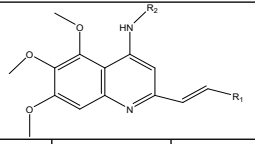
Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supplementary Material

Table S1. The structure and activity value



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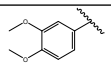
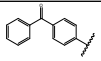
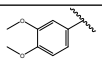
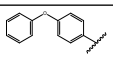
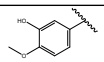
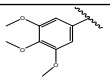
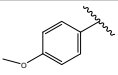
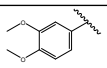
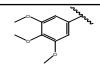
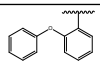
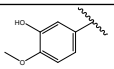
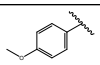
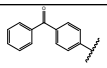
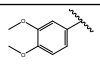
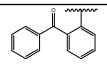
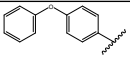
01			5.123	25			5.642
02*			5.254	26			4.885
03			5.662	27			5.395
04*			5.480	28*			5.149
05			4.179	29*			5.403
06			4.992	30			5.541
07*			4.971	31			5.827
08			5.038	32			5.710
09*			5.339	33			4.845
10			5.514	34			4.595
11			5.879	35*			5.385
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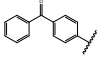
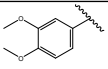
13			4.527	37			5.896
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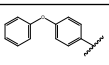
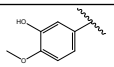
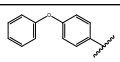
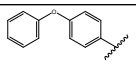
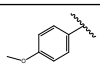
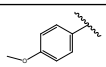
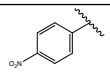
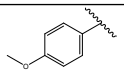
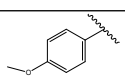
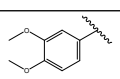
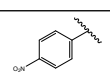
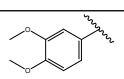
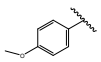
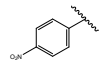
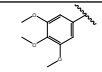
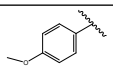
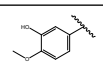
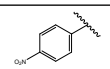
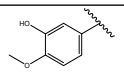
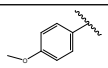
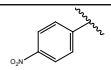
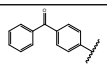
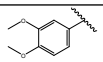
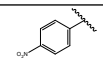
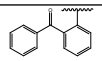
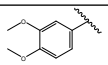
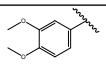
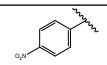
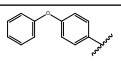
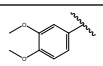
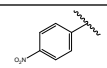
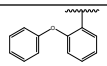
15*			5.141	39*			5.932
16			4.992	40			4.931
17			5.358	41			5.499
18*			5.461	42			5.842
19*			5.658	43			6.420
20			5.463	44*			5.130

21*			5.057	45*			5.039
22*			5.519	46			5.016
23			5.770	47			5.424
24			6.301	48*			4.734

"*" means test set

Table S2. 31 possible combinations of CoMSIA molecular fields

COMSIA	LOO		Non-Cross-Validation			Field contribution				
	q2	N	r2	SEE	F	S	E	H	A	D
S	0.788	8	0.918	0.176	29.455	1.000				
E	0.826	5	0.941	0.139	76.793		1.000			
H	0.778	1	0.828	0.221	134.955			1.000		
A	0.424	4	0.568	0.370	9.209				1.000	
D	0.081	2	0.186	0.489	3.077					1.000
S+E	0.837	4	0.943	0.135	103.317	0.220	0.780			
S+H	0.778	2	0.868	0.197	89.159	0.302		0.698		
S+A	0.834	7	0.946	0.140	54.729	0.603			0.397	
S+D	0.76	10	0.929	0.172	24.796	0.893				0.107
E+H	0.839	3	0.936	0.140	125.760		0.609	0.391		
E+A	0.822	5	0.936	0.145	70.264		0.685		0.315	
E+D	0.813	6	0.930	0.155	50.925		0.839			0.161
H+A	0.797	4	0.902	0.177	57.380			0.669	0.331	
H+D	0.753	4	0.850	0.218	35.327			0.926		0.074
A+D	0.552	3	0.656	0.324	16.493				0.537	0.463
S+E+H	0.846	3	0.938	0.138	130.986	0.143	0.527	0.330		
S+E+A	0.826	5	0.914	0.140	75.983	0.172	0.546		0.282	
S+E+D	0.819	5	0.924	0.158	58.743	0.152	0.651			0.196
S+H+A	0.817	5	0.930	0.152	63.923	0.240		0.476	0.384	
S+H+D	0.765	3	0.858	0.208	52.459	0.263		0.611		0.127
S+A+D	0.823	8	0.946	0.143	46.026	0.598			0.243	0.158
E+H+D	0.828	3	0.910	0.166	87.229		0.551	0.285		0.165
E+H+A	0.811	3	0.916	0.160	94.887		0.441	0.228	0.271	
E+A+D	0.803	5	0.922	0.160	56.970		0.573		0.207	0.219
H+A+D	0.777	6	0.906	0.180	36.787			0.618	0.263	0.119
S+E+H+A	0.812	3	0.924	0.152	105.964	0.111	0.394	0.252	0.243	
S+E+H+D	0.83	3	0.913	0.163	90.874	0.105	0.479	0.249		0.167
S+E+A+D	0.815	5	0.930	0.152	63.833	0.122	0.476		0.193	0.208
S+H+A+D	0.805	10	0.966	0.118	54.665	0.274		0.508	0.166	0.052
E+H+A+D	0.803	5	0.928	0.154	62.003		0.437	0.233	0.184	0.147
S+E+H+A+D	0.812	5	0.933	0.149	66.827	0.097	0.383	0.202	0.174	0.145

Table S3. Errors and Prediction pIC50 in the Training and Test Sets of the 3D-QSAR Model

NO.	Exp.*pIC50*	CoMFA		CoMSA	
		pIC50	Error	pIC50	Error
01	5.123	5.27	0.147	5.236	0.113
02	5.254	5.291	0.037	5.445	0.191
03	5.662	5.718	0.056	5.812	0.150
04	5.480	5.304	-0.176	5.422	-0.058
05	4.179	4.427	0.248	4.441	0.262
06	4.992	4.822	-0.170	4.802	-0.190
07	4.971	5.131	0.160	5.076	0.105
08	5.038	4.873	-0.165	4.994	-0.045
09	5.339	5.416	0.077	5.249	-0.090
10	5.514	5.438	-0.076	5.458	-0.056
11	5.879	5.868	-0.011	5.825	-0.054
12	5.635	5.450	-0.185	5.436	-0.199
13	4.527	4.576	0.049	4.454	-0.073
14	4.962	4.677	-0.285	4.748	-0.214
15	5.141	4.882	-0.259	4.915	-0.226
16	4.922	4.874	-0.048	4.972	0.050
17	5.358	5.413	0.055	5.304	-0.054
18	5.461	5.435	-0.026	5.512	0.051
19	5.658	5.863	0.205	5.882	0.224
20	5.463	5.449	-0.014	5.491	0.028
21	5.057	4.873	-0.184	5.033	-0.024
22	5.519	5.804	0.285	5.636	0.117
23	5.770	5.826	0.056	5.845	0.075
24	6.301	6.257	-0.044	6.214	-0.087
25	5.642	5.841	0.199	5.822	0.180
26	4.885	4.959	0.074	4.841	-0.044
27	5.395	5.269	-0.126	5.302	-0.093
28	5.149	5.012	-0.137	5.278	0.129
29	5.403	5.629	0.226	5.458	0.055
30	5.541	5.654	0.113	5.668	0.127
31	5.827	6.078	0.251	6.037	0.210
32	5.710	5.665	-0.045	5.646	-0.064
33	4.845	4.785	-0.060	4.665	-0.180
34	4.595	4.644	0.049	4.664	0.069
35	5.385	5.094	-0.291	5.124	-0.261
36	5.493	5.418	-0.075	5.394	-0.099
37	5.896	5.753	-0.143	5.664	-0.232
38	5.967	5.866	-0.101	5.972	0.005
39	5.932	5.454	-0.478	5.581	-0.351
40	4.931	4.881	-0.050	5.060	0.129
41	5.499	5.719	0.2197	5.627	0.128
42	5.842	5.746	-0.096	5.835	-0.007
43	6.420	6.170	-0.250	6.205	-0.215
44	5.130	5.760	0.630	5.814	0.684
45	5.039	4.877	-0.162	4.832	-0.207
46	5.016	4.925	-0.091	5.036	0.020
47	5.424	5.584	0.160	5.467	0.619
48	4.734	5.099	0.365	5.353	0.043