SUPPORTING INFORMATION

Combination of multiple methods and views for recognition, transportation, structural-guided modify of lysine-specific demethylase phenylcyclopropylamine inhibitor

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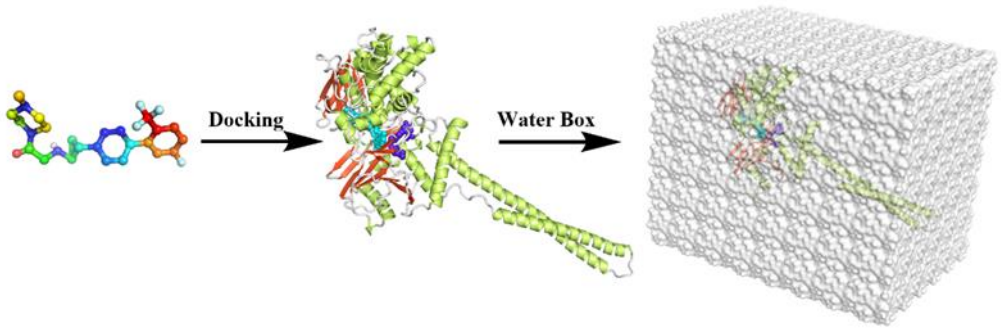


Figure S1. The docking process of compound 52 with the LSD1 protein and the water box of the building model.

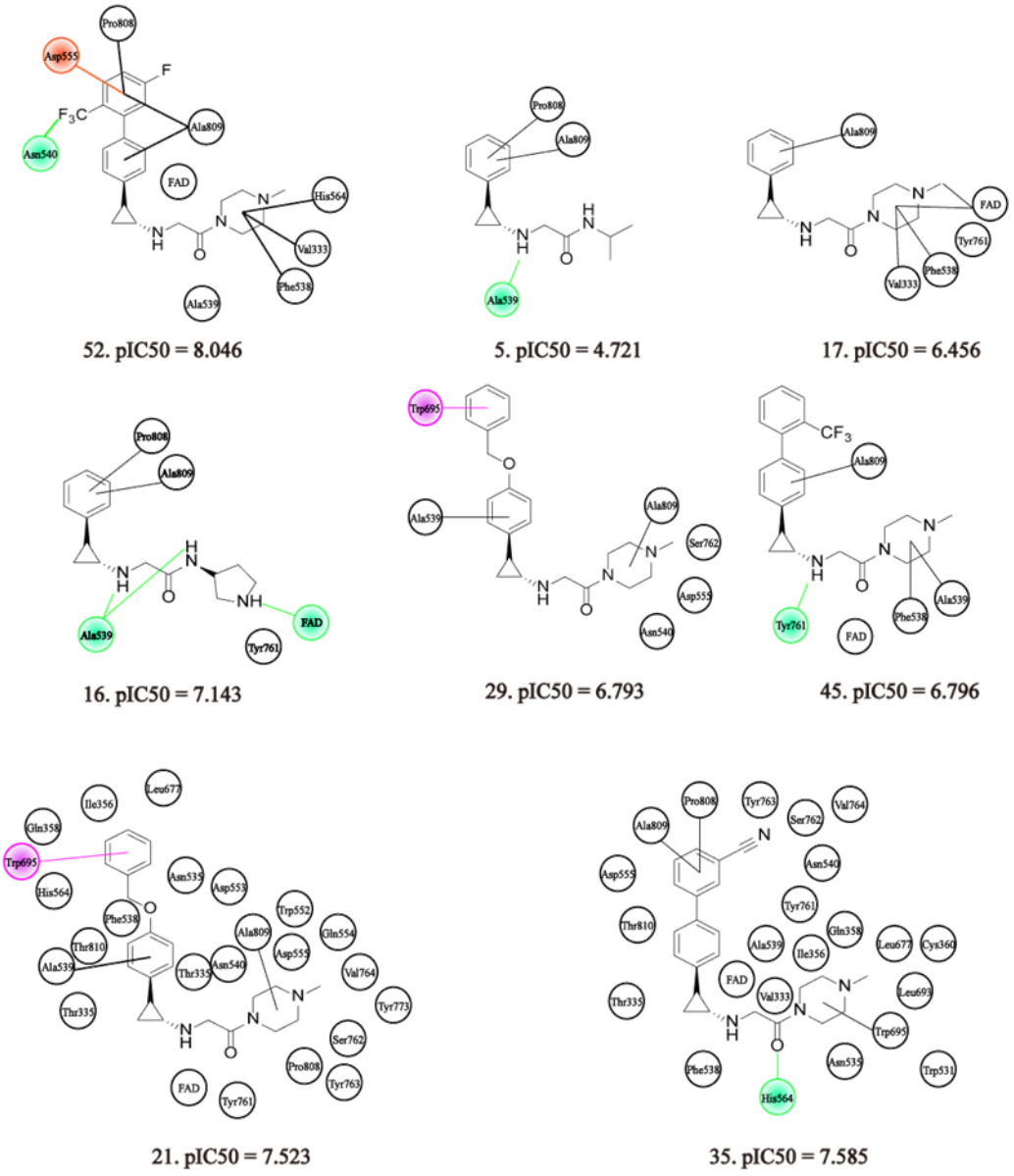


Figure S2. The interaction mode of the best docking configuration.

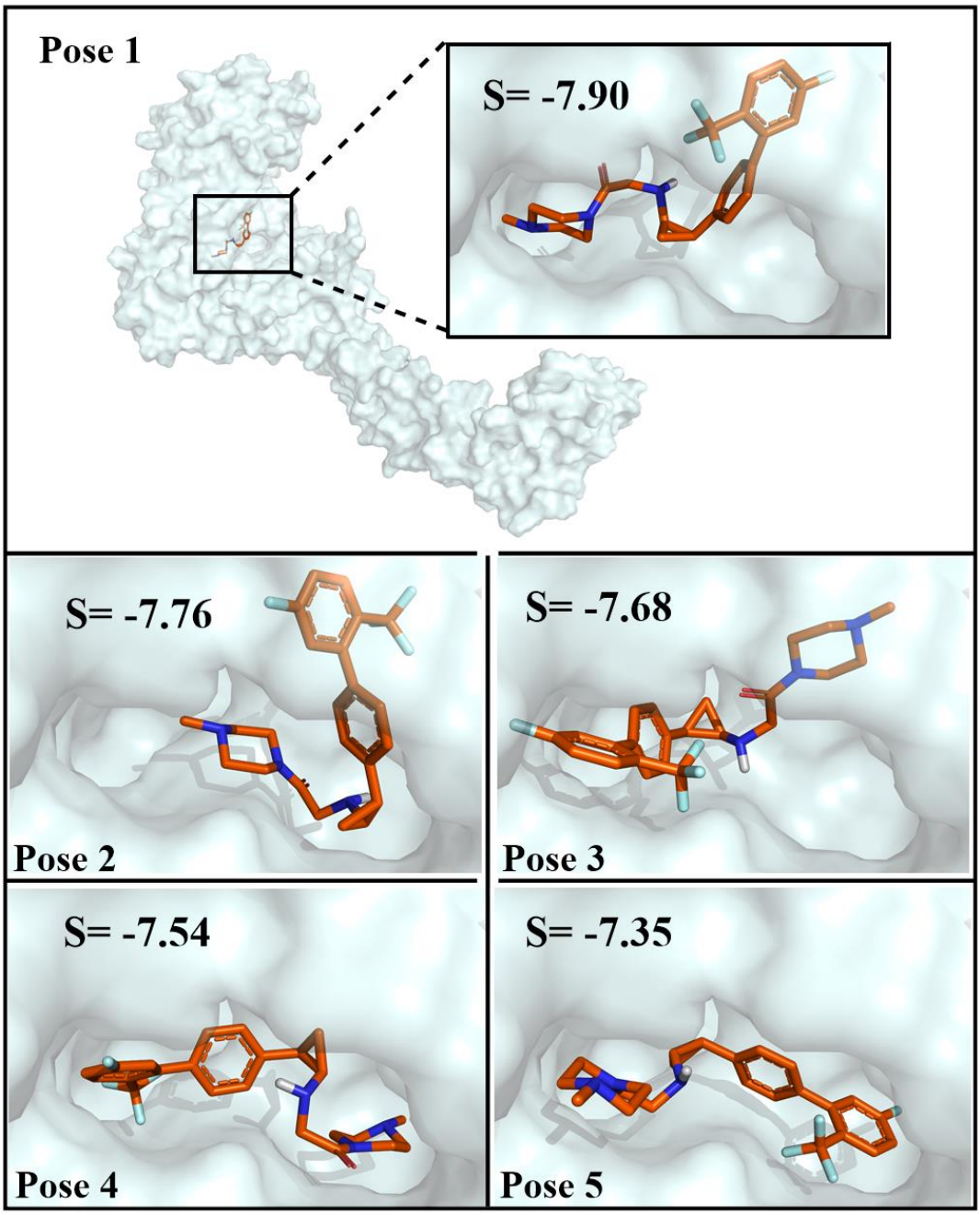


Figure S3. Docking scoring of different conformations of ligand 52 with LSD1.

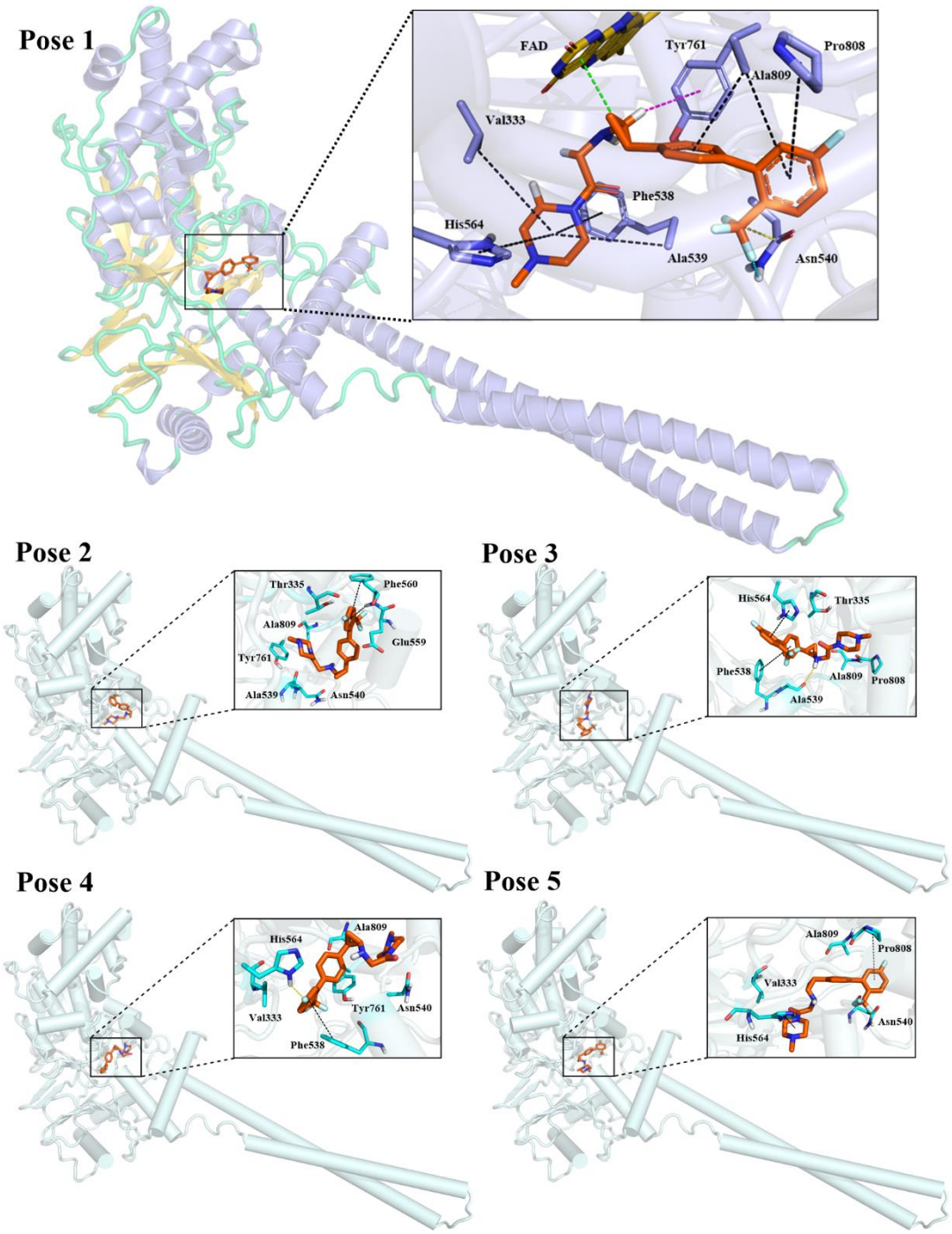


Figure S4. The interaction mode of the best docking configuration.

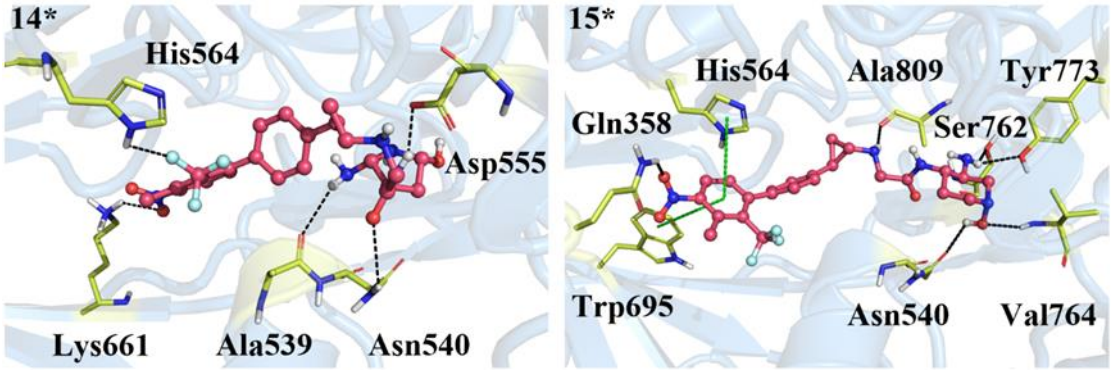


Figure S5. Docking interaction diagram of compounds of 14* and 15* with LSD1.

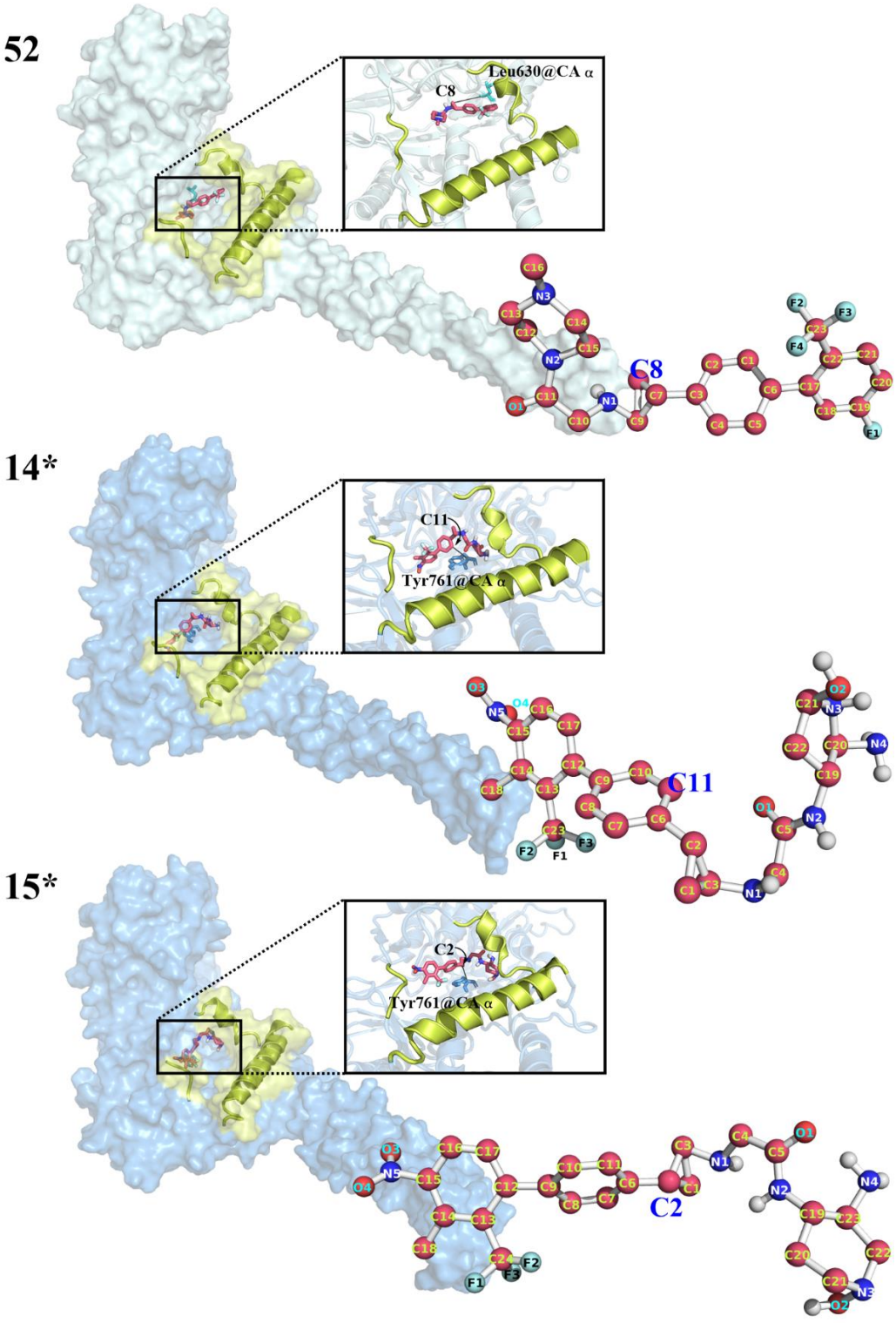


Figure S6. The pulling coordinates of P1 channel.

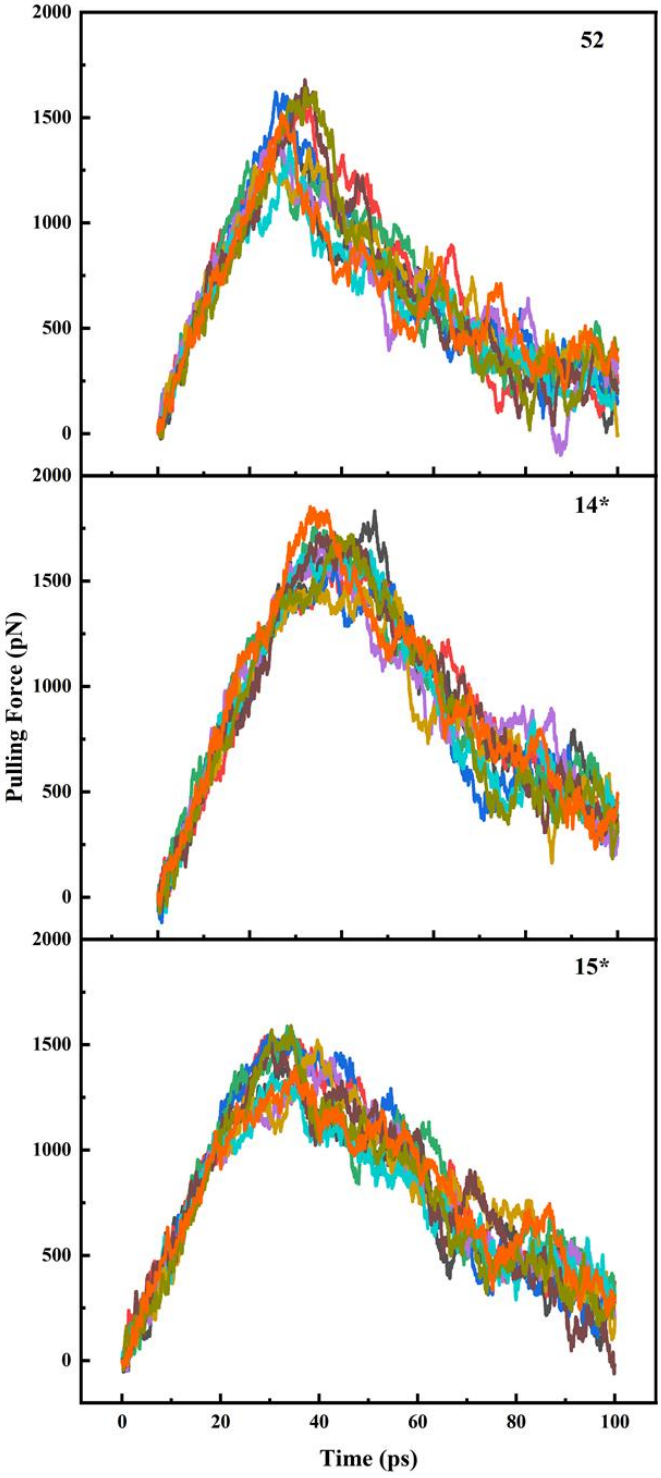


Figure S7. Pulling force in the release of ligands through the P1 channel.

Table S1. The molecular structure, corresponding experimental activity, and predicted activities obtained by 3D-QSAR for phenylcyclopropylamine class of LSD1 inhibitors selected in testing set.

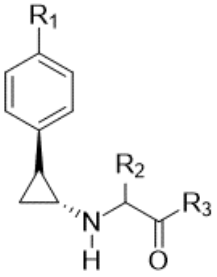
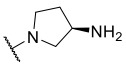
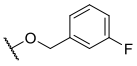
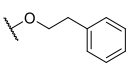
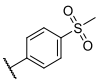
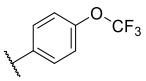
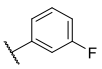
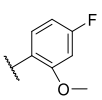
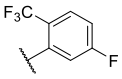
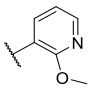
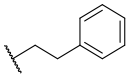
The structures' actual and predicted pIC_{50} values of the test set							
					Bioactivity(pIC_{50})		
No.	Inhibitor structure	R_1	R_2	R_3	Experi-mental data	Predicted by CoMFA	Predicted by CoMSIA
14		H	H		8.046	7.896	8.172
23			H		7.745	7.280	7.281
29			H		6.793	7.260	7.248
39			H		7.620	8.002	7.760
43			H		7.538	7.354	7.359
46			H		7.009	7.335	7.295
47			H		7.398	7.383	7.383
48			H		6.873	7.237	7.274
52			H		8.046	7.603	7.551
53			H		7.328	7.298	7.330
54			H		7.602	7.349	7.345

Table S2. Detail of MM/GBSA decomposition for 52 (All data units are kcal/mol)

Component	Energy	Component	Energy
ΔG_{vdW}	-51.54 ± 2.30	ΔG_{ele}	-10.36 ± 5.72
ΔG_{GB}	30.35 ± 3.68	ΔG_{SURF}	-6.20 ± 0.24
ΔGgas	-61.90 ± 6.55	ΔGsolv	24.15 ± 3.74
		ΔTotal	-37.75 ± 3.93

Table S3. Detail of MM/GBSA decomposition for 14* (All data units are kcal/mol)

Component	Energy	Component	Energy
ΔG_{vdW}	-51.12 ± 3.35	ΔG_{ele}	-59.09 ± 8.91
ΔG_{GB}	78.63 ± 7.31	ΔG_{SURF}	-7.23 ± 0.18
ΔGgas	-110.20 ± 7.67	ΔGsolv	71.40 ± 7.32
		ΔTotal	-38.80 ± 3.35

Table S4. Detail of MM/GBSA decomposition for 15* (All data units are kcal/mol)

Component	Energy	Component	Energy
ΔG_{vdW}	-49.33 ± 2.74	ΔG_{ele}	-29.51 ± 5.66
ΔG_{GB}	53.87 ± 6.01	ΔG_{SURF}	-7.00 ± 0.34
ΔGgas	-78.84 ± 6.30	ΔGsolv	46.87 ± 5.88
		ΔTotal	-31.97 ± 3.66