Supplementary Information

The effect of various atomic partial charge schemes to elucidate consensus activity-correlating molecular regions: A test case of diverse QSAR models

Sivakumar Prasanth Kumar^a, Prakash C. Jha^b, Yogesh T. Jasrai^{a,*} and Himanshu A. Pandya^a

^a*Department of Bioinformatics, Applied Botany Centre (ABC), University School of Sciences, Gujarat University, Ahmedabad – 380 009, India.*

^b*School of Chemical Sciences, Central University of Gujarat, Sector-30, Gandhinagar-382030, India.*

Tel: +91 079 26302578; Fax: +91 079 26306194; E-mail: yjasrai@yahoo.com

Supplementary Figure 2. Representative structures and scaffolds used for modeling QSAR of ten selected datasets. Refer reference for complete list of molecules.

Supplementary Figure 3. Relative contributions (expressed in fractions) of steric and electrostatic fields in explaining the variance of selected QSAR models (CoMFA models) for COX-2 inhibitors dataset.

Supplementary Figure 4. Relative contributions (expressed in fractions) of steric and electrostatic fields in explaining the variance of selected QSAR models (CoMFA models) for ten selected datasets. Charge schemes: H – Hückel, GH – Gasteiger- Hückel and P – Pullman.

Supplementary Figure 5. Scatter plot of observed and predicted activities of the QSAR models from ten selected datasets. (A) Apoptosis inducing 4-aryl-4H-chromenes, (B) Azaaurones derivatives with anti-malarial activity, (C) Azole antifungal dataset, (D) CDK2 inhibitors, (E) CYP2B6 inhibitors, (F) CYP19 inhibitors, (G) HIV-1 Reverse Transcriptase (HIV-1 RT) inhibitors, (H) LpxC inhibitors, (I) PfPK7 inhibitors and (J) Phosphodiesterase IV inhibitors

Supplementary Table 1. Descriptor contribution chart of various atomic partial charge-based QSAR models developed from VLife MDS software.

Target	VLifeMDS charge- based QSAR models	Electrostatic descriptors	Regression coefficients from the respective PLS model	Steric descriptors	Regression coefficients from the respective PLS model	Intercept of the model
COX-2 inhibitors	Gasteiger- Marsili	E_2034	+0.0912	S_1472	-0.0266	6.3236
		E_1986	-0.2392			
		E_1254	-0.2818			
		E_1200	-0.1272			
		E_1227	+0.0853			
	Del Re	E_2306	-0.3258	S_2517	-0.0587	5.6217
		E_1998	-0.0844	S_1726	-0.0411	
		E_1202	+0.0941	S_942	-0.0326	
	MMFF	E_1190	+0.1750	S_2553	+0.0511	5.4665
		E_1751	-0.0886	S_942	-0.0350	
	E_2281	+0.0735				
Apoptosis inducing 4- aryl-4 <i>H</i> - chromenes	Gasteiger- Marsili	E_156	-0.1446	S_235	0.0275	6.4970
				S_295	-0.0293	
	Del Re	-	-	S_235	0.0244	6.5555
				S_295	-0.0424	
				S_484	0.1455	
				S_944	0.0262	
	MMFF	E_683	0.1099	S_235	0.0227	6.1818
				S_295	-0.0389	
				S_484	0.1227	
	Azaaurones derivatives with anti- malarial activity	Gasteiger- Marsili	E_632	0.1099	S_664	-0.0234
E_1100			0.0871	S_509	-0.0194	
E_796			-0.0267			
Del Re		E_1099	0.0612	S_664	-0.0217	10.2125
		E_979	-0.0525			
MMFF		E_1100	0.0850	S_664	-0.0222	10.3542
		E_524	0.1229	S_509	-0.0161	
Azole antifungal dataset	Gasteiger- Marsili	E_1996	0.0596	S_1411	0.0698	8.5783
		E_1436	-0.0681	S_2822	-0.1276	

				S_1762	-0.0318	
	Del Re	E_1996	0.0713	S_1411	0.0633	8.1987
		E_1775	-0.1286	S_2822	-0.1848	
				S_1689	0.0246	
				S_2308	0.0576	
	MMFF	E_2278	0.1042	S_1411	0.0623	7.9329
		E_2526	0.2243	S_2822	-0.1847	
		E_2015	0.1105			
CDK2 inhibitors dataset	Gasteiger-Marsili	E_984	0.2364	S_1015	0.0392	4.6966
		E_626	0.2799			
		E_527	0.4099			
	Del Re	E_567	0.1183	S_1407	-0.0352	5.1959
		E_1106	0.2142			
		E_946	-0.1416			
		E_496	0.1911			
		E_827	-0.0571			
	MMFF	E_476	0.4964	S_716	0.0571	5.3215
		E_555	-0.2061			
		E_1235	-0.4106			
		E_856	-0.0514			
		E_989	-0.2762			
CYP2B6 inhibitors	Gasteiger-Marsili	E_809	0.6104	-	-	4.5271
	Del Re	E_688	0.5271	S_401	0.0528	4.4338
		E_786	0.1611	S_1015	0.0268	
		E_906	-0.0567			
	MMFF	E_689	0.1843	S_886	0.0603	3.9790
		E_403	0.2328			
		E_883	0.1165			
		E_642	-0.0548			
CYP19 inhibitors	Gasteiger-Marsili	E_1990	-0.2918	S_2060	-0.0467	3.6946
		E_1084	0.1824	S_1852	0.0448	
		E_1830	-0.1064	S_2331	-0.0598	
		E_826	-0.0841	S_2058	0.0171	
		E_1321	0.0467			
		E_1096	-0.1514			
	Del Re	E_1084	0.2553	S_2261	-0.0686	4.2715
		E_2010	-0.1337	S_2060	-0.0319	
		E_1560	-0.0484	S_1852	0.0486	
		E_1592	0.1119	S_1336	-0.0196	
				S_1866	-0.0247	
				S_2045	-0.0301	
	MMFF	E_780	-0.1310	S_2060	-0.0555	3.2455

		E_1560	-0.0682	S_1302	-0.1598	
		E_1835	0.0268	S_2059	0.0218	
		E_2262	-0.0630	S_2262	-0.0189	
		E_1753	0.1158			
		E_1820	0.0465			
HIV-1 Reverse Transcriptase (HIV-1 RT) inhibitors	Gasteiger- Marsili	E_562	0.4215	S_532	0.0529	5.3804
		E_643	-0.0273	S_332	-0.1404	
	Del Re	E_562	0.1765	S_532	0.0390	1.9888
		E_643	-0.0417	S_176	0.1071	
				S_752	0.0837	
	MMFF			S_525	-0.0160	
		E_574	0.4622	S_532	0.0686	-0.6784
		E_544	0.1132	S_656	0.0407	
		E_550	0.1471	S_666	-0.0275	
		E_393	-0.1528	S_797	0.1342	
LpxC inhibitors	Gasteiger- Marsili	E_1762	0.0625	S_1190	0.0400	5.3812
				S_2479	0.0488	
				S_1347	0.0502	
				S_1711	-0.0152	
	Del Re			S_1916	-0.0117	
		E_1762	0.0980	S_1190	0.0450	4.8874
		E_2308	0.0332	S_2479	0.0478	
		E_1710	0.0197	S_1347	0.0512	
	MMFF			S_1935	0.0171	
		E_1737	-0.0418	S_1190	0.0439	4.9234
		E_1554	0.0315	S_2479	0.0386	
				S_1347	0.0460	
				S_2321	0.0163	
PfPK7 inhibitors	Gasteiger- Marsili	E_729	0.0997	S_569	-0.0436	4.8280
		E_846	0.0912			
		E_419	0.1762			
	Del Re	E_609	-0.3036	-	-	5.3013
		E_861	-0.2608			
		E_679	0.0897			
	MMFF	E_679	0.0842	S_849	-0.0390	4.7249
		E_417	-0.0808			
		E_572	0.0576			
Phospho- diesterase IV inhibitors	Gasteiger- Marsili	E_720	-0.0375	S_832	0.0272	6.1722
		E_567	0.0638	S_314	-0.0518	
		E_446	0.0661	S_862	0.0064	
		E_965	0.0616			

	Del Re	E_964	0.0249	S_951	-0.0905	5.7697
		E_844	-0.0196	S_576	-0.0192	
		E_876	0.0200	S_709	0.0334	
				S_456	-0.0324	
				S_597	0.0058	
	MMFF	E_720	-0.0433	S_832	0.0194	6.9715
		E_435	0.1664	S_314	-0.0479	
				S_709	0.0160	
				S_1107	-0.0133	

Supplementary Table 2. Observed and predicted activities of the QSAR models from ten selected datasets.

Dataset 1: Apoptosis inducing 4-aryl-4 <i>H</i> -chromenes								
Compounds ^a	Observed pIC ₅₀	Predicted pIC ₅₀						
		Open3DQSAR	Atomic partial charge-based models (VLife MDS)				Atomic partial charge-based models (CoMFA)	
			Conventional model	Gasteiger- Marsili	Del Re	MMFF	Hückel	Gasteiger- Hückel
1	7.14	7.0554	6.489	6.451	6.4	6.672	6.679	6.682
2	7.35	6.9	7.469	7.11	7.001	7.19	7.188	7.194
4	7.74	7.0873	7.244	7.013	6.924	6.998	7.029	7.099
5	7.74	7.9397	6.345 ^b	6.219 ^b	6.197 ^b	7.193	7.234	7.184
6	6.61	6.9797	7.088	6.708	6.646	6.913	6.945	6.945
7	7.39	7.7316	7.406	7.14	7.065	7.431	7.495	7.537
8	5.5	5.8328	6.25	5.921	5.954	5.899	5.864	5.911
10	5.58	5.3192	6.58 ^b	6.583 ^b	6.5	6.243	6.258	6.26
11	7.64	7.076	7.47	7.053	6.993	7.642	7.685	7.679
12	7.51	7.8892	6.944	7.224	7.091	7.581	7.577	7.598
14	6.6	6.5002	6.403	7.224	7.124	7.143	7.174	7.235
15	5.99	5.7547	6.454	6.417 ^b	6.322	6.359	6.37	6.352
19	7.09	6.5245	6.593	6.617	6.574	7.145	7.136	7.16
20	6.95	6.7463	6.599	6.631	6.549	6.453	6.483	6.471
22	6.57	6.0256	6.605	6.589	6.473	6.92	6.89	6.904
23	6.35	6.4494	6.633	6.622	6.547	6.759	6.791	6.833
24	5.6	5.1594	5.731	5.793	5.713	6.341	6.298	6.254
26	5.8	5.6579	6.594	6.582	6.939 ^b	6.451	6.453	6.41
27	6.55	6.6914	6.512	6.582	6.443	6.55	6.559	6.523
28	7.17	6.595	6.768	6.67	6.629	6.651	6.607	6.629
29	6.33	5.9514	6.579	6.609	7.012	6.548	6.594	6.537
30	6.42	6.5595	6.564	6.599	6.475	6.312	6.255	6.179
31	7.48	7.9453	6.62	6.596	6.973	6.738	6.8	6.809
32	7.96	7.0178	7.364	7.229	7.608	7.244	7.282	7.261
33	6.61	7.0308	7.265	7.222	7.084	7.337	7.314	7.303
34	6.54	6.6779	6.55	6.577	6.484	6.889	6.814	6.769
35	6.37	6.2765	6.489	6.496	6.393	6.239	6.193	6.218
36	5.74	6.2672	5.619	5.462	5.427	5.563	5.566	5.564
37	6.7	6.9585	7.283	7.23	7.058	6.709	6.737	6.708
38	6.82	7.429	6.536	6.489	6.372	6.131	6.163	6.132
39	5.14	5.4502	6.519 ^b	6.491 ^b	6.4 ^b	6.449 ^b	6.515 ^b	6.478 ^b
40	5.92	7.2318 ^b	7.212 ^b	7.01	6.914	7.081 ^b	7.101 ^b	7.108 ^b
41	6.48	6.8064	6.482	6.449	6.477	6.438	6.437	6.438
44	5.24	5.7443	6.131	5.909	5.988	6.203	6.131	6.168

47	6.51	6.7106	6.243	6.099	6.274	6.472	6.43	6.462
49	7.85	7.0867	7.125	7.667	7.654	7.168	7.195	7.176
50	7.77	6.8352	6.774	6.983	7.137	7.127	7.159	7.147
51	7.19	7.2321	7.217	7.207	7.201	7.132	7.086	7.129
52	6.89	6.5585	7.31	7.294	7.288	7.384	7.387	7.417
54	6.8	6.8243	7.189	7.009	7.123	7.054	7.06	7.085
55	7.47	7.4703	7.209	7.652	7.64	7.148	7.17	7.19
56	7.59	7.4672	7.08	7.292	7.35	7.154	7.164	7.134
57	7.38	6.9541	7.182	7.097	7.211	7.07	7.083	7.085
58	7.21	6.9557	7.075	7.711	7.81	7.186	7.18	7.164
59	5.77	5.321	7.135 ^b	6.994 ^b	6.742	7.071 ^b	6.983 ^b	6.99 ^b
60	7.59	6.9095	7.139	7.349	7.077	7.073	7.082	7.073
61	7.82	7.547	7.462	7.411	7.402	7.706	7.672	7.687
62	7.28	6.9396	6.946	7.222	7.178	7.317	7.326	7.312
64	7.28	6.7547	6.578	6.595	6.599	6.811	6.723	6.751
66	7.05	7.0873	6.519	6.517	6.609	7.149	7.079	7.11
67	6.44	6.9397	6.593	6.588	6.567	6.527	6.452	6.473
68	6.77	6.9797	6.562	6.596	6.595	6.721	6.708	6.705
69	7.33	6.7316	7.548	7.225	7.294	7.632	7.622	7.617
70	7.31	7.8328	6.96	7.309	7.152	7.248	7.274	7.251
71	7.26	7.0513	7.094	7.441	7.289	7.522	7.576	7.539
73	6.92	7.076	6.58	6.698	7.23	6.725	6.718	6.715
75	7.62	7.1126	7.126	7.378	7.426	7.051	7.083	7.112
76	5.31	6.5002 ^b	5.277	6.159	6.338 ^b	7.152 ^b	7.123 ^b	7.08 ^b
78	7.04	6.265	6.93	7.228	7.285	7.349	7.361	7.316
79	6.82	6.6308	6.587	6.605	6.581	6.745	6.726	6.715
80	6.41	6.5477	6.474	6.458	6.5	6.479	6.499	6.479
3	7.72	7.1721	7.212	7.01	7.914	7.08	7.101	7.108
9	5.75	5.0513	5.936	5.363	5.442	6.362	6.374	6.393
13	7.12	7.1126	7.403	7.224	7.124	7.143	7.174	7.235
16	7.19	6.265	5.936 ^b	6.363	5.442 ^b	7.362	7.374	7.393
17	7.19	7.6308	6.614	6.623	6.529	6.714	6.725	6.71
18	7.2	6.5477	6.59	6.537	7.444	6.693	6.709	6.71
21	6.87	6.5977	6.613	6.628	6.544	6.625	6.632	6.636
42	6.32	6.4206	6.471	6.196	7.041	6.409	6.41	6.389
43	6.8	6.8647	6.549	6.483	6.854	6.411	6.479	6.442
45	5.96	5.4943	6.141	5.953	5.746	6.335	6.349	6.355
46	6.68	5.8013	6.851	7.334	7.392	6.688	6.72	6.676
48	7.48	7.5667	6.357 ^b	6.265 ^b	6.305 ^b	7.5	6.463 ^b	6.474 ^b
53	6.85	6.8468	7.147	6.708	7.359	7.105	7.079	7.059
63	7.28	7.0554	6.543	6.575	6.628	6.9	6.814	6.869
65	7.1	7.1721	6.577	6.598	6.604	6.691	6.619	6.657

72	6.96	7.3192	6.309	6.506	6.966	6.609	6.62	6.598
74	6.96	5.8892 ^b	6.508	6.555	7.171	6.858	6.893	6.879
77	7.64	6.7547	7.378	7.213	7.467	7.298	7.296	7.339

Dataset 2: Azaaurones derivatives with anti-malarial activity								
Compounds ^a	Observed pIC ₅₀	Predicted pIC ₅₀						
		Open3DQSAR	Atomic partial charge-based models (VLife MDS)			Atomic partial charge-based models (CoMFA)		
			Conventional model	Gasteiger- Marsili	Del Re	MMFF	Hückel	Gasteiger- Hückel
1	10.975	10.6445	10.651	10.66	10.517	10.746	10.713	10.715
2	10.802	10.7733	10.38	10.696	10.509	10.954	10.968	10.963
3	10.322	10.4259	10.643	10.548	10.501	10.355	10.268	10.251
5	10.447	10.4173	10.555	10.641	10.512	10.79	10.791	10.741
6	10.123	10.0525	10.493	10.63	10.477	10.019	10.009	9.984
7	10.071	10.0735	10.461	10.093	10.468	9.907	10.142	10.093
8	10.697	10.8633	10.468	10.411	10.545	10.634	10.637	10.732
9	10.802	10.886	10.344	10.945	10.473	10.691	10.8	10.765
11	11.113	11.0717	11.13	10.336	11.258	11.128	11.079	11.012
12	10.041	10.0736	9.987	9.979	10.075	10.181	10.087	10.198
13	11.369	11.4101	11.308	11.299	11.382	11.351	11.374	11.352
15	10.697	10.4058	10.344	10.188	10.29	10.347	10.268	10.306
16	10.23	10.4553	10.445	10.215	10.334	10.355	10.258	10.352
17	9.995	9.9291	10.057	9.988	9.962	9.988	9.987	9.975
19	9.954	9.9291	10.057	9.988	9.962	9.988	9.987	9.975
20	9	9.2563	9.294	9.57	9.6	9.308	9.419	9.359
22	9.959	9.895	9.878	10.246	9.881	10.043	9.944	10.005
23	9.556	9.7611	9.589	9.814	9.826	9.877	9.924	9.943
24	9.748	9.7769	9.85	10.201	9.792	9.819	9.653	9.685
26	9.643	9.5714	9.386	9.566	9.603	9.582	9.651	9.611
27	9.857	9.6663	9.845	9.569	9.623	9.73	9.807	9.853
28	9.612	9.6332	9.484	9.566	9.596	9.523	9.55	9.548
29	10.127	10.2758	10.387	10.233	10.311	10.072	9.965	10.013
31	9.278	9.2522	9.224	9.373	9.462	9.264	9.303	9.253
32	9.278	9.2124	9.39	9.546	9.157	9.328	9.271	9.264
33	9.826	9.789	9.94	9.568	9.668	9.563	9.645	9.613
34	9.949	10.002	9.908	9.587	9.646	9.888	9.975	9.978
35	9.568	9.5363	9.539	9.583	9.609	9.727	9.832	9.815
4	11.054	10.4011	10.529	10.464	10.847	11.004	10.972	10.543
10	10.938	11.0186	10.558	11.159	10.63	10.893	10.936	10.936
14	10.929	11.1249	11.315	10.572	11.418	11.333	11.561	11.07
18	9.924	10.1164	9.699	9.97	9.688	9.904	9.923	9.887

21	10.107	10.0545	10.27	10.256	10.319	10.013	10.024	10.03
25	9.949	9.3009	8.846 ^b	9.666	9.516	9.522	9.832	9.886
30	9.698	10.0519	10.11	10.18	10.438	9.713	9.584	9.536

Dataset 3: Azole Antifungal Dataset

Compounds ^a	Observed pIC ₅₀	Predicted pIC ₅₀						
		Open3DQSAR	Atomic partial charge-based models (VLife MDS)				Atomic partial charge-based models (CoMFA)	
			Conventional model	Gasteiger- Marsili	Del Re	MMFF	Hückel	Gasteiger- Hückel
1	10.174	10.0797	10.384	10.221	10.088	10.036	10.249	10.176
2	7.9031	7.7896	8.1	7.879	8.165	7.97	7.842	7.986
3	9.6776	9.3293	9.662	9.024	9.016	9.223	9.182	9.149
4	8.207	8.2571	7.985	8.24	8.333	8.141	8.159	8.185
5	7.9591	8.0064	7.844	8.256	7.937	7.946	8.044	7.957
6	7.699	7.6637	7.563	7.509	7.695	7.692	7.673	7.751
7	8.207	8.2099	8.815	8.654	8.608	8.211	8.102	8.292
8	7.23	7.3019	7.399	7.304	7.721	7.205	7.226	7.161
9	7	7.0475	7.258	7.018	7.169	6.998	7.05	6.935
10	7	6.8744	6.812	7.034	6.642	6.896	6.893	6.845
11	8	8.0263	7.671	7.919	7.646	7.868	7.971	7.912
12	9.4318	9.6316	9.271	9.518	9.473	9.479	9.46	9.545
13	8.2879	8.3675	8.727	8.289	8.069	8.415	8.492	8.308
14	9.5312	9.5174	9.069	9.297	9.506	9.608	9.57	9.575
15	9.4424	9.3448	8.827	9.405	8.871	9.461	9.47	9.432
16	8.2742	8.2279	8.513	8.167	8.283	8.285	8.263	8.397
17	7.699	7.7408	7.825	7.402	7.939	7.708	7.657	7.726
18	8	8.3377	8.194	8.521	8.673	8.444	8.554	8.516
19	11	11.0826	10.874	10.992	11.066	11.029	10.981	10.968
20	8	7.8873	7.931	8.074	7.822	7.965	7.921	7.988
21	8.1004	8.1484	9.005	8.559	8.487	8.033	8.082	8.102
22	8.1904	8.9054	8.835	8.953	8.036	8.034	8.508	8.031
23	9.9935	9.4757	8.515	9.505	9.35	9.899	9.766	9.67
24	8.6021	8.6113	8.49	8.576	8.874	8.761	8.496	8.703

Dataset 4: CDK2 Inhibitors Dataset

Compounds ^a	Observed pIC ₅₀	Predicted pIC ₅₀						
		Open3DQSAR	Atomic partial charge-based models (VLife MDS)			Atomic partial charge-based models (CoMFA)		
			Conventional model	Gasteiger- Marsili	Del Re	MMFF	Hückel	Gasteiger- Hückel
1	4.229	4.2443	5.441	4.939	5.124	4.472	3.555	3.838

3	6.301	6.4927	6.059	6.036	5.706	6.395	6.36	6.595
4	6.658	6.6402	6.002	6.296	6.459	6.371	6.55	6.693
5	6.921	7.1146	6.602	6.651	6.194	6.743	6.408	6.639
7	8.959	9.1412	6.751 ^b	9.329	8.429	9.504	9.471	9.152
8	5.658	5.5146	4.838	5.098	5.927	5.264	5.184	5.443
10	4.187	4.3953	4.774	3.936	4.202	4.5	4.542	4.649
12	4.569	4.4076	4.473	4.871	4.783	5.088	5.07	4.962
13	4.469	4.763	5.569	5.423	4.637	4.597	4.598	4.733
14	4.585	5.118	5.367	5.264	5.501	5.896	5.883	5.431
15	6	5.4292	5.319	5.651	5.25	5.866	5.945	5.706
17	5.301	5.2475	5.853	5.34	6.191	4.852	5.12	5.196
19	6.155	5.782	5.91	5.938	4.901	6.125	5.994	6.107
20	5.699	5.8537	5.364	5.393	4.977	5.092	5.363	5.49
21	5.523	5.3983	5.602	4.509	6.161	5.126	5.333	5.495
22	4.921	4.4943	5.9	4.544	5.604	5.144	5.032	4.62
23	5.155	5.2785	5.015	5.469	5.711	5.025	5.162	5.316
24	5.097	5.8758	6.182	5.873	4.705	6.292	6.015	5.994
26	6.523	5.8758	6.182	5.873	8.268	6.292	6.015	5.994
27	6.699	6.6045	5.48	6.399	7.456	6.434	6.31	6.239
29	5.155	5.227	5.324	5.271	5.103	5.77	5.74	5.245
30	5.398	5.2305	5.42	5.396	5.293	5.778	5.627	5.223
32	5.301	5.0763	5.363	5.685	5.519	4.575	4.687	4.928
34	4.444	4.6111	5.669	5.093	4.117	4.685	4.786	5.01
35	5.398	5.2459	4.907	5.02	4.722	5.221	5.187	5.048
36	5.538	5.2345	4.423	5.297	2.949	4.96	5.092	4.905
37	4.022	4.5523	4.702	5.258	4.707	4.87	4.951	4.734
38	7.441	7.4576	7.381	7.548	5.134	7.411	7.386	7.72
39	7.495	7.5623	7.379	7.613	5.674	6.908	7.323	7.852
42	8.097	7.6655	7.492	6.483	7.847	7.282	7.299	7.68
43	6.222	6.6205	6.676	6.365	6.808	6.074	6.282	6.346
44	6	6.0796	6.143	6.524	4.359	6.734	6.784	6.074
46	8.523	8.4089	9.081	8.257	10.202	8.277	8.139	8.483
2	5.538	5.9757	6.815	7.206	6.834	5.6	5.36	5.759
6	7.469	6.704	6.741	4.864 ^b	6.344	6.557	7.121	7.218
9	4.886	4.8992	3.474	5.334	6.967 ^b	4.692	4.451	4.619
11	5.301	4.8895	2.516 ^b	5.917	5.433	5.008	5.244	5.026
16	5.699	5.1737	5.328	5.204	5.308	5.89	5.858	5.349
18	6	5.603	5.098	5.509	4.861	5.563	5.705	5.94
25	6.301	5.8684	5.936	5.87	5.84	6.1	5.918	6.06
28	5.222	5.9376	5.337	5.064	5.346	5.994	5.839	5.421
31	4.824	5.3302	5.524	4.968	1.949 ^b	4.852	4.9	4.944
33	4.745	4.9341	5.148	5.464	5.45	4.677	4.674	4.877

40	4.495	5.2399	5.531	5.256	2.853	5.095	4.582	4.541
41	8.222	6.4483	8.299	7.596	75.803	7.072	7.561	7.696
45	6.222	8.5567 ^b	8.975 ^b	7.095	8.996	6.643	7.195	7.177

Dataset 5: CYP2B6 Inhibitors Dataset								
Compounds ^a	Observed pIC ₅₀	Predicted pIC ₅₀						
		Open3DQSAR	Atomic partial charge-based models (VLife MDS)			Atomic partial charge-based models (CoMFA)		
			Conventional model	Gasteiger- Marsili	Del Re	MMFF	Hückel	Gasteiger- Hückel
1	6.523	6.2491	6.305	6.367	6.339	6.346	6.589	6.895
3	6.398	5.8578	5.966	6.3	6.378	6.421	6.418	6.152
4	5.824	5.4193	5.524	5.596	5.813	5.088	5.323	5.507
5	5.357	5.351	4.803	5.361	5.285	5.188	5.217	5.103
6	5.301	5.231	5.135	4.948	5.594	5.543	5.48	5.432
8	5.167	4.4208	4.979	5.783	5.795	5.53	5.252	5.333
11	4.658	4.2444	4.4	4.595	4.626	4.641	4.373	4.528
12	4.456	4.2577	4.742	4.977	4.425	4.487	4.192	4.618
14	4.432	4.1607	4.714	4.83	4.448	4.147	4.124	4.338
15	4.409	3.7496	4.125	4.754	4.669	4.69	4.582	4.689
16	4.347	3.5143	4.55	3.781	4.476	3.845	4.005	4.108
17	4.301	3.535	4.264	3.724	4.308	3.83	3.774	3.739
18	4.174	3.3106	4.479	4.116	4.88	3.95	4.087	4.139
20	4.018	4.0952	4.294	3.666	3.834	3.881	3.879	3.966
23	3.824	3.9755	3.058	3.463	3.885	3.626	3.764	3.842
24	3.509	4.8708	4.156	3.44	3.563	3.472	3.558	3.639
28	3.377	3.4792	4.31	3.411	3.72	3.644	3.501	3.323
31	3.319	4.1869	4.455	3.651	3.84	3.707	3.6	3.502
32	3.201	4.085	4.089	3.262	3.885	3.344	3.119	3.136
33	3.174	4.0634	4.769	3.905	3.606	3.782	3.396	3.452
35	2.959	3.1678	2.261	2.841	3.874	3.23	2.865	3.184
36	2.959	2.9696	5.098 ^b	2.465	2.939	3.37	3.027	2.999
38	2.553	2.7517	3.259	3.718	2.982	2.181	2.386	2.76
39	2.328	5.3142	2.021	5.21 ^b	4.737 ^b	2.176	2.046	2.187
41	1.553	2.0702	1.135	1.977	2.179	1.399	1.519	1.279
42	5.41	4.5306	4.61	5.209	5.029	5.185	5.088	5.08
43	5	4.8207	4.137	4.406	4.999	5.587	5.33	4.383
45	4.55	4.1788	4.461	4.516	3.762	4.739	4.767	4.824
46	4.43	3.5015	4.696	4.367	4.455	3.657	3.834	4.028
2	6.398	6.1942	6.119	5.409	6.461	5.875	6.126	6.198
7	5.284	4.6144	4.553	4.622	5.899	5.349	5.58	5.641
9	5.041	4.1575	4.386	4.571	4.933	4.678	4.545	4.675

10	4.886	4.1129	4.464	5.528	5.582	5.034	5.151	5.087
13	4.432	3.9265	3.821	4.357	3.76	4.079	4.432	4.216
19	4.022	5.01	3.081	4.345	4.37	4.211	4.299	4.087
21	3.854	2.949	4.5	4.216	3.411	3.954	4.082	4.008
22	3.824	4.4031	4.81	3.712	3.648	3.91	4.156	3.837
25	3.456	4.0426	4.329	3.595	4.44	2.972	3.033	2.97
26	3.432	4.39	4.205	3.73	4.236	3.645	3.868	3.587
27	3.409	4.186	4.536 ^b	4.148	3.875	3.999	4.109	4.126
29	3.377	4.2471	4.118	4.177	3.772	3.414	3.247	3.254
30	3.357	4.4166 ^b	3.952	5.118 ^b	5.301 ^b	3.331	3.654	3.386
34	3.086	3.877	3.563	3.543	4.014	3.612	3.372	3.458
37	2.796	1.808	3.5978	3.397	2.65	2.99	2.934	3.118
40	2.194	2.588	3.086	2.557	2.13	2.295	2.625	2.317
44	4.7	4.2823	4.851	4.815	3.895	4.162	4.332	4.247
47	3.96	3.5309	4.081	4.474	3.453	4.139	3.977	4.053
48	2.85	3.9878 ^b	4.221 ^b	4.085 ^b	3.198	3.531	3.252	3.44

Dataset 6: CYP19 / Aromatase Inhibitors Dataset

Compounds ^a	Observed pIC ₅₀	Predicted pIC ₅₀						
		Open3DQSAR	Atomic partial charge-based models (VLife MDS)			Atomic partial charge-based models (CoMFA)		
			Conventional model	Gasteiger- Marsili	Del Re	MMFF	Hückel	Gasteiger- Hückel
1	2.446	2.8377	2.83	3.193	3.44	3.273	3.318	3.22
2	4.003	3.5926	3.545	3.486	3.805	3.724	3.666	3.566
5	3.699	3.5883	3.851	3.752	3.876	3.772	3.715	3.688
7	3.928	4.1345	3.169	4.118	3.632	3.743	3.628	3.533
11	3.959	4.0533	4.016	3.332	2.885	4.03	3.849	3.931
12	4.046	3.9865	3.744	4.021	3.722	4.03	4.081	4.086
13	4.222	4.0826	4.013	4.338	4.617	4.029	4	4.034
15	4.222	4.096	3.788	4.302	3.237	4.018	4.053	4.099
16	3.77	3.8988	3.25	4.295	3.215	4.091	3.898	3.988
17	4.222	4.0754	4.515	4.3	3.8214	4.092	4.046	4.16
18	4.155	4.1501	3.403	4.314	3.189	4.141	4.038	4.126
19	3.699	3.9738	3.486	4.389	3.167	4.055	4.195	4.197
20	4.222	3.9405	3.515	4.604	4.007	4.061	4.12	4.088
21	4.097	4.3947	3.55	4.676	4.574	3.845	3.973	3.911
22	4.301	4.1155	3.676	3.461	4.695	4.326	4.508	4.462
23	4.301	4.0487	3.697	3.42	4.25	4.208	4.095	4.239
24	4.301	4.0885	3.497	4.042	4.147	4.133	4.328	4.102
25	3.678	3.9982	3.927	3.553	3.527	3.877	4.086	4.002
26	4.398	4.079	4.123	3.508	4.64	4.323	4.33	4.402

28	4.523	4.1224	4.092	3.587	4.168	3.745	3.562	3.569
29	4.301	4.0327	3.688	3.538	3.606	4.08	4.088	4
31	3.854	3.7088	4.039	4.244	3.272	4.104	4.102	3.99
32	3.824	3.984	4.076	4.25	3.261	4.072	4.053	4.022
34	3.62	3.7186	3.54	4.301	3.216	3.773	3.912	3.896
35	3.387	3.3419	3.543	4.338	3.17	3.086	3.186	3.164
36	3.377	3.3952	3.637	4.336	3.179	2.972	3.121	3.066
37	3.027	2.9506	3.561	3.417	3.399	3.158	2.991	3.173
39	2.485	2.5153	3.001	3.309	2.143	2.51	2.662	2.597
40	2.461	2.6354	3.088	2.018	2.362	2.369	2.586	2.514
41	3.495	3.4196	3.659	2.58	3.81	3.828	3.776	3.964
42	3.469	3.6375	3.742	2.792	3.832	3.802	3.778	3.8
43	3.523	4.3264	3.531	3.461	3.842	4.042	3.962	4.038
44	4.071	4.4745	3.78	3.126	4.083	4.134	4.547	4.418
45	5.222	4.8296	4.9	4.353	4.373	5.245	5.462	5.163
47	5.398	5.0216	4.76	4.98	5.224	5.068	5.141	4.947
48	4.949	4.9321	4.789	4.308	4.085	5.134	5.155	5.236
49	4.921	5.0204	4.271	4.362	4.268	5.165	4.956	4.94
50	6	5.3856	5.579	5.304	5.257	5.94	5.542	5.629
51	5.046	5.0095	4.704	4.275	5.211	5.115	4.784	5.039
52	4.745	5.4179	4.895	4.288	3.924	5.103	4.781	4.771
55	4.523	4.828	4.256	4.199	3.752	4.767	4.239	4.367
56	5.222	5.3769	4.949	4.401	4.762	4.912	4.912	4.797
58	3.638	3.9139	3.62	3.837	3.843	3.988	4.301	4.229
59	5.699	4.4026 ^b	3.666 ^b	4.509 ^b	2.201 ^b	4.431	4.725	4.566
60	4.155	4.374	3.744	4.063	4.999	4.327	4.552	4.582
61	4.921	4.9891	4.841	4.182	4.327	4.626	4.548	4.723
63	4.678	4.4567	3.701	4.257	4.811	4.896	4.784	4.749
64	5.097	5.2796	4.195	4.236	5.252	4.828	5.211	5.288
65	4.678	4.8249	4.395	4.27	3.951	4.302	4.609	4.615
67	5.097	5.3704	5.153	4.272	4.301	5.015	4.987	5.069
70	2.959	3.2015	2.903	2.286	2.884	2.724	2.549	2.673
71	2.678	3.1588	2.177	2.284	2.661	3.766	3.505	3.803
72	3.26	3.1417	3.01	3.281	3.719	3.768	3.69	3.883
73	4.745	5.082	4.532	4.411	4.866	4.966	4.988	4.845
75	4.602	4.7036	4.559	4.556	4.623	3.969	3.98	4.064
77	4.431	4.7171	3.681	4.363	3.983	4.453	4.3	4.352
79	4.58	4.5488	3.69	4.293	4.01	4.705	4.827	4.902
80	4.347	4.3907	3.685	4.244	4.41	4.633	4.551	4.661
82	4.527	4.1664	3.674	3.908	4.246	4.531	4.611	4.669
84	4.714	4.662	4.662	4.032	4.524	4.75	4.887	4.893
86	2.529	3.0106	3.648	2.532	3.194	3.06	3.013	3.042

88	3.334	3.076	3.609	3.344	3.304	3.255	3.093	3.161
89	2.658	2.8056	3.627	3.308	3.312	3.163	3.079	3.157
90	2.926	2.9486	2.513	3.284	3.189	3.32	3.44	3.356
93	2.815	2.8461	3.689	3.317	3.208	3.136	3.071	3.164
94	2.438	2.7758	3.458	3.308	2.96	3.062	2.966	3.062
95	3.453	3.1382	4.233	4.319	2.859	3.281	3.057	3.168
97	3.023	3.0519	3.631	3.258	3.127	2.917	2.881	2.881
98	2.983	3.1187	3.682	3.25	3.353	3.243	2.994	3.051
99	2.963	3.1648	3.701	2.315	3.514	2.532	2.503	2.459
100	2.863	3.1507	3.705	2.287	3.55	2.462	2.828	2.645
101	2.879	2.932	3.67	3.231	3.446	2.811	2.719	2.762
102	3.947	3.884	3.357	4.211	3.282	3.386	3.817	3.583
103	3.291	3.3751	3.627	4.248	3.053	3.169	2.64	2.887
104	2.774	2.8981	2.987	2.249	3.275	2.673	2.678	2.573
105	2.907	3.2006	3.666	3.28	3.224	3.234	3.159	3.214
106	3.59	3.1595	3.622	4.28	3.233	3.319	3.194	3.195
107	2.338	2.1322	3.162	3.276	3.239	2.605	2.583	2.529
108	1.885	1.8575	2.767	1.283	1.23	1.898	2.13	2.018
110	2.666	2.5366	3.663	3.261	3.284	2.616	2.473	2.446
111	2.818	2.5178	3.709	3.273	3.197	2.896	2.791	2.729
112	3.237	2.8981	3.716	3.313	3.094	3.016	3.007	3.006
114	2.296	2.1819	2.667	2.259	3.285	1.982	1.945	2.032
116	5.495	4.763	5.661	4.89	5.446	4.893	4.986	4.913
3	4.144	3.9937	3.375	3.375	3.943	3.685	3.799	3.595
4	3.509	3.684	3.915	3.915	3.793	3.833	3.651	3.705
6	4	4.4314	4.137	4.137	3.332	3.648	3.675	3.623
8	2.52	3.095	2.7	2.07	2.609	2.869	3.022	2.937
9	3.162	3.1354	3.58	3.58	2.727	3.158	3.135	3.023
10	4.222	3.9653	3.69	3.69	3.758	3.948	3.933	3.942
14	3.301	4.1568	3.753	3.753	3.249	3.974	3.718	3.806
27	4.523	3.7682	4.577	5.057	4.889	4.248	4.089	4.028
30	4.222	3.9487	4.122	4.122	3.339	4.204	4.174	4.128
33	3.921	3.4506	4.598	4.598	3.183	3.262	3.437	3.336
38	2.726	2.6315	3.585	3.585	2.336	2.459	2.671	2.576
46	5	4.4765	4.2	4.2	5.524	4.637	4.978	4.58
53	4.886	5.418	4.158	4.158	4.083	5.103	4.781	4.772
54	4.678	5.0391	4.239	4.239	3.936	4.559	4.815	4.583
57	5.523	5.0323	5.546	5.546	4.4	5.806	5.652	5.675
62	5	4.8495	4.774	4.774	4.011	4.759	4.674	4.212
66	4.357	4.2879	5.094	5.094	4.017	4.4	4.581	4.626
68	4.456	3.8569	4.962	4.962	4.161	4.117	4.647	4.351
69	3.62	3.2328	2.819	3.019	3.086	4.115	3.698	3.88
83	4.625	4.2533	3.665	3.665	3.847	4.624	4.392	4.558

85	2.919	2.8839	3.741	3.741	2.513	3.238	3.19	3.231
87	3.521	2.8287	3.351	3.351	3.32	3.121	2.991	3.072
91	3.712	2.6643	3.941	3.941	3.245	3.306	3.2	3.311
92	2.82	2.6619	2.29	2.29	3.229	2.847	1.912	2.937
96	3.001	3.0449	3.684	3.684	2.843	3.093	2.958	2.96
109	2.398	2.8443	3.204	3.204	3.156	2.68	2.942	2.939
113	1.766	2.279	2.757	2.757	2.48	2.517	2.537	2.556
115	4.469	4.9824	3.67	3.67	4.887	4.513	4.094	4.049

Dataset 7: HIV-1 Reverse Transcriptase (HIV-1 RT) Inhibitors Dataset

Compounds ^a	Observed pIC ₅₀	Predicted pIC ₅₀						
		Open3DQSAR	Atomic partial charge-based models (VLife MDS)				Atomic partial charge-based models (CoMFA)	
			Conventional model	Gasteiger- Marsili	Del Re	MMFF	Hückel	Gasteiger- Hückel
1	2.061	1.7502	1.834	1.906	2.028	2.226	2.482	2.406
3	2.824	2.6739	2.824	1.998	2.015	2.695	2.769	2.846
6	2.244	1.766	1.793	1.85	1.943	2.118	2.2	2.161
7	2.143	2.1735	1.915	1.896	2.024	2.505	2.731	2.739
8	1.796	1.5832	2.478	2.044	2.058	2.022	1.904	1.805
11	1.824	1.9099	2.481	1.959	2.048	2.052	2.023	2.152
12	1.921	1.7647	2.207	2.038	2.049	1.989	1.785	1.822
14	0.959	1.1667	1.674	1.909	1.306	0.688	0.941	0.663
16	2.149	2.5985	1.753	2.202	2.293	1.817	2.177	2.21
18	2.456	2.7119	2.342	2.638	2.225	2.649	2.316	2.31
19	2.959	3.4158	3.384	2.888	3.505	3.125	2.974	3.104
20	3.921	3.6295	3.933	3.807	4.062	3.475	3.225	3.256
22	3.854	4.0944	3.675	3.488	3.881	3.731	3.429	3.373
24	1.921	1.7797	2.043	1.82	1.643	1.795	1.713	1.726
25	1.721	1.7039	2.038	1.737	1.939	2.159	2.293	2.125
27	2	2.0041	2.061	2.137	1.552	2.129	2.172	2.256
32	2.004	2.1714	2.447	2.019	2.452	2.142	2.039	2.103
36	2.208	2.3508	2.378	2.152	1.916	1.919	2.019	2.115
37	3.284	3.4328	3.89	3.482	3.312	3.422	3.228	3.087
38	3.046	3.2281	4.344 ^b	3.351	3.25	2.969	2.758	2.9
39	2.161	2.1752	2.412	2.537	2.474	2.55	2.597	2.568
40	2.854	2.6088	2.174	1.901	2.809	2.765	2.788	2.832
41	3.222	3.1277	3.601	3.727	2.91	2.786	2.917	2.972
43	2.347	2.4572	2.233	2.126	2.142	2.33	2.472	2.524
44	3.699	3.6366	3.223	3.362	3.542	3.861	3.875	3.727
45	2.137	2.4056	2.281	2.47	2.739	1.957	1.886	1.908
46	2.229	2.2496	2.004	2.418	2.251	2.359	2.313	2.152

47	3.398	3.452	3.036	3.489	3.505	3.865	3.934	3.857
49	1.921	2.1407	2.021	2.237	1.972	2.214	2.406	2.294
52	2.301	2.1376	2.039	2.293	1.918	2.484	2.512	2.525
54	2.222	2.1518	1.872	2.179	1.705	1.861	1.861	2.012
55	2.745	2.816	2.831	2.975	3.269	2.562	2.934	3.276
58	3.523	3.5208	3.48	3.458	3.208	3.053	2.867	2.803
60	5.155	5.2436	3.641 ^b	5.114	5.261	5.25	5.168	4.907
62	5.301	4.732	4.466	4.475	5.176	4.343	4.404	4.372
63	5	4.951	4.048	4.542	5.034	5.154	5.082	4.95
68	3.398	3.1928	4.052	4.284	2.514	3.464	3.373	3.356
2	2.569	1.8643	3.202	2.848	2.101	2.696	2.708	2.802
5	3.018	2.0535	2.517	2.888	2.915	2.469	2.534	2.645
9	1.921	1.1737	1.724	1.696	1.279	2.028	1.922	2.024
13	2.041	2.0769	1.839	1.892	2.397	2.135	2.068	2.014
21	2.77	3.6106	3.63	3.383	3.71	3.456	3.502	3.445
23	1.886	1.4903	1.784	2.306	1.078	2.12	1.977	1.883
30	2.319	2.4822	2.462	2.023	2.066	2.126	2.165	2.003
35	3.301	2.4193	2.785	2.877	3.382	3.513	3.546	3.526
42	1.886	2.063	2.079	2.494	1.654	1.562	1.471	1.421
50	3.699	3.9126	3.032	3.494	3.709	4.095	4.261	4.069
57	2.276	2.9077	2.741	2.403	2.23	2.987	3.024	3.756
59	4.523	4.0685	3.84	3.533	4.187	3.759	3.535	3.801
61	5.523	4.9686	4.136	4.586	5.156	5.122	5.079	4.727
64	4.398	5.2308	4.22	5.061	4.068	4.483	4.68	4.729

Dataset 8: LpxC Inhibitors Dataset								
Compounds ^a	Observed pIC ₅₀	Predicted pIC ₅₀						
		Open3DQSAR	Atomic partial charge-based models (VLife MDS)			Atomic partial charge-based models (CoMFA)		
			Conventional model	Gasteiger- Marsili	Del Re	MMFF	Hückel	Gasteiger- Hückel
5	6.3	6.3557	6.302	6.36	6.347	5.951	6.027	6.146
19	4.69	4.8331	4.71	4.765	5.002	5.112	5.005	5.003
21	6.6	6.5961	6.318	6.698	6.621	6.575	6.555	6.738
22	6.45	6.4995	6.308	6.367	6.354	5.981	6.027	6.139
25	5.22	5.072	4.828	5.24	4.932	5.47	5.306	5.254
27	4.52	4.8075	5.025	4.96	5.04	5.403	5.295	5.263
30	5.25	5.2049	5.239	5.27	4.857	5.486	5.301	5.353
32	6.55	6.6094	6.394	6.333	6.59	6.415	6.689	6.384
34	6.25	6.2744	6.222	6.319	6.17	6.146	6.499	5.868
36	5.88	5.3559	5.073	5.033	5.073	5.045	5.362	5.423
40	6.07	6.1434	6.232	6.072	5.99	6.442	6.323	6.404

42	5.04	4.986	5.167	5.089	5.094	5.216	5.265	5.278
43	5.48	5.3847	5.161	5.003	5.188	5.301	5.335	5.249
44	6	5.6128	6.374	6.115	6.094	5.798	5.7	5.865
45	5.3	5.3248	4.889	4.927	4.917	5.217	5.186	5.26
46	4.6	4.9144	5.099	4.901	5.014	4.928	5.171	5.21
48	5.65	5.8077	5.303	5.226	5.367	5.108	5.218	5.285
49	5.1	4.7871	5.026	5.163	5.047	4.783	5.077	5.213
50	5	5.0081	5.205	5.127	5.141	5.172	5.177	5.104
52	5.3	5.1505	4.989	5.229	5.316	5.481	5.118	5.245
56	4.74	4.807	4.923	4.99	5.086	5.148	5.098	5.162
57	4.52	4.6067	5.084	4.74	4.833	4.657	4.477	4.599
58	4.52	4.5901	4.624	4.472	4.455	4.43	4.519	4.339
59	4.52	4.5969	4.363	4.55	4.313	4.586	4.412	4.415
60	5.25	5.168	5.258	5.144	5.226	5.304	5.199	5.101
61	5	5.1916	5.23	5.137	5.214	5.429	5.354	5.219
62	4.92	5.0274	4.864	5.079	4.634	4.523	4.641	4.664
64	6.52	6.6652	6.601	6.467	6.602	6.231	6.733	6.606
66	5.4	5.2971	5.344	5.114	5.495	5.58	5.601	5.601
68	4.33	4.3004	4.58	4.687	4.54	4.623	4.594	4.58
70	5.12	5.0032	5.217	5.44	4.9	5.289	5.322	5.353
71	4.3	4.3727	4.374	4.282	4.561	4.545	4.62	4.457
72	4.88	4.8794	4.752	4.793	4.842	4.513	4.601	4.603
76	4.41	4.3282	4.516	4.627	4.352	4.164	4.236	4.177
77	4.23	4.3975	4.191	3.928	4.521	4.687	4.722	4.77
80	4.74	4.5829	4.769	4.897	4.773	4.313	4.344	4.359
81	4.22	4.328	4.318	4.325	4.366	4.352	4.372	4.226
20	6.79	5.9192	5.98	6.201	6.169	6.136	5.943	6.084
26	5.3	4.7796	5.569	6.088	5.897	5.263	5.179	5.164
28	5	4.777	4.391	4.062	5.136	4.888	4.871	4.901
29	5.13	4.9633	4.78	4.842	5.049	5.249	5.207	5.179
31	5.25	5.8787	4.808	4.661	4.828	5.661	5.412	5.331
33	6	5.8194	5.267	5.756	5.808	5.957	5.897	6.279
35	5.22	5.1226	4.843	4.989	4.946	5.05	5.032	5.092
37	5.92	5.2236	5.36	5.215	4.995	5.364	5.268	5.373
38	6.01	5.4158	6.597	6.224	6.203	6.41	6.312	6.346
47	5.6	5.1746	4.889	4.818	4.796	5.533	5.428	5.5
53	4.52	5.1367	4.817	4.935	4.993	5.073	4.887	4.785
65	4.3	4.5281	4.503	4.632	4.751	4.552	4.586	4.526
67	4.3	4.6685	4.77	4.585	4.655	4.411	4.417	4.284
69	5.81	4.9612	5.509	5.473	5.699	5.07	5.098	5.263

Dataset 9: PfPK7 Inhibitors Dataset								
Compounds ^a	Observed pIC ₅₀	Predicted pIC ₅₀						
		Open3DQSAR	Atomic partial charge-based models (VLife MDS)				Atomic partial charge-based models (CoMFA)	
			Conventional model	Gasteiger- Marsili	Del Re	MMFF	Hückel	Gasteiger- Hückel
1	4.936	5.0079	4.697	4.851	4.565	4.769	4.829	4.975
5	5.102	5.1318	5.828	5.661	5.28	5.233	5.072	5.218
7	5.9	6.0616	5.786	5.391	6.154	6.174	6.224	6.173
9	6.125	6.0026	6.281	6.554	6.862	6.231	6.113	6.197
10	6.237	6.2077	6.11	5.42	6.212	6.215	6.109	6.125
11	6.553	6.3463	6.637	5.545 ^b	6.219	6.295	6.196	6.275
13	6.114	5.813	5.767	5.695	5.494	6.154	6.061	6.105
14	5.131	4.8992	4.813	5.015	4.606	4.596	4.789	4.754
15	4.602	4.8878	4.847	5.208	4.674	4.539	4.594	4.426
16	4.469	4.702	4.672	4.809	4.786	4.65	4.655	4.72
17	3.983	4.552	4.153	4.233	4.506	4.33	4.271	4.29
18	3.955	3.5823	3.59	4.15	4.057	3.795	3.843	3.732
19	5.959	6.0782	5.686	5.903	5.543	5.935	5.884	6.041
21	4.377	4.403	4.793	4.606	4.8	4.389	4.321	4.245
22	4.469	4.358	4.406	4.386	4.539	4.443	4.372	4.342
23	4.252	4.4128	4.79	4.303	4.337	4.34	4.352	4.445
24	3.987	3.9181	3.984	3.768	3.92	4.045	3.899	3.907
31	6	5.8898	6.268	6.586	6.961	6.066	6.123	6.11
32	5.854	5.8844	6.523	6.276	6.232	5.941	5.802	5.94
34	6.886	6.9135	6.416	6.257	5.863	6.593	6.592	6.653
35	6.585	6.5105	6.222	6.14	6.635	6.439	6.484	6.401
37	6.469	6.4889	5.405 ^b	5.45 ^b	6.281	6.463	6.536	6.544
39	5.097	5.1182	4.771	4.6	5.228	5.174	5.172	5.146
41	4.367	4.2281	4.752	5.157	4.47	4.349	4.499	4.567
42	5.319	5.3081	5.289	5.411	5.427	5.258	5.263	5.264
43	4.602	4.5142	5.111	4.542	4.639	4.614	4.627	4.68
6	6.092	5.62	6.294	5.95	5.518	6.188	6.195	5.925
8	5.971	5.8293	5.988	5.625	5.934	6.029	6.225	6.039
29	6.357	6.2646	5.906	6.083	6.082	6.351	6.391	6.294
30	6	5.239	6.303	5.889	6.076	5.991	5.998	5.986
33	6.086	5.8168	6.195	6.547	5.658	5.976	6.038	6.012
36	6.658	6.1799	5.792	6.675	6.341	6.438	6.488	6.838
38	5.678	5.3007	6.289	5.71	5.158	6.069	6.153	6.205

Dataset 10: Phosphodiesterase IV Inhibitors Dataset								
Compounds ^a	Observed pIC ₅₀	Predicted pIC ₅₀						
		Open3DQSAR	Atomic partial charge-based models (VLife MDS)				Atomic partial charge-based models (CoMFA)	
			Conventional model	Gasteiger- Marsili	Del Re	MMFF	Hückel	Gasteiger- Hückel
1	6.05	5.9344	5.864	6.019	5.919	6.01	6.008	6.005
3	4.85	5.0827	4.895	4.826	4.858	4.893	4.906	4.897
4	5.64	5.5756	5.747	5.79	5.873	5.745	5.735	5.736
5	5.82	5.7337	5.667	5.811	5.792	5.932	5.906	5.901
6	5.96	5.962	5.936	5.95	5.931	5.841	5.834	5.843
8	5.82	5.8081	5.862	5.797	5.789	5.821	5.818	5.808
9	5.64	5.7317	5.505	5.639	5.508	5.778	5.77	5.765
10	5.33	5.359	5.399	5.35	5.497	5.368	5.368	5.375
11	5.52	5.53	5.739	5.581	5.509	5.537	5.533	5.524
12	6.22	6.3347	6.195	6.016	6.239	6.088	6.138	6.148
13	5.88	5.9129	5.823	5.763	5.885	5.894	5.899	5.909
14	4.19	4.1235	4.142	4.172	4.196	4.234	4.21	4.22
15	6.15	6.1289	6.068	6.141	6.053	6.09	6.133	6.098
16	5.85	5.9315	5.853	5.841	5.883	6.021	5.98	6.013
17	5.82	5.8641	5.905	5.986	5.9	5.848	5.862	5.858
20	6	6.0187	6.031	6.013	5.929	6.148	6.138	6.147
22	6.22	6.251	6.136	6.255	6.303	6.271	6.266	6.269
23	6	6.1195	6.202	6.188	6.13	6.105	6.098	6.1
25	5.57	5.5844	5.696	5.578	5.555	5.554	5.563	5.561
26	6.1	6.0608	6.158	6.09	6.151	6.113	6.111	6.109
27	5.6	5.5137	5.584	5.599	5.673	5.434	5.439	5.436
28	5.4	5.3495	5.422	5.436	5.328	5.254	5.256	5.258
29	6.4	6.1195	6.202	6.188	6.129	6.105	6.099	6.1
2	5.96	5.825	5.528	6.159	5.846	5.791	5.809	5.801
7	5.4	5.6213	5.344	5.583	5.567	5.511	5.517	5.512
18	6	5.9125	5.704	6.23	5.964	6.07	6.045	6.037
19	6.07	5.8829	5.78	6.351	6.172	6.004	6.031	6.039
21	6.22	6.137	5.766	5.932	5.935	6.153	6.154	6.161
24	6.22	6.2248	5.987	6.143	5.928	6.288	6.277	6.272

^a The test set molecules are shown in bold face

^b Outliers; Non-compliance of field variables with activity when chemical groups aligned in respective positions.

Note: The parameters, r^2 and q^2 , were calculated after removing the outliers.