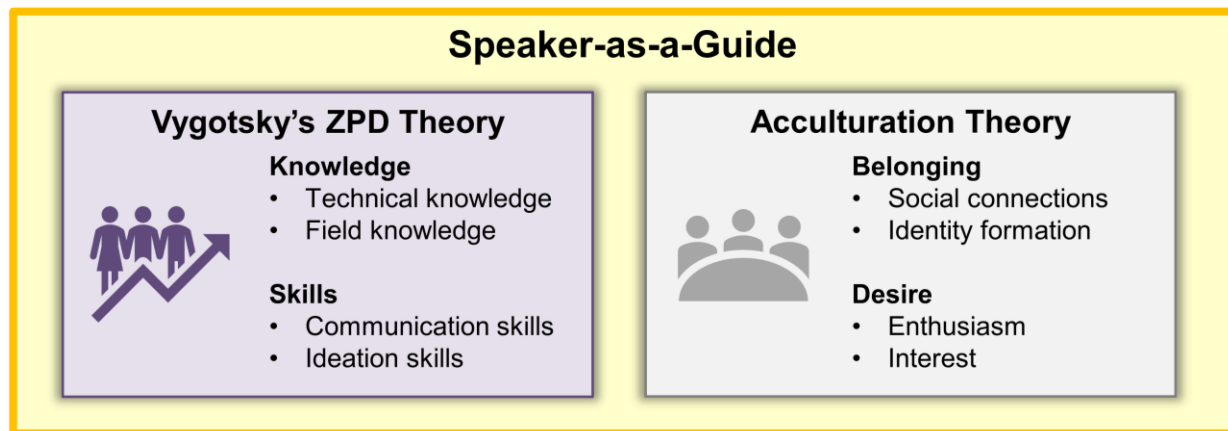


Figure 6.1.2. ZPD and acculturation theories formed a Speaker-as-a-Guide conceptual framework for survey creation (example item topics shown).

6.1.5 Survey

A mixed-methods survey with Likert ratings and free-response questions was therefore designed to enable respondents to both indicate their degree of agreement with prescribed impact statements and to write generatively about their beliefs regarding seminar attendance. A short cross-sectional survey was

selected as the most appropriate type of instrument logistically; convenience and a low time commitment should facilitate participation from people regardless of their role and schedules (i.e., from students to faculty). Since it was reasonable that advanced researchers' responses might vary from novices', being able to compare their responses was prioritized. The mixed-methods approach, meanwhile, enabled collection of qualitative data for concurrent triangulation of the quantitative.³⁸¹

The survey asked about the perceived value and impact of attending seminars using Likert ratings. There were three qualitative questions which asked respondents to describe the valuable features of seminars, nonvaluable features, and suggestions for improving seminars. To provide contextual information, data was also gathered regarding norms (e.g., attendance expectations). Respondents were shown questions tailored to their situation (e.g., Principal Investigators (PIs) were asked about their expectations for their group members' attendance – see **Appendix F**).

6.1.6 Validity

To promote content validity, two chemistry faculty and a lecturer were consulted as content experts by the graduate student author during the initial study design to brainstorm items. Topics which appeared in literature about conferences were also incorporated for content validity and construct validity. A faculty member in the sample department evaluated the survey positively for face validity. However, without an existing validated instrument about seminars, criterion validity could not be established. Finally, the free-response descriptions that respondents would provide were intended as additional validity checks for the quantitative items via concurrent triangulation.³⁸¹

6.1.7 Ethics

The author's IRB office determined this study to be exempt. The sample institution's department chair approved recruitment. Participants completed an online consent form accessed via email before viewing the anonymous survey. The institution is not identified by name here.

6.1.8 Data Collection

In the spring of 2021, the survey was emailed to department members and advertised at several department meetings. Meetings and seminars were remote via Zoom for the 2020-2021 academic year due to the COVID-19 pandemic. The instructions said to answer in terms of a normal year. The survey took most people between 5 – 10 minutes to complete.

6.1.9 Data Processing

100 responses were recorded. After removing those with less than 50 % completion, 78 remained. Most of the eliminated respondents abandoned the survey at or after the first question, which requested their role (e.g., faculty, postdoc). Respondents who skipped questions but proceeded to the end were recorded as completed; the skipped questions were overwhelmingly free-response options.

Quantitative data was analyzed using Microsoft Excel or IBM SPSS 28.0.0.0. A critical value of $p = .05$ was used for all significance tests. Dunn-Bonferroni corrections were applied for all multiple comparisons to mitigate Type I error.³⁸²

Qualitative data was analyzed using MAXQDA Analytics Pro 20.4.1 with constant comparative thematic analysis via iterative inductive open coding.¹³² Open codes for each free-response question were developed by analyzing a random subsample of 15 responses before expanding to analyze all the remaining responses for the question. The subsample was re-randomized between each question. Count data was tabulated for each axial code. Respondents could contribute only once to a code count / question so that verbose respondents would not overshadow the succinct. For example, a respondent who wrote that seminars are valuable for meeting researchers (code “Networking: People”) and for learning about places they could work at in the future (code “Networking: Places”) would count once toward the axial code “Networking” rather than twice. Several months later, coding was repeated with random subsamples of 15 to estimate intrarater reliability. The three free-response questions were coded again without the codebook. Cohen’s kappa indicated substantial agreement with $\kappa = .719$ (valuable features), $.855$ (nonvaluable features), and $.851$ (suggestions) and $p < .001$ for all three.

6.I.10 Sample Institution

This study focused on one R1 chemistry department in the midwestern United States during the spring of 2021. The university was a large, majority graduate institution with very high doctoral research activity and an undergraduate profile listed as more selective.¹⁶⁵

6.I.11 Demographic Comparison

Demographic data for the department and university were obtained from administrators and public websites. The survey collected similar data to compare the composition of the survey sample to the department population (i.e., departmental affiliation, educational role, domestic vs. international status, gender). Most respondents (85 %) self-affiliated with the department; the others (13 %) may be from overlapping spheres who encountered the survey as a consequence of their relationship to departmental communication outlets (e.g., a non-major undergraduate who works in a chemistry research lab). 28 % of respondents were undergraduate students, 50 % graduate students, 8 % postdoctoral researchers, and 14 % faculty/staff. 67 % identified as domestic students/staff and 29 % as international (4 % did not answer). 46 % identified as female, 47 % as male, and 3 % as other (n.b., although male and female are sexes, the term “gender” was used to align with the university’s data). These percentages were reasonably similar to the department’s demographics, indicating approximate similarity between the composition of the survey sample and the departmental community.

6.I.12 Role Groups

Respondents were mostly undergraduate and graduate students, but there were also a considerable number of postdoctoral researchers and faculty / staff, especially considering their lower representation in the department. The breakdown of student years and faculty positions shows that each group was well-represented by both junior and senior members (see **Appendix F**). Undergraduate students reported whether they were in a research group and go to seminars to determine if they had relevant experiences to enable them to answer the questions; those who did not were screened out. Faculty / staff were sometimes split into PI and non-PI groups for analysis as were the graduate students and postdoctoral researchers who self-identified as mentors of other students. Similarly, due to the different activities

engaged in by first-year graduate students vs. non-first-year graduate students in this department, the first-year and non-first-year students were analyzed as separate groups. The department operates a PhD program with an intermediate Master's degree granted after the first year. The first-year students earn the Master's after taking classes, serving as teaching assistants, joining a research group, and preparing for candidacy. In contrast, students past their first year focus on research, having obtained the Master's and passing candidacy in the second year.

6.I.13 Context Overview

In addition to demographics, characterizing the atmosphere that attendees operate in could help contextualize beliefs. Therefore, before probing for respondents' beliefs about seminars, data was collected regarding the seminars, attendance, and associated activities (e.g., socialization within groups).

6.I.14 Departmental Seminars

The department hosted weekly seminars (sometimes multiple a week) from outside speakers on a variety of disciplinary topics. Speakers were typically invited by faculty, but some were selected by students. In addition to seminars hosted by the chemistry department, seminars could also be joint ventures with other departments with overlapping interests. Occasionally, a seminar was arranged by specialty departmental subgroups. Seminars were announced via email from administrators and flyers posted in the laboratory buildings. There was no official department requirement for student attendance. Before COVID-19, speakers were often taken to lunch by selected individuals (faculty or students) and might also observe research presentations by selected graduate students / postdocs.

6.I.15 Attendance Expectations

Although the department did not have an official policy requiring attendance, PIs might have required attendance, or students may have felt pressured to attend seminars. Therefore, respondents were asked whether they were required to attend. A minority of undergraduates (9 %), graduate students (15 %), and postdocs (33 %) felt required to attend seminars. Instead, the vast majority of students and postdocs

reported being encouraged, not required, to attend seminars. PIs' responses about their expectations for group members' closely mirrored these percentages.

The 8 PIs were also asked to report their expectations for how often their group members should attend seminars per academic session. PI responses varied from faculty who did not monitor attendance (1 response), who promoted only certain talks without a specific frequency (1), who expected approximately 1 seminar / week (3), at least 2 – 3 / week (1), and as many as possible (2). Ultimately, although PIs reported not *requiring* attendance, they did *expect* frequent attendance.

Relatedly, all respondents reported how often they themselves attend seminars (**Table 6.I.1**). The data suggests an increase in frequency as educational level within a group increases. Means were higher than corresponding medians due to a handful of individuals who reported much higher attendance than their peers. It appears that group members may not be meeting PI expectations if PIs expect them to attend 1 seminar / week (approximately 10 seminars / session), although this cannot be definitively determined without matched PI-group member responses.

Table 6.I.1. Self-reported attendance frequency by [Role] per academic session.

By [Role] ^a	N	Median	Mean	Std. Dev.
Undergraduates	17	1.5	2.79	3.197
Graduate Students (year 1)	6	3.5	7.33	8.881
Graduate Students (years 2+)	29	5.0	8.00	7.372
Postdocs	6	2.5	4.88	5.060
PIs (Faculty/Staff)	8	12.5	19.50	14.852
Non-PI (Faculty/Staff)	2	3.0	3.00	1.414

^a68 of 78 cases after excluding ambiguous and skipped responses

Graduate students and postdocs were also asked, if they were responsible for mentoring someone, to report their expectations for their mentee. 14 of the 19 graduate students and postdocs who identified as mentors also wrote about expectations they have for their mentees' attendance and learning. Overall, mentors reported no expectations for mentees to attend (5 respondents) or, if they did attend, to just try to learn a little something (6) or broaden their horizons (4). Alternatively, a few mentors wanted mentees to learn how to process new information (3), how to present (2) and become aware of potential future collaborators/employers (1). In general, mentors emphasized that their expectations for mentees (undergraduates or younger graduate students) were low or nonexistent.

6.1.16 Social Systems

Finally, seminars do not occur in a vacuum: attendees might discuss the seminars with others. Therefore, students, postdocs, and PIs were asked about social interactions regarding seminars (**Figure 6.1.3**). The questions asked whether anyone in the group was:

- helping prepare group members beforehand with tips about what to listen for or other preparatory discussion/guidance
- advising group members on how to best listen, take notes, question, evaluate, or otherwise follow along
- discussing or debriefing group members afterward

The percentage of respondents who indicated that they (or, in the PIs' case, their group members) never received any assistance from their group was high (71 % for preparation, 83 % for processing, 40 % for debriefing). PIs and senior group members were the primary sources of support.

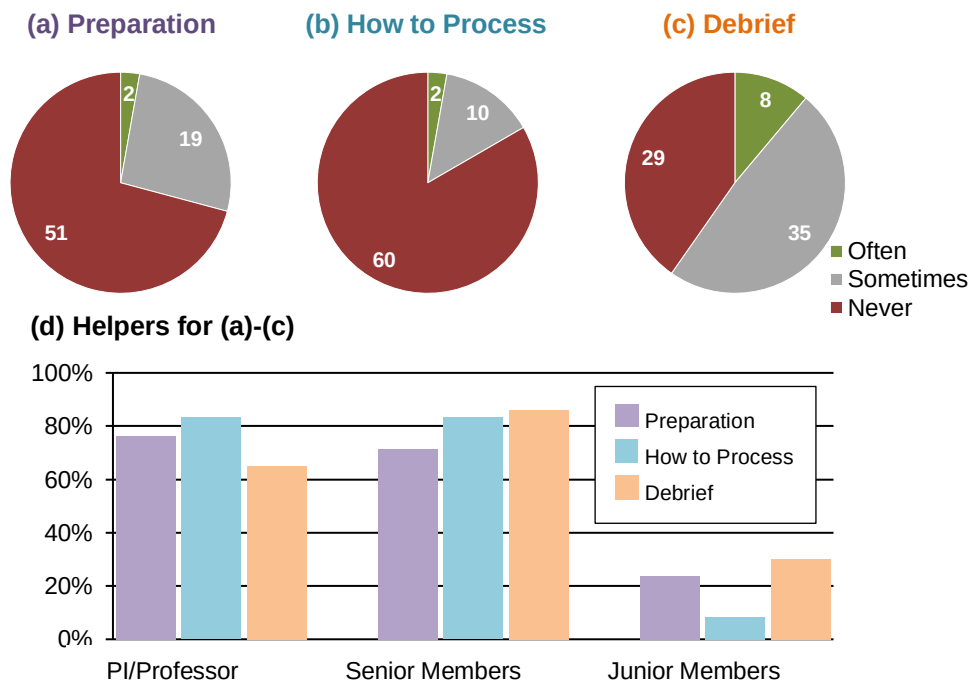


Figure 6.1.3. Most respondents reported receiving no guidance in (a) preparing (purple), (b) learning how to process (blue), or (c) debriefing (orange). Raw Helper counts were adjusted to display the percentage of affirmative responses (d). Respondents displayed similar distributions across Role (e.g., the PI respondents gave similar answers as graduate students). Since research groups vary in their composition, the terms “senior members” and “junior members” were used despite the inherent vagueness of what constitutes seniority.

6.I.17 Quantitative Perceptions Overview

After generating a contextual outline, the next question to address was whether the community felt that there was value to attending seminars (and, if so, what the associated impacts might be).

6.I.18 Perceived Value for Roles

Respondents rated the value of attending seminars (“Value”) for five major educational positions (“Roles”). The Likert ratings (**Table 6.I.2**) exhibited normal distributions (histograms not shown) with slightly lower means than medians and all skews and kurtosis smaller than -1 (not shown). Due to the ordinal nature of the data and the use of each respondent to rat each Role levels, a Friedman related-samples two-way analysis of variance by ranks test was pursued as a nonparametric alternative to a repeated measures ANOVA. A statistically significant result, $\chi^2(4) = 73.098$, $p < .001$, indicated differences in how the community rated the value of attending seminars for people in different positions with a moderate Kendall’s W effect size of .24. Subsequently, post hoc Dunn-Bonferroni pairwise comparisons (**Appendix F**) indicated that the community felt that seminars were less valuable for undergraduate students compared to others ($p_{adj} < .005$ for all four Undergraduate pairwise comparisons). This could provide an alternative narrative about the value of departmental seminars in contrast to literature who shows that attending conferences is valuable for undergraduates.

Table 6.I.2. Perceived value of seminars for [Role].

For [Role] ^a	Median	Mean	Std. Dev.
Undergraduates	4	4.49	1.709
Graduate Students (year 1)	6	5.42	1.543
Graduate Students (years 2+)	6	5.66	1.150
Postdocs	6	5.76	1.130
Faculty	6	5.68	1.298

^a76 of 78 cases

^ball item responses on a 1 to 7 ordinal positive agreement response format (i.e., “not at all valuable” to “extremely valuable”)

6.I.19 Perceived Value by Roles

A related question was whether people from different Role groups rated Value differently. Visual analysis of the Value rating means via a clustered horizontal bar chart, split by respondent Role group,

suggested that upper-level graduate students may have been more negative in general (**Figure 6.I.4**). A series of Kruskal-Wallis H tests (**Appendix F**) found a statistically significant difference in the Value ratings among groups for the Role group Graduate Student (years 2+), $\chi^2(4) = 9.610$, $p = .048$ with a moderate effect size of $\eta^2[H] = .079$. However, subsequent post hoc Dunn-Bonferroni tests failed to yield significant pairwise comparisons (not shown; $p > .05$ for all comparisons). The lack of post hoc significance suggests that the Role groups did not statistically significantly differ in how they rated Value, despite the Kruskal-Wallis significance. Therefore, the null hypothesis was not rejected, concluding that the community members held similar opinions as each other about the value of attending seminars.

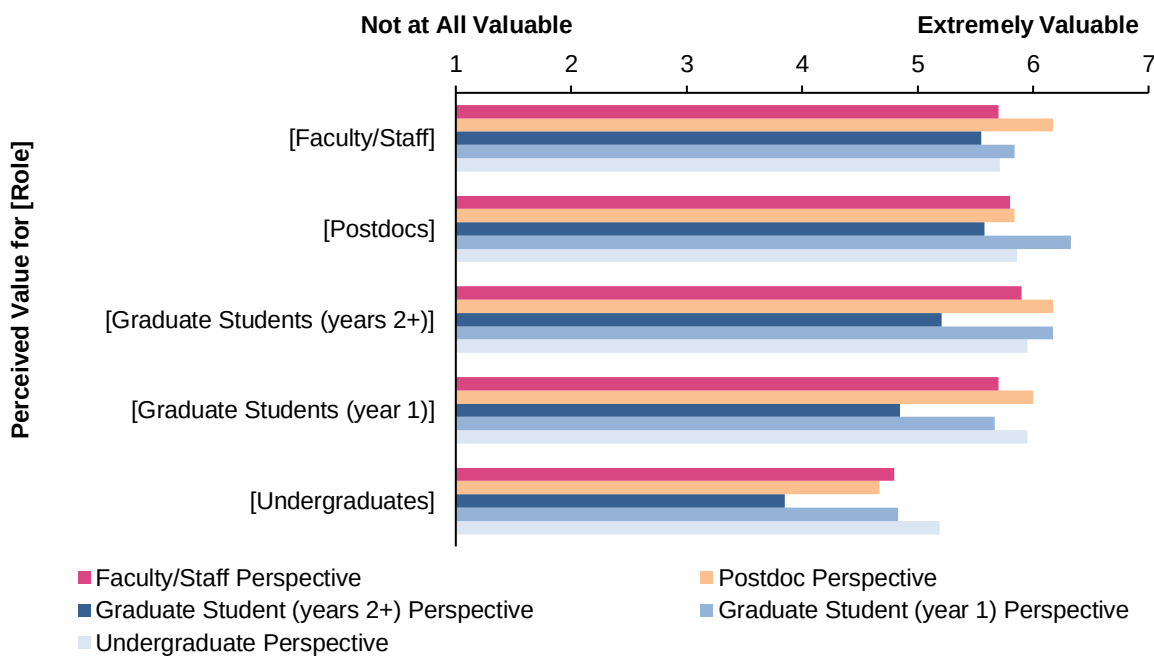


Figure 6.I.4. Average Value scores for [Role] as perceived by the respondents in each Role group.

6.I.20 Perceived Impact by Items

In conversations with students and faculty before this study began, several themes recurred regarding how people explained the value of attending a seminar. These themes were combined with related literature to write items which might hypothetically be impacted by attending seminars (**Table 6.I.3**). At the end of the survey, respondents rated how important seminars are for improving each item. Item “Awareness” was rated the highest whereas items “Confidence” and “Identity” tied as the lowest. Note that,

for Awareness, most respondents selected the highest rating possible. With a wider response format, even greater differentiation may have manifested between Awareness and the other items.

Table 6.I.3. Perceived improvement of respondent's own _____ from attending seminars.

Tier ^a	Item ^b	Label	Median ^c	Mean	Std. Dev.
Highest	Awareness of the broader scientific / research community	Awareness	7 ^d	6.13	1.189
Middle	Ability to form new ideas for projects	Ideating	5	5.15	1.531
	Interest in research	Research	5	5.15	1.850
	Communication / presentation skills	Communicating	5	5.00	1.507
	Career / education interests	Career	5	4.99	1.689
	Social connections / networking	Networking	5	4.84	1.534
	Enthusiasm about chemistry	Enthusiasm	5	4.84	1.860
	Ability to critically evaluate another's work	Evaluating	5	4.83	1.663
	Technical / content knowledge	Knowledge	5	4.61	1.723
Lowest	Self-identity as a chemist	Identity	4	3.67	1.735
	Self-confidence as a chemist	Confidence	4	3.67	1.803

^astatistically significant differences between the 3 levels but not within each level; items organized by descending mean

^b75 of 78 cases

^call item responses on a 1 to 7 ordinal positive agreement response format (i.e., "not at all important" to "extremely important")

^dmaximum rating possible

A Friedman test demonstrated significant differences among the impact items' ratings, $\chi^2(10) = 217.274$, $p < .0005$ with a moderate Kendall's W effect size of .29. Post hoc Dunn-Bonferroni tests (**Appendix F**) illuminated the significant pairwise comparisons, leading to a 3-tier hierarchy. It is interesting that Confidence and Identity place in the lowest tier when they are frequently mentioned for why undergraduates should attend conferences. The results appear to suggest that seminars play a different role than conferences do.

6.I.21 Perceived Impact by Roles

Kruskal-Wallis tests investigated whether Role groups gave significantly different ratings for the impact items (**Appendix F**). Two tests were significant: Confidence ($\chi^2(4) = 15.295$, $p = .004$, effect size $\eta^2[H] = .16$) and Identity ($\chi^2(4) = 18.209$, $p = .001$, $\eta^2[H] = .21$). However, despite these large effect sizes,

subsequent post hoc Dunn-Bonferroni pairwise comparisons (**Appendix F**) for Confidence and Identity revealed only a few differences between Roles: Confidence from Graduate Student (years 2+) vs. Undergraduate ($p = .014$) and Identity from Graduate Student (years 2+) vs. Undergraduate ($p = .008$) and Postdoc ($p = .042$). In other words, upper-level graduate students reported lower improvement of their self-confidence and scientific identity than the undergraduate students and postdocs reported (**Table 6.1.4**).

Table 6.1.4. Significant perceived improvement in own confidence and identity for [Role].

[Role Group] Rating Improvement of Own [Confidence/Identity] ^a	N ^b	Confidence Median	Confidence Mean	Identity Median	Identity Mean
Undergraduates	21	4	4.48	4	4.38
Graduate Students (years 2+)	33	3	2.85	3	2.82
Postdocs	5			5	5.00

^aonly significant comparisons ($p_{adj} = .014, .008, \text{ and } .042$) shown; nonsignificant comparisons excluded
^b75 of 78 cases

By this point, it was surprising to not see more significant differences arise between the novice and expert groups; it was presumed that faculty would rate some items differently than undergraduates, for example. However, since the Role groups are smaller subsamples, significance may be attained for some nonsignificant comparisons if conducted with larger sample sizes in future studies. Additionally, Dunn-Bonferroni corrections can be criticized as overly conservative and may be masking significant results for the sake of mitigating Type I error.³⁸²

6.1.22 Qualitative Perceptions

Since the 11 impact items stemmed from literature about conferences and seminar-like experiences, important features about attending seminars could be missing from the quantitative data. Therefore, respondents were asked three free-response questions about what they believe is and is not valuable about attending seminars as well as suggestions for improving the experience. The free-response questions were shown after respondents rated perceived value but before the impact items to avoid cuing the respondents. The responses largely mirrored the quantitative data and added some additional perspectives. Major takeaways are highlighted below.

6.1.23 Valuable and Nonvaluable Components

Thematic analysis yielded strong consensus from 48 respondents that improving one's awareness of developments in the field is an important outcome of attending seminars. Many respondents explicitly mentioned learning about fields outside their specialty (28 of the 48):

Undergraduate: If the topic is not exactly within my field, that's the best.

Faculty / Staff: Seeing the latest research in the field, getting a better understanding of related or peripheral fields, better understanding the contextualization of a given area or field [is valuable].

Networking (18 respondents), observing presentation styles (15), generating new ideas (15), and gaining insights into the research process (14) were the next most common themes about what makes attending seminars valuable. Respondents articulated not only the importance of networking with speakers and attendees but also learning whether certain institutions, fields, or careers would be good fits for them. Several people stated that attendance improves their technical knowledge (7), but more people complained that seminars can be difficult to comprehend (24) and too focused on the “nitty-gritty” (11):

Graduate Student (years 2+): I think in general as a scientific community we need to be more comfortable presenting at a lower (i.e. first year graduate student level). Like I understand my field, but I feel like as soon as I attend a talk even one bit removed from my area of research, there is a tendency to me to get lost in the weeds.

Faculty/Staff: Even for a faculty member when the presenter goes too quickly or doesn't give even a bit of background I will struggle to follow along.

Speakers' poor presentation skills (9 respondents) and lack of connection to the “big picture” (5) also induced frustration. Some respondents resented feeling required to attend seminars irrelevant to their research (11) or when they felt their time could have been better spent elsewhere (8):

Faculty / Staff: I also have to go to a certain number of seminars for departmental service reasons (my colleague invited someone, tenure talk, etc.), and when it's outside my interests, I often come away with little benefit.

A few respondents also specified interpersonal issues such as a distaste for people who make Q&A sessions inhospitable: “faculty bickering or asking gotcha questions” (Graduate Student, years 2+). A few respondents noted how a seminar could show them how *not* to behave: “learn how to (and how not to) ask questions by watching others; learn how to (and how not to) present research...” (Undergraduate).

Overall, suggestions for improving the experience revolved around fixing issues stated in the above paragraphs or reflecting on the earlier contextual data by suggesting that speakers / departments / groups should facilitate learning by distributing notes (7 respondents), prepping students before a seminar (6), or holding debriefs afterward (6). Most suggestions were compatible, but a few respondents wanted presenters to focus more on technical details (4), a key complaint against seminars. Notably, several respondents indicated that they could not think of anything that detracts value from a seminar (5).

6.1.24 Additional Perspectives

Finally, respondents were offered additional space at the end of the survey to supply additional perspectives, such as a couple faculty / staff who discussed problems with overscheduling:

Faculty / Staff: At [institution name] we have way too many seminars, so the audiences are usually small. This gives a bad overall feel to the experience and emphasizes the divergent interests of our units.

Another respondent raised their desire to see more student-selected seminars and networking:

Graduate Student (years 2+): I think the [student-selected seminar series] in particular are an excellent way to engage students... I was much more engaged in lectures when I was meeting with the speaker for either lunch or dinner (as a bit of accountability, to make sure I had something to discuss with them, and also because it was easier to connect with them as people).

However, a different respondent described how attending seminars makes them feel like they do not belong in research:

Graduate Student (years 2+): Attending research talks can actually be very damaging to one's self-confidence as a chemist; whether the audience (typically faculty) create a hostile environment for the speaker, or if the presentation is simply too specific/poorly done to be followed by anyone outside of the field, attending research talks often makes me feel like I am not cut out for research.

A respondent also portrayed seminars as an integral component of science:

Undergraduate: What does it mean to be a scientific community if there isn't going to be lively discussion of research and interdisciplinary dialogue? What is science without research talks? Like honestly, what is it? Pieces of paper with data that get published, and people who individually and separately collect that data? That doesn't constitute "science" for me, no.

Similarly, a respondent shared how a seminar fueled their own work:

Graduate Student (years 2+): One of my papers came out of my advisor saying 'hey can we do something kinda like what that seminar speaker did?' to which I said 'maybe, but I'm not quite sure and would never think about doing it and probably not spend that much time on it unless I'm unexpectedly kicked out of lab for several months but we know that is never going to happen'. Ended up being a pretty important paper if I do say so myself. (n.b., Student is referring to how the COVID-19 pandemic shut down university research labs.).

6.1.25 Discussion and Implications

This paper explored practices and beliefs regarding seminars within one R1 chemistry department. Overall, the data asserts that there was perceived value for attending seminars while also highlighting areas that respondents felt should be improved to maximize the benefits. When reflecting on their practices, most people felt encouraged to attend seminars but not officially required. Student mentors did not expect mentees to attend seminars or had low expectations for what mentees should learn. Group members overall might be attending seminars less frequently than PIs expect, although this cannot be conclusively determined without matched responses. Qualitative data indicates that some respondents (from students to faculty) may feel obligated to attend seminars which offer minimal value for them and that too many seminars are offered in general. Additionally, the community reported minimal support for facilitating seminar-based learning. When support was provided, the PI and senior group members were often involved. ZPD theory would suggest that increasing scaffolding from these experts could help novices extract greater value from seminars.

When reflecting on their beliefs, the community believed that attending seminars was valuable for everyone but less so for undergraduates. Regardless of the differences in their experience levels, novices

and experts were similar in how they viewed seminars. However, upper-level graduate students might feel more negatively about the impact on self-confidence and self-identity than other groups. Seminars were highly valued for helping attendees stay aware of field developments, including those outside the attendee's area of expertise. Similarly, frustration with overly detailed technical presentations suggests that seminar speakers should prioritize broad strokes of research agendas and emphasize the "big picture". Respondents also valued networking and the impact on their own project ideas, presentation skills, and insights into the research process. A desire for better presentation skills from speakers, greater comprehensibility for non-specialist attendees, the use of structured learning activities, and positive interactions also featured markedly.

Interestingly, several respondents appeared either unaware of or did not agree with key complaints. For example, a few people felt that seminars should focus more on technical details, but more people wanted less technicality. Several respondents also stated that there was nothing detracting from seminars. While the data did support that seminars were considered valuable, aligning seminars with respondents' common suggestions could improve acculturation and knowledge/skill development. For example, Confidence and Identity were the lowest rated impact items, but perhaps better presentations, moderated Q&A sessions with positive socialization, and more support would booster the affective domain. Since conferences often support positive affective experiences for undergraduates,^{366–372} this discrepancy suggests that seminars may differ from how conferences contribute to positive acculturation into a disciplinary culture.

Finally, a few excerpts point to potential difficulties that may be encountered in enacting reforms of seminars. Firstly, some people might not believe that reforms are advisable due to their belief that there is nothing nonvaluable about attending seminars: "It's a win-win. Nothing not valuable." (*Graduate Student, year 1*). Other people may believe that responsibility for extracting value lies solely with the attendee: "I think of the value of my attending a research presentation for me to be my responsibility: I can look up the speaker, read their publications, ask any mentors or teachers for more information." (*Undergraduate*). On the other hand, a respondent stated that other people obtain more value out of seminars than they do themselves, indicating that people can falsely assume that their complaints are not shared: "[It is not valuable to have] Very technical details about methodology for those talks about very interesting topics outside my

direct line of work. Of course, that is valuable for other people in the audience, so I can't fairly complain." (*Graduate Student, years 2+*). Similarly, people can downplay their criticisms by assuming that the traditional format is appropriate: "The biggest problem is the lack of interaction, which makes the presentation feel like it drags on. I don't think this is really a fair criticism since the point of a research talk is to just talk about your research, but that's the biggest reason why I don't enjoy them so much." (*Graduate Student, year 1*). Not only might reforms be opposed by some people due to perceptions that no issues exist, others may not believe their own criticisms possess merit because they do not think their opinions are shared by others or valid. A similar reflection was shared by Busby and Harshman in their interviews with four chemistry graduate students (ref 375, p. 356):

Colloquium, despite being commonly described as boring and / or overly complex, was still seen as a benefit for those participants with faith in the system. They felt that invited speakers must be good examples of presenters because they were prominent people who came from prestigious universities. Similarly, there was recognition that professors in the audience were able to ask questions despite the topic of the presentation because they were experts, and that this was something that the students should strive for...

Even though the students in the Busby and Harshman study felt frustrated with seminars later, saying that reading the paper would accomplish the same goals or that attending is minimally valuable after learning how to present and use scientific language, the students' assumptions that seminars and speakers must be good since they were selected by more knowledgeable people emphasizes how junior members of a community might defer to senior members.

6.1.26 Limitations

This data reflects one department at a more selective R1 institution and may not represent other institutions. Also, the sample could potentially skew toward the champions of seminars or their detractors; the unimodal distributions of data, however, suggest that this was unlikely. Unfortunately, many people skipped the free-response questions: 14 % skipped all three whereas 17 % skipped one or two. However, a Kruskal-Wallis test for the Value ratings of the all-skipped, partially-skipped, and all-answered

respondents' own Role groups failed to detect a significant difference, $\chi^2(2) = 4.658$, $p = .097$, indicating that the qualitative data was not skewed toward unrepresentative respondents.

The use of Role groups with small subsamples and Dunn-Bonferroni post hoc tests may mean that some nonsignificant results would reach significance under more favorable conditions such as larger samples. While the Dunn-Bonferroni correction can be overly conservative in reducing Type I errors (thereby inducing Type II errors), it was selected to compensate for false positives that could arise from small subsamples. p -values with small subsamples should be considered cautiously. Additionally, criterion validity of the instrument was not established nor was response process; subject area experts, prior literature, and generative free-responses served as alternative validation checks.

Notably, this study does not ascertain whether, after attending a seminar, an attendee actually evaluates the experience based on the items presented here; it is uncertain whether seminars do indeed provide the perceived benefits. This study also investigated neither the associated networking nor the value for the speaker in presenting. Additionally, while avenues for scaffolding were proposed (e.g., debriefs afterward), there was no indication whether one type is most advisable. It would be interesting to compare the value of attending seminars to other activities such as reading literature. Finally, a few qualitative responses indicate that some respondents assumed that other people found seminars more valuable than they themselves did; their quantitative responses may therefore inaccurately reflect their own opinions and, instead, follow a social desirability effect.

6.1.27 Conclusion

This study used a short, cross-sectional, intergenerational mixed-methods survey to capture beliefs about attending seminars in an R1 chemistry department, from undergraduate students to faculty. With the goal of inspiring future research and community dialogue, several areas were identified for how seminars are (or are not) valuable for attendees. Future research should continue to consider the experiences and needs of people at different educational stages within a community.

Part II: Factors Predicting the Perceived Value of Remote Seminar Talks in an R1 Chemistry Department

6.II.1 Abstract

Seminar talks are a long-standing tradition in chemistry departments and are believed to play a key role in disseminating research results, kickstarting innovative ideas, and brokering professional connections. However, despite these anecdotal attributes, the seminar's role in promoting these benefits is underinvestigated empirically. Recent work in Part I revealing a potential social desirability bias in how some people view seminars underscores the need to better elucidate how the chemistry community experiences this widespread scientific activity. Greater clarity regarding a seminar's impact on attendees could enable institutions to optimize this learning environment. Therefore, this paper reports characteristics which predict whether a departmental seminar talk was reported as having been valuable to attendees.



Figure 6.II.1. Perceptions of the value of seminar talks may be subject to social desirability bias and may actually hinge upon only two of five recognized factors.

6.II.2 Introduction

In 2008, the American Chemical Society discovered 96 % of PhD-granting chemistry departments host colloquia.³⁶⁵ This high prevalence reflects the historical robustness of the tradition: the earliest reports about seminars in the *Journal of Chemical Education* trace back almost 100 years.^{364,366,383} Likewise, accounts from other disciplines reiterate the widespread nature of colloquia / seminars (two phrases which are often used interchangeably).^{374,384} Prior work has shown that seminars and conferences are appreciated for helping attendees learn about new developments, cultivate new ideas, and network, among other benefits.^{364,366–372,374} Such findings support the continued investment of resources into these events.

However, the recent work from Part I has also highlighted that a social desirability bias may manifest in how individuals perceive the value of attending a seminar, leading individuals to downplay their personal criticisms of norms associated with some seminar series.³⁷⁵ Unfortunately, a social desirability bias could cloud institutions' understanding of the role that seminars play in the continuing development of department members.³⁸⁵ Understanding clearly how individuals experience seminars could enable optimization of these experiences. For example, uncovering low-impact or negative aspects of seminars could provide a roadmap for improving the positive impact of talks.

Concurrently, literature asserts the need for the scientific community to improve communication skills, positive climates, and graduate education.^{88,311,376,377,386,387} How should seminars factor into conversations about institutional reform, scientific communication skills, challenges with graduate education, or chilly department climates? Considering the prevalence of seminars in the academic ecosystem and exposure potential across educational levels (from student to faculty audiences), the seminar's role in the macrocosm of learning and professional development could be deliberately leveraged to address contemporary issues.

Therefore, to better understand how seminars contribute to attendees' development, this paper investigates how individuals in an R1 chemistry department experienced seminars. The study was conducted with an eye toward minimizing social desirability bias. Factors were uncovered which predicted whether an attendee reported a seminar as a valuable experience. These factors were then contrasted with how the department expected seminars to be beneficial. The results clarify the types of impact that seminars have on attendees and how these experiences compare to general perceptions.

6.II.3 Methods

The primary goal of this study was to determine which characteristics predict whether a departmental chemistry seminar talk is rated by attendees as being a valuable experience.

6.II.4 Research Question

The research question was “What makes a seminar a valuable (or not a valuable) experience for attendees?”. In light of a potential social desirability bias from Part I, note that the seminars investigated here were exclusively remote, thus maximizing independence of participants’ observations. This compromise notably induces a trade-off in the types of value maximally derivable from in-person vs. remote experiences. For example, networking options were more limited due to the remote format.

6.II.5 Frameworks

Prior literature about conferences and seminars suggested that the goals of attending events such as seminars could be viewed as (1) improving knowledge / skills and (2) participating in a disciplinary culture.^{366–372,374} Using a bespoke conceptual framework dubbed and in Part I as “Speaker-as-a-Guide”,¹⁶¹ the two theoretical frameworks of Vygotsky’s Zone of Proximal Development (ZPD) and acculturation theory were used to explore beliefs about the value of attending a departmental seminar. ZPD asserts that attendees improve their knowledge and skills with the assistance of the speaker as a “more expert other”.³⁷⁸ Acculturation theory helps describe how attendees transition from being a member of the general public into a member of the academic field.³⁷⁹ The recent prior study supported the theoretical validity of these frameworks for this context and sample while revealing the possibility of a social desirability effect.

Therefore, this paper builds on the prior work to evaluate how seminars function to promote learning and disciplinary belonging in line with these same frameworks. However, this time, the data collection from this article was explicitly paired with specific seminars while utilizing a remote environment to help control for desirability bias. The paired aspect of this work contrasts with the prior work’s collection of general, holistic perceptions of seminars as a whole.

6.II.6 Survey and Validity

Use in Part I: The survey was a modified version of a short cross-sectional, multi-generational survey previously used with this sample department (**Appendix F**). That survey drew from literature about the impact of conference attendance on undergraduate students (as seen through the lenses of the ZPD and acculturation) and featured a concise collection of both Likert ratings and free-response questions. The Likert ratings asked respondents to reflect on seminars' impacts on an attendee's knowledge, skills, and feelings of belonging in science. The free-response questions asked respondents to generatively write about what makes a seminar a valuable or nonvaluable experience. The brevity of the 5-10-minute survey was anticipated to be crucial to encourage participation across the education spectrum (i.e., from students to faculty). Since it seemed reasonable that novices and experts would perceive seminars differently, the survey traded comprehensiveness for brevity to prioritize the ability to compare groups by collecting adequate subsample sizes. In addition to its literature base, the survey content validity and face validity were also supported using feedback from chemistry faculty and staff as content area experts. Respondents in the prior study also provided triangulating data via the qualitative free-response questions which supported the content validity of the quantitative items.

Use in Part II: The survey was here revised to remove existing free-response questions, focus on the most relevant questions by trimming less relevant items, and add additional quantitative items for evaluating characteristics specific to each seminar (e.g., the content of the talk; the speaker's communication skills). Some of the original positively-worded response labels were adjusted to reflect different types of impact, such as negative impact (e.g., decrease in self-confidence). Additionally, a few short optional free-response questions were added to gather preliminary data for future work and not discussed further here.

Subsequent factor analysis revealed pertinent internal structure validity data. Finally, whereas the prior study asked respondents to report their beliefs about seminars in general, this survey evaluated perceptions of a seminar shortly after the talk concluded, thus capturing more authentic, immediate reactions. Separately, the speakers themselves wrote short descriptions of the anticipated impact of the talk on attendees within a week before the seminar, separately from the survey to attendees.

6.II.7 Ethics

The author's IRB office determined this study to be exempt. The chair of the sample department approved recruitment. Each participating speaker approved recruitment at their talk with the understanding that the study was not an evaluation of them; this non-evaluative message was also delivered to the department's faculty and students at the study's commencement and during each recruitment cycle. Participants completed online consent forms before viewing the anonymous survey (attendees) / before writing the description (speakers). The institution is not identified by name.

6.II.8 Data Collection

In the spring of 2021, the department's seminars were remote via Zoom due to the COVID-19 pandemic. The department hosted a formal, traditional seminar(s) most weeks, both before and during the pandemic. Speakers were usually external to the department and invited to lecture about their recent research by either the faculty as a whole, by the initiative of individual faculty or specialty subgroups, or by student vote. Permission was granted to recruit at 9 of the spring seminars, roughly half of the advertised seminars. All participating seminars were hosted by the chemistry department.

The Qualtrics survey was announced at the beginning of each seminar, and the link was posted in the chat box at the end. The survey took approximately 5 minutes. Additionally, attendees were emailed the link within 1 – 2 days afterward. Most of the attendees' institutional email addresses were saved by Zoom to the seminar host's account and provided to the author for recruitment and descriptive analysis before deletion (n.b., personal identifiers were not linked to surveys). Emails missing from the Zoom report were often discoverable by searching publicly accessible websites using an attendee's name. An average 91.1 % of attendees at each seminar were recruitable via email (**Appendix F**).

The seminar speakers also wrote a few descriptive sentences to the author approximately a week before the seminar to state what they hoped attendees would gain from their presentation. Finally, the seminars themselves were observed to capture descriptive data (e.g., audience size, duration).

6.II.9 Data Processing

8 of the 9 speakers submitted descriptive statements which underwent iterative inductive coding with thematic analysis. The emergent codes were categorized hierarchically to indicate what the speaker's expectations were for how their seminar talk would impact the attendees.

Consent for 104 responses was logged for the survey. After removing 12 blank responses (all abandoned immediately after granting consent), 92 were retained. The remaining responses contained almost complete Likert data with the free-response and demographic questions occasionally skipped. Based on the observed audiences, 23.5 % of the audiences across all seminars submitted responses retained for analysis (n.b., 23.5 % of the *audience* sizes – percentage of total *attendees* cannot be calculated since audiences contained duplicate attendees who were present at other seminars).

Since Zoom logs individuals iteratively if their internet cuts out, the attendance spreadsheets were evaluated to eliminate duplicates within each seminar and to remove in-and-out attendees who departed after fewer than 5 minutes. This trimming enabled accurate audience size calculations and avoided redundancies in survey recruitment via email. Attendees who stayed for longer than a few minutes typically remained for a substantial portion of the talk and so were recruited even if they were late or left early.

Quantitative data was analyzed using Microsoft Excel or IBM SPSS 28.0.1.1. A critical value of $p = .05$ was used for significance tests except where noted.

6.II.10 Sampling Methodology

This study focused on remote seminars at one R1 chemistry department in the United States during the spring of 2021. Purposeful sampling was employed to target a chemistry department which offered (1) many seminars to recruit, (2) many potential participants from each level of the education spectrum (i.e., large faculty, postdoc, graduate, and undergraduate student bodies), and (3) remote seminars, thus reducing the potential for attendees' body language or conversations to influence others' perceptions.¹³⁵ Convenience sampling was employed in that the seminars were recruited regardless of subdiscipline, topic, etc.

6.II.11 Institution

The university was a large, majority graduate institution with very high doctoral research activity and an undergraduate profile listed as more selective.¹⁶⁵ Since seminar practices vary across institutions, the department is the same as the one in the prior study from Part I, thus enabling comparison.

6.II.12 Seminars

4 of the 9 participating seminars were on physical chemistry, 3 on organometallic / inorganic chemistry, 1 biochemistry, and 1 materials science. 5 of the speakers were faculty. 4 were either PhD candidates near their defense or postdoctoral researchers. The speakers were all from R1 academic institutions and mostly based in the United States, although a couple were based in other countries.

Seminar talks were 49 minutes on average, excluding introductions and Q&A sessions. 82.1 % of attendees were present at the start of the seminar and 87.8 % at the end. These high percentages indicated that most people were present for the entirety of each talk, despite occasional internet connectivity issues, early departures, and late arrivals. Each talk was followed immediately by a Q&A session which featured an average of 3.3 questions, spread across 2 different undergraduates, 7 graduate students, 2 postdocs, and 11 faculty / staff out of 274 total attendees. 73.0 % of attendees were present throughout the Q&A sessions. The speaker sometimes then left for a remote social event with selected individuals (and / or engaged in social activities before the seminar).

6.II.13 Attendees

The cumulative estimated audience size across all 9 seminars was 392 (excluding people who departed within 5 minutes), generating an average audience size of 44 attendees / seminar. This number is estimated since there was no way to know if individuals used different email addresses or profile nicknames across seminars, whether they were actually in attendance (versus leaving the meeting unattended on their computer), or whether multiple people were watching on the same screen. The logged attendees were mostly upper-level students and professional researchers (**Appendix F**), although one seminar had many undergraduate students due to targeted advertising.

An estimated 274 attendees were unique, meaning that 30.1 % of the audience sizes were comprised of people attending multiple seminars. Since attendees submitted survey responses for separate seminars, the use of repeat attendees was deemed acceptable for this study. After accounting for duplicates, 15.0 % of attendees were undergraduate students, 43.8 % graduate students, 17.2 % postdocs, and 15.0 % faculty / staff. Roles for 9.1 % were nonidentifiable. Since the seminars were remote and open to the public, some attendees were not officially in the department (e.g., recent PhD graduates in postdoctoral roles at other institutions; non-major undergraduate research students). 75.5 % of the attendees (duplicates accounted for) were identified based on their email address domains as being a member of the university whereas 16.1 % used domains from other institutions. Affiliations for 8.4 % were nonidentifiable (e.g., generic domain; undiscoverable emails).

Of the institutionally affiliated attendees, 18.8 % were undergraduates, 45.4 % graduate students, 20.3 % postdocs, and 14.5 % faculty / staff. Based on administrative data (not shown), these percentages mirrored the department's own relative compositions moderately well but with lower percentages of undergraduates and graduate students in attendance and higher percentages of postdocs and faculty. A substantial portion of the department attended at least one of the 9 seminars, but the seminars attracted postdocs and faculty / staff disproportionately. For example, 38.4 % of the department's graduate students attended at least one of the seminars compared to 63.6 % of the postdocs.

6.II.14 Respondents

Since the survey was administered at multiple seminars and 30.1 % of the audiences were duplicate attendees, it is likely that some people submitted multiple surveys. Therefore, the 92 survey responses likely reflect fewer than 92 people. 57.6 % of the retained responses came from people who identified as being from the university's chemistry department and 17.4 % from a different chemistry department, indicating that the sample should be representative of a chemistry community (16.3 % did not answer). Additionally, 17.4 % of the responses were from undergraduates, 58.7 % graduate students, 16.3 % postdoctoral researchers, and 7.6 % faculty / staff. Additional data indicates an even distribution of common demographic metrics among respondents: 38.0 % responses were from females, 41.3 % males, and 3.3 %

other (17.4 % did not answer). 48.9 % were from domestic students / researchers and 33.7 % from international (17.4 % did not answer).

Finally, respondents identified whether their attendance was mandatory or voluntary to gauge potential affective predispositions. 3.3 % of responses were from people who were attending the seminar because they felt required to. However, 59.8 % were from those who had been actively encouraged to attend while 37.0 % attended purely on their own initiative. These breakdowns indicated that most respondents were likely positively predisposed toward the seminars.

6.II.15 Data Analysis Overview

The Likert items constituted the backbone of the analysis. First, the items were analyzed to visualize how respondents characterized their experiences attending seminars. Then, the data was compared to the speakers' expectations. Afterward, the data was processed further to generate a model for the relationship between impact and perceptions of value.

6.II.16 Attendee Perspective

The attendee respondents reported moderately favorable experiences overall (**Tables 6.II.1** and **6.II.2**). They felt that the seminars were valuable uses of their time, being both relevant and understandable (**Table 6.II.1**). Respondents reported moderately positive feelings about the quality of the research itself and the speakers' communication skills. While it is important to remember that attendees were likely positively predisposed given attendance was mostly self-driven, the items' histograms (not shown) displayed unimodal normality, standard deviations remained in the positive range, and the skews and kurtoses were almost all within accepted normality ranges. The noted exception was the item "Language" which displayed a high mean with a low standard deviation, was substantially skewed left, and manifested similarly across seminars, indicating that respondents did not register substantial language barriers in comprehending the speakers.

Table 6.II.1. Perceived characteristics of seminars.

Item	Label	N ^a	Median	Mean ^b	Std. Dev.	
(-6) <i>Very negative</i> ----- <i>Very positive</i> (+6)						
Positive or negative experience overall for you	Positive	92	4	3.54	2.078	
			0	+2	+4	+6
(0) <i>Not at all</i> ----- <i>Extremely</i> (+6)						
Valuable experience overall for you	Valuable	92	4	4.27	1.276	
Worthwhile experience overall for you	Worthwhile	92	5	4.59	1.259	
How much the presentation related to your area(s) of research	Relevant	92	4	3.64	1.559	
How much you conceptually understood the presentation	Understood	92	5	4.34	1.328	
How much you linguistically understood the presenter (for example, no language barriers) ^e	Language	92	6	5.57 ^d	0.684	
			0	+2	+4	+6
(-6) <i>Poor</i> ----- <i>Excellent</i> (+6)						
The “novelty” of the work	Novel	91	4	4.02	1.874	
The “impactfulness” of the work	Impactful	91	4	3.60	2.154	
The presenter’s communication skills	Presenter	92	4	4.13	2.254	
The professionalism and attractiveness of the slides	Slides	90	4	4.07 ^e	2.171	
			0	+2	+4	+6

^a92 cases from 9 seminars; missing data excluded pairwise; 89 cases contained complete data for all items in **Tables 6.II.1** and **6.II.2**

^bAll item responses originally rated by respondents on a 1 to 7 ordinal positive agreement response format before being transformed to make visualizations intuitive and zeroed for the reader (e.g., “not at all worthwhile, 1” to “extremely worthwhile, 7” → “not at all worthwhile, 0” to “extremely worthwhile, 7”; “significantly worsened, 1” to “significantly improved, 7” → “significantly worsened, -6” to “significantly improved, +6”); graphs illustrate transformed means and standard deviation bars; all skews within ± 1 and kurtosis ± 2 except where noted

^cIncluded to ensure that native language differences did not impair comprehension

^dSkew of -1.713 and kurtosis of 3.077

^eSkew of -1.213

However, while respondents reflected favorably on the characteristics of the seminars, they were not as positive in their evaluation of how the seminar impacted themselves (**Table 6.II.2**). They reported that the experience somewhat to moderately improved their own knowledge and skills and somewhat impacted their interests. However, many people felt that the seminars either did not contribute to any improvement in their disciplinary belonging or actually caused harm (e.g., damaging their self-confidence for which the standard deviation extends into the negative range). The contrast between the various items in tandem with the perceived value of the seminars appears to indicate that items possessed different weights in the respondents' determinations of what makes a seminar valuable.

Table 6.II.2. Perceived impacts of seminars on respondents.

Item	Label	N ^a	Median	Mean ^b	Std. Dev.			
(0) Not at all improved ----- Extremely improved (+6)								
Technical / content knowledge	Knowledge	92	4	3.57	1.385			
Awareness of the broader scientific / research community	Awareness	92	4	4.30	1.373			
Communication / presentation skills	Communicating	92	3	3.18	1.735			
Ability to critically evaluate another's work	Evaluating	92	3	3.12	1.759			
Ability to develop new project ideas	Ideating	92	4	3.39	1.785			
		0	+2	+4	+6			
(-6) Significantly worsened ----- Significantly improved (+6)								
Social connections / networking	Networking	91	0	0.62	1.993			
Self-confidence as a scientist	Confidence	91	0	0.86	1.958			
Self-identity as a scientist	Identity	91	0	1.23	2.082			
Enthusiasm about science	Enthusiasm	91	2	2.37	2.365			
Interest in research	Research	91	2	2.55	2.212			
		-6	-4	-2	0	+2	+4	+6
(0) Not at all impacted ----- Extremely impacted (+6)								
Career / education interests	Career	91	3	2.40	2.027			
		0	+2	+4	+6			

^a92 cases from 9 seminars; missing data excluded pairwise; 89 cases contained complete data for all items in **Tables 6.II.1** and **6.II.2**

^bAll item responses underwent transformations as described in **Table 6.II.1**; all skews within ± 1 and kurtosis ± 2

Note, while all items on the survey presented 7-point response formats¹⁷⁴ (1 → 7) to respondents (**Appendix F**), they are visualized transformed here for intuitive comparison (i.e., -6 → +6 or 0 → +6). The untransformed data was used in subsequent analyses (e.g., factor analysis).

6.II.17 Speaker Perspective

For general comparison purposes and to supplement the attendees' perspectives, the speakers also provided qualitative snapshots of how they hoped seminars would impact their audience (**Table 6.II.3**). Most speakers aimed for attendees to gain new foundational knowledge ("Conceptual") whereas a couple focused on them learning a new method to use ("Methods"). A few speakers hoped that attendees would leave with new ideas for future work ("Ideas"), questions to ponder ("Questions"), improved communication skills ("Communication"), and / or improved realization of how to manage a team ("Management"). Several speakers expected that their talk would increase interest in the topic ("Interest"). One speaker hoped that their presence would help gender visibility ("Representation"). Most speakers hoped to improve awareness overall of key developments and potential applications in their field ("Field"). One speaker aimed to make attendees aware of their own institution ("Institution"). It is interesting to note that the foci on learning new knowledge, a better awareness of the field, and generating interest in a topic are reflected in the survey data with somewhat to moderately positive responses; the speakers appear to have been at least partially successful in achieving their aims.

Table 6.II.3. Speakers' expectations for impact on attendees.^a

Seminar ID ^b	Technical Knowledge	Ideation	People Skills	Socioemotional Impact	Awareness
	Conceptual Methods	Ideas Questions	Communication Management	Representation Interest	Field Institution
1					
2					
3					
4					
5					
6					
7					
8					
Total	6	2	2	2	1

^aA colored cell indicates that the speaker mentioned the theme as an expectation for what their audience would take away from the seminar.

^bSurvey not completed by speaker 9; seminar IDs organized by chronological order

6.II.18 Factors Characterizing Seminar Experience

Exploratory Factor Analysis (EFA) can be used to discover common factors between items, enabling them to be combined and reduced into their underlying themes for subsequent predictive analyses.^{172,177} After describing the data from the attendees' and speakers' perspectives, EFA reduced the Likert items down to factors characterizing the overall experience.

6.II.19 Assumption Testing for EFA

First, in order to evaluate the suitability of the data for factor analysis, a Pearson r correlation matrix was generated (not shown). The matrix indicated very strong correlations ($r > .8$, $p < .001$) among three items: Positive, Valuable, and Worthwhile, as anticipated. Therefore, they were not included in the factor analysis due to redundancy but instead were averaged into a composite target score of "Perceived Value" for subsequent regressions.

Significant correlations among the remaining items ranged from low to moderate which indicated that the data could be factorable and appropriate for EFA. An exception was Language which displayed low correlations across all items and therefore was removed before EFA. The original purpose of the item was to flag seminars producing invalid data due to language barriers between the speaker and attendees. χ^2 Tests of Independence failed to show statistically significant associations with either Role ($\chi^2(9) = 11.812$, $p = .224$) or Seminar ($\chi^2(24) = 22.674$, $p = .539$) which, combined with a high mean (**Table 6.II.1**), left skew, sharp leptokurtic distribution, and low standard deviation, indicated that language barriers were not presenting barriers for respondents. Therefore, its descriptive statistics and removal before EFA were both encouraging signs that the seminars were linguistically accessible in this multinational sample.

After removing the four items, Kaiser-Meyer-Olkin's Measure of Sampling adequacy was executed to verify sampling adequacy ($KMO = .837$) while Bartlett's Test of Sphericity ($\chi^2(136) = 985.09$, $p < .001$) indicated that correlations between items were sufficiently large for factor analysis.

6.II.20 Exploratory Factor Analysis to Characterize Seminar Experiences

Since the items were expected to represent unobservable latent constructs of learning, belonging, and value, Principal Axis Factoring was selected as the most appropriate EFA method per the common factor

model theory.¹⁷² Since some factors were expected to be correlated, oblique rotation was executed using Direct Oblimin rotation. Therefore, with the data having passed assumptions for normality and factorability, the eigenvalues-of-one condition and scree plot (not shown) were used to discover factors.

Since the number of responses was fewer than 200 (which is frequently invoked for EFA), a factor loading value of .45 was set as a removal condition, constituting a stricter cut-off value than often used.^{172,176,177} After the first EFA with the untransformed Likert data (**Appendix F**), two items (Enthusiasm and Research) were removed since they cross-loaded across 4 of 5 emergent factors. The second EFA yielded a cleaner 5-factor model with factor loadings ranging from |.459| – |.920| and 66.0 % cumulative variance explained (**Table 6.II.4**, color-coded to match **Figure 6.II.3**). The factors appeared reasonable according both to factor loading values and face validity (see **Appendix F** for complete loading values).

Table 6.II.4. Factor loadings^a for Exploratory Factor Analysis.

Item ^b	Knowledge & Skills Impact	Presentation Quality	Socioemotional Impact	Expertise Relevance	Research Quality
Novel					-.920
Impactful					-.645
Relevant				.785	
Understood				.539	
Confidence			.885		
Identity			.709	-.251	-.236
Networking		.243	.576	.268	
Slides		.821			
Presenter		.678			-.252
Evaluating	.894			.202	
Ideating	.819				
Communicating	.747	.202			
Knowledge	.570	.300			
Career	.472		.273		
Awareness	.459	.277			
% of Variance ^c	38.5	9.0	7.8	6.0	4.6

^aPattern matrix from Principal Axis Factoring and Direct Oblimin rotation ($\delta = 0$) with Kaiser normalization converged in 9 iterations; missing data excluded pairwise

^bFor clarity, pattern coefficients less than $\pm .2$ not shown; items organized by descending factor loading value; factor loading cut-off value of .45 for factor inclusion; color-coded to match **Figure 6.II.3**

^c66.0 % cumulative variance accounted for

The factors were then named based on the perceived similarities between their items. Notably, one factor (Knowledge & Skills Impact) aligns well with the ZPD framework while another (Socioemotional

Impact) aligns with acculturation. The remaining three describe characteristics of a seminar itself. Interestingly, the factor Research Quality was inversely related to the others (i.e., as the perceived novelty and impactfulness of the speaker's research increased, all other attributes decreased).

6.II.21 Factor Scores

Next, with both theoretical and statistical soundness established, the raw scores of each retained item passing the cut-off condition were multiplied by the corresponding absolute loading value (**Table 6.II.4**) and summed with the factor's other items to generate a weighted sum score for each factor. This type of "non-refined / coarse method" for estimating factor scores is considered appropriate with (1) simpler factor structures, (2) data that, when on the same response format range, produce similar standard deviations (**Appendix F**), and (3) factors which are not highly correlated, as in this case (see **Appendix F** for factor correlations).¹⁷³ The weighted sum factor scores were then averaged according to their respective total weights (e.g., Presentation Quality weights = .821 + .678 = 1.499) to scale each factor according to its respective summed weight (**Table 6.II.5**). This scaling enables the reader to intuitively compare the factor scores while ensuring that the stronger loading items contribute more to the scores than the weaker.

Table 6.II.5. Descriptive statistics and internal consistency of composite Perceived Value and factor scores.

Factor ^a	# of Items	Scaling Weight ^b	N ^c	Mean	Std. Dev.	Skew	Kurtosis	Cronbach's α ^d
Perceived Value	3	3 items	92	5.54	1.134	-0.569	0.061	.948
Knowledge & Skills Impact	6	3.961	91	4.31	1.374	-0.097	-0.655	.873
Presentation Quality	2	1.499	90	6.06	1.007	-1.007	0.486	.829
Socioemotional Impact	3	2.170	91	4.46	0.858	0.429	2.030	.797
Expertise Relevance	2	1.342	92	4.92	1.299	-0.432	-0.301	.697
Research Quality	2	1.565	91	5.92	0.911	-0.565	-0.428	.800

^aAll factor scores are scaled weighted sums of the items' raw Likert scores (1 → 7 response format)

^bScaled per sum of the factor loadings except for Perceived Value which was averaged across 3 items

^cTotal 92 cases across 9 seminars; missing data excluded pairwise; 89 cases had complete data

^dMissing data excluded pairwise; reliability analyses are for the items' raw Likert scores

The five factors and the composite score for Perceived Value displayed acceptable skewness, kurtoses, and unimodal histograms (not shown) for claiming normality, albeit with some moderate skewness. Internal consistencies ranged from Acceptable-Good to Excellent according to Cronbach's α .¹⁷⁸ The scores were treated as continuous interval data for subsequent significance testing.

6.II.22 Predicting Perceived Value of Attending Seminars

The factor scores were then analyzed alongside the respondents' roles (e.g., undergraduate, postdoc) and the seminar IDs to detect whether patterns existed regarding the experiences (**Figure 6.II.2**).

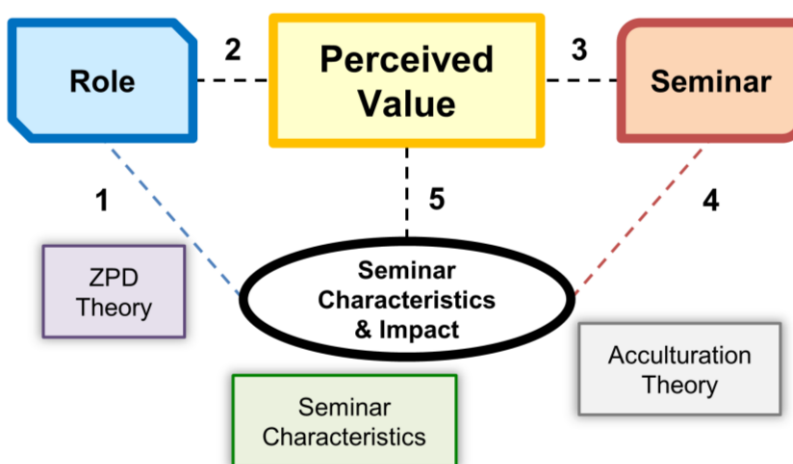


Figure 6.II.2. Major analytical pathways. Significance testing probed whether relationships existed between the Perceived Value of attending a seminar and the characteristics of the experience, the respondents' education level, and / or the individual seminars.

Before evaluating whether the factors predicted Perceived Value (**Figure 6.II.2**, line 5), it was important to test whether the education level of the respondents influenced their perceptions of the seminar experience (line 1) and / or their personal priorities (i.e., how they decided the seminar was valuable or not, line 2). Novices and experts might manifest different perceptions. Concurrently, it was also prudent to test whether respondents viewed the individual seminars differently, in terms of either value (line 3) and / or particular characteristics (line 4). Therefore, Two-Way Multivariate Analysis of the Variance (MANOVA) was selected to analyze paths 1-4 followed by multiple regression for path 5.

6.II.23 Assumption Testing for MANOVA

MANOVA assumptions were first checked in preparation for the procedure. A Pearson's r correlation matrix (not shown) revealed moderate correlations between the factor scores and the Perceived Value composite score, $r = .208 - .601$, $p < .001$ for all (n.b., scaled scores were used throughout the remaining analyses – correlations are unchanged regardless of whether scaled or unscaled scores are used). Next, scatterplots (not shown) supported the presence of linear relationships between variables. Univariate normality was previously described with skew and kurtosis (**Table 6.II.5**). Quartile-Quartile (Q-Q) plots were visually determined to be linear (not shown) for all 6 dependent variables (Perceived Value and the 5 factor scores) per Role and Seminar, suggesting multivariate normality. No multivariate outliers were found per Mahalanobis distances with the commonly-accepted critical value of $\alpha = .001$ for this highly sensitive test ($p > .001$ for $N = 89$ complete entries).¹⁷²

Additionally, since subsample sizes between Role levels and Seminar levels were unequal, Levene's and Box's M tests were executed. Brown & Forsythe's median-based modification to Levene's test was used due to the moderate skew of some of the factor scores. The modified Levene's Test of Equality of Variance failed to find unequal variances between the variables (**Appendix F**) while Box's M Test of Equality of Covariance Matrices failed to find unequal covariance matrices between the variables across groups, Box's $M = 148.161$, $F(63,1930.928) = 148.161$, $p = .010$, indicating homogeneity of variance-covariance matrices (since Box's M is considered highly sensitive, $\alpha = .001$ is often advised¹⁷²).

Finally, although using duplicate respondents could threaten the independence of observations assumption between seminars, respondents would likely have forgotten their prior survey response for a preceding week's seminar. Also, crucially, social desirability bias was mitigated by the study design: participants with videos off in a webinar are unlikely to affect others' responses since they cannot signal opinions. Independence of observation between individuals was therefore deemed adequate.

6.II.24 MANOVA to Probe Effects of Role and Seminar

Two-Way MANOVA proceeded to reveal a nonsignificant interaction between a respondent's education level and the seminar they attended, $F(78, 331.413) = 1.047$, $p = .383$; Wilks' $\lambda = .297$. In other words, perceptions did not vary significantly by Role between Seminars. Note, although Pillai's trace is often

recommended for uneven cell sizes, small sample sizes, and significant Box's M tests, increasing degrees of freedom decreases Pillai's power.¹⁷² Therefore, both Wilks' λ and Pillai's trace are reported in **Appendix F** for transparency, but λ guided significance decisions.

The variable Role was also nonsignificant for how the seminars were perceived, $F(18, 167.362) = 1.292, p = .199$; Wilks' $\lambda = .692$, indicating similar perspectives manifested across the education spectrum. Considering the prior work showing the department believed undergraduates obtain less value from attending seminars than others, a power analysis had been conducted to determine if the sample size would be adequate to detect a significant difference for the Perceived Value means between Role levels. The contraindicated post hoc ANOVA result for Perceived Value in this study exhibited nonsignificance, $F(3, 64) = 1.325, p = .274$. A power of .751 for One-Way ANOVA was approximated based on a hypothetical moderate effect size of $\eta^2 = .1$, $\alpha = .05$, and the subsample sizes for the respondents' Role levels. Therefore, although there was room for nonsignificance arising from an underpowered sample, the nonsignificance seen was more likely believable than not.

Conversely, a significant result for Seminar indicated differences in how the 9 seminars were perceived, $F(48, 294.367) = 1.436, p = .039$; Wilks' $\lambda = .355$. Post hoc ANOVA specified significant differences between seminars for Presentation Quality, $F(8, 64) = 2.481, p = .021$; $\omega^2 = .131$, and Expertise Relevance, $F(8, 64) = 2.219, p = .037$; $\omega^2 = .096$. While η^2 is often reported for ANOVA, ω^2 was computed due to its lower bias for small sample sizes.³⁸⁸ Further post hoc Tukey HSD Multiple Comparisons (not shown) did not continue to identify differences between specific seminars ($p > .05$).

In sum, the large effect size for Presentation Quality and moderate effect size for Expertise Relevance reveal substantial variation in (1) speakers' communication skills and (2) alignment between the seminar topics and the respondents' own backgrounds. Ultimately, however, the specific seminars were not rated significantly differently in either Perceived Value nor the other 3 factors. Meanwhile, it appears that novices and experts alike share similar perspectives when attending seminars.

6.II.25 Assumption Testing for Multiple Linear Regression

Finally, multiple linear regression was executed to evaluate the effect of the seminar experience itself on Perceived Value (**Figure 6.II.2**, line 5). Additional assumptions for multiple regression were checked. Descriptive statistics, visualizations, and correlation coefficients previously described indicated normality, linear relationships between Perceived Value and each factor, and a lack of strong multicollinearity between variables. Additionally, all Variance Inflation Factors (VIF) were below 1.6 for each factor, further rejecting problematic multicollinearity. A linear Predicted-Probability (P-P) plot showed a normal distribution of residuals (not shown) while a shotgun scatterplot of the residuals demonstrated homoscedasticity (not shown). These traits indicated suitability for multiple regression.

6.II.26 Multiple Linear Regression to Probe Effects of Factors

The first multiple regression model significantly predicted Perceived Value, $F(5,83) = 16.544, p < .001$. Within the model, two factors were significant predictors: Presentation Quality ($p < .001$) and Expertise Relevance ($p = .022$). Therefore, the other three factors were removed, and the regression was rerun. The adjusted R^2 of .428 indicates that the final regression model accounted for 42.8 % of the variance in Perceived Value (**Table 6.II.6**). Every scale unit increase for Presentation Quality (Poor, 1 → Excellent, 7) corresponded to a .585 scale unit increase in Perceived Value whereas every scale unit increase for Expertise Relevance (Not at all, 1 → Extremely, 7) corresponded to a .256 unit increase.

Table 6.II.6. Multiple linear regression predicting Perceived Value.

Model Fit	Variable ^b	Unstandardized Coefficient ^a	Standardized Coefficient	p^c
R = .664	Presentation Quality	.585	.520	< .001
R ² = .441	Expertise Relevance	.256	.293	< .001
R _{adj} ² = .428				

^aCoefficients provided for significant variables only
^bMissing data excluded pairwise
^cOne-tailed

6.II.27 Discussion

Seminars are a long-standing tradition in chemistry departments, but they have historically been uninvestigated empirically. Greater clarity regarding the impact on attendees could enable institutions to optimize this learning environment and leverage its attributes in promoting the professional development of students and researchers. Through factor analysis, the seminar experience in an R1 chemistry department was characterized. Significance testing revealed which characteristics contributed significantly to perceptions of whether attending a seminar was valuable.

6.II.28 Implications

When investigating long-cherished practices, it is important to stay aware of pre-existing experiences and potential biases. The popularity of seminars among some is attested to by the duplicate attendees in the audiences: 30.1 % were duplicates. At the same time, the differentiation in audience composition reveals an imbalance in who the seminars were attracting. For example, even though graduate students were the largest attendee population, 38.4 % of the department's graduate students attended at least one of the seminars versus 63.6 % of the postdocs. While this ratio might not be replicated in the non-participating seminars, the discrepancy is intriguing. When combined with the voluntary nature of attendance as well as literature showcasing complaints against seminars, it is natural to wonder whether different perceptions exist between attendees and non-attendees.

Ultimately, Likert data revealed that the respondents viewed the seminars positively overall which, considering their voluntary attendance, is unsurprising. Of greater interest is the variation between items: while respondents rated characteristics highly (e.g., the novelty of the research), the impact items received lower ratings (e.g., impact on career interests). In particular, socioemotional items scored noticeably lower with a substantial portion of responses reflecting a neutral or negative effect. This contrast dovetails with prior reports suggesting seminars may not result in positive affective reactions previously seen in conference attendees or may be accompanied by feelings of frustration.³⁷⁵ This contrast also suggests that, even for enthusiasts, seminars play distinct roles in professional development and that respondents discriminate between different considerations when evaluating the value of the experience. Fortunately,

the speakers would likely be pleased that their major goals for attendees (e.g., learn new knowledge, gain awareness of the field, build interest in the topic) appeared moderately well-achieved.

Factor analysis, MANOVA, and multiple linear regression subsequently revealed that the Likert items represented 5 underlying factors describing the seminar experience, in addition to marking perceptions of overall value. Respondents' education levels did not significantly affect experiences, contradicting Part I's data showing that a chemistry department expects undergraduate students to obtain less value out of a seminar than graduate students, postdocs, and faculty. However, the undergraduate students at these seminars might be unrepresentative of their peers (e.g., perhaps they were engaged in undergraduate research while non-attending undergraduates were not). Finally, only two characteristics functioned as significant predictors of Perceived Value: Expertise Relevance and Presentation Quality (**Figure 6.II.3**). These characteristics also varied among the seminars with moderate to large effect sizes respectively. These results show (1) that the quality of presentation and the seminar's relevance were important predictors of whether respondents felt the seminar was a valuable experience for them and (2) that these attributes did not manifest positively in every seminar talk.

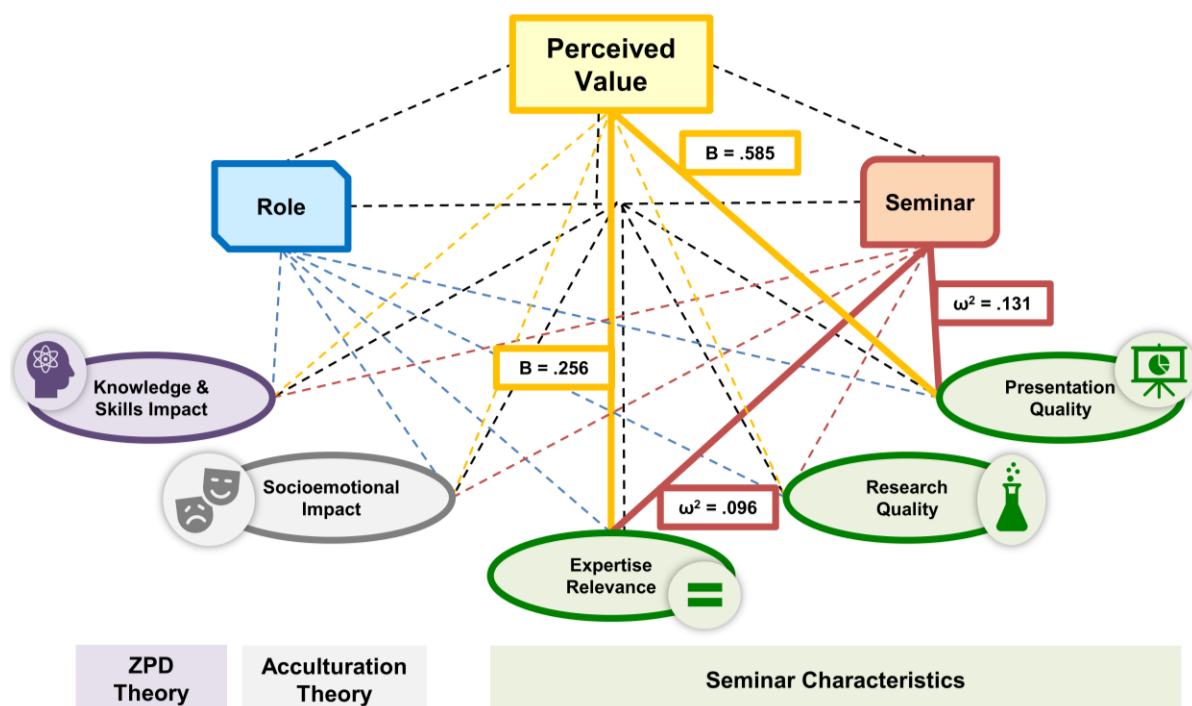


Figure 6.II.3. Four significant effects were discovered via MANOVA (black lines), post hoc ANOVA (blue and red lines), and multiple regression (yellow lines): Perceived Value – Expertise Relevance, Perceived Value – Presentation Quality, Seminar – Expertise Relevance, and Seminar – Presentation Quality. Insignificant effects are denoted with dashed lines and significant effects with solid lines.

Interestingly, the desire for the seminar to be relevant to respondents' own expertise contrasts beliefs previously evinced by the department in Part I. The prior respondents overwhelmingly indicated that seminars are most valuable when they expand attendees' awareness of the research field, especially of fields outside their own expertise. However, other findings in that work (e.g., low improvement of socioemotional aspects; moderate improvement of technical knowledge and project skills) are corroborated here, despite their lack of significance with Perceived Value. The potential contradictions illustrated between these two studies open the door for future, more in-depth research regarding the role of the departmental seminar. Counterintuitively, the two theoretical frameworks used for this study were not reflected in the multiple regression model. This omission raises the specter that perhaps different frameworks should be employed in future work.

6.II.29 Limitations

As with all single-institution studies, greater generalizability will be achieved with replication experiments. Especially considering the self-selected nature of most of the attendees, future work at institutions with different seminar policies could yield substantially different results. The national representativeness of these undergraduate attendees at a selective institution in particular is worth questioning.

Fortunately, power analysis and sampling adequacy tests indicated sufficient sample sizes and data traits for this study. However, EFA typically utilizes larger samples, although the stricter factor cut-off of .45 and the good to excellent internal consistencies help compensate for the suboptimal sample size.^{176,177} Accepting duplicate respondents across seminars, the shortness of the survey, and the remote format likely helped boost response rates and combat biases, but these were trade-offs which introduced the possibility for repeated-measures dependence of observations, limited item options, and limited social interactions, respectively.

Finally, with only 42.8 % of the variance accounted for in the regression model, more work should be done to better understand the nature of the departmental seminar experience. Additionally, "Perceived Value" is not the same thing as "Actual Value". Attendees may be benefiting downstream from these experiences in ways beyond what they consciously perceive in the moment.

6.II.30 Conclusion

As widespread as seminars are in the chemistry community, the unknowns surrounding their impact are empirically murky. This paper helped clarify the role that departmental seminars play in a chemistry community and what aspects of the experience contribute to their value. Going forward, considerations were highlighted for future work to be conducted in this area.

Epilogue

This dissertation presented original research in synthetic organic chemistry (**Chapter 1**), the nature of chemistry research itself (**Chapters 2 – 3**), modern issues in the teaching and learning of laboratory chemistry (**Chapter 4**), and contemporary analyses of traditional support systems for training research chemists (**Chapters 5 – 6**). Together, these six chapters wove a narrative about the progression of individuals' chemical knowledge and their experiences in the field of chemistry. In the process, they provided implications for redesigning training programs for the next generation of chemists. Furthermore, the following additional implications manifest from the interplay between the chapters, supplemental to those already derived from each individually.

The importance of relationships and the team environment, for example, shows up in every chapter in complementary ways. In **Chapter 1**, it was observed how the rate of progress (and ultimately success) of a research project is heavily impacted by the ability to collaborate across the initial and final stages of a synthetic strategy. Meanwhile, in **Chapters 2 – 3**, the way in which an individual chemist conducts their day-to-day benchwork was shown to intersect with (1) their relationships with PIs and group members and (2) the individual's desire to maintain positive relationships by displaying considerate behavior. The decrease in these types of positive relationships during the COVID-19 pandemic appeared to harm some undergraduate students' chemical learning and motivation in **Chapter 4**. That finding further parallels the emphases in **Chapters 5 – 6** on the importance of positive mentoring relationships and socially situated research activities. Across this dissertation as a whole, therefore, it can be concluded that relationships are crucial for learning and doing chemistry.

Also crucial for learning and doing chemistry is the opportunity to acquire and reinforce essential skills and knowledge. **Chapters 1 – 3** demonstrated how bench chemistry is a challenging, failure-filled endeavor conducted in complex environments filled with diverse hazards and staffed by highly specialized scientists. The ability to safely, quickly, and effectively execute chemical projects therefore depends on trainees acquiring a strong toolkit of specific skills. These skills draw upon the cognitive, affective, and psychomotor domains which, as shown in **Chapter 4**, require deliberate exposure to and practice with in order to develop competency. Moreover, as shown in **Chapters 5 – 6**, these competencies must be continuously developed after acquisition via effective mentorship and professional development to continue nurturing chemists'

abilities and interests. **Chapter 1** and **Chapter 6** emphasize how science is not as streamlined an endeavor as it may appear from the outside perspective while **Chapters 2, 4, and 6** illustrate how sharing stories about failure, learning how to be original, and learning how to handle set-backs are important types of ongoing lifelong lessons that extend beyond traditional undergraduate coursework. However, it should also be noted that the reviewed environments were especially tailored to the chemistry graduate student experience and, consequently, may reveal misalignment between current chemistry experiences at the undergraduate level and the non-chemical career routes that most undergraduates take.

In addition to the research presented in this dissertation, I also had the good fortune to engage in multiple published curriculum development projects^{199,389–391}, action-based research as a high school teacher (not shown), mentorship in research and education, K-16 classroom teaching, STEM outreach, institutional leadership, higher education administration, nationally competitive grants (e.g., National Science Foundation Graduate Research Fellowship), and independent consulting studies as part of my PhD portfolio. As of August 2023, these endeavors yielded almost 20 public presentations, 5 published single-author peer-reviewed articles,^{199,389,390,392,393} and 2 white papers^{394,395} and as well as other manuscripts in preparation. I am gratified these contributions have already begun influencing on-going scholarly discussions, as evidenced by ~ 100 citations and 15,000+ views of my published articles, 4 invited speakerships, and recognitions such as nomination to the international Schmidt Science Fellowship postdoctoral competition and receipt of the American Association for Colleges & Universities K. Patricia Cross Future Leaders Award. Moving forward, future efforts will hopefully continue to build on this work by generating and evaluating best practices in next-generation laboratory instruction for hands-on skills and in research training programs for improving alignment between individuals' goals and programmatic elements.

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Appendix A

Corresponding to **Chapter 1.** Studies Toward the Asymmetric Total Syntheses of Dankasterone A and B, Illisimonin A, Obtusenol, and Substituted Piperidines

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A.1 General Procedures

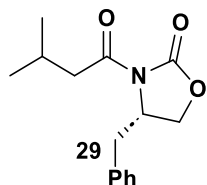
Unless otherwise noted, the following procedures were followed.

Conditions. Reactions were carried out in anhydrous, oxygen-free environments using a positive Ar atmosphere in flame-dried glassware with magnetic stirring. Magnetic stir bars were dried concurrently under vacuum within glassware while flaming the glassware. Cannulas and NMR tubes were maintained dry in ovens until use. Round-bottom borosilicate glass flasks were utilized for reaction vessels. Reaction temperatures refer to the temperature of the hot / cold bath that the reaction vessel was suspended in. All hot bath temperatures were continuously monitored automatically by an external hot plate probe. Overnight cold baths were continuously cooled by a CryoCooler with stirring. Solvents and reagents were purchased anhydrous and with > 99 % purity where possible. Infrequently, when purity was $\leq$ 99 %, mmol calculations were adjusted accordingly. For example, HOBt was purchased as an 82 % mixture wetted with H₂O, so the 4.279 g measured out was calculated as 25.97 mmol, not 31.67 mmol. THF, CH₂Cl₂, and toluene (tol) solvents were obtained anhydrously by passing commercially available pre-dried, oxygen-free formulations through activated alumina columns with positive Ar flow. Commercial reagents were purchased with $\geq$ 95 % purity, used as received, and stored according to the supplier's directions with Ar used as an inert headspace where warranted. Addition of liquids into reaction flasks was accomplished using a fresh syringe and needle through a sealed septum. Literature precedents which guided the experimental conditions used are cited in this Appendix.

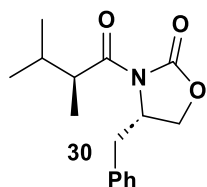
Purification. Saturated (sat.) aqueous (aq.) NaCl solution ("brine") was used for washing reaction mixtures. After purification, samples were concentrated via reduced pressure on a rotatory evaporator and then a high vacuum pump. Flash column chromatography was performed using SiliCycle silica gel (60, academic grade, particle size 0.040–0.063 mm). Most samples were loaded as solutions in minimal CH₂Cl₂ onto columns packed and flushed with EtOAc and hexanes (hex). Samples loaded onto Et₂O / pentanes (pent) columns were loaded with pent. Preparatory thin-layer chromatography (TLC) was performed on 0.50 mm E. Merck silica gel plates (60F-254). Synthesized compounds were stored under an Ar atmosphere in a freezer.

Analysis. Analytical TLC was performed on 0.25 mm E. Merck silica gel plates (60F-254). Visualization was accomplished with UV light and an aq. solution of KMnO_4 and NaHCO_3 followed by heating. Yields refer to compounds judged to be homogeneous by ^1H spectroscopy unless otherwise noted to be mixtures. NMR spectra were recorded on a 500 MHz Bruker spectrometer and are reported in ppm using solvent as an internal standard (e.g., CDCl_3 ^1H δ 7.26 ppm). The following abbreviations were used to denote spectral multiplicities: s = singlet (1), d = doublet (2), t = triplet (3), q = quartet (4), p = pentet (5), sx = sextet (6), h = heptet (7), m = multiplet, br = broad.

A.2 Experimental Details for Dankasterone Project

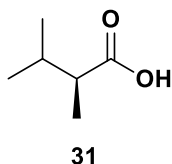


(S)-4-benzyl-2-oxazolidinone (24.302 g, 134.40 mmol, 1.05 equiv.) was dissolved in CH_2Cl_2 (192 mL).¹¹ Et_3N (28.6 mL, 205 mmol, 1.6 equiv.) was added dropwise via cannula to the yellow solution, followed by addition of DMAP (1.720 g, 14.08 mmol, 0.1 equiv.). The mixture was cooled to 0 °C in an ice bath. Isopentanoyl chloride, **18**, (15.9 mL, 128 mmol) was slowly added dropwise via cannula over 20 min with gas evolution. After 3.5 h, the chunky, opaque yellow suspension was diluted with CH_2Cl_2 (200 mL) and washed with brine (200 mL). The aq. washing was further extracted with CH_2Cl_2 (200 mL), and the combined organic layers were dried over Na_2SO_4 and concentrated to yield a dark orange liquid. The sample was purified via silica plug (20 % EtOAc / hex) to afford oxazolidinone **29** as a white-ish / yellow-ish crystalline solid (32.76 g, 125.4 mmol, 98 % yield): TLC (20% EtOAc / hex) R_f = 0.40 (UV / KMnO_4); the spectral data is in agreement with published literature.¹¹

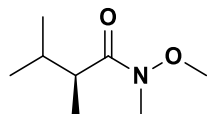


Oxazolidinone **29** (13.470 g, 51.546 mmol) was dissolved in THF (515 mL) and cooled to -78 °C in an acetone dry ice bath.¹¹ NaHMDS as a 1 M solution in THF (77.3 mL, 77.3 mmol, 1.5 equiv.) was slowly added dropwise via cannula over 1 h. After stirring for an additional 15 min, MeI (13.0 mL, 207 mmol, 4 equiv.) was added slowly over 20 min. After stirring overnight, the yellow solution was quenched with sat. aq. NH_4Cl (400 mL) to reach pH 5 and warmed to rt. The reaction mixture was extracted with Et_2O (3 x 200 mL). The combined organic layers were washed with brine (100 mL), dried over Na_2SO_4 , and concentrated to yield a red liquid with solid yellow clumps. The sample was purified via flash column chromatography

(40 % EtOAc / hex) to afford oxazolidinone **30** as a white-ish / yellow-ish crystalline solid (13.68 g, 49.68 mmol, 96 % yield, *dr* 10:1): TLC (10 % EtOAc / hex) R_f = 0.36 (UV / KMnO_4); the spectral data is in agreement with published literature.¹¹

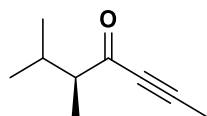


Oxazolidinone **30** (3.97 g, 14.4 mmol) was dissolved in THF (206 mL) and cooled to 0 °C in an ice bath.¹¹ H_2O_2 as a 30 % w / w aq. solution (5.9 mL, 58 mmol, 4 equiv.) was added dropwise. $\text{LiOH} \cdot \text{H}_2\text{O}$ (1.21 g, 28.8 mmol, 2 equiv.) was dissolved in H_2O (72 mL), and the resulting solution was poured into the reaction mixture at ambient atmosphere. The reaction mixture was raised to rt, and white precipitate began forming. After 2 h, the opaque white suspension was washed with CH_2Cl_2 (2 x 100 mL). Analytical TLC confirmed the absence of the desired product in the organic washings. The aq. phase was acidified to pH 1 and turned yellow with 10 % aq. HCl (50 mL). The mixture was extracted with CH_2Cl_2 (4 x 50 mL) until TLC confirmed the absence of product in the aq. layer. The combined organic phases were dried over Na_2SO_4 and concentrated in a dry flask at a dry rotatory evaporator under an Ar atmosphere with a 0 °C ice bath and an applied vacuum strength slightly less than 700 torr. TLC was used to monitor for the presence of product in the collection flask. The concentrated and highly volatile carboxylic acid **31** was carried on to the subsequent reaction without further purification as a colorless liquid with small amounts of solvent (1.73 g). A portion of **31** was purified with stronger vacuum for analytical purposes: TLC (40 % EtOAc / hex) R_f = 0.49 (KMnO_4); the spectral data is in agreement with published literature.¹¹



32

Concentrated carboxylic acid **31** from the previous step (1.73 g) was dissolved in CH₂Cl₂ (50. mL) and cooled to 0 °C in an ice bath.³⁹⁶ Weinreb's salt (1.933 g, 19.82 mmol, 1.3 equiv.) was added to the colorless solution, followed by Et₃N (3.5 mL, 25 mmol, 1.7 equiv.), EDC•HCl (2.776 g, 17.88 mmol, 1.2 equiv.), and DMAP (182.0 mg, 1.490 mmol, 0.1 equiv.). The white suspension was raised to rt and allowed to stir overnight. The reaction mixture was diluted with CH₂Cl₂ (100 mL) and then washed with 1 % aq. HCl (2 x 100 mL), sat. aq. NaHCO₃ (100 mL), and brine (100 mL). The organic layer was dried over Na₂SO₄ and concentrated at a dry rotatory evaporator with a 0 °C ice bath. TLC was used to monitor for the presence of product in the collection flask. Concentration afforded the volatile amide **32** as a yellow liquid (2.18 g, 13.7 mmol, 95 % yield over 2 steps): TLC (30 % EtOAc / hex) R_f = 0.47 (UV / KMnO₄); ¹H NMR (500 MHz, CDCl₃) δ 3.68 (s, 3H), 3.19 (s, 3H), 2.61 (br, 1H), 1.94 – 1.83 (m, 1H), 1.09 (d, J = 6.9 Hz, 3H), 0.93 (d, J = 6.8 Hz, 3H), 0.89 (d, J = 6.7, 3H).

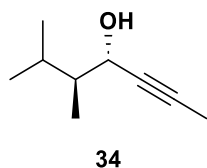


33

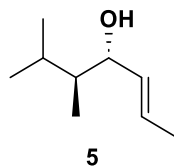
The following reaction was split into 2 equal batches due to glassware size constraints.

Amide **32** (1st batch: 2.30 g, 14.4 mmol; 2nd batch: 2.10 g, 13.2 mmol) was dissolved in THF (1st: 57.6 mL; 2nd: 52.8 mL) and cooled to -78 °C in an acetone dry ice bath.³⁹⁷ 1-propynyl-MgBr as a 0.5 M solution in THF (1st: 57.8 mL, 28.9 mmol, 2 equiv.; 2nd: 52.8 mL, 26.4 mmol, 2 equiv.) was slowly added dropwise by hand to the colorless solution over 45 min. The resulting yellow mixture was raised to rt. After stirring for an additional 2 h, the reaction mixture was added to an addition funnel and quenched under ambient atmosphere by quickly dripping the reaction mixture into a vigorously stirring mixture of Et₂O (2 L), H₂O (1 L), and dibasic (77.5 g) and monobasic (29.1 g) sodium phosphate dihydrate to form a 0.5 M phosphate

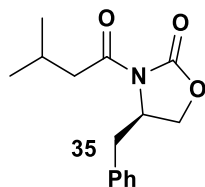
buffer at pH 7³⁹⁸. After vigorous stirring for 0.5 h, the organic phase was collected, partially concentrated at 0 °C, and dried over Na₂SO₄. The sample was purified via silica plug (5 % Et₂O / pent), and the combined batches were again partially concentrated at 0 °C. By carefully holding the rotatory evaporator's applied vacuum strength at 720 torr in a 0 °C ice bath for a long period of time, a slightly less polar impurity was fortunately susceptible to removal without compromising the desired product. This careful concentration afforded volatile ketone **33** as a yellow solution in THF (5.15 g total, 1.6 **33** : 1 THF). The concentrated solution was carried on to the subsequent reaction without further purification (calculated 3.88 g **33**, 28.1 mmol, quantitative yield). A portion of **33** was purified with stronger vacuum for analytical purposes: TLC (5 % EtOAc / hex) R_f = 0.42 (UV / KMnO₄); the spectral data is in agreement with its enantiomer in published literature.²¹



Ketone **33** (0.790 g, 5.72 mmol) was dissolved in THF (28.6 mL) and cooled to -30 °C in an *i*-PrOH bath maintained by a CryoCooler.³⁹⁹ (S)-CBS as a 1 M solution in tol (11.5 mL, 11.5 mmol, 2 equiv.) was slowly added dropwise to the yellow solution, followed by BH₃•Me₂S as a 2 M solution in THF (14.3 mL, 28.6 mmol, 5 equiv.). After stirring for an additional 1 h, the reaction mixture was quenched with dropwise addition of EtOH (30 mL). After the prolonged gas evolution subsided, the mixture was diluted with H₂O (40 mL) and extracted with Et₂O (2 x 50 mL). The combined organic layers were washed with brine (30 mL), dried over Na₂SO₄, and concentrated at 0 °C. The sample was purified via flash column chromatography (15 % → 100 % CH₂Cl₂ / pent) and carefully concentrated with the rotatory evaporator's applied vacuum strength at 700 torr in a 0 °C to afford the volatile alcohol **34** as a colorless liquid (0.74 g, 5.3 mmol, 92 % yield): TLC (100 % CH₂Cl₂) R_f = 0.33 (UV / KMnO₄); ¹H NMR (500 MHz, CDCl₃) δ 4.35 – 4.29 (m, 1H), 1.85 (d, *J* = 2.2 Hz, 3H), 1.86 – 1.75 (m, 1H), 1.66 (br, 1H), 1.50 (sx, *J* = 6.7 Hz, 1H), 0.92 (d, *J* = 6.8 Hz, 6H), 0.86 (d, *J* = 6.8 Hz, 3H).

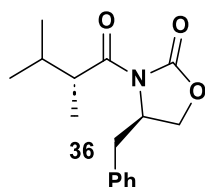


Alcohol **34** (3.28 g, 23.4 mmol) was added to a flask fitted with a water condenser.⁴⁰⁰ The alcohol was dissolved in THF (117 mL) and cooled to 0 °C in an ice bath. LiAlH₄ as a 1 M solution in THF (93.6 mL, 43.6 mmol, 4 equiv.) was added dropwise via cannula over 0.5 h. After gas evolution subsided, the yellow reaction mixture was heated to reflux at 66 °C. Reaction progress was monitored via NMR aliquots. After 7 h, the mixture was cooled to 0 °C. A gas outlet was added to the condenser septum, and the reaction was quenched slowly with dropwise addition of sat. aq. Na₂SO₄ (5 mL) until gas evolution subsided. The mixture was warmed to rt and filtered over celite with Et₂O (1 L). The resulting filtrate was dried over Na₂SO₄ and concentrated at 0 °C with an applied vacuum strength less than 740 torr. The sample was purified via flash column chromatography (0 % → 60 % Et₂O / pent) to afford the volatile alcohol **5** as a yellow liquid (2.30 g, 16.2 mmol, 69 % yield): TLC (100 % CH₂Cl₂) R_f = 0.41 (KMnO₄); ¹H NMR (500 MHz, CDCl₃) δ 5.72 – 5.61 (m, 1H), 5.47 (dd, *J* = 15.5, 7.7 Hz, 1H), 3.92 (td, *J* = 7.8, 3.3 Hz, 1H), 1.95 – 1.88 (m, 1H), 1.88 – 1.82 (m, 1H), 1.71 (dd, *J* = 6.5, 1.6 Hz, 3H), 1.46 – 1.38 (m, 1H), 0.92 (d, *J* = 6.8 Hz, 3H), 0.83 (d, *J* = 6.9 Hz, 3H), 0.73 (d, *J* = 6.9 Hz, 3H).

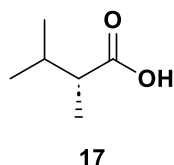


(*R*)-4-benzyl-2-oxazolidinone (34.174 g, 189.00 mmol, 1.05 equiv.) was dissolved in CH₂Cl₂ (270 mL). Et₃N (40.2 mL, 288 mmol, 1.6 equiv.) was added dropwise via cannula to the yellow solution, followed by addition of DMAP (2.419 g, 19.80 mmol, 0.1 equiv.). The mixture was cooled to 0 °C in an ice bath. Isopentanoyl chloride, **18**, (22.4 mL, 180. mmol) was added dropwise via cannula over 10 min with gas evolution. After 3.5 h, the chunky, opaque yellow suspension was diluted with CH₂Cl₂ (100 mL) and washed with brine (100 mL). The aq. washing was further extracted with CH₂Cl₂ (2 x 100 mL), and the combined organic layers

were dried over Na₂SO₄ and concentrated to yield an orange mixture of liquid and solid. The sample was purified via flash column chromatography (10 % → 20 % EtOAc / hex) to afford oxazolidinone **35** as a white crystalline solid (43.66 g, 167.1 mmol, 93 % yield). See enantiomer **29** for analytical data.



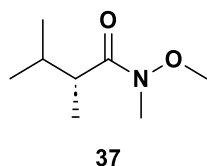
Oxazolidinone **35** (21.62 g, 82.73 mmol) was dissolved in THF (830 mL) and cooled to -78 °C in an acetone dry ice bath. NaHMDS as a 1 M solution in THF (124.1 mL, 124.1 mmol, 1.5 equiv.) was slowly added dropwise via cannula over 1 h. After stirring for an additional 15 min, MeI (20.8 mL, 331 mmol, 4 equiv.) was added slowly over 1 h. After stirring for an additional 3 h, the yellow solution was quenched with sat. aq. NH₄Cl (450 mL) to reach pH 5 and warmed to rt. The reaction mixture was extracted with Et₂O (2 x 300 mL). The combined organic layers were washed with brine (200 mL), dried over Na₂SO₄, and concentrated to yield a dark yellow liquid with solid white clumps. The sample was purified via flash column chromatography (10 % → 30 % EtOAc / hex) to afford oxazolidinone **36** as an almost-white crystalline solid (20.73 g, 75.29 mmol, 91 % yield, *dr* 20:1). See enantiomer **30** for analytical data.



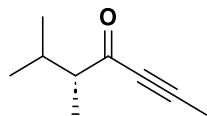
After the reaction, the mixture was split into multiple batches for purification due to glassware size constraints.

Oxazolidinone **36** (42.32 g, 153.7 mmol) was dissolved in THF (2.2 L) at ambient atmosphere and cooled to 0 °C in an ice bath. H₂O₂ as a 30 % w / w aq. solution (62.8 mL, 615 mmol, 4 equiv.) was added dropwise to the colorless solution over 20 min. LiOH•H₂O (12.899 g, 307.41 mmol, 2 equiv.) was dissolved in H₂O

(770 mL), and the resulting solution was added to the reaction mixture dropwise via a suspended addition funnel over 1 h. The reaction mixture was raised to rt, and yellow precipitate began forming. After an additional 3 h, the opaque yellow suspension was washed with CH₂Cl₂ (2 x 800 mL). Analytical TLC confirmed the presence of the desired product in the organic washings, so the combined organic washings were extracted with H₂O (200 mL) basified beforehand with 1 M NaOH. The combined aq. phases were then acidified to pH 1 and turned yellow with 3 % aq. HCl (40 mL). The mixture was extracted with CH₂Cl₂ (2 x 300 mL) until TLC confirmed the absence of product in the aq. layer. The combined organic phases were dried over Na₂SO₄ and concentrated in a dry flask at a dry rotatory evaporator with a 0 °C ice bath and an applied vacuum strength slightly less than 700 torr. TLC was used to monitor for the presence of product in the collection flask. The concentrated and highly volatile carboxylic acid **17** was carried on to the subsequent reaction without further purification as a colorless liquid with small amounts of solvent (19.73 g). See enantiomer **31** for analytical data.

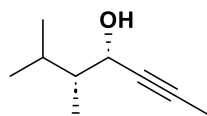


Concentrated carboxylic acid **17** from the previous step (19.73 g) was dissolved in CH₂Cl₂ (770 mL) and cooled to 0 °C in an ice bath. Weinreb's salt (19.489 g, 199.81 mmol, 1.3 equiv.) was added to the colorless solution, followed by Et₃N (36.4 mL, 261 mmol, 1.7 equiv.), EDC•HCl (35.351 g, 184.40 mmol, 1.2 equiv.), and DMAP (1.878 g, 15.37 mmol, 0.1 equiv.). The white suspension was raised to rt and allowed to stir overnight. The reaction mixture was washed with 1 % aq. HCl (4 x 200 mL), sat. aq. NaHCO₃ (2 x 200 mL), and brine (200 mL). The organic layer was dried over Na₂SO₄ and concentrated at a dry rotatory evaporator with a 0 °C ice bath. TLC was used to monitor for the presence of product in the collection flask. Concentration afforded the volatile amide **37** as a yellow liquid (23.16 g, 145.4 mmol, 95 % yield over 2 steps). See enantiomer **32** for analytical data.



38

Amide **37** (17.06 g, 107.1 mmol) was dissolved in THF (500. mL) and cooled to -78 °C in an acetone dry ice bath. 1-propynyl-MgBr as a 0.5 M solution in THF (504 mL, 252 mmol, 2.4 equiv.) was slowly added dropwise via cannula to the colorless solution over 3 h. The resulting yellow solution was raised to rt. After stirring for an additional 2 h, the reaction mixture was cooled to 0 °C in an ice bath and quenched with sat. aq. NH₄Cl (300 mL). The mixture was extracted with Et₂O (2 x 300 mL), and the combined organic layers were washed with brine (200 mL), dried over Na₂SO₄, and partially concentrated at 0 °C. The sample was purified via flash column chromatography (0 % → 10 % Et₂O / pent), and the eluate was partially concentrated at 0 °C to afford volatile ketone **38** as a yellow solution in pentanes (14.55 g). The concentrated solution was carried on to the subsequent reaction without further purification. See enantiomer **33** for analytical data.

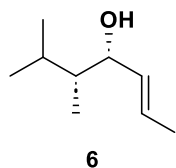


39

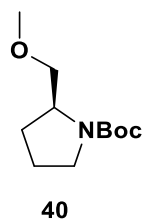
After extraction and reduction, the mixture was split into 2 batches for chromatographic separation due to glassware size constraints.

Concentrated ketone **38** from the previous step was dissolved in THF (530 mL) and cooled to -30 °C in an *i*-PrOH bath maintained by a CryoCooler. (S)-CBS (61.444 g, 210.60 mmol, 2 equiv.) was dissolved in toluene (211 mL) via sonication and then added quickly dropwise to the yellow solution over 40 min, followed by BH₃•Me₂S as a 2 M solution in THF (200. mL, 400. mmol, 3.8 equiv.) over 1 h until TLC showed complete conversion of the ketone. After stirring for an additional 15 min, the reaction mixture was quenched with dropwise addition of EtOH (75 mL). After the prolonged gas evolution subsided, the mixture was allowed to warm to rt, diluted with H₂O (500 mL), and extracted with Et₂O (2 x 500 mL). The combined organic

layers were washed with brine (250 mL), dried over Na₂SO₄, and concentrated at 0 °C. The sample was purified via flash column chromatography (0 % → 25 % Et₂O / pent) to afford the slightly volatile alcohol **39** as a colorless liquid (12.23 g, 87.21 mmol, 81 % yield over 2 steps): TLC (100 % CH₂Cl₂) R_f = 0.42 (KMnO₄); ¹H NMR (500 MHz, CDCl₃) δ 4.35 – 4.24 (m, 1H), 1.85 (s, 3H), 1.56 – 1.49 (m, 1H), 1.49 – 1.38 (m, 1H), 0.97 (d, *J* = 7.0 Hz, 3H), 0.94 (d, *J* = 7.0 Hz, 3H), 0.85 (d, *J* = 6.9 Hz, 3H).

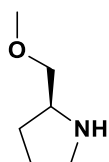


Alcohol **39** (800. mg, 5.71 mmol) was added to a flask fitted with a water condenser. The alcohol was dissolved in THF (28.5 mL) and cooled to 0 °C in an ice bath. LiAlH₄ as a 1 M solution in THF (22.8 mL, 22.8 mmol, 4 equiv.) was added dropwise. After gas evolution subsided, the reaction mixture was heated to reflux at 66 °C and allowed to stir overnight. The mixture was then cooled to 0 °C and quenched dropwise addition of 1 N aq. Rochelle's salt (30 mL). The mixture was warmed to rt and extracted with Et₂O (3 x 30 mL). The combined organic layers were washed with brine (20 mL), dried over Na₂SO₄, and concentrated at 0 °C with an applied vacuum strength less than 740 torr. The sample was purified via flash column chromatography (0 % → 20 % Et₂O / pent) to afford the volatile alcohol **6** as a colorless liquid (0.690 g, 4.85 mmol, 85 % yield): TLC (20 % Et₂O / pent) R_f = 0.49 (KMnO₄); the spectral data is in agreement with published literature.²¹



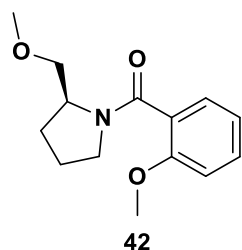
Light-sensitive *N*-Boc-L-prolinol, **16**, (20.000 g, 97.382 mmol) was added to a flask covered with Al foil in a darkened room, dissolved in THF (390 mL), and cooled to -78 °C in an acetone dry ice bath.¹⁴ NaH as a

60 % dispersion in oil (5.064 g, 126.6 mmol, 1.3 equiv.) was added portionwise. After stirring for 15 min, MeI (7.88 mL, 127 mmol, 1.3 equiv.) was added dropwise, and the reaction mixture was allowed to warm to rt overnight. The yellow solution was later cooled to 0 °C and quenched with sat. aq. NH₄Cl (200 mL) to reach pH 4. The mixture was extracted with EtOAc (3 x 200 mL), and the combined organic layers were washed with brine (200 mL), dried over Na₂SO₄, and concentrated to yield a red liquid. The sample was purified via flash column chromatography (0 → 50 % EtOAc / hex) to afford methoxy **40** as a yellow liquid (19.57 g) with stubborn trace grease which was carried on to the subsequent reaction without further purification. A portion of **40** was purified further for analytical purposes: TLC (10 % EtOAc / hex) R_f = 0.24 (KMnO₄); the spectral data is in agreement with published literature.^{14,15}

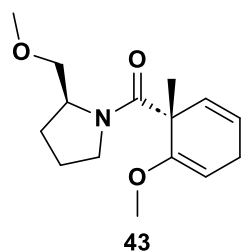


41

Concentrated methoxy **40** from the previous step (19.57 g) was dissolved in CH₂Cl₂ (165 mL) and cooled to 0 °C.¹⁵ TFA (98 mL, 1,300 mmol, 14 equiv.) was quickly added dropwise to the off-white solution via an additional funnel over 1 h. The pink-ish reaction mixture was then raised to rt and subsequently cooled again to 0 °C in an ice bath after 1 h at rt. The mixture was quenched with quick dropwise addition of 10 % aq. NaOH (1.1 L) via an addition funnel until the pink color disappeared and the pH reached 13. The mixture was extracted with CH₂Cl₂ (9 x 400 mL). The combined organic layers were dried over Na₂SO₄ and concentrated at 0 °C to afford volatile amine **41** as a yellow liquid (quantitative yield over 2 steps): TLC (70 % EtOAc / hex) R_f = 0.08 (KMnO₄); the spectral data is in agreement with published literature.⁴⁰¹

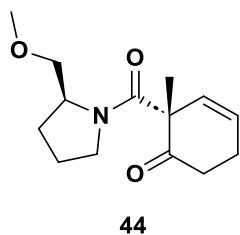


o-Anisic acid (3.991 g, 25.97 mmol, 1 equiv.) dried under vacuum was dissolved in CH₂Cl₂ (200. mL) and cooled to 0 °C.⁴⁰² NMM (5.8 mL, 52 mmol, 2 equiv.) was added, followed by DCC (5.626 g, 27.27 mmol, 1.05 equiv.) and HOBt wetted with 14 % w / w H₂O (4.279 g, 25.97 mmol, 1 equiv.). After stirring for 20 min, amine **41** (25.97 mmol) was dissolved in CH₂Cl₂ (36.6 mL), and the resulting solution was added to the white suspension. The reaction mixture was then raised to rt. After stirring overnight, the white precipitate was filtered off from the orange mixture via a frit. The mixture was diluted with H₂O (200 mL) and extracted with CH₂Cl₂ (4 x 200 mL). The combined organic layers were washed with brine (200 mL), dried over Na₂SO₄, and concentrated to yield a grainy yellow liquid. The sample was purified via flash column chromatography (10 % → 90 % EtOAc / hex) to afford amide **42** as a yellow liquid (5.657 g, 22.69 mmol, 87 % yield): TLC (70 % EtOAc / hex) R_f = 0.28 (UV / KMnO₄); the spectral data is in agreement with published literature.¹⁶



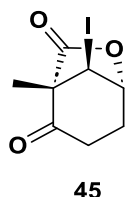
Amide **42** (4.000 g, 16.04 mmol) was warmed slightly to decrease its viscosity, and a widened pipette was used to transfer it to a very dry 1 L 3-necked round-bottom flask with an externally marked 300-mL volume line and a dry ice condenser.^{10,16} THF (15.1 mL) was added, and the flask was sonicated to dissolve the amide. Then, the flask was fitted with a mechanical stirrer instead of a stir bar. *t*-BuOH (1.52 mL, 16.0 mmol, 1 equiv.) was added as a warm liquid to the colorless solution. The reaction mixture was cooled to -72 in a 1.5 L 35 % H₂O / MeOH dry ice bath. An *i*-PrOH dry ice bath was prepared in the flask condenser.

NH₃ was then condensed quickly dropwise from a gas cylinder while the flask was under a strong Ar flow for 1 h until the overall reaction mixture just passed the 300-mL line. The flask was temporarily fitted with an Al foil skirt to completely cover the cold bath during K addition. Small chunks of K stored in mineral oil were rinsed with hex and added portionwise to the reaction mixture under a strong Ar flow for 1 h until the reaction mixture retained a dark blue color for 0.5 h uninterrupted. Isoprene (5 drops) was added dropwise until the mixture retained a yellow color for 0.5 h uninterrupted. MeI (1.51 mL, 24.0 mmol, 1.5 equiv.) was slowly added dropwise. The reaction mixture turned colorless after an additional 0.5 h and was allowed to continue stirring for 3.5 h more. Solid NH₄Cl (60 g) was added slowly to quench the reaction. The mixture was raised to rt, and the septum was removed to enable atmospheric exchange within the fume hood. The mechanical stirrer was replaced with a conventional magnetic stir bar, and the mixture was allowed to stir overnight. H₂O (400 mL) was added to dissolve the resulting NH₄Cl. The mixture was extracted with EtOAc (2 x 400 mL), and the combined organic layers were washed with brine (400 mL), dried over Na₂SO₄, and concentrated to yield concentrated methoxy **43** as a dark red liquid (4.39 g) which was carried on to the subsequent reaction without further purification. A portion of **43** was purified further for analytical purposes: TLC (50 % EtOAc / hex) R_f = 0.43 (UV / KMnO₄); the spectral data is in agreement with published literature.^{10,16}

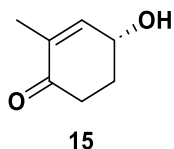


Concentrated methoxy **43** from the previous step (4.39 g) was dissolved in MeOH (8.0 mL) under ambient atmosphere at rt.¹⁰ 6 N aq. HCl (8.0 mL) was added dropwise to the red solution. After 2 h, the reaction mixture was extracted with CH₂Cl₂ (3 x 30 mL), and the combined organic layers were washed with brine (20 mL), dried over Na₂SO₄, and concentrated to yield a dark red liquid. The sample was purified via flash column chromatography (0 → 100 % EtOAc / hex) to afford ketone **44** as a yellow oil (3.374 g, 13.42 mmol,

84 % yield over 2 steps): TLC (50 % EtOAc / hex) R_f = 0.23 (KMnO_4); the spectral data is in agreement with published literature.¹⁰

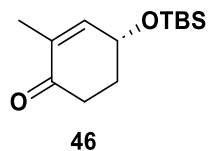


Ketone **44** (3.890 g, 15.48 mmol) was dissolved in non-anhydrous THF (86 mL) and H_2O (86 mL) under ambient atmosphere at rt.¹⁰ I_2 (23.574 g, 92.881 mmol, 6 equiv.) was added to the colorless solution. After stirring for 2.5 h, sat. aq. $\text{Na}_2\text{S}_2\text{O}_3$ (150 mL) was added to the black reaction mixture until it turned yellowish / white-ish. The reaction mixture was extracted with EtOAc (3 x 300 mL) until analytical TLC confirmed absence of the desired product in the aq. layer. The combined organic layers were washed with brine (200 mL), dried over Na_2SO_4 , and concentrated to yield a yellow solid. The sample was purified via flash column chromatography (10 % $\rightarrow$ 80 % EtOAc / hex) to afford iodolactone **45** as a white solid (4.03 g, 14.4 mmol, 93 % yield): TLC (30 % EtOAc / hex) R_f = 0.38 (UV / KMnO_4); the spectral data is in agreement with published literature.¹⁰

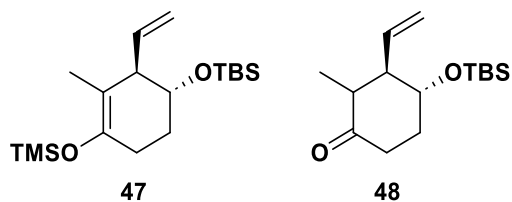


Iodolactone **45** (4.03 g, 14.4 mmol) was dissolved in non-anhydrous THF (96 mL) and H_2O (96 mL) with a strict 1 : 1 THF : H_2O ratio under ambient atmosphere at rt.¹⁰ $\text{LiOH} \cdot \text{H}_2\text{O}$ (1.812 g, 43.18 mmol, 3 equiv.) was added to the colorless solution, turning it into a dark yellow colloidal suspension which subsided to lime green and then later light brown after stirring overnight. The reaction mixture was quenched with 10 % aq. HCl (3 mL), stopping immediately upon reaching a pH range of 6 – 7 and dissolving the precipitate. The orange solution was extracted with EtOAc (7 x 150 mL) until analytical TLC confirmed absence of the

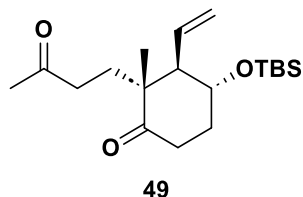
desired product in the aq. layer. The combined organic layers were washed with brine (600 mL), and the brine washing was again extracted with EtOAc until analytical TLC confirmed absence of the desired product in the brine layer. The combined organic layers were dried over Na₂SO₄ and concentrated briefly under strong vacuum to yield a dark orange liquid. The sample was purified via flash column chromatography (15 % → 100 % EtOAc / hex) to afford slightly volatile cyclohexenone **15** as a yellow oil (1.19 g, 9.43 mmol, 66 % yield): TLC (50 % EtOAc / hex) R_f = 0.20 (UV / KMnO₄); the spectral data is in agreement with published literature.¹⁰



Cyclohexenone **15** (200.0 mg, 1.585 mmol) was dissolved in CH₂Cl₂ (9.3 mL) and cooled to 0 °C.⁴⁰³ *i*-Pr₂NEt (0.97 mL, 5.5 mmol, 3.5 equiv.) was added to the yellow solution, followed by DMAP (58.1 mg, 0.476 mmol, 0.3 equiv.) and TBSCl (716.7 mg, 4.755 mmol, 3 equiv.). The reaction mixture was raised to rt and allowed to stir overnight. The reaction was diluted with H₂O (10 mL) and stirred vigorously. The mixture was extracted with CH₂Cl₂ (3 x 10 mL), and the combined organic layers were washed with brine (20 mL), dried over Na₂SO₄, and concentrated with an applied vacuum strength slightly less than 740 torr to yield a yellow liquid. The sample was purified twice via flash column chromatography (10 % → 100 % CH₂Cl₂ / pent) to afford slightly volatile ketone **46** as an impure yellow liquid (478.9 mg) with a stubborn TBS-containing impurity which, after further drying very briefly under strong vacuum, was carried on to the subsequent reaction without further purification: TLC (5 % EtOAc / hex) R_f = 0.27 (UV / KMnO₄); the spectral data is in agreement with published literature.²¹



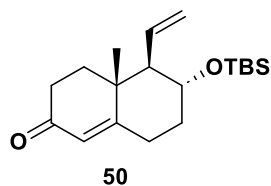
LiCl (13.6 mg, 0.317 mmol, 0.2 equiv.) was added to an oven-dried flask and flame-dried under vacuum to form a glass.⁴⁰⁴ CuI (30.8 mg, 0.159 mmol, 0.1 equiv.) and THF (9.2 mL) were added, creating a yellow-green solution. The mixture was cooled to -40 °C in a MeCN dry ice bath. Impure volatile ketone **46** from the previous step (478.9 mg) was briefly dried under strong vacuum before dissolution in THF (2.2 mL) and subsequent addition to the reaction flask. TMSCl (0.22 mL, 1.7 mmol, 1.1 equiv.) was added dropwise. After stirring for 15 min, vinyl-MgBr as a 1 M solution in THF (1.9 mL, 1.9 mmol, 1.2 equiv.) was added dropwise to the yellow solution. After stirring for an additional 2.5 h, the black solution was quenched with sat. aq. NH₄Cl (5 mL). The reaction mixture was extracted with EtOAc (3 x 10 mL), and the combined organic layers were washed with brine (10 mL), dried over Na₂SO₄, and concentrated to yield a grainy yellow liquid. The sample was purified via silica plug (5 % EtOAc / hex) to afford desired silyl enol ether **47** in a 5.6:1 ratio with its co-eluting hydrolyzed by-product **48** as a yellow liquid and brown solid (458.9 mg total, theoretical 1.181 mmol **47**, theoretical 75 % yield over 2 steps) which was carried on to the subsequent reaction without further purification: TLC (5 % EtOAc / hex) R_f = 0.71 (KMnO₄); ¹H NMR (500 MHz, CDCl₃) δ 5.62 – 5.46 (m, 1H), 5.11 – 5.00 (m, 2H), 3.76 – 3.64 (m, 1H), 2.60 – 2.53 (m, 1H), 2.29 – 2.18 (m, 1H), 1.98 – 1.86 (m, 1H), 1.81 – 1.71 (m, 1H), 1.66 – 1.56 (m, 1H), 1.49 (s, 3H), 0.87 (s, 9H), 0.18 (s, 6H), 0.08 – 0.02 (m, 9H).



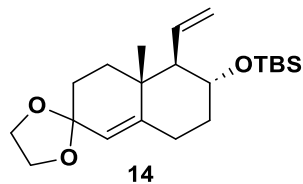
Silyl enol ether **47** in a 5.6:1 ratio with hydrolyzed by-product **48** from the previous step (458.9 mg) was dissolved in CH₂Cl₂ (6.4 mL) and cooled to -78 °C in an acetone dry ice bath.⁴⁰⁴ MeNO₂ (0.22 mL, 4.1

mmol, 3 equiv.) was added to the light brown suspension, followed by *i*-PrOH (0.31 mL, 4.1 mmol, 3 equiv.). After stirring for an additional 3 h, 3-buten-2-one freshly distilled at 115 °C (0.56 mL, 6.7 mmol, 5 equiv.) was added. After stirring for an additional 10 min, BF₃•OEt₂ with 53 % BF₃ basis (0.20 mL, 1.6 mmol, 1.2 equiv.) was added dropwise. The reaction mixture was raised to -65 °C and allowed to stir for 2 h more. The reaction was quenched with sat. aq. NaHCO₃ (5 mL) and raised to rt. After gas evolution subsided, the mixture was extracted with CH₂Cl₂ (3 x 10 mL), and the combined organic layers were washed with brine (5 mL), dried over Na₂SO₄, and concentrated to yield a yellow liquid. The sample was purified via flash column chromatography (5 % → 40 % EtOAc / hex) to afford ketone **49** as a colorless liquid (91.4 mg, 0.270 mmol, theoretical 23 % yield over 1 step, isolated 17 % yield over 3 steps) and, separately, hydrolyzed by-product **48** (253.9 mg, 0.9457 mmol, TLC (20 % EtOAc) R_f = 0.65 (KMnO₄)).

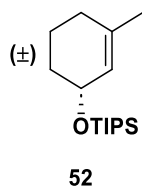
For 49: TLC (20 % EtOAc) R_f = 0.43 (KMnO₄); ¹H NMR (500 MHz, CDCl₃) δ 5.57 (dt, *J* = 16.9, 10.1 Hz, 1H), 5.15 (dd, *J* = 10.2, 1.8 Hz, 1H), 5.07 (dd, *J* = 16.9, 1.8 Hz, 1H), 3.97 (td, *J* = 8.2, 4.1 Hz, 1H), 2.54 – 2.44 (m, 2H), 2.44 – 2.39 (m, 1H), 2.39 – 2.28 (m, 2H), 2.18 – 2.08 (m, 1H), 2.12 (s, 3H), 1.93 – 1.80 (m, 2H), 1.80 – 1.69 (m, 1H), 1.04 (s, 3H), 0.88 (s, 9H), 0.07 (d, *J* = 4.2 Hz, 6H).



Ketone **49** (91.0 mg, 0.269 mmol) was dissolved in MeOH (2.7 mL) at rt.⁴⁰⁴ NaOMe as a colorless 0.5 M solution in MeOH (0.70 mL, 0.35 mmol, 1.3 equiv.) was added dropwise to the colorless solution, turning it yellow and then eventually pink. The reaction mixture was allowed to stir overnight. The pink solution was diluted with H₂O (5 mL) and extracted with EtOAc (3 x 10 mL). The combined organic layers were washed with brine (10 mL), dried over Na₂SO₄, and concentrated to yield a yellow liquid. The sample was purified via flash column chromatography (5 % → 40 % EtOAc / hex) to afford α,β-unsaturated ketone **50** as a yellow liquid (73.1 mg, 0.228 mmol, 85 % yield): TLC (20 % EtOAc) R_f = 0.39 (UV / KMnO₄); the spectral data is in agreement with published literature.²¹

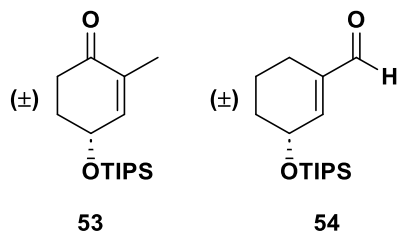


α,β -Unsaturated ketone **50** (73.1 mg, 0.228 mmol) was dissolved in CH_2Cl_2 (0.20 mL) at rt.⁴⁰⁵ $\text{CH}(\text{OEt})_3$ (0.06 mL, 0.35 mmol, 1.5 equiv.) and $(\text{CH}_2\text{OH})_2$ (0.13 mL, 2.3 mmol, 10 equiv.) were added. The reaction mixture was cooled to $-15\text{ }^\circ\text{C}$ in a $(\text{CH}_2\text{OH})_2$ dry ice bath. TMSOTf as a freshly prepared 0.163 M solution in CH_2Cl_2 (0.07 mL, 0.011 mmol, 0.05 equiv.) was added dropwise, and the reaction mixture was allowed to stir overnight. The reaction was quenched with Et_3N (0.01 mL) and raised to rt. The mixture was diluted with CH_2Cl_2 (5 mL) and sat. aq. NaHCO_3 (5 mL) and extracted with CH_2Cl_2 (3 x 5 mL). The combined organic layers were dried over Na_2SO_4 and concentrated to yield a yellow oil. The sample was purified via flash column chromatography (0 % $\rightarrow$ 40 % EtOAc / hex) to afford ketal **14** as a colorless liquid (42.0 mg, 0.115 mmol, 51 % yield): TLC (20 % EtOAc / hex) R_f = 0.52 (KMnO_4); ^1H NMR (500 MHz, CDCl_3) δ 5.56 (dt, J = 16.9, 10.0 Hz, 1H), 5.27 (s, 1H), 5.11 (dd, J = 10.3, 2.2 Hz, 1H), 5.02 (dd, J = 17.0, 2.2 Hz, 1H), 4.06 – 3.92 (m, 3H), 3.91 – 3.83 (m, 1H), 3.75 (td, J = 10.5, 4.6 Hz, 1H), 2.27 (tdd, J = 14.2, 4.8, 2.0 Hz, 1H), 2.09 (ddd, J = 14.2, 4.6, 2.8 Hz, 1H), 1.98 (dtd, J = 12.2, 4.7, 2.7 Hz, 1H), 1.83 (t, J = 9.9 Hz, 1H), 1.79 – 1.67 (m, 2H), 1.66 – 1.52 (m, 2H), 1.46 – 1.31 (m, 1H), 1.02 (s, 3H), 0.83 (s, 9H), 0.02 (s, 3H), 0.00 (s, 3H).



3-methyl-2-cyclohexenol (0.85 mL, 6.9 mmol) was dissolved in CH_2Cl_2 (20.1 mL).⁴⁰⁶ Imidazole (941.4 mg, 13.69 mmol, 2 equiv.) was added, and the reaction mixture was cooled to $0\text{ }^\circ\text{C}$ in an ice bath. TIPSCl (2.3 mL, 10. mmol, 1.5 equiv.) was added dropwise to the colorless solution. The reaction mixture was raised to rt and allowed to stir overnight. The white suspension was washed with H_2O (2 x 20 mL), washed with brine (20 mL), dried over Na_2SO_4 , and concentrated to yield a colorless liquid. The sample was purified via

flash column chromatography (0 % $\rightarrow$ 2 % EtOAc / hex) to afford silyl ether **52** as a colorless liquid (1.739 g, 6.478 mmol, 94 % yield): TLC (100 % hex) R_f = 0.58 (KMnO₄); ¹H NMR (500 MHz, CDCl₃) δ 5.43 (s, 1H), 4.33 – 4.23 (m, 1H), 1.99 – 1.89 (m, 1H), 1.87 – 1.74 (m, 3H), 1.66 (s, 3H), 1.59 – 1.46 (m, 2H), 1.07 (br, 21H).

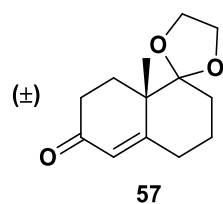


*Conditions from entry 7, **Scheme 1.7***

SeO₂ (20.7 mg, 0.186 mmol, 1 equiv.) was added to a flask, and H₂O (0.04 mL, 1.96 mmol, 10.5 equiv.) and AcOH (2 drops) were added.⁴⁰⁷ Silyl ether **52** (50.0 mg, 0.186 mmol) was dissolved in 1,4-dioxane (1.1 mL) and added to the reaction mixture. The mixture was heated to 40 °C and monitored by NMR aliquots (filtered over silica) as the temperature was repeatedly increased by 10 °C stepwise over 3 h until reaching reflux with an air condenser at 80 °C. The reaction mixture was allowed to stir overnight. The mixture was then cooled to rt, filtered over silica with EtOAc, and concentrated to yield a yellow-orange film. The sample was purified via flash column chromatography (2 % $\rightarrow$ 20 % EtOAc / hex) to afford desired ketone **53** in a 1.6:1 mixture with co-eluting aldehyde **54** as a yellow liquid (21.5 mg total, calculated 0.0497 mmol **53**, 27 % yield).

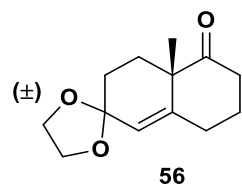
*For **53**:* TLC (20 % EtOAc / hex) R_f = 0.53 (UV / KMnO₄); ¹H NMR (500 MHz, CDCl₃) δ 6.66 (s, 1H), 4.62 – 4.54 (m, 1H), 2.60 (dt, J = 17.2, 4.8 Hz, 1H), 2.36 – 2.21 (m, 2H), 2.07 – 1.95 (m, 1H), 1.78 (s, 3H), 1.17 – 0.97 (m, 21H).

*For **54**:* TLC (20 % EtOAc / hex) R_f = 0.56 (UV / KMnO₄); ¹H NMR (500 MHz, CDCl₃) δ 9.47 (s, 1H), 6.64 (s, 1H), 4.57 – 4.50 (m, 1H), 2.19 – 2.12 (m, 2H), 2.04 – 1.93 (m, 1H), 1.92 – 1.81 (m, 1H), 1.69 – 1.60 (m, 1H), 1.59 – 1.49 (m, 1H), 1.17 – 0.97 (m, 21H).



Conditions from entry 1, **Scheme 1.8**

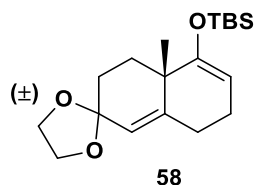
Wieland-Miescher ketone (500. mg, 2.67 mmol) was dissolved in CH₂Cl₂ (1.8 mL) and cooled to -78 °C in an acetone dry ice bath.^{19,20} (CH₂OTMS)₂ (2.0 mL, 8.0 mmol, 3 equiv.) was added to the yellow solution, followed by TMSOTf (0.01 mL, 0.053 mmol, 0.02 equiv.), turning the solution colorless and then pink. The reaction mixture was allowed to stir overnight. The reaction was quenched with H₂O (3 mL) and raised to rt with incomplete conversion indicated by analytical TLC. The mixture was extracted with CH₂Cl₂ (3 x 3 mL), and the combined organic layers were washed with brine (5 mL), dried over Na₂SO₄, and concentrated to yield a yellow liquid. The sample was purified via flash column chromatography (10 % → 80 % EtOAc / hex) to afford undesired ketal **57**, a colorless liquid, as the major isomer (131.4 mg, 0.5911 mmol, 22 % yield): TLC (40 % EtOAc / hex) R_f = 0.27 (UV, Anisaldehyde); the spectral data is in agreement with published literature.⁴⁰⁸



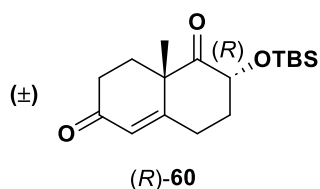
Conditions from entry 4, **Scheme 1.8**

Wieland-Miescher ketone (500. mg, 2.67 mmol) was dissolved in CH₂Cl₂ (3.3 mL) and cooled to -40 °C in a MeCN dry ice bath. (CH₂OTMS)₂ (2.0 mL, 8.0 mmol, 3 equiv.) was added dropwise to the yellow solution, followed by dropwise addition of CH(OEt)₃ (0.50 mL, 3.0 mmol, 1.1 equiv.). After stirring for 1 h, TMSOTf (2 drops) was added, turning the solution pink. After stirring for an additional 3 h, the reaction was quenched with Et₃N (0.4 mL) and raised to rt. The mixture was diluted with sat. aq. NaHCO₃ (10 mL) and extracted with CH₂Cl₂ (3 x 10mL). The combined organic layers were washed with brine (5 mL), dried over Na₂SO₄, and concentrated to yield a yellow liquid. The sample was purified via flash column chromatography (18 % → 100 % EtOAc / hex) to afford desired ketal **56** as a colorless liquid (507.7 mg, 2.284 mmol, 86 % yield):

TLC (60 % EtOAc / hex) R_f = 0.56 (KMnO_4); the spectral data is in agreement with its enantiomer in published literature.⁴⁰⁹



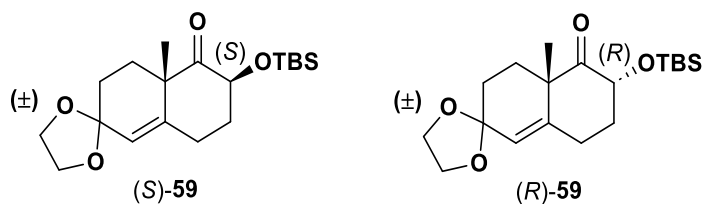
Ketal **56** (50. mg, 0.22 mmol) was dissolved in CH_2Cl_2 (0.75 mL) and cooled to 0 °C in an ice bath.⁴¹⁰ Et_3N (0.16 mL, 1.1 mmol, 5 equiv) was added dropwise to the colorless solution, followed by dropwise addition of TBSOTf (148.6 mg, 0.5623 mmol, 2.5 equiv). The yellow solution was raised to rt. After stirring for 2 h, the reaction mixture was cooled to 0 °C in an ice bath and quenched with sat. aq. NaHCO_3 (5 mL). The mixture was extracted with CH_2Cl_2 (3 x 5 mL), and the combined organic layers were washed with brine (3 mL), dried over Na_2SO_4 , and concentrated to yield immiscible yellow and red liquids. The sample was purified via flash column chromatography (1 % $\rightarrow$ 10 % EtOAc / hex) to afford silyl enol ether **58** as a colorless liquid (50.2 mg, 0.149 mmol, 66 % yield): TLC (5 % EtOAc / hex) R_f = 0.31 (KMnO_4); ^1H NMR (500 MHz, CDCl_3) δ 5.26 (t, J = 1.5 Hz, 1H), 4.67 – 4.60 (m, 1H), 4.05 – 3.96 (m, 2H), 3.96 – 3.92 (m, 1H), 3.92 – 3.83 (m, 1H), 2.34 – 2.23 (m, 1H), 2.13 – 2.02 (m, 3H), 1.95 – 1.80 (m, 3H), 1.73 – 1.58 (m, 1H), 1.22 (s, 3H), 0.92 (s, 9H), 0.15 (s, 3H), 0.13 (s, 3H).



Conditions from entry 1, **Scheme 1.9**

Silyl enol ether **58** (28 mg, 0.083 mmol) was dissolved in CH_2Cl_2 (1.3 mL) and cooled to 0 °C in an ice bath.⁴¹⁰ Acetone (3.25 mL), NaHCO_3 (4.411 g), and H_2O (7.5 mL) were added to a large separate flask. Oxone (6.25 g) was added to the large flask slowly, causing gas evolution in a white suspension. A cannula

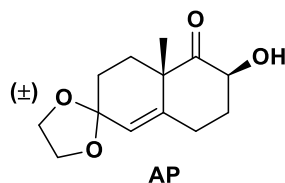
was positioned to connect the two flasks, and positive Ar pressure forced the *in situ* dioxirane gas to bubble through the silyl enol ether solution. Analytical TLC was used to closely monitor the reaction progress. Acetone and Oxone were periodically replenished as needed. After stirring for 2.5 h, the colorless reaction mixture was concentrated. The residue was dissolved in CH₂Cl₂ (1.3 mL) and cooled to 0 °C in an ice bath. CSA (1.0 mg, 0.0042 mmol, 0.05 equiv.) was added to the colorless solution. After stirring for 0.5 h, the yellow solution was quenched with 5 % w / w aq. NaHCO₃ (3 mL). The mixture was extracted with CH₂Cl₂ (3 x 5 mL), and the combined organic layers were washed with brine (5 mL), dried over Na₂SO₄, and concentrated to yield a yellow liquid. The sample was purified via preparatory TLC (40 % EtOAc / hex) to afford deprotected ketone **60** (5.7 mg, 0.018 mmol, 22 % yield, *dr* 3.5 (*R*)-**60** : 1 (*S*)-**59**) with the desired relative stereochemistry in the major isomer confirmed by NOESY: TLC (20 % EtOAc / hex) R_f = 0.30 (KMnO₄); ¹H NMR (500 MHz, CDCl₃) δ 5.85 (s, 1H), 4.60 (dd, *J* = 12.4, 6.2 Hz, 1H), 2.82 (td, *J* = 14.8, 3.9 Hz, 1H), 2.59 – 2.33 (m, 3H), 2.33 – 2.26 (m, 1H), 2.22 (td, *J* = 13.9, 5.3 Hz, 1H), 2.11 (dq, *J* = 14.4, 4.3 Hz, 1H), 1.76 (qd, *J* = 13.2, 3.9 Hz, 1H), 1.44 (s, 3H), 0.92 (s, 9H), 0.16 (s, 3H), 0.06 (s, 3H).



*Conditions from entry 2, **Scheme 1.9***

Silyl enol ether **58** (22 mg, 0.065 mmol) and NaHCO₃ (6.0 mg, 0.072 mmol, 1.1 equiv.) were dissolved in CH₂Cl₂ (0.65 mL) and cooled to 0 °C in an ice bath.⁴¹¹ *m*-CPBA (16.1 mg, 0.0718 mmol, 1.1 equiv.) was added to the colorless solution. After stirring for 0.5 h, the white suspension was washed with sat. aq. Na₂CO₃ (5 mL), sat. aq. Na₂S₂O₃ (5 mL), and brine (5 mL), dried over Na₂SO₄, and concentrated to yield a colorless liquid. The sample was purified via flash column chromatography (40 % EtOAc / hex) to afford ketone **59** (13.4 mg, 0.0380 mmol, 58 % yield, *dr* 2.7 (*S*)-**59** : 1 (*R*)-**59**) with the undesired relative stereochemistry in the major isomer: TLC (20 % EtOAc / hex) R_f = 0.35 (KMnO₄); ¹H NMR (500 MHz,

CDCl₃) δ 5.41 (s, 1H), 4.17 (dd, J = 7.2, 5.6 Hz, 1H), 4.06 – 3.80 (m, 4H), 2.79 – 2.68 (m, 1H), 2.34 – 2.13 (m, 2H), 2.00 – 1.72 (m, 5H), 1.36 (s, 3H), 0.88 (s, 9H), 0.08 (s, 3H), 0.04 (s, 3H).



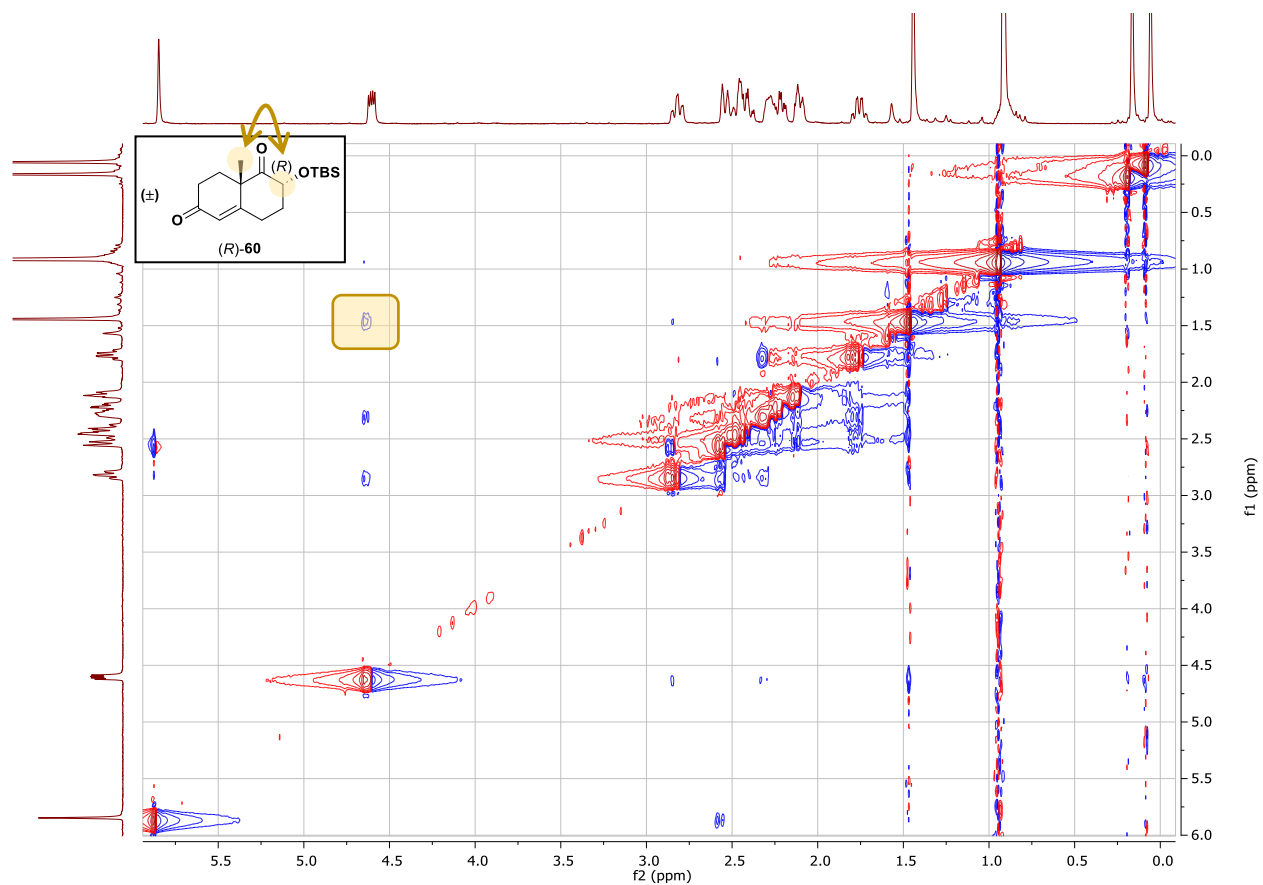
Conditions from entry 4, **Scheme 1.10**

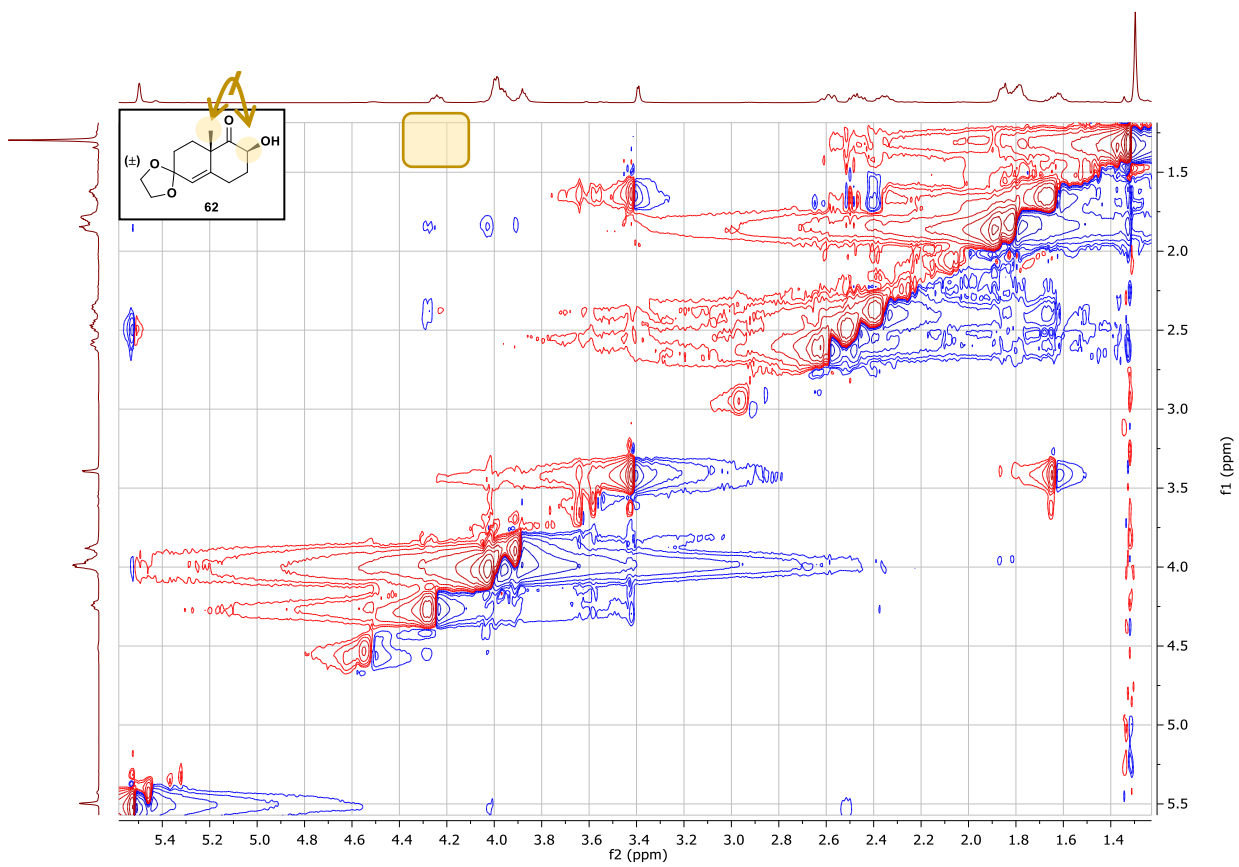
Ketal **56** (150. mg, 0.675 mmol) was dissolved in THF (6.7 mL) and cooled to -78 °C in an acetone dry ice bath.⁴¹² LiHMDS as a 1.5 M solution in THF (0.54 mL, 0.81 mmol, 1.2 equiv.) was added dropwise to the colorless solution. After stirring for 0.5 h, Davis's oxaziridine (215.9 mg, 0.8098 mmol, 1.2 equiv.) was dissolved in THF (0.95 mL) and added dropwise to the reaction mixture. After stirring for an additional 1 h, the reaction was quenched with sat. aq. NH₄Cl (10 mL) and raised to rt. The mixture was extracted with EtOAc (3 x 10 mL), and the combined organic layers were washed with brine (10 mL), dried over Na₂SO₄, and concentrated to yield a yellow liquid. The sample was purified via flash column chromatography (20 % → 100 % EtOAc / hex) to afford α -hydroxyketone **62** as a yellow liquid (60.7 mg, 0.255 mmol, 38 % yield) with the undesired relative stereochemistry confirmed by NOESY: TLC (60 % EtOAc / hex) R_f = 0.27 (KMnO₄); ¹H NMR (500 MHz, CDCl₃) δ 5.49 (s, 1H), 4.24 (ddd, J = 11.8, 7.9, 3.4 Hz, 1H), 4.03 – 3.91 (m, 3H), 3.91 – 3.80 (m, 1H), 3.41 (d, J = 3.6, 1H), 2.66 – 2.53 (m, 1H), 2.53 – 2.40 (m, 1H), 2.40 – 2.29 (m, 1H), 1.93 – 1.55 (m, 5H), 1.29 (s, 3H).

Cited below are the literature precedents which guided the experimental conditions for...

- entry 1, **Scheme 1.7**⁴¹³
- entry 2, **Scheme 1.7**⁴¹⁴
- entries 3 and 4, **Scheme 1.7**⁴¹⁵
- entry 5, **Scheme 1.7**⁴¹⁶
- entry 6, **Scheme 1.7**⁴¹⁷
- entry 1, **Scheme 1.8**⁴¹⁸
- entry 2, **Scheme 1.8**⁴¹⁹
- entry 3, **Scheme 1.8**⁴²⁰

A.3 NOESY NMR Spectra for Selected Intermediates





Appendix B

Corresponding to **Chapter 2. A Day in the Life: Characterization of Doctoral Bench Research in Synthetic Chemistry Using Phenomenological Case Studies**

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B.1 Coding Descriptions

After data collection, Meaningful Actions (MA) were classified with one code each from the Equipment, Technique, and Purpose list.

Some codes were deemed “secondary”, meaning that they were only assigned if no other “primary” code applied. This clarified the coding process for situations where potential overlap might cause inconsistencies during coding.

Primary vs. Secondary examples:

- Manipulating a bump trap did not fall under the secondary “standard glassware” Equipment code but rather the primary “rotatory evaporator” Equipment code.
- Manipulating a separatory funnel did not fall under any primary Equipment codes and so was assigned to “standard glassware”.
- Most chemical additions could technically be classified as a “dissolution” Technique, so an action was only classified as “dissolution” if the action could not be classified under other primary Technique codes (for example, “sonication”).

Meaningful Action = a specific, basic psychomotor action related to accomplishing a task while working in a laboratory

- Coded using sentence-like descriptive text articulating the action and the apparent rationale

Equipment = a tangible object, its integral components, and/or a set of highly related objects used in conjunction with the meaningful action to accomplish a technique or purpose

Technique = a cohesive sequence of meaningful actions to complete a specific procedure in a discrete span of time or a series of repeated meaningful actions spread out across time to meet a common objective

Purpose = an objective that possess value in the macrocosm of the “real-world”, regardless of a specific technique or equipment

Example photos are cropped, grainy, and zoomed in both to focus on the applicable MA and to exclude potentially identifying information about the participants. An example video is also provided to demonstrate the coding process.

B.2 Codebook for Equipment

Table B.1. Codebook for Equipment codes.

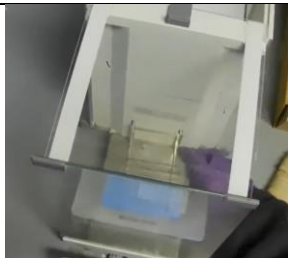
#	Equipment Code	Definition	Primary / Secondary	Applicable MA Example	Image of Applicable MA Example	NOT an Applicable MA Example
E1	Automated column	operating the automated column machine – does not include the column itself	Primary	Adjusting column conditions to finish up faster		Packing frit to be flush - Column
E2	Balance	operating the balance machine – does not include the associated transfer tools (e.g., spatulas, syringes)	Primary	Fixing crooked balance tray to measure mass		Using static gun to stabilize balance measurement - Static gun
E3	Calculator	operating a calculator	Primary	Calculating amounts to determine starting materials		Drawing in chemical drawing software to get molar mass for calculations - Computer
E4	Column	manipulating the components of a column (e.g., frits and attachments) – does not include the automated column machine	Primary	Packing frit to be flush		Adjusting column conditions to finish up faster - Automated column

Table B.1. Codebook for Equipment codes. *[continued]*

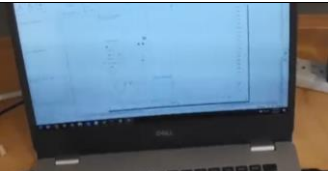
E5	Computer	operating a computer and scientific software	Primary	Calibrating NMR integrals' proton count		Removing safety glasses while working at computer - PPE
E6	Fridge	using a fridge	Primary	Storing compound in fridge to prevent decomposition		Labeling container to keep track of compound identity - Records
E7	Fume hood	operating a fume hood and its built-in utilities (e.g., vacuum line, air line)	Primary	Decreasing air flow to reduce loud annoying sound		Switching line needle to enable a greater flow of inert gas - Schlenk line
E8	Glovebox	operating a glovebox and its built-in components (e.g., antechamber, glovebox gloves)	Primary	Evacuating glovebox chamber to ensure a tight door seal		Taking notes to enable distant work at glovebox - Records

Table B.1. Codebook for Equipment codes. *[continued]*

E9	Heat gun	operating a heat gun	Primary	Warming vial with heat gun to promote evaporation		Warming item with hand so compound melts and is easier to handle - Human body
E10	Human body	using the human body itself directly as the primary tool (e.g., using a hand to test the temperature of hot glass or tapping a finger against a flask to dislodge a stuck chemical)	Secondary	Warming item with hand so compound melts and is easier to handle		Washing hands at sink - In-house utilities
E11	In-house utilities	using a room's non-scientific infrastructure (e.g., cabinets, sinks) – does not include glovebox, fume hood, oven, etc.	Primary	Washing hands at sink		Putting NMR tubes in oven to dry them - Oven
E12	Monkey bars & clamps	adjusting monkey bar, rod clamps, etc.	Primary	Adjusting clamps to hold flask to not fall over		Adjusting thermometer to confirm reaction is at correct temperature - Temperature bath

Table B.1. Codebook for Equipment codes. *[continued]*

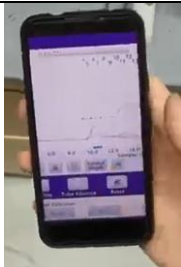
E13	Oven	using an oven	Primary	Putting NMR tubes in oven to dry them		Putting on thermal gloves to prevent hand burn - PPE
E14	Phone	operating a phone for scientific purposes (e.g., as a camera or a timer) – does not include recreational phone use	Primary	Referencing phone photo to decide which fractions to TLC		Removing gloves to protect non-lab materials - PPE
E15	PPE	adjusting personal protective equipment (e.g., lab coat, safety glasses, gloves)	Primary	Putting new gloves on to protect hands		Lowering fume hood sash to conserve energy - Fume hood
E16	Propane torch	operating a hand-held propane torch	Primary	Flaming flask to remove water		Putting on lab coat to work safely with flammable material - PPE

Table B.1. Codebook for Equipment codes. *[continued]*

E17	Records	using or creating records to communicate information to others or to future self	Primary	Labeling NMR cap to prevent sample mix-up		Calculating amounts to determine starting materials - Calculator
E18	Rotatory evaporator	operating a rotatory evaporation machine and its built-in components (e.g., vacuum pump, water bath, bump trap) – does not include the attached flask/vial itself	Primary	Attaching collection flask to collect condensation		Holding magnet to keep stir bar from moving during rotatory evaporation - Stir plate and bar magnet
E19	Schlenk line	operating a Schlenk line and its integral components (e.g., Dewar trap, needles in lines) – does not include the attached flask/vial itself	Primary	Switching line needle to enable a greater flow of inert gas		Preparing septum hookup to use Schlenk line - Sundry items
E20	Solvent system	operating a solvent system (e.g., pump, stopcock) – does not include the associated transfer tools (e.g., syringe)	Primary	Draining solvent flask to get dry solvent		Drawing inert gas into needle to make headspace barrier - Transfer tools – gas

Table B.1. Codebook for Equipment codes. *[continued]*

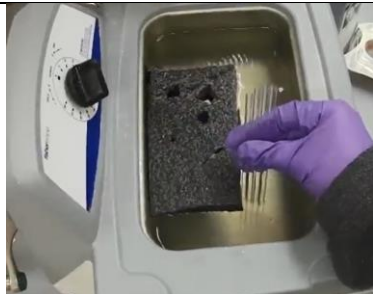
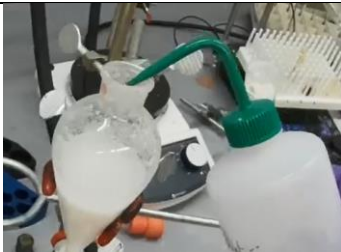
E21	Sonicator	operating a sonicator	Primary	Operating sonicator to dislodge insoluble contaminant		Swirling to dissolve solute - Human body
E22	Standard glassware	adjusting glassware and its integral components (e.g., stopcocks in separatory funnel) – does not include attachments or other connected equipment (e.g., caps, Schlenk line adaptors, rotatory evaporator bump trap)	Secondary	Opening stopcock to drain emulsion onto vacuum filter funnel		Capping flask to prevent a possible spill - Sundry items
E23	Static gun	operating a static gun	Primary	Using static gun to stabilize balance measurement		Fixing crooked balance tray to measure mass - Balance

Table B.1. Codebook for Equipment codes. *[continued]*

E24	Stir plate & bar magnet	operating a stir plate or another magnet to manipulate a stir bar	Primary	Holding magnet to keep stir bar from moving during rotatory evaporation		Rinsing stir bar to retrieve every bit of reaction mixture - Transfer tools – liquid
E25	Sundry items	using (typically small) items not accounted for under other categories and often in conjunction with managing glassware (e.g., caps, tape)	Secondary	Capping flask to prevent a possible spill		Opening stopcock to drain emulsion onto vacuum filter funnel - Standard glassware
E26	Temperature bath	using a cold or hot bath and its integral accessories (e.g., thermometer, dry ice evaporation cover) – does not include when bath is part of another machine (e.g., rotatory evaporator)	Primary	Adjusting thermometer to confirm reaction is at correct temperature		Touching bath and flask to doublecheck temperature - Human body
E27	TLC chamber and stain	using a thin-layer chromatography elution / development chamber or stain solution	Primary	Placing plate in chamber to confirm presence of product in mixture		Using UV light to confirm spotting is heavy enough - UV lamp

Table B.1. Codebook for Equipment codes. [continued]

E28	Transfer tools – gas	using items to move a gas from one location to another (e.g., via syringe headspace)	Primary	Drawing inert gas into needle to make headspace barrier		Drawing solvent into syringe to obtain reagent for reaction - Transfer tools - liquid
E29	Transfer tools – liquid	using items to move a liquid from one location to another (e.g., via syringes, squirt bottles)	Primary	Adding solvent to try to dissolve solid		Drawing inert gas into needle to make headspace barrier - Transfer tools – gas
E30	Transfer tools – solid	using items to move a solid from one location to another (e.g., via spatulas, weigh paper, wipes)	Primary	Scraping mass out of filter with spatula to collect product		Adding solvent to try to dissolve solid - Transfer tools – liquid
E31	UV lamp	using an ultraviolet lamp	Primary	Using UV light to confirm spotting is heavy enough		Dipping TLC plate in stain to reveal non-UV spots - TLC chamber & stain
E32	Waste collector	using a waste collector to segregate hazardous waste	Primary	Collecting used silica in jar to dispose of safely		Preparing cleaning solution to clean TLC spotter - Transfer tools – liquid

B.3 Codebook for Techniques

Table B.2. Codebook for Technique codes.

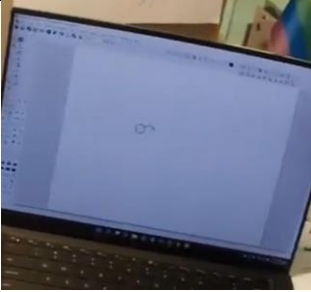
#	Technique Code	Definition	Primary / Secondary	Applicable MA Example	Image of Applicable MA Example	NOT an Applicable MA Example
T1	Air-free mass transfer	preventing a chemical from being exposed to air while transferring from one location to another location	Primary	Drawing inert gas into needle to make headspace barrier		Scraping spatula on flask mouth to get residual to fall off - Mass transfer – solid
T2	Airstream evaporation	using airflow to evaporate a chemical	Primary	Decreasing air flow to reduce loud annoying sound		Switching line needle to enable a greater flow of inert gas - Schlenk line operation
T3	Chemical drawing software usage	operating chemical drawing software to draw and obtain information about chemicals	Primary	Drawing in chemical drawing software to get molar mass for calculations		Calculating amounts to determine starting materials - Notebook management
T4	Cleaning and waste disposal	cleaning up and disposing of hazardous waste	Primary	Collecting used silica in jar to dispose of safely		Attaching collection flask to collect condensation - Rotatory evaporation

Table B.2. Codebook for Technique codes. *[continued]*

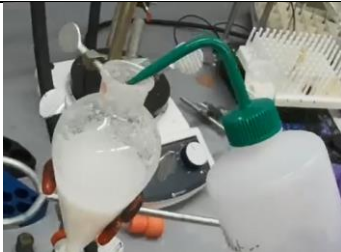
T5	Column chromatography	separating chemicals via column chromatography	Primary	Adjusting column conditions to finish up faster		Pouring fraction into flask for collection - Rotatory evaporation
T6	Dissolution	trying to dissolve a substance, especially one that is not dissolving easily – does not include when a reagent immediately dissolves after addition	Secondary	Adding solvent to try to dissolve solid		Operating sonicator to dislodge insoluble contaminant - Sonication
T7	Glassware drying	removing trace water from glassware	Primary	Putting NMR tubes in oven to dry them		Waving plate to dry it after elution - Thin-layer chromatography
T8	Glovebox operation	operating a glovebox	Primary	Evacuating glovebox chamber to ensure a tight door seal		Adjusting clamps to hold flask to not fall over - Laboratory and workspace management

Table B.2. Codebook for Technique codes. *[continued]*

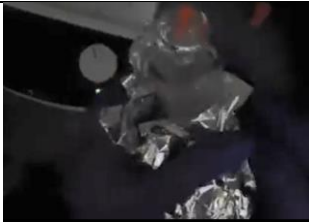
T9	Inventory management	managing lab materials and stock supplies in accordance with accepted conventions	Secondary	Storing compound in fridge to prevent decomposition		Putting NMR tubes in oven to dry them - Glassware drying
T10	Laboratory and workspace management	managing lab infrastructure and general workspace in accordance with accepted conventions	Secondary	Adjusting clamps to hold flask to not fall over		Evacuating glovebox chamber to ensure a tight door seal - Glovebox operation
T11	Light-sensitive reaction management	preventing a chemical from being exposed to light	Primary	Covering flask in aluminum foil to protect light-sensitive reaction		Capping flask to prevent a possible spill - Inventory management
T12	Liquid-liquid extraction	separating chemicals via liquid-liquid extraction	Primary	Adding solvent to make a larger phase		Opening stopcock to drain emulsion onto vacuum filter funnel - Vacuum filtration

Table B.2. Codebook for Technique codes. *[continued]*

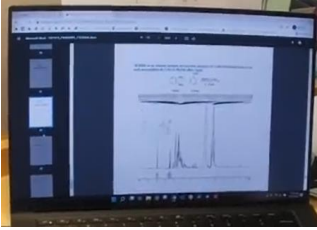
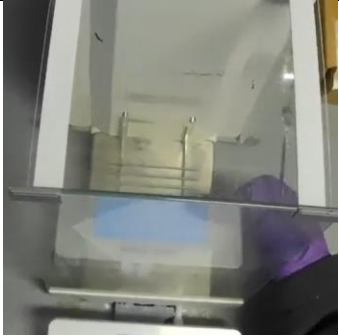
T13	Literature searching	finding information in the literature	Primary	Retrieving NMR data from an article to reference		Drawing in chemical drawing software to get molar mass for calculations - Chemical drawing software usage
T14	Mass measurement – liquid	measuring amount of a liquid	Primary	Pouring solvent into cylinder to measure amount for addition		Pumping cleaning solvent through used syringe before discarding - Cleaning and waste disposal
T15	Mass measurement – solid	measuring amount of a solid	Primary	Getting mass of weigh paper to see how much was not transferred		Scraping spatula on flask mouth to get residual to fall off - Mass transfer – solid
T16	Mass transfer – liquid	moving a liquid from one location to another	Secondary	Depressing pipette bulb repeatedly to get every bit out		Draining solvent flask to get dry solvent - Solvent system operation

Table B.2. Codebook for Technique codes. *[continued]*

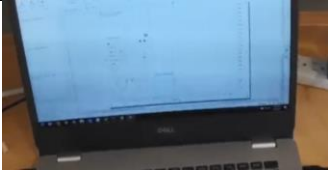
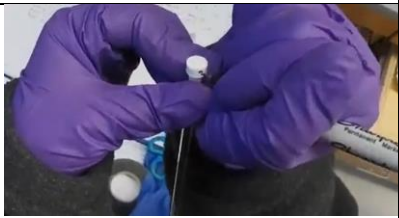
T17	Mass transfer – solid	moving a solid from one location to another	Secondary	Scraping spatula on flask mouth to get residual to fall off		Collecting used silica in jar to dispose of safely - Cleaning and waste disposal
T18	Mass transfer – phase change	manipulating the phase of a chemical to enable mass transfer in a different phase	Secondary	Warming item with hand so compound melts and is easier to handle		Warming vial with heat gun to promote evaporation - Schlenk line operation
T19	NMR analysis	analyzing NMR data	Primary	Calibrating NMR integrals' proton count		Retrieving NMR data from an article to reference - Literature searching
T20	NMR sample preparation	making an NMR solution in an NMR tube	Primary	Labeling NMR cap to prevent sample mix-up		Depressing pipette bulb repeatedly to get every bit out - Mass transfer – liquid
T21	Notebook management	setting up or recording data in experimental notebook	Primary	Calculating amounts to determine starting materials		Drawing in chemical drawing software to get molar mass for calculations - Chemical drawing software usage

Table B.2. Codebook for Technique codes. *[continued]*

T22	PPE management	managing own personal protective equipment	Primary	Putting new gloves on to protect hands		Decreasing air flow to reduce loud annoying sound - Airstream evaporation
T23	Rotatory evaporation	operating a rotatory evaporator to evaporate a substance	Primary	Attaching collection flask to collect condensation		Adding silica to solution for later dry loading - Column chromatography
T24	Schlenk line operation	operating a Schlenk line to apply vacuum or manage inert atmosphere	Primary	Switching line needle to enable a greater flow of inert gas		Drawing inert gas into needle to make headspace barrier - Air-free mass transfer
T25	Solution drying and gravity filtration	removing trace water or filtering off solids from a solution	Primary	Adding sodium sulfate to dry solution		Opening stopcock to drain emulsion onto vacuum filter funnel - Vacuum filtration

Table B.2. Codebook for Technique codes. *[continued]*

T26	Solvent system operation	operating a solvent system to collect dry solvent	Primary	Draining solvent flask to get dry solvent		Depressing pipette bulb repeatedly to get every bit out – Mass transfer – liquid
T27	Sonication	sonicating a mixture to improve homogeneity	Primary	Operating sonicator to dislodge insoluble contaminant		Swirling to dissolve solute - Dissolution
T28	Temperature bath manipulation	monitoring, lowering, or raising the temperature of a reaction – does not include when bath is part of another machine (e.g., rotatory evaporator's warm water bath, Schlenk line vacuum pump's cold dewar)	Secondary	Adjusting thermometer to confirm reaction is at correct temperature		Checking water bath temperature to ensure it is good – Rotatory evaporation

Table B.2. Codebook for Technique codes. *[continued]*

T29	Thin-layer chromatography	separating chemicals via thin-layer chromatography	Primary	Placing plate in chamber to confirm presence of product in mixture		Using phone to take photo of TLC plate for notebook later - Notebook management
T30	Vacuum filtration	applying a vacuum to separate solid and liquid components of a mixture	Primary	Opening stopcock to drain emulsion onto vacuum filter funnel		Applying vacuum to help pack column silica - Column chromatography

B.4 Codebook for Purposes

Table B.3. Codebook for Purpose codes.

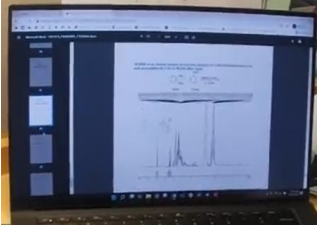
#	Purpose Code	Definition	Primary / Secondary	Applicable MA Example	Image of Applicable MA Example	NOT an Applicable MA Example
P1	Analyze results	using a qualitative or quantitative test to try to determine whether synthesis or purification was successful	Primary	Retrieving NMR data from an article to reference		Labeling NMR cap to prevent sample mix-up - Optimization – analyze results
P2	Avoid contamination	avoiding the potential for contamination to occur, including atmospheric contamination of oxygen, introduction of trace water to glassware, or other avenues for chemical contamination – does not include actively engaging in purification	Primary	Drawing inert gas into needle to make headspace barrier		Applying air to dry out column so silica can be removed - Optimization – avoid contamination
P3	Enable next step only	executing an action with no other Purpose than to operate specialized equipment in order to do the next step of a Technique	Secondary	Switching vacuum to nitrogen to release vial		Writing in notebook to record work - Enable repetition via records

Table B.3. Codebook for Purpose codes. *[continued]*

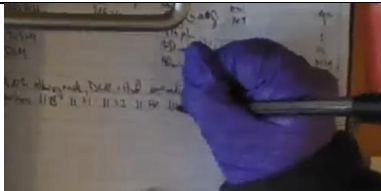
P4	Enable repetition via measurements	measuring materials so as to accurately record what was used or so as to completely use what was recorded as being used	Primary	Pouring solvent into cylinder to measure amount for addition		Writing on glove to remind self of the needed amount – Optimization – enable repetition via measurements
P5	Enable repetition via records	enabling a procedure to be repeated in the future through record-keeping	Primary	Writing in notebook to record work		Labeling NMR cap to prevent sample mix-up - Optimization – analyze results
P6	Maintain work relationships	maintaining positive work relationships by engaging in considerate behaviors for the benefit of labmates	Primary	Cleaning up spilled material under the balance tray		Decreasing air flow to reduce loud annoying sound - Reduce personal annoyance
P7	Maximize product yield	maximizing the amount of product that can be collected or prevent loss of formed product	Primary	Adding solvent to try to dissolve solid		Feeling for a leak from the running column - Optimization – maximize product yield

Table B.3. Codebook for Purpose codes. *[continued]*

P8	<i>Optimization – analyze results</i>	doing something to facilitate analyzing results or to avoid needing to redo a task – does not include actions necessary on the surface to analyze results	Primary	Labeling NMR cap to prevent sample mix-up		Retrieving NMR data from an article to reference – Analyze results
P9	<i>Optimization – avoid contamination</i>	doing something to facilitate avoiding contamination or to avoid needing to redo a task – does not include actions necessary on the surface to avoid contamination	Primary	Applying air to dry out column so silica can be removed		Drawing inert gas into needle to make headspace barrier – Avoid contamination
P10	<i>Optimization – enable repetition via measurements</i>	doing something to facilitate measuring accurately or to avoid needing to redo a task – does not include actions necessary on the surface to measure accurately	Primary	Writing on glove to remind self of the needed amount		Pouring solvent into cylinder to measure amount for addition – Enable repetition via measurements

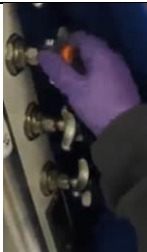
Table B.3. Codebook for Purpose codes. *[continued]*

P11	<i>Optimization – maximize product yield</i>	doing something to facilitate maximizing yield or to avoid needing to redo a task – does not include actions necessary on the surface to maximize product yield	Primary	Feeling for a leak from the running column		Adding solvent to try to dissolve solid – Maximize product yield
P12	<i>Optimization – purify product</i>	doing something to facilitate purifying product or to avoid needing to redo a task – does not include actions necessary on the surface to purify product	Primary	Adjusting column conditions to finish up faster		Applying vacuum to remove residual solvent – Purify product
P13	<i>Optimization – synthesize product</i>	doing something to facilitate synthesizing product or to avoid needing to redo a task – does not include actions necessary on the surface to synthesize product	Primary	Warming item with hand so compound melts and is easier to handle		Calculating amounts to determine starting materials – Optimization – synthesize product

Table B.3. Codebook for Purpose codes. *[continued]*

P14	Preserve amount of supply	avoiding unnecessary loss of expendable materials (e.g., silica gel, starting material, argon atmosphere)	Primary	Trying to recover material stuck in pipette to not waste		Storing compound in fridge to prevent decomposition - Preserve product integrity
P15	Preserve product integrity	preventing product from degrading after formation	Primary	Storing compound in fridge to prevent decomposition		Applying vacuum to remove residual solvent - Purify product
P16	Protect equipment	safeguarding the functionality of equipment	Primary	Hammering dry ice to make sizes fit for rotatory evaporator's condenser		Storing compound in fridge to prevent decomposition - Preserve product integrity
P17	Protect people	safeguarding the health of people	Primary	Collecting used silica in jar to dispose of safely		Cleaning up spilled material under the balance tray - Maintain work relationships

Table B.3. Codebook for Purpose codes. *[continued]*

P18	Purify product	separating desired product from contaminants – does not include avoidance of contamination in general	Primary	Applying vacuum to remove residual solvent		Adjusting column conditions to finish up faster - Optimization – purify product
P19	Reduce personal annoyance	managing a personal source of vexation to be less annoying	Primary	Decreasing air flow to reduce loud annoying sound		Cleaning up spilled material under the balance tray - Maintain work relationships
P20	Synthesize product	initiating a chemical change to try to create a desired product	Primary	Calculating amounts to determine starting materials		Warming item with hand so compound melts and is easier to handle - Synthesize product

B.5 Textual Analysis of Supplemental File “Video Clip with Example Coding”

Table B.4. Textual analysis of coded segments in example video clip.

Meaningful Action	ETP Coding	Rationale
using tweezers to pick up TLC plate to avoid contamination	E: transfer tools – solid T: thin-layer chromatography P: optimization - avoid contamination	A transfer tool (tweezers) is being used to manipulate a TLC plate. This process is the beginning of preparing the materials for thin-layer chromatography. If the tweezers weren't used, the participant would find it harder to keep the TLC plate clean and free of contaminants from their gloves.
marking plate as contaminated to avoid using	E: records T: thin-layer chromatography P: optimization - analyze results	A TLC plate is being marked as contaminated. If the plate wasn't marked, the participant might make a mistake and run TLC using the contaminated plate, meaning they would have to then redo the TLC when they realize it was contaminated upon analysis.
marking a TLC plate to keep track of spots	E: records T: thin-layer chromatography P: analyze results	If the spots' loading locations weren't marked, the participant wouldn't be able to analyze the results accurately.
spotting a TLC plate with standard to determine compound presence	E: transfer tools – liquid T: thin-layer chromatography P: analyze results	If the plate wasn't spotted with standard, the participant wouldn't be able to analyze the results accurately.
spotting a TLC spotter with clean solvent to remove contamination	E: transfer tools – liquid T: cleaning and waste disposal P: avoid contamination	The TLC spotter is being cleaned. If the spotter wasn't cleaned out, future samples would be contaminated the next time the spotter is used.
re-spotting a TLC spotter with solvent to ensure de-contamination	E: transfer tools – liquid T: cleaning and waste disposal P: optimization - avoid contamination	If the spotter wasn't cleaned multiple times, the participant wouldn't be confident about whether it is / isn't actually clean.
marking a TLC plate to keep track of conditions	E: records T: thin-layer chromatography P: enable repetition via records	If the plate wasn't marked with the conditions, the participant wouldn't have a record of the conditions that they should use again in the future.
spotting a TLC plate with mixture to determine composition	E: transfer tools – liquid T: thin-layer chromatography P: analyze results	If the plate wasn't spotted with the crude mixture, the participant wouldn't be able to analyze the results.
waving plate to dry it before elution	E: human body T: thin-layer chromatography P: optimization - analyze results	The participant is using their own body as a tool to provide airflow and encourage the spots to dry quickly. If the plate wasn't waved around, the participant would have to wait longer before beginning elution.

Examples of what was not coded:

- Waiting for the spots to dry
 - This was an unseen cognitive decision. Since it did not physically manifest in a specific psychomotor action within the clip, it did not meet the criteria for coding.
- Rubbing gloved fingers against each other
 - This did not readily offer clear meaning as a separate meaningful action, and so it did not meet the criteria for coding.
- Emptying the spotter of remaining solvent after picking it up from the vial of cleaning solvent
 - Emptying the spotter is a natural and necessary next-step for using the spotter, and so it did not meet the criteria for coding.
- Moving head in closer to view the spot sizes more closely while spotting
 - The action was not directly viewable on the screen (only implied), and so it did not meet the criteria for coding.

B.6 Example Inter- and Intra-Coder Reliability

Figure B.1.

Example temporal analysis of intra- & inter-coder reliability for MA coding.

This is a sample 10-minute video clip's temporal analysis (bottom → top). The clip was coded by the author twice and by a participant once for qualitative intra- & inter-coder reliability in MA coding. Items which aren't physical (i.e., "considering") and therefore couldn't be coded by the author are crossed out.



B.7 Cluster Silhouette Analysis

Figure B.2. Cluster sizes for an 8-cluster model

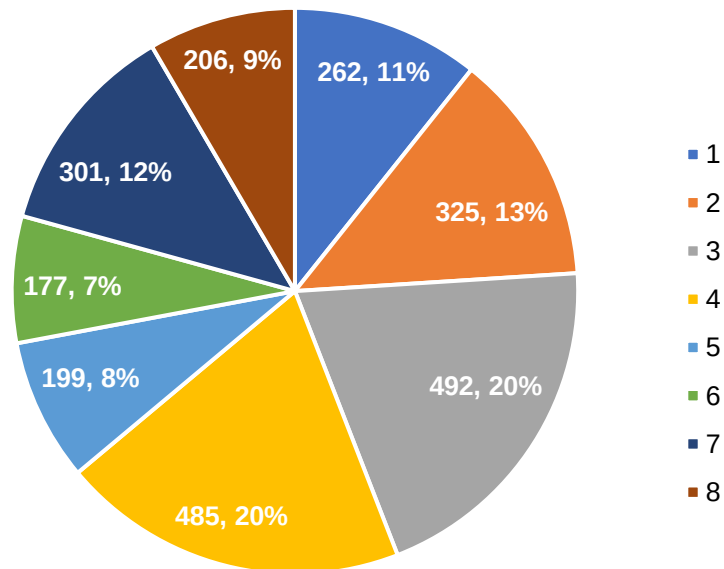
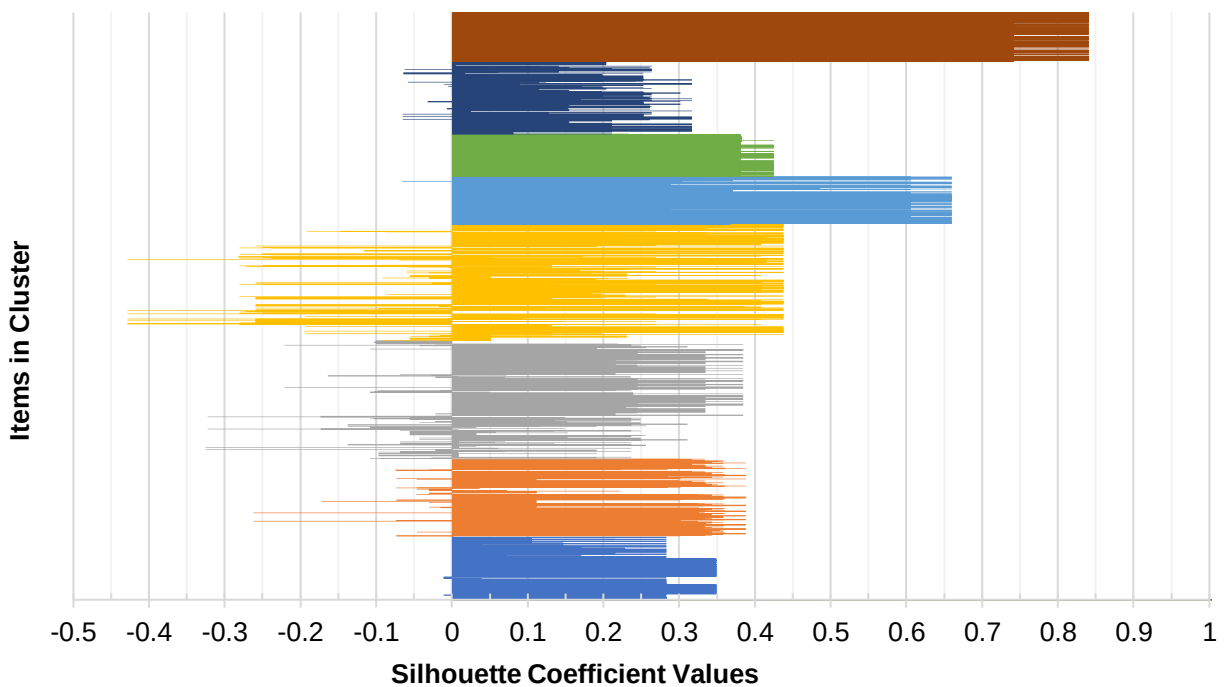


Figure B.3. Silhouette values for an 8-cluster model.



Average $k = .2670$ (8-cluster local maximum k after testing up to 10 clusters)

B.8 Cluster Compositions

Dark blue bars indicate an item's count within the cluster. Light blue backgrounds indicate the item's overall presence in the total data.

Figure B.4. Summary of cluster 1 (“Analyzing NMRs and Preparing Chemicals”).

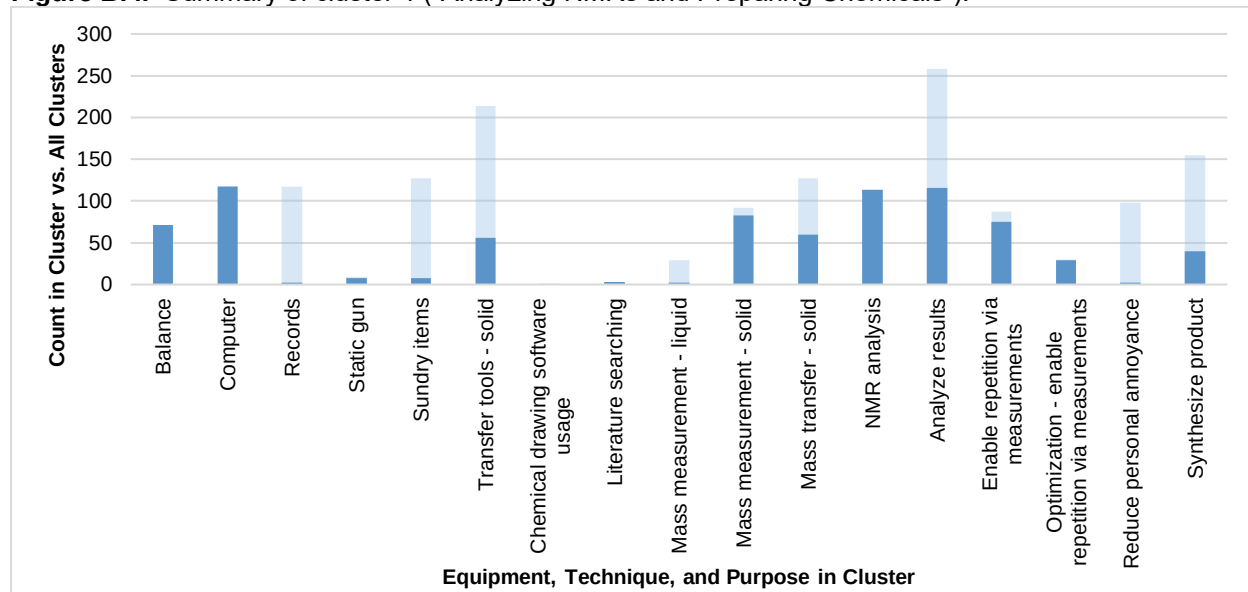


Figure B.5. Summary of cluster 2 (“Making NMRs and Running TLCs”).

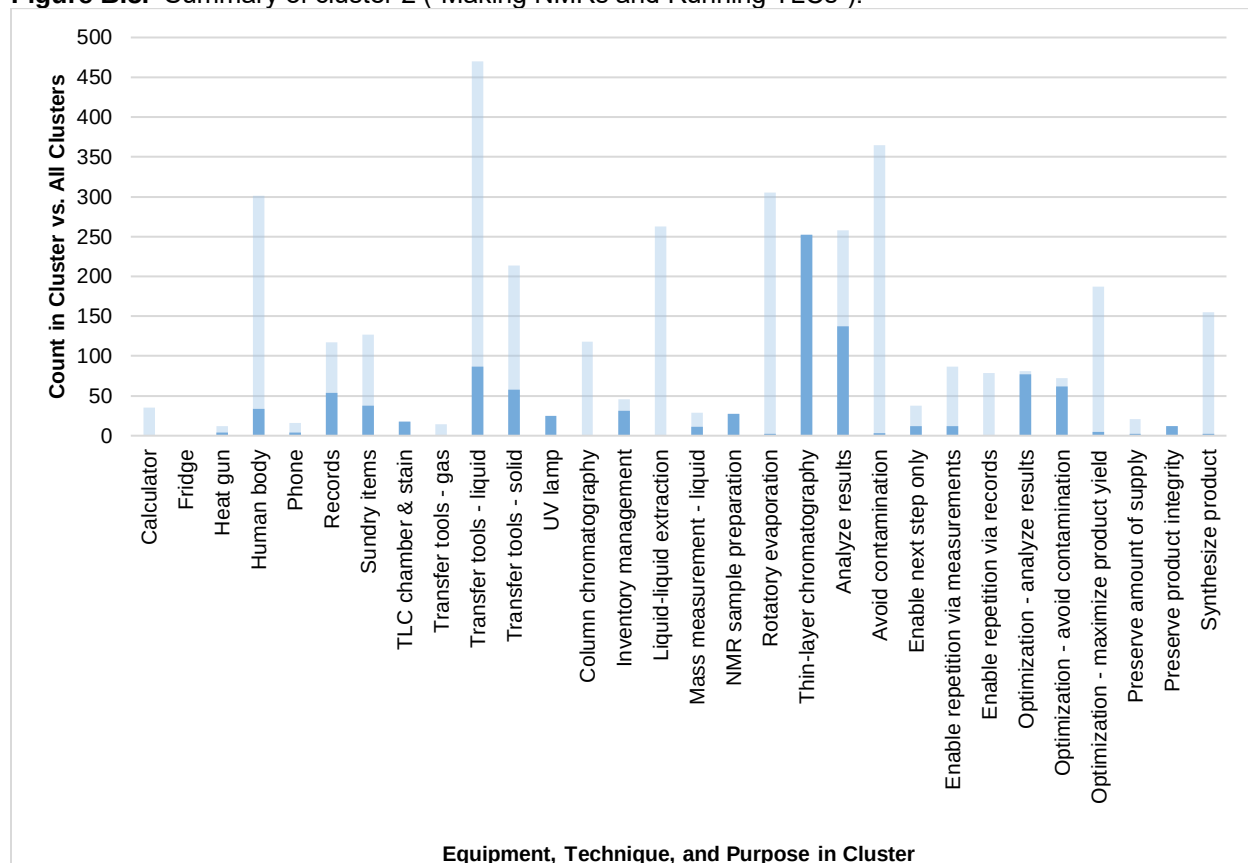


Figure B.6. Summary of cluster 3 (“Purifying Crude Mixtures”).

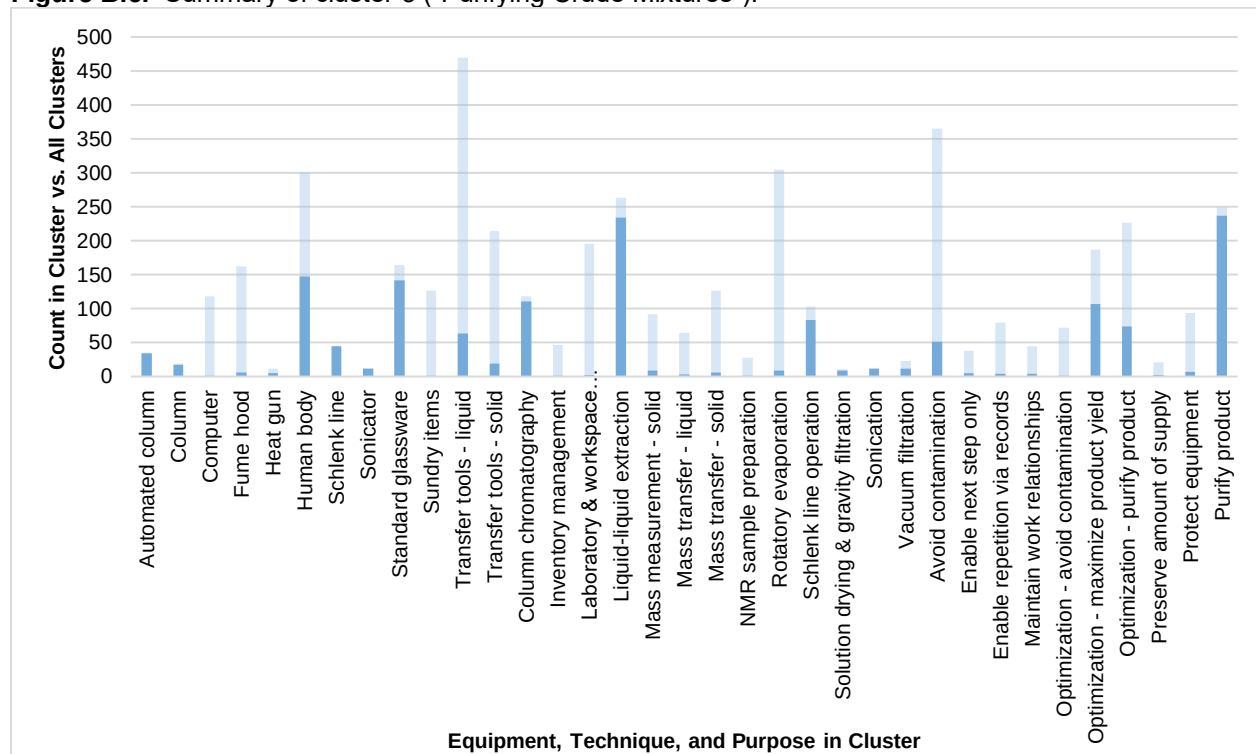


Figure B.7. Summary of cluster 4 (“Using Scientific Equipment and Room Infrastructure”).

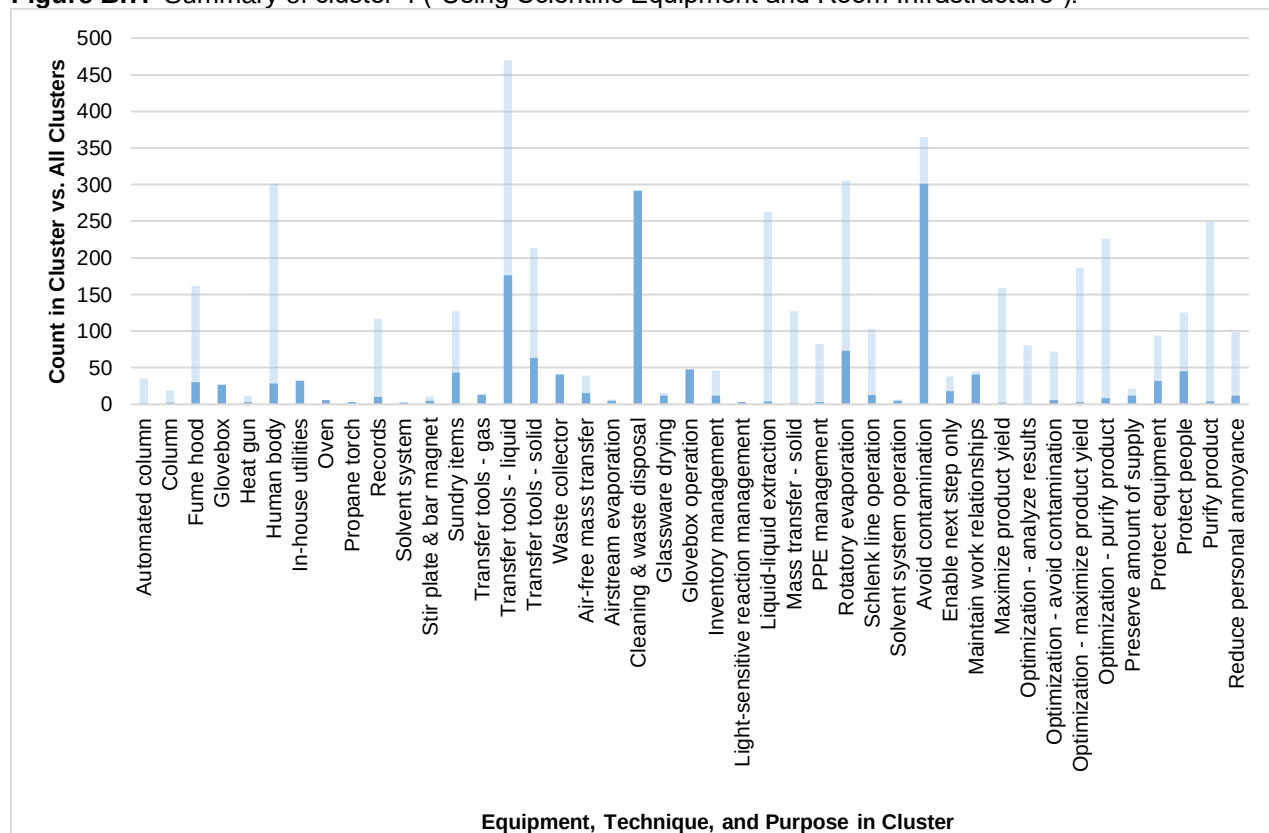


Figure B.8. Summary of cluster 5 (“Working in a Fume Hood”).

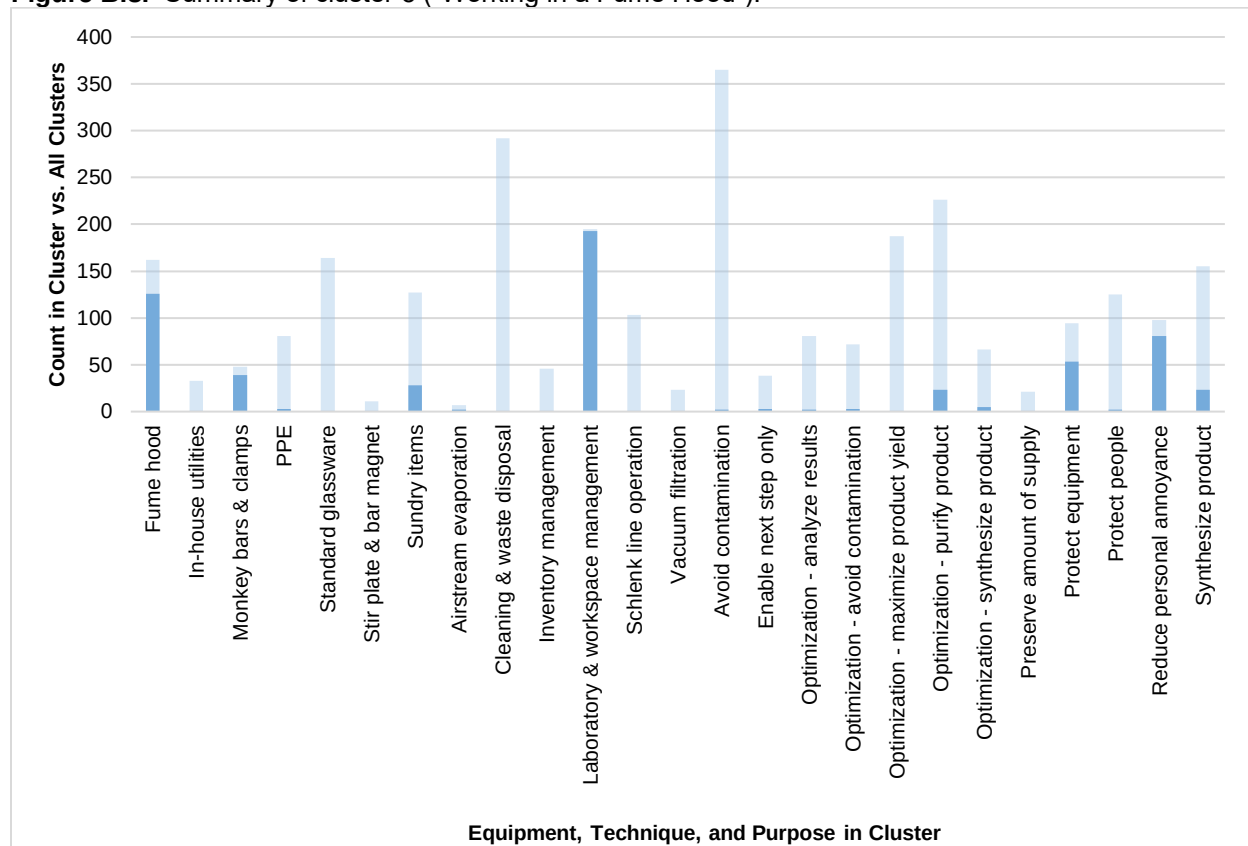


Figure B.9. Summary of cluster 6 (“Staying Safe and Using a Notebook”).

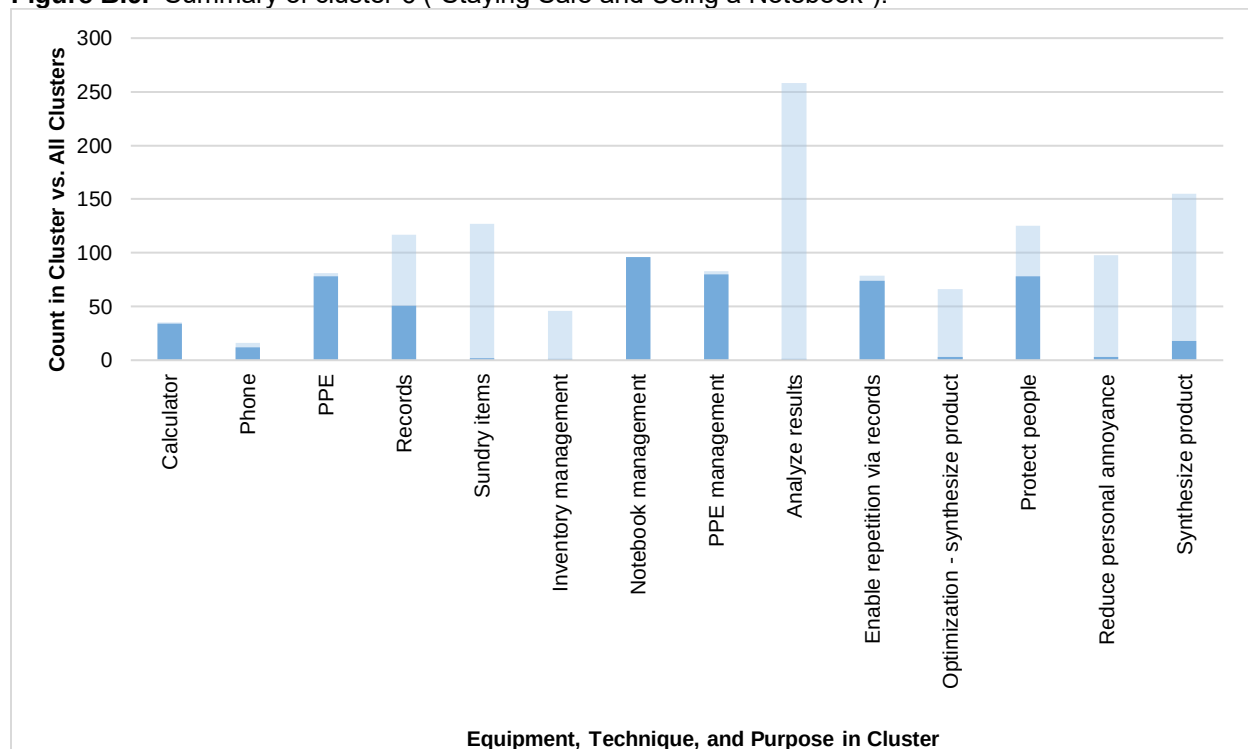


Figure B.10. Summary of cluster 7 (“Setting Up and Monitoring Reactions”).

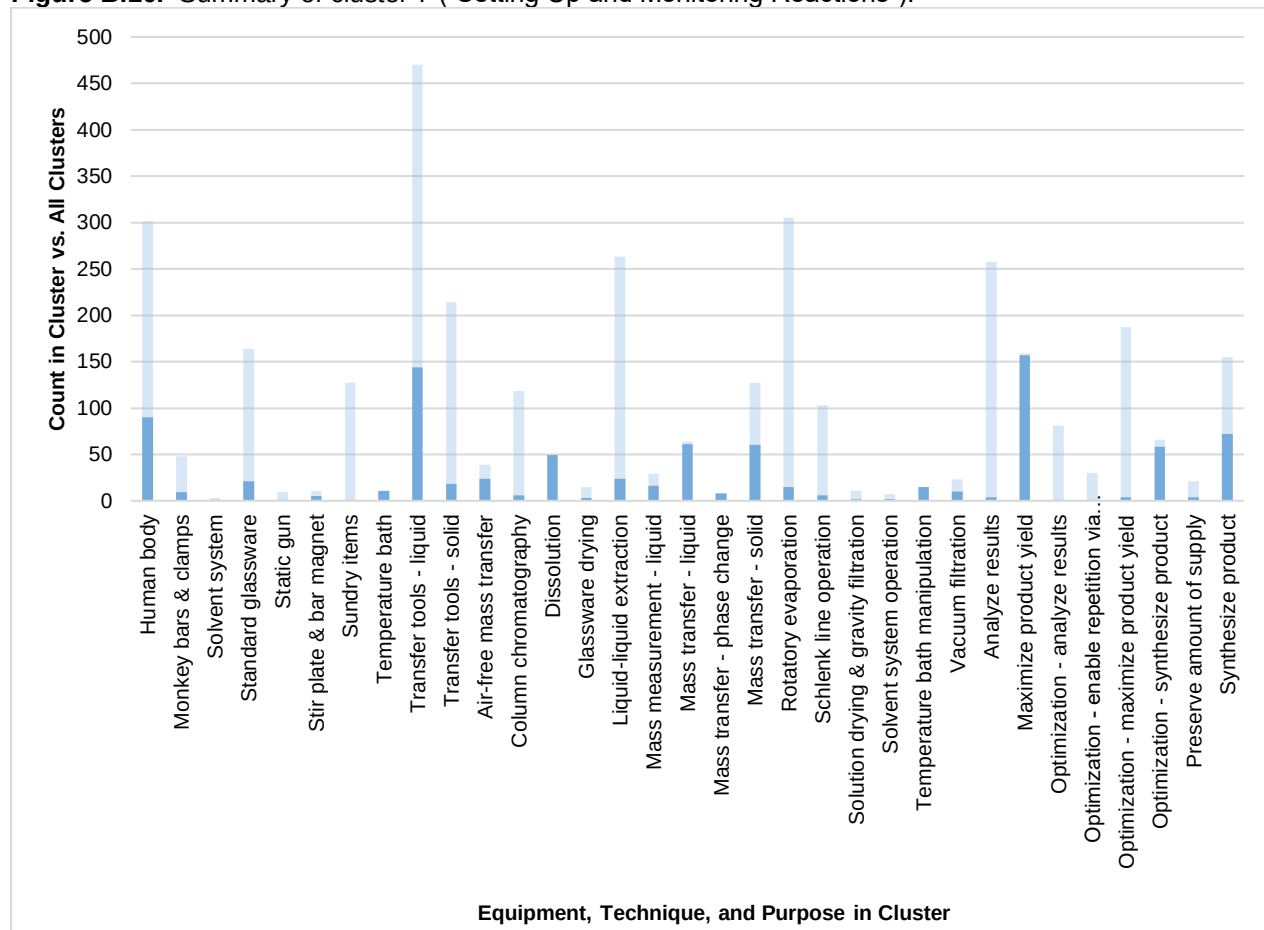
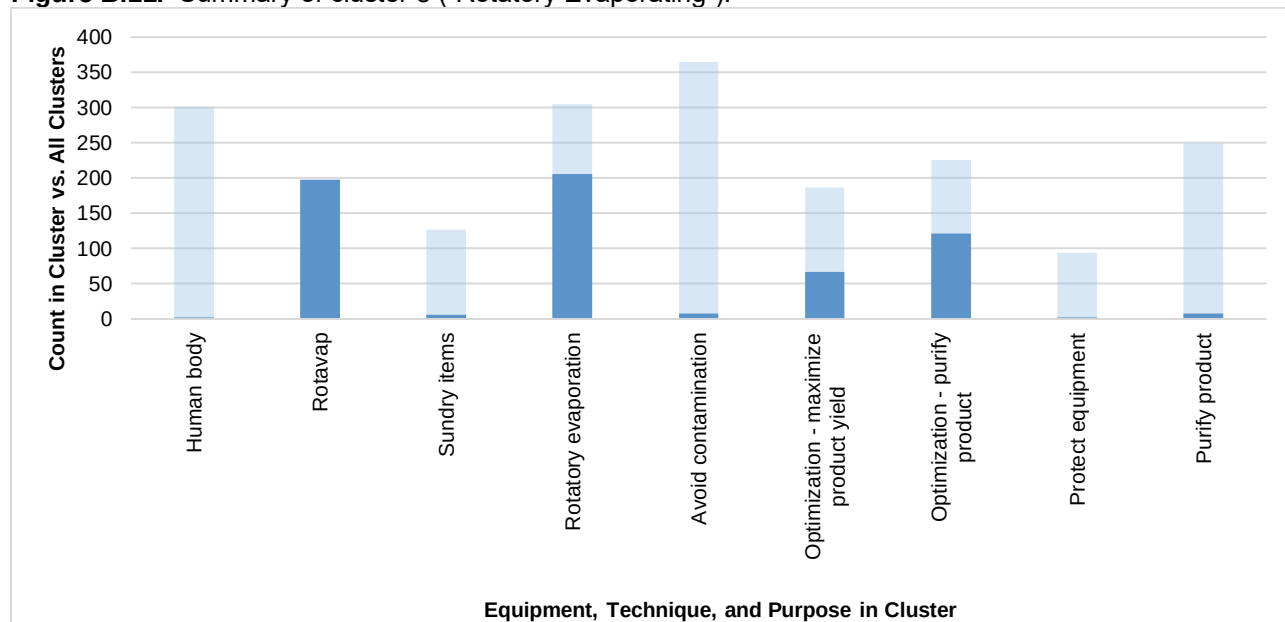


Figure B.11. Summary of cluster 8 (“Rotatory Evaporating”).



Appendix C

Corresponding to **Chapter 3.** Structural Predictors of Safety Behavior in Graduate Student Chemical Researchers

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C.1 Key Informant Interview Guide for Safety Professionals

Discussion Goal

To identify the safety needs/concerns and assets/programs/services that are most salient to safety professionals who have administrative-level perspectives about chemical safety issues facing academic researchers.

Facilitator Instructions - DO NOT READ TO PARTICIPANT

- Be in the Zoom room **10 minutes early** to test your equipment, prepare your timer, prepare your script, and set up your recording (but don't start recording yet).
 - Be in a private and quiet place, booking a conference room or equivalent if necessary.
 - Have the slides ready to screenshare before the participant arrives
 - Have a private timer set that the interviewee cannot see or hear but which you will not miss.
 - Bring and use headphones to keep the interview private.
 - Confirm ahead of time that your **AUDIO ONLY** Zoom recording is set up correctly and working. Be sure to change your Zoom settings so that video recording is turned off and audio recording is on for cloud recording.
 - Practice this before your first interview.
 - Try not to cue certain responses from the interviewee, but don't be a robot.
 - Read the script in a normal voice, and react to what they say. Use a warm tone of voice and smile to appear relatable and friendly.
 - The questions are intended to serve as a **flexible guide, not a rigid script**.
 - Modify/adapt questions as appropriate to the graduate student's focus.
 - Interviews will be recorded so focus on directing the conversation.
 - For each item, probe as indicated and if appropriate.
 - **"Probe:"** questions are only meant to serve as additional possible probes to ask interviewees if they are struggling to articulate a response to the main question. The interviewee may answer the main question fully anyway. If so, do not make the conversation redundant by asking the Probe questions.
 - Keep within the allotted time. Never go over, even if you haven't finished all the questions.
 - Show items in the order on the list. Log which ones you asked immediately afterward.
-

Interviewer Script

[START 60-MINUTE TIMER ONCE THEY ARRIVE]

1) Hi [NAME]! How are you doing today? [PAUSE - RESPOND] Well, thank you for agreeing to be interviewed. I really appreciate your time.[PAUSE]

- So, let me start by introducing myself:
- My name is _____ and I'm a _____ from _____, and today I'm going to be running our interview. But first, just a little background:
- As I mentioned in my email, I'm working with a team of researchers that's exploring how to support the safe research work of graduate students in the chemical sciences.
- Which ultimately will help institutions improve safety outcomes in research labs.

2) As part of our exploration, we are conducting interviews with graduate students and safety professionals to understand different perspectives.

- And then, what we learn through these interviews will help guide the development of a survey which will be sent to universities throughout the U.S.
- Sp the survey—we believe—will help to improve the safe working conditions in research labs by helping us determining which types of safety programs work and which don't.

The purpose of this particular interview is to hear about your experiences and to get feedback on how things function at your university.

- Since we only have so many people on our research team, we can only represent so many perspectives.
- So we need to talk to others, like you, to make sure that we're asking the right questions and providing the right answer choices in our survey.
- Your candid answers will help us improve our survey,
- So we greatly appreciate your help with this! [PAUSE]

3) Our interview will last no more than 60 minutes,

- And you will be compensated for your time with a \$20 Amazon gift card which will be sent via email.

4) We don't expect that there is any risk for you in participating in this study.

- No names or organizations will be connected to anything that anyone says in these discussions.
- We may discuss key themes of aggregated data or share completely anonymized quotes in a journal publication, and your de-identified data may be kept for use in future research.
- Now, before we begin, I'd like to just remind you that your participation is completely voluntary. You may stop at any time, and you will be compensated for your time.

5) Do you have any questions, or would you like me to repeat any of the information I just provided?

IF YES...

[[Answer questions, address concerns]]

IF NO...

Okay great! If you think of anything later, just let me know.

6) So, would you like to continue on and participate in this study?

IF YES...

Great, thank you so much!

IF NO...

Okay not a problem! Thank you so much for your time, we can stop the call now. Have a good day! **[[STOP]]**

7) If you need a moment to change location or to grab headphones, please let me know. Are you in a location where you feel comfortable speaking freely about your experiences at your university? [PAUSE]

IF NO...

Would you like a moment to change your location? We can also reschedule for a different time if you'd prefer.

IF YES...

Great! Alright, one last thing before we begin the interview.

8) As mentioned in the email, we would like to record audio of our session today so that we can make sure our notes are accurate.

- This recording is only for my research team and will be erased once we complete our notes. No one else will have access to it.
- Is this okay with you? [PAUSE]

IF NO...

Okay, I understand, not a problem. Since recording helps us take detailed and accurate notes, we won't be able to proceed with the interview. Thank you so much for your time, though! We can go ahead and end the call. Have a good day! **[[STOP]]**

IF YES...

Great, thank you! We'll start recording now. If you'd like me to stop recording at any point during the interview, feel free to let me know.

- One little note though: because one of our researchers is in California (and they have some very specific regulations about research over there), we're supposed to ask you to try to not use names. So please do your best to say "my university" or "my PI" instead of using their names. It's not a problem if you forget or accidentally slip up, though, we won't keep any of that information in our notes.
- Okay, let's get started! [DELETE THEIR LAST NAME FROM DISPLAYED NAME ON ZOOM CALL - START RECORDING]

Okay, great thanks, let's get started!

Their Work Environment

To begin, can you tell me a bit about what a typical day of work looks like for you?

Probes

- What are your responsibilities?
- Can you tell me a bit about the size and composition of administrative safety departments who deal with laboratories at your institution?
- What kind of management software do you use to organize things like trainings, inspection reports, and lab hazard assessments?

Oftentimes there are liaison-type positions within research groups who serve as a point-of-contact between safety administrators and research groups. If positions like these exist at your institution, can you tell me a little about them?

- **Probes:**
 - What types of people can fill these roles? [student, PI, staff, undergraduate, _____]
 - Is there training for this position?
 - How do people get into this position? [PI appoints them, institution requires someone to be listed, they are voted for by peers, _____]
 - Can you list out what the responsibilities of this position are?
 - What is the term for this position at your institution?
 - Have you heard of any of these other terms? Do they mean something different than _____ **[[THEIR TERM]]**?
 - Lab Safety Officer
 - Lab Safety Contact
 - Lab Safety Delegate
 - Lab Safety Liaison
 - Lab Safety Coordinate
 - Are there any other people within research groups that safety professionals at your university coordinate discussions with on a regular basis who *aren't* the **[[TERM FOR SAFETY LIAISON POSITION]]**? These could include people who have information about controlled substances or radioactive materials that might not be the **[[TERM]]**.
 - Is there a term used to refer to people in these positions?
 - Same position for different hazard groups in admin
-

Training

Can you describe any **general** university-mandated training requirements that students must complete before being able to conduct work in their labs?

- Who provides these trainings?
- What is your opinion of these trainings? Why?
 - **Probe:** As they are, would you feel confident recommending these trainings as a resource? Why or why not?
- Are you aware of any new training initiatives in research department themselves or anywhere else?

Are you aware of any PI-mandated training requirements for students being able to conduct work in their lab, if any?

- Who provides these trainings?
- What is your opinion of these trainings? Why?
 - **Probe:** As they are, would you feel confident recommending these trainings as a resource? Why or why not?

Are there any other entities that have training requirements for students being able to conduct work in a lab?

- Who provides these trainings?
- What is your opinion of these trainings? Why?
 - **Probe:** As they are, would you feel confident recommending these trainings as a resource? Why or why not?

Can you describe any additional training that is available for **lab-specific work**, if any?

- Who provides this training?
- What is your opinion of this training?
- Is this training required?

Can you describe any additional training or other administrative support available for graduate students to access when they start working with **new procedures**, if any?

- What is the format of these trainings?
 - Who provides this training?
 - What is your opinion of this training?
 - Is this training required?
-

Reporting

What reporting resources are available to graduate students? These can be at any level, including the university, department, or group levels.

- What types of things can graduate students use this system to report?
 - Who can make reports using this system?
 - Where do these reports go to?
 - Have you ever received a report for something you didn't expect?
 - What was it for?
 - Why didn't you expect it?
 - What happens when a report is submitted?
 - Follow-up
 - Procedural changes
 - Lab shutdown
 - Changes in social environment
 - What is your opinion of the reporting process? Why?
 - What do you think could be improved?
 - What do you think works well?
 - Are there any special initiatives run by the university, the safety office, individual departments, or anyone else that is meant to encourage students to submit reports?
 - If yes, can you explain them?
-

Relationships

Are there any avenues for students to provide feedback about _____ **[[TERM BELOW]]** of some sort?

- **About safety policies** If so, what are those avenues, and who do they provide the feedback to?
- **About the safety liaison position** If so, what are those avenues, and who do they provide the feedback to?
- **About interacting with EHS professionals** If so, what are those avenues, and who do they provide the feedback to?
- **About inspection reports or findings** If so, what are those avenues, and who do they provide the feedback to?
- **About safety in their lab, other than incident reporting** If so, what are those avenues, and who do they provide the feedback to?

Are there any other ways in which graduate students can be directly involved in organizing or managing safety on a broad level? This could be a student-led safety program or team, a committee of some sort, a social initiative, or anything else.

Can you list the ways that your office stays in contact with graduate students? This could be at your current institution or any other institution that you have experience with.

- Are there any other ways that you think **could** be used to stay in touch with graduate students, but maybe aren't?
-

Encouragement

How do you know who else to contact besides PI?

Does the safety office at your university ever do any inspections or walkthroughs of research lab spaces?

IF YES...

- What do you call these interactions with research groups? (**walk-through, audit, inspection, _____**)
- Can you explain, from beginning to end, the process of one of these **[[NAME]]**?
 - What is the process of followup like?
- What types of value, if any, do you think these **[[NAME]]** provide research groups?
 - **Probe:** Do you feel like they're a good use of your time? WHY/WHY NOT?
- If you could do anything to improve how the **[[NAME]]** works, what would it be?
- Are you aware of any other group that conducts events similar to these? (student groups, PIs, peer labs, _____.)

IF YES...

- Can you explain what this typically entails?
- What types of value, if any, do these events provide research groups?

IF NO...

- Are you aware of any other group that conducts events similar to these? (student groups, PIs, peer labs, _____.)
 - **IF YES...**
 - Can you explain what this typically entails?
 - What types of value, if any, have these events ever provided research groups?

Does the safety office do anything that is meant to encourage graduate students to engage more with safety? This could be some sort of program, an award, or anything.

- Can you tell me a little bit about any programs that other groups might be using to encourage students to be safe, if any?
-

Addressing Top Issues

What do you think are the top issues facing graduate students that contribute to a lack of chemical safety?

IF NONE OR UNSURE...

- Continue to next question

[[Thinking about the top issues you've mentioned,]] what is currently being done to address **[[these issues/chemical safety issues]]** by your safety office or other groups?

- What programs or services are available to graduate students to support their safe research?
- What organizations do you or your university work with to address these issues?

[[Still thinking about the top issues you've mentioned,]] are there any strengths or assets that your university, department, or safety office has that COULD be leveraged to address **[[these issues/chemical safety issues]]** but currently aren't?

If you had all of the resources you needed at your disposal, what would you like to do to help improve safety outcomes for graduate student chemical researchers?

Visions of Assets and Services

What do you see as the biggest **barrier** to addressing the top issues that you mentioned?

- What factors do you think contribute most to this barrier?
 - **Probes:**
 - Cost
 - Infrastructure
 - Legislation/Regulation
 - Access
 - Communication
 - Culture
 - Lack of interest
 - Inequities
- Who do you think has the ability to address these factors?

Thinking about the future, if you could change or implement a new program, service, or policy to address the top issues that you mentioned, what would it be?

- What individuals/organizations do you think should lead this effort?
-

Closing

Thank you so much for your time and for sharing your opinions. We really value your feedback and help in understanding the experiences of graduate students in the chemical sciences. Before we end the discussion, is there anything that you wanted to add that you did not get a chance to bring up earlier, or is there something you think that I should have asked but I didn't?

Alright—well thank you!—those were all my questions.

- After we hang up here, I will send you an email with a PDF that contains the gift card. And in that PDF is a Claim Code; you'll just simply enter that code into your Amazon account, and \$20 will be added to your account.
- If in the future you have any questions about this study, you can contact the project coordinator, Dr. Zinn

[COPY/PASTE IN ZOOM CHAT]

Sarah Zinn

szinn@ucla.edu

- Or if you have any questions about your rights as a research participant, you can contact the UCLA Office of Human Research Protection

[COPY/PASTE IN ZOOM CHAT]

UCLA Office of Human Research Protection

(310) 825-5344

- I've put the contact info in the chat.
- And that's everything I have! Again, thank you so much! We really appreciate your time and feedback today.
- Do you have any other thoughts you'd like to share before we hang up? [PAUSE]

Have a great day, and thanks again!

[STOP RECORDING - ENSURE IT UPLOADED TO ZOOM CLOUD]

[EMAIL THE INTERVIEWEE THEIR GIFT CARD - LOG THAT YOU SENT THE FOLLOW-UP EMAIL]

[TRANSCRIBE THE AUDIO - UPLOAD TRANSCRIPTION - DELETE RE

C.2 Key Informant Interview Guide for Graduate Students

Discussion Goal

To identify the safety needs/concerns and assets/programs/services that are most salient to graduate students who have ground-level perspectives about chemical safety issues facing academic researchers.

Facilitator Instructions - DO NOT READ TO PARTICIPANT

- Be in the Zoom room **10 minutes early** to test your equipment, prepare your timer, prepare your script, and set up your recording (but don't start recording yet).
 - Be in a private and quiet place, booking a conference room or equivalent if necessary.
 - Have the slides ready to screenshare before the participant arrives
 - Have a private timer set that the interviewee cannot see or hear but which you will not miss.
 - Bring and use headphones to keep the interview private.
 - Confirm ahead of time that your **AUDIO ONLY** Zoom recording is set up correctly and working. Be sure to change your Zoom settings so that video recording is turned off and audio recording is on for cloud recording.
 - Practice this before your first interview.
 - Try not to cue certain responses from the interviewee, but don't be a robot.
 - Read the script in a normal voice, and react to what they say. Use a warm tone of voice and smile to appear relatable and friendly.
 - The questions are intended to serve as a **flexible guide, not a rigid script**.
 - Modify/adapt questions as appropriate to the graduate student's focus.
 - Interviews will be recorded so focus on directing the conversation.
 - For each item, probe as indicated and if appropriate.
 - **"Probe:"** questions are only meant to serve as additional possible probes to ask interviewees if they are struggling to articulate a response to the main question. The interviewee may answer the main question fully anyway. If so, do not make the conversation redundant by asking the Probe questions.
 - Keep within the allotted time. Never go over, even if you haven't finished all the questions.
 - Show items in the order on the list. Log which ones you asked immediately afterward.
-

Interviewer Script

[START 60-MINUTE TIMER ONCE THEY ARRIVE]

1) Hello! Thank you for being here today. I really appreciate your time.

- My name is _____ and I'm a _____ from _____.
- How are you doing today? [OR OTHER "How's the weather?" type question to establish conversational tone - THEN PAUSE]
- [RESPOND IF NEEDED - "Oh that's great to hear!", "Oh, I'm sorry to hear that, I hope things turn around soon."]
- Well, as I mentioned in my email, I'm working with a team of researchers who are exploring how to support the safe research work of graduate students in the chemical sciences.
- Which ultimately will help institutions improve safety outcomes in research labs.

2) As part of our exploration, we are conducting interviews with graduate students and safety professionals to understand different perspectives.

- What we learn through these interviews will help guide the development of a survey which will be sent to universities throughout the U.S.
- We expect that the findings from this survey will help to improve the safe working conditions in research labs by determining which types of safety programs work and which don't.

The purpose of this particular interview is to hear about your experiences and to get feedback on how things function at your university or in your research group.

- Since we only have so many people on our research team, we can only represent so many perspectives.
- So we need to talk to others, like you, to make sure that we're asking the right questions and providing the right answer choices in our survey.
- Your candid answers will help us improve our survey,
- So we greatly appreciate your help with this! [PAUSE]

3) Our interview will last no more than 60 minutes,

- And you will be compensated for your time with a \$20 Amazon gift card.

4) We don't expect that there is any risk for you in participating in this study.

- No names or organizations will be connected to anything that anyone says in these discussions.
- We may discuss key themes of aggregated data or share completely anonymized quotes in a journal publication, and your de-identified data may be kept for use in future research.
- Now, before we begin, I'd like to just remind you that your participation is completely voluntary. You may stop at any time, and you will be compensated for your time.

5) Do you have any questions, or would you like me to repeat any of the information I just provided?

IF YES...

[[Answer questions, address concerns]]

IF NO...

Okay great! If you think of anything later, just let me know.

6) So, would you like to continue on and participate in this study?

IF YES...

Great, thank you so much!

IF NO...

Okay not a problem! Thank you so much for your time, we can stop the call now. Have a good day! **[[STOP]]**

7) If you need a moment to change location or to grab headphones, please let me know. Are you in a location where you feel comfortable speaking freely about your experiences at your university or within your group? [PAUSE]

IF NO...

Would you like a moment to change your location? We can also reschedule for a different time if you'd prefer.

IF YES...

Great! Alright, one last thing before we begin the interview.

8) As mentioned in the email, we would like to record audio of our session today so that we can make sure our notes are accurate.

- This recording is only for my research team and will be erased once we complete our notes. No one else will have access to it.
- Is this okay with you? [PAUSE]

IF NO...

Okay, I understand, not a problem. Since recording helps us take detailed and accurate notes, we won't be able to proceed with the interview. Thank you so much for your time, though! We can go ahead and end the call. Have a good day! **[[STOP]]**

IF YES...

Great, thank you! We'll start recording now. If you'd like me to stop recording at any point during the interview, feel free to let me know.

- One little note though: because one of our researchers is in California (and they have some very specific regulations about research over there), we're supposed to ask you to try to not use names. So please do your best to say "my university" or "my PI" instead of using their names. It's not a problem if you forget or accidentally slip up, though, we won't keep any of that information in our notes.
- Okay, let's get started! [DELETE THEIR LAST NAME FROM DISPLAYED NAME ON ZOOM CALL - START RECORDING]

Okay, great thanks, let's get started!

Their Group Environment

To begin, can you tell me a bit about what a typical day of work looks like in your lab?

- Just imagine you walk into the lab, what do you do next?
- What type of hazards do you work with?
- Can you tell me a bit about the size and composition of your research group?
- Is your PI new to your university?

Do you have a person in your group who is in charge of managing safety in your group?

- What is their position in your group? (student, PI, staff, undergraduate, _____)?
 - What kind of training, if any, is provided for this position?
 - How do people get into this position? (PI appoints them, volunteer, institution requires someone to be listed, they are voted for by peers, _____)
 - Can you list out what the responsibilities of this position are?
 - What is the term for this position at your institution?
 - Have you heard of any of these other terms? Lab Safety Officer (LSO), Lab Safety Contact (LSC), Lab Safety Coordinator (LSC)?
-

Training

Are there any general university-mandated training requirements for being able to work in your lab?

- Who provides these trainings?
- What is your opinion of these trainings? Why?
 - **Probe:**
 - Have you ever been working in your lab space and thought specifically about what you learned in these trainings?
 - Would you recommend these trainings as a resource? Why?

Can you describe any PI-mandated training requirements for being able to work in your lab, if any?

From your perspective, what is the most hazardous procedure that you've worked with in your lab?

- Can you describe any additional training or knowledge-gathering procedures, both formal and informal, that you went through when you started working with this procedure, if any?
 - **IF FORMAL...**
 - Who provided this training?
 - What is your opinion of this training?
 - **Probe:** Would you recommend it to someone else, why or why not?
 - **IF INFORMAL...**
 - What did this training look like?
 - Who provided it?
 - What resources, if any, did you access to help you get oriented with the safety aspects of the procedure?
 - **Probes:**
 - Other lab members
 - Other labs
 - Youtube
 - Peer-reviewed literature
 - Books, manuals
 - Existing protocol documents created by others
- When you have questions about working safely with this hazard, who would you go to?
 - **Probes:**
 - Other students
 - Principal investigator
 - Safety professionals
 - Online resources
 - External organizations or contacts
 - Why do you choose to go to this resource with questions?

Have you ever needed to work with a protocol that was new to your lab group?

- Can you explain what the process was like to start this new protocol?
 - Can you describe any processes that were triggered by starting this new protocol, if any?
Perhaps through the university or your research group?

If there is anything that you work with that you still feel unsure of how to handle appropriately, what do you think would help better prepare you? This can be on any level, be it in your group, at your university, within the safety department, or anywhere else.

Reporting

What reporting resources are available to you? These can be at any level, including the university, department, or group levels.

- Have you ever used any of these systems? **WHY?**

IF YES or SOMEONE ELSE REPORTS...

- What happened after the report was submitted?

■ **Probes:**

- Follow-up
- Procedural changes
- Lab shutdown
- Changes in social environment

IF NO & HAS EXPERIENCED INCIDENT...

- Why didn't you report your **[[INCIDENT/INJURY]]**?
 - Is there anything that could be done differently at your university, department, or group that would encourage you to submit reports, even minor ones?
-

Relationships

In what ways, if any, are students at your university involved in safety?

• **Probes:**

- Are there any avenues for students to provide feedback of some sort?
- Are there any student-led safety programs?
- Are they on any sort of committees?

Often at universities there are various groups that are interested in maintaining communication with graduate students. These groups might be student groups, ombudspeople, departmental administration, university administration, external companies, or anyone else that is interested in maintaining an ongoing relationship with the graduate student body.

- Can you list the ways in which these groups, people, or organizations stay in contact with graduate students? This could be at your current institution or any other institution that you have experience with.
 - Are there any other ways that you think **could** be used to stay in touch with graduate students, but maybe aren't?
-

Encouragement

Does anyone from the safety office at your school ever check out your lab space or walk through it?

IF YES...

- What do you call these interactions with the safety office? (**walk-through, audit, inspection,** _____)
- Can you explain what the **[[NAME]]** typically entails?
- What value, if any, have these **[[NAME]]** ever provided you or your group?
 - **Probe:** Do you feel like they're a good use of your time? WHY/WHY NOT?
- Are you aware of any other group that conducts events similar to these? (student groups, PIs, peer labs, _____.)

IF YES...

- Can you explain what this typically entails?
- What value, if any, have these events ever provided you or your group?

IF NO...

- Are you aware of any other group that conducts events similar to these? (student groups, PIs, peer labs, _____.)
 - **IF YES...**
 - Can you explain what this typically entails?
 - What value, if any, have these events ever provided you or your group?

What types of verbal OR nonverbal interactions have you experienced that have encouraged you to engage more in safety behavior? **WHY?**

- **Probes:**
 - Official award by university, department, group, or outside organization
 - Reporting procedures
 - Interpersonal interactions
 - **[[IF RELEVANT AND NOT EXPLAINED ALREADY]]:** Who was this interaction with?
 - (PI, post-doc, peer graduate student, university leadership, department leadership, safety professional, outside organization, _____)
- What other types of recognition do you feel would encourage you to engage more with safety?

What types of verbal OR nonverbal interactions have you experienced that have **discouraged** you? **WHY?**

- **Probes:**
 - Official award by university, department, group, or outside organization
 - Reporting procedures
 - Interpersonal interactions
 - **[[IF RELEVANT AND NOT EXPLAINED ALREADY]]:** Who was this interaction with?
(PI, post-doc, peer graduate student, university leadership, department leadership, safety professional, outside organization, _____)
-

Addressing Top Issues

What do you think are the top issues facing graduate students that contribute to a lack of chemical safety?

IF NONE OR UNSURE...

- Continue to next question

[[Thinking about the top issues you've mentioned,]] what is currently being done to address **[[these issues/chemical safety issues]]** in your university, department, or research group?

- What programs or services are available to graduate students to support their safe research?
- What organizations do you or your university, department, or research group work with to address these issues?

[[Still thinking about the top issues you've mentioned,]] what are the strengths or assets that your university, department, or research group has that could be leveraged to address **[[these issues/chemical safety issues]]**?

Vision of Assets and Services

What do you see as the biggest **barrier** to addressing the top issues that you mentioned?

- What factors do you think contribute most to this barrier?
 - **Probes:**
 - Cost
 - Infrastructure
 - Legislation/Regulation
 - Access
 - Communication
 - Culture
 - Lack of interest
 - Inequities
- Who do you think has the ability to address these factors?

Thinking about the future, if you could change or implement a new program, service, or policy to address the top issues that you mentioned, what would it be?

- What individuals/organizations do you think should lead this effort?
-

Closing

Thank you so much for your time and for sharing your opinions. We really value your feedback and help in understanding the experiences of graduate students in the chemical sciences. Before we end the discussion, is there anything that you wanted to add that you did not get a chance to bring up earlier, or is there something you think that I should have asked but I didn't?

Alright, those were all my questions.

- After we hang up here, I will send you an email with a PDF that contains the gift card. In the PDF is a Claim Code; simply enter the code into your Amazon account, and \$20 will be added to your account.
- If in the future you have any questions about this study, you can contact the project coordinator, Dr. Zinn
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- Or if you have any questions about your rights as a research participant, you can contact the UCLA Office of Human Research Protection
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UCLA Office of Human Research Protection
(310) 825-5344
- I've put the contact info in the chat.
- And that's everything I have! Again, thank you so much! We really appreciate your time and feedback today.
- Do you have any other thoughts you'd like to share before we hang up? [PAUSE]

Have a great day, and thanks again!

[STOP RECORDING - ENSURE IT UPLOADED TO ZOOM CLOUD]

[EMAIL THE INTERVIEWEE THEIR GIFT CARD - LOG THAT YOU SENT THE FOLLOW-UP EMAIL]

[TRANSCRIBE THE AUDIO - UPLOAD TRANSCRIPTION - DELETE RECORDING]

C.3 Cognitive Interview Guide

Discussion Goals

For scale: To identify how chemistry graduate students interpret a set of questions about safety behavior.

For survey: To identify how chemistry graduate students & safety professionals interpret a set of questions about safety training, laboratory groups, etc. on our overall survey (minus the scale questions).

Interviewer Instructions - DO NOT READ TO PARTICIPANT

- Be in the Zoom room **10 minutes early** to test your equipment, prepare your timer, prepare your script, and set up your recording (but don't start recording yet).
 - Be in a private and quiet place, booking a conference room or equivalent if necessary.
 - Have the slides ready to screenshare before the participant arrives.
 - Have the list of questions ready (don't show to participant).
 - Have a private timer set that the interviewee cannot see or hear but which you will not miss.
 - Bring and use headphones to keep the interview private.
 - Confirm ahead of time that your **AUDIO ONLY** Zoom recording is set up correctly and working. Be sure to change your Zoom settings so that video recording is turned off and audio recording is on for cloud recording.
 - Practice this before your first interview.
 - Keep your video on to help promote a human connection.
 - Try not to cue certain responses from the interviewee, but don't be a robot.
 - Read the script in a normal voice, and react to what they say. Use a warm tone of voice and smile to appear relatable and friendly.
 - The questions are intended to serve as a **flexible guide, not a rigid script**.
 - Modify/adapt questions as appropriate to the graduate student's focus.
 - Interviews will be recorded so focus on directing the conversation.
 - For each item, probe as indicated and if appropriate.
 - **"Probe:"** questions are only meant to serve as additional possible probes to ask interviewees if they are struggling to articulate a response to the main question. The interviewee may answer the main question fully anyway. If so, do not make the conversation redundant by asking the Probe questions.
 - Keep within the allotted time. Never go over, even if you haven't finished all the questions.
 - Show items in the order on the list. Log which ones you asked immediately afterward.
-

Interviewer Script

[START 60-MINUTE TIMER ONCE THEY ARRIVE, DELETE THEIR LAST NAME]

1) Hello! Thank you for being here today. I really appreciate your time.

- My name is _____ and I'm a _____ from _____.
- How are you doing today? [OR OTHER "How's the weather?" type question to establish conversational tone - THEN PAUSE]
- [RESPOND IF NEEDED - "Oh that's great to hear!", "Oh, I'm sorry to hear that, I hope things turn around soon."]
- Well, as mentioned in the email, I'm working with a team of researchers who are exploring how to support the safe research work of graduate students in the chemical sciences.
- Which ultimately will help institutions improve safety outcomes in research labs.

2) As part of our exploration, we are conducting interviews with graduate students and safety professionals to understand different perspectives.

- What we learn through these interviews will help guide the development of a survey which will be sent to universities throughout the U.S.
- The survey will help to improve the safe working conditions in research labs by determining which types of safety programs work and which don't.

The purpose of this particular interview is to get some information on how graduate students and safety professionals interpret questions that are currently under development for the survey.

- People who write survey questions already know what they think questions mean, which can sometimes make it difficult to notice when questions are unclear or imprecise.
- So, one way to find out whether survey questions are working how we intended is to have other people test drive the questions.
- I'll ask you to read and answer some of our survey questions, just as you would on any survey that you would take. But then, after each survey question, I will ask you questions like how hard or easy it was to answer and what you thought the question was asking about so that I can discover whether the question has any problems that need fixing.
- Rest assured that this is a test of the questions I've written, not a test of you or your responses.
- I really appreciate your help with this! [PAUSE]

3) Our interview will last no more than 60 minutes,

- And you will be compensated for your time with a \$20 Amazon gift card.

4) We don't expect that there is any risk for you in participating in this study.

- No names or organizations will be connected to anything that anyone says in these discussions.
- We may discuss key themes of aggregated data or share completely anonymized quotes in a journal publication, and your de-identified data may be kept for use in future research.
- Now, before we begin, I'd like to just remind you that your participation is completely voluntary. You may stop at any time, and you will be compensated for your time.

5) Do you have any questions, or would you like me to repeat any of the information I just provided?
[PAUSE]

IF YES...

[[Answer questions, address concerns]]

IF NO...

Okay great! If you think of anything later, just let me know.

6) So, would you like to continue on and participate in this study? [PAUSE]

IF YES...

Great, thank you so much!

IF NO...

Okay not a problem! Thank you so much for your time, we can stop the call now. Have a good day! **[[STOP]]**

7) If you need a moment to change location or to grab headphones, please let me know. Are you in a location where you feel comfortable speaking freely about your experiences at your university or within your group? [PAUSE]

IF NO...

Would you like a moment to change your location? We can also reschedule for a different time if you'd prefer.

IF YES...

Great! Alright, one last thing before we begin the interview.

8) As mentioned in the email, we would like to record audio of our session today so that we can make sure our notes are accurate.

- This recording is only for my research team and will be erased once we complete our notes. No one else will have access to it.
- Is this okay with you? [PAUSE]

IF NO...

Okay, I understand, not a problem. Since recording helps us take detailed and accurate notes, we won't be able to proceed with the interview. Thank you so much for your time, though! We can go ahead and end the call. Have a good day! **[[STOP]]**

IF YES...

Great, thank you! We'll start recording now. If you'd like me to stop recording at any point during the interview, feel free to let me know.

- One little note though: because one of our researchers is in California (and they have some very specific regulations about research over there), we're supposed to ask you to try to not use names. So please do your best to say "my university" or "my PI" instead of using their names. It's not a problem if you forget or accidentally slip up, though, we won't keep any of that information in our notes.
 - Okay, let's get started! [DELETE THEIR LAST NAME FROM DISPLAYED NAME ON ZOOM CALL - START RECORDING]
-

9) I will now share my screen to show you the questions one-by-one. [SCREENSHARE SLIDES, STARTING ON BLUEPRINTS SLIDE]

- Here are the blueprints for how we will format our discussion today. First, I'd like you to do your best to answer the question that is presented to you, and then I will ask you follow-up questions about how you arrived at your answer.
- I will ask you...
 - *what* the item meant to you,
 - *what* the item made you think of,
 - *why* you decided on your specific answer, and
 - finally how *easy or difficult* the question was to answer.
- A couple things for you to keep in mind:
 - Sometimes my questions may seem a little redundant, as if you feel you already answered that question. My reason for asking similar questions is to try to probe what you are thinking from multiple angles. So please be patient with me and just answer the question again even if it seems redundant :)
 - Also, please try to answer as honestly as you can. Your answers help us improve the questions and the survey overall, so answering truthfully is very helpful to us.
 - Finally, as much as possible, voice out loud what is going through your mind as you are trying to answer. Sometimes, this might even be something that you might think sounds a little rude, like "What a stupid question!" or "How should I know?," but if this is truly your immediate reaction, please do say so! We are evaluating the questions, not you, and if this is what the item makes you feel, we really do want to know that!
- Any questions so far? [PAUSE]

10) Okay, great. Let's start with a practice question, which I'll go through myself to show you how things work.

- Okay, "How many bathrooms do you have in your house?"
 - Hmm, I'll say 1 bathroom.
 - And now I'll respond to the follow-up questions:
 - ***What does this item mean to you?*** Well, I took it to mean, what is the number of full-sized bathrooms that are in the place that I'm currently living in.
 - ***What were you thinking about when you decided on your answer?*** Well, it made me think about my current living situation and some of my past living situations, too. It also made me think about what is generally considered a "bathroom".
 - ***How did you decide to pick that answer over the other possible answers?*** Well, really in my current living situation there is a full sized bathroom as well as a powder room so really I think it's more accurate to say that I have one and a half bathrooms, but since that wasn't an option, I just choose 1 bathroom.
 - ***Did you have any difficulty answering the question, and why?*** Well, I thought this question was actually pretty unclear and difficult to answer. I wasn't sure if half bathrooms counted, and the answer choices didn't really contain what I needed to answer the question accurately. Plus, I actually just rent a room in someone else's house, so when the question said "your house" it didn't really apply to me.
 - Okay, do you have any questions about how I answered those questions?
-

11) Now let's do our real questions.

- Just so you know, the slides are organized randomly, and each interviewee will only see a random subset of slides. So, for the purposes of my notes, I'll say the slide number out loud.
 - [SPEAK THE SLIDE NUMBER OUT LOUD]
- Please read and then say which answer you would select for the following item.
 - [AFTER THEY READ & ANSWER THE ITEM: FOR EACH ITEM, ASK THE FOLLOWING FOUR TYPES OF QUESTION, A-D]

(A) What does this item mean to you? [FOR "UNDERSTANDING"]

- **Probe:** How would you rephrase this item in your own words? What does this item refer to? What does it mean?
- **If instructions slide:** What does this item mean to you?

(B) What were you thinking about when you decided on your answer? [FOR "RETRIEVAL"]

- **Probe:** What thoughts or memories did this item (or the answer options) bring into your head?
- **If instructions slide:** What do you expect you will be thinking about when you answer the upcoming questions?

(C) How did you decide to pick that answer over the other possible answers? [FOR "JUDGMENT"]

- **Probe:** What about this item (or the answer options) made your answer seem like the best option?
- **If instructions slide:** [SKIP]

(D) Did you have any difficulty answering the question, and why? [FOR "RESPONSE"]

- **Probe:** Would you change anything about this item (or the answer options) to make answering the item easier or clearer? If so, what and why?
 - **If instructions slide:** [SKIP]
-

[STOP SCREEN-SHARING BY THE 55-MINUTE MARK]

12) Alright, those were all my questions.

- After we hang up here, I will send you an email with a PDF that contains the gift card. In the PDF is a Claim Code; simply enter the code into your Amazon account, and \$20 will be added to your account.
- If in the future you have any questions about this study, you can contact the project coordinator, Dr. Zinn

[COPY/PASTE IN ZOOM CHAT]

Sarah Zinn

szinn@ucla.edu

- Or if you have any questions about your rights as a research participant, you can contact the UCLA Office of Human Research Protection

[COPY/PASTE IN ZOOM CHAT]

UCLA Office of Human Research Protection
(310) 825-5344

- I've put the contact info in the chat.
- And that's everything I have! Again, thank you so much! We really appreciate your time and feedback today.
- Do you have any other thoughts you'd like to share before we hang up? [PAUSE]

Have a great day, and thanks again!

[STOP RECORDING - ENSURE IT UPLOADED TO ZOOM CLOUD]

[LOG WHICH QUESTIONS YOUR INTERVIEWEE ANSWERED]

[EMAIL THE INTERVIEWEE THEIR GIFT CARD - LOG THAT YOU SENT THE FOLLOW-UP EMAIL]

[TRANSCRIBE THE AUDIO - UPLOAD TRANSCRIPTION - DELETE RECORDING]

C.4 Example Slides for Cognitive Interviews

Practice slides:

For each item:

1. Answer to the best of your ability.
2. I will ask you follow-up questions about...
 - What the item meant to you
 - What the item made you think of
 - Why you decided on your specific answer
 - How *easy or difficult* the item was to answer

1

Practice: How many bathrooms do you have in your house?

0 1 2 3 4

2

Example slides: *Scale* (students)

Do you know where you stand with your PI and do you usually know how satisfied your PI is with what you do?

Rarely Occasionally Sometimes Fairly Often Very Often

3

Helping to teach safety procedures to new group members

Strongly Disagree Neither Agree nor Disagree Strongly Agree

A B C D E F G

12

Example slides: *Survey* (SPs)

Are you familiar with the research safety operations and policies involving research laboratories in the Department of Chemistry at your current institution?

☐ Yes ☐ No

8

Select all that apply. Under what conditions do labs utilize an LSC?

☐ Every chemistry lab is required to have one regardless of the type of hazard present.

☐ Certain specialized safety units in the safety administration department require it (e.g. Chemical Safety, Radiation Safety, etc.).

☐ They are required if a lab has experienced safety violations in the past.

☐ They are required according to some other factor not listed here.

☐ They are only on a volunteer basis.

☐ Safety administration doesn't require it, but some individual professors require it.

☐ I don't know.

15

Example slides: *Survey* (students)

What **best** characterizes your type of research work?

☐ Inorganic Chemistry ☐ Organic Chemistry ☐ Computational Chemistry ☐ Physical Chemistry ☐ Analytical Chemistry

☐ Polymer Chemistry ☐ Nuclear Chemistry ☐ Biochemistry ☐ Chemical Biology ☐ Materials Chemistry

☐ Chemical Engineering ☐ Chemistry Education

6

A **hazard** is anything that has the **potential** to cause harm.

How do you think the following people view the **hazards** in your research lab?

	Very low	Low	Moderate	High	Very high
You	☐	☐	☐	☐	☐
Your Fellow Group Members	☐	☐	☐	☐	☐
Your PI	☐	☐	☐	☐	☐
Safety professionals	☐	☐	☐	☐	☐

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C.5 Scales Before and After Testing

The chemistry versions of the scales are displayed below in their pilot form (i.e., after KI and cognitive interviews), followed by the final short forms (i.e., for the national survey). These questions were issued to survey-takers after formatting in Qualtrics.

Leader-Member Exchange 7 – After Cognitive Testing (for Pilot Survey)

These next few questions ask about your **basic, overall relationship with your PI** to understand your general working relationship, which impacts safety.

1. Do you usually know **how** satisfied or unsatisfied your PI is with what you do?
Almost Never
Rarely
Occasionally
Often
Usually
Almost Always
2. How well does your PI understand your job problems and needs?
Almost not at all
Slightly
Somewhat
Moderately
Very
Extremely
3. How well does your PI recognize your potential?
Almost not at all
Slightly
Somewhat
Moderately
Very
Extremely
4. What are the chances that your PI would try to use their power to help you solve problems in your work, to the extent possible?
Almost definitely not
Very unlikely
Unlikely
Likely
Very likely
Almost definitely

5. What are the chances that your PI would try to get you out of trouble even when it impacts them negatively?
- Almost definitely not
 - Very unlikely
 - Unlikely
 - Likely
 - Very likely
 - Almost definitely
6. I have enough confidence in my PI **as a manager** that I would defend and justify my PI's decisions **about the group** if they were not present to do so.
- Strongly disagree
 - Moderately disagree
 - Slightly disagree
 - Slightly agree
 - Moderately agree
 - Strongly agree
7. How would you characterize your working relationship with your PI?
- Extremely ineffective
 - Moderately ineffective
 - Slightly ineffective
 - Slightly effective
 - Moderately effective
 - Extremely effective
-

Leader-Member Exchange₂ – Short Form (for National Survey)

These next few questions ask about your **basic, overall relationship with your PI** to understand your general working relationship, which impacts safety.

1. Do you usually know **how satisfied / unsatisfied** your PI is with what you do?

Almost Never
Rarely
Occasionally
Often
Usually
Almost Always

2. How well does your PI understand your job problems and needs?

Almost not at all
Slightly
Somewhat
Moderately
Very
Extremely

3. How well does your PI recognize your potential?

Almost not at all
Slightly
Somewhat
Moderately
Very
Extremely

4. How would you characterize your working relationship with your PI?

Extremely ineffective
Moderately ineffective
Slightly ineffective
Slightly effective
Moderately effective
Extremely effective

Safety Citizenship – After Cognitive Testing (for Pilot Survey)

The following list contains actions you might take regarding safety.

Please rate each of the following items on the degree to which you feel it is part of **your job**

Response format for each item:

Strongly disagree
Moderately disagree
Slightly disagree
Slightly agree
Moderately agree
Strongly agree

1. Volunteering for safety committees or other safety initiatives
 2. Helping to teach safety procedures to new group members
 3. Assisting others to make sure they perform their work safely
 4. Getting involved in safety activities to help my group work more safely
 5. Helping other group members learn about safe work practices
 6. Helping others with safety-related responsibilities

 7. Voicing safety-related recommendations concerning work activities
 8. Encouraging others to get involved in safety issues
 9. Expressing opinions on safety matters even if others disagree
 10. Raising safety concerns within the group during group meetings

 11. Dealing with safety hazards in the lab
 12. Going out of my way to look out for the safety of other group members
 13. Taking action to protect other group members from risky lab-related situations
 14. Trying to prevent other group members from being injured on the job
 15. Taking action to stop safety violations in order to protect the well-being of other group members

 16. Explaining to other group members that I will report safety violations
 17. Telling other group members to follow safe working procedures
 18. Monitoring new group members to ensure they are performing safely
 19. Reporting group members that violate safety procedures
 20. Telling new group members that violations of safety procedures will not be tolerated

 21. Attending mandatory safety-oriented meetings
 22. Attending non-mandatory safety-oriented meetings
 23. Keeping informed of changes in safety policies and procedures

 24. Trying to improve safety procedures
 25. Trying to change the way the job is done to make it safer
 26. Trying to change policies and procedures to make them safer
 27. Making suggestions to improve the safety of an experiment
-

Safety Citizenship₂ – Short Form (for National Survey)

The following list contains actions you might take regarding safety.

Please rate each of the following items on the degree to which you feel it is part of **your job**

Response format for each item:

- Strongly disagree
- Moderately disagree
- Slightly disagree
- Slightly agree
- Moderately agree
- Strongly agree

1. Getting involved in safety activities to help my group work more safely
 2. Helping other group members learn about safe work practices
 3. Voicing safety-related recommendations concerning work activities
 4. Encouraging others to get involved in safety issues
 5. Telling other group members to follow safe working procedures
 6. Trying to improve safety procedures
-

Safety Climate – After Cognitive Testing (for Pilot Survey)

The following list contains actions describing potential group behaviors.

For each of the items, indicate the degree to which you think the item is true **for your PI's group**.

Response format for each item:

Strongly disagree
Moderately disagree
Slightly disagree
Slightly agree
Moderately agree
Strongly agree

1. My PI negatively evaluates group members who behave recklessly
2. A group member who violates safety regulations will receive a negative evaluation by my PI even when no harm was caused by the violation
3. In my group, compliance with safety regulations is part of determining a group member's graduation readiness
4. In my group, causing an accident would have an adverse effect on a member's reputation
5. In my group, a member's safety record is one of the main factors impacting how their performance in lab is viewed.
6. The best researchers in my group expect other members to behave safely
7. Members in my group comply with safety regulations
8. The best researchers in my group care about safety
9. Members in my group who work safely try to emphasize it and make sure others do the same
10. Members in my group remind each other of the need to follow safety regulations
11. Group members who violate safety regulations irritate other members in my group even when no harm has resulted
12. My PI is well-informed about safety problems in our lab
13. My PI gets personally involved in safety activities
14. Reporting minor safety violations is a common practice in my group
15. My PI would tell group members who are doing something unsafe to stop
16. My PI views safety regulation violations very seriously even if they don't result in apparent damage
17. My PI would act quickly to correct safety issues
18. My PI is willing to invest time and effort to improve safety
19. My PI values group members' suggestions for correcting safety hazards
20. My PI is willing to implement new ideas for improving safety
21. Lab safety practices are important to my PI
22. My PI seems to care about my safety
23. My PI emphasizes safe practices on the job

Note: The original Safety Climate scale included an additional four questions about upward communication. Since Hofmann and Morgeson did not use them in their article, we also omitted them.

Safety Climate₂ – Short Form (for National Survey)

The following list contains actions describing potential group behaviors.

For each of the items, indicate the degree to which you think the item is true **for your PI's group**.

Response format for each item:

- Strongly disagree
- Moderately disagree
- Slightly disagree
- Slightly agree
- Moderately agree
- Strongly agree

1. Members in my group comply with safety regulations
 2. My PI views safety regulation violations very seriously even if they don't result in apparent damage
 3. My PI would act quickly to correct safety issues
 4. My PI is willing to invest time and effort to improve safety
 5. Lab safety practices are important to my PI
 6. My PI seems to care about my safety
-

C.6 Cluster Silhouette Analysis

Figure C.1. Cluster sizes for a 2-cluster model.

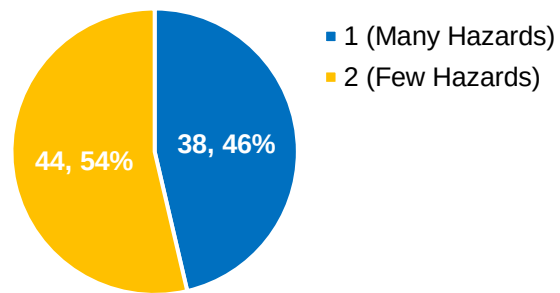
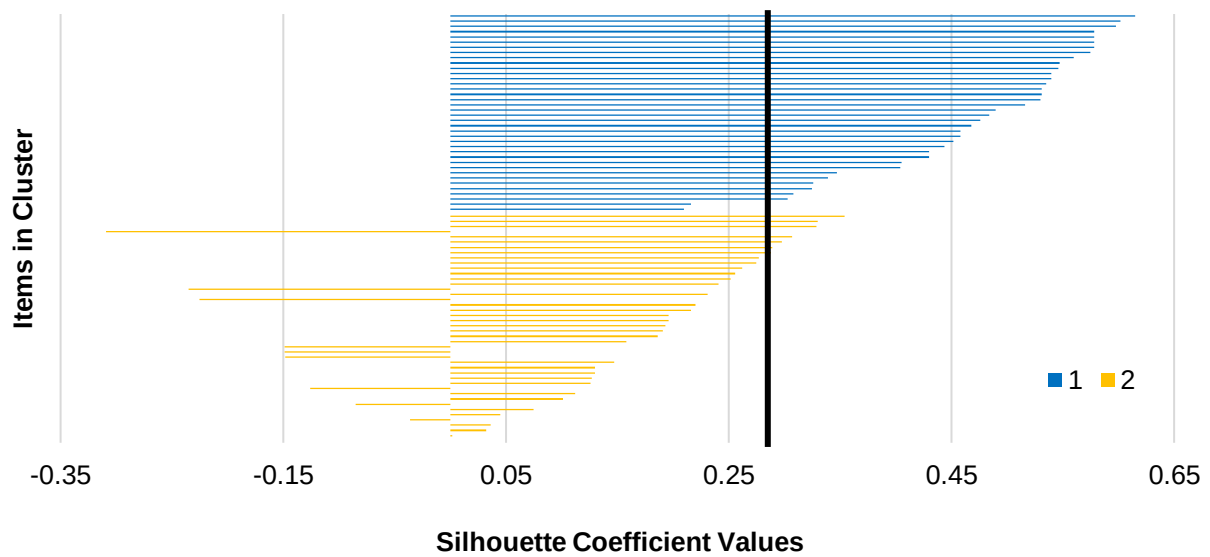


Figure C.2. Silhouette values for a 2-cluster model.



C.7 Supplemental Statistical Data

Table C.1. Descriptive statistics for complete list of anti-saboteur items.

#	Item ^a	Mean ^b	Std. Dev.	Skew	Kurtosis
1	I think that overall, safety in my lab could be improved.	4.37	1.139	-0.457	0.208
2	My lab does a good job of mitigating the hazards associated with our lab work.	4.62	1.151	-1.253	1.987
3	I personally feel that lab safety rules and regulations... <i>Prevent experiments from being done.</i>	2.35	1.382	0.974	0.165
4	I personally feel that lab safety rules and regulations... <i>Negatively impact my lab productivity.</i>	2.10	1.253	1.084	0.351
5	I personally feel that lab safety rules and regulations... <i>Make my lab a safe place to work.</i>	5.20	1.048	-1.857	4.165
6	I personally feel that lab safety rules and regulations... <i>Are to keep me and my peers from harm.</i>	5.26	1.081	-2.120	5.296
7	I personally feel that lab safety rules and regulations... <i>Are to protect the university from litigation.</i>	5.34	0.971	-1.982	5.119
8	If the following people watched me work in the lab, they would probably evaluate my lab behavior as being... <i>I would evaluate myself as...</i>	4.88	0.880	-1.203	1.992
9	If the following people watched me work in the lab, they would probably evaluate my lab behavior as being... <i>My fellow group members would evaluate me as...</i>	4.88	0.992	-1.163	1.290
10	If the following people watched me work in the lab, they would probably evaluate my lab behavior as being... <i>My PI would evaluate me as...</i>	4.93	0.966	-1.452	3.231
11	If the following people watched me work in the lab, they would probably evaluate my lab behavior as being... <i>Safety professionals would evaluate me as...</i>	4.38	1.183	-1.101	1.072
12	How hazardous do you think the following people view your research lab as?: <i>You</i>	3.58	1.257	-0.067	-0.551
13	How hazardous do you think the following people view your research lab as?: <i>Your Fellow Group Members</i>	3.21	1.243	-0.149	-0.719
14	How hazardous do you think the following people view your research lab as?: <i>Your PI</i>	3.15	1.247	0.120	-0.576
15	How hazardous do you think the following people view your research lab as?: <i>Safety Professionals</i>	3.82	1.337	-0.191	-0.824

Table C.1. Descriptive statistics for complete list of anti-saboteur items. [continued]

16	How risky do you think the following people view your research lab as?: <i>You</i>	2.92	1.187	0.381	-0.180
17	How risky do you think the following people view your research lab as?: <i>Your Fellow Group Members</i>	2.60	1.043	0.296	-0.515
18	How risky do you think the following people view your research lab as?: <i>Your PI</i>	2.43	0.973	0.729	0.637
19	How risky do you think the following people view your research lab as?: <i>Safety Professionals</i>	3.19	1.207	0.381	-0.720

^aAll item responses on a 1 to 6 ordinal positive agreement response format (i.e., “; “Strongly disagree” → “Strongly agree”; “Very unsafe” → “Very safe”; “Not at all hazardous” → “Extremely hazardous; “Not at all risky” → “Extremely risky”)

^bTotal 87 cases; missing data excluded pairwise; 79 cases contained complete data for all items

Table C.2. Factor loadings^a for Exploratory Factor Analysis^b of full-length scales.

Code ^c	F1	F2	F3
LMX7_1	.474		-.437
LMX7_2	.657		-.452
LMX7_3	.543		-.493
LMX7_4	.505		-.345
LMX7_5	.351	.242	-.230
LMX7_6	.675		
LMX7_7	.707		-.390
Safety Citizenship_1		.465	.466
Safety Citizenship_2		.346	-.364
Safety Citizenship_3		.520	
Safety Citizenship_4		.633	.250
Safety Citizenship_5		.591	
Safety Citizenship_6		.606	-.206
Safety Citizenship_7		.703	
Safety Citizenship_8		.683	.383
Safety Citizenship_9		.635	
Safety Citizenship_10		.504	
Safety Citizenship_11		.231	
Safety Citizenship_12		.646	
Safety Citizenship_13		.594	
Safety Citizenship_14		.632	-.205
Safety Citizenship_15		.721	
Safety Citizenship_16		.596	.259
Safety Citizenship_17		.742	
Safety Citizenship_18		.290	

Table C.2. Factor loadings^a for Exploratory Factor Analysis^b of full-length scales. [continued]

Safety Citizenship_19		.482	.293
Safety Citizenship_20	.308	.488	
Safety Citizenship_21		.487	
Safety Citizenship_22		.522	.506
Safety Citizenship_23		.395	
Safety Citizenship_24		.833	
Safety Citizenship_25		.790	
Safety Citizenship_26		.801	
Safety Citizenship_27		.868	
Safety Climate_1	.577		
Safety Climate_2	.517		
Safety Climate_3	.557		.420
Safety Climate_4			
Safety Climate_5	.398		.364
Safety Climate_6	.560		
Safety Climate_7	.694	-.254	
Safety Climate_8	.504		
Safety Climate_9	.473	.326	
Safety Climate_10	.501		
Safety Climate_11	.260		
Safety Climate_12	.811		
Safety Climate_13	.655		
Safety Climate_14	.448		.283
Safety Climate_15	.690		
Safety Climate_16	.846		
Safety Climate_17	.789		
Safety Climate_18	.835		
Safety Climate_19	.697		
Safety Climate_20	.682		
Safety Climate_21	.882		
Safety Climate_22	.865		
Safety Climate_23	.827		
% of Variance ^d	28.3	41.4	46.1

^aPattern matrix from Principal Axis Factoring and Direct Oblimin rotation ($\delta = 0$) with Kaiser normalization converged in 9 iterations; missing data excluded pairwise

^bKMO = .666; Bartlett's Test of Sphericity $\chi^2(1596) = 4025.851, p < .001$

^cFor clarity, pattern coefficients less than $\pm .2$ not shown

^d46.109% cumulative variance accounted for

Table C.3. Factor correlation matrix for scales' full-length forms.

Factor	F1	F2	F3
F1	---		
F2	.277	---	
F3	.007	.055	---

Table C.4. Levene's Test of Homogeneity of Variance for short forms.

Variable ^a	Levene Statistic ^b	df1	df2	p
Safety Climate ₂	1.967	12	44	.052
Safety Citizenship ₂	3.988	12	44	< .001
LMX ₂	.902	12	44	.552

^aScaled weighted sum factor scores^bBased on trimmed mean**Table C.5.** Multivariate tests.^a

Effect	Pillai's Trace	F	Hypothesis df	Error df	p
Institution [prestigious three R1s vs. other four schools]	.068	1.020	3	42.000	.068
Tenure in Research Group [years 1, 2, 3, 4]	.051	.254	9	132.000	.985
Program Year [years 2, 3, 4, 5]	.296	1.606	9	132.000	.120
English Status [ELLs vs. native English speakers]	.154	2.548	3	42.000	.069

^aInteraction effects not listed for conciseness; all were $p > .05$ **Table C.6.** Kruskal-Wallis tests of how different groups scores on the Safety Citizenship short form.

Group Comparison	Short Form	N ^a	df	$\chi^2(df)$	p^b
Institution [prestigious three R1s vs. other four schools]	Safety Climate ₂	79	1	1.887	.170
	Safety Citizenship ₂	79	1	.965	.326
	LMX ₂	81	1	3.166	.075
Tenure in Research Group [years 1, 2, 3, 4]	Safety Climate ₂	69	3	.509	.917
	Safety Citizenship ₂	69	3	.966	.810
	LMX ₂	70	3	1.867	.600
Program Year [years 2, 3, 4, 5]	Safety Climate ₂	76	3	.501	.919
	Safety Citizenship ₂	76	3	6.185	.103
	LMX ₂	78	3	3.826	.281
English Status [ELLs vs. native English speakers]	Safety Climate ₂	79	1	.118	.731
	Safety Citizenship ₂	79	1	1.630	.202
	LMX ₂	79	1	.830	.362

^aprogram years > 5 and research years > 4 were treated as missing data^basymptotic, two-tailed

Appendix D

Corresponding to **Chapter 4.** LAB Theory, HLAB Pedagogy, and Review of Laboratory Learning in Chemistry during the COVID-19 Pandemic

D.1 Overview of Reviewed Articles	354

D.1 Overview of Reviewed Articles

Table D.1. Contextual, performance, competency, and engagement data for reviewed articles.

Ref.	Cohort Comparison ^a	Activity Comparison ^b	Sample	Context	Performance Evidence	Performance Results	Competency Evidence	Competency Results	Engagement Evidence	Engagement Results
218	Same	At-school vs. at-home hands-on labs	Preservice teacher training in nonmajors general chemistry with 20 students at California State Polytechnic University–Pomona, USA during Spring 2020	Students did a series of simple at-home, hands-on kitchen labs and follow-up creative assignments which built on the lab results. The course's core experimental learning objectives appeared unchanged.	Lab grades before vs. during remote learning in that semester.	Grades dropped a little but not by much.	Quality of lab assignments	Students interpreted data correctly. Instructor believed hands-on labs are valuable for student learning.	Comparison of submission rates before vs. during remote learning in that semester. Student feedback (methods unspecified).	Most students continued submitting assignments. Students reported that, with more heads-up, they could have obtained all the materials and done all the labs.
390	Same	At-school vs. at-home hands-on labs	Introductory high school organic chemistry with 7 students at the University of Chicago Laboratory Schools, USA during Fall 2020	Students used a DIY lab kit made by the instructor to complete several hands-on labs at home with a mix of laboratory supplies and household materials.			Quality of lab work.	Students mostly successfully executing the experiments and appeared to learn the desired information. They could accurately predict outcomes of procedures, interpret results, and troubleshoot experiments.	Student feedback via non-anonymous mid-semester and end-of semester surveys (86 % response rate for each) and exit interviews. Parent feedback during Parent-Teacher Conferences.	Students and parents were happy to have hands-on labs to do. Students valued the labs and saw nuances between what the lab and the lecture contributed to their learning. Students mostly reported preferring hands-on labs over other popular alternatives.
199	Same	At-school vs. at-home hands-on labs AND Hands-on labs vs. videos	Introductory high school general chemistry with 59 students in 3 class sections at the University of Chicago Laboratory Schools, USA during Spring 2020	Students did (1) a lab at school before closure and then analysis at home, (2) a classroom lab at home with school-provided supplies, and (3) a kitchen lab at home with home supplies. Students had the option of doing a parallel video-based alternative assignment instead of the hands-on, wet labs, but all students answered the same	Averages and standard deviations for lab assignment grades between (1) hands-on vs. video groups and (2) different labs.	Completing the labs (vs. the video alternative) appeared to result in better grades for lab assignments; hands-on lab grades were comparable to earlier in the semester. The standard deviation for the video assignments was much higher than for the labs, indicating a possible	Student feedback from multiple anonymous and non-anonymous surveys (65 %, 81 %, and 85 % response rates) and class discussions in focus group format.	Students commented that it helped them to learn with their hands.	Submission rates of hands-on lab vs. alternative video assignments. Supply distribution of lab materials. Historical grade distribution of students who chose hands-on vs. video assignments. Student feedback from multiple anonymous and non-anonymous surveys (65 %, 81 %, and 85 % response rates) and	Lack of supplies appeared to drive student selection to do the alternative video assignment more than student choice did. Labs appeared to be viewed favorably and boosted morale. At-risk students were more likely to not complete the lab and to do the video assignment instead. Students and instructor reported pros and cons of at-

				post-lab questions. The lecture component did not differ much other than the new remote modality.		performance gap between strong and weak students who did the video alternative.			class discussions in focus group format.	home, hands-on labs, but the positives outweighed the negatives for both students and instructor.
210	Same	At-school vs. at-home hands-on labs AND At-school hands-on labs vs. at-home videos	IT Academy Project with 20 middle and high school general chemistry teachers at different institutions and 78 of their students in Slovakia during Spring 2020	Teachers had been receiving training on using data logging equipment for inquiry-based experiments. Most teachers implemented their training during remote learning but made different decisions as to how to do labs in remote learning. 10 teachers showed pictures with captions, 11 showed videos, 10 did live demos, and 11 had students conduct at-home, hands-on experiments.			Teacher feedback on non-anonymous survey. Student feedback on anonymous survey paired with teacher (average 13 students per teacher responded for 17 teachers)	Teachers felt that experiments made problems easier to understand/discuss but did not enable students to develop manual skills. 33 % of students said they didn't understand the lessons. 20 % reported struggles with time management and focus.	Teacher feedback on non-anonymous survey. Student feedback on anonymous survey paired with teacher (average 13 students per teacher responded for 17 teachers)	Teachers felt that experiments increased student interest but did not make up for personal contact with students. 26 % of students disliked remote learning, but 70 % preferred working at home. 46 % said that experiments were what they most missed about f2f learning; 100 % of the students who did hands-on, at-home labs reported missing experiments whereas 34 % of students who didn't do labs reported missing labs (presumed that the absence of labs during remote learning made them think less about doing the labs). 10 % did not like online experimentation due to lower "coolness"

									relative to f2f labs. 28 % missed interacting with teachers and classmates.	
221	Same	At-school hands-on lab proposals vs. at-home hands-on labs	Introductory undergraduate food chemistry course at the College of the Ozarks, USA during Spring 2020	Students had learned the course content knowledge and proposed two experimental projects each before the transition. The instructor developed three at-home, hands-on labs for students to do instead, or the students could develop their own at-home procedures. Each student did two labs of their choice.			Student notebooks. Student-instructor email correspondence.	Students actively worked on their projects and frequently contacted the instructor to troubleshoot experimental issues. Students generated creative projects and procedures instead of just following the provided procedures.	Perceived student attitude.	The instructor reflected that students appeared interested and invested in their projects.

234	Same	At-school hands-on labs vs. remote control of hands-on labs	Introductory noncredit optional supplemental high school course for 17 students at Sekolah Pelita Harapan School, Indonesia through Covenant College, USA during Summer 2020	The instructor did any wet benchwork live during the class while student volunteers used their computers to control the instructor's computer and run software programs to operate instruments.				Background survey after day 1 (100 % response rate). Attendance records. End-of-course survey (response rate unspecified).	A third of the students had not taken chemistry before. Students valued taking real-time measurements using the remote sensors and seeing the data appear as it was collected. 98 % attendance rate was excellent, possibly due to attendance requirements for receiving the financial deposit back afterward. Students enjoyed the course and felt it increased their interest in chemistry. Students were fascinated by the ability to run experiments remotely. Students did not feel lost during the class sessions and felt that their connection to collecting the data was important. Students also reported that they felt more involved and interested when their peers were collecting the data rather than when an instructor collects data.

208	Same	At-home mobile app vs. hands-on dry simulation	Upper-level undergraduate materials science course with 23 students at the Hochschule Bremen–City University of Applied Sciences, Germany during Spring 2020	Students investigated the structures of metals using a smartphone AR mobile app and manually building mock unit cells from table tennis balls at home.	Pre/post-quiz grades.	Students performed statistically significantly better on quiz questions at the end of the lab than before.	Student feedback on anonymous survey at end of lab (74 % response rate).	Students were evenly split as to whether the app helped them build the models. Only 9 students agreed that using the app helped them understand the concept, although 13 students agreed that building the model helped (remainder were neutral or disagreed). Only 7 students felt the hands-on activity helped them do better on the quiz, and only 8 students felt the app helped (remainder were neutral or disagreed). Students overwhelmingly agreed that the app was easy to use and cited visualization and interaction as the most important features for AR.	Student feedback on anonymous survey at end of lab (74 % response rate).	Students expressed gratefulness for and enjoyment of the hands-on activity.
280	Same	At-school hands-on labs vs. at-home modeling	Upperlevel undergraduate biochemistry course with 56 students, graduate bioinformatics course with 15 students, and summer high school course with 24 students at Kean University, USA during Spring	After the transition, all labs were remote as the students conducted bioinformatics analyses and modeling of the COVID-19 virus.	Grades for the activities in the undergraduate course.	The activity grades were considered satisfactory.			Student feedback (methods unspecified).	Students reported favorably on the experience, and several high school students expressed interest in minoring in Bioinformatics in the future.

240	Same	At-school hands-on labs vs. at-home videos, simulations, data	Introductory undergraduate general chemistry course with 26 students in 2 class sections at St. John's University, USA during Spring 2020	Before the transition, student groups planned their own experiments but, after the transition, collected data through simulations and experimental videos. The final course project challenged students to address how science could be used to address COVID-19 social issues.			Student feedback after end of course (38 % response rate)	Students were either neutral or agreed somewhat that the simulations and activities during remote learning were effective at promoting their learning. Students overwhelmingly felt that f2f labs gave greater educational growth compared to remote.	Student feedback after end of course (38 % response rate)	Students overwhelmingly felt that f2f labs gave the greatest emotional satisfaction whereas remote labs gave the greatest anxiety.
255	Same	At-school hands-on labs vs. at-home videos, simulations, data	11 Department of Chemistry faculty and their undergraduate students in various chemistry courses at Davidson College, USA during Spring 2020	The department faculty surveyed students to inform how they would transition to remote learning, and each faculty member did something different with their course. However, none of them made at-home, hands-on labs, instead focusing on the thought process of experimentation. Students read procedures, watched videos, attended lab lectures about techniques or theory, recorded observations, analyzed sample data, did computational and thought experiments, used modeling, and/or wrote reports.			Quality of student work in class.	Synchronous lab sessions seemed to help students conduct data analysis.	Student feedback on surveys from multiple courses (methods unspecified). Attendance records. Peer tutor feedback from informal conversations.	Students responded negatively to asynchronous lab work. Students enjoyed the creative remote lab assignments but still missed hands-on labs.

272	Same	At-school hands-on labs vs. at-home videos, simulations, data	Introductory undergraduate nonmajors general/biochemistry course with 73 students in 4 class sections at New York University, USA during Spring 2020	Four f2f labs into remote group activities, and two virus-related activities were added. Students watched experimental videos, did simulations, collected and analyzed simulated data, watched and wrote about a documentary, and analyzed genome sequencing data. Students who lived outside the New York time zone were permitted to do asynchronous work instead of synchronous.			Student feedback on anonymous end-of-semester survey (91.8 % response rate).	Each remote activity was rated as useful for learning by a majority of students, and ratings were consistent across the activities.	Attendance records. Student survey about time zones. Student feedback on anonymous end-of-semester survey (91.8 % response rate).	71 % of students outside the New York time zone chose to participate in the optional-for-group lab activities. Students preferred the virus-related documentary and genome sequencing activity the most. Students commented that they preferred hands-on labs to remote but also appreciated the structure and content of the remote labs.
250	Same	At-school hands-on labs vs. at-home videos, simulations, data	Upper-level undergraduate/graduate applied biopharmaceuticals at Columbia University, USA during Spring 2020	Student groups had completed 3 of 6 lab modules (different from other groups due to a rotation schedule) before closure. f2f labs were replaced with fully virtual exercises: modeling, simulations, experimental videos and photographs, literature reviews, additional lectures, and analyzing shared student data from groups who had completed other modules. Students completed different tasks depending on which modules they had left to finish.	Grades of (1) individual prelab quizzes and (2) formal group lab reports from before vs. during remote learning in that semester.	Performance on quizzes and lab reports were consistent with earlier in the semester.	Quality of lab reports	The quality of data interpretation in lab reports suggests that students struggled with handling and understanding the data that they did not collect.		

253	Same	At-school hands-on labs vs. at-home videos, simulations, data	Introductory undergraduate analytical chemistry course at Lander University, USA during Spring 2020	For 2 labs, students watched experimental videos and were provided with sample data from past students to analyze for lab reports. For the next 2 labs, students did simulations and gathered simulated data to analyze.			Student-instructor discussions.	Students appeared confused about the data, where it came from, what it meant, and how to analyze it when simply provided with it; students did not appear as confused for the simulated data.		
277	Same	At-school hands-on lab vs. at-home simulations, data	Introductory undergraduate biochemistry course with 180 students at the University of Oxford, UK during Spring 2020	Students completed a Michaelis-Menten enzyme kinetics simulation instead of the corresponding hands-on lab. Students planned and conducted their simulated experiment, gathered data, and generated conclusions about their assigned enzyme.			Student feedback on survey (response rate unspecified). Quality of assignment responses.	Students said the simulation helped build their experimental design skills and that mistakes had fewer consequences than they would have had in the real world. Students also learned that statistical analysis of data is important. The most common miscomprehensions related to how enzymes work and the relationship to the data.	Student feedback on survey (response rate unspecified).	Students reflected favorably on the simulation, saying that it was enjoyable.
207	Same	At-school hands-on labs vs. at-home simulations, data	Introductory undergraduate biochemistry course with 96 students at the University of South Australia, Australia during Spring 2020	58 of 96 students had already completed 2 of the 3 labs before the transition. Students were provided with 5 simulations and sample data to analyze to complete worksheets. Before the semester ended, restrictions were eased so that students could choose to come in to school to do hands-on labs.	Worksheet grade averages and standard deviations for the first and second labs.	There was very little difference between the worksheet grades for the f2f vs. simulation students.			Optional hands-on lab attendance. Student feedback (methods unspecified).	12 students choose to come in to do hands-on labs. Students appeared to highly value getting the chance to do hands-on work.

273	Same	At-school hands-on labs vs. at-home simulations, data	Introductory undergraduate organic chemistry course with 24 students at Alfred University, USA during Spring 2020	Students had completed their standard labs at school and were planning a final research project. Instead of doing the project, students did five click-through "Choose Your Own Adventure" games to virtually conduct a set of standard experiments. The games featured safety, preparation, choosing proper steps, handling mistakes, and receiving data to analyze.			Simulation statistics, including number of clicks, time stamps, and selected answers. Student reflection responses	Students appeared to repeatedly make the same errors both within and across labventures and struggled to determine how to fix mistakes. Students very rarely completed a labventure in the optimal decision pathway. Students appeared to overwhelmingly struggle with making proper experimental decisions (such as deciding in what order to do steps and which analytical techniques to use) and interpreting data/observations provided.		
262	Same	At-school hands-on labs vs. at-home simulations, data	Introductory undergraduate general chemistry course with 131 students at Rice University, USA during unspecified semester (presumably Spring 2020)	Students completed a prelab quiz, watched lecture and experimental videos, and made procedural decisions that led to new experimental videos showing the expected results stemming from those decisions.	Pre/post-test (reduced number of answer options and different grading policies between the pretest and post test).	Students' scores improved dramatically after the virtual lab.				

283	Same	At-school hands-on labs vs. at-home simulations, data	Upperlevel graduate biochemistry/analytical chemistry course with 58 students at Sheffield Hallam University, UK	Cross-disciplinary students used multiple simulations of analytical techniques, kept lab notebooks, and conducted data analysis in synchronous class sessions.			Student feedback on end-of-semester survey (81 % response rate).	Students felt both supported and challenged by the simulations. Students felt the simulations helped them learn. Only 39 % of the students mentioned that they felt the virtual lab experience helped their data analysis abilities, and only 3.7 % discussed their ability to use the equipment in the context of what the simulation helped them learn. Students reported that the simulations were useful but that they do not replace the learning from hands-on labs.	Student feedback on end-of-semester survey (81 % response rate).	Students were frustrated by glitches with the website. Students appeared to think the simulations were interesting and informative. Most students felt that breakout rooms made it easier to receive help.
269	Same	At-school hands-on labs vs. at-home videos, data, simulations, data	Upperlevel undergraduate forensic chemistry course in the spring and an upperlevel undergraduate forensic biochemistry course and upperlevel graduate forensic biology course in the fall at Towson University, USA during Spring and Fall 2020	Students were given pre-recorded lectures in a flipped classroom model. In the spring, students watched experiment videos, made observations, wrote reports, and analyzed a mock case using a decision-dependent PowerPoint. In the fall, most students were in-person, but a few were remote. All students continued in the flipped classroom model, but in-person students conducted hands-on labs when at school. Remote students analyzed pictures and data from the experiment. Students used			Quality of lab notebooks.	The quality of lab notebooks was comparable between the f2f and the remote students in the fall, although there were very few remote students to compare.	Student self-selection into f2f or remote registration option for fall. Student feedback (methods unspecified).	Almost all students chose to be in-person in the fall. Students reportedly gave positive feedback about the decision-dependent PowerPoint slides, the simulation software, and the mock case trial. Students liked being able to exert some control over the synchronous video stream.

				simulations for several labs, interacted with a live-stream video for one lab to direct the instructor's actions (if remote - in-person students did the lab themselves), and reported the results in a final paper and a mock criminal trial.						
244	Same	At-school hands-on labs vs. at-home videos, data	Upper-level undergraduate experimental physical chemistry with 95 students in 5 class sections at Pennsylvania State University, USA during Spring 2020	After 7 f2f labs before closure, 3 remaining labs were replaced with short experimental videos, lectures connecting theory with data, prelab quizzes, graded notes, graded during-lab questions, and raw sample data to analyze. Students answered questions and wrote reports based on the provided data. The end-of-semester research projects were eliminated.	Paired sample t test comparison of lab report grades before vs. during remote learning in that semester.	Grades on the lab reports were not significantly different.	Quality of lab reports	Students did not fully understand the experiments. They copied mistakes out of the lab manual, even when the experiment in the video differed from the manual.	Zoom attendance records. Student feedback on end-of-course survey (methods unspecified).	No student missed a class. Students were reported apparently satisfied with the remote transition.

252	Same	At-school hands-on labs vs. at-home videos, data	Introductory undergraduate analytical chemistry course with 51 students in 3 class sections at Ohio State University, USA during Spring 2020	Students did 2 remote labs and were given notebook pages which included sample data and details about the procedural set-up. They watched explanatory prelab videos and completed prelab quizzes. They wrote a lab report for the first lab but, based on student feedback, did a short answer-style assignment focused on data analysis and discussions for the second lab.	Grades for both labs and a t-test analysis.	Students performed better on the short answer-styled assignment than the lab report.	Student feedback mid-semester (methods unspecified) and on end-of-semester survey (21.6 % response rate).	8 of 11 respondents preferred the short answer assignment over the lab report, and 7 either said the short answer was easier or didn't provide a comment about its difficulty. Students found understanding the procedure, analyzing the data, considering sources of error, and writing the lab report to be very challenging without having conducted the experiment themselves. Students suggested using more experimental videos in future remote iterations, but some comments emphasized that students believe labs could never be effectively taught remotely.

246	Same	At-school hands-on labs vs. at-home videos, data	Introductory undergraduate analytical chemistry courses for pharmacy careers with 188 students in 2 class sections and for food science careers with 118 students at Complutense University, Spain during Spring 2020	The pharmacy students had completed all labs already, but the food science students had not and so did four labs during remote learning (except the students repeating the food science course). These students read procedures, watched experimental videos, attended lectures, and were assigned more homeworks. Students received sample data, answered questions, and gave presentations about the data.			Student feedback on survey at end of course (46 % response rate – 72 % were pharmacy and 28 % were food science).	31.7 % did the remote labs; of them, 79.6 % of these students felt the labs required additional effort, 100 % preferred labs f2f, and they gave neutral ratings to the quality of the remote lab education.	Student feedback on survey at end of course (46 % response rate – 72 % were pharmacy and 28 % were food science). Attendance records, Submission rates.	Students had better attendance and higher submission rates for remote classes vs. f2f, although students repeating the courses (17 %) were very likely to not submit assignments in both situations. The pharmacy students had statistically significantly better attendance and submission rates than the food science students during both f2f and remote learning. 81 % preferred f2f learning over remote, without much difference between the two courses. The most common advantage listed for remote learning was saving time and schedule flexibility. Students favorably rated teachers and teaching during remote learning in general.
245	Same	At-school hands-on labs vs. at-home videos, data	Introductory undergraduate general chemistry course with 88 students in 2 class sections at Missouri University of Science and Technology, USA during Spring 2020	Students watched synchronous, live-streamed videos of the instructor doing the labs without any editing and including any mistakes that may have occurred naturally. Students made observations, recorded data, and worked with peers on data analysis.					Student feedback (methods unspecified).	Some students commented that the labs were well-done despite the occasional video blurriness but that the videos did not substitute for hands-on labs in training chemists. Many students did not appear to continue paying attention to

				Attendance was incorporated into the overall grade.						the class session after checking in for attendance.
270	Same	At-school hands-on labs vs. at-home videos, data	Introductory undergraduate honors general chemistry course with 128 students in 7 class sections at Duke University, USA during Fall 2020	Near the end of the semester, students were given prelab resources and watched a pre-recorded video of a polymer lab experiment. Students used observations, data, and a published article to answer post-lab questions.	Grades on post-lab discussion questions between class sections.	Students did well overall on answering the post-lab questions, although there was noticeable differences in performance between sections.	Quality of post-lab discussion question responses. Student feedback from post-lab survey (response rate unspecified).	Students felt that the virtual lab and resources helped improve their understanding of polymer chemistry, which they were previously unfamiliar with. Students met expectations for answering conceptual, reasoning, and calculation questions but showed some difficulty in interpreting the UV-Vis spectra for the experiment, although they had learned about UV-Vis analysis and Beer's Law.	Student feedback from post-lab survey (response rate unspecified)	Students reported positively on the virtual lab experience. Several students comments indicated that they felt it was cool to watch the experiment video. They were interested in the real-life applicability of polymers and looked forward to doing similar hands-on labs in the future. Students liked being in breakout rooms with peers and TAs to answer the questions.

259	Same	At-school hands-on labs vs. at-home videos, data, literature reviews AND At-home readings vs. videos vs. lectures	Upper-level undergraduate chemical environmental engineering courses with 104 students and 20 instructors at the National Institute of Science and Technology of Toulouse, France during Spring 2020	At first, instructors sent students class materials to read alone, then later sent videos of lectures, then later sent audio-commented slideshows, then later hosted virtual class sessions. For labs, students worked in small groups on literature reviews, data analysis of existing or sample data, and/or unspecified projects. Some labs were abandoned.		Student feedback on end-of-semester survey (85 % response rate).	61.9 % felt they learned less effectively in virtual classes than f2f and needed to spend more time out of class learning than before. 43.5 % felt they covered comparable amounts of knowledge to f2f, but 44.7 % felt it was less knowledge. 51.2 % felt it was difficult to do group projects remotely, although some students felt groupwork was easier due to simplified logistics. Only 21.5 % felt that continuing groupwork was useful during remote learning. 44.7 % agreed that processing sample data live with the instructor was useful vs. only 16.5 % for asynchronous data analysis. 72.0 % felt the labs were less effective when remote, and 81.9 % felt they accomplished less when remote vs. f2f labs.	Student feedback on end-of-semester survey (85 % response rate).	Students did not like solely reading materials, considered an explanatory instructor more beneficial, and felt that synchronous classes were helpful with live Q&A. Students reported that the personal interaction with live sessions was helpful and encouraged them to stay at the session. Motivation and participation in groupwork were felt to be unequal. Students appeared to feel more positively about short-term, low-stakes groupwork than larger projects. Some students were frustrated to not do hands-on labs whereas others appreciated the greater emphasis on theory. 33.3 % students agreed with cancelling some labs, 38.1 % were neutral, and 28.6 % disagreed. Students felt that trying to continue labs was exhausting and time consuming, even without experiments.

233	Same	At-school hands-on labs vs. at-home videos, data, procedure writing	Introductory undergraduate organic chemistry and biochemistry CUREs (respectively 15 students & 55 students in 3 class sections) and upper-level undergraduate biochemistry CURE (7 students) with 3 instructors at the University of New England, USA during Spring 2020	The organic chemistry students had reviewed literature and finished their first research project; the second experimental project was replaced with an instructor-selected research question. Students revised the question as a class, designed experiments for the instructor to run, watched the instructor's filmed videos of their designed experiments, analyzed the data, presented posters, and did peer review.....For both biochemistry courses, students had reviewed literature, designed research projects, and were collecting data. The instructor finished running their experiments and distributed the data. The introductory class wrote a manuscript and presented results orally. The upper-level class wrote, pitched, and peer reviewed mock grants.		Student feedback on surveys (methods unspecified).	Lack of hands-on labs appeared to hinder student knowledge of procedures, troubleshooting skills, data analysis, ownership of projects, and motivation. It was harder for them to understand their experiments and outcomes as well as to propose new experiments to try.	Student feedback on surveys (methods unspecified).	Students reported various types of frustrations surrounding not being able to do their own experiments at school. Many of the students and instructors were burnt out by the end of the semester.

268	Same	At-school hands-on labs vs. at-home data	Upperlevel undergraduate biochemistry course with 12 students at College of St. Benedict/St. John's University, USA during Spring 2020	Students watched prelab videos and analyzed real and simulated ELISA data.	Pre/post-lab quiz grades (before lab vs. end of semester).	Grades on the same prelab quiz given at the end of the semester during finals week improved 67.5-70 %, but the instructor notes this was not a rigorous analysis.	Student feedback (methods unspecified).	Students self-reported that they understood chemical principles and the steps of the ELISA afterward but struggled with the math.	Student feedback (methods unspecified).	Students felt that they would have liked to do a wet lab.
288	Same	At-school hands-on lab vs. at-home data, presentations	Introductory undergraduate analytical chemistry course with 87 students in 5 class sections at the University of Wisconsin – Madison, USA during Spring 2020	Students performed an extraction and collected data via HPLC for a project before the transition. The second experimental portion of the project was replaced with a more in-depth statistical analysis of the class's pooled data. Groups presented their results orally and provided peer feedback.			Student feedback on end-of-semester survey (response rate unspecified).	Some students found satisfaction in handling the raw, real data, but other students felt the opposite way. Despite contributing to the class's pooled data set, students struggled to trust their classmates' data, expressed uncertainty with nonideal data, struggled with the statistical analysis tools, and expressed discontent at the lack of one correct answer. Students needed more coaching than expected by the instructors to successfully complete data analysis. TAs sometimes gave incorrect or misleading feedback to students.	Student feedback on end-of-semester survey (response rate unspecified).	Students liked that the remote activities related to their previous work in the project. Some students liked determining their own work schedule. Students appeared connected to their groups. The majority of students enjoyed the project, were satisfied with their group members, and felt they accomplished their goals.

289	Same	At-school hands-on labs vs. at-home literature reviews, data	Upper-level undergraduate synthetic chemistry course with 16 students at Georgia Gwinnett College, USA during Spring 2020	Students were conducting experiments to modify literature reactions before the transition. Further experimentation was abandoned, and students instead attended mini-lectures, searched literature, and completed guided-inquiry assignments. Students analyzed data they collected from earlier in the semester and data from published sources to evaluate environmental impacts and lifecycles. Students kept notebooks, wrote papers, and made a poster.			Student feedback at start of remote learning (methods unspecified) and on end-of-semester survey (56.3 % response rate) and final exam questions.	Groups did not appear to communicate well with each other. Students struggled to write lab reports for their incomplete projects, make predictions about experiments, and make assumptions from literature precedents.	Attendance rate. Estimated in-class participation rate. Student feedback at start of remote learning (methods unspecified) and on end-of-semester survey (56.3 % response rate) and final exam questions.	91 % of students attended class. ~ 50 % participated in class by speaking or using the chat box, but students did not turn on their video. Students wished they could have completed their experiments, but they still reported positive experiences with the course overall.
274	Same	At-school hands-on labs vs. at-home literature reviews, data, procedure writing, outreach	Upper-level undergraduate biochemistry course at Southwestern University, USA during Spring 2020	Students had already completed technique-building labs, reviewed literature, and generated a research project hypothesis in small groups. The hands-on lab projects were then replaced with more literature reviews, investigating methods, proposed a protocol for solving a presented research question, and orally presented their final protocol. Students generated publication-level figures from data and analyzed raw sample data provided from original research.			Student feedback (methods unspecified).	The instructor reported that students indicated they learned a lot during remote learning.	Student feedback (methods unspecified). Student self-reflection assignment.	The instructor reported that students showed increased levels of pride and confidence in their ideas. Students reported enjoying the public outreach project.

				Students made public outreach projects related to the pandemic.					
292	Same	At-school hands-on lab vs. at-home literature reviews, procedure writing	Unspecified (presumed introductory undergraduate chemical engineering course at Graz University of Technology, Austria during either Spring or Fall 2020)	Students searched the literature and proposed their hypothetical procedure. They did not conduct their proposed procedure.				Student feedback (methods unspecified).	Students reportedly gave positive feedback by the end and felt the experience was valuable for their education. Students felt it took more work than they initially expected it would, and they were overwhelmed at first.

238	Same	At-school hands-on labs vs. at-home presentations	Introductory undergraduate organic chemistry course with 82 students at Wesleyan University, USA during Spring 2020	Students worked in small groups to write and make presentations about a published paper about COVID-19. They reviewed their peers' submissions, received multiple types of feedback, and completed other activities meant to scaffold their development in this symposium-styled project which also featured prize-giving.		Student feedback on survey at end of project (91 % response rate).	The class was split evenly regarding their past experience with symposium-styled presentations. Many students reported the general, chemistry, organic chemistry, and assorted biology courses were helpful for completing the project. 88 % agreed the project increased their awareness about the pandemic, 92 % agreed it helped them correlate concepts to the real-world, and 83 % agreed the project was relevant to the course. Students were fairly familiar with some of the paper's techniques but not universally so. Many students utilized the university's independent mentoring service for practicing presentations. Students reported improvement in public speaking and connecting concepts to the real world. 59 % felt they learned more during the f2f labs vs. the remote project.	Student feedback on survey at end of project (91 % response rate).	71 % agreed they enjoyed the project. Students reported positively on the project experience. 68 % felt they were more engaged.

226	Same AND Different	At-school vs. at-home hands- on labs	Upperlevel undergraduate biochemistry course with > 80 students at Arizona State University-Tempe, USA during Summer 2020	At the end of the course (having done simulations until then), students wrote and conducted a procedure at home to determine amylase activity on starch in multiple substances. They were given guidance on a general protocol and relative ratios to consider using with household supplies. Students watched a video to learn how to use a computer program to analyze results.	Historical comparison of grades on Methods section of lab report (with related but not identical lab).	Grades were comparable between prior f2f lab and at-home lab.	Discussions during office hours. Historical comparison of quality of lab reports and data. Discussion board activity. Poll about time workload (27 % response rate).	Students wanted a procedure that provided specific amounts of material that should be used. Resources from the f2f lab version and a video about dilutions was thought to be helpful by the instructors. Students struggled to write the experimental section of the lab reports and couldn't directly compare to other students since they wrote separate procedures. Students struggled to analyze and interpret data properly; less than half were perceived to understand why they were analyzing the linearity of their plot. Students appropriately recognized multiple experimental limitations caused by the at-home format. The lab took the standard amount of time as a f2f lab.	Student feedback (methods unspecified).	Students valued the hands-on lab experience despite the challenges.

225	Same AND Different	At-school vs. at-home hands- on labs, videos	Introductory undergraduate organic chemistry course with 30 students at the University of Pennsylvania, USA during Summer 2020	Students completed pre-laboratory work, including readings, practice problems, lectures, watching videos of standard liquid-liquid extractions, and a pre-lab write-up. Students then conducted acid-base liquid-liquid extractions of food dyes to separate and analyze mixtures. This was one of five at-home hands-on labs.		Assignment responses. Pictures from experiment. Historical comparison of quality of conceptual development to previous cohorts (methods unspecified).	Students required further guidance on the difference between overall vs. functional group-specific pKa values. 2 students had dye on their bare hands at the end, indicating inadequate safety practices with gloves. Students overwhelmingly conducted the experiment and analyzed results correctly. 83 % made a correct separation tree diagram afterward. In a later assessment, the majority of students correctly answered separation questions. Instructors believe that students had similar or superior conceptual understanding than prior cohorts.	End-of-course survey (93 % response rate).	The majority of students rated this lab as their favorite or second favorite of the five experiments.

211	Same AND Different	At-school vs. at-home hands-on labs AND At-school hands-on labs vs. at-home videos	Introductory undergraduate general chemistry with 987 students across 3 campuses at Deakin University, Australia during Spring 2020	21.5 % of students did the first lab f2f before closure. After closure, the first lab was filmed for students who hadn't done the f2f lab yet, and then they filled out the worksheet based on the video. Later, students did two at-home, hands-on kitchen labs. The lecture component did not differ much other than the new remote modality.	Averages and Kruskal-Wallis rank sum test for grades on (1) first lab between historical, f2f, and video groups and (2) the three labs during the semester.	Grades for the first lab were significantly worse for the video group compared to (1) the f2f group and (2) prior students. There appeared to be a greater spread in performance for the remote labs, but accurate historical comparison was not possible. Grades were considered acceptable.	Historical comparison of LMS usage. TA feedback (6 of 18 TAs), non-anonymous. Student feedback through an anonymous discussion forum (response rate of 1.3 %) & non-anonymous emails.	Students struggled to learn and fill out the worksheets. A large disparity was noted between adept and weaker students in the video group. Students posted in the Lab section of LMS to seek help much more frequently than historically. TAs and staff believed hands-on labs were very valuable to students and not replaceable by videos or simulations. A few students said kitchen chemistry was inauthentic and therefore less valuable than videos, but other students reported that the labs were valuable.	Historical comparison of submission rates for remote vs. historical labs. Student feedback through an anonymous discussion forum (response rate of 1.3 %) & non-anonymous emails.	Students and staff did not like the video alternative. Submission of remote lab assignments was comparable to historical submission f2f submission rates. Pros and cons appeared in student feedback.

215	Same AND Different	At-school vs. at-home hands-on labs AND At-school hands-on labs vs. at- home simulations, data	Introductory undergraduate general chemistry course with 43 students and biochemistry course with 10 students at SUNY College at Old Westbury, USA during Spring 2020	For each course, after completing 5 hands-on experiments at school before the transition, students did 5 remote labs (hands-on kitchen labs and simulations) to replace the originally planned experiments. Students collected simulated data and wrote lab reports.	Historical comparison of lab report grades for remote vs. earlier in the semester and past years.	General chemistry students received better grades on remote lab assignments compared to labs earlier in the semester; instructors attribute this improvement to the use of easier questions for the remote assignments. Biochemistry students received slightly better grades on remote lab assignments compared to similar labs from past years.	Student feedback on anonymous end- of-semester surveys (53 % response rate for general chemistry). Historical comparison of self- reported study hours vs. computer logs of time spent on remote assignments.	General chemistry students rated f2f labs as more efficient for learning (4.1/5 Likert) compared to remote (3.4/5) and hands- on kitchen labs (3.2/5). Freshmen spent about the same amount of time on assignments as before. Students commented positively on the ability to use real equipment and interact closely with people for f2f labs but also appreciated the simpler and clearer structure to remote labs. Students reported negatively on experiencing software issues with remote labs. 66.7 % rated f2f teaching as the most effective mode for learning, and 20 % preferred a combination of f2f and remote. The majority of biochemistry students rated the remote labs as effective.	Student feedback on anonymous end- of-semester survey.	The majority of biochemistry students reported satisfaction with their remote learning experience.

228	Same AND Different	At-school vs. at-home hands-on labs AND At-school hands-on labs vs. at-home simulation, data	Undergraduate forensic science course in the spring and an upperlevel undergraduate/graduate serology course with 43 students, upperlevel undergraduate forensic biology course, and upperlevel graduate forensic biology course in the fall at Virginia Commonwealth University, USA during Spring and Fall 2020	In the spring, undergraduate forensic science students had one final, major lab remaining which they did at home by creating and analyzing a crime scene. In the fall, students in the serology course had the option to conduct a supplemental virtual simulated serology lab on PowerPoint in a choose-your-own-adventure style. In the forensic biology course, students analyzed sample data. In the graduate forensic biology course, students watched a screenshare to remotely see how to use a program usually done in a computer lab at school.	Historical grade comparison on various assessments.	Students did better on certain assessments compared to prior years, but it was very obvious there was widespread cheating going on. Cheating was a huge, flagrant problem for some courses.	Student feedback via serology survey (60 % response rate).	Students felt the virtual serology lab was very helpful for their understanding of how to do the lab. A few students said it was just like doing the hands-on lab, which they also did at school.	Student feedback (methods unspecified). Student feedback via serology survey (60 % response rate).	Students enjoyed the crime scene lab for the undergraduate forensic science course. Students highly enjoyed the virtual serology lab. Screen-sharing the graduate forensic biology software was better than clustering many students around one computer in the lab.
230	Same AND Different	At-school vs. at-home hands-on labs AND At-school hands-on labs vs. at-home simulation	Introductory forensic science course and upperlevel forensic science course with 24 students at Teesside University, UK during Fall 2020	Students collected forensic data from their local environment and compared data from other sources. Students also conducted other activities such as simulations.	Historical comparison of final exam grades.	Students in the upperlevel course achieved a higher average exam grade than the prior two years' of students, although statistical analysis was not provided.	Student feedback (methods unspecified).	Students felt that they learned better doing the hands-on data collection than they would have from simulations or other formats and felt that it played a significant role in helping them learn and retain knowledge.	Student feedback (methods unspecified). Perceived engagement with course activities (methods unspecified).	Students appreciated the break from a computer screen. Students enjoyed the hands-on work. More students engaged with the hands-on activities than the non-hands-on activities (method of measurement not specified).

229	Same AND Different	At-school vs. at-home hands-on labs AND At- school hands- on labs vs. data	Introductory undergraduate biophysics course with > 100 students at the University of Bologna, Italy during Spring 2020	Students completed two hands-on labs about kinematics and optics in their homes using household supplies. Those who could not obtain the supplies were given sample data to analyze.			Student feedback on end-of-semester survey (response rate unspecified).	Some students commented that the hands-on labs were helpful for learning and reinforcing the lecture concepts.	Submission rates. Historical comparison of student feedback on end-of-semester survey (response rate unspecified).	Approximately 3/4 of the students did the hands-on kinematics experiment and 1/4 did the optics. Students expressed appreciation for the hands-on labs. 79 % of students gave positive feedback about the course compared to 81 % from the previous year.
248	Same AND Different	At-school hands-on labs vs. at- home videos, data AND At-school hands-on practical lab exam vs. at- home paper exam	Introductory undergraduate general chemistry course with ~1,400 students and 30 TAs and organic chemistry with 104 students and 9 TAs in 20- 24-person class sections at the University of California–Irvine, USA during Spring 2020	General chemistry students had no prior college chemistry lab course, and the academic quarter had not yet started. The physical learning objectives for both courses were abandoned, and focus was placed on data analysis, theory, concepts of techniques, and safety. Students in both courses watched experimental videos and analyzed provided sample data from past students ("good" data for general chemistry, imperfect data for organic)..... General chemistry students took a final exam with essays describing techniques instead of doing a lab practical. Organic students were supposed to take a final exam about safety, concepts, data analysis, and			Student feedback from general chemistry students on mid-quarter and post-quarter surveys (79 % mid- quarter, 67 % post- quarter response rates). Student feedback from organic chemistry students on mid- quarter survey (84 % response rate). TA feedback from general chemistry TAs on mid-quarter and post-quarter surveys (64 % mid- quarter, 82 % post- quarter response rates). TA feedback from organic chemistry TAs on post-quarter survey (100 % response rate) and weekly informal discussions. Historical comparison of general chemistry discussion board usage.	General chemistry students struggled with the electronic laboratory notebook. Organic chemistry students felt it was easier to ask questions when remote, liked the lack of time pressure to finish experiments, liked watching the videos with the TA and classmates, and wanted more structure to the video discussions. Organic students felt the lab lecture was helpful and thought it was similar to f2f lab lectures. TAs felt the labs required less time when remote. TAs felt students required more guidance to analyze data than in previous courses but discussed the theory and concepts more. TAs struggled to assess	Student feedback from general chemistry students on mid-quarter and post-quarter surveys (79 % mid- quarter, 67 % post- quarter response rates). Student feedback from organic chemistry students on mid- quarter survey (84 % response rate). TA feedback from general chemistry TAs on mid-quarter and post-quarter surveys (64 % mid- quarter, 82 % post- quarter response rates). TA feedback from organic chemistry TAs on post-quarter survey (100 % response rate) and weekly informal discussions. Historical comparison of general chemistry discussion board usage.	General chemistry students appreciated the experimental videos and quizzes. Students were stressed about communication and expectations as evidenced by higher activity on the discussion board than in the previous year. Students attended TA office hours much more than when f2f. General chemistry TAs worried they had lower personal connection to students regardless of higher office hour attendance rates. TAs felt insufficiently prepared for office hours, where students primarily asked about grading rather than theory. Organic chemistry students felt connected to their instructors but not their classmates. Fewer organic students attended

		thin layer chromatography (previously a hands-on lab) instead of an exam with experimental project component (for f2f) but instead took the technique part of the exam and then were offered creative work pass/fail assignment options to finish the exam (the instructor's response to sudden social upheaval)..... Instead of discussing tips for labs, TA staff meetings focused on contextualizing the lab and the underlying theory. TAs filmed videos of experiments and supported students in different capacities based on experience and assigned role. TA office hours featured TAs playing the experimental videos and discussing them with students.		gaps in student learning.	and organic chemistry student attendance at TA office hours.	office hours than for f2f courses the TAs had previously worked for. TAs felt there was an overall decrease in student participation even though some students increased and contacted TAs more. Overall, students, TAs, and instructors felt the remote transition was a success.

282	Same AND Different	At-school hands-on labs vs. at-home simulations	Introductory and accelerated introductory undergraduate general chemistry courses (2 different tracks) with 154 students combined at Georgia Institute of Technology, USA during Summer 2020	Students watched videos and did simulations online to collect data. TAs facilitated breakout room sessions to foster peer-to-peer learning (based on prior experiences in Spring 2020).		Modified version of the Meaningful Learning in the Laboratory Instrument as end-of-semester survey (80 % response rate between both tracks).	Cognitive learning scores were similar between the two groups and with other, previously reported uses of the MLLI. TA presence and synchronous (vs. asynchronous) sessions were perceived as helpful for learning. Students were reasonably confident (although not highly confident) in their ability to do physical labs in the future, although the students who were likely to take organic chemistry next were much less confident.	Modified version of the Meaningful Learning in the Laboratory Instrument as end-of-semester survey (80 % response rate between both tracks). Demographics of student populations.	For the standard course, the lowest scoring items were mostly affective items, but the overall affective scores were similar to literature. For the accelerated course, there were more low-scoring affective items, and the average affective score was noticeably lower than the standard course. The accelerated course had almost 50:50 split in incoming freshmen versus returning students, a much higher ratio of incoming students than the standard course. The incoming students were much more likely to give low ratings than returning students. Students appreciated that the remote labs were done during synchronous sessions rather than asynchronous.

242	Same AND Different	At-school hands-on labs vs. at- home videos, data	Introductory undergraduate biochemistry course with 98 students in 7 class sections at Gonzaga University, USA during Spring 2020	Halfway through the course, students had already done many experiments with most of the techniques and equipment before the transition occurred. The procedure design and observation activities were abandoned, and students instead attended prelab lectures, watched experimental videos, and analyzed the provided raw sample data from the instructor.	Historical grade comparison to previous years (methods unspecified)	Instructors reported student performance was comparable to previous semesters.	Student feedback on survey at end of course (44 % response rate).	90.7 % agreed that they became comfortable with doing labs when f2f vs. 16.3 % who agreed for remote. 90.7 % agreed they learned how to organize a lab notebook when f2f vs. 7.0 % for remote. 90.6 % agreed they learned how to analyze data when f2f vs. 81.4 % for remote. 86.1 % agreed they learned how to work collaboratively with peers when f2f vs. 79.1 % for remote. 95.4 % agreed that f2f labs increased their understanding of the discipline vs. 53.5 % for remote. 76.7 % agreed that that f2f labs made them more competitive professionally vs. 42.8 % for remote.	Student feedback on survey at end of course (44 % response rate).	Students overwhelmingly contrasted f2f labs and remote learning in terms of the ability to manually perform experiments and gain hands-on experience, but the majority also reported the videos and Zoom data discussion sessions were helpful and provided a much- needed sense of normalcy, motivation, and accountability.

287	Same AND Different	At-school hands-on labs vs. at-home procedure writing, data prediction	Upper-level undergraduate biochemistry and synthetic chemistry CUREs (10-20 & 6-9 students respectively) at Sonoma State University, USA during Spring 2020	Students had reviewed literature, developed a research plan, and were in the initial experiment stages of their group projects before the transition. Instead of conducting more experiments, students wrote theoretical procedures and predicted the data that should result. Students wrote journal-style manuscripts, made posters for the experiments they had already completed, attended group meetings, and did peer review.			Historical comparison of quality of lab notebooks. Percent-matches with literature via Turn-It-In plagiarism detection software. Student feedback (methods unspecified).	Students struggled to write realistic procedures, understand literature experimental sections, engage in experimental design, make appropriate practical decisions, and predict the expected raw data. Students drew heavily on examples of published data and experimental sections, although students who followed the rubric guidelines had fewer instances of Turn-It-In percent-matches and appeared to understand the procedures and data better. The quality of the manuscripts, posters, and presentations appeared unchanged. Students reported learning that hands-on bench work is only one part of the research process.	Attendance records. In-class behavior.	Although synchronous meetings were not mandatory, most students attended; no students requested alternative asynchronous assignments. Student participation in class appeared much worse, and students often had their cameras and audio off.

294	Same AND Different	At-school hands-on labs vs. unspecified	Introductory undergraduate general chemistry with 57 students and general chemistry CURE with 29 students at the University of Nebraska at Omaha, USA during Spring 2020	Students had self- selected into the traditional or CURE lab sections. CURE students had completed several traditional experiments and were working in small groups to develop a research question about food chemistry and use the literature to develop a procedure. They had started preparing their samples before the transition. Traditional lab students were conducting cookbook experiments. After the transition, both groups did "online laboratories" of an unspecified type which supposedly followed the traditional lab manual (the Supporting Information files could not be accessed for further investigation due to an apparent website glitch).	Final exam grades.	Performance on the final exam was not statistically significantly different between the two groups, although the CURE group scored a little higher on average.	Two-tailed paired t test with equal variances analysis of pre/post-survey responses (given at start and end of course) on modified CLASS-Chem instrument to evaluate expert-like thinking for both CURE and traditional lab (~ 50 % response rate). Semistructured focus group interviews (n =3 for each course).	There were no significant differences between the pre/post scores for the CURE course or for the traditional lab course. Students in both courses mostly already somewhat agreed with expert- like thinking statements at the start of the courses. In the focus group interviews, CURE students focused on "thinking like a scientist" topics whereas traditional students focused on "thinking like a student" topics. However, CURE students tended to already have somewhat better CLASS-Chem scores at the start of the semester than traditional students, and the traditional course had more first-generation students than the CURE did.	Two-tailed paired t test with equal variances analysis of pre/post-survey responses (given at start and end of course) on modified CLASS-Chem instrument to evaluate expert-like thinking for both CURE and traditional lab (~ 50 % response rate). Demographic comparison of CURE vs. traditional students. Semistructured focus group interviews (n =3 for each course).	The demographic composition of the CURE and traditional lab sections were roughly comparable except for the ratio of 1st generation students. The instructors suspect that scheduling registration into one or the other. CURE students discussed their morale more than traditional students did.
209	Different	At-school hands-on labs vs. at- home videos AND At-school vs. at-home hands-on labs	Introductory undergraduate organic chemistry with 61 students in 3 class sections at the Autonomous University of Nuevo León, Mexico during Spring 2020	At first, experimental videos replaced labs but were then replaced with an at- home, hands-on column chromatography experiment.			Quality of student lab reports for remote vs. previous semesters.	Videos were felt to be ineffective at promoting interaction and learning outcomes. There appeared to be no significant difference between student comprehension of separation and chromatography		

							concepts compared to previous years.		
216	Different	At-school vs. at-home hands-on labs	Introductory undergraduate physical chemistry with 23 students at the University of Santiago de Compostela, Spain during Spring 2020	One of the two planned experiments was converted to an at-home, hands-on kitchen lab. Students made photometers out of smartphones to collect data on dyed solutions. Students who failed to get data were supplied with sample data.	Historical comparison of lab report grades for remote vs. previous semesters.	Lab report grades were similar to previous years.		Perceived student attitude. Student feedback (methods unspecified).	The experiment was optional, but everyone did them. Students were keen and motivated to make the lab work. Students reported positive feedback.
212	Different	At-school hands-on labs vs. at-home videos, simulations, data, procedure writing	Introductory undergraduate organic chemistry for health careers at the University of Michigan – Dearborn, USA during Spring 2020	12 labs were replaced with instructor demonstrations, experimental videos, simulations, readings, more writing-based assignments, and sample data. Students wrote lab reports based on the sample data and determined structures of unknown molecules. They also analyzed journal articles to write a lab procedure and made videos about techniques.	Historical grade comparison of similar lab reports for remote vs. previous semesters.	Lab report grades were similar to historical grades.	Quality of lab reports and student-made videos explaining lab techniques. Student feedback (methods unspecified).	Students learned new concepts, did simple calculations, and analyzed spectra and TLC results without noted difficulty. They appeared to struggle to build on knowledge, connect topics across questions, and use all relevant data to make conclusions. Students incorrectly assumed that incomplete simulated reactions were complete and showed lower comprehension regarding safety, troubleshooting, how to execute practical techniques, and waste disposal. Students gave	

								positive feedback about the digital resources in general but reported that they struggled to make connections between simulations and lab reports.		
254	Different	At-school hands-on labs vs. at-home videos, simulations, data	Upper-level undergraduate biochemistry/computational BASIL CURE with 6 courses at 5 institutions in USA during Spring 2020	Students had almost finished collecting experimental data for a multi-stage lab. The remaining computational modules of the curriculum and experimental videos replaced the remaining f2f labs. Students used data from students at other schools or historical student data to complete their analysis and then present results.			Paired pre/post-Participant Perception Indicator survey (9 students with paired responses). Student feedback on end-of-semester survey (methods unspecified)	Students reported it was hard to write about experiments they didn't do themselves and data that wasn't perfectly aligned with their projects. A survey at one school showed learning gains but not as much as a previous f2f precedent; learning gains were higher for computational techniques than biochemical.	Student feedback on end-of-semester survey (methods unspecified)	Students were glad to have data to analyze but were sad to not gather it themselves. Students were excited to still do projects computationally. Motivation decreased for students who couldn't analyze their own data.

236	Different	At-school hands-on labs vs. at-home videos, procedure writing, data	Introductory undergraduate organic and analytical chemistry at the University of Connecticut, USA during Spring 2020	Experimental videos were made for organic labs, for which students already had prior experience with. Organic students also designed a guided-inquiry lab practical to rank reaction rates, a modified version of a similar guided-inquiry f2f lab..... Readings, notes, and data were given to analytical students, and the course shifted to focus heavily on data analysis rather than experimentation. Analytical students were anticipated to poorly understand the experiments and so grading and lectures expected mistakes.	Historical grade comparison of organic postlab assignments for remote vs. previous semester.	For organic chemistry, students got 10 – 15 % higher grades on organic postlab assignments, leading the instructors to suspect cheating.	Historical comparison of quality of organic inquiry lab for remote vs. previous semester. Quality of analytical chemistry data analysis. Student feedback (methods unspecified).	For organic chemistry, instructors and students felt students did not understand organic labs and gave superficial responses. The final organic guided-inquiry lab activity was considered much less successful. For analytical chemistry, students frequently made mistakes with data analysis.	Attendance at office hours.	Very few students came to the added office hours for either course.
239	Different	At-school hands-on labs vs. at-home videos	Introductory undergraduate general chemistry with ~ 150 students at Brown University, USA during Spring 2020	After 3 f2f labs before closure, the remaining labs were replaced with pre-made first-person experimental videos with embedded interactive questions. Lab reports were revised to focus around critical thinking questions.			Student feedback from multiple surveys during the semester. Historical comparison of student perceptions of one lab for remote vs. previous semester.	Students reported the lab videos were well-done and helpful but not as effective as f2f labs. By the end of the semester, students reported much lower levels of learning than previous, f2f students had. Students commented that they felt that hands-on labs were irreplaceable.	Historical comparison of student perceptions of one lab for remote vs. previous semester.	Students reported much lower levels of enjoyment than previous, f2f students had.

232	Different	At-school vs. at-home hands-on labs AND At-school hands-on labs vs. at-home videos, professional development, presentations	Introductory noncredit optional supplemental high school program with professional development activities with 35 students at University of Michigan - Ann Arbor, USA during Summer 2020	Students virtually took tours of the campus, socialized, learned about foundational general and organic chemistry topics, focused on specific organic chemistry reactions, spoke with university and research personnel, attended information sessions, investigated careers, watched live videos of experiments, did hands-on experiments at home, and gave class presentations.				Student feedback on end-of-course survey (100 % response rate). Historical comparison of experiment ratings.	Students rated the hands-on kitchen labs, the lessons, and the career prep higher than the video experiment labs and the virtual tours. The program increased 91.4 % students interest in pursuing STEM careers. The 2020 remote students ranked the two hands-on labs higher than the 2019 in-person students did for the corresponding lab experiment, although a statistical analysis was not provided.

^a"Same" = remote learning is contrasted within the group of students; "Different" = remote learning is contrasted with a different group of students;

^b"Activity Comparison" = general sketch of activities contrasted or implied in the evidence for before vs. during remote learning

Appendix E

Corresponding to **Chapter 5. Which Attributes Matter Most in the Mentors of Early Career Chemists?: Instrument Development for Assessing Mentorship**

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E.1 Interview Protocol for Key Informants (Phase 2)

Key informant interviewees discussed their beliefs about mentorship and prior experiences in chemistry research environments during semi-structured interviews (10 participants for 20 – 30 minutes each). In the final part of the interview, participants were asked for their impressions of a few purposefully selected items under development (such as the list of Content examples) from the draft survey. Participants were not asked all the questions in each interview. Question selections were partially guided by participant responses and the available remaining time.

[consent process, then the following questions]

I will ask you questions about your experiences and opinions regarding mentorship in chemistry research labs. I hope that you will feel you can speak freely in front of me and express your full opinion without any concerns. Our discussion today will help me to develop a survey for future use about chemistry mentorship, so I really appreciate your help with this.

Questions:

1. In thinking about current and prior chemistry research mentors you have had, what types of positions have they held (e.g., faculty, grad student, etc.)?
2. Were these mentors good, bad, or just mediocre, and why do you say so?
 - **[Probe]** Can you give me some examples of situations that demonstrate the type of mentor they were?
 - **[Follow up if bad or mediocre]** What should they have done differently to be a better research mentor?
3. In thinking about any current or prior chemistry research mentors you have had, what did they teach you or help you to do?
 - **[Probe]** How did your research mentor factor into your day-to-day work in the lab?
 - **[Follow up if they didn't factor into the day-to-day]** Your overall, long-term work?
4. What do you feel makes someone a good or bad “research mentor” in chemistry?
 - **[Follow up]** Do you feel like this is any different from what makes someone a good or bad mentor in general, for things outside of the chemistry research lab?
5. Is a chemistry research mentor more important (A) for helping you with practical / technical / experimental work OR (B) for helping you in a social / career / advising capacity? Or are the categories equal in importance?
6. I'm going to present you with a couple questions that might show up on the survey I am developing. I will put the link in the chat box now. Please go to question #__, and submit answers to it. Please talk out loud while you are reading and answering the question so that I can hear what's going on in your head.
 - **[Prompt if participant falls silent]** Please speak aloud whatever you are thinking right now, even if it's just a half-formed thought.
 - **[Follow up]:**
 - Does this question make sense? What do you think this question is asking?
 - Can you walk me through your response? Why did you answer the way you did?
 - Is there anything else, either in terms of question wording or answer options, that you think should or should not be in this question for it to make sense? What would you add, remove, modify?

- **[For Likert questions]** What does a 1 or 4 or 7 mean to you for this question?

[wrap-up and incentive distribution]

E.2 Category Descriptions

The categories were adjusted slightly as a result of cognitive testing and the item classification data. The category “Awareness” was removed due to poor performance (namely, cross-loading with “Emotion” and “Life”), and slight revisions were made to some items to minimize confusion (e.g., changing “Professional Conventions” to “Norms” due to participants interpreting “conventions” as referring to academic conferences).

Descriptions used for pilot survey

- A (conceptual) = improving conceptual knowledge and conceptual skills
- B (technical) = improving technical knowledge and technical skills
- C (project) = guiding the development and progress of a research project
- D (advising) = providing advice and guidance on academic and career topics
- E (professional and conventions) = showcasing professionalism and scientific conventions used in the field
- F (professional socialization) = facilitating professional socialization in the field
- G (emotion) = providing emotional support and a sense of belonging
- H (awareness) = being aware of differences between people, their backgrounds, and their abilities
- I (life) = supporting life goals outside of research and the professional world

Descriptions for final survey

- Conceptual = improving conceptual knowledge and conceptual skills
- Technical = improving technical knowledge and technical skills
- Project = guiding the development and progress of a research project
- Advising = providing guidance on academic and career topics
- Norms = showcasing professionalism and scientific norms used in the field
- Professional Socialization = facilitating professional socialization in the field
- Emotion = providing emotional support and a sense of belonging
- Life = supporting life goals outside of research and the professional world

The Awareness category was removed due to the category’s poor performance overall.

E.3 Pilot Survey (Phase 3A)

The drafted survey underwent revisions based on the key informant interviews, and the resulting version was submitted to piloting. This pilot survey was used for classifying example activity items into the mentorship Content domains and for soliciting written response process data for the survey items. Respondents were randomly assigned to portions of the survey. The displayed items were selectively chosen from the drafted survey such that the more methodologically questionable items were prioritized for the sake of time and to minimize survey fatigue (e.g., questions about race or gender were not tested). Some survey logic is shown here for the reader's convenience.

[consent form, then the following questions]

You may pause the survey if you need a break and return to finish later (after 48 hours of no activity from you, the survey will close permanently without distributing a gift card). Your responses are anonymous and confidential, so please be honest. We will ask you to provide feedback on questions we are developing to use _____ in _____ a _____ future _____ survey.

[Parts were randomly assigned]

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[PART I]

Instructions: We will show you a list of actions that a mentor/PI might engage in to support someone (such as a student mentee) working in a research group. We would like you to sort each of these actions into 1 of _____ 9 _____ possible _____ categories.

*Q1 Choose the category you think each action best fits based on the provided descriptions of the categories.

Categories of how a mentor might support a student:

- A (conceptual) = improving conceptual knowledge and conceptual skills
- B (technical) = improving technical knowledge and technical skills
- C (project) = guiding the development and progress of a research project
- D (advising) = providing advice and guidance on academic and career topics
- E (professional and conventions) = showcasing professionalism and scientific conventions used in the field
- F (professional socialization) = facilitating professional socialization in the field
- G (emotion) = providing emotional support and a sense of belonging
- H (awareness) = being aware of differences between people, their backgrounds, and their abilities
- I (life) = supporting life goals outside of research and the professional world



Define terminology	▼ A (conceptual) ... I (life)
Provide important conceptual facts	▼ A (conceptual) ... I (life)
Explain how techniques work theoretically on the abstract level	▼ A (conceptual) ... I (life)
Show how to solve conceptual problems	▼ A (conceptual) ... I (life)
Explain how standard concepts relate to their application in research	▼ A (conceptual) ... I (life)
Teach advanced concepts not learned in courses	▼ A (conceptual) ... I (life)
Explain how to handle research equipment	▼ A (conceptual) ... I (life)
Explain how to conduct research techniques	▼ A (conceptual) ... I (life)
Show how to conduct standard techniques using research equipment	▼ A (conceptual) ... I (life)
Show how to complete group chores	▼ A (conceptual) ... I (life)
Give tips on troubleshooting technical research problems	▼ A (conceptual) ... I (life)
Show how to do advanced research techniques	▼ A (conceptual) ... I (life)
Explain how to develop a project	▼ A (conceptual) ... I (life)
Show how to search the literature	▼ A (conceptual) ... I (life)
Provide a research idea	▼ A (conceptual) ... I (life)
This question detects people not reading the questions. Select "Life".	▼ A (conceptual) ... I (life)
Give advice on a research project	▼ A (conceptual) ... I (life)
Evaluate a project's progress	▼ A (conceptual) ... I (life)
Enable a mentee to make a significant contribution to a project	▼ A (conceptual) ... I (life)
Give advice on academic decisions	▼ A (conceptual) ... I (life)
Advise the mentee on careers	▼ A (conceptual) ... I (life)
Prepare the mentee for future department expectations	▼ A (conceptual) ... I (life)
Help the mentee set career goals	▼ A (conceptual) ... I (life)
Give the mentee feedback on their professional progress	▼ A (conceptual) ... I (life)
Help the mentee navigate an institution's policies	▼ A (conceptual) ... I (life)
Be professional	▼ A (conceptual) ... I (life)
Be a role model as a chemist	▼ A (conceptual) ... I (life)
Demonstrate good workplace behavior	▼ A (conceptual) ... I (life)

Teach important professional skills for a chemist	▼ A (conceptual) ... I (life)
Give advice on how to meet professional expectations	▼ A (conceptual) ... I (life)
Explain field-specific conventions for presenting research	▼ A (conceptual) ... I (life)
Introduce the mentee to other people in chemistry	▼ A (conceptual) ... I (life)
Help the mentee build positive social relationships with other group members	▼ A (conceptual) ... I (life)
Suggest social events for meeting other chemists	▼ A (conceptual) ... I (life)
Suggest activities to participate in for professional advancement	▼ A (conceptual) ... I (life)
Speak up for the mentee on their behalf	▼ A (conceptual) ... I (life)
Give advice on how to collaborate with other people	▼ A (conceptual) ... I (life)
Make the mentee feel like they belong	▼ A (conceptual) ... I (life)
Show the mentee they are welcome in the group	▼ A (conceptual) ... I (life)
Be encouraging	▼ A (conceptual) ... I (life)
Be positive	▼ A (conceptual) ... I (life)
Show sympathy	▼ A (conceptual) ... I (life)
Show kindness	▼ A (conceptual) ... I (life)
This question detects people not reading the questions. Select "Conceptual".	▼ A (conceptual) ... I (life)
Be patient	▼ A (conceptual) ... I (life)
Listen to what the mentee thinks	▼ A (conceptual) ... I (life)
Consider what the mentee does/doesn't know	▼ A (conceptual) ... I (life)
Try to understand the mentee's background	▼ A (conceptual) ... I (life)
Be non-judgmental	▼ A (conceptual) ... I (life)
Ask the mentee what they think about things	▼ A (conceptual) ... I (life)
Get to know the mentee as a person	▼ A (conceptual) ... I (life)
Discuss life events outside of research	▼ A (conceptual) ... I (life)
Encourage a healthy work-life balance	▼ A (conceptual) ... I (life)
Discuss long-term life goals (excluding career or professional goals)	▼ A (conceptual) ... I (life)
Be a role model as a person in general, outside of research	▼ A (conceptual) ... I (life)
Suggest fun social activities outside of the research group	▼ A (conceptual) ... I (life)

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[PART II]

Instructions: You will be presented a randomly selected portion of 6-7 shorter survey questions. Write down what you think each question is asking you to do in your own words without copying the question's wording. You do NOT need to actually answer the sample survey questions! Do NOT answer the actual survey questions.

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[PART IIA]

***Q2A.1 Answer This:**

What do you think the question below is asking? Please use "your own words" (instead of just copying the question) to describe what you think the question is asking.

Also, state whether you would be able to answer the question. If you are uncertain what the question is asking or if you have any suggestions for how the question or answer choices should be modified, please also say that. Do not bother actually answering the question below.

Sample Question (Don't Answer This):

What is your experience with working in a chemistry research group? Select all that apply.

This includes any research group that is interdisciplinary or works jointly in chemistry and another academic area, such as chemical education, chemical engineering, computational chemistry, etc.

- ☐ Currently working in a chemistry research group now
- ☐ Previously worked in a chemistry research group in the past
- ☐ Will start working in a chemistry group in the future
- ☐ None of the above

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***Q2A.2 Answer This:**

What do you think the question below is asking? Please use "your own words" (instead of just copying the question) to describe what you think the question is asking.

Also, state whether you would be able to answer the question. If you are uncertain what the question is asking or if you have any suggestions for how the question or answer choices should be modified, please also say that. Do not bother actually answering the question below.

Sample Question (Don't Answer This):

Do you have a PI?

"PI" (Principal Investigator) refers to the person (usually a professor) who leads the research group.

- ☐ Yes
- ☐ Yes, more than one PI
- ☐ No

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***Q2A.3 Answer This:**

What do you think the question below is asking? Please use "your own words" (instead of just copying the question) to describe what you think the question is asking.

Also, state whether you would be able to answer the question. If you are uncertain what the question is asking or if you have any suggestions for how the question or answer choices should be modified, please also say that. Do not bother actually answering the question below.

Sample Question (Don't Answer This):

Do you have an official mentor within the research group (not including your PI)?

A "mentor" is someone who advises or trains you (they might also be a friend, a supervisor, an older or younger colleague, etc. and could hold any position ranging, for example, from undergraduate to faculty). You might have a positive or negative relationship with them; they might be a good or bad mentor. This question refers specifically to a person within the group who was assigned, "voluntold" / volunteered, or otherwise expected to mentor you (perhaps by your PI or another senior member of the group).

- ☐ Yes, I have an official mentor.
- ☐ Yes, I have a mentor, but it's more like a semi-official mentorship.
- ☐ No, I do not have an official mentor.

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***Q2A.4 Answer This:**

What do you think the question below is asking? Please use "your own words" (instead of just copying the question) to describe what you think the question is asking.

Also, state whether you would be able to answer the question. If you are uncertain what the question is asking or if you have any suggestions for how the question or answer choices should be modified, please also say that. Do not bother actually answering the question below.

Sample Question (Don't Answer This):

Describe (in ~2-4 sentences) what you typically do on a day-to-day basis for your research, whether conducted inside or outside a physical laboratory space.

Please describe in simple terms so that a chemist outside your specialty could understand. For example, are you writing computer codes? Are you growing cell cultures? Are you planning reactions?

----- page break -----

***Q2A.5 Answer This:**

What do you think the question below is asking? Please use "your own words" (instead of just copying the question) to describe what you think the question is asking.

Also, state whether you would be able to answer the question. If you are uncertain what the question is asking or if you have any suggestions for how the question or answer choices should be modified, please also say that. Do not bother actually answering the question below.

Sample Question (Don't Answer This):

Indicate the ratio of time you yourself spend doing "wet" work (i.e., chemicals, organisms, fume hoods) vs. doing "dry" (i.e., computers, analysis, instruments) in your research.

	1 = Almost Only Wet	2	3	4 = Equal	5	6	7 = Almost Only Dry
Time spent doing "wet" vs. "dry" work	☐	☐	☐	☐	☐	☐	☐

----- page break -----

***Q2A.6 Answer This:**

What do you think the question below is asking? Please use "your own words" (instead of just copying the question) to describe what you think the question is asking.

Also, state whether you would be able to answer the question. If you are uncertain what the question is asking or if you have any suggestions for how the question or answer choices should be modified, please also say that. Do not bother actually answering the question below.

Sample Question (Don't Answer This):

Describe (in ~1-2 sentences) the goal of your research project in simple terms so that a chemist outside your specialty could understand.

For example, are you synthesizing a natural product? Are you developing a new laser methodology?

----- *page break* -----

***Q2A.7 Answer This:**

What do you think the question below is asking? Please use "your own words" (instead of just copying the question) to describe what you think the question is asking.

Also, state whether you would be able to answer the question. If you are uncertain what the question is asking or if you have any suggestions for how the question or answer choices should be modified, please also say that. Do not bother actually answering the question below.

Sample Question (Don't Answer This):

Describe (in ~1-2 sentences) your general career path goals and the type of future job(s) you think you want. If you aren't sure yet, describe whatever you are currently most interested in.

For example, do you want to become a research-focused professor? A government forensic scientist? A science journalist?

----- *page break* -----

[PART IIB]

***Q2B.1 Answer This:**

What do you think the question below is asking? Please use "your own words" (instead of just copying the question) to describe what you think the question is asking.

Also, state whether you would be able to answer the question. If you are uncertain what the question is asking or if you have any suggestions for how the question or answer choices should be modified, please also say that. Do not bother actually answering the question below.

Sample Question (Don't Answer This):

For each category, rate how important it would be for an ideal PI (hypothetical – not your current, real PI) to provide you with that type of support currently.

Answer based on how you think a PI should support you. For example, do not answer based on how you think a PI should support other people. Do not answer based on what you wish your PI would do more of. Do not answer what you wish other mentors would do.

	1 = not at all important	2	3	4	5	6 = moderately important	7	8	9	10	11 = extremely important
Conceptual	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
Technical	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
Project	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
Advising	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
Professionalism and Conventions	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
Professional Socialization	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
Emotion	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
Awareness	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
Life	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐

----- page break -----

***Q2B.2 Answer This:**

What do you think the question below is asking? Please use "your own words" (instead of just copying the question) to describe what you think the question is asking.

Also, state whether you would be able to answer the question. If you are uncertain what the question is asking or if you have any suggestions for how the question or answer choices should be modified, please also say that. Do not bother actually answering the question below.



Sample Question (Don't Answer This):

Rank the categories in order of importance for the type of support that an ideal PI would provide to you currently. Click and drag to move the categories around.

1 (top) = most important, 9 (bottom) = least important

- Conceptual
- Technical
- Project
- Advising
- Professionalism and Conventions
- Professional Socialization
- Emotion
- Awareness
- Life

----- page break -----

***Q2B.3 Answer This:**

What do you think the question below is asking? Please use "your own words" (instead of just copying the question) to describe what you think the question is asking.

Also, state whether you would be able to answer the question. If you are uncertain what the question is asking or if you have any suggestions for how the question or answer choices should be modified, please also say that. Do not bother actually answering the question below.



Sample Question (Don't Answer This):

For each category, rate how often an ideal PI should provide you with that type of support currently.

	Daily	Every couple days	Weekly	Every couple weeks	Monthly	Less frequently than monthly	Never
Conceptual	☐	☐	☐	☐	☐	☐	☐
Technical	☐	☐	☐	☐	☐	☐	☐
Project	☐	☐	☐	☐	☐	☐	☐
Advising	☐	☐	☐	☐	☐	☐	☐
Professionalism and Conventions	☐	☐	☐	☐	☐	☐	☐
Professional Socialization	☐	☐	☐	☐	☐	☐	☐
Emotion	☐	☐	☐	☐	☐	☐	☐
Awareness	☐	☐	☐	☐	☐	☐	☐
Life	☐	☐	☐	☐	☐	☐	☐

----- page break -----

***Q2B.4 Answer This:**

What do you think the question below is asking? Please use "your own words" (instead of just copying the question) to describe what you think the question is asking.

Also, state whether you would be able to answer the question. If you are uncertain what the question is asking or if you have any suggestions for how the question or answer choices should be modified, please also say that. Do not bother actually answering the question below.



Sample Question (Don't Answer This):

Rank the categories in order of how often an ideal PI should provide you with that type of support currently. Click and drag to move the categories around.

1 (top) = most often, 9 (bottom) = least often

- Conceptual
- Technical
- Project
- Advising
- Professionalism and Conventions
- Professional Socialization
- Emotion
- Awareness
- Life

----- page break -----

***Q2B.5 Answer This:**

What do you think the question below is asking? Please use "your own words" (instead of just copying the question) to describe what you think the question is asking.

Also, state whether you would be able to answer the question. If you are uncertain what the question is asking or if you have any suggestions for how the question or answer choices should be modified, please also say that. Do not bother actually answering the question below.



Sample Question (Don't Answer This):

For each category, rate how satisfied you are with how your current, real PI provides you with that type of support currently.

	1 = not at all satisfied	2	3	4	5	6 = moderately satisfied	7	8	9	10	11 = extremely satisfied
Conceptual	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
Technical	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
Project	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
Advising	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
Professionalism and Conventions	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
Professional Socialization	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
Emotion	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
Awareness	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
Life	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐

----- page break -----

*Q2B.6 **Answer This:** What do you think the question below is asking? Please use "your own words" (instead of just copying the question) to describe what you think the question is asking.

Also, state whether you would be able to answer the question. If you are uncertain what the question is asking or if you have any suggestions for how the question or answer choices should be modified, please also say that. Do not bother actually answering the question below.



Sample Question (Don't Answer This):

Rank the categories in order of your satisfaction for the type of support that your PI provides to you currently. Click and drag to move the categories around.

1 (top) = most satisfied, 9 (bottom) = least satisfied

- _____ Conceptual
- _____ Technical
- _____ Project
- _____ Advising
- _____ Professionalism and Conventions
- _____ Professional Socialization
- _____ Emotion
- _____ Awareness
- _____ Life

----- *page break* -----

[PART IIC]

***Q2C.1 Answer This:**

What do you think the question below is asking? Please use "your own words" (instead of just copying the question) to describe what you think the question is asking.

Also, state whether you would be able to answer the question. If you are uncertain what the question is asking or if you have any suggestions for how the question or answer choices should be modified, please also say that. Do not bother actually answering the question below.

Sample Question (Don't Answer This):

Select the major subfield(s) of chemistry that you are currently conducting research in. Select all that apply.

- ☐ Analytical chemistry
- ☐ Biochemistry
- ☐ Chemical education
- ☐ Chemical engineering
- ☐ Computational chemistry
- ☐ Inorganic chemistry
- ☐ Organic chemistry
- ☐ Physical chemistry
- ☐ Other _____

----- page break -----

*Q2C.2 **Answer This:** What do you think the question below is asking? Please use "your own words" (instead of just copying the question) to describe what you think the question is asking.

Also, state whether you would be able to answer the question. If you are uncertain what the question is asking or if you have any suggestions for how the question or answer choices should be modified, please also say that. Do not bother actually answering the question below.

Sample Question (Don't Answer This):

Select _____ the _____ position _____ your _____ chemistry _____ research mentor _____ holds.

A "mentor" is someone who advises or trains you (they might also be a friend, a supervisor, an older or younger colleague, etc. and could hold any position ranging, for example, from undergraduate to faculty). You might have a positive or negative relationship with them; they might be a good or bad mentor. This question refers specifically to a person within a research group who was assigned, "voluntold" / volunteered, or otherwise expected to mentor you (perhaps by your PI or another senior member of the group).

- ☐ 1st-year undergraduate student ("freshman")
- ☐ 2nd-year undergraduate student ("sophomore")
- ☐ 3rd-year undergraduate student ("junior")
- ☐ 4th-year or more undergraduate student ("senior")
- ☐ 1st-year graduate student
- ☐ 2nd-year graduate student
- ☐ 3rd-year graduate student
- ☐ 4th-year graduate student
- ☐ 5th-year graduate student
- ☐ 6th-year or more graduate student
- ☐ Postdoc
- ☐ Staff scientist / research associate
- ☐ Professor
- ☐ Other _____

----- page break -----

***Q2C.3 Answer This:**

What do you think the question below is asking? Please use "your own words" (instead of just copying the question) to describe what you think the question is asking.

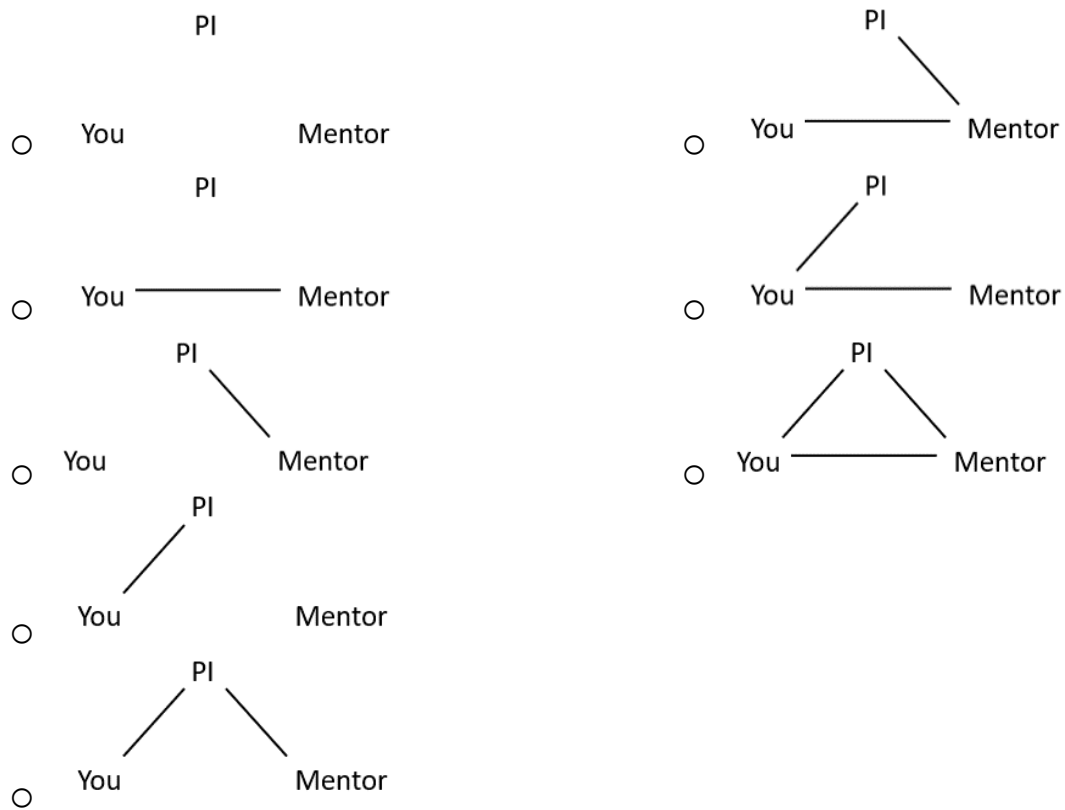
Also, state whether you would be able to answer the question. If you are uncertain what the question is asking or if you have any suggestions for how the question or answer choices should be modified, please also say that. Do not bother actually answering the question below.

Sample Question (Don't Answer This):

The following images display ways in which you, your mentor, and your PI might interact in order to support you and your research work.

"PI" (Principal Investigator) refers to the person (usually a professor) who leads the research group. The lines indicate that interactions occur between the people in order to support you and your work; no line means that interactions do not occur between the people (in terms of supporting you and your work).

Select the best image that currently illustrates your mentoring structure.



----- *page break* -----

***Q2C.4 Answer This:**

What do you think the question below is asking? Please use "your own words" (instead of just copying the question) to describe what you think the question is asking.

Also, state whether you would be able to answer the question. If you are uncertain what the question is asking or if you have any suggestions for how the question or answer choices should be modified, please also say that. Do not bother actually answering the question below.



Sample Question (Don't Answer This):

Rate the degree to which you currently agree with the following statements for your PI.

	-5 = Strongly Disagree	-4	-3	-2	-1	0 = Neutral	+1	+2	+3	+4	+5 = Strongly Agree
My PI and I are a good fit.	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
My PI and I see things in the same way.	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
My PI and I are not similar in our outlook, perspective, and values.	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐

----- page break -----

***Q2C.5 Answer This:**

What do you think the question below is asking? Please use "your own words" (instead of just copying the question) to describe what you think the question is asking.

Also, state whether you would be able to answer the question. If you are uncertain what the question is asking or if you have any suggestions for how the question or answer choices should be modified, please also say that. Do not bother actually answering the question below.

Sample Question (Don't Answer This):

Rate the current quality of mentorship that you feel you receive from your...

	-5 = Extremely negative / unfavorable	-4	-3	-2	-1	0 = Neutral	+1	+2	+3	+4	+5 = Extremely positive / favorable
Pl.	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
mentor.	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐

----- page break -----

***Q2C.6 Answer This:**

What do you think the question below is asking? Please use "your own words" (instead of just copying the question) to describe what you think the question is asking.

Also, state whether you would be able to answer the question. If you are uncertain what the question is asking or if you have any suggestions for how the question or answer choices should be modified, please also say that. Do not bother actually answering the question below.

Sample Question (Don't Answer This):

Has COVID-19 impacted the responses that you gave on this survey about your PI, your mentor, or your needs? If so, please briefly describe which responses were impacted and how. If not, write "NA" or skip this question.

----- page break -----

[incentive distribution]

E.4 Item Performance from Pilot Survey

Participants sorted each item into a category during the pilot survey. Items were presented in a random order in the pilot survey. Percent selection data was calculated for each item's most common subcategory (and corresponding parent category). 3 – 4 of the best performing items for each subcategory were selected for use in the final survey to provide concrete examples contextualizing what each category refers to in a chemistry research environment.

The following items were especially inspired by specific prior literature:

- Hernandez, P. R. *Landscape of Assessments of Mentoring Relationship Processes in Postsecondary STEMM Contexts: A Synthesis of Validity Evidence from Mentee, Mentor, Institutional/Programmatic Perspectives*; The National Academies Press, **2018**.^{340,351}
- Ceyhan, G. D.; Tillotson, J. W. Mentoring Structures and the Types of Support Provided to Early-Year Undergraduate Researchers. *CBE Life Sci. Educ.* **2020**, *19*:ar26 (3), 1–14.³⁵¹
- Tenenbaum, H. R.; Crosby, F. J.; Gliner, M. D. Mentoring Relationships in Graduate School. *J. Vocat. Behav.* **2001**, *59* (3), 326–341.³³⁹

Table E.1. Percent selection for the items from the pilot survey.

#	Original Pilot Item <i>Revisions after pilot in italics</i>	Parent / Subcategory ^a	% Selection with Subcat.	% Selection with Parent	Retained in Final?
1	Define terminology	Intellectual / Conceptual			
2	Provide important conceptual facts	Intellectual / Conceptual	89.6	95.8	Y
3	Explain how techniques work theoretically on the abstract level	Intellectual / Conceptual	68.8	95.8	Y
4	Show how to solve conceptual problems	Intellectual / Conceptual	85.4	93.8	Y
5	Explain how standard concepts relate to their application in research	Intellectual / Conceptual			
6	Teach advanced concepts not learned in courses	Intellectual / Conceptual	75.0	89.6	Y
7	Explain how to handle research equipment	Intellectual / Technical	89.6	93.8	Y
8	Explain how to conduct research techniques	Intellectual / Technical	87.5	97.9	Y
9	Show how to conduct standard techniques using research equipment	Intellectual / Technical	87.5	95.8	Y
10	Show how to complete group chores	Intellectual / Technical			
11	Give tips on troubleshooting technical research problems	Intellectual / Technical			
12	Show how to do advanced research techniques	Intellectual / Technical	81.3	95.8	Y

Table E.1. Percent selection for the items from the pilot survey. *[continued]*

13	Explain how to develop a project	Intellectual / Project			
14	Show how to search the literature	Intellectual / Technical			
15	Provide a research idea	Intellectual / Project	68.8	83.3	Y
16	Give advice on a research project	Intellectual / Project	68.1	70.2	Y
17	Evaluate a project's progress	Intellectual / Project	64.6	66.7	Y
18	Enable a mentee to make a significant contribution to a project	Intellectual / Project			
19	Give advice on academic decisions	Professional / Advising	89.6	95.8	Y
20	Advise the mentee on careers <i>Advise you on careers</i>	Professional / Advising	75.0	89.6	Y
21	Prepare the mentee for future department expectations	Professional / Advising			
22	Help the mentee set career goals <i>Help you set career goals</i>	Professional / Advising	72.3	85.1	Y
23	Give the mentee feedback on their professional progress <i>Give you feedback on your professional progress</i>	Professional / Advising	66.7	81.3	Y
24	Help the mentee navigate an institution's policies	Professional / Advising			
25	Be professional <i>Show how to be professional</i>	Professional / Norms	72.3	97.9	Y
26	Be a role model as a chemist	Professional / Norms			
27	Demonstrate good workplace behavior	Professional / Norms	72.7	95.5	Y
28	Teach important professional skills for a chemist	Intellectual / Technical			
29	Give advice on how to meet professional expectations	Professional / Norms			
30	Explain field-specific conventions for presenting research <i>Explain field-specific norms for presenting research</i>	Professional / Norms	72.9	75.0	Y
31	Introduce the mentee to other people in chemistry <i>Introduce you to other people in chemistry</i>	Professional / Socialization	80.4	93.5	Y

Table E.1. Percent selection for the items from the pilot survey. *[continued]*

32	Help the mentee build positive social relationships with other group members <i>Help you build positive social relationships with other group members</i>	Professional / Professional Socialization	73.9	80.4	Y
33	Suggest social events for meeting other chemists	Professional / Professional Socialization	85.4	93.8	Y
34	Suggest activities to participate in for professional advancement	Professional / Professional Socialization			
35	Speak up for the mentee on their behalf	Professional / Advising			
36	Give advice on how to collaborate with other people	Professional / Professional Socialization			
37	Make the mentee feel like they belong <i>Make you feel like you belong</i>	Psychosocial / Emotion	85.4	87.8	Y
38	Show the mentee they are welcome in the group	Psychosocial / Emotion			
39	Be encouraging	Psychosocial / Emotion			
40	Be positive	Psychosocial / Emotion	87.2	95.7	Y
41	Show sympathy	Psychosocial / Emotion	95.6	100.0	Y
42	Show kindness	Psychosocial / Emotion	91.3	95.7	Y
43	Be patient	Psychosocial / Emotion			
44	Listen to what the mentee thinks	Psychosocial / Emotion			
45	Consider what the mentee does/doesn't know	Psychosocial / Awareness			
46	Try to understand the mentee's background	Psychosocial / Awareness			
47	Be non-judgmental	Psychosocial / Awareness			
48	Ask the mentee what they think about things	Psychosocial / Awareness			
49	Get to know the mentee as a person	Psychosocial / Emotion			
50	Discuss life events outside of research	Psychosocial / Life	86.7	93.3	Y

Table E.1. *Percent selection for the items from the pilot survey. [continued]*

51	Encourage a healthy work-life balance	Psychosocial / Life	77.8	91.1	Y
52	Discuss long-term life goals (excluding career or professional goals)	Psychosocial / Life	77.1	79.2	Y
53	Be a role model as a person in general, outside of research	Psychosocial / Life			
54	Suggest fun social activities outside of the research group	Psychosocial / Life	72.9	91.7	Y

^aThe parent and subcategory designations shown here are according to what the plurality of respondents selected, which did not match the expected categories for 6 items.

E.5 Interview Protocol for Response Process (Phase 3B)

The survey was revised after Phase 3A, and 4 cognitive interviewees were asked about their process of answering the refined survey using Tourangeau's full 4-stage response process model during 30-60-minute interviews.

[consent process, then the following questions]

Our discussion today will help me to develop a survey for future use about chemistry mentorship, so I really appreciate your help with this. I will ask you questions about portions of that survey which is currently under development. I just want to get your in-depth thoughts on how you interpret certain items so I can make sure I am using the appropriate wording when I finalize the overall survey for future participants.

Questions, Part I [item classification]:

The survey asks you to sort a list of items into one of nine categories about how a PI or mentor might support a mentee. *[share screen of slide with instructions]*. I will present you with some of the items in a random order. I'd like you to describe to me how you interpret each item. Then, I will show you the nine categories and ask you to describe your thought process in how you decide to categorize the item. Some of my questions might seem a little repetitive, but bear with me. I will ask questions that try to get at different angles of what you think. Any questions so far?

For each item shown, ask the following:

1. What does this item mean to you in the context of mentorship in chemistry research settings?
[probing for Understanding of Item]
 - **[Probe]** How would you rephrase this item in your own words? What does this item refer to? What does it mean?
2. Now, here are the nine categories. Which category do you think you would categorize this item into?
3. What were you thinking about when you categorized this item? *[probing for Retrieval of Item and Category]*
 - **[Probe]** What thoughts or memories did this question bring into your head?
4. How did you decide to pick that category for this item over other categories? *[probing for Judgment of Item and Category]*
 - **[Probe]** What about this item or the category made that category seem like the best option?
5. How easy or hard was it to categorize this item, and why? *[probing for Response of Item and Category]*
 - **[Probe]** Would you change anything about this item to make categorizing it easier or clearer? If so, what would you change and why?

Sample slides (each item has a slide):

Part I of II: We will show you a list of actions that a mentor/PI might engage in to support someone (such as a student mentee) working in a research group. We would like you to sort each of these actions into 1 of 9 possible categories.

Choose the category you think each action best fits based on the provided descriptions of the categories.

Categories of how a mentor might support a student:

- A = improving conceptual knowledge and conceptual skills
- B = improving technical knowledge and technical skills
- C = guiding the development and progress of a research project
- D = providing advice and guidance on academic and career topics
- E = showcasing professionalism and scientific conventions used in the field
- F = facilitating professional socialization in the field
- G = providing emotional support and a sense of belonging
- H = being aware of differences between people, their backgrounds, and their abilities
- I = supporting life goals outside of research and the professional world

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Be a role model as a chemist

- A (conceptual) = improving conceptual knowledge and conceptual skills
- B (technical) = improving technical knowledge and technical skills
- C (project) = guiding the development and progress of a research project
- D (advising) = providing advice and guidance on academic and career topics
- E (professionalism & conventions) = showcasing professionalism and scientific conventions used in the field
- F (professional socialization) = facilitating professional socialization in the field
- G (emotion) = providing emotional support and a sense of belonging
- H (awareness) = being aware of differences between people, their backgrounds, and their abilities
- I (life) = supporting life goals outside of research and the professional world

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Questions, Part 2 [all other survey items]:

I'm going to present you with some questions that might show up on the final survey. I will put the link in the chat box now. Please go to question #____, and submit answers to it.

6. What does this question mean to you? [probing for *Understanding*]
 - **[Probe]** How would you rephrase this question in your own words? What does this question refer to? What does it mean?
7. What were you thinking about when you were reading and answering this question? [probing for *Retrieval*]
 - **[Probe]** What thoughts or memories did this question bring into your head?
8. How did you decide on your answer? [probing for *Judgment*]
 - **[Probe]** What about this question made that answer seem like the best option?
9. Was it easy or hard to answer this question, and why? [probing for *Response*]
 - **[Probe]** Would you change anything about this question to make answering it easier or clearer? If so, what and why?

[wrap-up and incentive distribution]

E.6 Final Survey

This final version of the survey is ready to be used with a larger population. Based on demographics (e.g., whether the respondent is a postdoc, graduate student, etc.), the survey flow will change as needed. However, the core survey items remain the same across all respondent subsamples. Information about survey logic (e.g., display logic) is shown here for the utility of future researchers. The branching logic controls the eligibility criteria and the blocks shown based on whether a respondent has a peer mentor or not.

The following items were either borrowed directly from or highly inspired by specific prior literature:

- Q9.4
 - Aikens, M. L.; Sadselia, S.; Watkins, K.; Evans, M.; Eby, L. T.; Dolan, E. L. A Social Capital Perspective on the Mentoring of Undergraduate Life Science Researchers: An Empirical Study of Undergraduate-Postgraduate-Faculty Triads. *CBE Life Sci. Educ.* **2016**, *15*:ar16 (2), 1–15.³⁵²
 - Q9.5
 - Hernandez, P. R.; Estrada, M.; Woodcock, A.; Schultz, P. W. Mentor Qualities That Matter: The Importance of Perceived (Not Demographic) Similarity. *J. Exp. Educ.* **2017**, *85* (3), 450–468.³⁴¹
 - Ensher, E. A.; Murphy, S. E. Effects of Race, Gender, Perceived Similarity, and Contact on Mentor Relationships. *J. Vocat. Behav.* **1997**, *50* (3), 460–481.³⁴⁶
 - Q9.6
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 - Demographic questions
 - Office of Management and Budget. *Standards for the Classification of Federal Data on Race and Ethnicity*; Executive Office of the President; Washington, D.C.; **1995**. https://obamawhitehouse.archives.gov/omb/fedreg_race-ethnicity (accessed 5/2023).³⁵⁶
-

Block: Consent Form (2 Questions)

Branch: New Branch

If

If Consent: You can either agree (“consent”) or not agree to participate in the study. I do NOT agree to participate in the research. The form will now close, and no further information will be collected. Is Selected

EndSurvey:

Standard: Screening (7 Questions)

Branch: New Branch

If

If Select the option that best describes your position. None of the above Is Selected

EndSurvey: Advanced

Branch: New Branch

If

If How long ago did you stop working in your most recent group? 2 or more months ago Is Selected

EndSurvey: Advanced

Standard: Mentorship Status (8 Questions)

Standard: Categories (5 Questions)

Standard: Overall Ratings (5 Questions)

Standard: PI Ratings (5 Questions)

Branch: New Branch

If

If Do you have a mentor within the research group (not including\${q://QID13/ChoiceTextEntryValue})? A “mentor” is someone wh... Yes, I have a mentor in the group. Is Selected

Standard: Mentor Ratings (5 Questions)

Standard: Ranking (6 Questions)

Standard: Mentoring Structure (9 Questions)

Standard: Past Experiences (7 Questions)

Standard: Demographics (23 Questions)

Standard: Gift Card (1 Question)

Branch: New Branch

If

If Thank you for completing this survey! Your response has been recorded. We greatly appreciate yo... Yes, enter me Is Selected

EndSurvey: Advanced

Start of Block: Consent Form

Q1.1 Greetings! We would like your help to improve mentorship and related resources available to chemists. We are researchers investigating how people view mentorship in the chemistry research setting. Your input is very important to make sure that experiences of students and postdocs like you are properly represented. Your candid answers on our survey would help us understand nuances in mentorship nationwide and potentially make general recommendations for how to adjust trainings, policies, and/or other resources related to mentoring.

We would greatly appreciate your help with our research! Please read below to learn more.

Participation: You have been asked to participate because of your chemistry connections. Participation is voluntary.

What You'd Do: Complete a **survey (estimated 20-40 minutes)**.

- The estimated time may be a wide range because of individuals' desire to carefully consider questions about personal experiences. Once you start, you will be able to pause the survey and return to it over the course of 72 hours.
- It will be easier to complete the survey on a computer rather than a phone.

Eligibility: undergraduate students, graduate students, and postdoctoral researchers in chemistry research groups

- **Including** interdisciplinary chemistry groups (i.e., chemical engineering, chemical education, computational chemistry, etc.)
- **Excluding** people who have never been in a chemistry research group OR who left their group more than 2 months ago
- **Excluding** people who joined their group less than 2 months ago

Benefits:

- [incentive info]
- This study may help institutions make mentorship more effective.

Risks: There are no significant anticipated risks beyond that of everyday life.

Confidentiality: The survey is anonymous.

- Data will be reported in aggregate. We will keep data protected in secure digital storage.
- If you withdraw or do not finish the survey, the data already collected might be used. Any personally-identifiable data (e.g., email addresses in the drawing) will be destroyed at the end of data collection.
- Your email address is (optionally) collected after the survey on a separate form for the gift card drawing. Your email is not connected to your survey responses.

Questions or Concerns?

- [insert contact & IRB info]

***Q1.2 Consent:** You can either agree ("consent") or not agree to participate in the study.

- ☐ I agree to participate in the research.
- ☐ I do NOT agree to participate in the research. The form will now close, and no further information will be collected.

End of Block: Consent Form

Start of Block: Screening

Q2.1 Instructions: You may pause the survey if you need a break and return to finish later (after 72 hours of no activity from you, the survey will restart).

First, we will ask questions to confirm that you are eligible to participate. Next, we will ask about ways that people can support you in chemistry research settings. Finally, we will ask about the type of research you do and about your experiences.

*Q2.2 Select the option that best describes your position.

- ☐ Undergraduate student
- ☐ Graduate student
- ☐ Postdoctoral researcher
- ☐ None of the above

*Q2.3 Do you currently work in a chemistry research group?

This includes any research group that is interdisciplinary or works jointly in chemistry and another academic area, such as chemical education, chemical engineering, computational chemistry, etc.

- ☐ Yes
- ☐ No

*Display This Question:
If Q2.3 = Yes*

*Q2.4 How long ago did you join your current group?

- ☐ Less than 2 months ago
- ☐ 2 or more months ago

*Display This Question:
If Q2.3 = No
Or Q2.4 = Less than 2 months ago*

*Q2.5 Have you previously worked in a chemistry research group?

- ☐ Yes
- ☐ No

*Display This Question:
If Q2.5 = Yes*

*Q2.6 How long ago did you stop working in your most recent group?

- ☐ Less than 2 months ago
- ☐ 2 or more months ago

End of Block: Screening

Start of Block: Mentorship Status

Q3.1 Great, you are eligible to participate in this study!

Mentorship is a very broad concept. The following questions refer specifically to your experiences being mentored in your current chemistry (or interdisciplinary chemistry) research group.

We want to hear only about your recent experiences. Please answer all questions exclusively based on your recent experiences (aka within the past month or two) in chemistry research. Do not answer based on other experiences. If you are not currently in a chemistry research group, answer based on your most recent experiences in your past chemistry research group.

*Q3.2 Do you have a PI?

"PI" (Principal Investigator) refers to the person (usually a professor) who leads the research group.

- ☐ Yes, one PI
- ☐ Yes, more than one PI
- ☐ No

Display This Question:
If Q3.2 = No

Q3.3 Please briefly explain how it is that you do not have a PI and who supervises you instead (you do not need to use their name - just describe the general situation).

Also, for any future questions referring to "your PI", answer those questions based on your opinions about whoever you consider to be your primary supervisor.

Display This Question:
If Q3.2 = Yes, more than one PI

Q3.4 For any future questions referring to "your PI", please consistently answer based on the PI who would most likely be considered your primary chemistry PI.

*Q3.5 [Note to reader: piped text references Q3.5 as QID13]

What is your PI's name?

Note: this data is **NOT** used to identify you / your PI and will be deleted before analysis. Some of the upcoming questions are complex, so we ask for a name because then the computer can put your PI's name

into the questions to make questions easier for you to read. You may provide a nickname, initials, or write "PI" if you are uncomfortable with writing their name.

----- page break -----

*Q3.6 Do you have a mentor within the research group (not including \${q://QID13/ChoiceTextEntryValue})?

A “mentor” is someone who advises or trains you. They might also be a friend, a supervisor, an older or younger colleague, etc. They could hold any position ranging, for example, from undergraduate to faculty. You might have a positive or negative relationship with them; they might be a good or bad mentor.

This question refers specifically to a person within the group who was assigned, “voluntold”, volunteered, or expected to mentor you (perhaps by \${q://QID13/ChoiceTextEntryValue} or another senior member of the group) or is otherwise perceived to be mentoring you.

- ☐ Yes, I have a mentor in the group.
- ☐ No, I do not have a mentor in the group.

Display This Question:

If Q3.6 = Yes, I have a mentor in the group.

Q3.7 How many of these mentors do you currently have in the group? Ignore prior mentors. Enter as a number.

Display This Question:

If Q3.6 = Yes, I have a mentor in the group.

And And How many of these mentors do you currently have in the group? Ignore prior mentors. Enter as a... Text Response Is Not Equal to 1

And And How many of these mentors do you currently have in the group? Ignore prior mentors. Enter as a... Text Response Is Not Empty

Q3.8 Please consistently answer all following questions about “your (non-PI) mentor” in terms of the one person you think \${q://QID13/ChoiceTextEntryValue} most considers to currently be your primary mentor.

Display This Question:

If Q3.6 = Yes, I have a mentor in the group.

*Q3.9 [Note to reader: piped text references Q3.9 as QID17]

What is your mentor's name?

You may provide a nickname, initials, or write "Mentor" if you are uncomfortable with writing their name.

End of Block: Mentorship Status

Start of Block: Categories

Q4.1 Next, here are 8 categories of common types of support that \${q://QID13/ChoiceTextEntryValue} or \${q://QID17/ChoiceTextEntryValue} might provide with examples of actions that belong to each category. For example, \${q://QID13/ChoiceTextEntryValue} might support you by "providing important conceptual facts" or by "providing a research idea".

Please take a moment to become familiar with each category's examples. The next questions will ask you about your experiences with these types of mentoring. You will be shown the category definitions again.

Q4.2 **Conceptual** = improving conceptual knowledge and conceptual skills

- Provide important conceptual facts
- Show how to solve conceptual problems
- Teach advanced concepts not learned in courses
- Explain how techniques work theoretically on the abstract level

Technical = improving technical knowledge and technical skills

- Explain how to handle research equipment
- Explain how to conduct research techniques
- Show how to conduct standard techniques using research equipment
- Show how to do advanced research techniques

Project = guiding the development and progress of a research project

- Provide a research idea
- Give advice on a research project
- Evaluate a project's progress

Advising = providing guidance on academic and career topics

- Give advice on academic decisions
- Advise you on careers
- Help you set career goals
- Give you feedback on your professional progress

Norms = showcasing professionalism and scientific norms used in the field

- Explain field-specific norms for presenting research
- Show how to be professional
- Demonstrate good workplace behavior

Professional Socialization = facilitating professional socialization in the field

- Suggest social events for meeting other chemists
- Introduce you to other people in chemistry
- Help you build positive social relationships with other group members

Emotion = providing emotional support and a sense of belonging

- Show sympathy
- Show kindness
- Be positive
- Make you feel like you belong

Life = supporting life goals outside of research and the professional world

- Discuss life events outside of research
- Discuss long-term life goals (excluding career or professional goals)
- Encourage a healthy work-life balance
- Suggest fun social activities outside of the research group

Q4.3 Click the arrow button to go to the next page after you have looked over the category definitions and example actions.

----- page break -----

Q4.5 For the following questions, answer based on your opinions about your recent experiences (i.e., this past month or two) in chemistry research only.

For example, do not...

- guess what other people might say (We only want to hear about your opinion)
- guess what you might think in the future (We only want to hear about your recent experiences)
- reflect on what you used to think a year ago (We only want to hear about your recent experiences)
- reflect on something happening in another aspect of your life, like classes (We only want to hear about chemistry research)

End of Block: Categories

Start of Block: Overall Ratings

Q5.1 Rate the amount of each type of support you currently receive **overall** related to chemistry research (from all possible sources: \${q://QID13/ChoiceTextEntryValue}, \${q://QID17/ChoiceTextEntryValue}, family, etc.). The category definitions are provided again below. Don't overthink the question; just answer with your first, gut reaction.

Note: People can support you positively (i.e., the support is good or helpful) or negatively (i.e., the "support" is bad or damaging). For example, someone could be hurting you emotionally about your research or sabotaging your work; these would be classified as negative (-1 to -5).

	-5 = a lot of negative "support"	-4	-3	-2	-1	0 = no support at all	+1	+2	+3	+4	+5 = a lot of positive support
Conceptual	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
Technical	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
Project	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
Advising	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐

Norms	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
Professional Socialization	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
Emotion	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
Life	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐

Q5.2 Conceptual = improving conceptual knowledge and conceptual skills
Technical = improving technical knowledge and technical skills
Project = guiding the development and progress of a research project
Advising = providing guidance on academic and career topics
Norms = showcasing professionalism and scientific norms used in the field
Professional Socialization = facilitating professional socialization in the field
Emotion = providing emotional support and a sense of belonging
Life = supporting life goals outside of research and the professional world

Display This Question:

If Q5.1 [0 = no support at all] (Count) >= 1
 Or Q5.1 [+1] (Count) >= 1
 Or Q5.1 [+2] (Count) >= 1
 Or Q5.1 [+3] (Count) >= 1
 Or Q5.1 [+4] (Count) >= 1
 Or Q5.1 [+5 = a lot of positive support] (Count) >= 1

Q5.3 You indicated you are receiving some positive or no support in certain areas. Rate the degree of change you would like to see in each.

For example, if you are receiving positive “Conceptual” support but want more, you would choose between +1 and +5. Conversely, if you are receiving more positive “Conceptual” support than you want (for example, perhaps someone is overwhelming you or you want to test yourself), you would choose between -1 and -5.

Display This Choice:

If Q5.1 = Conceptual [0 = no support at all]
 Or Q5.1 = Conceptual [+1]
 Or Q5.1 = Conceptual [+2]
 Or Q5.1 = Conceptual [+3]
 Or Q5.1 = Conceptual [+4]
 Or Q5.1 = Conceptual [+5 = a lot of positive support]

Display This Choice:

If Q5.1 = Technical [0 = no support at all]
 Or Q5.1 = Technical [+1]
 Or Q5.1 = Technical [+2]
 Or Q5.1 = Technical [+3]
 Or Q5.1 = Technical [+4]
 Or Q5.1 = Technical [+5 = a lot of positive support]

Display This Choice:

If Q5.1 = Project [0 = no support at all]
 Or Q5.1 = Project [+1]
 Or Q5.1 = Project [+2]
 Or Q5.1 = Project [+3]
 Or Q5.1 = Project [+4]
 Or Q5.1 = Project [+5 = a lot of positive support]

Display This Choice:

If Q5.1 = Advising [0 = no support at all]
 Or Q5.1 = Advising [+1]
 Or Q5.1 = Advising [+2]
 Or Q5.1 = Advising [+3]
 Or Q5.1 = Advising [+4]
 Or Q5.1 = Advising [+5 = a lot of positive support]

Display This Choice:

If Q5.1 = Norms [0 = no support at all]
 Or Q5.1 = Norms [+1]
 Or Q5.1 = Norms [+2]
 Or Q5.1 = Norms [+3]
 Or Q5.1 = Norms [+4]
 Or Q5.1 = Norms [+5 = a lot of positive support]

Display This Choice:

If Q5.1 = Professional Socialization [0 = no support at all]
 Or Q5.1 = Professional Socialization [+1]
 Or Q5.1 = Professional Socialization [+2]
 Or Q5.1 = Professional Socialization [+3]
 Or Q5.1 = Professional Socialization [+4]
 Or Q5.1 = Professional Socialization [+5 = a lot of positive support]

Display This Choice:

If Q5.1 = Emotion [0 = no support at all]
 Or Q5.1 = Emotion [+1]
 Or Q5.1 = Emotion [+2]
 Or Q5.1 = Emotion [+3]
 Or Q5.1 = Emotion [+4]
 Or Q5.1 = Emotion [+5 = a lot of positive support]

Display This Choice:

If Q5.1 = Life [0 = no support at all]
 Or Q5.1 = Life [+1]
 Or Q5.1 = Life [+2]
 Or Q5.1 = Life [+3]
 Or Q5.1 = Life [+4]
 Or Q5.1 = Life [+5 = a lot of positive support]

	-5 = a lot less	-4	-3	-2	-1	0 = no change	+1	+2	+3	+4	+5 = a lot more
L Conceptual	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
L Technical	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
L Project	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
L Advising	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐

L Norms	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
L Professional Socialization	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
L Emotion	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
L Life	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐

Display This Question:

If Q5.1 [-5 = a lot of negative "support"] (Count) >= 1

Or Q5.1 [-4] (Count) >= 1

Or Q5.1 [-3] (Count) >= 1

Or Q5.1 [-2] (Count) >= 1

Or Q5.1 [-1] (Count) >= 1

Q5.4 You indicated you are receiving some negative "support" in certain areas. Rate the degree of change you would like to see in each.

For example, if you are receiving negative "Conceptual" support and want the negativity to decrease or want someone to leave you alone, you would choose between -1 and -5. Conversely, if you see the adversity as a good test that you want to try overcoming, you would choose between +1 and +5.

Display This Choice:

If Q5.1 = Conceptual [-5 = a lot of negative "support"]

Or Q5.1 = Conceptual [-4]

Or Q5.1 = Conceptual [-3]

Or Q5.1 = Conceptual [-2]

Or Q5.1 = Conceptual [-1]

Display This Choice:

If Q5.1 = Technical [-5 = a lot of negative "support"]

Or Q5.1 = Technical [-4]

Or Q5.1 = Technical [-3]

Or Q5.1 = Technical [-2]

Or Q5.1 = Technical [-1]

Display This Choice:

If Q5.1 = Project [-5 = a lot of negative "support"]

Or Q5.1 = Project [-4]

Or Q5.1 = Project [-3]

Or Q5.1 = Project [-2]

Or Q5.1 = Project [-1]

Display This Choice:

If Q5.1 = Advising [-5 = a lot of negative "support"]

Or Q5.1 = Advising [-4]

Or Q5.1 = Advising [-3]

Or Q5.1 = Advising [-2]

Or Q5.1 = Advising [-1]

Display This Choice:

If Q5.1 = Norms [-5 = a lot of negative "support"]

Or Q5.1 = Norms [-4]

Or Q5.1 = Norms [-3]

Or Q5.1 = Norms [-2]

Or Q5.1 = Norms [-1]

Display This Choice:

If Q5.1 = Professional Socialization [-5 = a lot of negative "support"]

Or Q5.1 = Professional Socialization [-4]

Or Q5.1 = Professional Socialization [-3]

Or Q5.1 = Professional Socialization [-2]

Or Q5.1 = Professional Socialization [-1]

Display This Choice:

If Q5.1 = Emotion [-5 = a lot of negative "support"]

Or Q5.1 = Emotion [-4]

Or Q5.1 = Emotion [-3]

Or Q5.1 = Emotion [-2]

Or Q5.1 = Emotion [-1]

Display This Choice:

If Q5.1 = Life [-5 = a lot of negative "support"]

Or Q5.1 = Life [-4]

Or Q5.1 = Life [-3]

Or Q5.1 = Life [-2]

Or Q5.1 = Life [-1]

	-5 = a lot less	-4	-3	-2	-1	0 = no change	+1	+2	+3	+4	+5 = a lot more
L Conceptual	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
L Technical	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
L Project	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
L Advising	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
L Norms	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
L Professional Socialization	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
L Emotion	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
L Life	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐

End of Block: Overall Ratings

Start of Block: PI Ratings

Q6.1 Rate the amount of each type of support you currently receive specifically from \$(q://QID13/ChoiceTextEntryValue) related to chemistry research.

	-5 = a lot of negative “support”	-4	-3	-2	-1	0 = no support at all	+1	+2	+3	+4	+5 = a lot of positive support
Conceptual	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
Technical	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
Project	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
Advising	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
Norms	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
Professional Socialization	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
Emotion	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
Life	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐

Q6.2 Conceptual = improving conceptual knowledge and conceptual skills
Technical = improving technical knowledge and technical skills
Project = guiding the development and progress of a research project
Advising = providing guidance on academic and career topics
Norms = showcasing professionalism and scientific norms used in the field
Professional Socialization = facilitating professional socialization in the field
Emotion = providing emotional support and a sense of belonging
Life = supporting life goals outside of research and the professional world

Display This Question:

If Q6.1 [0 = no support at all] (Count) >= 1
 Or Q6.1 [+1] (Count) >= 1
 Or Q6.1 [+2] (Count) >= 1
 Or Q6.1 [+3] (Count) >= 1
 Or Q6.1 [+4] (Count) >= 1
 Or Q6.1 [+5 = a lot of positive support] (Count) >= 1

Q6.3 You indicated you are receiving some positive or no support in certain areas from \${q://QID13/ChoiceTextEntryValue}. Rate the degree of change you would like to see in each.

For example, if you are receiving positive “Conceptual” support but want more, you would choose between +1 and +5. Conversely, if you are receiving more positive “Conceptual” support than you want (for example, perhaps someone is overwhelming you or you want to test yourself), you would choose between -1 and -5.

Display This Choice:

If Q6.1 = Conceptual [0 = no support at all]
Or Q6.1 = Conceptual [+1]
Or Q6.1 = Conceptual [+2]
Or Q6.1 = Conceptual [+3]
Or Q6.1 = Conceptual [+4]
Or Q6.1 = Conceptual [+5 = a lot of positive support]

Display This Choice:

If Q6.1 = Technical [0 = no support at all]
Or Q6.1 = Technical [+1]
Or Q6.1 = Technical [+2]
Or Q6.1 = Technical [+3]
Or Q6.1 = Technical [+4]
Or Q6.1 = Technical [+5 = a lot of positive support]

Display This Choice:

If Q6.1 = Project [0 = no support at all]
Or Q6.1 = Project [+1]
Or Q6.1 = Project [+2]
Or Q6.1 = Project [+3]
Or Q6.1 = Project [+4]
Or Q6.1 = Project [+5 = a lot of positive support]

Display This Choice:

If Q6.1 = Advising [0 = no support at all]
Or Q6.1 = Advising [+1]
Or Q6.1 = Advising [+2]
Or Q6.1 = Advising [+3]
Or Q6.1 = Advising [+4]
Or Q6.1 = Advising [+5 = a lot of positive support]

Display This Choice:

If Q6.1 = Norms [0 = no support at all]
Or Q6.1 = Norms [+1]
Or Q6.1 = Norms [+2]
Or Q6.1 = Norms [+3]
Or Q6.1 = Norms [+4]
Or Q6.1 = Norms [+5 = a lot of positive support]

Display This Choice:

If Q6.1 = Professional Socialization [0 = no support at all]
Or Q6.1 = Professional Socialization [+1]
Or Q6.1 = Professional Socialization [+2]
Or Q6.1 = Professional Socialization [+3]
Or Q6.1 = Professional Socialization [+4]
Or Q6.1 = Professional Socialization [+5 = a lot of positive support]

Display This Choice:

If Q6.1 = Emotion [0 = no support at all]
Or Q6.1 = Emotion [+1]
Or Q6.1 = Emotion [+2]
Or Q6.1 = Emotion [+3]
Or Q6.1 = Emotion [+4]
Or Q6.1 = Emotion [+5 = a lot of positive support]

Display This Choice:

If Q6.1 = Life [0 = no support at all]
Or Q6.1 = Life [+1]
Or Q6.1 = Life [+2]
Or Q6.1 = Life [+3]
Or Q6.1 = Life [+4]
Or Q6.1 = Life [+5 = a lot of positive support]

	-5 = a lot less	-4	-3	-2	-1	0 = no change	+1	+2	+3	+4	+5 = a lot more
L Conceptual	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
L Technical	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
L Project	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
L Advising	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
L Norms	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
L Professional Socialization	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
L Emotion	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
L Life	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐

Display This Question:

If Q6.1 [-5 = a lot of negative "support"] (Count) >= 1
 Or Q6.1 [-4] (Count) >= 1
 Or Q6.1 [-3] (Count) >= 1
 Or Q6.1 [-2] (Count) >= 1
 Or Q6.1 [-1] (Count) >= 1

Q6.4 You indicated you are receiving some negative "support" in certain areas from \${q://QID13/ChoiceTextEntryValue}. Rate the degree of change you would like to see in each.

For example, if you are receiving negative "Conceptual" support and want the negativity to decrease or want someone to leave you alone, you would choose between -1 and -5. Conversely, if you see the adversity as a good test that you want to try overcoming, you would choose between +1 and +5.

Display This Choice:

If Q6.1 = Conceptual [-5 = a lot of negative "support"]
 Or Q6.1 = Conceptual [-4]
 Or Q6.1 = Conceptual [-3]
 Or Q6.1 = Conceptual [-2]
 Or Q6.1 = Conceptual [-1]

Display This Choice:

If Q6.1 = Technical [-5 = a lot of negative "support"]
 Or Q6.1 = Technical [-4]
 Or Q6.1 = Technical [-3]
 Or Q6.1 = Technical [-2]
 Or Q6.1 = Technical [-1]

Display This Choice:

If Q6.1 = Project [-5 = a lot of negative "support"]
 Or Q6.1 = Project [-4]
 Or Q6.1 = Project [-3]

Or Q6.1 = Project [-2]

Or Q6.1 = Project [-1]

Display This Choice:

If Q6.1 = Advising [-5 = a lot of negative "support"]

Or Q6.1 = Advising [-4]

Or Q6.1 = Advising [-3]

Or Q6.1 = Advising [-2]

Or Q6.1 = Advising [-1]

Display This Choice:

If Q6.1 = Norms [-5 = a lot of negative "support"]

Or Q6.1 = Norms [-4]

Or Q6.1 = Norms [-3]

Or Q6.1 = Norms [-2]

Or Q6.1 = Norms [-1]

Display This Choice:

If Q6.1 = Professional Socialization [-5 = a lot of negative "support"]

Or Q6.1 = Professional Socialization [-4]

Or Q6.1 = Professional Socialization [-3]

Or Q6.1 = Professional Socialization [-2]

Or Q6.1 = Professional Socialization [-1]

Display This Choice:

If Q6.1 = Emotion [-5 = a lot of negative "support"]

Or Q6.1 = Emotion [-4]

Or Q6.1 = Emotion [-3]

Or Q6.1 = Emotion [-2]

Or Q6.1 = Emotion [-1]

Display This Choice:

If Q6.1 = Life [-5 = a lot of negative "support"]

Or Q6.1 = Life [-4]

Or Q6.1 = Life [-3]

Or Q6.1 = Life [-2]

Or Q6.1 = Life [-1]

	-5 = a lot less	-4	-3	-2	-1	0 = no change	+1	+2	+3	+4	+5 = a lot more
L Conceptual	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
L Technical	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
L Project	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
L Advising	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
L Norms	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
L Professional Socialization	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
L Emotion	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
L Life	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐

End of Block: PI Ratings

Start of Block: Mentor Ratings

Q7.1 Rate the amount of each type of support you currently receive specifically from related to chemistry research.

	-5 = a lot of negative "support"	-4	-3	-2	-1	0 = no support at all	+1	+2	+3	+4	+5 = a lot of positive support
Conceptual	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
Technical	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
Project	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
Advising	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
Norms	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
Professional Socialization	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
Emotion	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
Life	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐

Q7.2 **Conceptual** = improving conceptual knowledge and conceptual skills
Technical = improving technical knowledge and technical skills
Project = guiding the development and progress of a research project
Advising = providing guidance on academic and career topics
Norms = showcasing professionalism and scientific norms used in the field
Professional Socialization = facilitating professional socialization in the field
Emotion = providing emotional support and a sense of belonging
Life = supporting life goals outside of research and the professional world

Display This Question:

If Q7.1 [0 = no support at all] (Count) >= 1
 Or Q7.1 [+1] (Count) >= 1
 Or Q7.1 [+2] (Count) >= 1
 Or Q7.1 [+3] (Count) >= 1
 Or Q7.1 [+4] (Count) >= 1
 Or Q7.1 [+5 = a lot of positive support] (Count) >= 1

Q7.3 You indicated you are receiving some positive or no support in certain areas from

#{q://QID17/ChoiceTextEntryValue}. Rate the degree of change you would like to see in each.

For example, if you are receiving positive “Conceptual” support but want more, you would choose between +1 and +5. Conversely, if you are receiving more positive “Conceptual” support than you want (for example, perhaps someone is overwhelming you or you want to test yourself), you would choose between -1 and -5.

Display This Choice:

*If Q7.1 = Conceptual [0 = no support at all]
Or Q7.1 = Conceptual [+1]
Or Q7.1 = Conceptual [+2]
Or Q7.1 = Conceptual [+3]
Or Q7.1 = Conceptual [+4]
Or Q7.1 = Conceptual [+5 = a lot of positive support]*

Display This Choice:

*If Q7.1 = Technical [0 = no support at all]
Or Q7.1 = Technical [+1]
Or Q7.1 = Technical [+2]
Or Q7.1 = Technical [+3]
Or Q7.1 = Technical [+4]
Or Q7.1 = Technical [+5 = a lot of positive support]*

Display This Choice:

*If Q7.1 = Project [0 = no support at all]
Or Q7.1 = Project [+1]
Or Q7.1 = Project [+2]
Or Q7.1 = Project [+3]
Or Q7.1 = Project [+4]
Or Q7.1 = Project [+5 = a lot of positive support]*

Display This Choice:

*If Q7.1 = Advising [0 = no support at all]
Or Q7.1 = Advising [+1]
Or Q7.1 = Advising [+2]
Or Q7.1 = Advising [+3]
Or Q7.1 = Advising [+4]
Or Q7.1 = Advising [+5 = a lot of positive support]*

Display This Choice:

*If Q7.1 = Norms [0 = no support at all]
Or Q7.1 = Norms [+1]
Or Q7.1 = Norms [+2]
Or Q7.1 = Norms [+3]
Or Q7.1 = Norms [+4]
Or Q7.1 = Norms [+5 = a lot of positive support]*

Display This Choice:

*If Q7.1 = Professional Socialization [0 = no support at all]
Or Q7.1 = Professional Socialization [+1]
Or Q7.1 = Professional Socialization [+2]
Or Q7.1 = Professional Socialization [+3]
Or Q7.1 = Professional Socialization [+4]
Or Q7.1 = Professional Socialization [+5 = a lot of positive support]*

Display This Choice:

*If Q7.1 = Emotion [0 = no support at all]
Or Q7.1 = Emotion [+1]
Or Q7.1 = Emotion [+2]
Or Q7.1 = Emotion [+3]
Or Q7.1 = Emotion [+4]*

Or Q7.1 = Emotion [+5 = a lot of positive support]

Display This Choice:

If Q7.1 = Life [0 = no support at all]

Or Q7.1 = Life [+1]

Or Q7.1 = Life [+2]

Or Q7.1 = Life [+3]

Or Q7.1 = Life [+4]

Or Q7.1 = Life [+5 = a lot of positive support]

	-5 = a lot less	-4	-3	-2	-1	0 = no change	+1	+2	+3	+4	+5 = a lot more
L Conceptual	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
L Technical	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
L Project	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
L Advising	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
L Norms	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
L Professional Socialization	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
L Emotion	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
L Life	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐

Display This Question:

If Q7.1 [-5 = a lot of negative "support"] (Count) >= 1

Or Q7.1 [-4] (Count) >= 1

Or Q7.1 [-3] (Count) >= 1

Or Q7.1 [-2] (Count) >= 1

Or Q7.1 [-1] (Count) >= 1

Q7.4 You indicated you are receiving some negative "support" in certain areas from \${q:/QID17/ChoiceTextEntryValue}. Rate the degree of change you would like to see in each.

For example, if you are receiving negative "Conceptual" support and want the negativity to decrease or want someone to leave you alone, you would choose between -1 and -5. Conversely, if you see the adversity as a good test that you want to try overcoming, you would choose between +1 and +5.

Display This Choice:

If Q7.1 = Conceptual [-5 = a lot of negative "support"]

Or Q7.1 = Conceptual [-4]

Or Q7.1 = Conceptual [-3]

Or Q7.1 = Conceptual [-2]

Or Q7.1 = Conceptual [-1]

Display This Choice:

If Q7.1 = Technical [-5 = a lot of negative “support”]
 Or Q7.1 = Technical [-4]
 Or Q7.1 = Technical [-3]
 Or Q7.1 = Technical [-2]
 Or Q7.1 = Technical [-1]

Display This Choice:

If Q7.1 = Project [-5 = a lot of negative “support”]
 Or Q7.1 = Project [-4]
 Or Q7.1 = Project [-3]
 Or Q7.1 = Project [-2]
 Or Q7.1 = Project [-1]

Display This Choice:

If Q7.1 = Advising [-5 = a lot of negative “support”]
 Or Q7.1 = Advising [-4]
 Or Q7.1 = Advising [-3]
 Or Q7.1 = Advising [-2]
 Or Q7.1 = Advising [-1]

Display This Choice:

If Q7.1 = Norms [-5 = a lot of negative “support”]
 Or Q7.1 = Norms [-4]
 Or Q7.1 = Norms [-3]
 Or Q7.1 = Norms [-2]
 Or Q7.1 = Norms [-1]

Display This Choice:

If Q7.1 = Professional Socialization [-5 = a lot of negative “support”]
 Or Q7.1 = Professional Socialization [-4]
 Or Q7.1 = Professional Socialization [-3]
 Or Q7.1 = Professional Socialization [-2]
 Or Q7.1 = Professional Socialization [-1]

Display This Choice:

If Q7.1 = Emotion [-5 = a lot of negative “support”]
 Or Q7.1 = Emotion [-4]
 Or Q7.1 = Emotion [-3]
 Or Q7.1 = Emotion [-2]
 Or Q7.1 = Emotion [-1]

Display This Choice:

If Q7.1 = Life [-5 = a lot of negative “support”]
 Or Q7.1 = Life [-4]
 Or Q7.1 = Life [-3]
 Or Q7.1 = Life [-2]
 Or Q7.1 = Life [-1]

	-5 = a lot less	-4	-3	-2	-1	0 = no change	+1	+2	+3	+4	+5 = a lot more
L Conceptual	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
L Technical	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
L Project	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
L Advising	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐

L Norms	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
L Professional Socialization	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
L Emotion	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
L Life	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐

End of Block: Mentor Ratings

Start of Block: Ranking

Q8.1 Pretend you are in a world where you could get exactly the type and amount of positive support you want. Rank the categories in order of amount for positive support you think you would want to receive **overall** _____ for _____ chemistry _____ research.

It is ok if this reflects what you are indeed receiving! For example, if you are receiving positive "Conceptual" support more than any other category but you also think that "Conceptual" support is what you need the most _____ of, _____ then _____ place "Conceptual" _____ at _____ the _____ top.

Click _____ and _____ drag _____ to _____ move _____ the _____ categories _____ around.
1 (top) = the largest amount of support you would want, 8 (bottom) = the smallest amount

- _____ Conceptual
- _____ Technical
- _____ Project
- _____ Advising
- _____ Norms
- _____ Professional Socialization
- _____ Emotion
- _____ Life

Q8.2 **Conceptual** = improving conceptual knowledge and conceptual skills
Technical = improving technical knowledge and technical skills
Project = guiding the development and progress of a research project
Advising = providing guidance on academic and career topics
Norms = showcasing professionalism and scientific norms used in the field
Professional Socialization = facilitating professional socialization in the field
Emotion = providing emotional support and a sense of belonging
Life = supporting life goals outside of research and the professional world

Q8.3 Rank the categories in order of amount for positive support you think you would want to receive from **specifically**.
QID13/ChoiceTextEntryValue}

1 (top) = largest amount, 8 (bottom) = smallest amount

- _____ Conceptual
- _____ Technical

- _____ Project
- _____ Advising
- _____ Norms
- _____ Professional Socialization
- _____ Emotion
- _____ Life

Display This Question:

If Q3.6 = Yes, I have a mentor in the group.

Q8.4 **Conceptual** = improving conceptual knowledge and conceptual skills
Technical = improving technical knowledge and technical skills
Project = guiding the development and progress of a research project
Advising = providing guidance on academic and career topics
Norms = showcasing professionalism and scientific norms used in the field
Professional Socialization = facilitating professional socialization in the field
Emotion = providing emotional support and a sense of belonging
Life = supporting life goals outside of research and the professional world

Display This Question:

If Q3.6 = Yes, I have a mentor in the group.

Q8.5 Rank the categories in order of amount for positive support you think you would want to receive from **\$(q://QID17/ChoiceTextEntryValue)** **specifically.**

1 (top) = largest amount, 8 (bottom) = smallest amount

- _____ Conceptual
- _____ Technical
- _____ Project
- _____ Advising
- _____ Norms
- _____ Professional Socialization
- _____ Emotion
- _____ Life

End of Block: Ranking

Start of Block: Mentoring Structure

Q9.1 You are doing great! You are over halfway through the survey.

Display This Question:

If Q3.6 = Yes, I have a mentor in the group.

Q9.2 Select the **position \$(q://QID17/ChoiceTextEntryValue)** currently holds. Make your best guess. Do not include any skipped years, high school college credits, leaves of absence, or gap years.

- ☐ 1st-year undergraduate ("freshman")
- ☐ 2nd-year undergraduate ("sophomore")
- ☐ 3rd-year undergraduate ("junior")
- ☐ 4th-year undergraduate ("senior")
- ☐ 5th-year or more undergraduate ("super senior")
- ☐ 1st-year Master's student
- ☐ 2nd-year Master's student
- ☐ 3rd-year or more Master's student
- ☐ 1st-year PhD student
- ☐ 2nd-year PhD student
- ☐ 3rd-year PhD student
- ☐ 4th-year PhD student
- ☐ 5th-year PhD student
- ☐ 6th-year PhD student
- ☐ 7th-year PhD student
- ☐ 8th-year or more PhD student
- ☐ 1st-year MD student
- ☐ 2nd-year MD student
- ☐ 3rd-year MD student
- ☐ 4th-year MD student
- ☐ 5th-year or more MD student
- ☐ Postdoc
- ☐ Staff scientist / research associate
- ☐ Medical resident / fellow / doctor
- ☐ Professor
- ☐ Something else not listed here

Display This Question:

If Q9.2 = 1st-year Master's student
Or Q9.2 = 2nd-year Master's student
Or Q9.2 = 3rd-year or more Master's student
Or Q9.2 = 1st-year PhD student
Or Q9.2 = 2nd-year PhD student
Or Q9.2 = 3rd-year PhD student
Or Q9.2 = 4th-year PhD student
Or Q9.2 = 5th-year PhD student
Or Q9.2 = 6th-year PhD student
Or Q9.2 = 7th-year PhD student
Or Q9.2 = 8th-year or more PhD student
Or Q9.2 = 1st-year MD student
Or Q9.2 = 2nd-year MD student
Or Q9.2 = 3rd-year MD student

Or Q9.2 = 4th-year MD student
 Or Q9.2 = 5th-year or more MD student

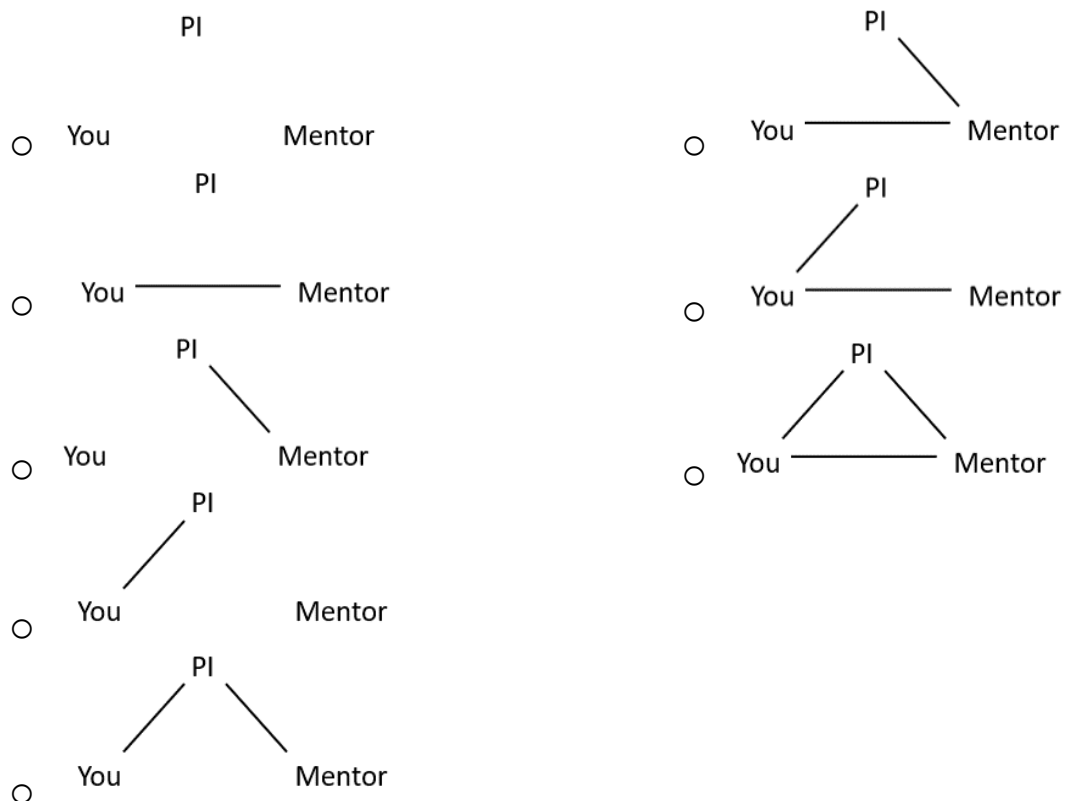
Q9.3 Select the highest degree (or international equivalent) \${q://QID17/ChoiceTextEntryValue} had **completed before** entering their current graduate program. Make your best guess.

- ☐ Bachelor's
- ☐ Master's
- ☐ PhD
- ☐ MD
- ☐ JD
- ☐ Something else not listed here

Display This Question:
 If Q3.6 = Yes, I have a mentor in the group.

Q9.4 The following images display ways in which you, \${q://QID17/ChoiceTextEntryValue}, and \${q://QID13/ChoiceTextEntryValue} might interact in order to support you and your research. The lines indicate that interactions occur between the people in order to support you and your work; no line means that interactions do not occur between the people (in terms of supporting you and your work). Interactions might be about the project or you (e.g., emotional support, project support, etc.).

Select the best image that currently illustrates your mentoring structure.



----- page break -----

Q9.5 Rate the degree to which you currently agree with the following statements on a **personal** level.

Display This Choice:

If Q3.6 = Yes, I have a mentor in the group.

Display This Choice:

If Q3.6 = Yes, I have a mentor in the group.

Display This Choice:

If Q3.6 = Yes, I have a mentor in the group.

	-5 = Strongly Disagree	-4	-3	-2	-1	0 = Neutral	+1	+2	+3	+4	+5 = Strongly Agree
\${q://QID13/ChoiceText EntryValue} and I are a good fit.	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
\${q://QID13/ChoiceText EntryValue} and I see things in the same way.	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
This question helps us ensure that a real person is taking our survey. Select "+2".	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
\${q://QID13/ChoiceText EntryValue} and I are similar in our outlook, perspective, and values.	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
└ \${q://QID17/ChoiceText EntryValue} and I are a good fit.	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
└ \${q://QID17/ChoiceText EntryValue} and I see things in the same way.	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
└ \${q://QID17/ChoiceText EntryValue} and I are similar in our outlook, perspective, and values.	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐

----- page break -----

Q9.6 Rate how you feel about the current quality of chemistry research mentorship overall that you feel you receive from...

Display This Choice:

If Q3.6 = Yes, I have a mentor in the group.

	-5 = Extremely negative / unfavorable	-4	-3	-2	-1	0 = Neutral	+1	+2	+3	+4	+5 = Extremely positive / favorable
{q://QID13/ChoiceTextEntryValue}.	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
⌞ {q://QID17/ChoiceTextEntryValue}.	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
This question helps us ensure that a real person is taking our survey. Select “-4”.	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
other support systems.	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐

End of Block: Mentoring Structure

Start of Block: Past Experiences

Q10.1 Excellent, you are over two-thirds done with this survey! Now, please answer questions about your personal experiences.

Q10.2 Select the option that **best** characterizes your **current** research.

- ☐ Analytical chemistry
- ☐ Biochemistry
- ☐ Chemical education
- ☐ Chemical engineering
- ☐ Computational chemistry
- ☐ Inorganic chemistry
- ☐ Organic chemistry
- ☐ Physical chemistry
- ☐ Nothing here comes close to what I do

Display This Question:

If Q10.2 = Nothing here comes close to what I do

Q10.3 What phrase do you think best describes the type of chemistry you are currently conducting research on?

Q10.4 Your answers to the following three questions must add up to 100 % combined. The website will stop you from going over 100 %.

Indicate the percentage of time you yourself spend doing _____ in your current research.

____[slider bar]____ "wet" work (e.g., manipulating chemicals, culturing cells, operating fume hoods)

____[slider bar]____ "dry" work (e.g., deriving complex computations, manipulating lasers)

____[slider bar]____ "auxiliary" work (e.g., literature searching, doing simple calculations, preparing presentations, planning a project, reporting results)

----- page break -----

Q10.5 Write a keyword(s) that describe the subfield of research you currently do. Use a ; symbol to separate sets of keywords.

For example: "natural product total synthesis; organic synthesis"
For example: "inorganic methodology; single atom deletion"

Please be specific. For example, "organic chemistry" is somewhat vague, but "natural product total synthesis; organic synthesis" is more specific.

Q10.6 Write a keyword(s) that describe the type of future job(s) you think you want. If you aren't sure yet, describe whatever you are currently most interested in. Use a ; symbol to separate sets of keywords.

For example: "mass spectrometry technician; pharmaceutical industry"
For example: "science journalist; media; communications"

Please be specific. For example, "academia" is somewhat vague, but "research professor; R1 university" is more specific.

End of Block: Past Experiences

Start of Block: Demographics

Display This Question:
If Q2.2 = Undergraduate student

Q11.1 Do you plan to major or minor in chemistry?

- ☐ Yes, major
- ☐ Yes, minor
- ☐ No

Display This Question:
If Q2.2 = Undergraduate student

Q11.2 Select your current year in college. Do not include any skipped years, high school college credits, leaves of absence, or gap years.

- ☐ 1st ("freshman")

- ☐ 2nd ("sophomore")
 - ☐ 3rd ("junior")
 - ☐ 4th ("senior")
 - ☐ 5th+ ("super senior")
-

Display This Question:
If Q2.2 = Graduate student

Q11.3 Select the highest degree (or international equivalent) you had **completed before** you entered your current graduate program.

- ☐ Bachelor's
 - ☐ Master's
 - ☐ PhD
 - ☐ MD
 - ☐ JD
 - ☐ Something else not listed here
-

Display This Question:
If Q2.2 = Graduate student

Q11.4 Select the type of graduate program you are **currently** in. If you are in a joint program, select the stage you are currently at.

- ☐ Master's
 - ☐ PhD
 - ☐ MD
 - ☐ JD
 - ☐ Something else not listed here
-

Display This Question:
If Q2.2 = Graduate student

Q11.5 Select your year in your **current** graduate program. Do not include any skipped years, leaves of absence, or gap years.

- ☐ 1st
- ☐ 2nd
- ☐ 3rd
- ☐ 4th
- ☐ 5th
- ☐ 6th
- ☐ 7th

☐ 8th+

Display This Question:
If Q2.2 != Postdoctoral researcher

Q11.6 Name the school you are currently enrolled at. This information is not used to identify you. We will enter the final list of school names into a website that will tell us general characteristics about the schools (such as whether the students are primarily undergraduates or primarily doctoral students).

Display This Question:
If Q2.2 = Graduate student

Q11.7 Name the school you earned your most recent degree from. This information is not used to identify you.

Display This Question:
If Q2.2 = Postdoctoral researcher

Q11.8 What is the total number of years you have been a postdoc (in any groups, combined)? Enter as a number. You can enter decimals (for example "0.5" for half a year).

Display This Question:
If Q2.2 = Postdoctoral researcher

Q11.9 Name the school you earned your most recent degree from.

This information is not used to identify you. We will enter the final list of school names into a website that will tell us general characteristics about the schools (such as whether the students are primarily undergraduates or primarily doctoral students).

Q11.10 What is the total number of years you have worked _____? Enter as a number. You can enter decimals (for example "0.5" for half a year).

Display This Choice:
If Q3.6 = Yes, I have a mentor in the group.

☐ in chemistry research (or closely related research).

☐ with \${q://QID13/ChoiceTextEntryValue}. _____

policies.

- ☐ Domestic
- ☐ International
- ☐ Prefer not to say

Display This Question:
If Q11.16 = International

Q11.17 Please name the country(ies) in which you were previously educated before your current program, including the USA if you were previously educated at an institution in the United States before your current program.

This information is not used to identify you, just to help us stay aware of the complexities of our respondents' backgrounds.

Q11.18 Select whether you are a native English speaker.

- ☐ Native English speaker
- ☐ Non-native English speaker
- ☐ Prefer not to say

Q11.19 Select whether you are a first-generation undergraduate / graduate student. Select all that apply.

“First-generation undergraduate” means that you do not have a parent who completed a four-year college degree. “First-generation graduate student” means that you do not have a parent who completed a graduate degree (e.g., Master’s, PhD, MD, JD).

- ☐ I am / was a first-generation undergraduate student.
- ☐ I am / was a first-generation graduate student.
- ☐ Neither, not first-generation
- ☐ Prefer not to say

Q11.20 Select the bracket that (in considering your childhood and teenage years) you most closely identify growing up in.

- ☐ Lowest-income class (sometimes called “poor” or “near-poor”)
- ☐ Lower-middle income class (“working class”)
- ☐ Middle income class
- ☐ Upper-middle income class (“upper class”)
- ☐ Highest-income class (“wealthy” or “rich”)
- ☐ Prefer not to say

End of Block: Demographics

Start of Block: Gift Card

Q12.1 Thank you for completing this survey! Your response has been recorded. We greatly appreciate your help. Would you like to enter the gift card drawing?

The form where you would enter your contact information does not connect your survey responses to your contact information. The confidentiality of your responses on this survey is therefore protected.

- ☐ Yes, enter me
- ☐ No, do not enter me

End of Block: Gift Card

Appendix F

Corresponding to **Chapter 6.** Comparative Analysis of a Department's Perceived Value of Seminar Talks

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F.I.1 Supplemental Statistical Data

Figure F.I.1. An overview of the survey components based on the respondent's role.

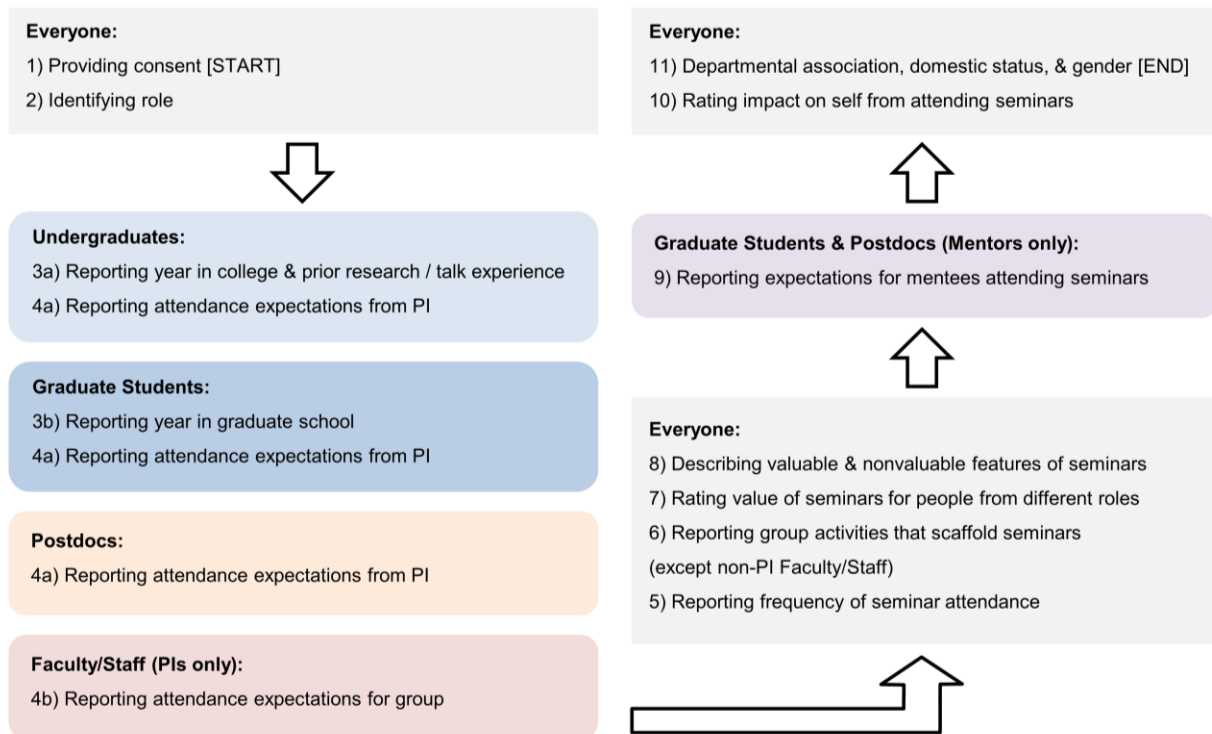


Table F.I.1. Breakdown of respondent Roles.^a

(a) Undergraduate Year (N = 22, 28 %)				(b) Graduate Student Year (N = 39, 50 %)				
1 st	2 nd	3 rd	4 th	1 st	2 nd	3 rd	4 th	5 th +
5	4	6	7	6	9	11	4	9
23 %	18 %	27 %	32 %	15 %	23 %	28 %	10 %	23 %
(c) Postdoctoral Researchers (N = 6, 8 %)								
(d) Mentor/PI Status				(e) Faculty/Staff Position ^b (N = 11, 14 %)				
Grad. Students & Postdocs		Faculty & Staff		Assistant Prof.	Full Prof.	Emeritus Prof.	Named Prof.	Lecturers & Staff
Mentor	Not a Mentor	PI	Not a PI					
19	26	8	3	3	4	1	2	3
42 %	58 %	73 %	27 %	27 %	36 %	9 %	18 %	27 %

^acomplete Role data for 78 of 78 cases

^bThe 11 Faculty/Staff could select or write-in multiple options to indicate their Role since overlap could exist. Therefore, some people indicated more than 1 position. No one selected "Associate Professor".

Table F.I.2. Post hoc Dunn-Bonferroni pairwise comparisons of community's Perceived Value for different Roles.

Perceived Value for [Role] ^a	adj. p^b				
	Undergraduates	Graduate Students (year 1)	Graduate Students (years 2+)	Postdocs	Faculty
Undergraduates	---				
Graduate Students (year 1)	< .0005	---			
Graduate Students (years 2+)	< .0005	1.000	---		
Postdocs	< .0005	.726	1.000	---	
Faculty	< .0005	1.000	1.000	1.000	---

^a76 of 78 cases

^basymptotic, two-tailed p after Dunn-Bonferroni correction following Friedman test with $p < .001$

Table F.I.3. Kruskal-Wallis tests of how different groups rate Perceived Value.

Perceived Value for [Role] ^a	$\chi^2(4)$	p^b
Undergraduates	8.736	.068
Graduate Students (year 1)	8.200	.085
Graduate Students (years 2+)	9.610	.048
Postdocs	3.269	.514
Faculty	1.840	.765

^a76 of 78 cases

^basymptotic, two-tailed

Table F.I.4. Post hoc Dunn-Bonferroni pairwise comparisons of impact items.

Item ^a	adj. <i>p</i> ^b										
	Knowledge	Awareness	Communicating	Evaluating	Ideating	Networking	Confidence	Identity	Enthusiasm	Research	Career
Knowledge	---										
Awareness	< .0005	---									
Communicating	1.000	< .0005	---								
Evaluating	1.000	< .0005	1.000	---							
Ideating	.245	.002	1.000	1.000	---						
Networking	1.000	< .0005	1.000	1.000	1.000	---					
Confidence	.016	< .0005	< .0005	< .0005	< .0005	< .0005	---				
Identity	.039	< .0005	< .0005	< .0005	< .0005	.001	1.000	---			
Enthusiasm	1.000	< .0005	1.000	1.000	1.000	1.000	< .0005	< .0005	---		
Research	.245	.002	1.000	1.000	1.000	1.000	< .0005	< .0005	1.000	---	
Career	1.000	< .0005	1.000	1.000	1.000	1.000	< .0005	< .0005	1.000	1.000	---

^a75 of 78 cases; listed by order presented to respondents^basymptotic, two-tailed *p* after Dunn-Bonferroni correction following Friedman test with *p* < .0005**Table F.I.5.** Kruskal-Wallis tests of how different groups rated the impact items.

Groups Rating Improvement of Own [Item] ^a	$\chi^2(4)$	<i>p</i> ^b
Knowledge	6.697	.153
Awareness	6.314	.177
Communicating	5.520	.238
Evaluating	8.018	.091
Ideating	7.861	.097
Networking	4.057	.398
Confidence	15.295	.004
Identity	18.209	.001
Enthusiasm	6.447	.168
Research	3.222	.521
Career	8.209	.084

^a75 of 78 cases; listed by order presented to respondents^basymptotic, two-tailed

Table F.I.6. Post hoc Dunn-Bonferroni pairwise comparisons of how different groups rated the impact items.

[Role Group] Rating Improvement of Own [Item]		adj. <i>p</i> ^b				
	N ^a	Undergraduates	Graduate Students (year 1)	Graduate Students (years 2+)	Postdocs	Faculty/Staff
<i>Confidence (p = .004)</i>						
Undergraduates	21	---				
Graduate Students (year 1)	6	1.000	---			
Graduate Students (years 2+)	33	.014	.435	---		
Postdocs	5	1.000	1.000	.085	---	
Faculty	10	1.000	1.000	1.000	1.000	---
<i>Identity (p = .001)</i>						
Undergraduates	21	---				
Graduate Students (year 1)	6	1.000	---			
Graduate Students (years 2+)	33	.008	.143	---		
Postdocs	5	1.000	1.000	.042	---	
Faculty/Staff	10	1.000	1.000	1.000	1.000	---

^a75 of 78 cases

^basymptotic, two-tailed p after Dunn-Bonferroni correction following Kruskal-Wallis test $p = .005$ and $.001$

F.II.1 Survey

After seminars, this survey was administered via Qualtrics and preceded by an online consent form.

Instructions: Answer the following questions about the presentation honestly with your gut reaction. **It is ok to give a negative or neutral response.**

1. Please select the option that *best* describes your role.

- ☐ Undergraduate student
- ☐ Graduate student
- ☐ Postdoc
- ☐ Faculty
- ☐ Staff
- ☐ Other _____

2. What was the presenter's name and/or presentation title?

It's ok if you don't remember the exact wording or spelling. This just helps to keep track of responses properly.

3. Were you required or encouraged by someone to attend this presentation?

- ☐ Yes, required
- ☐ Yes, encouraged
- ☐ No, neither required nor encouraged
- ☐ Not sure

4. Rate whether attending this presentation was a...

(a) positive or negative experience overall for *you*.

- ☐ 1 = Very negative
- ☐ 2
- ☐ 3
- ☐ 4 = Neutral
- ☐ 5
- ☐ 6
- ☐ 7 = Very positive

(b) valuable experience overall for *you*.

- 1 = Not at all valuable
- 2
- 3
- 4 = Moderately valuable
- 5
- 6
- 7 = Extremely valuable

(c) worthwhile experience overall for *you*.

- 1 = Not at all worthwhile
- 2
- 3
- 4 = Moderately worthwhile
- 5
- 6
- 7 = Extremely worthwhile

----- page break -----

5. Rate the following about the presentation and presenter.

	1 = Not at all	2	3	4 = Moderately	5	6	7 = Extremely
(a) how much the presentation related to your area(s) of research	☐	☐	☐	☐	☐	☐	☐
(b) how much you conceptually understood the presentation	☐	☐	☐	☐	☐	☐	☐
(c) how much you linguistically understood the presenter (for example, no language barriers)	☐	☐	☐	☐	☐	☐	☐

	1 = Poor	2	3	4 = Okay	5	6	7 = Excellent
(d) the "novelty" of the work	☐	☐	☐	☐	☐	☐	☐
(e) the "impactfulness" of the work	☐	☐	☐	☐	☐	☐	☐
(f) the presenter's communication skills	☐	☐	☐	☐	☐	☐	☐
(g) the professionalism and attractiveness of the slides	☐	☐	☐	☐	☐	☐	☐

[Optional] Explain further if you want.

----- page break -----

6. Rate how attending the presentation impacted you in the following areas.

	1 = Not at all improved	2	3	4 = Moderately improved	5	6	7 = Extremely improved
(a) Technical / content knowledge	☐	☐	☐	☐	☐	☐	☐
(b) Awareness of the broader scientific / research community	☐	☐	☐	☐	☐	☐	☐
(c) Communication / presentation skills	☐	☐	☐	☐	☐	☐	☐
(d) Ability to critically evaluate another's work	☐	☐	☐	☐	☐	☐	☐
(e) Ability to develop new project ideas	☐	☐	☐	☐	☐	☐	☐

[Optional] Explain further if you want.

	1 = Significantly worsened	2	3	4 = Not really affected	5	6	7 = Significantly improved
(f) Social connections / networking	☐	☐	☐	☐	☐	☐	☐
(g) Self-confidence as a scientist	☐	☐	☐	☐	☐	☐	☐
(h) Self-identity as a scientist	☐	☐	☐	☐	☐	☐	☐
(i) Enthusiasm about science	☐	☐	☐	☐	☐	☐	☐
(j) Interest in research	☐	☐	☐	☐	☐	☐	☐

[Optional] Explain further if you want.

	1 = Not at all impacted	2	3	4 = Moderately impacted	5	6	7 = Extremely impacted
(k) Career / education interests	☐	☐	☐	☐	☐	☐	☐

[Optional] Explain further if you want.

----- *page break* -----

7. [Optional] Briefly summarize the presentation in a sentence or two.

8. [Optional] Briefly describe what your main take-aways were in a sentence or two.

This could be about anything that the presentation/presenter caused you to think of.

9. [Optional] Briefly describe what you primarily gained from the presentation (Knowledge about a new reaction? Inspiration for a new project idea? Excitement? Constructive criticism? Ideas about making good slides? Etc.).

----- *page break* -----

10. Do you identify as...

(a) a person associated with the Chemistry Department (for example, a joint appointment professor or a chemistry major undergraduate)?

- ☐ Yes, associated with [*institution's name not provided here*] Chemistry Department
- ☐ Yes, associated with a different institution's chemistry department
- ☐ No, not associated with a chemistry department

(b) a domestic or international person at this school?

- ☐ Domestic
- ☐ International
- ☐ Prefer not to say

(c) female, male, or other?

- ☐ Female
- ☐ Male
- ☐ Other _____
- ☐ Prefer not to say

F.II.2 Supplemental Statistical Data

Table F.II.1. Reach of survey distribution after seminars.

Seminar ID	Attendees	Emailed (%) ^a
1	48	89.6
2	38	94.7
3	88	85.2
4	36	86.1
5	43	93.0
6	40	92.5
7	44	97.7
8	26	84.6
9	29	96.6

^aEmail addresses obtained from the Zoom spreadsheet of attendees or found via Internet searches of publicly available professional information based on attendee names displayed on Zoom seminar calls

Figure F.II.1. Percentage of audiences by Role in the education spectrum.

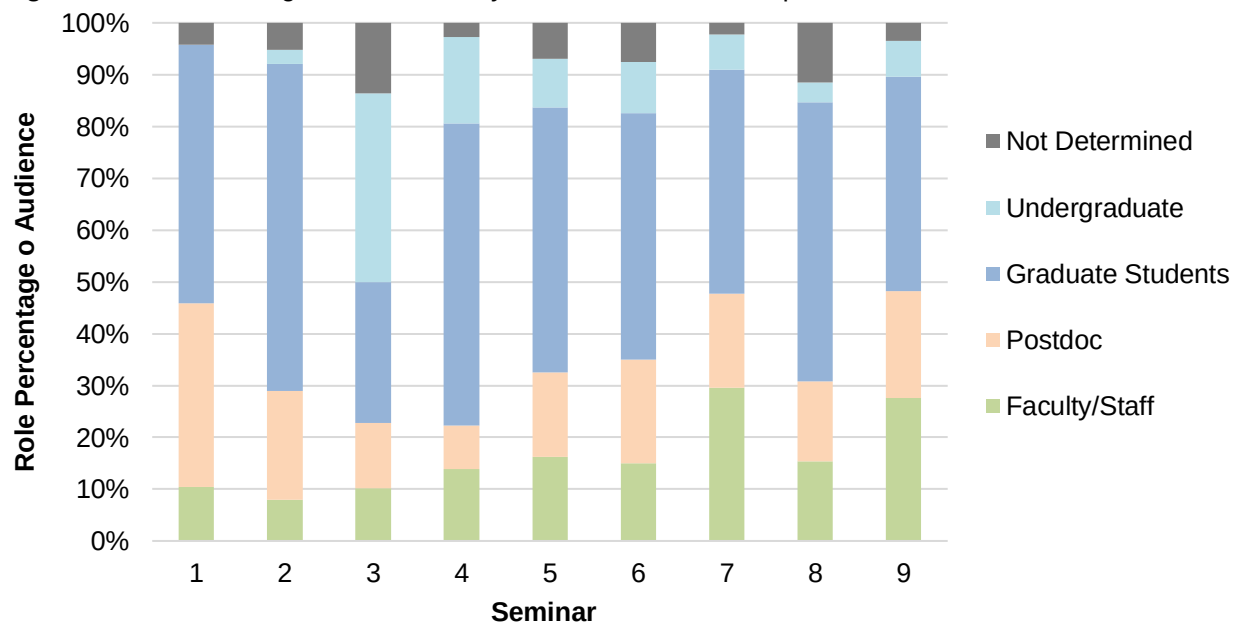


Figure F.II.2. Count of audiences by Role in the education spectrum

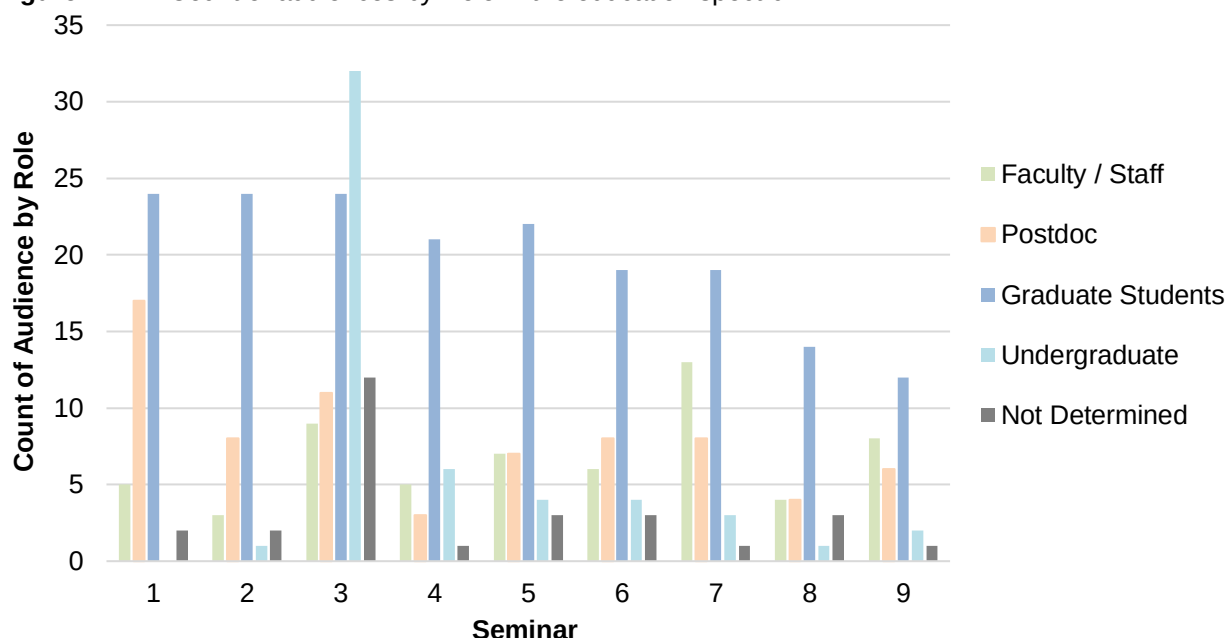


Table F.II.2. Perceived characteristics of seminars and perceived impacts of seminars on respondents with original response formats.

Item	Label	N ^a	Median	Mean ^b	Std. Dev.
Value of seminar: "Rate whether attending this presentation was a..."					
(1) <i>Very negative</i> -----					<i>Very positive (7)</i>
Positive or negative experience overall for you	Positive	92	6	5.77	1.039
(1) <i>Not at all valuable</i> -----					<i>Extremely valuable (7)</i>
Valuable experience overall for you	Valuable	92	5	5.27	1.276
(1) <i>Not at all worthwhile</i> -----					<i>Extremely worthwhile (7)</i>
Worthwhile experience overall for you	Worthwhile	92	6	5.59	1.259
Characteristics of seminar: "Rate the following about the presentation and presenter."					
(1) <i>Not at all</i> -----					<i>Extremely (7)</i>
How much the presentation related to your area(s) of research	Relevant	92	5	4.64	1.559
How much you conceptually understood the presentation	Understood	92	6	5.34	1.328
How much you linguistically understood the presenter (for example, no language barriers) ^e	Language	92	7	6.57 ^d	0.684

Table F.II.2. Perceived characteristics of seminars and perceived impacts of seminars on respondents with original response formats. **[continued]**

<i>(1) Poor</i> -----				<i>Excellent (7)</i>	
The “novelty” of the work	Novel	91	6	6.01	0.937
The “impactfulness” of the work	Impactful	91	6	5.80	1.077
The presenter’s communication skills	Presenter	92	6	6.07	1.127
The professionalism and attractiveness of the slides	Slides	90	6	6.03 ^e	1.086
Impact of seminar: “Rate how attending the presentation impacted you in the following areas.”					
<i>(1) Not at all improved</i> -----				<i>Extremely improved (7)</i>	
Technical / content knowledge	Knowledge	92	5	4.57	1.385
Awareness of the broader scientific / research community	Awareness	92	5	5.30	1.373
Communication / presentation skills	Communicating	92	4	4.18	1.735
Ability to critically evaluate another’s work	Evaluating	92	4	4.12	1.759
Ability to develop new project ideas	Ideating	92	5	4.39	1.785
<i>(1) Significantly worsened</i> -----				<i>Significantly improved (7)</i>	
Social connections / networking	Networking	91	4	4.31	0.997
Self-confidence as a scientist	Confidence	91	4	4.43	0.979
Self-identity as a scientist	Identity	91	4	4.62	1.041
Enthusiasm about science	Enthusiasm	91	5	5.19	1.182
Interest in research	Research	91	5	5.27	1.106
<i>(1) Not at all impacted</i> -----				<i>Extremely impacted (7)</i>	
Career / education interests	Career	91	4	3.40	2.027

^a92 cases from 9 observed seminars; missing data excluded pairwise; 89 cases contained complete data for all items

^bAll item responses on a 1 to 7 ordinal positive agreement response format; all skews within ± 1 and kurtosis ± 2 except where noted

^cIncluded to ensure that native language differences did not impair comprehension

^dSkew of -1.713 and kurtosis of 3.077

^eSkew of -1.213

Table F.II.3. Complete factor loadings^a for Exploratory Factor Analysis.

Item ^b	F1 Knowledge & Skills Impact	F2 Presentation Quality	F3 Socioemotional Impact	F4 Expertise Relevance	F5 Research Quality
Novel	-.067	-.016	.040	.098	-.920
Impactful	.016	.108	.021	.092	-.645
Relevant	.067	.002	-.025	.785	-.116
Understood	.186	.050	.036	.539	-.162
Confidence	.035	-.037	.885	-.022	.008
Identity	.178	-.052	.709	-.251	-.236
Networking	-.073	.243	.576	.268	.039
Slides	.001	.821	.059	.039	.017
Presenter	.064	.678	.026	.005	-.252
Evaluating	.894	-.139	.048	.202	.098
Ideating	.819	-.104	.009	.103	-.150
Communicating	.747	.202	.045	.002	.090
Knowledge	.570	.300	.077	.130	-.055
Career	.472	-.079	.273	-.141	-.162
Awareness	.459	.277	-.077	-.181	-.145
% of Variance ^c	38.5	9.0	7.8	6.0	4.6

^aPattern matrix from Principal Axis Factoring and Direct Oblimin rotation ($\delta = 0$) with Kaiser normalization converged in 9 iterations; missing data excluded pairwise

^bFor clarity, items organized by descending factor loading value; factor loading cut-off value of .45 for factor inclusion

^c66.0 % cumulative variance accounted for

Table F.II.4. Factor correlation matrix.

Factor	F1 Knowledge & Skills Impact	F2 Presentation Quality	F3 Socioemotional Impact	F4 Expertise Relevance	F5 Research Quality
F1 Knowledge & Skills Impact	---				
F2 Presentation Quality	.301	---			
F3 Socioemotional Impact	.383	.227	---		
F4 Expertise Relevance	.149	.191	.117	---	
F5 Research Quality	-.438	-.371	-.368	-.198	---

Table F.II.5. Levene's Test of Homogeneity of Variance.

Variable ^a	Levene Statistic ^b	df1	df2	<i>p</i>
Perceived Value	.947	15	64	.519
Knowledge & Skills Impact	.675	15	64	.799
Presentation Quality	1.018	15	64	.449
Socioemotional Impact	.586	15	64	.875
Expertise Relevance	1.081	15	64	.391
Research Quality	.794	15	64	.680

^aScaled weighted sum factor scores^bBased on median (Brown & Forsythe's modification)**Table F.II.6.** Multivariate tests.

Effect	Statistic	Value	<i>F</i>	Hypothesis df	Error df	<i>p</i>
Role	Pillai's Trace	.337	1.286	18.000	183.000	.201
	Wilks' Lambda	.692	1.292	18.000	167.362	.199
Seminar	Pillai's Trace	.881	1.377	48.000	384.000	.055
	Wilks' Lambda	.355	1.436	48.000	294.367	.039
Role * Seminar	Pillai's Trace	1.065	1.063	78.000	384.000	.350
	Wilks' Lambda	.297	1.047	78.000	331.413	.383