

**S3 Table.** Bioactive compound predictions for PI3K/AKT/mTOR pathway proteins: LIMK1, LIMK2, MDM2 and VEGFA; given as ChEMBL molecule identifiers and gene names of the corresponding targets.

Predicted Compound (ChEMBL id)	Target Protein (Gene Name)	Predicted Compound (ChEMBL id)	Target Protein (Gene Name)
CHEMBL1316589	LIMK1	CHEMBL505899	MDM2
CHEMBL1512352	LIMK1	CHEMBL506261	MDM2
CHEMBL516650	LIMK1	CHEMBL506263	MDM2
CHEMBL518653	LIMK1	CHEMBL506507	MDM2
CHEMBL1316589	LIMK2	CHEMBL506623	MDM2
CHEMBL1512352	LIMK2	CHEMBL506646	MDM2
CHEMBL516650	LIMK2	CHEMBL506647	MDM2
CHEMBL518653	LIMK2	CHEMBL506740	MDM2
CHEMBL1241424	MDM2	CHEMBL507004	MDM2
CHEMBL1241425	MDM2	CHEMBL507649	MDM2
CHEMBL1241426	MDM2	CHEMBL508126	MDM2
CHEMBL1243385	MDM2	CHEMBL508377	MDM2
CHEMBL1242922	MDM2	CHEMBL508398	MDM2
CHEMBL458791	MDM2	CHEMBL508486	MDM2
CHEMBL514738	MDM2	CHEMBL508491	MDM2
CHEMBL515347	MDM2	CHEMBL508564	MDM2
CHEMBL515848	MDM2	CHEMBL508902	MDM2
CHEMBL516172	MDM2	CHEMBL508983	MDM2
CHEMBL475670	MDM2	CHEMBL509409	MDM2
CHEMBL481213	MDM2	CHEMBL509666	MDM2
CHEMBL481421	MDM2	CHEMBL510017	MDM2
CHEMBL1791379	MDM2	CHEMBL510066	MDM2
CHEMBL1791380	MDM2	CHEMBL510233	MDM2
CHEMBL1791382	MDM2	CHEMBL510473	MDM2
CHEMBL219860	MDM2	CHEMBL510817	MDM2
CHEMBL434556	MDM2	CHEMBL511030	MDM2
CHEMBL427239	MDM2	CHEMBL524509	MDM2
CHEMBL1791381	MDM2	CHEMBL524659	MDM2
CHEMBL445253	MDM2	CHEMBL524691	MDM2
CHEMBL505051	MDM2	CHEMBL524856	MDM2
CHEMBL503520	MDM2	CHEMBL524887	MDM2
CHEMBL207341	MDM2	CHEMBL524908	MDM2
CHEMBL443697	MDM2	CHEMBL525014	MDM2
CHEMBL446284	MDM2	CHEMBL525018	MDM2
CHEMBL450322	MDM2	CHEMBL525040	MDM2
CHEMBL451424	MDM2	CHEMBL525045	MDM2
CHEMBL451944	MDM2	CHEMBL525060	MDM2

CHEMBL454229	MDM2	CHEMBL525201	MDM2
CHEMBL486090	MDM2	CHEMBL525263	MDM2
CHEMBL499121	MDM2	CHEMBL525265	MDM2
CHEMBL499749	MDM2	CHEMBL525594	MDM2
CHEMBL499766	MDM2	CHEMBL525614	MDM2
CHEMBL500441	MDM2	CHEMBL525624	MDM2
CHEMBL500788	MDM2	CHEMBL525635	MDM2
CHEMBL501541	MDM2	CHEMBL525636	MDM2
CHEMBL503191	MDM2	CHEMBL526187	MDM2
CHEMBL503489	MDM2	CHEMBL526336	MDM2
CHEMBL503730	MDM2	CHEMBL526337	MDM2
CHEMBL503983	MDM2	CHEMBL526381	MDM2
CHEMBL504226	MDM2	CHEMBL526861	MDM2
CHEMBL504266	MDM2	CHEMBL527080	MDM2
CHEMBL504423	MDM2	CHEMBL527084	MDM2
CHEMBL504493	MDM2	CHEMBL1089944	VEGFA
CHEMBL504855	MDM2	CHEMBL1689394	VEGFA
CHEMBL504919	MDM2	CHEMBL499790	VEGFA
CHEMBL505501	MDM2	CHEMBL501558	VEGFA
CHEMBL505622	MDM2	CHEMBL508411	VEGFA
CHEMBL505790	MDM2	CHEMBL509774	VEGFA