Identification of selective Lyn inhibitors from the chemical databases through integrated molecular modelling approaches

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Supplementary data

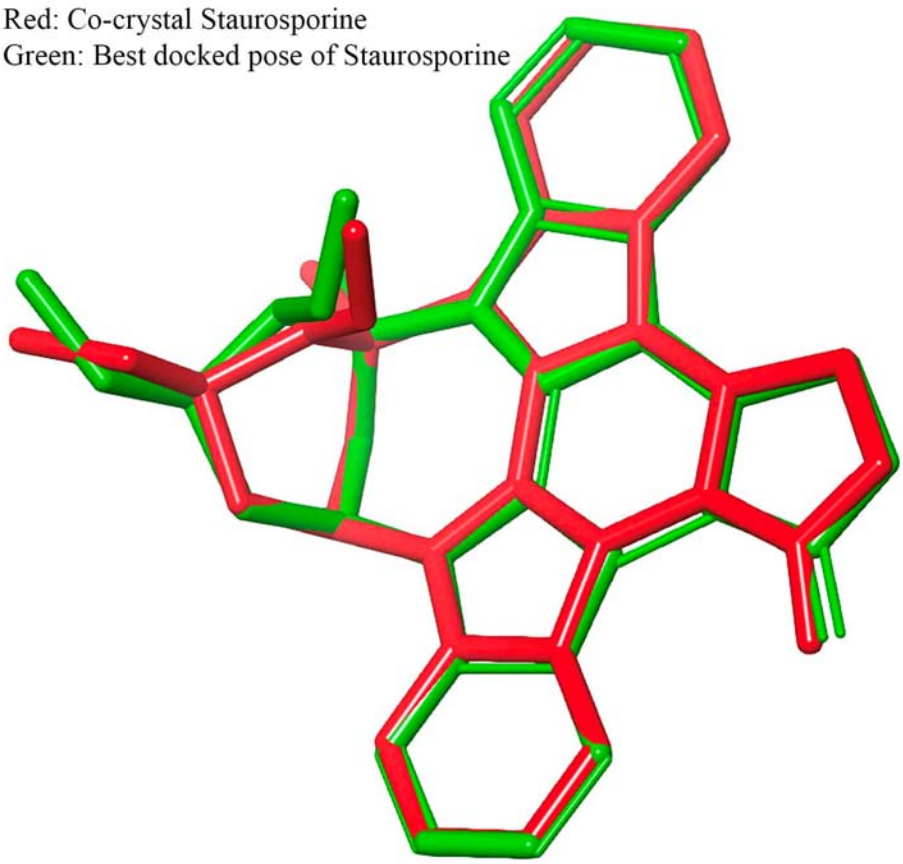

Figure S1. Superimposed structure between co-crystal Staurosporine and best docked pose of Staurosporine

Table S1. *In silico* pharmacokinetics and drug-likeness properties of 36 molecules

Molecule	MW	TPSA	Solubility Class	GI absorption	Synthetic Accessibility
Molecule1	470.5	93.13	Moderately soluble	High	3.93
Molecule2	467.56	80.12	Moderately soluble	High	3.66
Molecule3	456.51	76.8	Moderately soluble	High	4.11
Molecule4	393.39	84.07	Moderately soluble	High	2.63
Molecule5	420.42	189.68	Soluble	Low	3.96
Molecule6	435.29	98.13	Moderately soluble	High	3.52
Molecule7	322.31	92.34	Soluble	High	2.48
Molecule8	489.47	115.71	Moderately soluble	Low	3.37
Molecule9	373.36	83.91	Moderately soluble	High	2.52
Molecule10	383.42	110.69	Soluble	High	3.24
Molecule11	433.53	110.99	Moderately soluble	High	3.62
Molecule12	350.39	102.73	Soluble	High	3.62
Molecule13	400.45	107.36	Moderately soluble	High	2.96
Molecule14	324.33	62.82	Moderately soluble	High	2.62
Molecule15	376.45	67.74	Poorly soluble	High	3.62
Molecule16	455.35	144.1	Moderately soluble	Low	3.93
Molecule17	432.56	51.23	Soluble	High	3.19
Molecule18	359.44	85.75	Poorly soluble	High	3.4
Molecule19	374.39	51.44	Poorly soluble	High	2.44
Molecule20	396.87	67.74	Poorly soluble	High	3.53
Molecule21	392.41	172.61	Soluble	Low	3.85
Molecule22	426.42	104.35	Soluble	High	4.38
Molecule23	411.52	162.82	Moderately soluble	Low	2.99
Molecule24	388.42	73.47	Moderately soluble	High	3.43
Molecule25	376.45	144.1	Soluble	Low	3.87
Molecule26	369.32	104.93	Soluble	High	3.26
Molecule27	485.48	107.05	Moderately soluble	High	3.27
Molecule28	366.39	112.83	Moderately soluble	High	3.3
Molecule29	385.37	110.22	Soluble	High	3.42
Molecule30	298.25	111.9	Soluble	High	2.73
Molecule31	428.39	161.59	Moderately soluble	Low	4.68
Molecule32	431.57	62.3	Moderately soluble	High	4.29
Molecule33	438.5	147.21	Moderately soluble	Low	4.1
Molecule34	423.94	47.99	Moderately soluble	High	2.96
Molecule35	409.91	83.56	Moderately soluble	High	3.03
Molecule36	420.46	89.83	Moderately soluble	High	3.94

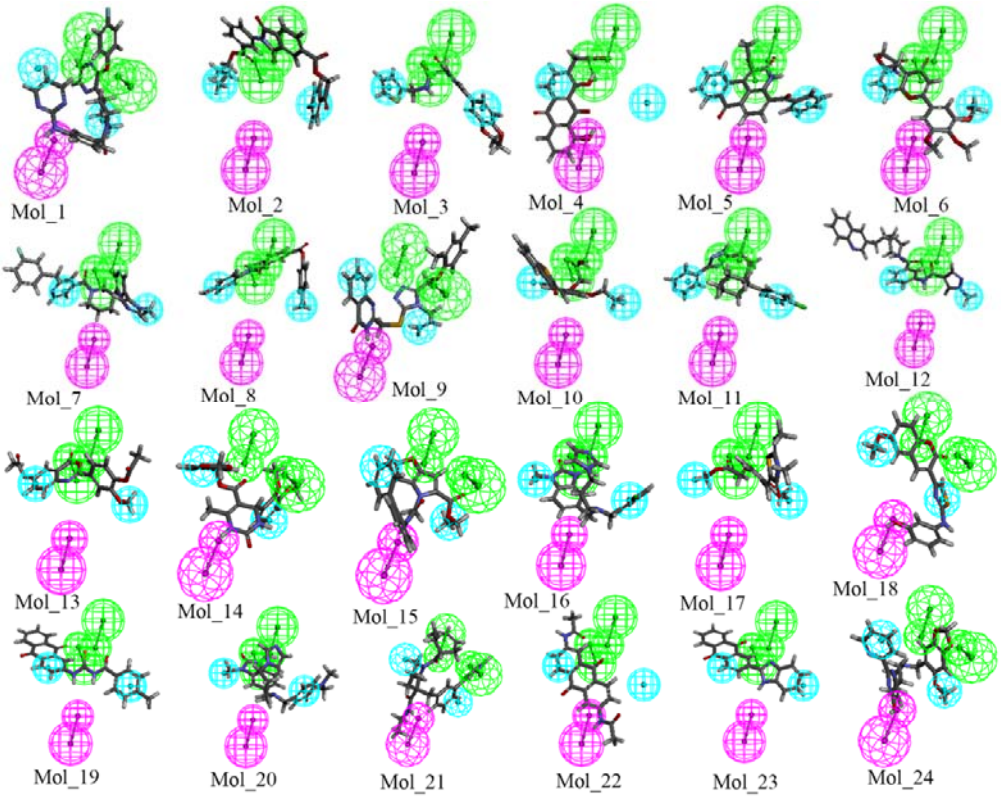

Figure S2. Ligand-pharmacophore mapped of best 24 molecules

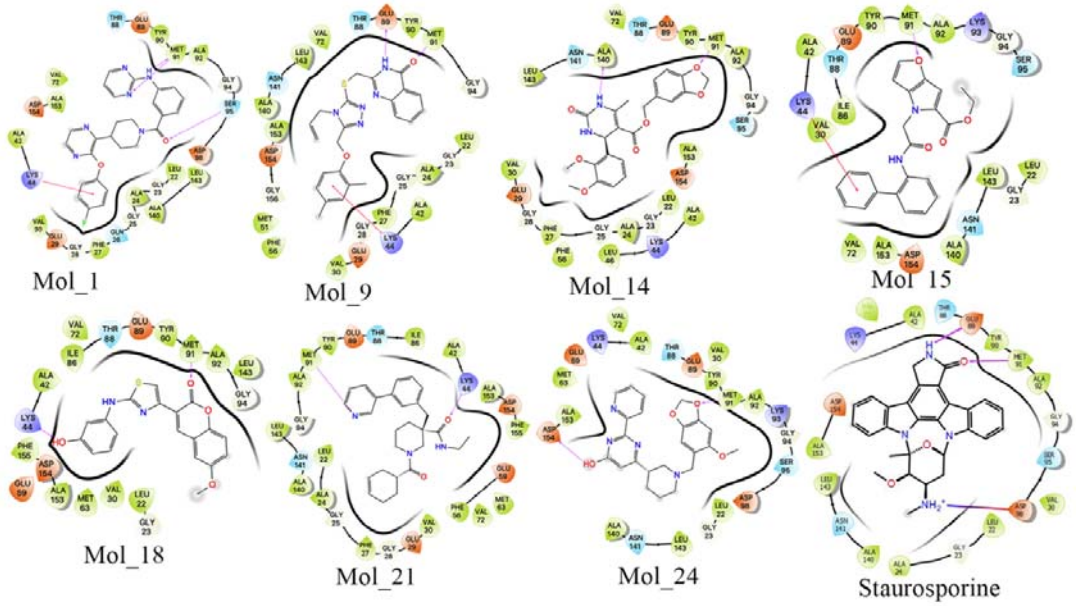

Figure S3. Binding interaction profile of best 7 molecules and Staurosporine

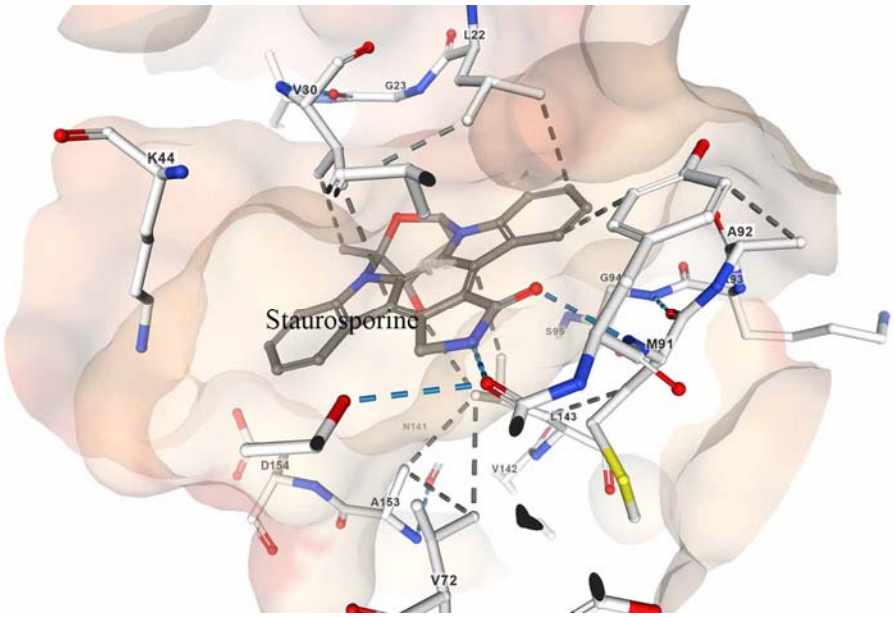

Figure S4. Binding interactions profile of the original co-crystallized Staurosporine

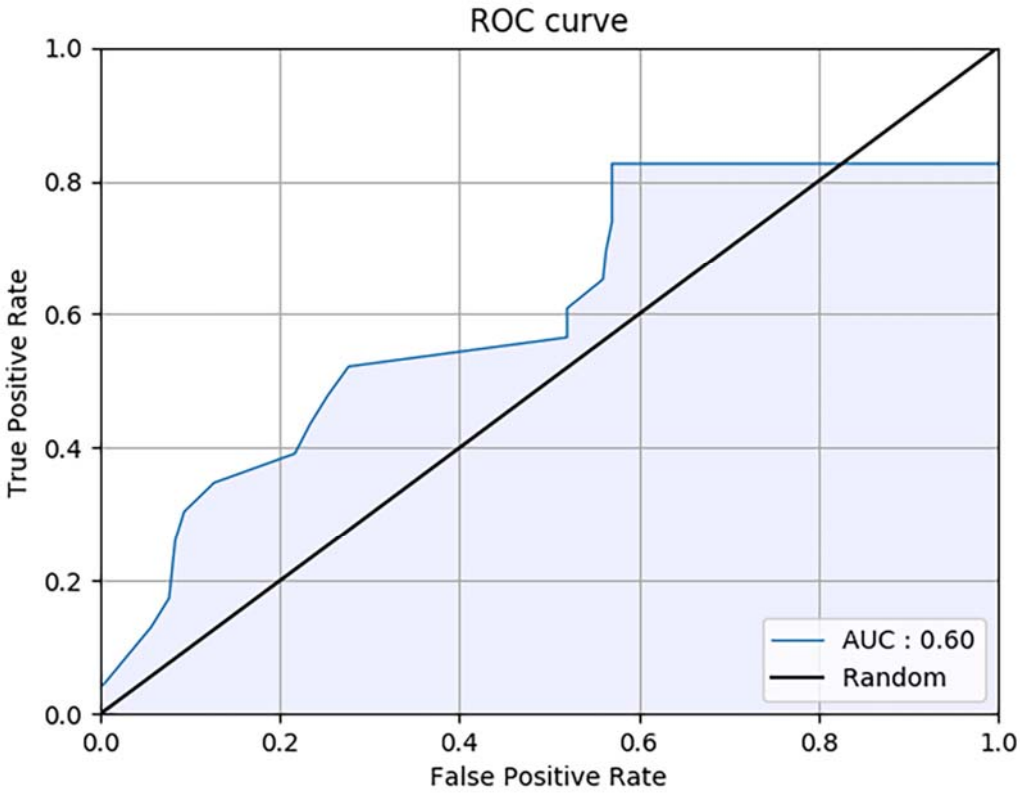

Figure S5. The ROC curve generated from the decoy set validation