Electronic Supplementary Material (ESI) for Molecular BioSystems.

Molecular modeling studies on SIRT2 inhibitors using 3D-QSAR and molecular dynamics simulations

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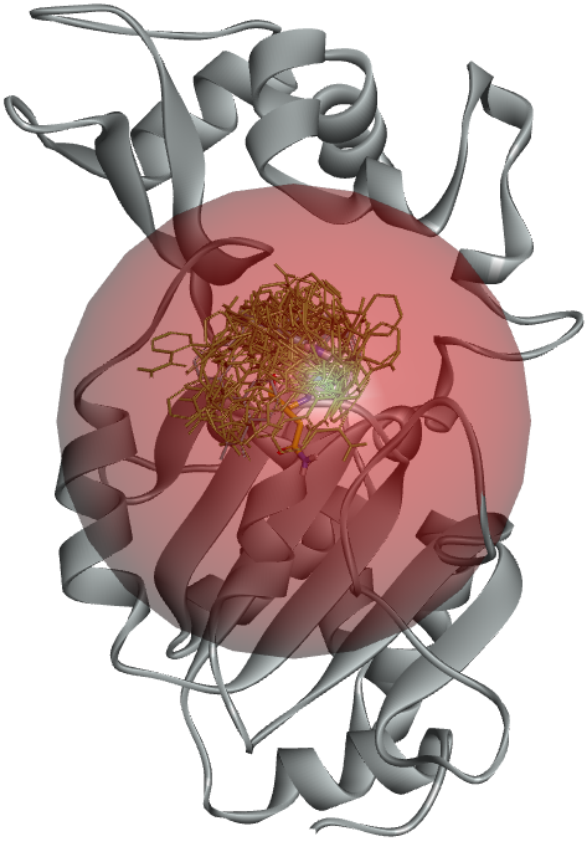

Figure S1. The docking sphere assigned to dock **39** and the obtained 35 docking conformations where conformation 1 (with the highest score) is presented in blue, the others are presented in green. Q267 is shown in atomic color.

Table S1. Docking scores of 35 collected conformation for **39** by LibDock.

Conformation #	LibDock score	Conformation #	LibDock score
1	**102.074**	19	75.009
2	101.684	20	72.578
3	100.547	21	71.439
4	93.713	22	69.891
5	92.258	23	68.836
6	89.914	24	67.451
7	87.365	25	66.518
8	86.847	26	64.766
9	85.732	27	64.412
10	85.010	28	62.615
11	84.689	29	62.179
12	84.344	30	59.829
13	82.258	31	59.028
14	81.721	32	58.033
15	80.511	33	56.419
16	78.347	34	56.273
17	77.207	35	54.942
18	76.297		

Table S2. The experimentally observed pIC_{50}, CoMFA predicted pIC_{50}, and their residuals of the studied molecules.

	pIC_{50}	CoMFA	
compound	Experimental	Predicted	Residual
1	4.481	4.496	-0.015
***2**	4.143	**4.270**	**-0.127**
3	4.000	4.035	-0.035
4	4.602	4.533	0.069
***5**	4.495	**4.137**	**0.358**
6	4.032	4.130	-0.098
***7**	4.222	**5.756**	**-1.534**
8	4.161	4.131	0.030
***9**	4.097	**4.043**	**0.054**
10	4.481	4.437	0.044
11	4.032	4.011	0.021
12	4.081	4.074	0.007
***13**	4.699	**5.881**	**-1.182**
***14**	4.056	**4.678**	**-0.623**
15	4.161	4.134	0.027
16	4.638	4.665	-0.027
17	4.770	4.753	0.017
18	4.114	4.094	0.019
***19**	4.602	**4.637**	**-0.035**
***20**	4.276	**5.691**	**-1.415**
***21**	4.420	**5.587**	**-1.167**
22	4.081	4.081	0.000
23	4.409	4.416	-0.007
24	4.398	4.390	0.008
25	4.244	4.258	-0.014
26	4.131	4.081	0.050
27	4.620	4.565	0.055
28	4.523	4.549	-0.026
29	4.268	4.354	-0.086
***30**	5.367	**4.230**	**1.137**
***31**	6	**5.878**	**0.122**
***32**	5.745	**4.660**	**1.085**
33	5.745	5.748	-0.003
34	5.796	5.894	-0.098

***35**	5.509	**5.788**	**-0.279**
***36**	5.678	**4.221**	**1.457**
37	5.854	5.859	-0.005
***38**	5.699	**5.896**	**-0.197**
***39**	6.244	**5.542**	**0.702**
40	5.569	5.646	-0.077
41	5.824	5.873	-0.049
42	5.699	5.688	0.011
43	6.081	5.872	0.209
44	5.959	5.870	0.089
45	5.469	5.583	-0.115
***46**	5.921	**4.356**	**1.565**