

S4 Table. Full-scale molecular docking results (including both local and online docking) of computationally predicted LIMK inhibitors and their derivatives against kinase domains of LIMK proteins in terms of binding free energy (ΔG).

LIMK1	Molecule file resource	Local Molecular Docking Results		Online Molecular Docking Results	
		AutoDock (Rigid)	AutoDock (Flexible)	MtiAutoDock	SwissDock
Native ligand (Staurosporine)	ZINC	-9.5	-10.6	-11.8	-9.9
LIMKi-2 (M-379)	ZINC	-9.1	-10.1	-9.8	-8.4
LIMKi-3 (M-395)	ZINC	-9.9	-10.0	-10.1	-8.5
Native ligand (Staurosporine)	Chemaxon	-9.8	-9.5	-8.9	-8.7
LIMKi-1	Chemaxon	-7.5	-7.7	-7.2	-7.9
LIMKi-1a	Chemaxon	-7.5	-7.4	-7.4	-7.8
LIMKi-2 (M-379)	Chemaxon	-8.4	-10.1	-8.4	-8.6
LIMKi-2a	Chemaxon	-8.8	-9.7	-8.9	-8.4
LIMKi-2b	Chemaxon	-8.0	-9.1	-8.3	-8.5
LIMKi-2c	Chemaxon	-9.0	-9.7	-9.8	-8.8
LIMKi-2d	Chemaxon	-9.5	-10.3	-9.4	-8.6
LIMKi-3 (M-395)	Chemaxon	-8.4	-9.3	-8.4	-8.6

LIMK2	Molecule file resource	Local Molecular Docking Results		Online Molecular Docking Results	
		AutoDock (Rigid)	AutoDock (Flexible)	MtiAutoDock	SwissDock
Native ligand (9D8)	ZINC	-12.4	-9.9	-15.0	-10.7
LIMKi2 (M-379) - ZINC	ZINC	-12.1	-11.4	-12.7	-9.6
LIMKi3 (M-395) - ZINC	ZINC	-11.9	-11.8	-13.1	-9.4
Native ligand (9D8)	Chemaxon	-12.4	-12.7	-12.0	-11.5
LIMKi-1	Chemaxon	-9.3	-9.9	-9.3	-8.8
LIMKi-1a	Chemaxon	-9.3	-9.0	-9.4	-8.6
LIMKi-2 (M-379)	Chemaxon	-10.8	-11.8	-11.7	-9.5
LIMKi-2a	Chemaxon	-11.1	-11.3	-11.1	-9.5
LIMKi-2b	Chemaxon	-11.0	-10.5	-11.3	-9.5
LIMKi-2c	Chemaxon	-11.4	-11.9	-11.6	-9.7
LIMKi-2d	Chemaxon	-11.6	-12.0	-11.6	-9.7
LIMKi-3 (M-395)	Chemaxon	-10.6	-10.5	-11.4	-10.5