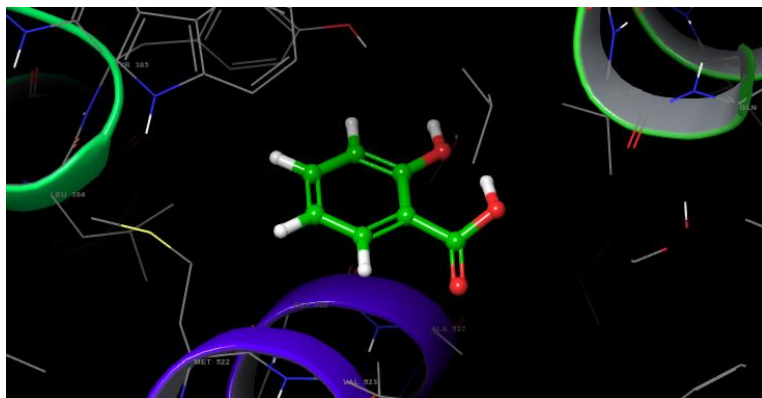


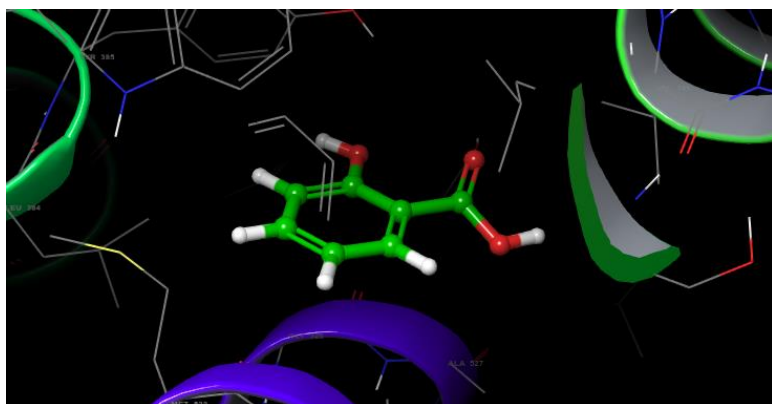
Ferulic acid



Co-crystallized



Salicylic acid



Supplementary Figure 1: 3D interactions of the top compounds and Co-crystallized ligand in the active site of Human cyclooxygenase-2.

Supplementary Table 1: Test and Train Dataset for the QSAR model.

ID Set	Y(Obs)	Y(Pred)	Error	Name
1 train	5.4800	5.9647	0.4847	CHEMBL223655
2 train	5.5900	5.9647	0.3747	CHEMBL387879
3 train	5.7300	6.6724	0.9424	CHEMBL388625
4 train	7.2200	7.0286	-0.1914	CHEMBL118
5 test	6.1600	5.8790	-0.2810	CHEMBL440001
6 train	4.4400	4.4865	0.0465	CHEMBL105350
7 train	5.0100	4.8757	-0.1343	CHEMBL180239
8 train	4.9700	4.8757	-0.0943	CHEMBL181529
9 test	6.7500	6.4906	-0.2594	CHEMBL270730
10 train	6.1100	5.8902	-0.2198	CHEMBL4091890
11 train	4.9300	6.2903	1.3603	CHEMBL1221678
12 train	7.7000	5.7715	-1.9285	CHEMBL4071983
13 train	6.1100	6.3117	0.2017	CHEMBL72515
14 train	7.9200	6.4613	-1.4587	CHEMBL358609
15 test	8.9200	7.2423	-1.6777	CHEMBL270078
16 train	5.4000	6.3297	0.9297	CHEMBL271572
17 test	7.0600	7.2508	0.1908	CHEMBL96947
18 train	7.0000	6.0682	-0.9318	CHEMBL92793
19 train	6.6000	6.7145	0.1145	CHEMBL364966
20 train	6.3000	6.9689	0.6689	CHEMBL122
21 train	6.5700	6.4350	-0.1350	CHEMBL281847
22 train	6.9600	6.4350	-0.5250	CHEMBL285828
23 test	5.9000	6.1871	0.2871	CHEMBL1221730
24 train	6.5200	5.5684	-0.9516	CHEMBL146703
25 train	5.1600	6.1665	1.0065	CHEMBL3127307
26 train	4.9500	5.2372	0.2872	CHEMBL3289925
27 train	4.7300	5.3244	0.5944	CHEMBL3309947
28 test	4.3300	4.9676	0.6376	CHEMBL3290193
29 train	5.0900	6.0500	0.9600	CHEMBL3322400
30 train	5.5400	5.7702	0.2302	CHEMBL3322412
31 train	5.6000	6.3339	0.7339	CHEMBL3322415
32 train	6.7200	7.0231	0.3031	CHEMBL126991
33 train	8.9000	7.0495	-1.8505	CHEMBL93372
34 train	5.2300	5.8790	0.6490	CHEMBL157720
35 test	6.2800	6.5149	0.2349	CHEMBL1630223
36 train	4.0200	6.7091	2.6891	CHEMBL1630245
37 train	6.8200	6.7262	-0.0938	CHEMBL1630226
38 test	7.0300	6.7091	-0.3209	CHEMBL1630228
39 train	7.0000	6.9660	-0.0340	CHEMBL278505
40 train	4.9600	5.8014	0.8414	CHEMBL212918
41 test	6.4300	6.2102	-0.2198	CHEMBL434520
42 train	5.8300	6.1572	0.3272	CHEMBL361504
43 test	7.8200	6.6210	-1.1990	CHEMBL56367
44 train	4.2900	5.8125	1.5225	CHEMBL326005
45 train	5.3800	5.7583	0.3783	CHEMBL419561
46 train	6.1600	6.6197	0.4597	CHEMBL375309

47 test	4.3100	6.1132	1.8032	CHEMBL101459
48 train	6.5100	6.8555	0.3455	CHEMBL274473
49 train	6.3600	6.0296	-0.3304	CHEMBL108452
50 test	8.1000	7.4762	-0.6238	CHEMBL117295
51 train	5.7400	6.0641	0.3241	CHEMBL321407
52 train	6.4600	6.4172	-0.0428	CHEMBL44468
53 train	7.1000	7.3267	0.2267	CHEMBL295032
54 train	7.2400	6.6261	-0.6139	CHEMBL17069
55 test	5.8900	5.8571	-0.0329	CHEMBL154422
56 train	6.0000	7.0286	1.0286	CHEMBL118
57 train	7.6200	6.2485	-1.3715	CHEMBL185621
58 train	5.7000	5.6869	-0.0131	CHEMBL307233
59 train	7.3800	7.1966	-0.1834	CHEMBL117306
60 train	6.6200	6.4199	-0.2001	CHEMBL46761
61 train	8.7000	8.6192	-0.0808	CHEMBL52020
62 test	6.1000	6.1800	0.0800	CHEMBL44466
63 train	7.6600	7.8841	0.2241	CHEMBL314297
64 train	6.7000	5.5205	-1.1795	CHEMBL155781
65 train	6.1600	6.4283	0.2683	CHEMBL154253
66 train	7.4000	6.3770	-1.0230	CHEMBL316866
67 test	6.8500	6.4452	-0.4048	CHEMBL327751
68 train	6.7000	6.3632	-0.3368	CHEMBL275376
69 train	6.3900	5.6246	-0.7654	CHEMBL158148
70 train	7.8900	6.8453	-1.0447	CHEMBL43461
71 test	7.2500	7.0286	-0.2214	CHEMBL118
72 train	4.4700	5.1337	0.6637	CHEMBL1275971
73 train	6.4800	5.2812	-1.1988	CHEMBL4454251
74 train	4.9600	5.8713	0.9113	CHEMBL16814
75 train	7.0300	6.7904	-0.2396	CHEMBL312221
76 test	6.4700	6.5112	0.0412	CHEMBL282084
77 train	7.2900	6.4543	-0.8357	CHEMBL117146
78 train	8.0300	7.7442	-0.2858	CHEMBL29887
79 train	4.7700	6.2304	1.4604	CHEMBL6
80 test	4.8200	5.5469	0.7269	CHEMBL3410346
81 train	4.7400	5.8825	1.1425	CHEMBL3410352
82 train	4.7900	5.6330	0.8430	CHEMBL3410364
83 train	6.7200	6.3419	-0.3781	CHEMBL4071061
84 train	6.2500	5.8902	-0.3598	CHEMBL4092847
85 train	5.0500	5.3195	0.2695	CHEMBL2333740
86 train	5.1000	5.3195	0.2195	CHEMBL2333739
87 train	5.9500	6.2773	0.3273	CHEMBL4074825
88 test	6.7000	5.6805	-1.0195	CHEMBL399878
89 test	6.5100	6.6958	0.1858	CHEMBL2347670
90 test	5.8600	6.1533	0.2933	CHEMBL4211316
91 train	5.5700	5.9452	0.3752	CHEMBL4206180
92 train	7.8500	6.9366	-0.9134	CHEMBL1221731
93 train	6.0000	6.6759	0.6759	CHEMBL2283181
94 test	7.6800	7.5174	-0.1626	CHEMBL1669033
95 train	7.1100	7.5737	0.4637	CHEMBL1669035

96 train	8.1000	6.4968	-1.6032	CHEMBL4084676
97 train	4.5000	5.7385	1.2385	CHEMBL179204
98 train	4.5000	5.7041	1.2041	CHEMBL2283168
99 train	7.5200	6.1683	-1.3517	CHEMBL2283154
100 train	5.7200	5.5090	-0.2110	CHEMBL1221677
101 test	6.9200	6.9689	0.0489	CHEMBL122
102 train	6.4000	6.1865	-0.2135	CHEMBL3127308
103 test	5.1000	5.8428	0.7428	CHEMBL1089958
104 train	5.0100	5.4758	0.4658	CHEMBL1939434
105 train	5.1200	5.3172	0.1972	CHEMBL1939435
106 train	6.2000	6.1871	-0.0129	CHEMBL2283150
107 train	6.7100	6.2163	-0.4937	CHEMBL4780951
108 train	5.7000	4.9609	-0.7391	CHEMBL266858
109 train	5.6800	5.3385	-0.3415	CHEMBL141113
110 train	8.0000	7.1739	-0.8261	CHEMBL148153
111 train	8.1000	6.9271	-1.1729	CHEMBL29839
112 train	6.8000	6.1000	-0.7000	CHEMBL400080
113 train	6.7200	7.0286	0.3086	CHEMBL118
114 train	4.8300	6.2933	1.4633	CHEMBL213267
115 test	5.6900	5.8958	0.2058	CHEMBL17161
116 test	6.5400	7.0286	0.4886	CHEMBL118
117 train	4.5000	6.0948	1.5948	CHEMBL1632406
118 test	6.9600	6.7546	-0.2054	CHEMBL19056
119 train	7.3700	6.8932	-0.4768	CHEMBL1288617
120 train	4.7300	7.4032	2.6732	CHEMBL1290434
121 test	7.8500	6.0048	-1.8452	CHEMBL104009
122 train	6.4700	7.8062	1.3362	CHEMBL52889
123 test	6.0000	5.7630	-0.2370	CHEMBL95479
124 train	4.4600	5.7109	1.2509	CHEMBL341298
125 train	7.4000	6.5008	-0.8992	CHEMBL330194
126 train	6.0200	5.7840	-0.2360	CHEMBL49011
127 test	4.2100	5.7885	1.5785	CHEMBL376583
128 test	6.3900	6.2304	-0.1596	CHEMBL6
129 test	7.0000	5.5035	-1.4965	CHEMBL521
130 train	6.5500	7.0286	0.4786	CHEMBL118
131 train	6.5100	5.5740	-0.9360	CHEMBL1242554
132 train	5.9200	5.8393	-0.0807	CHEMBL3265351
133 train	5.3600	5.4520	0.0920	CHEMBL3265355
134 train	5.1900	5.3691	0.1791	CHEMBL1242364
135 train	4.6000	6.0436	1.4436	CHEMBL1242459
136 train	4.2400	6.2868	2.0468	CHEMBL3265346
137 train	4.3200	5.3619	1.0419	CHEMBL224401
138 train	7.0500	5.4626	-1.5874	CHEMBL224400
139 test	4.8500	5.5838	0.7338	CHEMBL376143
140 train	6.0300	5.7157	-0.3143	CHEMBL1631308
141 train	4.3800	5.8499	1.4699	CHEMBL340717
142 train	4.7000	5.3141	0.6141	CHEMBL25
143 test	6.3200	6.3077	-0.0123	CHEMBL257103
144 test	6.3000	6.5189	0.2189	CHEMBL278231

145	train	7.4600	7.0286	-0.4314	CHEMBL118
146	train	6.0000	7.0286	1.0286	CHEMBL118
147	train	4.5600	5.5608	1.0008	CHEMBL2315854
148	test	5.6000	6.3455	0.7455	CHEMBL95659
149	train	6.8000	6.8327	0.0327	CHEMBL274893
150	test	6.4700	6.2644	-0.2056	CHEMBL300021
151	test	5.9800	5.8646	-0.1154	CHEMBL300687
152	train	6.7700	6.6925	-0.0775	CHEMBL126303
153	train	7.6400	6.9301	-0.7099	CHEMBL420628
154	test	5.3300	5.3195	-0.0105	CHEMBL2333755
155	train	5.1800	5.5357	0.3557	CHEMBL2333753
156	test	5.2400	6.0578	0.8178	CHEMBL323277
157	train	7.1000	7.3267	0.2267	CHEMBL295032
158	train	6.1200	6.4009	0.2809	CHEMBL29204
159	train	5.3400	5.7563	0.4163	CHEMBL568715
160	test	5.4600	6.0602	0.6002	CHEMBL568719
161	train	6.0500	5.7563	-0.2937	CHEMBL568723
162	train	5.6200	5.3141	-0.3059	CHEMBL25
163	train	5.3800	5.9591	0.5791	CHEMBL4799227
164	train	6.9200	7.0286	0.1086	CHEMBL118
165	train	6.9200	6.3920	-0.5280	CHEMBL4455511
166	train	6.6000	6.2847	-0.3153	CHEMBL273340
167	train	5.3300	6.3203	0.9903	CHEMBL2160146
168	train	7.3300	6.4937	-0.8363	CHEMBL4867950
169	train	7.8500	6.8835	-0.9665	CHEMBL282924
170	train	4.6800	6.6153	1.9353	CHEMBL268470
171	train	5.6600	5.1894	-0.4706	CHEMBL503071
172	train	5.2400	6.2304	0.9904	CHEMBL6
173	train	5.0700	4.8568	-0.2132	CHEMBL3400659
174	train	4.6700	5.4427	0.7727	CHEMBL2315016
175	test	5.9700	5.8988	-0.0712	CHEMBL3402597
176	train	6.4200	6.3862	-0.0338	CHEMBL18040
177	train	4.7100	4.9829	0.2729	CHEMBL517149
178	train	4.3300	4.8086	0.4786	CHEMBL465194
179	test	6.5700	5.7505	-0.8195	CHEMBL106255
180	train	6.0000	5.7505	-0.2495	CHEMBL106255
181	train	9.3500	6.9360	-2.4140	CHEMBL282093
182	train	4.7100	4.8644	0.1544	CHEMBL291501
183	test	4.7500	4.6092	-0.1408	CHEMBL471103
184	train	6.0900	4.2393	-1.8507	CHEMBL490482
185	train	4.6700	5.0488	0.3788	CHEMBL473518
186	train	7.2400	6.9689	-0.2711	CHEMBL122
187	train	8.4800	8.5008	0.0208	CHEMBL92107
188	train	8.7000	8.2542	-0.4458	CHEMBL329999
189	train	8.0500	6.5794	-1.4706	CHEMBL283178
190	train	8.5200	8.4766	-0.0434	CHEMBL54327
191	train	8.0000	7.8829	-0.1171	CHEMBL52760
192	train	7.5700	6.6570	-0.9130	CHEMBL89625
193	train	5.0100	5.7653	0.7553	CHEMBL69261

194 train	6.2200	6.7110	0.4910	CHEMBL51434
195 test	8.3300	6.5112	-1.8188	CHEMBL28881
196 train	6.3700	6.4797	0.1097	CHEMBL320926
197 train	6.8900	6.0514	-0.8386	CHEMBL42225
198 train	5.3000	5.4322	0.1322	CHEMBL145727
199 train	5.9200	6.2521	0.3321	CHEMBL596888
200 train	4.1100	5.2172	1.1072	CHEMBL1163237
201 test	6.2900	6.4872	0.1972	CHEMBL43957
202 train	6.0400	5.5663	-0.4737	CHEMBL1081855
203 train	5.5700	6.0087	0.4387	CHEMBL1081856
204 test	5.8000	5.7622	-0.0378	CHEMBL1079875
205 train	6.8000	5.8648	-0.9352	CHEMBL1079876
206 test	5.5700	6.1559	0.5859	CHEMBL1079877
207 test	6.1400	6.3819	0.2419	CHEMBL1078090
208 test	4.9200	6.5526	1.6326	CHEMBL1078376
209 train	5.8900	5.2071	-0.6829	CHEMBL5202074
210 train	7.1600	6.7040	-0.4560	CHEMBL347720
211 train	6.5200	5.8517	-0.6683	CHEMBL15039
212 train	6.1200	6.9689	0.8489	CHEMBL122
213 train	5.4000	6.4581	1.0581	CHEMBL100250
214 test	5.4700	5.6307	0.1607	CHEMBL122890
215 test	5.5400	5.3097	-0.2303	CHEMBL409627
216 train	6.8500	6.1191	-0.7309	CHEMBL276052
217 train	5.6800	6.2509	0.5709	CHEMBL2283165
218 train	6.8100	6.9311	0.1211	CHEMBL1814813
219 train	6.4700	6.9010	0.4310	CHEMBL287447
220 train	8.8200	8.5368	-0.2832	CHEMBL92102
221 train	5.6200	6.2761	0.6561	CHEMBL346697
222 test	8.0500	7.0628	-0.9872	CHEMBL118064
223 test	6.6200	6.6664	0.0464	CHEMBL298296
224 train	7.5200	6.2001	-1.3199	CHEMBL331278
225 test	8.7000	7.7143	-0.9857	CHEMBL111562
226 train	7.7700	7.1322	-0.6378	CHEMBL361472
227 train	5.6000	6.2668	0.6668	CHEMBL365033
228 train	5.3200	6.4003	1.0803	CHEMBL284914
229 test	7.4000	7.0286	-0.3714	CHEMBL118
230 train	4.3400	5.8274	1.4874	CHEMBL29075
231 train	4.7800	5.4444	0.6644	CHEMBL236433
232 train	6.5800	7.1772	0.5972	CHEMBL361494
233 train	5.7600	5.1248	-0.6352	CHEMBL482162
234 train	7.2200	6.1389	-1.0811	CHEMBL44244
235 train	6.9600	6.3547	-0.6053	CHEMBL109017
236 train	7.6800	8.3098	0.6298	CHEMBL300597
237 train	8.5200	8.6539	0.1339	CHEMBL558340
238 test	6.7500	6.0462	-0.7038	CHEMBL5279631
239 train	6.0400	6.0514	0.0114	CHEMBL5272130
240 train	7.0000	5.8149	-1.1851	CHEMBL5278506
241 train	6.4400	6.8200	0.3800	CHEMBL52454
242 test	7.6400	8.4807	0.8407	CHEMBL300601

243	test	5.3400	4.9517	-0.3883	CHEMBL270060
244	test	4.1400	4.6652	0.5252	CHEMBL464610
245	train	6.8200	6.6489	-0.1711	CHEMBL95572
246	train	5.2400	5.3195	0.0795	CHEMBL2333737
247	train	6.7700	6.4350	-0.3350	CHEMBL24874
248	train	7.8500	6.1132	-1.7368	CHEMBL42485
249	train	5.8200	6.7780	0.9580	CHEMBL94274
250	train	5.2500	6.2686	1.0186	CHEMBL3309824
251	train	5.6400	6.2564	0.6164	CHEMBL1689431
252	train	5.1700	5.4187	0.2487	CHEMBL2334136
253	test	7.0000	6.2628	-0.7372	CHEMBL374427
254	test	5.7000	6.4407	0.7407	CHEMBL1682231
255	train	7.4000	6.8024	-0.5976	CHEMBL107088
256	train	7.7000	7.1072	-0.5928	CHEMBL290192
257	train	6.5000	6.0376	-0.4624	CHEMBL104147
258	train	8.2200	6.5156	-1.7044	CHEMBL1288592
259	train	4.9100	5.6118	0.7018	CHEMBL386992
260	train	4.9100	5.2494	0.3394	CHEMBL1275941
261	train	6.9600	7.0286	0.0686	CHEMBL118
262	train	4.3900	5.8713	1.4813	CHEMBL274271
263	test	4.4500	5.8493	1.3993	CHEMBL129861
264	train	7.1000	5.9219	-1.1781	CHEMBL319306
265	train	7.5200	6.4185	-1.1015	CHEMBL229955
266	train	6.5000	6.0200	-0.4800	CHEMBL2283160
267	test	4.4400	5.6414	1.2014	CHEMBL407035
268	train	5.7000	5.6642	-0.0358	CHEMBL361848
269	train	5.4400	5.7041	0.2641	CHEMBL2283167
270	test	5.6200	6.9301	1.3101	CHEMBL420628
271	train	6.1700	6.2304	0.0604	CHEMBL6
272	train	4.5400	6.6047	2.0647	CHEMBL1630233
273	test	5.5900	6.1559	0.5659	CHEMBL1078091
274	train	5.0900	6.4018	1.3118	CHEMBL1078557
275	train	7.5200	6.2063	-1.3137	CHEMBL362093
276	train	6.4200	5.9360	-0.4840	CHEMBL183101
277	train	6.0300	6.0464	0.0164	CHEMBL184764
278	train	9.3600	7.3431	-2.0169	CHEMBL186632
279	train	4.0700	5.6796	1.6096	CHEMBL169
280	test	8.0500	8.1121	0.0621	CHEMBL111095
281	train	5.0800	6.4368	1.3568	CHEMBL45383
282	train	8.4000	7.5898	-0.8102	CHEMBL296384
283	train	8.7000	9.0577	0.3577	CHEMBL315585
284	train	8.4000	7.9414	-0.4586	CHEMBL90447
285	train	6.1400	6.5064	0.3664	CHEMBL327078
286	train	8.3000	8.3198	0.0198	CHEMBL443791
287	test	8.4000	7.5898	-0.8102	CHEMBL296384
288	train	4.4000	5.7109	1.3109	CHEMBL126418
289	train	6.5700	6.6271	0.0571	CHEMBL161590
290	test	7.5400	6.5961	-0.9439	CHEMBL287919
291	train	6.8400	6.3005	-0.5395	CHEMBL324957

292 test	5.9200	6.2304	0.3104	CHEMBL6
293 train	4.1900	6.6628	2.4728	CHEMBL129215
294 train	5.2400	6.4770	1.2370	CHEMBL289484
295 train	7.8000	6.5112	-1.2888	CHEMBL29439
296 test	7.1300	7.6609	0.5309	CHEMBL324275
297 train	5.4600	6.1662	0.7062	CHEMBL358372
298 train	6.7700	6.4842	-0.2858	CHEMBL296447
299 train	4.7000	5.4322	0.7322	CHEMBL144232
300 test	6.9200	6.1389	-0.7811	CHEMBL42409
301 train	6.3600	6.2582	-0.1018	CHEMBL108961
302 train	6.1700	6.9789	0.8089	CHEMBL127190
303 test	6.1900	5.7028	-0.4872	CHEMBL24429
304 test	7.2300	7.1396	-0.0904	CHEMBL3355608
305 train	5.5000	5.0844	-0.4156	CHEMBL16272
306 train	5.4000	5.2077	-0.1923	CHEMBL149335
307 test	5.5000	6.2170	0.7170	CHEMBL3427203
308 train	6.3600	5.6822	-0.6778	CHEMBL65793
309 train	7.1000	6.1549	-0.9451	CHEMBL107706
310 train	6.9200	6.0729	-0.8471	CHEMBL110822
311 train	6.4600	6.3891	-0.0709	CHEMBL108857
312 train	7.7000	6.9689	-0.7311	CHEMBL122
313 train	4.8200	4.9996	0.1796	CHEMBL279166
314 train	5.1600	5.8712	0.7112	CHEMBL357380
315 test	6.0200	6.3380	0.3180	CHEMBL295752
316 train	6.8700	8.3832	1.5132	CHEMBL89263
317 test	8.8200	8.7434	-0.0766	CHEMBL312822
318 train	6.3200	7.3414	1.0214	CHEMBL18264
319 train	7.6800	7.4781	-0.2019	CHEMBL405623
320 test	7.8200	6.9399	-0.8801	CHEMBL282085
321 train	4.8700	6.5276	1.6576	CHEMBL338097
322 train	6.7500	5.5897	-1.1603	CHEMBL347198
323 train	7.0500	7.1640	0.1140	CHEMBL290945
324 test	6.6600	7.1237	0.4637	CHEMBL111039
325 train	6.4000	6.3037	-0.0963	CHEMBL443278
326 train	5.8800	6.4766	0.5966	CHEMBL95021
327 train	8.2200	7.6718	-0.5482	CHEMBL363574
328 train	7.4900	7.4113	-0.0787	CHEMBL365603
329 train	6.2400	6.7680	0.5280	CHEMBL865
330 train	6.9600	6.4305	-0.5295	CHEMBL44516
331 train	6.1800	5.1772	-1.0028	CHEMBL70158
332 train	7.7000	6.7917	-0.9083	CHEMBL289561
333 test	7.8900	6.8104	-1.0796	CHEMBL155927
334 train	5.8100	6.1575	0.3475	CHEMBL71455
335 train	6.2900	6.2971	0.0071	CHEMBL71372
336 train	5.5400	5.5205	-0.0195	CHEMBL155781
337 train	6.2400	6.4710	0.2310	CHEMBL183294
338 train	4.8400	6.1953	1.3553	CHEMBL27733
339 train	5.1900	5.8855	0.6955	CHEMBL388756
340 test	7.2100	7.9414	0.7314	CHEMBL327900

341 train	6.1600	6.4881	0.3281	CHEMBL516680
342 train	6.9200	7.0286	0.1086	CHEMBL118
343 train	7.3000	5.9907	-1.3093	CHEMBL274990
344 train	7.0000	6.7141	-0.2859	CHEMBL7162
345 test	7.5200	7.0009	-0.5191	CHEMBL296662
346 train	6.9200	6.4275	-0.4925	CHEMBL95469
347 train	4.2700	5.2466	0.9766	CHEMBL1163243
348 train	5.4700	6.5584	1.0884	CHEMBL126244
349 train	8.5200	7.9890	-0.5310	CHEMBL185547
350 train	5.8300	6.6325	0.8025	CHEMBL158421
351 train	4.2000	6.4881	2.2881	CHEMBL29492
352 train	7.8900	8.5551	0.6651	CHEMBL418448
353 train	4.8400	6.1953	1.3553	CHEMBL27733
354 train	5.6400	6.5695	0.9295	CHEMBL159206
355 test	6.5200	5.7578	-0.7622	CHEMBL3113235
356 train	7.9000	5.6513	-2.2487	CHEMBL5283932
357 train	7.2500	6.5233	-0.7267	CHEMBL29533
358 train	6.5000	6.3862	-0.1138	CHEMBL18790
359 train	7.1600	6.7413	-0.4187	CHEMBL28599
360 test	8.0000	8.3455	0.3455	CHEMBL88550
361 train	4.0600	6.1003	2.0403	CHEMBL339221
362 train	8.0500	7.2143	-0.8357	CHEMBL97874
363 train	6.3600	5.7509	-0.6091	CHEMBL276976
364 test	6.0900	5.8820	-0.2080	CHEMBL222482
365 train	6.3500	5.7509	-0.5991	CHEMBL276976
366 train	7.4000	7.1769	-0.2231	CHEMBL289653
367 train	6.8500	6.7481	-0.1019	CHEMBL273815
368 train	6.3700	6.9689	0.5989	CHEMBL122
369 test	5.3000	5.2821	-0.0179	CHEMBL800
370 test	5.4000	6.3016	0.9016	CHEMBL91923
371 train	6.1400	5.2358	-0.9042	CHEMBL432782
372 train	6.5200	5.8790	-0.6410	CHEMBL158310
373 train	6.2700	7.0286	0.7586	CHEMBL118
374 train	4.4200	5.2372	0.8172	CHEMBL3289927
375 train	4.7100	5.1320	0.4220	CHEMBL3289931
376 test	4.8300	5.2286	0.3986	CHEMBL3289941
377 train	5.4900	6.2304	0.7404	CHEMBL6
378 test	5.7100	6.0915	0.3815	CHEMBL3309823
379 test	6.1700	6.9689	0.7989	CHEMBL122
380 test	7.4700	7.0026	-0.4674	CHEMBL524662
381 test	6.4000	6.2677	-0.1323	CHEMBL319825
382 train	6.0000	5.9922	-0.0078	CHEMBL153767
383 train	6.1600	5.8790	-0.2810	CHEMBL154480
384 train	4.7500	6.3361	1.5861	CHEMBL571852
385 train	5.3000	6.5800	1.2800	CHEMBL98903
386 train	6.1400	5.9527	-0.1873	CHEMBL282185
387 train	7.8900	7.9366	0.0466	CHEMBL118081
388 train	5.4100	6.1389	0.7289	CHEMBL44101
389 train	7.5200	6.6457	-0.8743	CHEMBL44152

390	train	5.1800	7.2009	2.0209	CHEMBL109486
391	test	8.2200	8.1200	-0.1000	CHEMBL52872
392	train	8.4000	7.1758	-1.2242	CHEMBL324509
393	test	6.2100	5.8780	-0.3320	CHEMBL156256
394	train	5.8200	5.7245	-0.0955	CHEMBL107600
395	train	6.5500	6.4842	-0.0658	CHEMBL296447
396	train	7.6800	7.2978	-0.3822	CHEMBL282839
397	train	6.1400	6.8427	0.7027	CHEMBL43331
398	train	6.4600	6.0259	-0.4341	CHEMBL416989
399	train	7.7200	8.1202	0.4002	CHEMBL52019
400	train	4.1900	5.7086	1.5186	CHEMBL497678
401	train	4.5200	5.7152	1.1952	CHEMBL355771
402	train	6.1900	6.3158	0.1258	CHEMBL319766
403	train	7.3000	6.4054	-0.8946	CHEMBL97179
404	train	5.9800	6.1099	0.1299	CHEMBL295068
405	train	8.0000	7.6605	-0.3395	CHEMBL111597
406	train	7.0000	6.0525	-0.9475	CHEMBL99933
407	train	8.9200	6.2200	-2.7000	CHEMBL91118
408	test	8.1500	6.3478	-1.8022	CHEMBL115752
409	test	7.7000	7.6539	-0.0461	CHEMBL117947
410	test	7.7200	7.4496	-0.2704	CHEMBL54039
411	train	8.2800	6.9567	-1.3233	CHEMBL280636
412	train	8.3000	7.5418	-0.7582	CHEMBL109623
413	train	6.1900	6.8994	0.7094	CHEMBL283388
414	train	5.5800	6.5516	0.9716	CHEMBL183977
415	train	5.9200	7.0286	1.1086	CHEMBL118
416	train	4.9300	5.0080	0.0780	CHEMBL1916948
417	train	5.0600	5.5870	0.5270	CHEMBL1916961
418	train	5.5800	5.3733	-0.2067	CHEMBL1916967
419	train	5.7000	5.4974	-0.2026	CHEMBL589812
420	test	5.8200	5.6495	-0.1705	CHEMBL70921
421	test	6.8500	5.8840	-0.9660	CHEMBL69998
422	train	7.1700	6.2903	-0.8797	CHEMBL94939
423	test	4.8400	4.9600	0.1200	CHEMBL1275921
424	train	6.6400	6.6607	0.0207	CHEMBL415895
425	test	4.7000	6.5285	1.8285	CHEMBL489899
426	train	6.4800	5.6605	-0.8195	CHEMBL157950
427	train	6.1700	6.9789	0.8089	CHEMBL127190
428	train	7.8200	7.1931	-0.6269	CHEMBL89578
429	train	6.2800	6.0100	-0.2700	CHEMBL109143
430	train	6.1900	6.4022	0.2122	CHEMBL157886
431	test	6.2200	5.8790	-0.3410	CHEMBL157720
432	train	6.4300	6.3460	-0.0840	CHEMBL155206
433	test	6.9600	6.4350	-0.5250	CHEMBL285828
434	train	6.3400	6.9474	0.6074	CHEMBL273420
435	train	8.0500	7.4535	-0.5965	CHEMBL328009
436	train	7.7500	7.6145	-0.1355	CHEMBL17075
437	train	6.9600	6.8555	-0.1045	CHEMBL16850
438	train	6.5700	5.3449	-1.2251	CHEMBL1917099

439	train	6.3000	5.7993	-0.5007	CHEMBL1917102
440	train	4.9500	6.4768	1.5268	CHEMBL743
441	train	6.7700	6.4350	-0.3350	CHEMBL279265
442	train	4.3500	6.0142	1.6642	CHEMBL1086757
443	test	4.0200	6.2249	2.2049	CHEMBL1076751
444	train	5.0800	5.4719	0.3919	CHEMBL2063855
445	train	6.0000	6.8453	0.8453	CHEMBL43461
446	train	5.5800	5.6580	0.0780	CHEMBL357262
447	test	6.0100	4.9912	-1.0188	CHEMBL356596
448	train	5.8700	5.5035	-0.3665	CHEMBL521
449	train	6.9400	6.1265	-0.8135	CHEMBL561888
450	train	8.1000	7.6911	-0.4089	CHEMBL551829
451	test	7.4000	7.0286	-0.3714	CHEMBL118
452	test	6.5700	6.4350	-0.1350	CHEMBL281847
453	train	9.2700	7.3560	-1.9140	CHEMBL500674
454	test	8.2900	6.3043	-1.9857	CHEMBL499347
455	train	10.7000	7.8567	-2.8433	CHEMBL525247
456	train	8.0000	6.7759	-1.2241	CHEMBL525020
457	train	8.8400	7.8790	-0.9610	CHEMBL502556
458	test	6.0000	6.2589	0.2589	CHEMBL49114
459	train	7.1200	7.0289	-0.0911	CHEMBL321182
460	train	4.2900	6.2438	1.9538	CHEMBL148691
461	train	4.1900	5.7109	1.5209	CHEMBL419777
462	train	4.6300	5.5062	0.8762	CHEMBL139
463	test	5.0300	6.0204	0.9904	CHEMBL1629743
464	train	6.1000	6.2757	0.1757	CHEMBL70588
465	test	7.6800	7.2102	-0.4698	CHEMBL411894
466	train	6.3400	6.9474	0.6074	CHEMBL273420
467	train	7.7000	7.2233	-0.4767	CHEMBL329919
468	test	7.1600	6.7419	-0.4181	CHEMBL1630230
469	train	6.2800	6.7777	0.4977	CHEMBL16797
470	train	6.5200	6.3402	-0.1798	CHEMBL96057
471	train	7.5200	7.5097	-0.0103	CHEMBL322949
472	train	8.0500	8.1121	0.0621	CHEMBL111095
473	train	7.4000	6.9969	-0.4031	CHEMBL316455
474	train	8.0500	7.4535	-0.5965	CHEMBL328009
475	test	7.8900	7.4644	-0.4256	CHEMBL319512
476	train	7.5200	6.9047	-0.6153	CHEMBL100422
477	train	5.0000	6.2094	1.2094	CHEMBL166156
478	train	6.0000	6.4424	0.4424	CHEMBL347705
479	train	7.2700	7.0286	-0.2414	CHEMBL118
480	test	8.0000	6.9230	-1.0770	CHEMBL144728
481	train	6.0000	7.1385	1.1385	CHEMBL37371
482	train	4.1800	5.6922	1.5122	CHEMBL146920
483	train	6.6800	6.6972	0.0172	CHEMBL279249
484	train	7.2200	6.1132	-1.1068	CHEMBL42485
485	train	5.4000	5.8278	0.4278	CHEMBL149134
486	train	5.3300	5.4631	0.1331	CHEMBL305505
487	test	7.5100	6.9010	-0.6090	CHEMBL27975

488	train	6.3000	6.3037	0.0037	CHEMBL111904
489	test	6.0700	6.8250	0.7550	CHEMBL28801
490	test	4.5800	4.8854	0.3054	CHEMBL277515
491	train	7.4400	7.0286	-0.4114	CHEMBL118
492	test	6.3600	6.2582	-0.1018	CHEMBL108961
493	train	6.0800	6.9428	0.8628	CHEMBL282838
494	train	8.2200	7.1108	-1.1092	CHEMBL52402
495	train	7.3000	5.8790	-1.4210	CHEMBL440001
496	train	6.5200	6.9689	0.4489	CHEMBL122
497	train	6.3200	6.9414	0.6214	CHEMBL289262
498	train	6.2600	6.0499	-0.2101	CHEMBL320273
499	train	5.1900	4.9909	-0.1991	CHEMBL3099221
500	train	7.3000	6.6202	-0.6798	CHEMBL151042
501	test	7.5800	5.1365	-2.4435	CHEMBL571
502	train	7.1600	7.0286	-0.1314	CHEMBL118
503	test	4.9600	6.5166	1.5566	CHEMBL101503
504	train	6.4800	5.6794	-0.8006	CHEMBL107938
505	test	8.3000	7.0769	-1.2231	CHEMBL76692
506	train	6.1700	6.3426	0.1726	CHEMBL323267
507	train	6.8500	6.7675	-0.0825	CHEMBL41405
508	train	8.0000	6.6266	-1.3734	CHEMBL1288533
509	train	8.1500	6.7091	-1.4409	CHEMBL1630251
510	test	6.1600	5.9219	-0.2381	CHEMBL319072
511	train	8.0000	6.7139	-1.2861	CHEMBL45192
512	test	6.3400	6.6061	0.2661	CHEMBL43089
513	train	7.2400	7.0286	-0.2114	CHEMBL118
514	train	7.1000	6.0658	-1.0342	CHEMBL350039
515	train	7.7000	5.8880	-1.8120	CHEMBL76376
516	train	6.3700	6.4797	0.1097	CHEMBL320926
517	train	8.2200	8.5463	0.3263	CHEMBL57837
518	train	7.8200	5.9219	-1.8981	CHEMBL328837
519	test	6.4900	6.4368	-0.0532	CHEMBL43933
520	test	7.2900	7.5054	0.2154	CHEMBL111657
521	train	4.2400	6.7594	2.5194	CHEMBL170780
522	test	6.1900	5.6101	-0.5799	CHEMBL496
523	train	6.0700	6.1461	0.0761	CHEMBL295640
524	train	6.1800	6.7934	0.6134	CHEMBL289447
525	train	5.0200	5.0101	-0.0099	CHEMBL3264687
526	train	4.1900	5.7992	1.6092	CHEMBL283425
527	train	6.3000	5.1042	-1.1958	CHEMBL3265358
528	train	7.3700	6.5245	-0.8455	CHEMBL3355603
529	train	5.1200	4.5665	-0.5535	CHEMBL1173685
530	train	5.8300	6.6266	0.7966	CHEMBL1630234
531	train	5.7000	6.9206	1.2206	CHEMBL1630238
532	test	4.6700	6.7091	2.0391	CHEMBL1630243
533	test	4.2100	4.9918	0.7818	CHEMBL5430086
534	test	5.2000	5.6922	0.4922	CHEMBL343865
535	train	9.6000	7.6911	-1.9089	CHEMBL551829
536	train	6.4700	7.0286	0.5586	CHEMBL118

537 train	6.5800	6.9689	0.3889	CHEMBL122
538 train	7.6400	6.3285	-1.3115	CHEMBL558230
539 train	6.6800	6.2206	-0.4594	CHEMBL70478
540 test	6.9200	6.9984	0.0784	CHEMBL283038
541 test	5.0800	6.6630	1.5830	CHEMBL285831
542 train	5.2800	6.3014	1.0214	CHEMBL73997
543 train	7.0000	6.5024	-0.4976	CHEMBL24957
544 train	6.5500	5.8824	-0.6676	CHEMBL2283148
545 train	6.9600	6.7698	-0.1902	CHEMBL2283180
546 train	7.5200	7.7397	0.2197	CHEMBL2283175
547 train	7.1800	8.0107	0.8307	CHEMBL1669039
548 train	4.4400	5.5280	1.0880	CHEMBL1814716
549 train	8.2900	7.5994	-0.6906	CHEMBL271932
550 train	6.5200	6.9041	0.3841	CHEMBL259678
551 train	6.8400	7.0658	0.2258	CHEMBL408216
552 train	7.6200	7.5270	-0.0930	CHEMBL408788
553 train	7.9600	7.7020	-0.2580	CHEMBL270305
554 train	6.6700	7.0570	0.3870	CHEMBL403827
555 train	6.2000	6.5222	0.3222	CHEMBL257300
556 test	5.7200	7.1615	1.4415	CHEMBL259469
557 test	6.1400	6.5934	0.4534	CHEMBL257491
558 train	6.0900	6.1615	0.0715	CHEMBL408897
559 train	4.0000	5.0113	1.0113	CHEMBL464006
560 train	7.5700	5.5333	-2.0367	CHEMBL414883
561 train	7.8000	6.6958	-1.1042	CHEMBL148708
562 train	7.1700	7.0286	-0.1414	CHEMBL118
563 test	9.5500	7.4437	-2.1063	CHEMBL551148
564 train	5.8200	6.3020	0.4820	CHEMBL286490
565 test	4.7100	6.4231	1.7131	CHEMBL35685
566 train	5.9200	7.0286	1.1086	CHEMBL118
567 test	6.5000	6.4350	-0.0650	CHEMBL25371
568 train	6.9600	6.5943	-0.3657	CHEMBL24798
569 test	7.5500	6.0286	-1.5214	CHEMBL407109
570 train	7.1900	6.2734	-0.9166	CHEMBL369492
571 test	6.3600	6.3455	-0.0145	CHEMBL26509
572 train	7.0300	7.1080	0.0780	CHEMBL271103
573 train	8.0100	6.7104	-1.2996	CHEMBL271104
574 train	7.3200	7.4339	0.1139	CHEMBL270510
575 train	8.3900	6.6760	-1.7140	CHEMBL270294
576 train	6.2800	6.1826	-0.0974	CHEMBL271312
577 train	7.5400	6.4906	-1.0494	CHEMBL270730
578 train	5.8300	5.9350	0.1050	CHEMBL270111
579 train	6.5300	6.4200	-0.1100	CHEMBL271763
580 train	7.3300	7.0434	-0.2866	CHEMBL272627
581 train	7.4300	8.0917	0.6617	CHEMBL257108
582 test	7.3100	7.5270	0.2170	CHEMBL269832
583 test	8.9200	7.0658	-1.8542	CHEMBL272433
584 test	7.9300	6.6240	-1.3060	CHEMBL269818
585 train	5.2400	6.9442	1.7042	CHEMBL272605

586 train	5.8900	5.0825	-0.8075	CHEMBL3331343
587 test	5.3300	5.4631	0.1331	CHEMBL305505
588 test	4.1000	4.9829	0.8829	CHEMBL480462
589 train	8.8400	7.8790	-0.9610	CHEMBL502556
590 test	4.3500	5.7086	1.3586	CHEMBL498529
591 train	5.7700	6.6977	0.9277	CHEMBL3290202
592 train	9.8500	6.2304	-3.6196	CHEMBL6
593 train	6.8400	6.6697	-0.1703	CHEMBL524304
594 train	6.8400	6.6697	-0.1703	CHEMBL524304
595 train	5.6200	5.0630	-0.5570	CHEMBL3087872
596 train	5.5600	5.2257	-0.3343	CHEMBL3087873
597 train	5.5700	5.1552	-0.4148	CHEMBL3087875
598 test	5.4000	7.2798	1.8798	CHEMBL410524
599 train	6.5400	6.9689	0.4289	CHEMBL122
600 train	5.7200	6.5880	0.8680	CHEMBL406528
601 test	6.6800	6.9689	0.2889	CHEMBL122
602 train	6.5300	6.3616	-0.1684	CHEMBL273118
603 train	5.5500	6.9125	1.3625	CHEMBL409468
604 train	5.4800	6.5880	1.1080	CHEMBL406528
605 test	7.2900	7.2404	-0.0496	CHEMBL408215
606 train	7.4700	7.4580	-0.0120	CHEMBL257677
607 train	7.6500	7.4592	-0.1908	CHEMBL257678
608 test	7.3500	8.0538	0.7038	CHEMBL257299
609 train	7.0400	7.5270	0.4870	CHEMBL272239
610 train	7.1100	6.8785	-0.2315	CHEMBL405841
611 train	6.2000	6.5222	0.3222	CHEMBL257300
612 train	5.0500	4.7124	-0.3376	CHEMBL1173450
613 train	4.8200	4.7284	-0.0916	CHEMBL517334
614 test	8.6000	8.4042	-0.1958	CHEMBL88549
615 train	4.4100	5.8967	1.4867	CHEMBL96842
616 train	5.5500	6.1397	0.5897	CHEMBL110145
617 train	7.4200	7.2925	-0.1275	CHEMBL17101
618 train	6.0000	7.0286	1.0286	CHEMBL118
619 test	6.3300	6.1172	-0.2128	CHEMBL421417
620 train	8.4000	8.2145	-0.1855	CHEMBL54370
621 train	7.3100	6.6669	-0.6431	CHEMBL282301
622 train	6.7000	6.5225	-0.1775	CHEMBL285335
623 test	4.4700	5.7883	1.3183	CHEMBL144658
624 train	5.7000	5.2494	-0.4506	CHEMBL19286
625 test	6.8100	7.4259	0.6159	CHEMBL117862
626 train	7.3000	6.5553	-0.7447	CHEMBL277115
627 train	5.9600	6.1987	0.2387	CHEMBL237208
628 test	5.2400	6.2442	1.0042	CHEMBL237400
629 test	5.3900	6.0440	0.6540	CHEMBL237399
630 train	5.4600	5.4667	0.0067	CHEMBL237204
631 test	7.1000	6.5658	-0.5342	CHEMBL42085
632 train	7.8500	6.5919	-1.2581	CHEMBL4465808
633 train	7.8500	6.5245	-1.3255	CHEMBL418859
634 test	5.0500	6.8410	1.7910	CHEMBL491477

635 train	6.3600	6.0296	-0.3304	CHEMBL108452
636 train	8.6600	7.0286	-1.6314	CHEMBL118
637 test	5.0100	6.2515	1.2416	CHEMBL127267
638 train	5.6000	5.7826	0.1826	CHEMBL2171253
639 train	8.3000	6.7680	-1.5320	CHEMBL865
640 train	5.3000	5.3905	0.0905	CHEMBL151658
641 train	5.7000	7.0202	1.3202	CHEMBL2283149
642 train	6.9200	6.8555	-0.0645	CHEMBL274473
643 test	7.4000	6.9086	-0.4914	CHEMBL43737
644 train	6.1800	6.4447	0.2647	CHEMBL416250
645 train	9.0000	8.7391	-0.2609	CHEMBL88717
646 test	6.8200	6.7253	-0.0947	CHEMBL42651
647 test	7.7000	6.9163	-0.7837	CHEMBL350422
648 train	5.6200	6.2304	0.6104	CHEMBL6
649 train	6.0500	6.0421	-0.0079	CHEMBL29562
650 train	5.3700	6.2167	0.8467	CHEMBL285975
651 train	6.2400	5.6033	-0.6367	CHEMBL433892
652 test	4.9600	6.7675	1.8075	CHEMBL434014
653 train	7.3300	5.9813	-1.3487	CHEMBL17229
654 train	6.6600	6.9665	0.3065	CHEMBL41739
655 train	7.6200	6.9665	-0.6535	CHEMBL281694
656 test	6.5500	6.5024	-0.0476	CHEMBL27784
657 train	7.2800	6.3222	-0.9578	CHEMBL283633
658 train	6.5400	6.5450	0.0050	CHEMBL29942
659 train	8.1700	6.9271	-1.2429	CHEMBL29583
660 train	7.2500	6.4985	-0.7515	CHEMBL283497
661 train	6.0500	6.5104	0.4604	CHEMBL436494
662 test	6.0400	6.3152	0.2752	CHEMBL373514
663 test	4.5300	6.2304	1.7004	CHEMBL6
664 test	5.6600	6.7141	1.0541	CHEMBL7162
665 train	7.1600	6.9136	-0.2464	CHEMBL290031
666 test	6.5200	7.3760	0.8560	CHEMBL3238415
667 train	5.2300	5.7121	0.4821	CHEMBL3234234
668 train	7.8900	8.5551	0.6651	CHEMBL418448
669 train	6.5500	6.2625	-0.2875	CHEMBL116253
670 train	6.0600	7.0286	0.9686	CHEMBL118
671 test	5.1200	5.1698	0.0498	CHEMBL1171257
672 train	4.8400	5.5711	0.7311	CHEMBL1210073
673 train	6.3000	6.2304	-0.0696	CHEMBL6
674 test	5.5500	6.2837	0.7337	CHEMBL5272219
675 train	5.9600	5.5062	-0.4538	CHEMBL139
676 train	4.5000	5.5533	1.0533	CHEMBL5271448
677 test	7.1600	7.0286	-0.1314	CHEMBL118
678 test	6.7700	5.7784	-0.9916	CHEMBL5287285
679 test	5.7800	6.5768	0.7968	CHEMBL5288533
680 train	5.0000	5.2326	0.2326	CHEMBL5270978
681 train	7.4000	7.0286	-0.3714	CHEMBL118
682 train	7.7500	7.6902	-0.0598	CHEMBL272862
683 test	7.3100	7.5270	0.2170	CHEMBL269832

684 test	7.0400	7.5270	0.4870	CHEMBL272239
685 train	7.9300	6.6240	-1.3060	CHEMBL269818
686 train	6.5200	6.4402	-0.0798	CHEMBL4062140
687 train	5.7400	5.3102	-0.4298	CHEMBL4067108
688 test	5.1800	5.5319	0.3519	CHEMBL4077764
689 train	5.3500	5.4231	0.0731	CHEMBL4064047
690 train	5.8900	6.0203	0.1303	CHEMBL4077191
691 train	5.4500	5.3694	-0.0806	CHEMBL3264694
692 test	5.6200	5.0740	-0.5460	CHEMBL3264699
693 train	5.3000	5.3406	0.0406	CHEMBL3264704
694 train	5.4800	5.8595	0.3795	CHEMBL1210074
695 train	5.6200	5.3141	-0.3059	CHEMBL25
696 train	5.3900	5.4719	0.0819	CHEMBL2063852
697 train	7.6400	6.8489	-0.7911	CHEMBL275601
698 train	5.9600	5.7564	-0.2036	CHEMBL323954
699 train	7.7000	6.9689	-0.7311	CHEMBL122
700 train	5.9700	5.6074	-0.3626	CHEMBL563

Supplementary Table 2: Results of the QSAR model.

S.D.	R ²	RMSE	Q ²
0.8870	0.4469	0.8714	0.4510