Supporting Information for
Coarse-grained Force Fields from the Perspective of Statistical Mechanics: Better Understanding the Origins of a MARTINI Hangover

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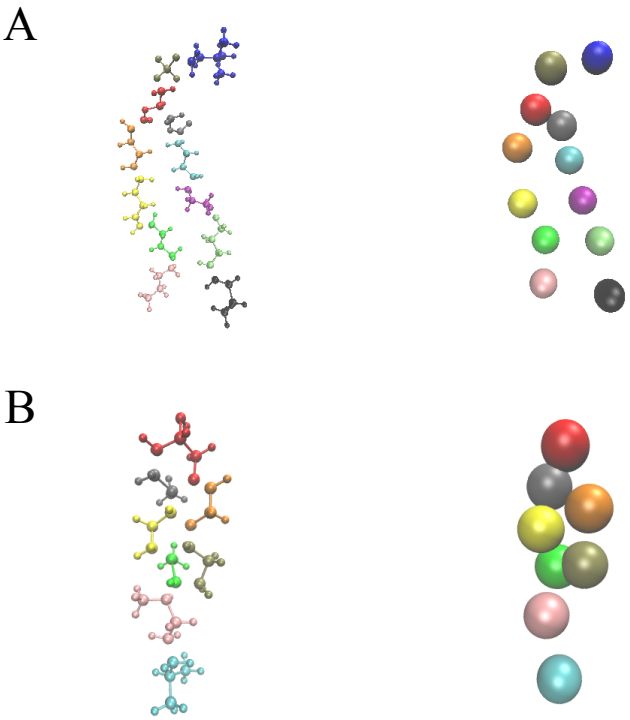
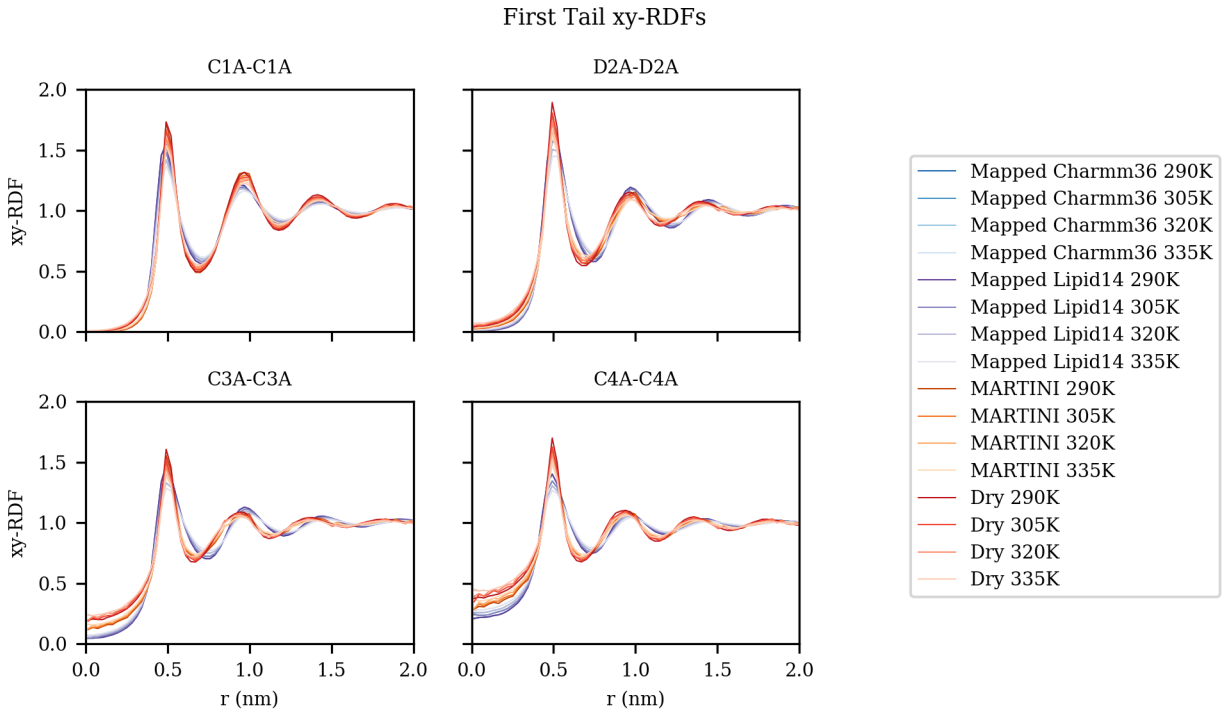
The mapping from all-atom lipids to the coarse-grained (CG) resolution use a center of mass mapping with approximately 4 heavy atoms per 1 CG bead shown in Figure S1. The main text presents the RDFs, PMFs, and enthalpy-entropy decompositions between head group beads NC3, PO4, GL1, and GL2 as well as GL1-ROH, GL2-ROH, C4A-C2, and C4B-C2. The remain SI figures are the RDFs, PMFs and enthalpy entropy decomposition between the tails of DOPC.

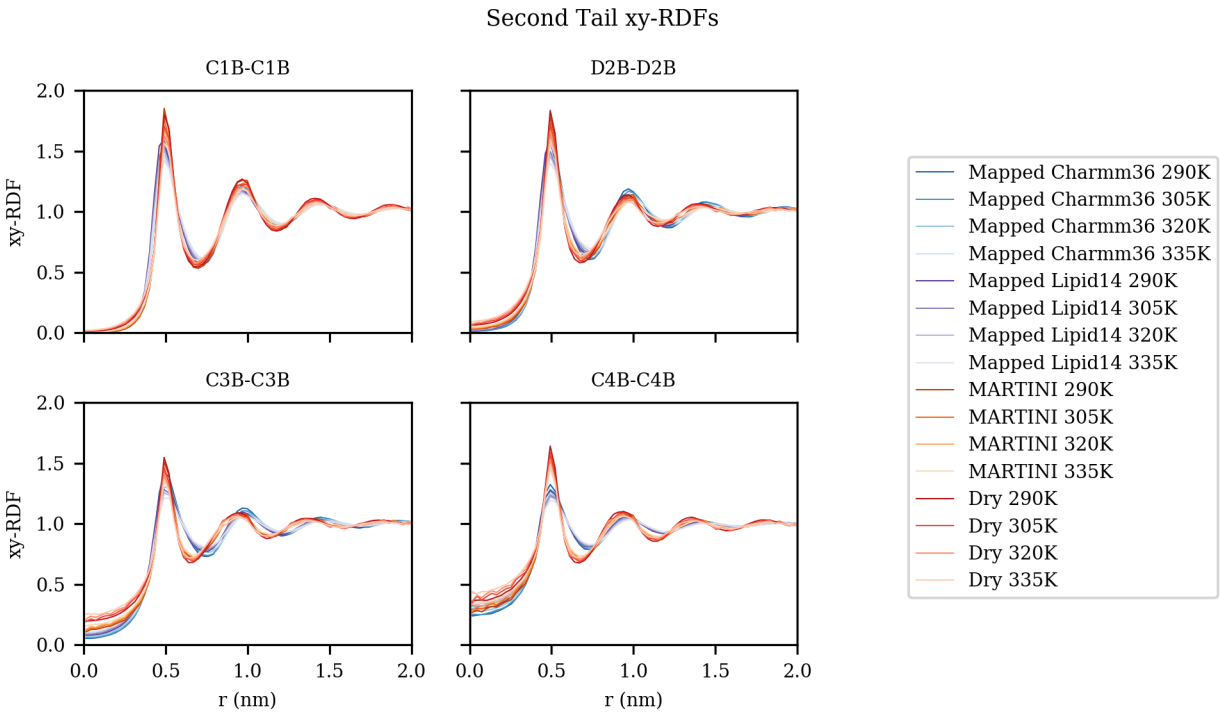


SI Figure 1: Snapshot of an atomistic (left) and CG mapped lipid (right) with each group of atoms corresponding to a CG bead a different color with DOPC shown in Panel A and cholesterol in Panel B. The DOPC bead names are NC3 (blue), PO4 (gold), GL1 (red), GL2 (gray), C1A (orange), D2A (yellow), C3A (green), C4A (pink), C1B (cyan), D2B (purple), C3B (light green), C4B (black). The cholesterol bead names are ROH (red), R1 (gray), R2 (orange), R3 (yellow), R4 (gold), R5 (green), C1 (pink), C2 (cyan).

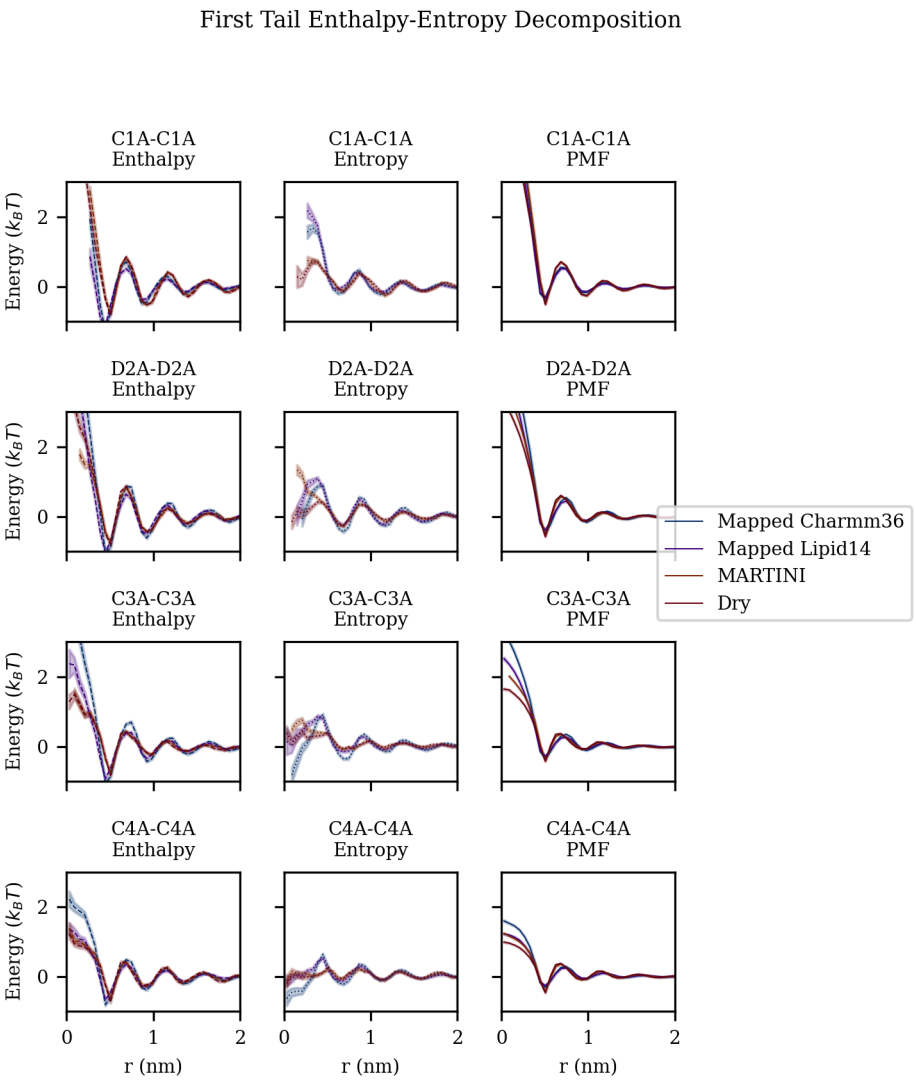
It has been discussed elsewhere that the entropy of the lipid tail groups is well captured by the MARTINI model.[1, 2] As such, we expect the radial distribution functions (RDFs) and the atomistic temperature behavior to be recapitulated. The following figures presenting the tail bead RDFs and corresponding enthalpy-entropy decompositions, which are calculated as described in the Methods section of the main document.



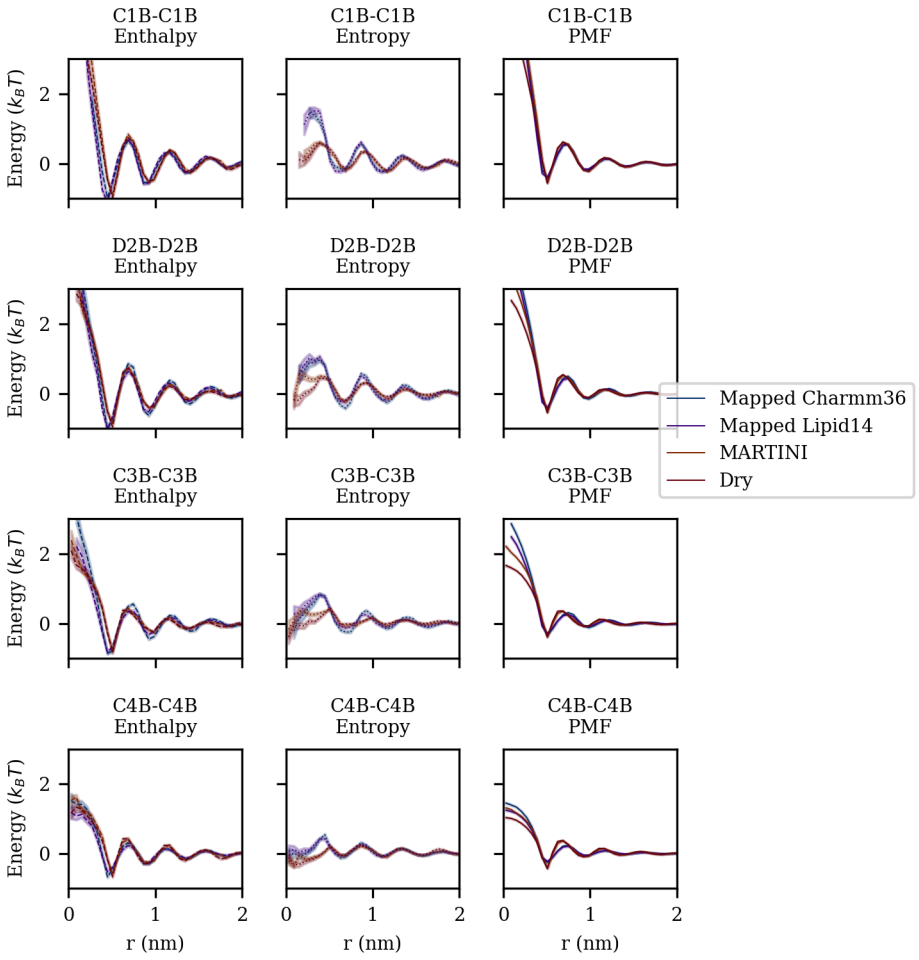
SI Figure 2: XY-projection of the radial distribution function for DOPC first tail beads comparing CG mapped Charmm36, CG mapped Lipid14, MARTINI, and Dry MARTINI models at various temperature averaged per leaflet.



SI Figure 3: XY-projection of the radial distribution function for DOPC second tail beads comparing CG mapped Charmm36, CG mapped Lipid14, MARTINI, and Dry MARTINI models at various temperature averaged per leaflet.



SI Figure 4: Entropy-enthalpy decomposition of potential of mean force between first tail beads of DOPC comparing CG mapped Charmm36, CG mapped Lipid14, MARTINI, and Dry MARTINI models



SI Figure 5: Entropy-enthalpy decomposition of potential of mean force between second tail beads of DOPC comparing CG mapped Charmm36, CG mapped Lipid14, MARTINI, and Dry MARTINI models.

Supplemental References

1. Baron, R., et al., *Configurational entropies of lipids in pure and mixed bilayers from atomic-level and coarse-grained molecular dynamics simulations.* J Phys Chem B, 2006. **110**(31): p. 15602-15614.
2. Hakobyan, D. and A. Heuer, *Comparing an All-Atom and a Coarse-Grained Description of Lipid Bilayers in Terms of Enthalpies and Entropies: From MD Simulations to 2D Lattice Models.* J Chem Theory Comput, 2019. **15**(11): p. 6393-6402.