Electronic Supplementary Material (ESI) for RSC Advances.

ADDITION INFORMATION FILE A

SCAFFOLD AND CELL LINE BASED APPROACHES FOR QSAR STUDIES ON ANTICANCER AGENTS

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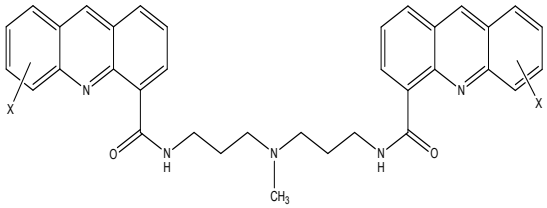
Table. S1. Structure and activity against various cancer cell lines for scaffold 1.

S.No.	Structure	P388	LLc	JLc
				
1	X= H	6.89	7.52	6.96
2	X= 1-Me	6.77	7.85	7.39
3	X= 1-Cl	6.40	7.38	6.90
4	X= 2-Me	6.66	7.17	6.59
5	X= 2-Cl	6.95	8.23	7.34
6	X= 3-Me	5.46	5.62	5.89
7	X= 3-Cl	-	5.53	6.05
8	X= 5-Me	7.64	8.75	7.96
9	X= 5-C_2H_5	6.77	7.57	6.95
10	X= 5-$CHMe_2$	5.56	5.98	5.68
11	X= 5-C_6H_5	5.91	5.97	5.60
12	X= 5-OMe	6.37	6.77	6.46
13	X= 5-F	7.80	7.46	7.31
14	X= 5-Cl	7.34	8.10	7.48
15	X= 5-Br	7.82	8.22	7.62
16	X= 5-CF_3	6.62	7.41	6.94
17	X= 5-NMe_2	5.67	6.17	6.75
18	X= 6-Me	6.46	7.25	6.75

19	X= 6-OMe	7.12	7.70	7.29
20	X= 6-F	7.62	7.70	7.28
21	X= 6-Cl	7.18	7.89	7.29
22	X= 6-Br	7.31	7.75	7.24
23	X= 6-CF_3	5.02	6.80	6.45
24	X= 6-NMe_2	6.12	6.50	6.65
25	X= 7-Me	6.57	7.14	6.56
26	X= 7-C_2H_5	5.97	6.12	5.79
27	X= 7-$CHMe_2$	5.84	5.68	5.68
28	X= 7-CMe_3	5.75	5.85	5.97
29	X= 7-C_6H_5	6.15	6.22	5.99
30	X= 7-OMe	6.88	7.70	6.83
31	X=7-F	6.85	7.50	7.02
32	X= 7-Cl	6.77	7.34	6.87
33	X= 7-Br	6.65	7.46	6.65
34	X= 7-NMe_2	6.01	6.74	6.12
35	X= 8-Me	6.75	7.80	7.15
36	X= 8-Cl	6.13	6.91	6.62
37	X= 5,7-di-Me	6.68	7.70	6.98
38	X= 5,8-di-Me	7.62	8.50	7.96
39	X= 1,5-di-Me	7.68	8.85	8.41
40	X= 5-Me,8-Cl	7.39	8.06	7.70
41	X= 1-Cl, 5-Me	7.32	8.22	7.92

Table S2: Structure and activity against various cancer cell lines for scaffold 2.

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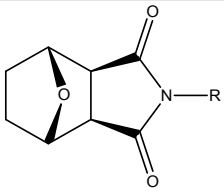
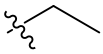
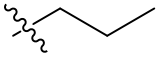
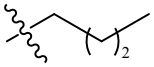
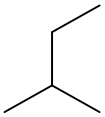
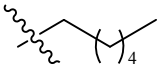
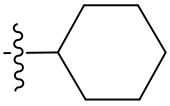
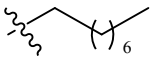
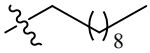
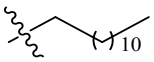
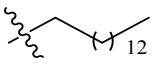
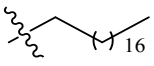
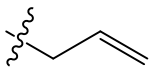
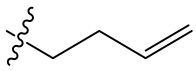
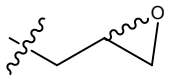
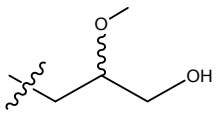
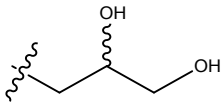
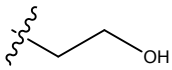
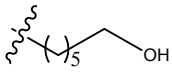
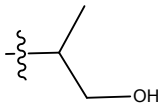
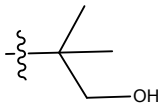
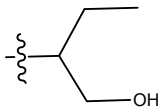
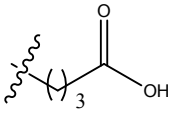
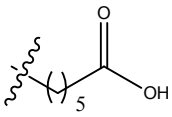
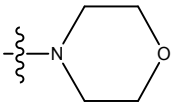
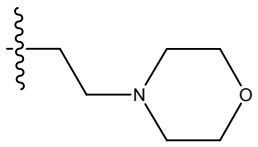
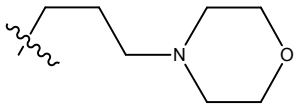
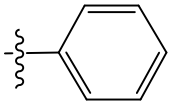
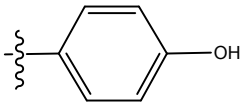
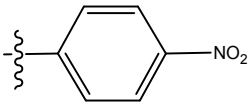
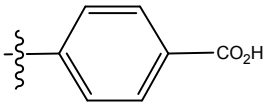
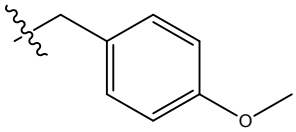
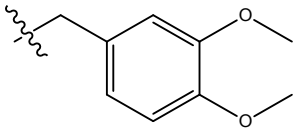
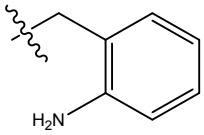
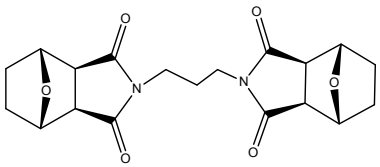
										
42		10	10	10	10	10	10	10	10	10
43		16	45	10	10	10	10	10	10	10
44		10	10	10	10	10	10	10	10	10
45		10	10	10	10	10	10	10	10	10
46		10	10	10	10	10	10	10	10	10
47		10	10	10	10	10	10	10	10	10
48		70	65	88	50	10	61	44	68	54
49		20	59	44	44	100	52	83	39	72
50		25	55	52	40	53	35	66	40	58
51		19	52	43	35	66	47	73	50	49
52		10	10	10	10	10	10	10	10	10
53		19	50	96	67	20	32	15	62	2

54		10	10	10	10	10	10	10	10	10
55		25	30	10	40	17	40	22	20	25
56		12	10	33	10	10	10	10	10	10
57		39	69	100	100	32	60	67	73	2
58		31	18	45	15	16	10	10	10	10
59		21	16	51	18	14	6	10	22	12
60		10	10	10	10	10	10	10	10	10
61		10	10	10	10	10	10	10	10	10
62		10	10	10	10	10	10	10	10	10
63		10	10	10	10	10	10	10	10	10
64		14	11	47	52	12	11	12	22	10
65		29	29	12	7	18	30	3	39	3

66		10	10	10	10	10	10	10	10	10
67		10	10	10	10	10	10	10	10	10
68		63	78	100	90	50	25	24	54	42
69		47	21	22	15	12	27	10	14	44
70		60	44	100	53	37	13	13	45	23
71		10	10	10	10	10	10	10	10	10
72		45	24	64	20	23	14	10	29	11
73		45	29	71	29	31	10	12	11	10
74		33	13	41	18	21	10	10	13	10
75		10	16	52	31	18	10	13	10	10

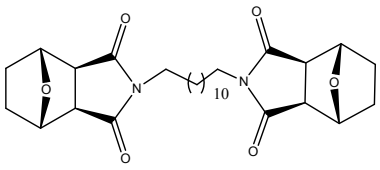
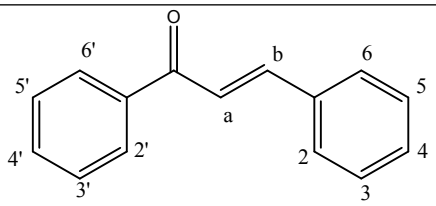
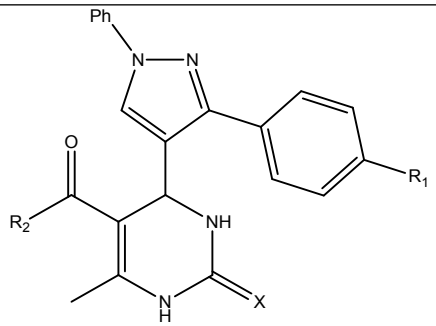
76		8.3	24	18	19	31	18	60	17	43

Table S3: Structure and activity against various cancer cell lines for scaffold 3.

S.NO.	Structure	ACHN	Panc1	Calu1	H460	HCT116
						
77	2',3',4',3,5 = H 2,4= OCH_3	93	94	91	92	95
78	2',3',3,5 = H 2,4= OCH_3, 4'= CH_3	44	45	37	34	31
79	2',3',3,5 = H 2,4,4'= OCH_3	45	36	31	38	37
80	2',3',3,5 = H 2,4= OCH_3, 4'= Cl	28	29	28	32	22
81	2',3',3,5 = H 2,4= OCH_3, 4'= Br	25	30	21	35	32
82	2',3',3,5 = H 2,4= OCH_3, 4'= F	35	36	30	22	37
83	2',4',3,5 = H 2,4= OCH_3, 3'= Cl	36	36	37	26	27
84	3',4',3,5 = H 2,4= OCH_3, 2'= Cl	30	37	38	29	25
85	3',3,5 = H 2,4= OCH_3, 2',4'= Cl	35	35	30	38	26

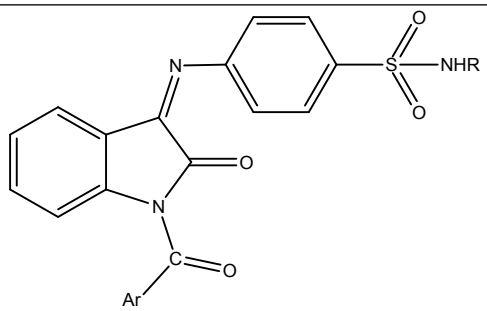
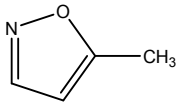
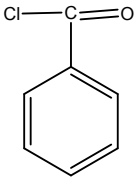
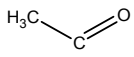
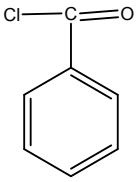
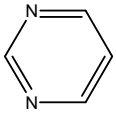
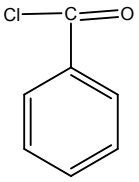
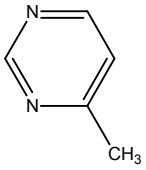
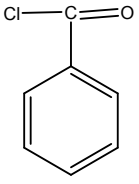
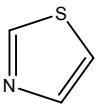
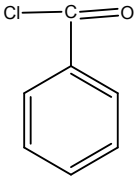
86	3’,3,5 = H 2’4’2,4= OCH_3	48	43	32	19	31
87	2’,3’,3,5 = H 2,4= OCH_3, 4’= NO_2	28	16	38	15	16
88	2’,3’,4’2 = H 3,4,5= OCH_3,	33	7	7	14	0
89	2’,3’,2 = H 3,4,5= OCH_3, 4’= CH_3	17	1	0	14	0
90	2’,3’,2 = H 4’,3,4,5= OCH_3	92	93	93	89	97
91	2’,3’,2 = H 3,4,5= OCH_3, 4’= OH	83	76	76	74	94
92	2’,3’,2 = H 3,4,5= OCH_3, 4’= Cl	57	66	67	54	92
93	2’,3’,2 = H 3,4,5= OCH_3, 4’= Br	48	57	57	44	86
94	3’,2 = H 2’,4’,3,4,5= OCH_3	79	62	58	57	84
95	2’,3’,2 = H 3,4,5= OCH_3, 4’= NO_2	99	100	100	100	99

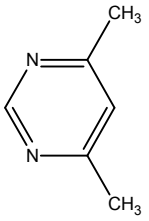
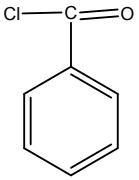
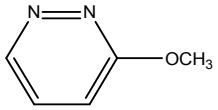
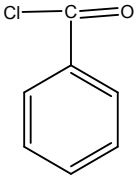
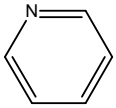
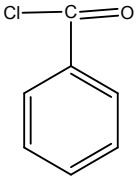
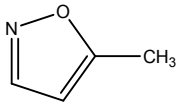
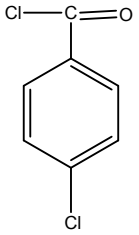
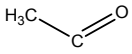
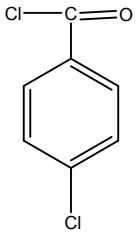
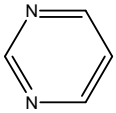
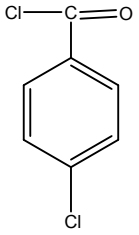
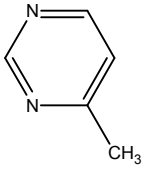
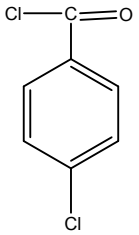
Table S4: Structure and activity against various cancer cell lines for scaffold 4.

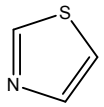
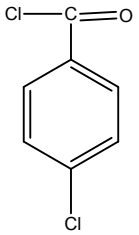
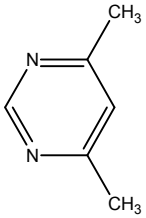
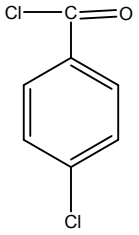
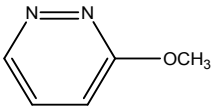
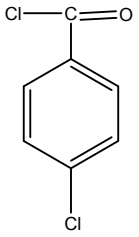
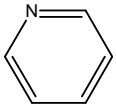
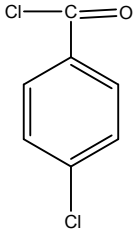
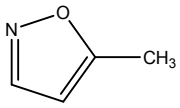
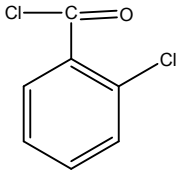
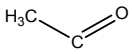
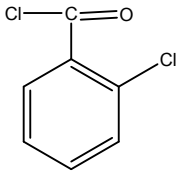
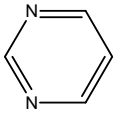
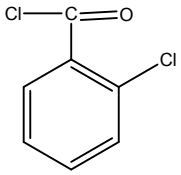
S.No.	Structure	MCF-7
		
96	R_1= H, R_2= OC_2H_5, X= O	<10
97	R_1= H, R_2= OC_2H_5, X= S	30.4
98	R_1= H, R_2= C_6H_5NH, X= O	<10
99	R_1= H, R_2= C_6H_5NH, X= S	<10
100	R_1= H, R_2= 4-$CH_3C_6H_4NH$, X= O	11.9
101	R_1= H, R_2= 4-$CH_3C_6H_4NH$, X= S	19.7
102	R_1= H, R_2= 4-$CH_3OC_6H_4NH$, X= O	-
103	R_1= H, R_2= 4-CH3OC6H4NH, X= S	<10
104	R_1= H, R_2= 4ClC_6H_4NH, X= O	-
105	R_1= H, R_2= 4-ClC_6H_4NH, X= S	48.6
106	R_1= H, R_2= 2-ClC_6H_4NH, X= O	13.9
107	R_1= H, R_2= 2-ClC_6H_4NH, X= S	16.5
108	R_1= H, R_2= 4-$NO_2C_6H_4NH$, X= O	27.3
109	R_1= H, R_2= 4-$NO_2C_6H_4NH$, X= S	48.4
110	R_1= Cl, R_2= OC_2H_5, X= O	17.1
111	R_1= Cl, R_2= OC_2H_5, X= S	70.6

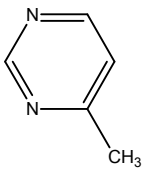
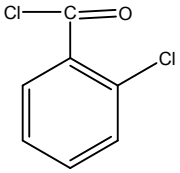
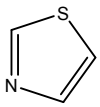
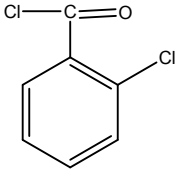
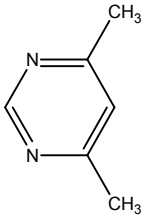
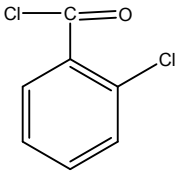
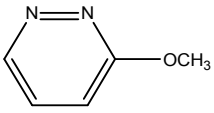
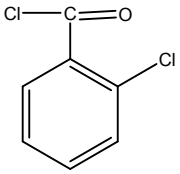
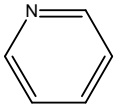
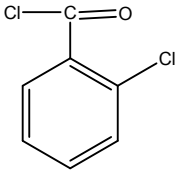
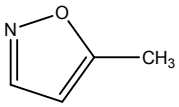
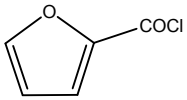
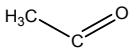
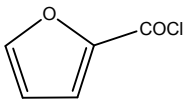
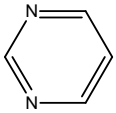
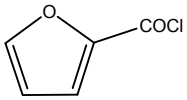
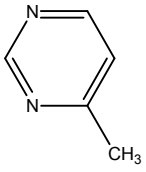
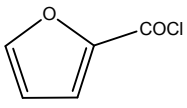
112	R_1= Cl, R_2= C_6H_5NH, X= O	19.6
113	R_1= Cl, R_2= C_6H_5NH, X= S	24.2
114	R_1= Cl, R_2= 4-$CH_3C_6H_4NH$, X= O	13.6
115	R_1= Cl, R_2= 4-$CH_3C_6H_4NH$, X= S	63.7
116	R_1= Cl, R_2= 4-$CH_3OC_6H_4NH$, X= O	<10
117	R_1= Cl, R_2= 4-$CH_3OC_6H_4NH$, X= S	<10
118	R_1= Cl, R_2= 4-ClC_6H_4NH, X= O	<10

Table S5: Structure and activity against various cancer cell lines for scaffold 5.

S.No.	Structure		HCT 116	MCF-7
				
	R	**Ar**		
119			-	1000
120			70	400
121			70	400
122			45	300
123			40	400

124			1000	250
125			120	300
126			50	500
127			35	500
128			150	450
129			50	450
130			120	500

131			280	190
132			400	200
133			500	150
134			300	110
135			200	190
136			210	90
137			210	200

138			480	170
139			70	100
140			400	140
141			110	110
142			260	100
143			200	150
144			120	160
145			210	100
146			500	200

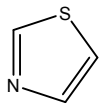
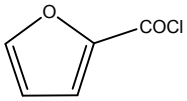
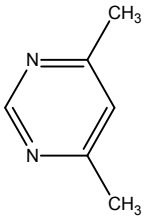
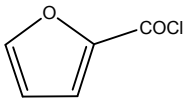
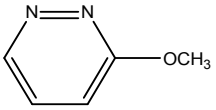
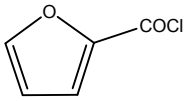
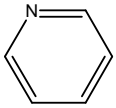
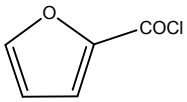
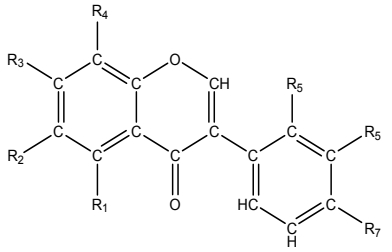
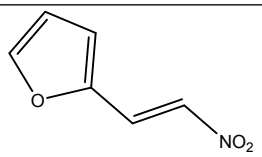
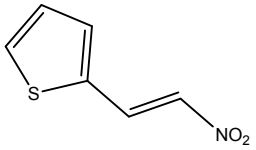
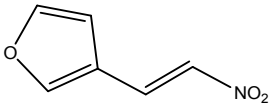
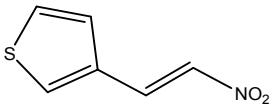
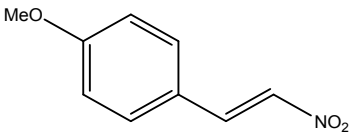
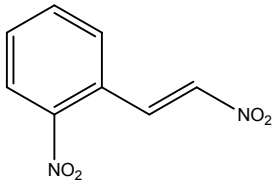
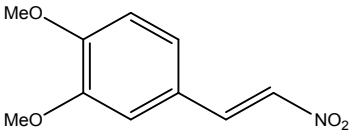
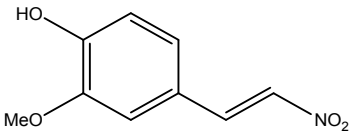
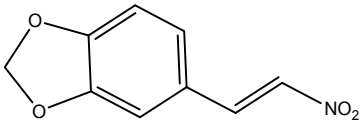
147			70	500
148			-	1000
149			90	450
150			80	500

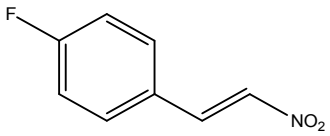
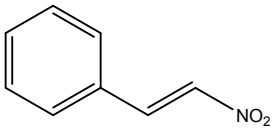
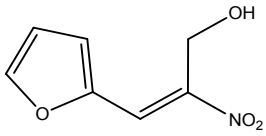
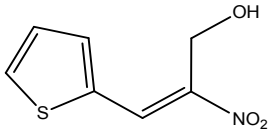
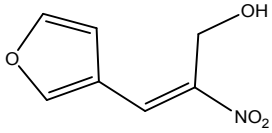
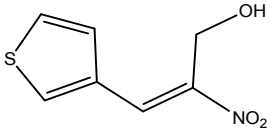
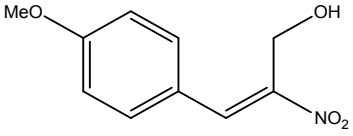
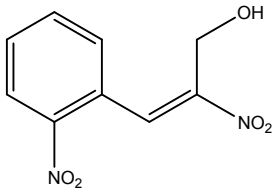
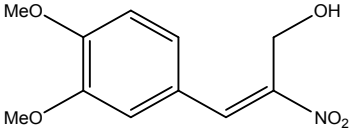
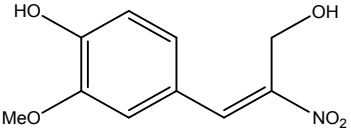
Table S6: Structure and activity against various cancer cell lines for scaffold 6.

S.No.	Structure	HCT116
		
151	R1,R2,R4,R5,R6,R7= H; R3= OCH_3	42.0
152	R1,R4,R5,R6,R7= H; R2,R3= OCH_3	91.3
153	R1,R7=OH; R2,R4,R5,R6,= H; R3= OCH_3	74.0
154	R1,R4,R5,R6= H; R3=OH; R2,R7= OCH_3	4.3
155	R1,R4,R5,R6,R7= H; R2=OCH_3; R3= OH	37.3
156	R2,R4,R5= H; R1,R3,R6,R7= OCH_3	22.3
157	R1,R4,R5= H; R2,R3,R6,R7= OCH_3	85.3
158	R1,R2,R5,R6= H; R3,R4,R7= OH	64.0
159	R1,R2,R5,R6= H; R3,R4,R7= OCH_3	70.0
160	R1,R2,R4,R5= H; R3,R6,R7= OH	35.7
161	R2,R4,R5,R6= H; R1,R3= OCH_3; R7= Br	13.7
162	R2,R4,R6,R7= H; R1,R3= OCH_3; R5= Cl	63.3
163	R2,R4,R5,R7= H; R1,R3= OCH_3; R6= Cl	82.7
164	R2,R4,R5,R6= H; R1,R3= OCH_3; R7= Cl	71.3
165	R1,R2,R5,R6= H; R4= CH_3,R3= OH; R7=Cl	46.3
166	R1,R2,R5,R6= H; R3= OCH_3; R4= CH_3; R7=Cl	58.3

167	R1,R4,R6, R7=H; R2=Cl; R3=OCH_3,	5.3
168	R1,R2,R5,R6= H; R3,R7=OCH_3; R4= CH_3	52.7
169	R1,R2,R5,R6,R7= H; R3=OH; R4=CH_3	27.7
170	R1,R2,R5,R6,R7= H; R3= OCH_3; R4= CH_3	54.0
171	R1,R4,R6= H; R2,R5,R7= Cl; R3= CH_3	12.7
172	R1, R4, R5, R6=H; R2= OCH_3; R3= OH, R7=OAc	26.7
173	R2,R4,R5,R6,R7=H; R1=CH_3; R3=OCH_3	55.3

Table S7: Structure and activity against various cancer cell lines for scaffold 7.

S.No.	Structure	HeLa
174		38
175		18
176		2
177		3
178		17
179		25
180		12
181		-
182		18

183		4
184		5
185		22
186		2
187		5
188		5
189		2
190		>50
191		3
192		-

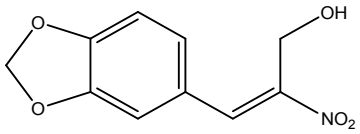
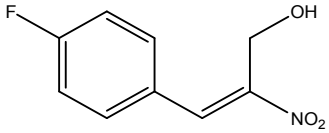
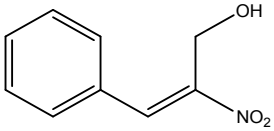
193		38
194		-
195		40

Table S8: Structure and activity against various cancer cell lines for scaffold 8.

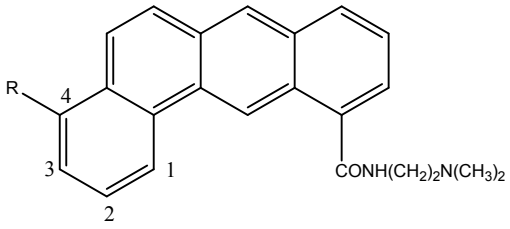
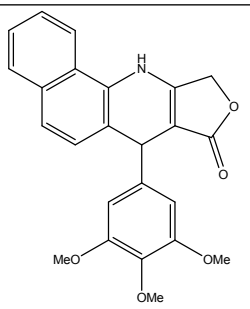
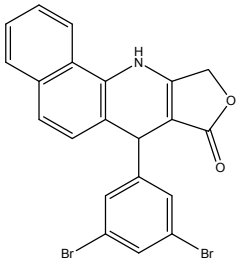
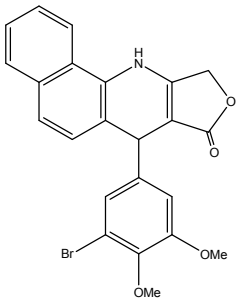
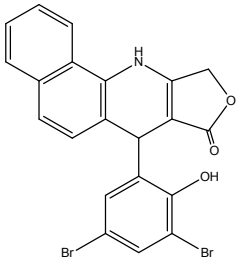
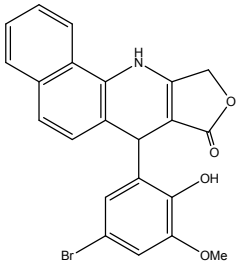
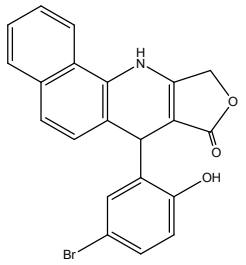
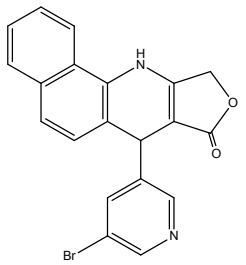
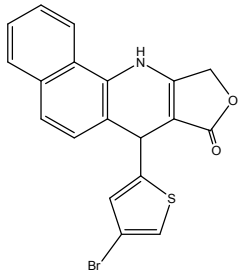
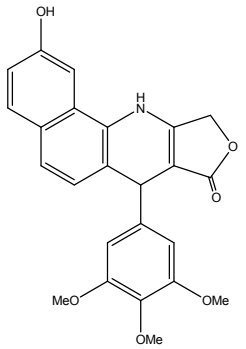
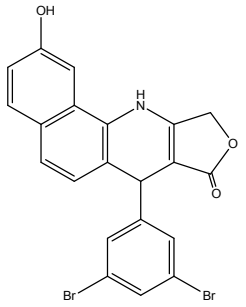
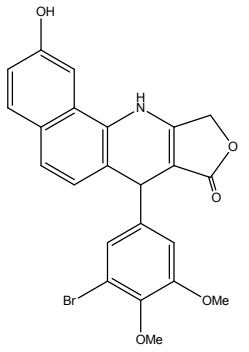
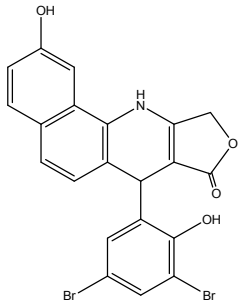
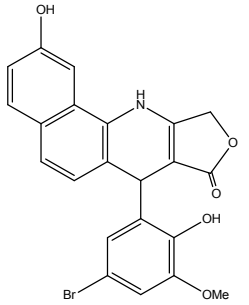
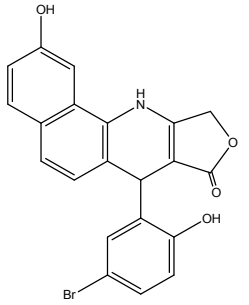
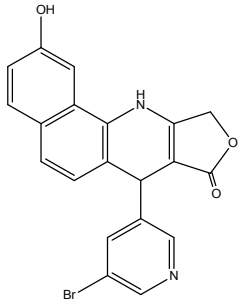
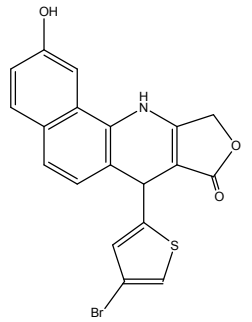
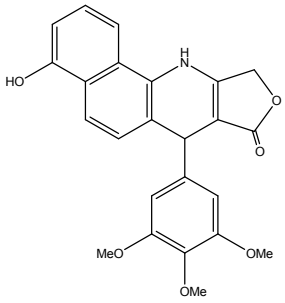
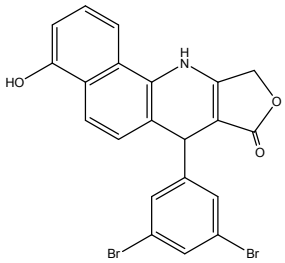
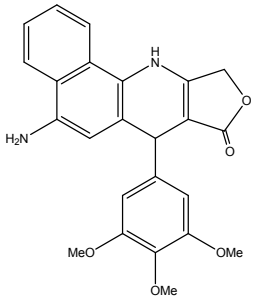
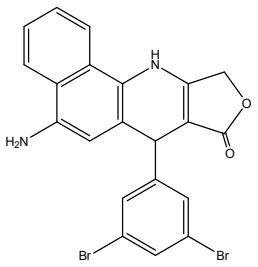
S.No.	Structure	H69
		
196	R= 4-OH	0.035
197	R= 4-OMe	0.035
198	R= 4-OEt	0.049
199	R= 4-O'Pr	0.420
200	R= 4-OBn	0.556
201	R= 4-OCH_2CCH	0.040
202	R= 4-OCH_2CN	0.028
203	R= 4-$OCH_2CH_2CH_2CN$	0.039
204	R= 4-OCOMe	0.024
205	R= 4-OCONHEt	0.064
206	R= 4-OCH_2CH_2OMe	0.090
207	R= 4-OCH_2CH_2OH	0.303
208	R= 4-OCH_2CO_2Et	0.587
209	R= 4-OCH_2COMe	0.045
210	R= 4-OCH_2CONH	0.089
211	R= 4-OCH_2CO_2H	3.844
212	R= 4-$OCH_2CH_2CH_2NMe_2$	0.116
213	R= 4-OCH_2CH_2morpholino	0.099

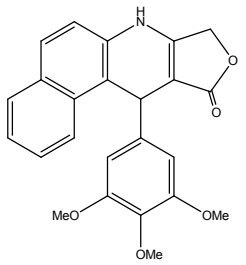
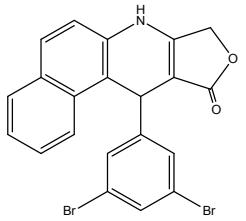
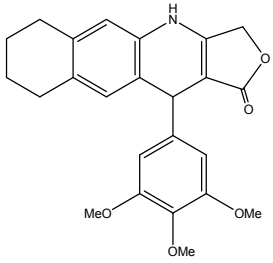
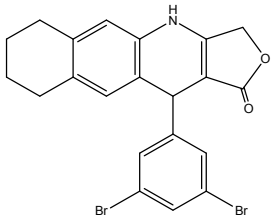
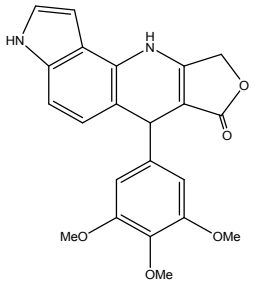
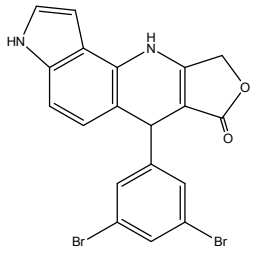
Table S9: Structure and activity against various cancer cell lines for scaffold 9.

S.No.	Structure	HeLa	MCF-7
214		3	3
S215		16	14
216		3	3
217		18	21
218		3	3

219		3	3
220		7	13
221		3	3
222		2	3
223		6	3

224		2	3
225		7	3
226		6	3
227		3	3
228		3	3

229		3	3
230		3	3
231		21	23
232		-	-
233		21	16

234		540	121
235		420	201
236		18	19
237		100	70
238		19	22
239		114	21

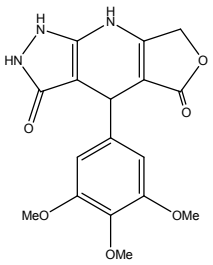
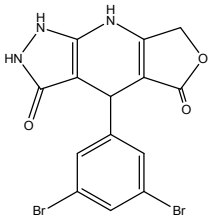
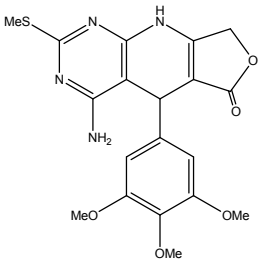
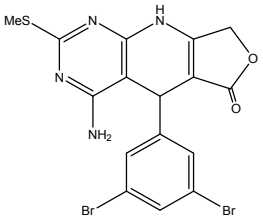
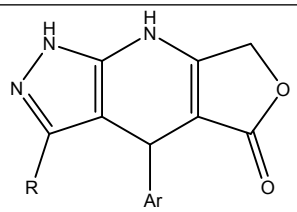
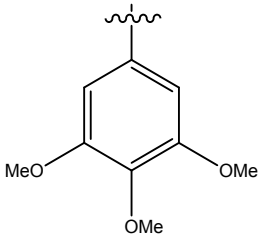
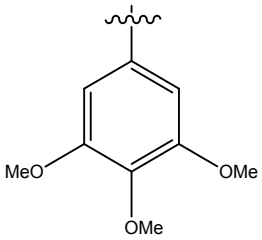
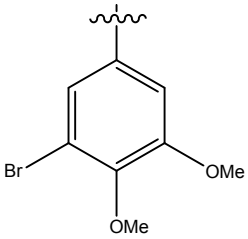
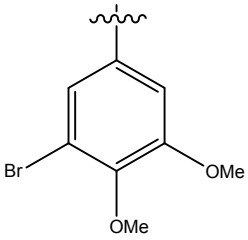
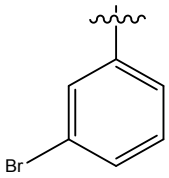
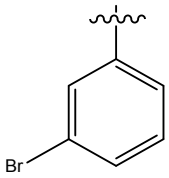
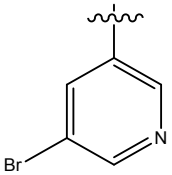
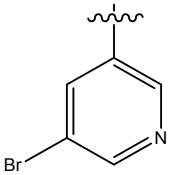
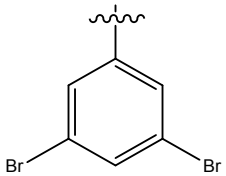
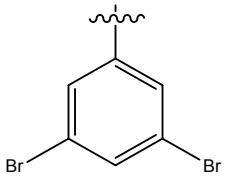
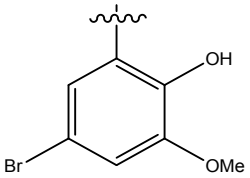
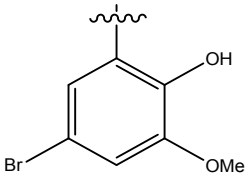
240		10000	10000
241		10000	10000
242		125	170
243		561	1020

Table S10: Structure and activity against various cancer cell lines for scaffold 10.

S.No.	Structure		HeLa	MCF-7
				
	Ar	**R**		
244		**Me**	5.0	5.0
245		**H**	3.0	0.25
246		**Me**	0.75	1.0
247		**H**	0.75	0.25

248		**Me**	3.0	4.0
249		**H**	0.075	0.10
250		**Me**	3.0	0.8
251		**H**	0.075	0.015
252		**Me**	0.075	0.074
253		**H**	0.025	0.025
254		**Me**	0.035	0.10
255		**H**	0.025	0.030

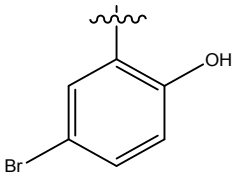
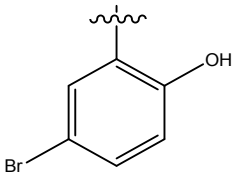
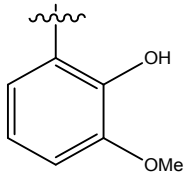
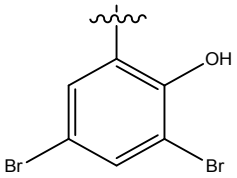
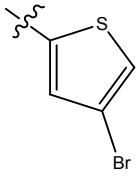
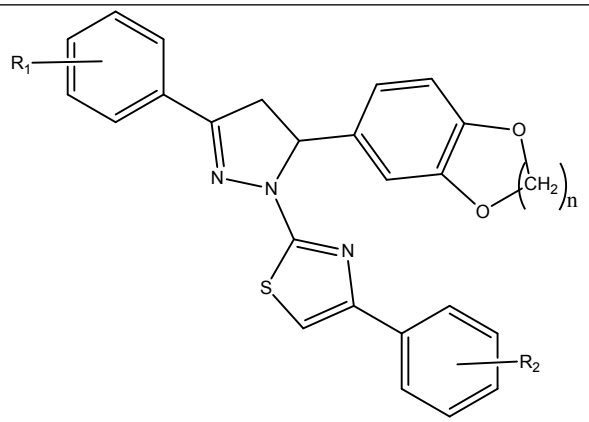
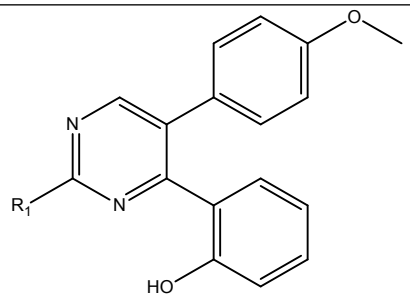
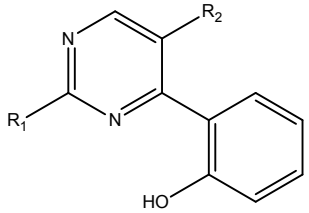
256		**Me**	0.30	0.25
257		**H**	0.050	0.025
258		**H**	2.0	0.50
259		**H**	0.020	0.010
260		**H**	1.15	0.74

Table S11: Structure and activity against various cancer cell lines for scaffold 11

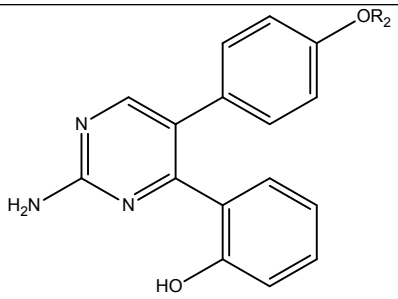
S.No.	Structure			MCF-7	B16-F10
					
	R1	**n**	**R2**		
261	F	1	OMe	3.65	3.98
262	F	1	Br	3.43	3.81
263	Cl	1	OMe	2.41	3.81
264	Cl	1	Br	1.72	1.51
265	Br	1	OMe	0.27	0.32
266	Br	1	Br	0.09	0.12
267	Me	1	OMe	1.43	1.52
268	Me	1	Br	1.41	1.39
269	OMe	1	OMe	2.73	2.67
270	OMe	1	Br	2.47	2.54
271	F	2	OMe	4.53	4.43
272	F	2	Br	4.20	4.11
273	Cl	2	OMe	3.03	3.12
274	Cl	2	Br	2.23	2.15

275	Br	2	OMe	0.87	1.1
276	Br	2	Br	0.32	0.4
277	Me	2	OMe	2.68	2.87
278	Me	2	Br	1.59	1.68
279	OMe	2	OMe	2.7	3.01
280	OMe	2	Br	2.54	2.5

Table S12: Structure and activity against various cancer cell lines for scaffold 12.

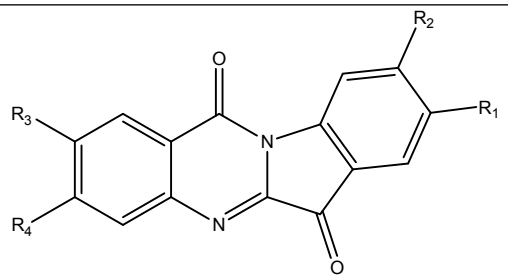
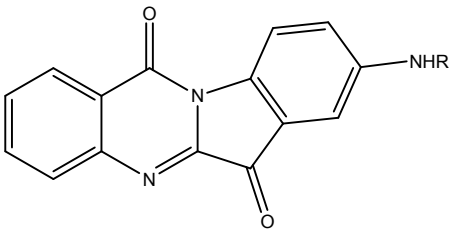
S. No.	Structure	BEL-7402
		
281	R_1= CH_3	1.02
282	R_1= H	1.43
283	R_1= OMe	6.00
284	R_1= NH_2	0.67
285	R_1= CO_2H	>10
286	R_1= CO_2Me	>10
287	R_1=CONHMe	>10
288	R_1= $CONMe_2$	>10
		
289	R_1= Me; R_2= 2-F-Ph	>10
290	R_1=NH2; R2= 2-F-Ph	>10
291	R_1= NH_2; R_2= 2-OMePh	>10

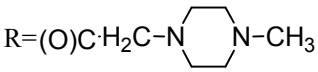
292	R_1= Me; R_2=OMePh	>10
293	R_1= Me; R_2= 3-CF_3Ph	>10
294	R_1= NH_2; R_2= 3-CF_3Ph	>10
295	R_1= Me; R_2= 4-ClPh	>10
296	R_1= Me; R_2= 4-NHBocPh	>10
297	R_1= NH2; R_2= 4-NHBocPh	>10
298	R_1= Me; R_2= 4-NH_2Ph	>10
299	R_1= NH_2; R_2= NH_2Ph	>10
300	R_1= Me; R_2= 4-OCF_3Ph	>10
301	R_1= NH_2; R_2= 4-OCF_3Ph	>10
302	R_1= NH_2; R_2= 4-OHPh	>10
303	R_1= NH_2; R_2= 4-SMePh	0.09
304	R_1= Me; R_2= 3-Me-4-OMePh	0.10
305	R_1= NH_2; R_2= 3-Me-4-OMePh	0.12
306	R_1= NH_2; R_2= 3,4-Di-OMePh	4.10
307	R_1= Me; R_2= 3,4,5-Tri-OMePh	>10
308	R_1= NH_2; R_2=3,4,5-Tri-OMePh	>10
309	R_1= Me; R_2= 3-Pyridinyl	>10
310	R_1= NH_2; R_2= 3-Pyridinyl	>10
311	R_1= Me; R_2= 4-Pyridinyl	>10
312	R_1=NH_2; R_2= 4-Pyridinyl	>10

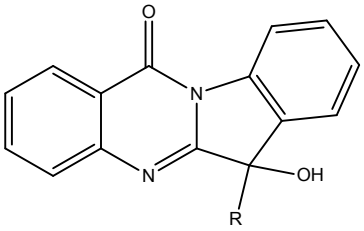


313	R_2= Et	0.24
314	R_2= Allyl	>10
315	R_2= Pr	>10
316	R_2= iPr	>10
317	R_2= Bu	>10
318	R_2= 2-Methylallyl	>10
319	R_2= iBu	>10
320	R_2= 3-Methylbut-2-enyl	>10
321	R_2= Isopentyl	>10
322	R_2= CH_2CN	>10
323	R_2= CH_2CO_2Et	>10
324	R_2= 2-(Pyrrolidin-1-yl)ethyl	>10
325	R_2= $CH_2CH_2CH_2OBn$	>10

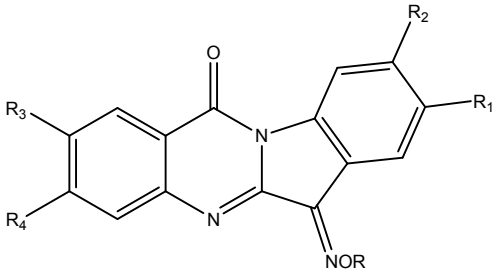
Table S13: Structure and activity against various cancer cell lines for scaffold 13.

S.No.	Structure	MCF-7	U251	SW260	H522	M14	SKOV3	DU145	A498
									
326	R_1,R_2,R_3,R_4= H	30	100	5	15	15.0	2.5	0.4	0.95
327	R_3= Br; R_1,R_2,R_4= H	100	100	100	100	100	100	100	100
328	R_3= NO_2; R_1,R_2,R_4= H	100	100	100	100	100	100	100	100
329	R_3,R_4= OMe; R_1,R_2= H	100	100	100	100	100	100	100	100
330	R_3= NH_2; R_1,R_2,R_4= H	40	70	60.0	60.0	60.0	40.0	60.0	80.0
331	R_1= Br; R_2,R_3,R_4= H	0.7	100	4.00	0.7	0.8	5.0	0.15	3.0
332	R_1= NO_2; R_2,R_3,R_4= H	1.0	4.5	25.0	4.8	15.0	25.0	8.0	2.0
333	R_1= NH_2; R_2,R_3,R_4= H	5.0	0.7	4.8	5.0	5.0	5.0	2.0	3.0
334	R_1,R_2= OCH_2O-;R_3, R_4= H	100	100	100	100	100	100	100	100
335	R_1= OMe; R_2,R_3,R_4= H	100	100	100	100	100	100	100	100
336	R_1= Me; R_2,R_3,R_4= H	0.4	20	100	0.15	60.0	100	100	60.0
337	R_1= Cl; R_2,R_3,R_4= H	100	100	100	100	100	100	100	100
									

338	R= $C(O)CH_3$	0.4	20	30.0	5.0	10.0	20.0	0.5	0.4
339	R= $C(O)CH_2CH_2CH_3$	10	12	10.5	18.2	18.5	6.0	20.0	20.0
340	R= $C(O)CH_2CH_3$	20	100	22.0	18.0	10.0	8.0	10.0	7.0
341	R=$C(O)CH_2Cl$	0.06	0.2	0.6	4.0	0.9	0.05	0.25	0.4
342		20	100	10	15.0	8.0	6.0	10.0	20.0
343	R= SO_2CH_3	100	100	100	100	100	100	100	100



344	R= $-CH_3$	100	100	100	100	100	100	100	100
345	R= $-CH=CH_2$	20	12	10	15	8.0	6.0	10.0	12.0
346	R= $-CH_2CH_2CH_2CH_3$	100	100	100	100	100	100	100	100
347	R= $-OCH_2CH_2O$-Ph	100	100	100	100	100	100	100	100



348	R_1,R_2,R_3,R_4, R = H	15	15	8	50.0	40.0	30.0	50.0	60.0
349	R_1,R_2,R_3,R_4, = H; R= $-CH_2CH_2OH$	0.01	1.0	20	7.0	30.0	20.0	3.0	40.0
350	R_1,R_2,R_3,R_4 = H; R= $-CH_2COOCH_3$	0.01	100	100	80.0	40.0	50.0	30.0	100

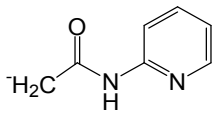
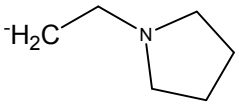
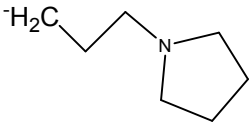
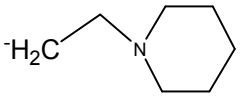
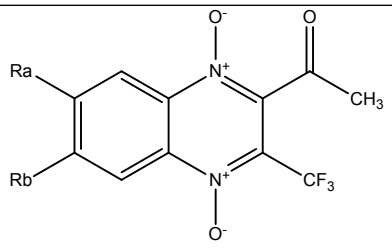
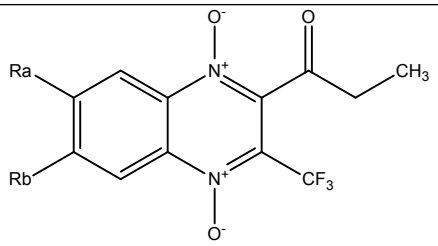
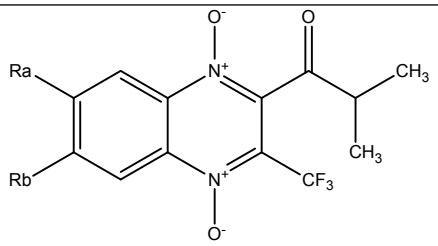
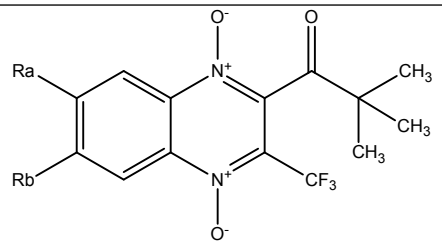
351	R1, R2, R3, R4 = H; R= 	8.0	8.5	100	25.0	95.0	52.0	10.0	20.0
352	R_1,R_2,R_3,R_4 = H; R= -C(O)CH=CH-Ph	7.5	20.0	60	45	90.0	6.0	100	10.0
353	R_1,R_2,R_3,R_4= H; R= $-CH_2CH_2CH_2-NMe_2$	7.5	0.7	4.0	0.6	5.0	2.0	3.5	4.0
354	R_1,R_2,R_3,R_4= H; R= $-CH_2CH_2-NMe_2$	0.4	0.8	0.75	0.7	2.0	2.0	2.5	0.6
355	R1, R2, R3, R4 = H; R= 	6.0	25.0	0.85	3	2.0	3.0	3.0	5.0
356	R1, R2, R3, R4 = H; R= 	5.0	6.0	4.5	4	6.0	4.0	5.0	7.0
357	R_1= NO_2;, R_2,R_3,R_4= H; R= $-CH_2CH_2-NMe_2$	4.0	7.5	0.75	9	7.5	9.0	100	100
358	R_1= NO_2;, R_2,R_3,R_4= H; R= $-CH_2CH_2CH_2-NMe_2$	4.0	2.5	0.5	0.4	0.4	0.6	2.0	0.09
359	R_1= NO_2;, R_2,R_3,R_4= H; R= $-CH_2CH_2OH$	0.4	0.8	0.75	0.7	2.0	2.0	2.5	0.6
360	R_1= Br;, R_2,R_3,R_4= H; R= $-CH_2CH_2-NMe_2$	0.06	0.45	3.0	2.0	2.0	3.0	0.2	1.5
361	R1, R2, R3, R4 = H; R= 	0.3	0.095	3.0	2.0	2.5	1.0	0.55	2.0

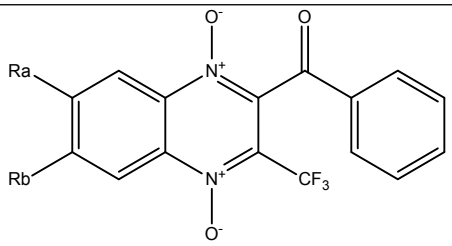
Table S14: Structure and activity against various cancer cell lines for scaffold 14.

S.No.	Structure	H460	MCF-7	SF-268
				
362	Ra= H; Rb= CH_3	18	0	16
363	Ra= Rb= H	29	9	61
364	Ra= Rb= Cl	-64	-49	-56
365	Ra= H; Rb= Cl	0	0	0
366	Ra= Rb= F	69	59	70
				
367	Ra= Rb= CH_3	63	98	110
368	Ra= H; Rb= CH_3	23	0	28
369	Ra= Rb= H	36	95	84
370	Ra= Rb= Cl	121	113	144
371	Ra= Rb= F	0	0	0
				

372	**Ra= Rb=** CH_3	107	96	99
373	Ra= Rb= H	0	0	0
374	Ra= Rb= Cl	102	101	101
375	Ra= Rb= F	28	100	100

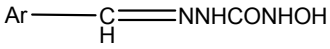
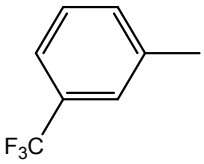
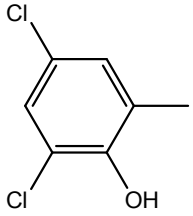
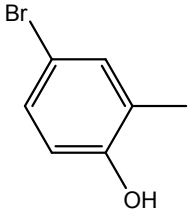
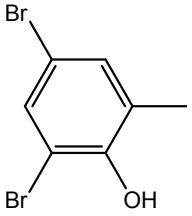
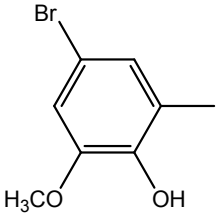


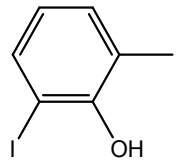
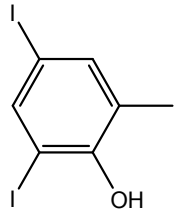
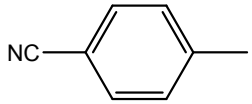
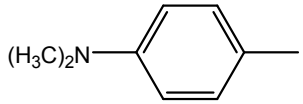
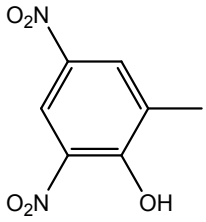
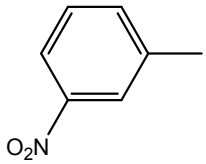
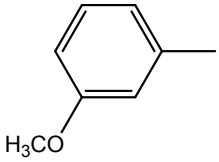
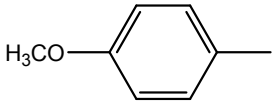
376	**Ra= Rb=** CH_3	1	28	71
377	Ra= Rb= H	0	0	0
378	Ra= Rb= Cl	67	27	96
379	Ra= Rb= F	106	106	100

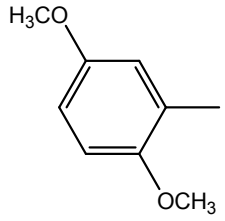
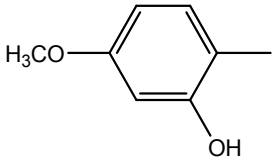
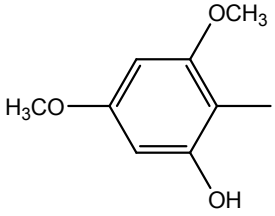
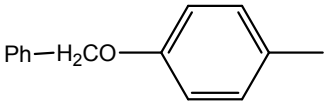
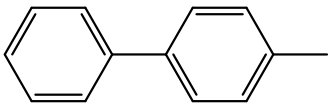
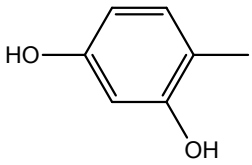
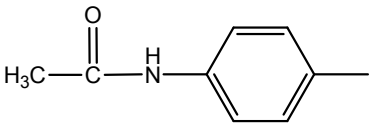
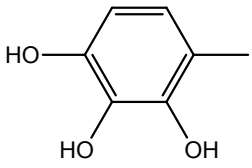
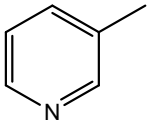


380	**Ra= Rb=** CH_3	-62	-32	-86
381	Ra= Rb= H	0	0	0
382	Ra= Rb= Cl	1	78	41
383	Ra= Rb= F	0	0	0

Table S15: Structure and activity against various cancer cell lines for scaffold 15.

S.No.	Structure	L120
		
	Ar	
384		39.5
385		6.5
386		10.1
386		7.2
387		37.7

388		80.4
389		4.7
391		208.5
392		446.3
393		820.6
394		399.3
395		368.8
396		316.7

397		30.1
398		60.2
399		91.4
400		48.1
401		42.7
402		130.8
403		944.1
404		2.7
405		607.0

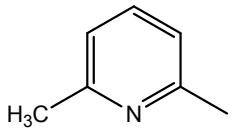
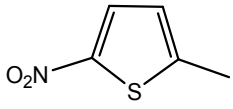
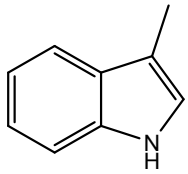
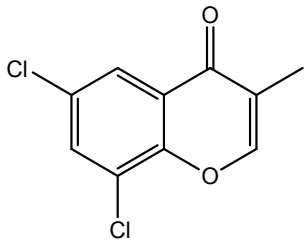
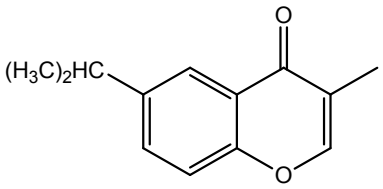
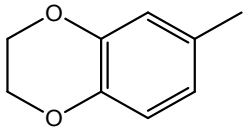
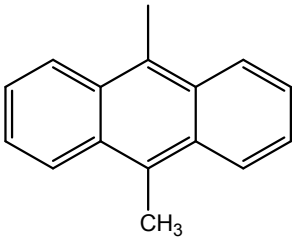
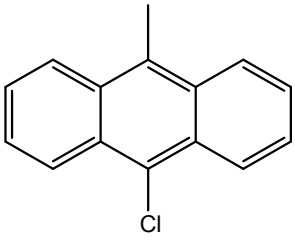
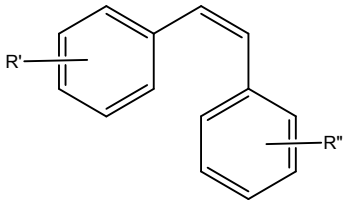
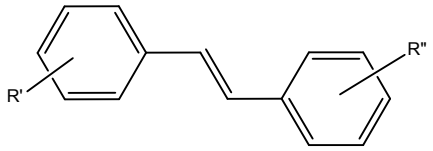
406		891.0
407		10.6
408		476.6
409		28.2
410		32.2
411		178.3
412		4.4
413		5.4

Table S16: Structure and activity against various cancer cell lines for scaffold 16.

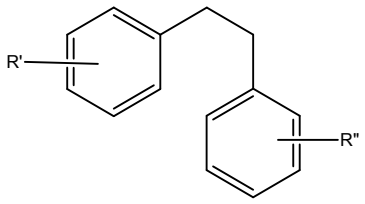
S.No.	Structure		A-549	MCF-7	HT-29	SKMEL-5	MLM
							
	R'	R"					
414	3,4,5-$(OMe)_3$	4-OMe	$2.2x10^{-5}$	$1.2x10^{-6}$	$2.7x10^{-6}$	$9.7x10^{-7}$	$9.3x10^{-6}$
415	3,4,5-$(OMe)_3$	3-OMe	$1.3x10^{-1}$	$1.4x10^{-1}$	$9.0x10^{-2}$	$6.0x10^{-2}$	1.4
416	3,4,5-$(OMe)_3$	2-OMe	1.1	1.3	8.7x10-1	1.2	8.6
417	2,3,4-$(OMe)_3$	4-OMe	$9.7x10^{-1}$	$2.3x10^{-1}$	1.0	1.1	10.9
418	3,4,5-$(OMe)_3$	2-Cl-4-OMe	$5.1x10^{-2}$	$4.6x10^{-2}$	$6.6x10^{-2}$	$1.7x10^{-2}$	$1.4x10^{-1}$
419	3,4,5-$(OMe)_3$	H	$1.7x10^{-1}$	$2.5x10^{-1}$	$8.4x10^{-2}$	$1.2x10^{-1}$	>25
420	3,4,5-$(OMe)_3$	4-Cl	$8.0x10^{-2}$	$1.8x10^{-1}$	$5.0x10^{-2}$	$1.0x10^{-2}$	$1.7x10^{-1}$
421	3,4,5-$(OMe)_3$	4-Br	$1.1x10^{-2}$	$1.6x10^{-2}$	$8.2x10^{-3}$	$6.7x10^{-3}$	$1.4x10^{-2}$
422	1-(4- Pyridyl)-2-(3,4,5-trimethpxyphenyl)ethene		14.2	17.0	12.9	14.4	>25
423	1-(3- Pyridyl)-2-(3,4,5-trimethpxyphenyl)ethene		13.7	14.7	9.8	6.0	>25
424	1-(2- Pyridyl)-2-(3,4,5-trimethpxyphenyl)ethene		>25	>25	>25	>25	>25
425	2,3,4-$(OMe)_3$	4-NO_2	>25	>25	>25	>25	>25
426	3,4,5-$(OMe)_3$	4-OSi(t-Bu)Me_2	10.95	7.29	10.60	7.59	17.23

427	3,4,5-$(OMe)_3$	4-NMe_2	$4.1x10^{-3}$	$5.8x10^{-3}$	$8.1x10^{-3}$	$1.5x10^{-4}$	$9.4x10^{-3}$
428	3,4,5-$(OMe)_3$	4-OH	12.70	5.70	1.75	2.27	12.60
429	3,4,5-$(OMe)_3$	4-OAc	1.7	$3.0x10^{-1}$	6.0	$6.0x10^{-1}$	6.3



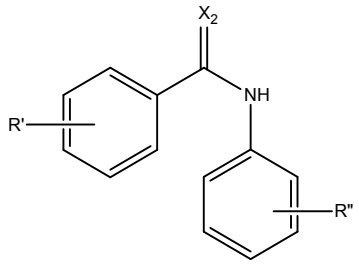
430	3,4,5-$(OMe)_3$	4-OMe	1.18	1.05	1.82	$8.1x10^{-1}$	2.07
431	3,4,5-$(OMe)_3$	3-OMe	9.8	12.2	7.3	10.5	>25
432	3,4,5-$(OMe)_3$	2-OMe	12.2	18.0	12.1	13.5	>25
433	3,4,5-$(OMe)_3$	2-Cl-4-OMe	>25	>25	>25	>25	>25
434	3,4,5-$(OMe)_3$	H	>25	>25	>25	>25	>25
435	3,4,5-$(OMe)_3$	4-Cl	>25	>25	>25	>25	>25
436	3,4,5-$(OMe)_3$	4-Br	6.47	9.14	12.69	6.53	5.13
437	1-(4- Pyridyl)-2-(3,4,5-trimethpxyphenyl)ethene		>25	>25	>25	>25	>25
438	1-(3- Pyridyl)-2-(3,4,5-trimethpxyphenyl)ethene		>25	>25	>25	>25	>25
439	2,3,4-$(OMe)_3$	4-NO_2	4-NO_2	>25	>25	>25	>25
440	3,4,5-$(OMe)_3$	4-OSi(t-Bu)Me_2	>25	>25	>25	>25	>25
441	3,4,5-$(OMe)_3$	4-NMe_2	$6.1x10^{-3}$	$8.2x10^{-2}$	$6.9x10^{-3}$	$4.6x10^{-3}$	$1.25x10^{-2}$
442	3,4,5-$(OMe)_3$	4-OH	>25	18.63	>25	11.55	24.15
443	3,4,5-$(OMe)_3$	4-OAc	9.7	9.6	5.4	4.6	13.0

444	3,4-$(OMe)_2$	H	>25	>25	>25	>25	>25
445	2,3,4-$(OMe)_3$	H	>25	>25	>25	>25	>25
446	3,4,5-$(OMe)_3$	3,5-$(OMe)_2$	>25	>25	>25	>25	>25
447	3,4,5-$(OMe)_3$	2,3,4-$(OMe)_3$	12.5	14.72	10.27	10.64	23.86
448	3,4,5-$(OMe)_3$	3,4,5-$(OMe)_3$	>25	>25	>25	>25	>25
449	3,4,5-$(OMe)_3$	2,4,5-$(OMe)_3$	>25	>25	>25	>25	>25
450	2,4,5-$(OMe)_3$	H	>25	8.5	>25	>25	>25
451	2,4,6-$(OMe)_3$	H	>25	>25	>25	>25	>25
452	3,4-$(OMe)_2$	3,5-$(OMe)_2$	>25	>25	>25	>25	>25
453	3,4,5-$(OMe)_3$	NH_2	>25	>25	>25	>25	>25



454	3,4,5-$(OMe)_3$	4-OMe	$1.8x10^{-4}$	$1.6x10^{-4}$	$2.5x10^{-4}$	$1.4x10^{-4}$	$1.8x10^{-4}$
455	3,4,5-$(OMe)_3$	3-OMe	11.7	12.4	7.6	9.2	>25
456	3,4,5-$(OMe)_3$	2-OMe	13.5	11.8	>25	20	>25
457	3,4,5-$(OMe)_3$	H	>25	>25	>25	>25	>25
458	1-(4- Pyridyl)-2-(3,4,5-trimethpxyphenyl)ethene		>25	>25	>25	>25	>25
459	1-(3- Pyridyl)-2-(3,4,5-trimethpxyphenyl)ethene		12.2	>25	>25	>25	>25

460	3,4,5-$(OMe)_3$	4-$OSi(t\text{-}Bu)Me_2$	>25	>25	>25	>25	>25
461	3,4,5-$(OMe)_3$	4-NMe_2	$8.3x10^{-2}$	$6.4x10^{-2}$	$7.7x10^{-2}$	$5.9x10^{-2}$	$1.2x10^{-1}$
462	3,4,5-$(OMe)_3$	4-OH	>25	>25	>25	>25	>25
463	3,4,5-$(OMe)_3$	4-OAc	19.0	>25	>25	>25	>25
464	3,4-$(OMe)_2$	H	>25	>25	>25	>25	>25
465	2,3,4-$(OMe)_3$	H	>25	>25	>25	>25	>25
466	3,4,5-$(OMe)_3$	3,5-$(OMe)_2$	>25	>25	>25	>25	>25
467	3,4,5-$(OMe)_3$	2,3,4-$(OMe)_3$	>25	>25	>25	>25	>25
468	3,4,5-$(OMe)_3$	3,4,5-$(OMe)_3$	>25	>25	>25	>25	>25
469	3,4,5-$(OMe)_3$	2,4,5-$(OMe)_3$	>25	>25	>25	>25	>25
470	3,4,5-$(OMe)_3$	NH_2	12.23	11.88	24.56	12.65	>25



	R'	**R"**	**X**					
471	3,4,5-$(OMe)_3$	4-OMe	O	14.07	12.21	22.65	>25	>25
472	3,4-$(OMe)_2$	3,4,5-$(OMe)_3$	O	>25	>25	>25	>25	>25
473	4-OMe	3,4,5-$(OMe)_3$	O	>25	>25	>25	>25	>25
474	3,5-$(OMe)_2$	4-OMe	O	9.02	5.47	14..52	11.88	>25
475	4-OMe	3,5-$(OMe)_2$	O	>25	>25	>25	>25	>25
476	3,4,5-$(OMe)_3$	3,4,5-$(OMe)_3$	O	>25	>25	>25	>25	>25

477	3,4,5-$(OMe)_3$	4-OMe	H_2	$1.9x1^{0-3}$	$2.4x10^{-3}$	$1.0x10^{-3}$	$7.0x10^{-4}$	$1.6x10^{-3}$
478	3,4-$(OMe)_2$	3,4,5-$(OMe)_3$	H_2	>25	>25	>25	>25	>25
479	4-OMe	3,4,5-$(OMe)_3$	H_2	$8.3x10^{-1}$	$8.6x10^{-1}$	2.24	1.13	>25
480	3,5-$(OMe)_2$	4-OMe	H_2	5.71	6.08	17.84	2.41	>25
481	4-OMe	3,5-$(OMe)_2$	H_2	>25	>25	>25	>25	>25
482	3,4,5-$(OMe)_3$	3,4,5-$(OMe)_3$	H_2	>25	>25	>25	>25	>25

Table S17: Details of the descriptors involved in the different combination in QSAR studies

No.	Descriptors	Full Name of the Descriptors	Nature	QSAR Model
1	MannRCN	Max n-n repulsion for a C-N bond	Quantum chemical	M1
2	ASIC1	Average Structural Information content (order 1)	Topological	M1, M20
3	$RNCS_z$	RNCS Relative negative charged SA(SAMNEG*RNCG)[Zefirov's PC]	Electrostatic	M1, S5
4	MaenACC	Max e-n attraction for a C-C bond	Quantum Chemical	M2, S16
5	$PNSA1_Q$	PNSA-1 Partial negative surface area[Quantum Chemical]	Quantum Chemical	M2
6	$PNSA2_Z$	PNSA-2 total charge weighted PNSA[Zefirov's PC]	Electrostatic	M2
7	MiNRIO	Min nucleoph.react.Index for a O atom	Quantum Chemical	M3
8	$HACA1_Q$	HACA-1 [Quantum Chemical]	Quantum Chemical	M3
9	$RPCS_z$	RPCS Relative Positive Charged SA (SAMPOS*RPCG)[Zefirov's PC]	Electrostatic	M3
10	$FPSA3_z$	FPSA-3 Fractional PPSA (PPSA-3/TMSA) [Zefirov's PC]	Electrostatic	M4, S3
11	$WNSA2_Z$	WNSA-2 Weighted PNSA (PNSA2*TMSA/1000) [Zefirov's PC]	Electrostatic	M4,M17, S3
12	BI	Balaban index	Topological	M4**,S3**
13	YZS	YZ Shadow	Geometrical	M5, M9
14	RI0	Randic index(Order 0)	Topological	M5
15	MiERIC	Min electroph.react.Index for a C atom	Quantum Chemical	M5, M7, S8, S15

16	$WPSA1_Q$	WPSA-1 Weighted PPSA(PPSA1*TMSA/1000)[Quantum-Chemical PC]	Quantum Chemical	M6
17	MiTICS	Min Total Interaction for C-S bond	Quantum Chemical	M6
18	MiNACN	Min net atomic charge for N atom	Quantum Chemical	M6
19	XYS/XYR	XY Shadow/XY rectangle	Geometrical	M7
20	RNO	Realative number of O atoms	Topological	M7
21	HLEG	HOMO-LUMO energy gap	Quantum Chemical	M8, S12
22	$WNSA3_Q$	WNSA-3 Weighted PNSA (PNSA3*TMSA/1000) [Quantum Chemical PC]	Quantum Chemical	M8
23	MiERIN	Min electroph.react.Index for a N atom	Quantum Chemical	M8,S9, S13
24	A1ERIC	Avg 1-electron react index for a C atom	Quantum Chemical	M9
25	SIC1	Structural Information Content(Order1)	Topological	M9
26	MiTICN	Min Total Interaction for C-N bond	Quantum Chemical	M10, M23, S14
27	$PNSA1_Z$	PNSA-1 Partial negative surface area[Zefirov's PC]	Electrostatic	M10
28	$CHaS_Z$	Count of H-acceptor sites [Zefirov's PC]	Electrostatic	M10
29	$FNSA2_Z$	FNSA-2 Fractional PNSA (PNSA-2/TMSA)[Zefirov's PC]	Electrostatic	M11
30	$ERPCG_Q$	ESP-RPCG Relative Positive Charge (QMPOS/QTPLUS) [Quantum Chemical]	Quantum Chemical	M11
31	MienACH	Min e-n attraction for C-H bond	Quantum Chemical	M11
32	$MiPCC_Z$	Min Partial charge for C atom [Zefirov's PC]	Electrostatic	M12
33	MiBOC(0.1)	Min (>0.1) bond order of a C atom	Quantum Chemical	M12, M18

34	THCMD	Toatal hybridization comp. of the molecular dipole	Quantum Chemical	M12
35	RE/T	Rot.entropy(300 K)	Thermodynamical	M13
36	LNMVF	Lowest normal mode vib frequency	Thermodynamical	M13, M24, S1
37	ACIC1	Average Complementry Information Content (Order 1)	Topological	M13
38	MaBON	Max bond order of a N atom	Quantum Chemical	M14
39	MaenACN	Max e-n attrction for a C-N bond	Quantum Chemical	M14
40	NN	Number of N atom	Constitutional	M14, M19
41	$FNSA2_Q$	FNSA-2 Fractional PNSA (PNSA-2/TMSA) [Quantum-Chemical PC]	Quantum Chemical	M15, S5
42	PP/SD	Polarity parameter / square distance	Electrostatic	M15
43	MaenAC	Max e-n attraction for a C atom	Quantum Chemical	M15, S2
44	EMaNACH	ESP-Max net atomic charge for a H atom	Quantum Chemical	M16
45	$HDSA2_Q$	HA dependent HDSA-2/TMSA [Quantum-Chemical PC]	Quantum Chemical	M16
46	MaeeRC	Max e-e repulsion for a C atom	Quantum Chemical	M16, M20
47	$HDCA2_Q$	HA dependent HDCA-2 [Quantum-Chemical PC]	Quantum Chemical	M17
48	MienANN	Min e-n attraction for a N-N bond	Quantum Chemical	M17
49	ZXS/ZXR	ZX Shadow / ZX Rectangle	Geometrical	M18, S4
50	$ERNCS_Q$	ESP-RNCS Relative negative charged SA (SAMNEG*RNCG) [Quantum-Chemical PC]	Quantum Chemical	M18, M25
51	RNBr	Relative number of Br atoms	Constitutional	M19

52	Mi1ERIC	Min 1-electron react. index for a C atom	Quantum Chemical	M19
53	$ERPCS_Q$	ESP-RPCS Relative positive charged SA (SAMPOS*RPCG) [Quantum-Chemical PC]	Quantum Chemical	M20
54	$EFPSA1_Q$	ESP-FPSA-1 Fractional PPSA (PPSA-1/TMSA) [Quantum-Chemical PC]	Quantum Chemical	M21
55	ANRIO	Avg nucleoph. react. index for a O atom	Quantum Chemical	M21
56	MaERC	Max electroph. react. index for a C atom	Quantum Chemical	M21
57	MiPC	Min partial charge (Qmin)	Electrostatic	M22
58	Ma1ERIC	Max 1-electron react. index for a C atom	Quantum Chemical	M22
59	MaenACO	Max e-n attraction for a C-O bond	Quantum Chemical	M22
60	ANRIN	Avg nucleoph. react. index for a N atom	Electrostatic	M23
61	$HDCA1_Q$	HA dependent HDCA-1/TMSA [Quantum-Chemical PC]	Quantum Chemical	M23
62	SIC2	Structural Information content (order 2)	Topological	M24
63	$FPSA3_Q$	FPSA-3 Fractional PPSA (PPSA-3/TMSA) [Quantum-Chemical PC]	Quantum Chemical	M24
64	ABOC	Avg bond order of a C atom	Quantum Chemical	M25, S9
65	EMaNAC	ESP-Max net atomic charge	Quantum Chemical	M25
66	CIC2	Complementary Information content (order 2)	Topological	M26
67	AVN	Avg valency of a N atom	Quantum Chemical	M26
68	MiRECN	Min resonance energy for a C-N bond	Quantum Chemical	M26
69	HOMO1E	HOMO-1 energy	Quantum Chemical	M27

70	MaTICH	Max total interaction for a C-H bond	Quantum Chemical	M27
71	$EFHDSA_Q$	ESP-FHDSA Fractional HDSA (HDSA/TMSA) [Quantum-Chemical PC]	Quantum Chemical	M27
72	$MiPCN_Z$	Min partial charge for a N atom [Zefirov's PC]	Electrostatic	M28
73	EE+eeR-CC	exch. eng. + e-e rep. for a C-C bond	Quantum Chemical	M28
74	$EFHDCA_Q$	ESP-FHDCA Fractional HDCA (HDCA/TMSA) [Quantum-Chemical PC]	Quantum Chemical	M28
75	MaASEN	Max atomic state energy for a N atom	Quantum Chemical	M29
76	RNCl	Relative number of Cl atoms	Constitutional	M29, S5
77	$HDSA_Q$	HDSA H-donors surface area [Quantum-Chemical PC]	Quantum Chemical	M29
78	IOKSE	Image of the Onsager-Kirkwood solvation energy	Quantum Chemical	M30
79	$EFHBSA_Q$	ESP-FHBSA Fractional HBSA (HBSA/TMSA) [Quantum-Chemical PC]	Quantum Chemical	M30
80	RNN	Relative number of N atoms	Constitutional	M30, S15
81	VE/T	Vib entropy (300K)	Thermodynamical	S1
82	$WPSA3_Q$	WPSA-3 Weighted PPSA (PPSA3*TMSA/1000) [Quantum-Chemical PC]	Quantum Chemical	S1
83	RNBR	Relative number of benzene rings	Constitutional	S2
84	PMIA	Principal moment of inertia A	Geometrical	S2
85	$PPSA3_Z$	PPSA-3 Atomic charge weighted PPSA [Zefirov's PC]	Electrostatic	S4
86	$RNCG_Q$	RNCG Relative negative charge (QMNEG/QTMINUS)	Quantum Chemical	S4

		[Quantum-Chemical PC]		
87	EMiNACC	ESP-Min net atomic charge for a C atom	Quantum Chemical	S6
88	$PNSA2_Q$	PNSA-2 Total charge weighted PNSA [Quantum-Chemical PC]	Quantum Chemical	S6
89	$EHBCA_Q$	ESP-HBCA H-bonding charged surface area [Quantum-Chemical PC]	Quantum Chemical	S6
90	PPIB	Principal moment of inertia B	Geometrical	S7
91	$EHDSA_Q$	ESP-HDSA H-donors surface area [Quantum-Chemical PC	Quantum Chemical	S7, S11
92	EMaNACC	ESP-Max net atomic charge for a C atom	Quantum Chemical	S7
93	$MaPCH_Z$	Max partial charge for a H atom [Zefirov's PC]	Electrostatic	S8
94	TE/#A-T	Tot entropy (300K) / # of atoms	Thermodynamical	S8
95	MaREHN	Max resonance energy for a H-N bond	Quantum Chemical	S9
96	MaenACH	Max e-n attraction for a C-H bond	Quantum Chemical	S10
97	HNMVF	Highest normal mode vib frequency	Thermodynamical	S10
98	MaPPBO	Max PI-PI bond order	Quantum Chemical	S10
99	1XGP	1X GAMMA Polarizability (DIP)	Quantum Chemical	S11
100	$DPSA2_Z$	DPSA-2 Difference in CPSAs (PPSA2-PNSA2) [Zefirov's PC]	Quantum Chemical	S11
101	MaeeRN	Max e-e repulsion for a N atom	Quantum Chemical	S12
102	KSI3	Kier shape index (order 3)	Topological	S12
103	MiAOEP	Min atomic orbital electronic population	Quantum Chemical	S13
104	MiBON(0.1)	Min (>0.1) bond order of a N atom	Quantum-Chemical	S13

105	MaTICC	Max total interaction for a C-C bond	Quantum Chemical	S14
106	$EPNSA3_Q$	ESP-PNSA-3 Atomic charge weighted PNSA [Quantum-Chemical PC]	Quantum Chemical	S14
107	MIA	Moment of inertia A	Geometrical	S15
108	FNSA1	FNSA-1 Fractional PNSA (PNSA-1/TMSA) [Quantum-Chemical PC]	Quantum Chemical	S16
109	AIC1	Average Information content (order 1)	Topological	S16

Table S18: Descriptors, experimental and predicted pIC_{50} values and their residuals for compounds in cell line based QSAR model against A498.

No.	MannRCN	ASIC1	$RNCS_z$	Exp.	Pred.	Res.
326	154.4330	0.5950	11.0535	-0.0223	0.467	0.4893
327	154.1900	0.6627	10.6527	2	`1.4358	-0.5642
328	153.6590	0.6642	9.3413	2	1.7758	-0.2242
329	154.5470	0.6851	2.8804	2	2.4345	0.4345
330	157.6390	0.6784	3.2651	1.9031	1.2665	-0.6366
331	154.4750	0.6627	10.3384	0.4771	1.3736	0.8965
332	154.6000	0.6642	9.2859	0.301	1.4643	1.1633
333*	158.9140	0.6784	3.5413	0.4771	0.8064	0.3293
334*	154.4430	0.7213	4.6920	2	2.7249	0.7249
335	154.3080	0.6871	4.3282	2	2.3831	0.3831
336	154.3960	0.6735	10.4984	1.7782	1.5179	-0.2603
337	154.4540	0.6627	9.7664	2	1.4426	-0.5574
338	158.4580	0.6947	8.7158	-0.3979	0.6034	1.0013
339	157.3900	0.6819	5.2913	1.301	1.1751	-0.1259
340	157.3850	0.6904	5.5157	0.8451	1.2585	0.4134

341	157.2250	0.7106	6.9432	-0.3979	1.4093	1.8072
342	159.2460	0.6330	0.8085	1.301	0.4243	-0.8767
343*	154.6180	0.6993	8.2728	2	2.0042	0.0042
344	153.8480	0.6703	7.6913	2	1.9656	-0.0344
345	153.8300	0.6272	7.1758	1.0792	1.4913	0.4121
346	153.8930	0.6300	4.3896	2	1.8051	-0.1949
347	154.3670	0.5932	0.9442	2	1.5593	-0.4407
348	153.6010	0.6451	6.5664	1.7782	1.8569	0.0787
349	153.6360	0.6776	8.0969	1.6021	2.0847	0.4826
350*	153.5790	0.6810	1.1981	2	2.8919	0.8919
351*	157.8590	0.6477	1.1987	1.301	1.0324	-0.2686
352	153.6150	0.5328	1.0196	1	1.0531	0.0531
353	159.6640	0.6260	1.4704	0.6021	0.1247	-0.4774
354	159.7700	0.6348	1.5167	-0.2218	0.1927	0.4145
355	158.1680	0.6178	0.7207	0.699	0.6082	-0.0908
356	157.0180	0.6002	0.3500	0.8451	0.8172	-0.0279
357	159.8050	0.6742	0.7928	2	0.7499	-1.2501

358	159.6770	0.6631	1.1022	-1.0458	0.6214	1.6672
359	152.2110	0.7227	7.4154	-0.2218	3.2003	3.4221
360	162.6270	0.6720	0.7295	0.1761	-0.2219	-0.398
361	157.3480	0.6310	0.5576	0.301	1.0672	0.7662

Table S19: Descriptors, experimental and predicted pIC_{50} values and their residuals for compounds in cell line based QSAR model against A549.

No.	MaenACC	$PNSA1_Q$	$PNSA2_z$	Exp.	Pred.	Res
414	261.423	171.2511	-91.3019	0.3424	0.593	0.2506
415	261.316	160.266	-85.2422	0.1139	0.531	0.4171
416	261.343	153.9007	-79.1007	0.0414	0.5042	0.4628
417	261.274	171.0708	-88.8451	0.9868	0.6299	-0.3569
418	260.658	206.3617	-115.592	0.7076	0.8969	0.1893
419	260.848	154.7965	-69.7081	0.2304	0.6532	0.4228
420	260.808	208.1646	-107.741	0.9031	0.9597	0.0566
421	260.817	135.274	-111.754	0.0414	0.105	0.0636
422	261.397	177.588	-64.2779	1.1523	0.8814	-0.2709
423	261.317	181.9742	-72.8172	1.1367	0.8738	-0.2629
424	261.139	150.4646	-66.0393	1.3979	0.5953	-0.8026
425*	261.208	200.5765	-97.1994	1.3979	0.9051	-0.4928
426	261.217	148.515	-81.4907	0.6128	0.4411	-0.1717
427	261.267	170.4401	-95.9602	1.1038	0.5674	-0.5364

428	261.27	209.9088	-141.704	0.2304	0.6506	0.4202
429	260.822	196.7997	-107.75	0.0719	0.8296	0.7577
430	260.835	204.8595	-108.047	0.9912	0.9165	-0.0747
431	260.66	191.6159	-95.4948	1.0864	0.8892	-0.1972
432	260.734	249.8832	-134.03	1.3979	1.232	-0.1659
433*	260.871	195.2115	-94.0402	1.3979	0.9136	-0.4843
434*	260.786	238.5806	-119.438	1.3979	1.2131	-0.1848
435	260.875	166.9031	-123.843	0.8109	0.3585	-0.4524
436	260.777	213.3736	-79.7869	1.3979	1.2433	-0.1546
437	260.515	224.7776	-90.7646	1.3979	1.3194	-0.0785
438	260.667	246.3548	-116.128	1.3979	1.3424	-0.0555
439	260.783	184.8005	-98.8033	0.7853	0.7701	-0.0152
440	260.693	215.358	-124.847	1.3979	0.9206	-0.4773
441	260.835	229.0678	-146.671	0.9867	0.8842	-0.1025
442*	260.923	206.1745	-88.4216	1.3979	1.0748	-0.3231
443*	260.765	191.0396	-95.774	1.3979	0.8668	-0.5311
444	260.83	190.5414	-107.976	1.3979	0.7562	-0.6417

445	260.488	235.8448	-86.4319	1.0969	1.4819	0.385
446	260.777	222.2045	-93.5186	1.3979	1.2344	-0.1635
447	260.457	236.5611	-79.9649	1.3979	1.5452	0.1473
448	260.676	190.8362	-86.2357	1.3979	0.9515	-0.4464
449	260.387	182.5772	-83.7233	1.3979	0.9159	-0.482
450*	260.835	203.2951	-114.341	1.3979	0.8491	-0.5488
451	260.816	195.2414	-102.667	0.4624	0.853	0.3906
452	257.672	170.9432	-86.5356	0.2553	1.1173	0.862
453	257.838	164.8768	-88.1404	1.0682	1.0145	-0.0537
454	257.888	151.1524	-75.3744	1.1303	0.9541	-0.1762
455	256.761	164.4297	-77.8796	1.3979	1.2313	-0.1666
456	255.789	183.7247	-63.8729	1.3979	1.6865	0.2886
457	256.828	175.5372	-64.0718	1.0864	1.4569	0.3705
458	258.192	191.3924	-118.9	1.3979	1.0242	-0.3737
459	257.628	155.2623	-82.7454	0.9191	0.9762	0.0571
460*	258.004	175.7417	-98.6644	1.3979	1.0322	-0.3657
461*	256.752	193.5108	-122.192	1.2788	1.2102	-0.0686

462	256.902	162.6538	-75.2191	1.3979	1.2139	-0.184
463	257.018	152.9572	-75.0975	1.3979	1.0903	-0.3076
464	255.721	172.4878	-82.0234	1.3979	1.4253	0.0274
465	258.002	158.9453	-66.7141	1.3979	1.0955	-0.3024
466	256.06	167.2496	-59.0152	1.3979	1.5037	0.1058
467	257.935	161.7632	-83.6558	1.0874	1.0022	-0.0852
468	259.016	211.1635	-129.276	1.1483	1.0575	-0.0908
469*	255.919	199.951	-107.308	1.3979	1.5093	0.1114
470*	257.42	215.8347	-129.988	1.3979	1.313	-0.0849
471	259.076	208.3198	-108.409	0.9552	1.1824	0.2272
472	257.415	220.5864	-110.494	1.3979	1.5213	0.1234
473	256.256	196.5063	-110.396	1.3979	1.402	0.0041
474	258.892	178.8875	-99.8534	0.2788	0.9422	0.6634
475	256.539	168.4693	-86.4938	1.3979	1.2378	-0.1601
476	257.503	171.3202	-91.6633	0.9191	1.1031	0.184
477	258.914	189.5578	-103.702	0.7566	1.0293	0.2727
478	257.514	178.436	-79.2919	1.3979	1.2797	-0.1182

479	256.451	162.2917	-69.6889	1.3979	1.3124	-0.0855

Table S20: Descriptors, experimental and predicted pIC_{50} values and their residuals for compounds in cell line based QSAR model against A2780.

No.	MiNRIO	$HACA1_Q$	RPCSz	Exp.	Pred.	Res.
42	2.02E-05	22.0842	0.4882	1	1.0421	0.0421
43	2.80E-05	21.8028	0.465	1	1.069	0.069
44	7.67E-05	20.5314	0.4429	1	1.2518	0.2518
45	5.35E-05	20.4226	0.0746	1	1.1637	0.1637
46	3.85E-05	21.5081	0.2692	1	1.1284	0.1284
47*	4.95E-05	20.5686	0.2092	1	1.1359	0.1359
48	1.11E-04	22.2463	0.1855	1.699	1.5691	-0.1299
49	1.15E-04	22.2491	0.1715	1.6435	1.5918	-0.0517
50	1.14E-04	21.8847	0.2659	1.6021	1.5541	-0.048
51	9.66E-05	20.7713	0.1025	1.5441	1.4103	-0.1338
52	9.70E-05	21.1664	0.1804	1	1.4278	0.4278
53	8.59E-05	21.5117	0.3213	1.8261	1.3744	-0.4517
54	8.82E-05	19.2939	0.1518	1	1.2694	0.2694
55	1.64E-04	21.4858	0.304	1.6021	1.7903	0.1882

56*	2.21E-08	26.9172	2.8236	1	0.9695	-0.0305
57	1.59E-05	38.2823	1.158	2	1.9368	-0.0632
58	3.69E-05	31.3476	3.5336	1.1761	1.3566	0.1805
59	2.78E-07	28.5397	3.2171	1.2553	1.0261	-0.2292
60	2.40E-05	26.3508	3.5375	1	0.9819	-0.0181
61	6.42E-05	20.8775	3.4873	1	0.8653	-0.1347
62	2.29E-05	25.8282	3.4599	1	0.9527	-0.0473
63	6.68E-09	24.1446	1.1651	1	0.9856	-0.0144
64*	1.41E-05	28.4044	2.5412	1.716	1.1671	-0.5489
65	6.04E-05	18.4866	0.1269	0.8451	1.0753	0.2302
66	1.07E-05	21.9549	0.1076	1	1.0267	0.0267
67	9.65E-07	20.4514	0.1554	1	0.8776	-0.1224
68*	5.12E-05	18.5475	0.4758	1.9542	0.9913	-0.9629
69	2.57E-05	26.9492	3.033	1.1761	1.0842	-0.0919
70	1.35E-04	17.3504	0.4285	1.7243	1.3658	-0.3585
71	8.54E-05	26.57	3.4867	1	1.3262	0.3262
72	7.27E-07	18.2531	0.2437	1.301	1.7317	0.4307

73	2.84E-07	16.5904	0.203	1.4624	0.9321	-0.5303
74*	3.88E-07	22.5529	0.0646	1.2553	1.0135	-0.2418
75	2.16E-05	41.2281	1.2086	1.4914	1.142	-0.3494
76	0.00E+00	38.683	0.1015	1.2788	0.9959	-0.2829

Table S21: Descriptors, experimental and predicted pIC_{50} values and their residuals for compounds in cell line based QSAR model against ACHN.

No.	FPSA3z	WNSA2z	BI	Exp.	Pred	Res
77	0.0171	-54.0101	2.2112	1.9685	1.8122	-0.1563
78	0.0171	-53.8129	2.2032	1.6435	1.5184	-0.1251
79	0.0192	-71.6674	2.1776	1.6532	1.6439	-0.0093
80	0.0165	-80.6252	2.2032	1.4472	1.4843	0.0371
81	0.016	-77.6961	2.2032	1.3979	1.4272	0.0293
82	0.0188	-63.6449	2.2032	1.5441	1.5246	-0.0195
83*	0.0165	-76.5074	2.2265	1.6812	1.5311	-0.1501
84	0.0166	-75.825	2.252	1.4477	1.4078	-0.0399
85	0.0162	-96.9422	2.2583	1.5441	1.5377	-0.0064
86	0.0214	-74.9107	2.2773	1.6812	1.7305	0.0493
87	0.0163	-73.2411	2.204	1.4472	1.4092	-0.038
88	0.0193	-68.0193	2.2941	1.5185	1.5044	-0.0141
89	0.019	-70.5591	2.2801	1.2304	1.1138	-0.1166
90*	0.021	-90.5589	2.251	1.9638	1.8493	-0.1145

91	0.0223	-88.9774	2.2801	1.9191	1.9027	-0.0164
92	0.0185	-102.932	2.2801	1.7559	1.7298	-0.0261
93	0.018	-102.775	2.2801	1.6812	1.6959	0.0147
94	0.0226	-92.3107	2.3342	1.8976	1.8969	-0.0007
95*	0.0184	-96.3458	1.7889	1.9956	2.0711	0.0755

Table S22: Descriptors, experimental and predicted pIC_{50} values and their residuals for compounds in cell line based QSAR model against A431.

No.	YZS	RI0	MiERIC	Exp.	Pred	Res
42	34.1804	9.8699	4.90E-08	1	1.0773	0.0773
43	36.1404	10.577	1.34E-08	1	1.0045	0.0045
44	40.0205	11.2841	1.29E-07	1	0.8041	-0.1959
45	34.9004	11.4472	1.70E-07	1	1.1937	0.1937
46	38.2805	12.6983	9.61E-10	1	1.0634	0.0634
47	36.4805	12.2757	2.87E-09	1	1.1509	0.1509
48	33.6804	14.1125	0.00E+00	1.7853	1.5388	-0.2465
49	33.8404	15.5267	0.00E+00	1.716	1.6702	-0.0458
50	39.3405	16.9409	0.00E+00	1.5441	1.4157	-0.1284
51	38.0405	18.0707	0.00E+00	1.6721	1.6239	-0.0482
52	50.4008	20.8991	0.00E+00	1	1.0165	0.0165
53	35.3204	10.9996	2.88E-06	1.5051	1.319	-0.1861
54	38.5205	11.7067	1.87E-07	1	0.9596	-0.0404
55	34.6204	10.8614	5.78E-09	1.6021	1.4426	-0.1595
56	40.5405	13.2841	1.52E-07	1	0.9705	-0.0295

57	34.9604	12.577	1.76E-06	1.7782	1.4214	-0.3568
58	34.6204	10.9996	2.74E-06	1	1.3595	0.3595
59	41.2406	13.8281	2.15E-09	0.7782	0.9638	0.1856
60	37.0005	11.8699	1.09E-06	1	1.1527	0.1527
61	39.5805	12.7925	1.39E-06	1	1.0821	0.0821
62	41.8206	12.577	8.09E-08	1	0.8012	-0.1988
63	39.9805	13.2841	5.16E-08	1	1.0035	0.0035
64*	40.9006	14.2757	1.25E-08	1.0414	1.0344	-0.007
65	38.1805	12.6983	4.98E-06	1.4771	1.44	-0.0371
66	36.1804	14.1125	1.18E-07	1	1.3669	0.3669
67*	39.2805	14.8196	1.08E-09	1	1.2056	0.2056
68	36.9005	12.6983	2.90E-06	1.3979	1.3779	-0.02
69	36.4605	13.5685	3.28E-06	1.4314	1.5262	0.0948
70	36.5405	15.1459	2.28E-06	1.1139	1.6054	0.4915
71	36.4005	15.1459	3.09E-06	1	1.6755	0.6755
72*	41.8006	14.9828	5.48E-08	1.1461	1.044	-0.1021
73*	45.1007	16.5601	5.73E-08	1	0.9651	-0.0349

74	41.4206	14.2757	1.97E-06	1	1.1422	0.1422
75*	48.8007	19.878	0.00E+00	1	1.0289	0.0289
76	70.0012	25.6561	0.00E+00	1.2553	1.0808	-0.1745

Table S23: Descriptors, experimental and predicted pIC_{50} values and their residuals for compounds in cell line based QSAR model againstB16-F10.

No.	WPSA1Q	MiTICS	MiNACN	Exp.	Pred	Res
261	338.7753	13.976	-0.1482	0.5999	0.6404	0.0405
262	380.6836	13.967	-0.1477	0.5809	0.3747	-0.2062
263	338.255	13.977	-0.1486	0.5809	0.5648	-0.0161
264	382.7879	13.969	-0.1484	0.179	0.2017	0.0227
265	405.1514	13.983	-0.149	-0.4949	-0.4116	0.0833
266	449.6217	13.974	-0.1492	-0.9208	-0.8204	0.1004
267	397.4221	13.96	-0.1481	0.1818	0.2327	0.0509
268*	404.5464	13.963	-0.1482	0.143	0.0777	-0.0653
269	409.921	13.945	-0.1466	0.4265	0.5879	0.1614
270	455.3469	13.937	-0.1463	0.4048	0.2301	-0.1747
271	379.1116	13.961	-0.1469	0.6464	0.6281	-0.0183
272	415.328	13.93	-0.1472	0.6138	0.6918	0.078
273	413.3936	13.934	-0.1485	0.4942	0.4359	-0.0583
274	411.8955	13.931	-0.1477	0.3324	0.6353	0.3029

275*	482.0564	13.933	-0.1492	-0.3492	-0.4862	-0.137
276	483.4664	13.936	-0.1486	-0.3665	-0.46	-0.0935
277	476.4405	13.905	-0.1476	0.4579	0.3333	-0.1246
278	476.2962	13.912	-0.147	0.2253	0.3075	0.0822
279	487.9049	13.892	-0.1465	0.4786	0.6015	0.1229
280*	483.3835	13.897	-0.146	0.4014	0.6478	0.2464

Table S24: Descriptors, experimental and predicted pIC_{50} values and their residuals for compounds in cell line based QSAR model against BE2-C.

No.	XYS/XYR	MiERIC	RNO	Exp.	Pred	Res
42	0.6727	4.90E-08	0.1111	1	1.1092	0.1092
43	0.697	1.34E-08	0.1	1	1.057	0.057
44	0.7091	1.29E-07	0.0909	1	1.0752	0.0752
45*	0.6717	1.70E-07	0.0909	1	1.2692	0.2692
46	0.6778	9.61E-10	0.0769	1	1.3084	0.3084
47	0.6803	2.87E-09	0.0811	1	1.2677	0.2677
48	0.6439	0.00E+00	0.0667	1.8325	1.5482	-0.2843
49	0.6345	0.00E+00	0.0588	1.5911	1.6486	0.0575
50	0.6336	0.00E+00	0.0526	1.6021	1.6954	0.0933
51*	0.6605	0.00E+00	0.05	1.699	1.5779	-0.1211
52	0.5372	0.00E+00	0.0417	1	1.2544	0.2544
53*	0.6429	2.88E-06	0.1071	1.7924	1.7094	-0.083
54	0.6638	1.87E-07	0.0968	1	1.2717	0.2717
55	0.6704	5.78E-09	0.0968	1.301	1.2114	-0.0896

56	0.6474	1.52E-07	0.1429	1	1.0363	0.0363
57*	0.6855	1.76E-06	0.1562	1.8633	1.9943	0.131
58	0.6398	2.74E-06	0.1429	1	1.4623	0.4623
59	0.6717	2.15E-09	0.1	1.3424	1.1825	-0.1599
60	0.6856	1.09E-06	0.129	1	1.0778	0.0778
61	0.7028	1.39E-06	0.1176	1	1.1146	0.1146
62	0.7274	8.09E-08	0.1176	1	0.7947	-0.2053
63	0.6998	5.16E-08	0.1471	1	1.329	0.329
64	0.6956	1.25E-08	0.1282	1.3424	1.5726	0.2302
65	0.7099	4.98E-06	0.1176	1.5911	1.6169	0.0258
66	0.7378	1.18E-07	0.1	1	0.8677	-0.1323
67	0.7168	1.08E-09	0.093	1	1.0029	0.0029
68	0.7013	2.90E-06	0.0968	1.7324	1.4892	-0.2432
69*	0.7164	3.28E-06	0.125	1.1461	1.2794	0.1333
70	0.7457	2.28E-06	0.1515	1.6532	1.8018	0.1486
71	0.7243	3.09E-06	0.1471	1	1.0604	0.0604
72	0.6712	5.48E-08	0.1053	1.4624	1.1573	-0.3051

73	0.6614	5.73E-08	0.119	1.0414	1.1135	0.0721
74	0.7306	1.97E-06	0.0833	1.1139	1.295	0.1811
75*	0.6278	0.00E+00	0.1224	1	1.2506	0.2506
76*	0.5067	0.00E+00	0.0789	1.2304	1.1545	-0.0759

Table S25: Descriptors, experimental and predicted pIC_{50} values and their residuals for compounds in cell line based QSAR model againstBEL-7402.

No.	HLEG	$WNSA3_Q$	MiERIN	Exp.	Pred	Res
281	8.451	-16.5582	1.71E-03	0.0086	0.0516	0.043
282	8.492	-15.1273	1.31E-03	0.1553	0.266	0.1107
283	8.452	-17.0474	3.28E-04	0.7782	0.7583	-0.0199
284	8.348	-19.9014	3.98E-04	-0.1739	0.6235	0.7974
285*	8.257	-29.489	3.80E-03	1	0.6874	-0.3126
286	8.273	-27.6389	3.61E-03	1	0.6665	-0.3335
287	8.304	-26.7546	4.36E-04	1	0.9071	-0.0929
288	8.336	-25.9124	3.54E-04	1	0.9799	-0.0201
289	8.92	-15.5706	1.65E-03	1	1.2594	0.2594
290	8.453	-17.9843	2.80E-04	1	0.8411	-0.1589
291	8.358	-16.0522	2.44E-04	1	0.4902	-0.5098
292*	8.686	-16.4072	1.89E-03	1	0.576	-0.424
293	8.659	-21.1402	1.36E-03	1	1.0511	0.0511
294	8.476	-24.7757	2.82E-04	1	1.3153	0.3153
295	8.598	-13.8158	1.52E-03	1	0.3657	-0.6343

296	8.297	-25.7868	5.53E-04	1	0.7727	-0.2273
297	8.227	-29.6726	4.24E-04	1	0.8877	-0.1123
298	8.131	-16.8907	1.20E-03	1	0.5219	-0.4781
299	8.128	-21.0037	3.41E-04	1	0.138	-0.862
300	8.632	-25.7867	1.20E-03	1	1.3435	0.3435
301	8.345	-29.6388	2.82E-04	1	1.2664	0.2664
302	8.35	-22.5543	3.63E-04	1	0.808	-0.192
303	7.759	-20.2057	3.66E-04	-1.0458	-0.8964	0.1494
304	8.392	-14.6859	1.73E-03	-1	-0.2273	0.7727
305*	8.309	-18.1568	3.67E-04	-0.9208	-0.4292	0.4916
306*	8.376	-19.9532	5.11E-04	0.6128	0.6455	0.0327
307	8.485	-16.877	1.79E-03	1	0.1242	-0.8758
308	8.393	-21.1348	4.69E-04	1	0.7829	-0.2171
309	8.764	-13.8101	8.80E-04	1	1.1152	0.1152
310	8.454	-16.8369	3.61E-04	1	0.7345	-0.2655
311*	8.77	-13.3731	1.77E-03	1	0.6719	-0.3281
312*	8.597	-16.9518	3.88E-04	1	1.1059	0.1059

313	8.319	-20.6027	5.00E-04	-0.6198	0.5404	1.1602
314	8.329	-25.6415	3.57E-04	1	0.9436	-0.0564
315	8.34	-20.8232	4.02E-04	1	0.657	-0.343
316	8.31	-23.1416	3.91E-04	1	0.7244	-0.2756
317	8.333	-21.7099	3.93E-04	1	0.6969	-0.3031
318	8.335	-25.0224	3.89E-04	1	0.9061	-0.0939
319*	3.977	-28.0261	4.10E-04	1	1.4199	0.4199
320	8.327	-24.0945	3.92E-04	1	0.827	-0.173
321	8.332	-23.0316	3.97E-04	1	0.7727	-0.2273
322	8.382	-22.6495	3.50E-04	1	0.9042	-0.0958
323*	8.378	-32.6649	3.98E-04	1	1.4813	0.4813
324*	8.327	-24.9202	2.12E-08	1	1.0682	0.0682
325*	8.324	-35.6386	5.26E-04	1	1.458	0.458

Table S26: Descriptors, experimental and predicted pIC_{50} values and their residuals for compounds in cell line based QSAR model against Calu1.

No.	A1ERIC	SIC1	YZS	Exp.	Pred	Res
77	3.58E-05	19.998	41.8006	1.959	1.9888	0.0298
78	-3.11E-05	22.5944	42.1206	1.5682	1.2465	-0.3217
79	4.08E-05	22.1541	42.5606	1.4914	1.5266	0.0352
80	-2.01E-05	21.7463	42.9406	1.4472	1.4926	0.0454
81	6.28E-05	21.7463	34.5804	1.3222	1.4251	0.1029
82	1.62E-05	21.7463	42.4006	1.4771	1.5591	0.082
83	-1.26E-06	21.7463	42.9006	1.5682	1.5346	-0.0336
84	3.43E-05	21.7463	46.2807	1.5798	1.7202	0.1404
85	-7.67E-06	22.6498	46.2207	1.4771	1.4137	-0.0634
86	6.97E-05	23.7544	54.5009	1.501	1.5913	0.0903
87	1.76E-04	23.5771	43.3406	1.5798	1.5321	-0.0477
88	-2.95E-04	22.1541	39.9605	0.8451	0.6771	-0.168
89	-2.79E-04	24.4248	39.8205	0	0.1855	0.1855
90	2.65E-04	23.7544	49.7008	1.9685	1.8915	-0.077
91*	-2.86E-04	24.2855	39.3805	1.8808	1.7905	-0.0903

92	2.98E-04	23.7834	39.1805	1.8261	1.6375	-0.1886
93	-3.00E-04	23.7834	39.0405	1.7559	1.5346	-0.2213
94*	2.61E-04	24.9572	48.3807	1.7634	1.5631	-0.2003
95*	-2.89E-04	25.6242	40.6405	2	1.8425	-0.1575

Table S27: Descriptors, experimental and predicted pIC_{50} values and their residuals for compounds in cell line based QSAR model against DU145.

No.	MiTICN	PNSA1Z	CHaSz	Exp.	Pred.	Res.
42	14.699	107.2981	3	1	1.7094	0.7094
43*	14.72	103.2483	3	1	1.7558	0.7558
44	14.718	92.2656	3	1	1.8403	0.8403
45*	14.569	106.5297	3	1	1.6242	0.6242
46*	14.744	108.1385	3	1	1.7343	0.7343
47	14.645	98.6991	3	1	1.7388	0.7388
48	14.747	112.8626	3	1.6435	1.6995	0.056
49	14.747	116.0671	3	1.9191	1.6744	-0.2447
50	14.748	114.2921	3	1.8195	1.689	-0.1305
51	14.706	164.1742	3	1.8633	1.2692	-0.5941
52	14.705	164.6286	3	1	1.265	0.265
53	14.716	183.5636	3	1.1761	1.1245	-0.0516
54	14.744	171.2901	3	1	1.2402	0.2402
55	14.89	124.665	3	1.3424	1.7074	0.365
56*	14.847	171.1443	4	1	1.0366	0.0366

57	14.689	192.5805	5	1.8261	0.4812	-1.3449
58*	14.842	178.0031	4	1	0.9794	-0.0206
59*	14.7	171.8004	4	1	0.9284	-0.0716
60*	14.656	166.9619	4	1	0.9354	-0.0646
61	14.364	149.9701	4	1	0.8637	-0.1363
62	14.685	164.2536	4	1	0.977	-0.023
63	14.681	196.5741	4	1	0.7213	-0.2787
64	14.878	165.4281	4	1.0792	1.1031	0.0239
65	13.898	161.7631	4	0.4771	0.4447	-0.0324
66	14.543	175.271	4	1	0.7912	-0.2088
67	14.447	168.8857	4	1	0.7739	-0.2261
68	16.018	205.2147	3	1.3802	1.8679	0.4877
69	15.937	227.086	4	1	1.3631	0.3631
70	14.463	232.9966	3	1.1139	0.5603	-0.5536
71	16.289	266.7717	4	1	1.2993	0.2993
72	14.702	197.2522	3	1	1.0076	0.0076
73	14.739	182.2387	3	1.0792	1.151	0.0718

74	14.571	205.2898	4	1	0.5759	-0.4241
75*	14.479	248.3546	7	1.1139	-0.6563	-1.7702
76*	14.709	267.8594	6	1.7782	-0.3707	-2.1489
326	15.963	227.6819	4	-0.0223	1.3766	1.3989
327*	16.04	270.646	4	2	1.0944	-0.9056
328	14.407	228.644	4	2	0.2782	-1.7218
329	15.973	184.9705	4	2	1.7179	-0.2821
330	15.734	208.0064	5	1.9031	1.0931	-0.81
331	15.886	264.9488	4	0.4771	1.031	0.5539
332	14.618	229.0827	4	0.301	0.4227	0.1217
333	16.064	223.0397	5	0.4771	1.2069	0.7298
334	15.9	204.8286	4	2	1.5113	-0.4887
335	16.046	200.4955	4	2	1.6476	-0.3524
336	15.979	218.9873	4	1.7782	1.4559	-0.3223
337	15.918	242.2251	4	2	1.2313	-0.7687
338	15.961	244.5868	6	-0.3979	0.6891	1.087
339*	16.045	228.6476	6	1.301	0.8727	-0.4283

340*	16.044	231.0631	6	0.8451	0.8531	0.008
341	16.015	288.9014	6	-0.3979	0.3802	0.7781
342*	14.446	240.1948	8	1.301	-1.5488	-2.8498
343*	15.715	254.6447	4	2	1.857	-0.143
344	16.146	204.7002	4	2	1.6848	-0.3152
345	16.138	204.0933	4	1.0792	1.6839	0.6047
346	16.125	174.4254	4	2	1.9069	-0.0931
347	16.204	247.158	4	2	1.3932	-0.6068
348	16.181	219.2268	4	1.7782	1.5956	-0.1826
349	16.183	212.7894	4	1.6021	1.6474	0.0453
350	16.188	222.2896	3	2	1.8535	-0.1465
351	16.101	277.2948	6	1.301	0.5313	-0.7697
352	16.228	329.3829	3	1	1.0435	0.0435
353	14.674	202.5498	4	0.6021	0.6696	0.0675
354	14.644	192.6776	4	-0.2218	0.7258	0.9476
355	14.346	191.3739	4	0.699	0.5271	-0.1719
356	14.382	199.4687	4	0.8451	0.489	-0.3561

357	14.569	205.8656	4	2	1.9347	-0.0653
358	14.573	212.4561	4	-1.0458	-0.9834	0.0624
359	14.559	238.4109	4	-0.2218	-0.1993	0.0225
360	15.562	245.075	4	0.1761	0.1356	-0.0405
361*	14.545	250.4525	4	0.301	0.2043	-0.0967

Table S28: Descriptors, experimental and predicted pIC_{50} values and their residuals for compounds in cell line based QSAR model against H69.

No.	FNSA2z	$ERPCG_Q$	MienACH	Exp.	Pred.	Res.
196	-0.2732	0.0683	66.929	-1.4559	-1.4226	0.0333
197	-0.2357	0.0621	66.958	-1.4559	-1.5004	-0.0445
198	-0.2306	0.061	66.946	-1.3098	-1.4883	-0.1785
199	-0.2299	0.0677	66.915	-0.3767	-0.8742	-0.4975
200	-0.29	0.0507	66.948	-0.2549	-0.2113	0.0436
201	-0.2758	0.0745	66.438	-1.3979	-1.4944	-0.0965
202	-0.3074	0.0742	66.558	-1.5528	-1.1837	0.3691
203	-0.295	0.0621	67.033	-0.2314	-0.194	0.0374
204	-0.2841	0.0738	66.935	-1.6198	-1.6237	-0.0039
205	-0.309	0.0677	67.007	-1.1938	-1.0198	0.174
206	-0.2698	0.0582	66.961	-1.0458	-0.8863	0.1595
207	-0.2991	0.0579	67.034	-0.5186	-0.5737	-0.0551
208*	-0.3411	0.0602	66.962	-1.4089	-1.5623	-0.1534
209	-0.3011	0.0747	67.036	-1.3468	-1.5326	-0.1858
210	-0.3613	0.0794	67.033	-1.0506	-1.1195	-0.0689

211	-0.3778	0.0635	66.196	0.5848	0.4385	-0.1463
212*	-0.2552	0.057	66.904	-0.9335	-0.9536	-0.0201
213*	-0.2865	0.0565	66.873	-1.0044	-1.1498	-0.1454

Table S29: Descriptors, experimental and predicted pIC_{50} values and their residuals for compounds in cell line based QSAR model against H522.

No.	MiPCCz	MiBOC(0.1)	THCMD	Exp.	Pred.	Res.
326	-0.0142	0.1024	0.986	1.1761	1.5301	0.354
327	-0.0142	0.1026	0.732	2	1.3438	-0.6562
328	-0.0142	0.1028	1.045	2	1.6813	-0.3187
329	-0.0142	0.1024	0.975	2	1.5211	-0.4789
330	-0.0142	0.1023	1.342	1.7782	1.8094	0.0312
331	-0.014	0.1023	1.17	-0.1549	-0.1386	0.0163
332*	-0.014	0.1017	1.008	0.6812	0.5964	-0.0848
333*	-0.014	0.1037	1.003	0.699	0.5843	-0.1147
334	-0.0139	0.1028	1.118	2	1.7803	-0.2197
335	-0.014	0.1034	1.326	2	2.0856	0.0856
336	-0.0281	0.1006	0.996	-0.8239	-0.9346	-0.1107
337	-0.014	0.1022	0.984	2	1.5167	-0.4833
338	-0.014	0.1009	0.654	0.699	0.8993	0.2003
339	-0.0316	0.1033	0.254	1.2601	1.4679	0.2078
340*	-0.0269	0.1033	0.248	1.2553	1.1404	-0.1149

341	-0.014	0.1032	0.328	0.6021	1.1602	0.5581
342	-0.0164	0.1015	0.684	1.1761	0.7124	-0.4637
343	-0.014	0.102	1.406	2	1.8258	-0.1742
344	-0.016	0.1045	1.36	2	2.0754	0.0754
345*	-0.0208	0.1045	1.339	1.1761	1.1264	-0.0497
346*	-0.033	0.1045	1.423	2	1.985	-0.015
347	-0.0165	0.1044	0.925	2	1.5978	-0.4022
348	-0.0148	0.104	0.679	1.699	1.5468	-0.1522
349	-0.0148	0.1041	1.029	0.8451	1.8623	1.0172
350	-0.0148	0.104	0.941	1.9031	1.7682	-0.1349
351	-0.0148	0.1037	1.091	1.3979	1.8383	0.4404
352	-0.0186	0.1041	1.349	1.6532	1.601	-0.0522
353	-0.0172	0.1042	1.438	-0.2218	-0.1956	0.0262
354*	-0.0164	0.1042	1.432	-0.1549	-0.1467	0.0082
355	-0.0234	0.1041	1.265	0.4771	0.8271	0.35
356	-0.0236	0.1042	0.702	0.6021	0.3023	-0.2998
357	-0.0164	0.1003	1.36	0.9542	1.0266	0.0724

358	-0.0172	0.1003	0.745	-0.3979	0.364	0.7619
359	-0.014	0.1004	1.312	-0.1549	-0.1357	0.0192
360*	-0.0164	0.1038	1.4	0.301	0.2976	-0.0034
361*	-0.0266	0.1038	1.746	0.3979	0.3865	-0.0114

Table S30: Descriptors, experimental and predicted pIC_{50} values and their residuals for compounds in cell line based QSAR model against HCT116.

No.	RE/T	LNMVF	ACIC1	Exp.	Pred.	Res.
119	38.7724	10.776	2.0814	-	1.9515	_
120	38.5168	10.566	2.1088	1.8451	1.8871	0.042
121	39.0466	9.824	2.3003	1.8451	2.0982	0.2531
122	39.2518	20.222	2.1346	1.6532	2.421	0.7678
123	38.9031	13.559	2.1122	1.6021	2.094	0.4919
124	39.4132	13.524	2.1872	3	2.2685	-0.7315
125	39.5012	9.429	2.1874	2.0792	2.1574	0.0782
126	39.0382	9.837	2.4748	1.699	2.1781	0.4791
127	38.9257	8.493	1.9328	1.5441	1.8486	0.3045
128*	39.3067	18.155	1.9893	2.1761	2.2996	0.1235
129	39.4705	19.163	2.051	1.699	2.4069	0.7079
130	39.5698	15.956	2.0427	2.0791	2.3243	0.2452
131	38.9283	18.432	1.9328	2.4472	2.1781	-0.2691
132	38.5782	19.65	1.9533	2.6021	2.1316	-0.4705
133	39.1055	18.394	2.145	2.699	2.3251	-0.3739

134	39.3105	19.006	1.9893	2.4771	2.3288	-0.1483
135	38.9164	18.581	1.9552	2.301	2.1902	-0.1108
136	39.4793	17.664	2.051	2.3222	2.3598	0.0376
137*	39.5682	13.483	2.0427	2.3222	2.2421	-0.0801
138*	39.107	18.808	2.3167	2.6812	2.4197	-0.2615
139*	39.3811	8.664	1.7847	1.8451	1.9102	0.0651
140	38.7469	10.012	1.9533	2.6021	1.8592	-0.7429
141	39.2767	22.882	2.145	2.0414	2.5207	0.4793
142	39.582	20.769	1.9893	2.415	2.4618	0.0468
143	39.2147	20.221	1.9552	2.301	2.3266	0.0256
144	39.7615	20.373	2.051	2.0792	2.5271	0.4479
145	39.702	14.313	2.0427	2.3222	2.3064	-0.0158
146	39.2872	9.811	2.3167	2.699	2.1717	-0.5273
147	38.4555	16.482	1.7332	1.8451	1.8898	0.0447
148	38.9777	15.174	1.9395	-	2.087	-
149*	38.841	13.984	1.7346	1.9542	1.9139	-0.0403
150*	38.99	12.65	2.1185	1.9031	2.0909	0.1878

151*	33.4883	47.94	1.9769	1.6232	1.6772	0.054
152*	34.23	45.2	1.9976	1.9605	1.8005	-0.16
153	34.3008	43.207	1.4749	1.8692	1.509	-0.3602
154	34.7942	22.308	1.7964	0.6335	1.1042	0.4707
155	33.9644	22.83	1.7238	1.5717	0.859	-0.7127
156	35.6838	24.426	2.3197	1.3483	1.6646	0.3163
157	35.6385	27.902	2.3197	1.9309	1.7671	-0.1638
158*	33.8792	49.44	1.8224	1.8062	1.762	-0.0442
159*	34.9326	36.869	2.1333	1.8451	1.782	-0.0631
160*	35.0246	32.453	2.1333	1.5527	1.6612	0.1085
161	35.7493	37.734	1.755	1.1367	1.858	0.7213
162	34.8425	56.219	1.755	1.8014	2.2199	0.4185
163	35.1459	30.475	1.755	1.9175	1.4518	-0.4657
164	35.1233	37.856	1.755	1.8531	1.6898	-0.1633
165	34.2996	49.216	1.4166	1.6656	1.6801	0.0145
166	34.6327	48.399	1.608	1.7657	1.8345	0.0688
167	34.9103	30.387	1.5457	0.7243	1.2859	0.5616

168	34.5926	38.002	1.9591	1.7218	1.6441	-0.0777
169	33.4424	52.504	1.9942	1.4425	1.8237	0.3812
170	33.8327	48.868	2.1305	1.7324	1.8748	0.1424
171	35.3259	45.654	1.7925	1.1038	2.0211	0.9173
172	35.377	29.245	1.8529	1.4265	1.5207	0.0942
173	33.8702	40.225	2.1305	1.7427	1.5992	-0.1435
77	34.7347	28.458	2.298	1.9777	1.5265	-0.4512
78	35.1493	22.007	2.2233	1.4914	1.3922	-0.0992
79	35.5189	23.351	2.3744	1.5682	1.6092	0.041
80	35.5899	26.487	2.047	1.3424	1.579	0.2366
81*	35.8617	22.013	2.047	1.5051	1.5058	0.0007
82*	35.2085	27.828	2.047	1.5682	1.5183	-0.0499
83	35.4729	16.612	2.047	1.4314	1.2201	-0.2113
84	35.1709	17.44	2.047	1.3979	1.1644	-0.2335
85	35.896	15.551	1.9172	1.415	1.2406	-0.1744
86	36.0544	15.425	2.512	1.4914	1.559	0.0676
87	35.8501	21.76	1.9919	1.2041	1.4684	0.2643

88	35.256	8.737	2.3744	0	1.0534	1.0534
89	35.626	22.669	2.344	0	1.6019	1.6019
90	36.0486	25.44	2.512	1.9868	1.8887	-0.0981
91	35.6455	26.186	2.1841	1.9731	1.6487	-0.3244
92	36.0329	25.753	2.1576	1.9638	1.7285	-0.2353
93*	36.6422	25.829	2.1576	1.9345	1.8988	-0.0357
94	36.4436	14.902	2.6811	1.9243	1.7281	-0.1962
95	36.2622	15.72	2.1025	1.9956	1.4339	-0.5617

Table S31: Descriptors, experimental and predicted pIC_{50} values and their residuals for compounds in cell line based QSAR model against HeLa.

No.	MaBON	MienACN	NN	Exp.	Pred.	Res.
214	1.1241	318.975	1	0.4771	0.9505	0.4734
215	1.1207	318.892	1	1.2041	0.9803	-0.2238
216	1.1267	319.342	1	0.4771	0.8992	0.4221
217	1.1194	318.895	1	1.2553	0.9885	-0.2668
218	1.1168	318.836	1	0.4771	1.0105	0.5334
219	1.1165	318.844	1	0.4771	1.0121	0.535
220	1.4343	318.918	2	0.8451	-0.2926	-1.1377
221*	1.1265	319.019	1	0.4771	0.5104	0.0333
222*	1.1342	319.461	1	0.301	0.2965	-0.0045
223*	1.1297	319.401	1	0.7782	0.8742	0.096
224*	1.1371	319.498	1	0.301	0.2876	-0.0134
225	1.1285	319.405	1	0.8451	0.8816	0.0365
226	1.1255	319.344	1	0.7782	0.9063	0.1281
227	1.1252	319.36	1	0.4771	0.9068	0.4297
228	1.4341	319.416	2	0.4771	-0.339	-0.8161

229	1.1358	319.5	1	0.4771	0.8255	0.3484
230	1.1246	319.188	1	0.4771	0.9269	0.4498
231	1.129	319.237	1	1.3222	0.8942	-0.428
232	1.1396	319.823	2	-	1.508	-
233	1.1358	319.694	2	1.3222	1.5443	0.2221
234	1.1303	320.382	1	2.7324	2.1457	-0.5867
235*	1.1365	320.396	1	2.6232	2.5689	-0.0543
236	1.1378	319.16	1	1.2553	0.9845	-0.2708
237	1.1371	319.086	1	2	0.8567	-1.1433
238	1.1398	317.549	2	1.2788	1.724	0.4452
239	1.141	317.407	2	2.0569	1.7297	-0.3272
240	1.1296	304.956	3	4	3.7294	-0.2706
241	1.1189	305.161	3	4	3.7778	-0.2222
242	1.3747	315.48	4	2.0969	1.8921	-0.2048
243	1.3733	315.443	4	2.749	2.4589	-0.2901
244*	1.5871	320.207	3	0.699	0.638	-0.061
245	1.6181	320.151	3	0.4771	0.3946	-0.0825

246	1.5865	320.211	3	-0.1249	-0.6532	-0.5283
247	1.6176	320.149	3	-0.1249	-0.846	-0.7211
248	1.5835	320.191	3	0.4771	-0.632	-1.1091
249	1.6155	320.144	3	-1.1249	-0.832	0.2929
250	1.5827	320.261	4	0.4771	0.1041	-0.373
251	1.6143	320.23	4	-1.1249	-0.0956	1.0293
252	1.5834	320.251	3	-1.1249	-0.6371	0.4878
253	1.6149	320.205	3	-1.6021	-0.8341	0.768
254	1.589	320.123	3	-1.4559	-0.6605	0.7954
255	1.6198	320.162	3	-1.6021	-0.8618	0.7403
256*	1.5869	320.191	3	-0.5229	-0.6536	-0.1307
257*	1.6171	320.135	3	-1.301	-1.2789	0.0221
258*	1.6216	320.079	3	0.301	0.2976	-0.0034
259	1.6169	320.18	3	-1.699	-0.8445	0.8545
260	1.6171	320.382	3	0.0607	-0.8655	-0.9262
174	1.4559	299.637	1	1.5798	0.6736	-0.9062
175	1.4564	299.891	1	1.2553	0.6459	-0.6094

176	1.4553	300.308	1	0.301	0.6135	0.3125
177*	1.4542	300.176	1	0.4771	0.5013	0.0242
178	1.4547	300.13	1	1.2304	1.178	-0.0524
179	1.4618	292.846	2	1.3979	1.6896	0.2917
180	1.4558	299.935	1	1.0792	0.6457	-0.4335
181	1.4563	299.838	1	-	0.652	-
182	1.4578	299.482	1	1.2553	0.6764	-0.5789
183	1.4574	299.502	1	0.6021	0.6767	0.0746
184	1.4564	299.604	1	0.699	0.6734	-0.0256
185	1.4653	296.797	1	1.3424	0.8848	-0.4576
186	1.4719	296.471	1	0.301	0.8739	0.5729
187	1.5013	295.033	1	0.699	0.8227	0.1237
188	1.4659	291.834	1	0.699	1.3548	0.6558
189	1.4635	296.697	1	0.301	0.9055	0.6045
190	1.4752	293.663	2	1.699	1.8578	0.1588
191	1.4638	296.592	1	0.4771	0.9141	0.437
192	1.5024	294.525	1	-	0.8641	-

193*	1.4649	296.201	1	1.5798	1.8543	0.2745
194	1.5035	294.169	1	-	0.8913	-
195	1.5023	294.305	1	1.6021	1.3567	-0.2454

Table S32: Descriptors, experimental and predicted pIC_{50} values and their residuals for compounds in cell line based QSAR model against HT29.

No.	$FNSA2_Q$	PP/SD	MaenAC	Exp.	Pred.	Res.
42	-0.5811	0.0267	160.966	1	1.186	0.186
43	-0.57	0.0267	160.937	1.2041	1.0973	-0.1068
44	-0.5406	0.0268	160.924	1	1.0838	0.0838
45	-0.5979	0.0267	160.856	1	1.1849	0.1849
46	-0.5942	0.0267	160.974	1	1.1085	0.1085
47	-0.565	0.0267	160.883	1	0.9972	-0.0028
48	-0.5978	0.0267	160.937	1.8451	1.1008	-0.7443
49*	-0.6049	0.0267	160.94	1.301	1.105	-0.196
50*	-0.5984	0.0267	160.941	1.3979	1.102	-0.2959
51	-0.8597	0.0226	161.456	1.2788	1.2512	-0.0276
52	-0.8514	0.0227	161.464	1	1.2447	0.2447
53	-0.9314	0.0227	161.438	1.2788	1.2948	0.016
54	-0.9169	0.0227	161.412	1	1.3202	0.3202
55	-0.7267	0.0175	160.149	1.3979	1.047	-0.3509
56	-0.9949	3.81E-03	161.201	1.0792	1.0715	-0.0077

57	-1.1216	6.36E-03	161.398	1.5911	1.1824	-0.4087
58	-0.9584	3.87E-03	161.416	1.4914	1.0518	-0.4396
59	-0.9486	2.88E-03	161.402	1.3222	1.0343	-0.2879
60	-0.9504	5.29E-03	161.353	1	1.1052	0.1052
61	-0.9155	4.28E-03	161.261	1	1.069	0.069
62	-0.9316	5.37E-03	161.347	1	1.0597	0.0597
63	-1.206	7.82E-03	161.237	1	1.2654	0.2654
64	-1.06	4.07E-03	160.177	1.1461	1.0173	-0.1288
65	-0.8709	0.0106	161.415	1.4624	1.0899	-0.3725
66*	-0.9473	4.94E-03	161.454	1	1.0555	0.0555
67*	-0.9225	4.11E-03	161.455	1	1.0339	0.0339
68	-1.0743	0.0229	161.239	1.7993	1.3914	-0.4079
69	-1.2104	3.15E-03	161.245	1.6721	1.2024	-0.4697
70	-1.559	0.0232	161.183	1.7782	1.6958	-0.0824
71	-1.5547	2.37E-03	159.547	1	1.4082	0.4082
72	-1.1083	0.0227	161.344	1.6532	1.4091	-0.2441
73	-1.0815	0.0228	161.328	1.6532	1.3909	-0.2623

74	-1.2127	0.0227	161.365	1.5185	1.4738	-0.0447
75	-1.6476	0.0111	160.854	1	1.6126	0.6126
76	-1.6172	9.93E-04	161.441	0.9191	1.4374	0.5183
414	-0.6887	3.93E-03	169.3	0.4314	0.8828	0.4514
415	-0.651	3.24E-03	169.361	0.9542	0.8354	-0.1188
416	-0.642	4.09E-03	169.283	0.9395	0.8628	-0.0767
417	-0.6958	4.22E-03	169.681	0	0.8351	0.8351
418	-0.7414	3.84E-03	169.867	0.8195	0.8568	0.0373
419	-0.5779	0.0407	171.14	0.9243	1.1869	0.2626
420	-0.735	0.0407	171.176	0.699	1.2866	0.5876
421*	-0.4809	0.0407	171.194	0.9138	1.118	0.2042
422	-0.7033	0.0366	169.184	1.1106	1.352	0.2414
423*	-0.7166	0.0366	169.178	0.9912	1.3606	0.3694
424	-0.6178	0.0365	169.358	1.3979	1.24	-0.1579
425	-0.9568	0.0366	169.232	1.3979	1.4964	0.0985
426	-0.6435	0.0366	169.414	0.9085	1.2691	0.3606
427	-0.7324	3.11E-03	169.349	0.243	0.8937	0.6507

428	-0.9446	2.54E-03	161.92	0.7782	1.1508	0.3726
429	-0.7681	2.00E-03	169.254	0.2601	0.8905	0.6304
430*	-0.7772	2.39E-03	169.959	0.8633	0.8255	-0.0378
431*	-0.7573	4.32E-03	169.329	1.0828	0.9149	-0.1679
432	-0.9124	1.99E-03	169.309	1.3979	0.9749	-0.423
433	-0.7409	0.0366	169.288	1.3979	1.3497	-0.0482
434	-0.8431	0.0366	169.323	1.3979	1.4103	0.0124
435	-0.609	0.0366	169.33	1.1035	1.2565	0.153
436	-0.7981	0.0365	169.954	1.3979	1.2375	-0.1604
437	-0.8251	0.0365	169.942	1.3979	1.2806	-0.1173
438	-1.089	0.0364	169.901	1.3979	1.3173	-0.0806
439	-0.7405	0.0366	169.782	0.8388	1.2587	0.4199
440*	-0.862	1.88E-03	169.948	1.3979	0.933	-0.4649
441*	-0.9684	1.69E-03	161.596	0.7324	1.0208	0.2884
442	-0.7256	0.0357	172.193	1.3979	1.0147	-0.3832
443	-0.7267	0.0378	169.658	1.3979	1.1383	-0.2596
444	-0.7643	2.38E-03	168.922	1.3979	1.0844	-0.3135

445	-0.9404	2.73E-03	169.015	1.0116	0.9745	-0.0371
446	-0.9277	2.32E-03	168.949	1.3979	1.2642	-0.1337
447	-0.9351	4.93E-03	169.988	1.3979	1.3017	-0.0962
448*	-0.7322	0.016	169.603	1.3979	1.0237	-0.3742
449*	-0.7836	0.0284	167.415	1.3979	1.5969	0.199
450*	-0.7823	2.37E-03	168.937	1.3979	1.097	-0.3009
451	-0.7775	0.0376	170.575	0.7404	1.3073	0.5669
452	-0.6639	2.05E-03	170.28	0.3979	0.7735	0.3756
453	-0.6513	2.64E-03	170.21	0.8808	0.7695	-0.1113
454	-0.6201	5.04E-03	170.286	1.3979	0.7814	-0.6165
455	-0.6215	0.0377	170.261	1.3979	1.2365	-0.1614
456	-0.6981	0.0377	170.251	1.3979	1.292	-0.1059
457*	-0.6721	0.0376	170.225	1.0864	1.2651	0.1787
458*	-0.8761	1.78E-03	161.395	1.3979	1.0736	-0.3243
459*	-0.6156	0.0377	170.257	0.8865	1.2315	0.345
460	-0.7135	1.95E-03	170.242	1.3979	0.8256	-0.5723
461	-0.8287	1.78E-03	161.631	1.2788	0.932	-0.3468

462	-0.608	0.0354	171.238	1.3979	1.1412	-0.2567
463	-0.5909	0.0376	171.166	1.3979	0.9815	-0.4164
464	-0.7167	2.43E-03	168.803	1.3979	0.9172	-0.4807
465	-0.6629	0.0403	169.226	1.3979	1.3649	-0.033
466	-0.6749	4.98E-03	169.694	1.3979	0.8151	-0.5828
467*	-0.6669	0.0377	170.267	1.3902	1.2651	-0.1251
468*	-0.9284	5.72E-03	159.418	1.3351	0.8909	-0.4442
469	-0.9526	7.43E-03	159.304	1.3979	1.3173	-0.0806
470	-1.0204	7.59E-03	159.187	1.3979	1.3691	-0.0288
471	-0.9732	5.69E-03	159.428	1.162	1.2214	0.0594
472	-1.0752	7.58E-03	159.193	1.3979	1.4405	0.0426
473	-0.9437	6.25E-03	159.339	1.3979	1.2923	-0.1056
474	-0.7022	2.09E-03	170.27	0	0.7346	0.7346
475*	-0.733	2.04E-03	167.809	1.3979	1.1131	-0.2848
476	-0.7589	2.08E-03	167.82	0.3502	1.134	0.7838
477*	-0.7727	6.16E-03	168.917	1.2514	1.1443	-0.1071
478	-0.8055	6.26E-03	167.563	1.3979	1.2552	-0.1427

479	-0.7138	2.46E-03	167.805	1.3979	1.1093	-0.2886

Table S33: Descriptors, experimental and predicted pIC_{50} values and their residuals for compounds in cell line based QSAR model against JLc.

No.	EMaNACH	$HDSA2_Q$	MaeeRC	Exp.	Pred.	Res.
1*	0.3347	0.0224	77.845	6.96	6.8861	-0.0739
2	0.3054	0.0228	77.877	7.39	8.177	0.787
3*	0.3361	0.021	77.839	6.9	6.5811	-0.3189
4	0.3345	0.0231	77.854	6.59	7.0097	0.4197
5	0.3277	0.0214	77.844	7.34	7.2184	-0.1216
6	0.344	0.0217	78.198	5.89	5.7717	-0.1183
7	0.3388	0.0199	77.944	6.05	6.1063	0.0563
8	0.3245	0.0249	77.875	7.96	7.9646	0.0046
9	0.3401	0.0191	78.744	6.95	5.8884	-1.0616
10	0.3042	0.0156	78.682	5.68	6.8135	1.1335
11*	0.316	0.0166	77.99	5.6	6.1438	0.5438
12	0.3261	0.0248	79.083	6.46	6.632	0.172
13	0.3232	0.0209	77.916	7.31	7.3942	0.0842
14	0.321	0.0211	77.938	7.48	7.5476	0.0676
15	0.3195	0.0212	77.968	7.62	7.6365	0.0165

16	0.319	0.0169	78.173	6.94	6.7919	-0.1481
17	0.3185	0.0261	78.816	6.75	7.6247	0.8747
18*	0.3364	0.0226	77.835	6.75	6.8066	0.0566
19	0.3368	0.0261	78.52	7.29	6.6507	-0.6393
20	0.3328	0.0226	77.872	7.28	7.0271	-0.2529
21	0.3226	0.0217	77.87	7.29	7.603	0.313
22	0.3244	0.0204	77.866	7.24	7.279	0.039
23	0.3386	0.02	77.85	6.45	6.2296	-0.2204
24	0.3382	0.0264	78.41	6.65	6.7027	0.0527
25*	0.3336	0.022	77.849	6.56	6.8998	0.3398
26*	0.3316	0.021	78.556	5.79	6.1787	0.3887
27*	0.3334	0.0193	78.597	5.68	5.7382	0.0582
28	0.3317	0.0184	78.508	5.97	5.8023	-0.1677
29	0.3341	0.0174	77.836	5.99	6.1551	0.1651
30	0.3325	0.0262	78.708	6.83	6.7679	-0.0621
31	0.3342	0.022	77.832	7.02	6.8793	-0.1407
32	0.3293	0.0217	77.842	6.87	7.1532	0.2832

33*	0.3281	0.0209	77.845	6.65	7.1149	0.4649
34*	0.3281	0.0283	77.828	6.12	7.2977	1.1777
35*	0.3315	0.0214	77.835	7.15	6.9633	-0.1867
36	0.3346	0.0223	77.836	6.62	6.8921	0.2721
37	0.3301	0.0232	77.866	6.98	7.3207	0.3407
38	0.3298	0.024	77.862	7.96	7.4758	-0.4842
39	0.3244	0.0237	77.859	8.41	7.7981	-0.6119
40	0.3267	0.0243	77.855	7.7	7.7412	0.0412
41*	0.3353	0.0243	77.866	7.92	7.1326	-0.7874

Table S34: Descriptors, experimental and predicted pIC_{50} values and their residuals for compounds in cell line based QSAR model against L120.

No.	$HDCA2_Q$	WNSA2z	MienAN	Exp.	Pred.	Res.
384	3.9808	-89.6236	428.819	1.5966	1.3884	-0.2082
385	4.7829	-94.5127	428.655	0.8129	0.9366	0.1237
386	4.7321	-68.6872	428.667	1.0043	1.4004	0.3961
387*	4.8003	-97.9285	428.731	0.8573	0.8584	0.0011
388	4.7032	-89.4058	428.595	1.5763	1.3718	-0.2045
389	4.7021	-67.4794	428.708	1.9053	1.4296	-0.4757
390	4.8029	-101.379	428.719	0.6721	0.8	0.1279
391	3.5951	-57.7053	426.685	2.3191	2.442	0.1229
392*	4.3273	-55.1808	428.777	2.6496	2.5127	-0.1369
393	3.9552	-116.721	426.256	2.9141	2.5228	-0.3913
394	3.5551	-54.0138	426.717	2.6013	2.5198	-0.0815
395	3.513	-55.0208	426.307	2.5668	2.5847	0.0179
396	3.5032	-56.5511	426.406	2.5006	2.5485	0.0479
397*	3.6394	-58.8494	425.565	1.4786	1.5687	0.0901
398*	3.5696	-78.5812	428.096	1.7796	1.8867	0.1071

399	3.5117	-89.293	428.212	1.9609	1.7148	-0.2461
400	3.4869	-105.177	426.464	1.6821	1.718	0.0359
401	3.5371	-77.9063	426.452	1.6304	2.1605	0.5301
402*	5.731	-65.2714	425.568	2.1166	2.134	0.0174
403	4.9015	-82.9205	426.43	2.975	2.6099	-0.3651
404	6.8007	-81.6654	426.579	0.4314	0.4787	0.0473
405	3.5722	-37.0913	426.553	2.7832	2.8247	0.0415
406	4.1573	-41.146	425.021	2.9499	2.6986	-0.2513
407	3.7019	-60.3837	427.407	1.0253	1.2357	0.2104
408	4.7299	-54.1322	426.689	2.6782	2.9465	0.2683
409	4.128	-125.322	425.067	1.4502	1.2696	-0.1806
410	4.5263	-73.7585	428.245	1.5079	1.478	-0.0299
411	4.3593	-45.2118	427.003	2.2512	2.2332	-0.018
412	3.6292	-79.083	425.699	0.6435	0.4083	-0.2352
413*	3.6546	-97.6324	426.981	0.7324	0.6871	-0.0453

Table S35: Descriptors, experimental and predicted pIC_{50} values and their residuals for compounds in cell line based QSAR model against LLc.

No.	ZXS/ZXR	$ERNCS_Q$	MiBOC(0.1)	Exp.	Pred.	Res.
1	0.5382	0.2075	0.1011	7.52	7.4608	-0.0592
2	0.5896	0.6509	0.1012	7.85	7.8435	-0.0065
3	0.5552	0.7527	0.101	7.38	8.0612	0.6812
4*	0.5393	0.1872	0.1013	7.17	7.2682	0.0982
5	0.533	0.2421	0.101	8.23	7.6923	-0.5377
6	0.6299	0.372	0.1012	5.62	6.4438	0.8238
7	0.6821	0.2464	0.1011	5.53	5.3696	-0.1604
8*	0.541	0.5748	0.1005	8.75	8.8433	0.0933
9*	0.5462	0.1486	0.1017	7.57	6.7789	-0.7911
10	0.5549	0.5092	0.1008	5.98	7.2469	1.2669
11	0.5798	0.107	0.1006	5.97	6.8435	0.8735
12	0.5732	0.1378	0.1017	6.77	6.3295	-0.4405
13	0.5721	0.0994	0.1002	7.46	7.2125	-0.2475
14	0.5443	0.5544	0.1007	8.1	8.5672	0.4672
15	0.5224	0.3818	0.1013	8.22	8.0542	-0.1658

16	0.5469	0.1402	0.101	7.41	7.2141	-0.1959
17	0.5547	0.1567	0.102	6.17	6.52	0.35
18	0.5447	0.1848	0.1017	7.25	6.9418	-0.3082
19*	0.5443	0.228	0.1005	7.7	7.8022	0.1022
20	0.547	0.2055	0.1013	7.7	7.1694	-0.5306
21*	0.5554	0.2307	0.1013	7.89	7.1118	-0.7782
22*	0.5671	0.439	0.1012	7.75	7.5751	-0.1749
23	0.5659	0.2014	0.1009	6.8	7.1688	0.3688
24	0.6131	0.1739	0.1004	6.5	6.6934	0.1934
25	0.5549	0.0912	0.1017	7.14	6.511	-0.629
26	0.5528	0.0969	0.1017	6.12	6.5727	0.4527
27	0.6305	0.1247	0.1017	5.68	5.4055	-0.2745
28	0.5677	0.0356	0.1017	5.85	6.1467	0.2967
29	0.5621	0.1696	0.1015	6.22	6.7493	0.5293
30	0.5028	0.1776	0.1011	7.7	7.9184	0.2184
31	0.5089	0.2082	0.1014	7.5	7.7206	0.2206
32	0.5345	0.0971	0.1014	7.34	7.026	-0.314

33	0.5817	0.425	0.1013	7.46	7.2651	-0.1949
34	0.547	0.0764	0.1015	6.74	6.7284	-0.0116
35*	0.5124	0.1863	0.1006	7.8	8.1356	0.3356
36*	0.5432	0.9355	0.1009	6.91	7.5481	0.6381
37	0.5237	0.1231	0.1018	7.7	6.9997	-0.7003
38	0.5197	0.0881	0.1001	8.5	8.0727	-0.4273
39	0.5366	0.4105	0.1006	8.85	8.3828	-0.4672
40	0.5462	0.2924	0.1005	8.06	7.9918	-0.0682
41*	0.5475	0.3684	0.1004	8.22	8.2009	-0.0191

Table S36: Descriptors, experimental and predicted pIC_{50} values and their residuals for compounds in cell line based QSAR model against M14.

No.	NN	RNBr	Mi1ERIC	Exp.	Pred.	Res.
326*	2	0.00E+00	-8.27E-03	1.1761	1.0965	-0.0796
327*	2	0.037	-0.0112	2	1.9654	-0.0346
328	3	0.00E+00	-6.13E-03	2	1.7972	-0.2028
329	2	0.00E+00	-0.013	2	1.8071	-0.1929
330	3	0.00E+00	-0.0133	1.7782	0.9579	-0.8203
331	2	0.037	-0.0115	-0.0969	0.1349	0.2318
332	3	0.00E+00	-9.13E-03	1.1761	1.4453	0.2692
333	3	0.00E+00	-9.51E-03	0.699	0.8435	0.1445
334	2	0.00E+00	-0.0117	2	1.9565	-0.0435
335	2	0.00E+00	-0.0131	2	1.8019	-0.1981
336	2	0.00E+00	-0.0119	1.7782	1.942	0.1638
337	2	0.00E+00	-0.0118	2	1.9492	-0.0508
338	3	0.00E+00	-9.11E-03	1	1.4477	0.4477
339*	3	0.00E+00	-7.81E-03	1.2672	1.6001	0.3329
340	3	0.00E+00	-0.014	1	0.8737	-0.1263

341	3	0.00E+00	-0.014	-0.0458	0.8773	0.9231
342	5	0.00E+00	-1.88E-03	0.9031	0.6587	-0.2444
343	2	0.00E+00	-0.0101	2	2.1478	0.1478
344*	2	0.00E+00	-0.0109	2	2.0588	0.0588
345*	2	0.00E+00	-0.0105	0.9031	1.1639	0.2608
346	2	0.00E+00	-0.0102	2	2.1344	0.1344
347	2	0.00E+00	-9.58E-03	2	2.2102	0.2102
348	3	0.00E+00	-9.43E-03	1.6021	1.4095	-0.1926
349	3	0.00E+00	-9.37E-03	1.4771	1.4164	-0.0607
350	3	0.00E+00	-9.46E-03	1.6021	1.406	-0.1961
351*	5	0.00E+00	-7.98E-03	1.9777	2.0567	0.079
352	3	0.00E+00	-9.09E-03	1.9542	1.4493	-0.5049
353	4	0.00E+00	-7.86E-03	0.699	0.7757	0.0767
354	4	0.00E+00	-9.32E-03	0.301	0.6048	0.3038
355	4	0.00E+00	-7.72E-03	0.301	0.7929	0.4919
356	4	0.00E+00	-9.46E-03	0.7782	0.588	-0.1902
357	5	0.00E+00	-8.75E-03	0.8751	1.0864	0.2113

358	5	0.00E+00	-0.0103	-0.3979	-0.3327	0.0652
359	4	0.00E+00	-8.88E-03	0.301	0.6562	0.3552
360	4	0.0233	-3.42E-05	0.301	0.5298	0.2288
361	4	0.02	-8.48E-03	0.3979	-0.2973	-0.6952

Table S37: Descriptors, experimental and predicted pIC_{50} values and their residuals for compounds in cell line based QSAR model against MCF7.

No.	MaeeRC	$ERPCS_Q$	ASIC1	Exp.	Pred.	Res.
42	79.539	2.0877	0.5474	1	0.7135	-0.2865
43	78.774	2.0975	0.5153	1	0.7183	-0.2817
44	78.802	1.8282	0.4865	1	0.8645	-0.1355
45	79.392	1.7727	0.4939	1	0.9084	-0.0916
46	78.725	1.5647	0.4385	1	1.0363	0.0363
47	77.655	1.6959	0.4378	1	0.9233	-0.0767
48	78.626	1.4288	0.4007	1.9445	1.1443	-0.8002
49	78.623	1.2783	0.3705	1.6435	1.25	-0.3935
50	78.636	1.0658	0.3459	1.716	1.3683	-0.3477
51*	78.941	0.00E+00	0.3793	1.6335	1.6963	0.0628
52	78.926	0.00E+00	0.3371	1	1.7707	0.7707
53	78.898	0.00E+00	0.723	1.9823	1.0794	-0.9029
54*	79.112	0.00E+00	0.6952	1	1.1428	0.1428
55*	78.497	0.2209	0.5142	1	1.3503	0.3503
56	78.897	0.00E+00	0.6179	1.5185	1.2672	-0.2513

57	78.827	0.00E+00	0.6561	2	1.1943	-0.8057
58	78.926	0.00E+00	0.6727	1.6532	1.171	-0.4822
59*	78.956	0.00E+00	0.5381	1.7076	1.4135	-0.2941
60*	79.304	0.00E+00	0.6477	1	1.2401	0.2401
61*	79.273	0.00E+00	0.615	1	1.2966	0.2966
62*	78.97	0.00E+00	0.615	1	1.2771	0.2771
63*	78.912	0.00E+00	0.6412	1	1.2264	0.2264
64	77.705	1.6107	0.5274	1.6721	0.7959	-0.8762
65*	78.933	0.00E+00	0.5875	1.0792	1.3238	0.2446
66	78.884	0.00E+00	0.5328	1	1.4184	0.4184
67	78.948	0.00E+00	0.5157	1	1.453	0.453
68	78.918	0.00E+00	0.6948	2	1.1311	-0.8689
69	78.906	0.00E+00	0.7522	1.3424	1.0278	-0.3146
70	78.78	0.00E+00	0.7378	2	1.0454	-0.9546
71	78.847	0.00E+00	0.7548	1	1.0192	0.0192
72	78.9	0.00E+00	0.684	1.8062	1.1492	-0.657

73	78.882	0.00E+00	0.6551	1.8513	1.1997	-0.6516
74	78.869	0.00E+00	0.7285	1.6128	1.0677	-0.5451
75	79.076	0.00E+00	0.6554	1.716	1.2117	-0.5043
76	78.936	0.00E+00	0.4589	1.2553	1.5537	0.2984
414	79.101	0.8306	0.512	0.0792	1.1827	1.1035
415	78.962	0.2115	0.512	0.1461	1.3876	1.2415
416	79.178	1.1382	0.512	0.1139	1.0815	0.9676
417	78.528	1.4362	0.512	0.3617	0.9367	0.575
418	78.478	0.3275	0.5935	0.6628	1.1706	0.5078
419	77.62	0.2003	0.5769	0.3979	1.1889	0.791
420	77.607	0.2593	0.6197	0.2553	1.0913	0.836
421	77.56	0.2772	0.6197	0.2041	1.0821	0.878
422*	79.141	0.3274	0.5808	1.2304	1.236	0.0056
423*	79.136	1.1773	0.5808	1.1673	0.9422	-0.2251
424*	78.553	0.3727	0.5829	1.3979	1.1789	-0.219
425*	78.953	2.3039	0.5852	1.3979	0.5336	-0.8643

426*	78.674	0.1931	0.5341	0.7634	1.3358	0.5724
427*	79.038	1.5079	0.5656	0.7559	0.849	0.0931
428	80.252	0.4166	0.5669	0.4771	1.3017	0.8246
429	78.928	0.3455	0.512	0.0212	1.3391	1.3179
430	78.142	0.4067	0.512	1.0864	1.2673	0.1809
431*	78.916	0.7971	0.512	1.2553	1.1824	-0.0729
432*	78.841	0.6141	0.5484	1.3979	1.1757	-0.2222
433*	78.87	0.3798	0.5237	1.3979	1.3025	-0.0954
434*	78.807	0.6883	0.5672	1.3979	1.1142	-0.2837
435*	78.78	0.7532	0.5672	0.9609	1.09	0.1291
436*	77.248	0.7694	0.5808	1.3979	0.9615	-0.4364
437*	77.526	0.6319	0.5808	1.3979	1.0268	-0.3711
438	76.247	2.4321	0.5852	1.3979	0.315	-1.0829
439*	77.94	0.2426	0.5341	0.9138	1.2714	0.3576
440	78.742	1.414	0.5656	1.2702	0.8624	-0.4078
441*	78.899	0.5093	0.5669	0.9823	1.1825	0.2002
442	75.693	0.5389	0.5217	1.3979	1.0465	-0.3514

443	76.634	0.4615	0.5237	1.3979	1.1302	-0.2677
444	80.891	0.3919	0.4935	1.3979	1.4825	0.0846
445*	78.557	0.3037	0.5154	1.1679	1.3236	0.1557
446*	80.659	0.8103	0.5154	1.3979	1.284	-0.1139
447	80.63	0.8315	0.5154	1.3979	1.2748	-0.1231
448	78.52	0.4239	0.5237	0.9294	1.2647	0.3353
449	82.314	0.4699	0.5237	1.3979	1.4932	0.0953
450	80.903	0.493	0.512	1.3979	1.4154	0.0175
451	78.047	0.5359	0.5852	0.4914	1.0858	0.5944
452	78.415	0.1507	0.4879	0.2041	1.4164	1.2123
453	78.367	0.9474	0.4879	1.0934	1.1382	0.0448
454	78.35	0.0304	0.4879	1.0719	1.4537	0.3818
455	78.345	0.4124	0.5036	1.3979	1.2934	-0.1045
456	78.412	0.275	0.5543	1.3979	1.2546	-0.1433
457	78.305	0.4407	0.5543	1.0864	1.1905	0.1041
458*	79.978	0.8802	0.5661	1.3979	1.1254	-0.2725

459	78.329	0.2347	0.5076	0.8062	1.3465	0.5403
460	78.61	1.7123	0.5419	1.3979	0.7932	-0.6047
461*	78.899	0.8534	0.5414	1.2788	1.1093	-0.1695
462*	77.778	0.383	0.5099	1.3979	1.2558	-0.1421
463	75.944	1.5914	0.5036	1.3979	0.7316	-0.6663
464*	79.477	0.4024	0.4675	1.3979	1.4343	0.0364
465	79.027	0.00E+00	0.4446	1.3979	1.5852	0.1873
466	78.341	0.0502	0.4446	1.3979	1.5237	0.1258
467	78.335	0.7926	0.5611	1.0748	1.0586	-0.0162
468	77.384	0.5484	0.5671	1.0867	1.071	-0.0157
469	81.311	0.5039	0.5409	1.3979	1.3862	-0.0117
470	81.371	0.5976	0.5671	1.3979	1.3108	-0.0871
471	80.432	0.3947	0.5883	0.738	1.2825	0.5445
472	81.739	0.8417	0.5883	1.3979	1.2124	-0.1855
473	81.28	0.4848	0.5124	1.3979	1.4417	0.0438
474	77.761	0.7135	0.5358	0.3802	1.0944	0.7142
475*	81.446	0.6303	0.5115	1.3979	1.4038	0.0059

476	81.483	0.5392	0.5358	0.9345	1.3943	0.4598
477	80.908	0.777	0.5555	0.7839	1.2398	0.4559
478*	81.816	0.6698	0.5555	1.3979	1.3353	-0.0626
479*	81.473	0.5447	0.4851	1.3979	1.4823	0.0844
214	77.252	0.6384	0.5993	0.4771	0.974	0.4969
215	77.105	1.3976	0.6361	1.1461	0.6365	-0.5096
216	76.53	0.4837	0.6447	0.4771	0.8997	0.4226
217	80.449	1.5572	0.6919	1.3222	0.6972	-0.625
218	77.49	0.8588	0.6866	0.4771	0.7571	0.28
219	78.796	0.8427	0.6674	0.4771	0.8813	0.4042
220	79.24	1.3153	0.6799	1.1139	0.7242	-0.3897
221	86.586	5.8544	0.7081	0.4771	-0.4204	-0.8975
222	78.163	0.6481	0.628	-	0.978	-
223	78.152	1.2085	0.6919	0.4771	0.6696	0.1925
224	78.147	0.4469	0.677	0.4771	0.9589	0.4818
225	80.447	1.5703	0.7143	0.4771	0.6524	0.1753
226*	78.208	0.7723	0.7037	0.4771	0.8028	0.3257

227	78.792	0.8466	0.6923	0.4771	0.8351	0.358
228*	79.233	1.2735	0.7341	0.4771	0.6413	0.1642
229	86.584	5.4373	0.764	0.4771	-0.3765	-0.8536
230*	79.35	0.8633	0.628	0.4771	0.9802	0.5031
231	79.307	1.4086	0.6919	1.3617	0.6749	-0.6868
232	78.953	0.6396	0.6251	-	1.037	-
233	79.216	1.1679	0.6793	1.2041	0.7746	-0.4295
234	77.966	0.745	0.5993	2.0828	0.9831	-1.0997
235	77.109	1.6771	0.6361	2.3032	0.5403	-1.7629
236	78.011	1.1676	0.5978	1.2788	0.8427	-0.4361
237	77.701	1.5021	0.6856	1.8451	0.5503	-1.2948
238	78.046	0.9954	0.6589	1.3424	0.7953	-0.5471
239	78.034	0.00E+00	0.7318	1.3222	1.008	-0.3142
240	77.334	0.00E+00	0.663	4	1.0858	-2.9142
241	77.099	0.00E+00	0.7808	4	0.8602	-3.1398
242	84.629	0.6479	0.678	2.2304	1.3052	-0.9252
243	84.68	0.00E+00	0.8032	3.0086	1.3085	-1.7001

244	76.588	2.488	0.6604	0.699	0.1832	-0.5158
245	76.369	2.7274	0.6855	-0.6021	0.0416	0.6437
246	77.116	2.5576	0.7296	0	0.0697	0.0697
247	77.081	2.6705	0.76	-0.6021	-0.0258	0.5763
248*	77.071	3.1221	0.7852	0.6021	-0.2276	-0.8297
249	77.047	3.3605	0.7987	-1	-0.3354	0.6646
250	79.286	3.2191	0.8364	-0.0969	-0.2099	-0.113
251	79.244	3.3813	0.8402	-1.8239	-0.2753	1.5486
252	77.136	1.4293	0.8008	-1.1308	0.3334	1.4642
253	77.103	1.9037	0.8189	-1.6021	0.135	1.7371
254	77.5	2.8821	0.7989	-1	-0.1415	0.8585
255	77.462	3.2297	0.8317	-1.5229	-0.3225	1.2004
256	78.8	3.1198	0.8326	-0.0602	-0.2	-0.1398
257	78.817	3.3822	0.8539	-1.6021	-0.3276	1.2745
258	76.516	3.1392	0.797	-0.301	-0.2902	0.0108
259	80.459	1.6205	0.8675	-2	0.3622	2.3622
260	86.488	7.7203	0.912	-0.1308	-1.4354	-1.3046

261	89.489	5.1946	0.6249	0.5623	0.1431	-0.4192
262	89.212	5.5704	0.6503	0.5353	-0.0499	-0.5852
263	89.485	4.7722	0.6249	0.382	0.2887	-0.0933
264	89.212	5.1176	0.6503	0.2355	0.1064	-0.1291
265	89.479	4.5294	0.6249	-0.5686	0.3722	0.9408
266	89.208	4.8238	0.6361	-1.0458	0.2329	1.2787
267	89.536	4.5529	0.6011	0.1553	0.4103	0.255
268	89.242	4.8906	0.6275	0.1492	0.2274	0.0782
269	89.528	4.4876	0.5905	0.4362	0.4512	0.015
270	89.261	4.7937	0.6249	0.3927	0.2669	-0.1258
271	89.431	4.6706	0.6156	0.6561	0.3369	-0.3192
272	89.204	5.0279	0.6419	0.6232	0.152	-0.4712
273	89.421	4.4357	0.6156	0.4814	0.4174	-0.064
274	89.187	4.6857	0.6419	0.3483	0.269	-0.0793
275	89.471	4.3152	0.6156	-0.0605	0.4622	0.5227
276	89.181	4.5158	0.6287	-0.4949	0.3509	0.8458
277	89.525	4.0613	0.5918	0.4281	0.596	0.1679

278	89.235	4.3307	0.6178	0.2014	0.4377	0.2363
279*	89.517	4.1268	0.5821	0.4362	0.59	0.1538
280*	89.234	4.3949	0.6156	0.4048	0.4194	0.0146
362	80.467	0.1685	0.7319	0	1.1064	1.1064
363*	80.468	0.00E+00	0.7422	0.9542	1.1463	0.1921
364*	80.469	0.2259	0.8076	1.6902	0.9514	-0.7388
365	80.465	0.2164	0.7953	0	0.9765	0.9765
366	80.468	0.233	0.8076	1.7709	0.9489	-0.822
367	78.719	0.00E+00	0.6836	1.9912	1.1383	-0.8529
368	78.612	0.00E+00	0.7233	0	1.0604	1.0604
369	78.656	0.00E+00	0.7277	1.9777	1.0555	-0.9222
370	78.539	0.00E+00	0.7845	2.0531	0.9465	-1.1066
371	78.543	0.00E+00	0.7845	0	0.9467	0.9467
372	78.655	0.1438	0.6547	1.9823	1.1361	-0.8462
373	78.59	0.00E+00	0.6975	0	0.1052	0.1052
374	78.527	0.00E+00	0.7475	2.0043	1.0118	-0.9925
375	78.534	1.7075	0.7475	2	0.4226	-1.5774

376	78.731	0.00E+00	0.6262	1.4472	1.2416	-0.2056
377	78.661	0.00E+00	0.6656	0	1.1668	1.1668
378	78.625	0.00E+00	0.7101	1.4314	1.0848	-0.3466
379	78.629	0.00E+00	0.7101	2.0253	1.0851	-0.9402
380	78.606	0.2181	0.6625	1.5051	1.0934	-0.4117
381	78.534	1.7588	0.5926	0	0.6816	0.6816
382*	78.379	5.7992	0.6753	1.8921	-0.8713	-2.7634
383	78.331	1.939	0.6753	0	0.4586	0.4586
326*	78.399	0.8028	0.595	1.4771	0.9988	-0.4783
327	78.362	0.9523	0.6627	2	0.8238	-1.1762
328	78.297	0.9869	0.6642	2	0.8049	-1.1951
329	78.401	0.8193	0.6851	2	0.8322	-1.1678
330*	78.379	0.8148	0.6784	1.6021	0.8442	-0.7579
331	78.618	0.6938	0.6627	-0.1549	0.9295	1.0844
332*	78.936	3.3983	0.6642	0	0.0134	0.0134
333	77.33	0.9501	0.6784	0.699	0.7299	0.0309
334	78.832	0.7627	0.7213	2	0.8148	-1.1852

335	77.189	0.7169	0.6871	2	0.786	-1.214
336	78.256	0.6955	0.6735	-0.3979	0.8863	1.2842
337	78.146	0.7461	0.6627	2	0.8811	-1.1189
338	79.609	0.9816	0.6947	-0.3979	0.8368	1.2347
339	78.709	0.5159	0.6819	1	0.9625	-0.0375
340	79.099	0.5643	0.6904	1.301	0.9557	-0.3453
341	77.432	0.8715	0.7106	-1.2219	0.7062	1.9281
342	77.575	0.2937	0.633	1.301	1.0535	-0.2475
343	107.94	2.2624	0.6993	2	2.2111	0.2111
344	78.072	0.00E+00	0.6703	2	1.1204	-0.8796
345	77.946	0.5202	0.6272	1.301	1.0096	-0.2914
346	78.585	0.6235	0.63	2	1.0102	-0.9898
347	78.32	1.5318	0.5932	2	0.7452	-1.2548
348	76.666	3.5852	0.6451	1.1761	-0.1632	-1.3393
349	76.683	0.8073	0.6776	-2	0.7391	2.7391
350	76.645	0.5286	0.681	-2	0.8268	2.8268
351	78.633	1.0547	0.6477	0.9031	0.8327	-0.0704

352	78.463	1.0666	0.5328	0.8751	1.0229	0.1478
353	77.967	0.7109	0.626	0.8751	0.9472	0.0721
354	76.708	0.6874	0.6348	-0.3979	0.8586	1.2565
355	77.264	0.7761	0.6178	0.7782	0.8941	0.1159
356	77.217	0.4952	0.6002	0.699	1.0195	0.3205
357	76.86	2.4285	0.6742	0.6021	0.1968	-0.4053
358	77.992	2.2873	0.6631	0.6021	0.3383	-0.2638
359	76.848	2.7684	0.7227	-3.9794	-8.044	-4.0646
360	78.058	0.4786	0.672	-1.2219	0.9511	2.173
361	78.074	1.1096	0.631	-0.5229	0.8075	1.3304
96	80.892	0.4146	0.6498	1	1.1954	0.1954
97	80.586	0.3079	0.6566	1.4829	1.2005	-0.2824
98	81.237	0.5085	0.5748	1	1.3192	0.3192
99	80.908	0.00E+00	0.5808	1	1.4629	0.4629
100	81.281	0.3892	0.5872	1.0755	1.3412	0.2657
101	80.895	0.00E+00	0.5928	1.2945	1.4406	0.1461
102	81.208	0.3043	0.6066	-	1.3311	-

103	80.845	0.00E+00	0.6122	1	1.4029	0.4029
104	81.338	0.3475	0.607	-	1.3238	-
105	81.006	0.00E+00	0.613	1.6866	1.4117	-0.2749
106	81.446	0.2604	0.607	1.143	1.3609	0.2179
107	81.471	0.5809	0.613	1.2175	1.2411	0.0236
108	81.668	0.3863	0.6098	1.4362	1.3266	-0.1096
109	81.334	0.00E+00	0.6156	1.6848	1.4282	-0.2566
110	80.179	0.291	0.6878	1.2323	1.1244	-0.1079
111	79.791	0.00E+00	0.6942	1.8488	1.1884	-0.6604
112	81.136	0.0496	0.607	1.2923	1.4137	0.1214
113	80.536	0.051	0.613	1.3838	1.3638	-0.02
114	80.849	0.0432	0.6168	1.1335	1.3799	0.2464
115	80.516	0.00E+00	0.6224	1.8041	1.3633	-0.4408
116	81.084	0.0466	0.6356	1	1.3602	0.3602
117	80.484	0.0486	0.6412	1	1.311	0.311
118	81.397	0.00E+00	0.6265	1	1.4127	0.4127
119	103.658	2.4627	0.64	3	1.9721	-1.0279

120	103.636	0.8963	0.6282	2.6021	2.5326	-0.0695
121	103.608	1.0261	0.6003	2.6021	2.5359	-0.0662
122	103.539	0.7647	0.634	2.4771	2.5614	0.0843
123	104.042	2.2442	0.6295	2.6021	2.0911	-0.511
124	103.466	0.7285	0.6297	2.3979	2.5769	0.179
125	103.769	1.0613	0.6266	2.4771	2.4871	0.01
126	103.617	0.6375	0.5719	2.699	2.7213	0.0223
127	103.705	2.6225	0.6657	2.699	1.874	-0.825
128	104.038	0.697	0.659	2.6532	2.5724	-0.0808
129	103.964	0.6679	0.6528	2.6532	2.5887	-0.0645
130	104.226	0.7527	0.6513	2.699	2.579	-0.12
131	103.701	2.4143	0.6657	2.2788	1.9457	-0.3331
132	103.65	1.0157	0.6557	2.301	2.4433	0.1423
133	103.663	0.7472	0.6273	2.1761	2.5876	0.4115
134	103.583	0.5256	0.659	2.0414	2.6023	0.5609
135	103.614	1.6645	0.657	2.2788	2.2145	-0.0643
136	103.518	0.3353	0.6528	1.9542	2.6749	0.7207

137	103.799	0.3827	0.6513	2.301	2.6792	0.3782
138	103.383	0.7521	0.5993	2.2304	2.6178	0.3874
139	104.094	1.7189	0.6899	2	2.1679	0.1679
140	103.578	0.8226	0.6557	2.1461	2.5053	0.3592
141	103.608	0.9499	0.6273	2.0414	2.514	0.4726
142	103.527	0.912	0.659	2	2.4653	0.4653
143	103.553	2.1484	0.657	2.1761	2.0435	-0.1326
144	103.437	0.8614	0.6528	2.2041	2.488	0.2839
145	103.754	0.9886	0.6513	2	2.4671	0.4671
146	103.611	0.9927	0.5993	2.301	2.5494	0.2484
147	104.009	1.1627	0.6897	2.699	2.3549	-0.3441
148	104.022	0.8506	0.6581	3	2.5199	-0.4801
149	103.513	1.9055	0.6911	2.6532	2.0639	-0.5893
150	104.025	0.6512	0.6284	2.699	2.6421	-0.0569

Table S38: Descriptors, experimental and predicted pIC_{50} values and their residuals for compounds in cell line based QSAR model against MLM.

No.	EFPSA1Q	ANRIO	EHDSAQ	Exp.	Pred.	Res.
414	0.7218	2.62E-03	110.694	0.9668	1.0439	0.0771
415	0.7345	2.26E-03	144.0931	0.1461	0.7496	0.6035
416	0.7392	2.49E-03	61.0726	0.9345	1.1034	0.1689
417	0.7136	3.01E-03	103.06	1.0374	1.1893	0.1519
418	0.7684	8.53E-04	120.7137	0.1461	0.4098	0.2637
419	0.6934	1.14E-03	59.164	1.3979	1.3308	-0.0671
420	0.7774	1.11E-03	117.851	0.2304	0.3789	0.1485
421	0.7897	1.10E-03	117.851	0.1461	0.276	0.1299
422	0.7445	5.37E-03	103.06	1.3979	1.2117	-0.1862
423	0.72	4.91E-03	135.0276	1.3979	1.2181	-0.1798
424	0.7601	4.61E-03	121.668	1.3979	0.9122	-0.4857
425	0.6592	2.54E-03	167.4724	1.3979	1.2987	-0.0992
426	0.7579	3.45E-04	100.1972	0.9731	0.5271	-0.446
427	0.6966	2.26E-03	201.3486	1.1004	0.8094	-0.291
428	0.6723	1.84E-03	121.1909	0.7993	1.3142	0.5149

429	0.6923	2.10E-03	119.7595	0.316	1.1854	0.8694
430	0.6934	1.17E-03	135.0276	1.3979	1.0006	-0.3973
431	0.6974	1.94E-03	67.7524	1.3979	1.3545	-0.0434
432	0.715	2.10E-03	125.485	1.3979	0.9736	-0.4243
433	0.6728	1.90E-03	109.7398	1.3979	1.3666	-0.0313
434	0.7353	2.34E-03	74.9093	1.3979	1.0572	-0.3407
435	0.7525	2.60E-03	101.6286	0.7101	0.8288	0.1187
436	0.7177	2.34E-03	107.3541	1.3979	1.0598	-0.3381
437	0.6822	1.40E-03	75.3864	1.3979	1.3822	-0.0157
438	0.6204	1.69E-03	127.8707	1.3979	1.6928	0.2949
439	0.7276	2.29E-04	114.9882	0.0969	0.6981	0.6012
440	0.656	1.72E-03	155.0671	1.3829	1.2842	-0.0987
441	0.6742	1.05E-03	189.4204	1.1139	0.9058	-0.2081
442	0.6479	1.11E-03	120.7137	1.3979	1.4309	0.033
443	0.6821	1.66E-03	88.2689	1.3979	1.3568	-0.0411
444	0.7165	1.47E-03	109.2626	1.3979	0.9593	-0.4386
445	0.6721	6.90E-04	120.2366	1.3777	1.185	-0.1927

446	0.6915	5.71E-03	165.0868	1.3979	1.4149	0.017
447	0.6933	5.85E-03	122.6223	1.3979	1.6029	0.205
448	0.6931	2.20E-03	98.7658	1.3979	1.2831	-0.1148
449	0.6909	2.56E-03	111.1712	1.3979	1.2891	-0.1088
450	0.6922	7.64E-04	150.7729	1.3979	0.8941	-0.5038
451	0.6969	2.45E-04	171.7666	0.1139	0.7024	0.5885
452	0.7354	3.63E-03	113.0797	0.2553	1.0393	0.784
453	0.7397	4.07E-03	71.5694	1.3979	1.2383	-0.1596
454	0.7511	3.96E-03	61.5497	1.3979	1.1758	-0.2221
455	0.7279	5.42E-03	69.6609	1.3979	1.5001	0.1022
456	0.7592	5.71E-03	60.1183	1.3979	1.3197	-0.0782
457	0.7695	5.63E-03	47.2358	1.3979	1.2824	-0.1155
458	0.7149	1.32E-03	96.8573	1.3979	1.0094	-0.3885
459	0.7673	7.35E-05	57.7327	0.0792	0.605	0.5258
460	0.7047	3.63E-03	110.2169	1.3979	1.3036	-0.0943
461	0.7157	3.20E-03	138.8447	1.3979	1.0369	-0.361
462	0.71	8.42E-03	95.903	1.3979	1.883	0.4851

463	0.7315	2.54E-03	57.7327	1.3979	1.1873	-0.2106
464*	0.7455	3.52E-03	52.9614	1.3979	1.2075	-0.1904
465*	0.7686	2.62E-03	80.6349	1.3979	1.1965	-0.2014
466*	0.7648	4.32E-03	67.7524	1.3979	1.2859	-0.112
467	0.7397	1.09E-04	135.0276	1.3979	0.8906	-0.5073
468*	0.66	2.92E-03	127.3936	1.3979	1.5136	0.1157
469*	0.6944	2.19E-03	144.5702	1.3979	1.0698	-0.3281
470*	0.6615	2.57E-03	146.0016	1.3979	1.3787	-0.0192
471*	0.6508	3.70E-03	178.4464	1.3979	1.456	0.0581
472*	0.6348	2.27E-03	156.0213	1.3979	1.5195	0.1216
473*	0.714	1.88E-03	105.9227	1.3979	1.0429	-0.355
474*	0.7113	2.37E-03	92.086	0.2041	1.1823	0.9782
475*	0.7451	1.56E-03	94.4716	1.3979	0.9064	-0.4915
476*	0.7212	1.91E-03	141.2303	1.3979	0.8313	-0.5666
477*	0.6851	3.18E-03	184.6491	1.3979	1.0854	-0.3125
478	0.6959	9.33E-04	153.1585	1.3979	0.8725	-0.5254
479	0.7679	1.29E-03	52.4842	1.3979	0.9034	-0.4945

Table S39: Descriptors, experimental and predicted pIC_{50} values and their residuals for compounds in cell line based QSAR model against H460.

No.	MiPC	Ma1ERIC	MaenACO	Exp.	Pred.	Res.
362	-0.1147	0.021	410.652	1.2553	1.0012	-0.2541
363	-0.1147	0.0214	410.651	1.4624	1.021	-0.4414
364	-0.1145	0.0211	410.622	1.8062	0.996	-0.8102
365	-0.1146	0.0215	410.632	0	1.025	1.025
366	-0.1442	0.021	410.612	1.8388	1.3699	-0.4689
367	-0.1144	0.0215	410.736	1.7993	1.0462	-0.7531
368	-0.1144	0.0209	410.727	1.3617	1.0083	-0.3534
369	-0.1144	0.0212	410.724	1.5563	1.028	-0.5283
370	-0.1143	7.28E-03	410.7	2.0828	0.138	-1.9448
371	-0.1442	7.08E-03	410.683	0	0.5104	0.5104
372	-0.1142	8.29E-03	410.628	2.0294	0.1827	-1.8467
373	-0.1142	8.20E-03	410.62	0	0.1755	0.1755
374	-0.114	0.021	410.598	2.0086	0.9765	-1.0321
375	-0.1442	0.0208	410.582	1.4472	1.3546	-0.0926
376	-0.114	8.78E-03	410.325	0	0.1359	0.1359

377	-0.114	0.0207	410.328	0	0.8918	0.8918
378*	-0.1138	7.33E-03	410.316	1.8261	0.0405	-1.7856
379*	-0.1442	7.25E-03	410.308	2.0253	0.4281	-1.5972
380	-0.1117	0.0214	408.408	1.7924	0.4321	-1.3603
381	-0.1117	0.0213	408.402	0	0.4228	0.4228
382	-0.1115	0.0209	408.388	0	0.3894	0.3894
383	-0.1442	7.31E-03	408.38	0	-0.0454	-0.0454
77	-0.18	0.0175	411.075	1.9638	1.729	-0.2348
78	-0.18	0.0154	411.05	1.5315	1.5919	0.0604
79	-0.1812	0.0174	410.938	3.5831	1.7069	-1.8762
80*	-0.18	0.0157	411.019	1.5051	1.6036	0.0985
81*	-0.18	0.0125	411.23	1.5441	1.4528	-0.0913
82	-0.18	0.0138	410.964	1.3424	1.4704	0.128
83	-0.18	0.0144	411.016	1.415	1.5231	0.1081
84	-0.18	0.0183	410.819	1.4624	1.7201	0.2577
85	-0.18	0.0167	410.783	1.5798	1.6088	0.029
86	-0.18	0.0187	410.348	1.2788	1.6269	0.3481

87*	-0.18	5.01E-03	411.076	1.1761	0.9422	-0.2339
88	-0.1753	0.0149	411.104	1.1461	1.5148	0.3687
89*	-0.1753	0.0149	411.082	1.1461	1.5059	0.3598
90	-0.1812	0.0208	410.977	1.9494	1.9352	-0.0142
91	-0.1753	0.0149	410.957	1.8692	1.4737	-0.3955
92	-0.1753	0.019	411.046	1.7324	1.7592	0.0268
93	-0.1753	0.0128	411.081	1.6435	1.3771	-0.2664
94	-0.1796	0.0225	410.379	1.7559	1.8699	0.114
95*	-0.1753	0.0103	411.09	2	1.2189	-0.7811
42*	-0.1793	1.85E-03	411.574	1	0.8568	-0.1432
43*	-0.1793	2.11E-03	411.578	1	0.8746	-0.1254
44	-0.1793	2.24E-03	411.595	1	0.8872	-0.1128
45	-0.1793	1.96E-03	411.499	1	0.8451	-0.1549
46	-0.1793	2.09E-03	411.578	1	0.8734	-0.1266
47	-0.1793	2.19E-03	411.493	1	0.8584	-0.1416
48	-0.1793	2.09E-03	411.576	1	0.8727	-0.1273
49	-0.1793	2.10E-03	411.574	2	0.8727	-1.1273

50	-0.1793	2.10E-03	411.574	1.7243	0.8727	-0.8516
51	-0.1819	2.07E-03	412.959	1.8195	1.2464	-0.5731
52	-0.1819	2.97E-03	412.957	1	1.3034	0.3034
53	-0.1819	2.96E-03	412.86	1.301	1.2787	-0.0223
54	-0.1819	2.92E-03	412.867	1	1.2779	0.2779
55	-0.1793	2.00E-03	411.102	1.2304	0.7495	-0.4809
56	-0.1818	2.07E-03	412.789	1	1.2041	0.2041
57	-0.1818	2.94E-03	412.983	1.5051	1.3071	-0.198
58*	-0.1818	2.07E-03	412.961	1.2041	1.2466	0.0425
59*	-0.1819	3.02E-03	412.911	1.1461	1.2947	0.1486
60	-0.1818	2.07E-03	412.881	1	1.2272	0.2272
61	-0.1818	2.07E-03	412.88	1	1.2266	0.2266
62	-0.1818	2.96E-03	412.888	1	1.2853	0.2853
63	-0.1819	1.86E-04	412.897	1	1.1122	0.1122
64	-0.1793	2.07E-03	414.05	1.0792	1.4837	0.4045
65*	-0.1829	2.90E-03	412.776	1.2553	1.2678	0.0125
66*	-0.1844	4.18E-04	412.946	1	1.1719	0.1719

67*	-0.1845	1.41E-04	413.016	1	1.1728	0.1728
68	-0.1818	6.70E-04	412.586	1.699	1.0652	-0.6338
69	-0.1818	6.72E-04	412.627	1.0792	1.0754	-0.0038
70	-0.1818	0.0114	412.432	1.5682	1.7054	0.1372
71	-0.1818	1.42E-03	412.486	1	1.0875	0.0875
72	-0.1818	8.78E-04	412.903	1.3617	1.1573	-0.2044
73	-0.1818	8.25E-04	412.899	1.4914	1.1529	-0.3385
74	-0.1818	5.42E-04	412.984	1.3222	1.1561	-0.1661
75*	-0.1817	3.00E-03	412.506	1.2553	1.192	-0.0633
76	-0.1819	2.98E-03	412.967	1.4914	1.306	-0.1854

Table S40: Descriptors, experimental and predicted pIC_{50} values and their residuals for compounds in cell line based QSAR model against P388.

No.	WPSA1z	MiTICN	$HDCA1_Q$	Exp.	Pred.	Res.
1	588.4211	14.647	0.0135	6.89	6.798	-0.092
2	572.2822	14.642	0.0142	6.77	6.5608	-0.2092
3	570.556	14.648	0.0129	6.4	6.8774	0.4774
4	699.0057	14.651	0.0145	6.66	6.7667	0.1067
5	603.8638	14.648	0.0133	6.95	6.7903	-0.1597
6	592.3561	14.706	0.0125	5.46	6.0516	0.5916
7	604.2498	14.647	0.0127	-	6.6757	-
8	632.6804	14.652	0.0161	7.64	7.1952	-0.4448
9	732.3254	14.653	0.0127	6.77	6.6486	-0.1214
10	797.2642	14.643	8.52E-03	5.56	5.3963	-0.1637
11	776.782	14.649	9.21E-03	5.91	5.9343	0.0243
12	706.3042	14.646	0.0168	6.37	6.5883	0.2183
13	595.455	14.659	0.0129	7.8	7.5441	-0.2559
14*	579.6463	14.66	0.0131	7.34	7.6843	0.3443
15*	553.3738	14.658	0.0129	7.82	7.6187	-0.2013

16	554.5101	14.662	0.0113	6.62	7.0585	0.4385
17	733.17	14.643	0.0134	5.67	6.0114	0.3414
18	694.676	14.648	0.014	6.46	6.5385	0.0785
19	724.0207	14.649	0.0174	7.12	6.7778	-0.3422
20	589.952	14.657	0.0134	7.62	7.4676	-0.1524
21	565.3438	14.658	0.0129	7.18	7.5839	0.4039
22*	563.3665	14.66	0.0121	7.13	7.6612	0.5312
23*	595.5165	14.659	0.0117	5.02	5.4505	0.4305
24	772.1777	14.641	0.014	6.12	6.7867	0.6667
25	713.9537	14.652	0.0136	6.57	6.7116	0.1416
26	794.0089	14.65	0.0128	5.97	6.238	0.268
27	836.8575	14.652	0.0113	5.84	6.1031	0.2631
28	914.6694	14.651	0.0107	5.75	5.7172	-0.0328
29	879.5561	14.65	0.0104	6.15	5.743	-0.407
30*	732.9794	14.647	0.0172	6.88	6.5998	-0.2802
31*	621.7991	14.64	0.0135	6.85	6.2003	-0.6497
32*	614.6342	14.643	0.013	6.77	6.3904	-0.3796

33	581.3491	14.642	0.0126	6.65	6.3997	-0.2503
34	822.4509	14.648	0.0155	6.01	6.2221	0.2121
35	680.7953	14.65	0.0131	6.75	6.651	-0.099
36	573.1866	14.641	0.0134	6.13	6.4294	0.2994
37	736.3275	14.65	0.0147	6.68	6.5899	-0.0901
38*	719.266	14.648	0.0157	7.62	6.9889	-0.6311
39*	751.6296	14.646	0.0152	7.58	7	-0.58
40	605.5173	14.643	0.0157	7.39	6.9416	-0.4484
41	623.9078	14.647	0.0158	7.32	6.8603	-0.4597

Table S41: Descriptors, experimental and predicted pIC_{50} values and their residuals for compounds in cell line based QSAR model against Panc1.

No.	SIC2	LNMVF	FPSA3Q	Exp.	Pred.	Res.
77	25.3578	28.458	0.0722	1.9731	1.6089	-0.3642
78	29.0346	22.007	0.0728	1.6532	1.7528	0.0996
79	26.6213	23.351	0.0699	1.5563	1.4074	-0.1489
80	26.7318	26.487	0.0638	1.4624	1.6422	0.1798
81	26.7318	22.013	0.0709	1.4771	1.3662	-0.1109
82	26.7318	27.828	0.069	1.5563	1.5952	0.0389
83*	27.6515	16.612	0.0629	1.5563	1.4937	-0.0626
84	27.2646	17.44	0.0655	1.5682	1.405	-0.1632
85	28.0657	15.551	0.0564	1.5441	1.6485	0.1044
86	28.1505	15.425	0.0698	1.6335	1.4232	-0.2103
87	28.4884	21.76	0.0965	1.2041	1.2259	0.0218
88	26.7632	8.737	0.0692	0.8451	0.9543	0.1092
89*	30.4124	22.669	0.0689	0	0.0957	0.0957
90	28.5168	25.44	0.0676	1.9685	1.8662	-0.1023
91	29.1385	26.186	0.072	1.8808	1.9264	0.0456

92*	28.0591	25.753	0.0615	1.8195	1.9006	0.0811
93	28.0591	25.829	0.0683	1.7559	1.7832	0.0273
94	30.1964	14.902	0.0671	1.7924	1.8268	0.0344
95	29.844	15.72	0.0629	2	1.8642	-0.1358

Table S42: Descriptors, experimental and predicted pIC_{50} values and their residuals for compounds in cell line based QSAR model against SF-468.

No.	ABOC	$ERNCS_Q$	EMaNAC	Exp.	Pred.	Res.
362*	1.0529	0.9528	0.3789	1.2404	1.4409	0.2005
363	1.0278	1.6144	0.3859	1.7853	1.3877	-0.3976
364	1.0627	2.0517	0.3563	1.7482	1.9888	0.2406
365*	1.0621	1.7237	0.3886	0	0.1815	0.1815
366	1.0609	1.9197	0.3701	1.8451	2.0308	0.1857
367	1.0392	0.8227	0.3924	2.0414	1.9944	-0.047
368	1.0456	1.0103	0.4049	1.4472	1.1041	-0.3431
369	1.0224	1.1128	0.4243	1.9243	1.5496	-0.3747
370	1.0537	1.5304	0.3863	2.1584	2.0487	-0.1097
371*	1.052	1.2399	0.401	0	0.1599	0.1599
372	1.0341	0.6145	0.2934	1.9956	1.7156	-0.28
373	1.018	1.249	0.26	2.0043	1.6682	-0.3361
374	1.0463	1.3807	0.2774	2.0043	1.6682	-0.3361
375	1.0448	1.3411	0.2682	2	1.6258	-0.3742
376	1.0299	0.7182	0.4924	1.8513	2.0497	0.1984

377	1.0144	0.6841	0.4766	0	0.6522	0.6522
378	1.0402	1.1903	0.4767	1.9823	2.0751	0.0928
379	1.0388	0.972	0.474	2	2.1218	0.1218
380*	1.0245	0.9943	0.3137	1.9345	1.3805	-0.554
381	1.0092	3.4266	0.2399	0	-0.13	-0.13
382	1.0334	0.6539	0.2138	1.6128	1.4918	-0.121
383	1.0321	3.2211	0.2715	0	0.5824	0.5824

Table S43: Descriptors, experimental and predicted pIC_{50} values and their residuals for compounds in cell line based QSAR model against SJ-G2.

No.	CIC2	AVN	MiRECN	Exp.	Pred.	Res.
42*	28.7549	3.2659	15.43	1	1.0673	0.0673
43*	36.2647	3.2686	15.452	1	1.1146	0.1146
44	44.7549	3.2689	15.456	1	1.1594	0.1594
45	45.0196	3.2664	15.07	1	1.077	0.077
46	65.7744	3.2674	15.476	1	1.2692	0.2692
47	74.0579	3.268	15.157	1	1.2466	0.2466
48	92.7549	3.2698	15.476	1.7324	1.4113	-0.3211
49	122.7032	3.2698	15.477	1.8573	1.5653	-0.292
50	154.794	3.2698	15.477	1.7634	1.73	-0.0334
51	149.3233	3.273	15.448	1.6902	1.7008	0.0106
52*	218.8606	3.273	15.448	1	1.0578	0.0578
53	10	3.2714	15.4	0.301	0.5734	0.2724
54	12	3.2742	15.485	1	1.0056	0.0056
55	42	3.2146	15.575	1.3979	1.0862	-0.3117
56	20.7549	3.2739	15.66	1	1.0863	0.0863

57	18	3.2692	15.518	0.301	0.0354	-0.2656
58*	14	3.2701	15.604	1	1.0342	0.0342
59	47.2193	3.2731	15.449	1.0792	1.1771	0.0979
60	16.7549	3.2686	15.207	1	0.9637	-0.0363
61	29.5098	3.2665	14.64	1	0.9084	-0.0916
62*	22.7549	3.2709	15.237	1	1.0043	0.0043
63*	21.5098	3.2724	15.447	1	1.0437	0.0437
64	51.2193	3.2121	15.623	1	1.1396	0.1396
65	31.5098	3.1226	14.081	0.4771	0.5809	0.1038
66	47.5098	3.1549	15.027	1	0.9089	-0.0911
67*	53.5098	3.1488	14.903	1	0.9045	-0.0955
68	24.3645	3.3063	16.701	1.6232	1.3705	-0.2527
69	18	3.3078	16.719	1.6435	1.3438	-0.2997
70	24	3.5583	14.554	1.3617	1.3126	-0.0491
71	18	3.3019	16.556	1	1.301	0.301
72*	24.7549	3.2724	15.358	1.0414	1.042	0.0006
73*	34.2647	3.2718	15.402	1	1.0989	0.0989

74	20	3.1884	15.235	1	0.8625	-0.1375
75	40	3.2531	14.767	1	0.9679	-0.0321
76	162.1075	3.268	15.443	1.6335	1.7577	0.1242

Table S44: Descriptors, experimental and predicted pIC_{50} values and their residuals for compounds in cell line based QSAR model against SKMEL-5.

No.	HOMO1E	MaTICH	$EFHDSA_Q$	Exp.	Pred.	Res.
414	-8.932	12.683	0.0393	0.9868	1.0059	0.0191
415	-8.945	12.675	0.05	0.7782	0.8468	0.0686
416	-8.898	12.686	0.0232	0.0792	1.1613	1.0821
417*	-8.85	12.665	0.038	0.5414	0.838	0.2966
418	-8.407	12.659	0.0419	0.2304	0.2082	-0.0222
419	-8.4	12.596	0.0233	0.0792	0.1171	0.0379
420	-8.456	12.583	0.0446	0	-0.1157	-0.1157
421*	-8.469	12.572	0.0441	0.8261	0.6404	-0.1857
422	-9.074	12.686	0.0422	1.1584	1.1824	0.024
423	-9	12.685	0.0515	0.7782	0.9501	0.1719
424	-8.942	12.686	0.0512	1.3979	0.9196	-0.4783
425	-9.222	12.677	0.0627	1.3979	1.0947	-0.3032
426	-8.827	12.651	0.0347	0.1761	0.7687	0.5926
427	-8.969	12.678	0.0771	0.356	0.6154	0.2594
428	-9.073	12.678	0.0427	0.7782	1.1346	0.3564

429*	-8.96	12.669	0.04	0.9085	0.9548	0.0463
430	-9.079	12.657	0.0459	1.0212	0.9946	-0.0266
431	-8.894	12.667	0.0228	1.1303	1.0552	-0.0751
432	-8.981	12.666	0.0408	1.3979	0.9601	-0.4378
433*	-8.985	12.667	0.038	1.3979	1.2828	-0.1151
434	-9.008	12.665	0.0272	1.3979	1.1508	-0.2471
435	-9.014	12.664	0.0358	0.8149	1.0474	0.2325
436	-9.292	12.658	0.0433	1.3979	1.3222	-0.0757
437*	-9.222	12.676	0.0301	1.3979	1.4535	0.0556
438	-9.448	12.588	0.0471	1.3979	1.1533	-0.2446
439	-8.928	12.634	0.0375	0.6628	0.7832	0.1204
440	-9.115	12.672	0.0586	1.0626	0.9936	-0.069
441*	-9.125	12.596	0.0586	0.6628	0.6077	-0.0551
442	-9.57	12.593	0.0446	1.3979	1.2967	-0.1012
443	-9.261	12.614	0.0317	1.3979	1.1607	-0.2372
444	-8.875	12.726	0.036	1.3979	1.1788	-0.2191
445*	-8.316	12.661	0.0374	1.0269	1.1618	0.1349

446	-8.668	12.897	0.0528	1.3979	1.5357	0.1378
447	-8.388	12.89	0.0394	1.3979	1.3078	-0.0901
448	-9.228	12.644	0.0354	1.3979	1.215	-0.1829
449*	-9.145	12.769	0.039	1.3979	1.6421	0.2442
450	-8.845	12.726	0.0503	1.3979	0.9762	-0.4217
451	-9.193	12.653	0.0689	0.5052	0.9582	0.453
452	-9.022	12.655	0.0371	0.1461	0.9993	0.8532
453*	-9.049	12.664	0.0246	0.9638	1.1238	0.16
454	-9.043	12.65	0.0212	1.301	1.1787	-0.1223
455	-9.26	12.642	0.0238	1.3979	1.3765	-0.0214
456	-9.352	12.668	0.0249	1.3979	1.6436	0.2457
457*	-9.328	12.673	0.0188	1.3979	1.1306	-0.2673
458	-8.95	12.641	0.0343	1.3979	0.9266	-0.4713
459	-8.922	12.64	0.0198	0.7709	1.0172	0.2463
460	-9.068	12.668	0.042	1.3979	1.1034	-0.2945
461*	-9.231	12.641	0.0423	1.3979	1.6864	0.2885
462	-9.439	12.619	0.0346	1.3979	1.3564	-0.0415

463	-9.45	12.601	0.0209	1.3979	1.4609	0.063
464	-8.941	12.706	0.0188	1.3979	1.3655	-0.0324
465*	-8.965	12.685	0.0244	1.3979	1.2062	-0.1917
466	-8.879	12.639	0.0207	1.3979	0.9378	-0.4601
467	-8.931	12.645	0.0565	1.1021	0.7413	-0.3608
468*	-9.358	12.623	0.0437	1.3979	1.2186	-0.1793
469	-8.995	12.724	0.0477	1.3979	1.1891	-0.2088
470	-8.959	12.726	0.0492	1.3979	1.1351	-0.2628
471	-9.118	12.705	0.0669	1.0748	1.0587	-0.0161
472*	-8.911	12.751	0.0561	1.3979	1.1232	-0.2747
473	-8.999	12.724	0.0338	1.3979	1.3511	-0.0468
474	-9.143	12.623	0.0342	0.8451	1.0743	0.2292
475	-8.942	12.741	0.0335	1.3979	1.3784	-0.0195
476	-8.908	12.742	0.0498	0.0531	0.1437	0.0906
477	-8.916	12.724	0.068	0.382	0.8817	0.4997
478	-8.833	12.77	0.0572	1.3979	1.1081	-0.2898
479*	-8.944	12.742	0.0191	1.3979	1.5452	0.1473

Table S45. Descriptors, experimental and predicted pIC_{50} values and their residuals for compounds in cell line based QSAR model against SKOV3.

No.	MiPCNz	EE+ee-CC	$EFHDCA_Q$	Exp.	Pred.	Res.
326	-0.0778	133.918	0.0595	0.3979	0.8495	0.4516
327	-0.0774	133.92	0.0498	2	1.726	-0.274
328	-0.0772	133.929	0.0651	2	1.9409	-0.0591
329*	-0.077	133.922	0.052	2	1.7674	-0.2326
330	-0.1178	133.989	0.0969	1.6021	1.2386	-0.3635
331	-0.0771	134.003	0.0467	0.699	1.6627	0.9637
332	-0.0767	134.147	0.0637	1.3979	1.8578	0.4599
333	-0.1179	134.344	0.0971	0.699	1.1139	0.4149
334	-0.0755	133.762	0.0499	2	1.8362	-0.1638
335*	-0.077	134.31	0.0643	2	1.8012	-0.1988
336	-0.0778	133.974	0.0544	2	1.7607	-0.2393
337	-0.0768	134.007	0.0468	2	1.67	-0.33
338*	-0.0973	134.269	0.0741	1.301	1.3903	0.0893
339	-0.097	134.296	0.0446	0.7782	0.9788	0.2006
340	-0.0971	134.296	0.0469	0.9031	1.0087	0.1056

341*	-0.0928	134.303	0.0774	-1.301	-1.5483	-0.2473
342	-0.122	134.259	0.0594	0.7782	0.5091	-0.2691
343	-0.0771	134.195	0.0814	2	2.0768	0.0768
344	-0.0814	134.075	0.0545	2	1.6265	-0.3735
345	-0.0811	137.847	0.091	0.7782	0.8121	0.0339
346	-0.0813	134.051	0.0486	2	1.5557	-0.4443
347*	-0.0773	134.121	0.057	2	1.7575	-0.2425
348	-0.0798	133.995	0.057	1.4771	1.7324	0.2553
349	-0.0799	134.002	0.0484	1.301	1.6082	0.3072
350*	-0.0798	133.996	0.0738	1.699	1.9649	0.2659
351	-0.088	133.991	0.0563	1.716	1.4973	-0.2187
352	-0.0796	136.758	0.0484	0.7782	0.6459	-0.1323
353*	-0.1247	134.006	0.0427	0.301	0.2913	-0.0097
354	-0.1221	134.004	0.0453	0.301	0.3991	0.0981
355	-0.12	133.988	0.0486	0.4771	0.5092	0.0321
356	-0.1226	133.982	0.0328	0.6021	0.2224	-0.3797
357	-0.1221	134.224	0.0558	0.9542	0.4673	-0.4869

358	-0.1247	134.227	0.0474	-0.2218	0.2783	0.5001
359	-0.0788	134.214	0.0543	0.301	0.6456	0.3446
360	-0.1221	134.074	0.0258	0.4771	0.1047	-0.3724
361	-0.1201	134.066	0.0404	0	0.3649	0.3649

Table S46. Descriptors, experimental and predicted pIC_{50} values and their residuals for compounds in cell line based QSAR model against SW480.

No.	MaASEN	RNCl	$HDSA_Q$	Exp.	Pred.	Res.
42	-185.08	0.00E+00	0.00E+00	1	1.3992	0.3992
43	-185.056	0.00E+00	0.00E+00	1.6532	1.4161	-0.2371
44	-185.06	0.00E+00	0.00E+00	1	1.4133	0.4133
45*	-185.113	0.00E+00	0.00E+00	1	1.3759	0.3759
46*	-185.061	0.00E+00	0.00E+00	1	1.4126	0.4126
47	-185.089	0.00E+00	0.00E+00	1	1.3928	0.3928
48	-185.031	0.00E+00	0.00E+00	1.8129	1.4338	-0.3791
49	-185.031	0.00E+00	0.00E+00	1.7709	1.4338	-0.3371
50	-185.031	0.00E+00	0.00E+00	1.7404	1.4338	-0.3066
51	-185.005	0.00E+00	6.2027	1.716	1.3825	-0.3335
52	-185.005	0.00E+00	6.2027	1	1.3825	0.3825
53	-185.018	0.00E+00	5.7256	1.699	1.3787	-0.3203
54	-184.995	0.00E+00	7.1569	1	1.3789	0.3789
55	-185.449	0.00E+00	0.00E+00	1.4771	1.1388	-0.3383
56	-184.972	0.00E+00	36.2618	1	1.0687	0.0687

57	-185.033	0.00E+00	38.1704	1.8388	1.0042	-0.8346
58	-184.991	0.00E+00	34.8304	1.2553	1.0713	-0.184
59	-185.003	0.00E+00	37.6932	1.2041	1.0307	-0.1734
60	-185.062	0.00E+00	34.8304	1	1.0212	0.0212
61	-185.139	0.00E+00	36.2618	1	0.9508	-0.0492
62	-185.043	0.00E+00	35.7847	1	1.0239	0.0239
63	-185.019	0.00E+00	16.2224	1	1.2603	0.2603
64	-185.452	0.00E+00	21.948	1.0414	0.8905	-0.1509
65	-185.205	0.00E+00	6.6798	1.4624	1.236	-0.2264
66*	-184.972	0.00E+00	6.2027	1	1.4058	0.4058
67*	-185.015	0.00E+00	6.6798	1	1.3701	0.3701
68	-184.627	0.00E+00	6.6798	1.8921	1.644	-0.2481
69	-184.594	0.00E+00	31.0134	1.3222	1.3943	0.0721
70	-184.721	0.00E+00	7.1569	1.6435	1.5723	-0.0712
71*	-184.688	0.00E+00	34.3533	1	1.2905	0.2905
72*	-185.038	0.00E+00	6.6798	1.3802	1.3539	-0.0263
73	-185.031	0.00E+00	6.6798	1.4624	1.3588	-0.1036

74	-185.466	0.00E+00	36.739	1.1139	0.7147	-0.3992
75	-185.43	0.00E+00	21.4708	1.2041	0.9113	-0.2928
76*	-185.09	0.00E+00	6.2027	1.3802	1.3226	-0.0576
326*	-184.398	0.00E+00	0.00E+00	0.699	0.8805	0.1815
327	-184.387	0.00E+00	0.00E+00	2	1.8882	-0.1118
328	-184.37	0.00E+00	10.4968	2	1.7825	-0.2175
329	-184.383	0.00E+00	0.00E+00	2	1.8911	-0.1089
330	-184.536	0.00E+00	49.6215	1.7782	1.2265	-0.5517
331	-184.414	0.00E+00	0.00E+00	-0.6021	-0.8692	-0.2671
332*	-184.458	0.00E+00	31.4905	1.3979	1.4849	0.087
333	-184.595	0.00E+00	48.6672	0.6812	1.1956	0.5144
334	-184.41	0.00E+00	15.2681	2	1.7008	-0.2992
335	-184.349	0.00E+00	0.00E+00	2	1.9151	-0.0849
336	-184.387	0.00E+00	0.00E+00	2	1.8882	-0.1118
337*	-184.403	0.037	0.00E+00	2	1.544	-0.456
338	-184.674	0.00E+00	19.0852	1.4771	1.4716	-0.0055
339	-184.471	0.00E+00	17.1767	1.0212	1.6363	0.6151

340	-184.468	0.00E+00	17.6538	1.3424	1.6331	0.2907
341	-184.357	0.0294	18.608	-0.2218	-0.2219	-1E-04
342	-184.764	0.00E+00	20.9937	1	1.3867	0.3867
343	-184.467	0.00E+00	0.00E+00	2	1.8318	-0.1682
344	-184.379	0.00E+00	20.9937	2	1.6584	-0.3416
345	-184.379	0.00E+00	19.5623	1	1.6745	0.6745
346*	-184.386	0.00E+00	22.4251	2	1.6374	-0.3626
347*	-184.338	0.00E+00	21.948	2	1.6767	-0.3233
348	-184.37	0.00E+00	33.3991	0.9031	1.5256	0.6225
349	-184.37	0.00E+00	28.6278	1.301	1.5791	0.2781
350	-184.371	0.00E+00	0.00E+00	2	1.8995	-0.1005
351	-184.493	0.00E+00	16.2224	2	1.6315	-0.3685
352	-184.364	0.00E+00	0.00E+00	1.7782	1.9045	0.1263
353	-186.423	0.00E+00	0.00E+00	0.6021	0.4514	-0.1507
354	-186.382	0.00E+00	0.00E+00	-0.1249	-0.4803	-0.3554
355	-186.685	0.00E+00	0.00E+00	-0.0706	0.2665	0.3371
356	-186.749	0.00E+00	0.00E+00	0.6532	0.2213	-0.4319

357	-186.367	0.00E+00	23.8565	-0.1249	0.2233	0.3482
358	-186.422	0.00E+00	22.9022	-0.301	0.1952	0.4962
359*	-184.436	0.00E+00	59.164	-0.1249	-0.1901	-0.0652
360*	-185.133	0.00E+00	0.00E+00	0.4771	0.3618	-0.1153
361*	-186.225	0.00E+00	0.00E+00	0.4771	0.5911	0.114

Table S47. Descriptors, experimental and predicted pIC_{50} values and their residuals for compounds in cell line based QSAR model against U251.

No.	IOKSE	$EFHBSA_Q$	RNN	Exp.	Pred.	Res.
326	0.0103	0.4794	0.0741	2	2.0546	0.0546
327	6.91E-03	0.4188	0.0741	2	1.7704	-0.2296
328	0.0994	0.669	0.1034	2	1.5904	-0.4096
329*	6.70E-03	0.4615	0.0571	2	2.2565	0.2565
330	0.0497	0.5739	0.1034	1.8451	1.6602	-0.1849
331	0.0188	0.4037	0.0741	2	1.5513	-0.4487
332	0.1587	0.6629	0.1034	0.6532	0.8691	0.2159
333*	0.0225	0.5814	0.1034	-0.1549	-0.3165	-0.1616
334	0.0106	0.4836	0.0667	2	2.1863	0.1863
335	0.0267	0.5073	0.0645	2	2.1583	0.1583
336	9.86E-03	0.4331	0.0667	1.301	1.9245	0.6235
337	0.0191	0.407	0.0741	2	1.5657	-0.4343
338	0.0542	0.5798	0.0882	1.301	1.8679	0.5669
339	0.0148	0.4001	0.075	1.0792	1.5647	0.4855
340	0.0144	0.4232	0.0811	2	1.6016	-0.3984

341*	6.67E-04	0.5208	0.0882	-0.699	-0.6749	0.0241
342	0.0386	0.4686	0.098	2	1.3072	-0.6928
343	0.1125	0.6842	0.0606	2	2.1658	0.1658
344	6.39E-04	0.3829	0.0625	2	1.8255	-0.1745
345*	8.48E-04	0.5663	0.0606	1.0792	1.8332	0.754
346	4.40E-04	0.3093	0.0488	2	1.6415	-0.3585
347	0.0134	0.3648	0.0426	2	1.882	-0.118
348	8.47E-03	0.4044	0.1034	1.1761	1.2319	0.0558
349*	8.43E-03	0.3695	0.0833	0	0.3494	0.3494
350	1.44E-03	0.49	0.0789	2	2.1413	0.1413
351	0.0142	0.3789	0.1111	0.9294	0.9132	-0.0162
352	0.0439	0.3644	0.0667	1.301	1.161	-0.14
353*	0.024	0.2901	0.087	-0.1549	-0.6891	-0.5342
354	0.0164	0.3004	0.093	-0.0969	0.7412	0.8381
355	0.014	0.3176	0.0851	1.3979	0.9799	-0.418
356	0.0239	0.2469	0.08	0.7782	0.564	-0.2142
357	0.1254	0.4789	0.1111	0.8751	0.1561	-0.719

358	0.1013	0.4296	0.1042	0.3979	0.2773	-0.1206
359	0.1802	0.5287	0.1053	-0.0969	-0.1257	-0.0288
360	0.0236	0.1989	0.093	-0.3468	0.1141	0.4609
361*	9.06E-03	0.2826	0.08	-1.0223	-0.9271	0.0952

Table S48. Descriptors, experimental and predicted pIC_{50} values and their residuals for compounds in scaffold based QSAR model against S1.

No.	VE/T	$WPSA3_Q$	LNMVF	Exp.	Pred.	Res.
1*	160.5771	74.2702	25.293	6.89	7.8323	0.9423
2	171.498	64.9869	22.416	6.77	6.8428	0.0728
3	173.66	66.9869	22.926	6.4	6.7717	0.3717
4	177.7117	80.8252	24.923	6.66	6.9069	0.2469
5	175.5511	67.9832	23.555	6.95	6.6982	-0.2518
6*	178.5283	67.4198	38.268	5.46	6.9893	1.5293
7	163.3616	71.1515	19.467	-	7.3933	-
8	173.2572	74.807	25.615	7.64	7.0673	-0.5727
9	174.9669	82.4356	28.075	6.77	7.2196	0.4496
10	192.137	85.1613	29.966	5.56	6.2784	0.7184
11*	207.515	98.2244	20.437	5.91	5.3083	-0.6017
12	182.8774	78.2397	25.76	6.37	6.5537	0.1837
13	164.5932	69.3788	26.831	7.8	7.5205	-0.2795
14	169.9603	67.4439	30.433	7.34	7.2619	-0.0781
15	176.1595	75.8059	38.716	7.82	7.3457	-0.4743

16*	187.9803	65.3201	47.89	6.62	6.6731	0.0531
17	190.3253	80.2993	21.741	5.67	6.0049	0.3349
18	179.7039	80.4102	24.9	6.46	6.7727	0.3127
19	174.9971	80.3645	25.101	7.12	7.0708	-0.0492
20	168.8236	67.391	24.988	7.62	7.1503	-0.4697
21*	172.9163	66.089	24.996	7.18	6.866	-0.314
22	177.5168	77.7544	35.825	7.13	7.2103	0.0803
23	191.9269	66.8857	9.117	5.02	5.1749	0.1549
24	191.0033	83.6009	24.098	6.12	6.1176	-0.0024
25	177.6772	82.3125	24.511	6.57	6.9298	0.3598
26*	179.7052	88.192	23.509	5.97	5.9066	-0.0634
27	192.2297	90.0034	20.884	5.84	6.0828	0.2428
28	201.1122	95.5295	21.382	5.75	5.6753	-0.0747
29	208.0452	112.4171	25.641	6.15	5.7772	-0.3728
30	187.6209	80.329	30.64	6.88	6.4696	-0.4104
31*	169.0597	69.9902	24.275	6.85	7.1721	0.3221
32	174.0242	68.2267	23.772	6.77	6.806	0.036

33	178.8614	79.9778	33.324	6.65	7.0951	0.4451
34	203.5241	88.3712	22.713	6.01	5.4038	-0.6062
35	176.4705	79.5424	23.449	6.75	6.9053	0.1553
36*	163.1201	69.0378	28.896	6.13	6.6729	0.5429
37	180.0255	80.1831	30.791	6.68	6.9433	0.2633
38	176.7187	79.2921	50.977	7.62	7.7994	0.1794
39	176.9818	81.4876	23.823	7.68	6.931	-0.749
40	175.1055	69.4312	36.002	7.39	7.1733	-0.2167
41*	187.6345	68.5562	22.771	7.32	6.9344	-0.3856

Table S49. Descriptors, experimental and predicted pIC_{50} values and their residuals for compounds in scaffold based QSAR model against S2.

No.	RNB	MaenAC	PMIA	Exp.	Pred.	Res.
42	0.00E+00	183.043	0.0432	1	1.1113	0.1113
43	0.00E+00	182.145	0.0362	1.2041	1.316	0.1119
44	0.00E+00	182.195	0.0293	1	1.209	0.209
45	0.00E+00	182.913	0.0406	1	1.1195	0.1195
46	0.00E+00	182.1	0.0271	1	1.2109	0.2109
47*	0.00E+00	181.08	0.0353	1	1.0562	0.0562
48	0.00E+00	181.99	0.0352	1.8451	1.3535	-0.4916
49	0.00E+00	181.984	0.0337	1.301	1.3356	0.0346
50*	0.00E+00	181.999	0.0273	1.3979	1.2475	-0.1504
51	0.00E+00	182.408	0.0271	1.2788	1.1085	-0.1703
52	0.00E+00	182.391	0.0144	1	0.9466	-0.0534
53*	0.00E+00	182.362	0.041	1.2788	1.308	0.0292
54	0.00E+00	182.753	0.0357	1	1.1086	0.1086
55	0.00E+00	181.891	0.0374	1.3979	1.4161	0.0182
56*	0.00E+00	182.361	0.0251	1.0792	1.0985	0.0193

57	0.00E+00	182.29	0.0369	1.5911	1.2771	-0.314
58	0.00E+00	182.393	0.0417	1.4914	1.306	-0.1854
59*	0.00E+00	182.423	0.024	1.3222	1.2626	-0.0596
60	0.00E+00	182.818	0.0329	1	1.05	0.05
61	0.00E+00	182.822	0.0315	1	1.0302	0.0302
62*	0.00E+00	182.441	0.0279	1	1.108	0.108
63	0.00E+00	182.38	0.0257	1	1.0991	0.0991
64	0.00E+00	181.264	0.0216	1.1461	1.4144	0.2683
65	0.00E+00	182.403	0.0303	1.4624	1.1526	-0.3098
66	0.00E+00	182.348	0.0302	1	1.1701	0.1701
67	0.00E+00	182.414	0.026	1	1.0931	0.0931
68*	0.0323	182.385	0.0325	1.7993	1.7832	-0.0161
69	0.0312	182.373	0.0319	1.6721	1.76	0.0879
70	0.0303	182.244	0.0293	1.7782	1.7508	-0.0274
71*	0.0294	182.313	0.0292	1	1.1109	0.1109
72	0.0263	182.364	0.0269	1.6532	1.6061	-0.0471
73	0.0238	182.347	0.021	1.6532	1.4879	-0.1653

74	0.0278	182.334	0.0263	1.5185	1.6357	0.1172
75	0.00E+00	182.56	0.015	1	0.8993	-0.1007
76	0.00E+00	182.402	6.79E-03	0.9191	0.8432	-0.0759

Table S50. Descriptors, experimental and predicted pIC_{50} values and their residuals for compounds in scaffold based QSAR model against S3.

No.	FPSA3z	WNSA2z	BI	Exp.	Pred.	Res.
77	0.0171	-54.0101	2.2112	1.9685	1.8542	-0.1143
78*	0.0171	-53.8129	2.2032	1.6435	1.5678	-0.0757
79	0.0192	-71.6674	2.1776	1.6532	1.6439	-0.0093
80	0.0165	-80.6252	2.2032	1.4472	1.4843	0.0371
81	0.016	-77.6961	2.2032	1.3979	1.4272	0.0293
82	0.0188	-63.6449	2.2032	1.5441	1.5246	-0.0195
83*	0.0165	-76.5074	2.2265	1.6812	1.7583	0.0771
84	0.0166	-75.825	2.252	1.4477	1.4078	-0.0399
85	0.0162	-96.9422	2.2583	1.5441	1.5377	-0.0064
86	0.0214	-74.9107	2.2773	1.6812	1.7305	0.0493
87	0.0163	-73.2411	2.204	1.4472	1.4092	-0.038
88	0.0193	-68.0193	2.2941	1.5185	1.5044	-0.0141
89*	0.019	-70.5591	2.2801	1.2304	1.2233	-0.0071
90*	0.021	-90.5589	2.251	1.9638	1.8493	-0.1145
91	0.0223	-88.9774	2.2801	1.9191	1.9027	-0.0164

92	0.0185	-102.932	2.2801	1.7559	1.7298	-0.0261
93	0.018	-102.775	2.2801	1.6812	1.6959	0.0147
94	0.0226	-92.3107	2.3342	1.8976	1.8969	-0.0007
95	0.0184	-96.3458	1.7889	1.9956	2.1711	0.1755

Table S51. Descriptors, experimental and predicted pIC_{50} values and their residuals for compounds in scaffold based QSAR model against S4.

No.	PPSA3z	ZXS/ZXR	$RNCG_Q$	Exp.	Pred.	Res.
96	-14.2167	0.5194	0.0929	1	0.9864	-0.0136
97	-10.0461	0.5238	0.0796	1.4829	1.4288	-0.0541
98	-11.7644	0.5319	0.0815	1	1.1014	0.1014
99*	-7.8886	0.5916	0.0851	1	0.9843	-0.0157
100*	-10.9597	0.5529	0.08	1.0755	1.144	0.0685
101	-7.6942	0.5835	0.0832	1.2945	1.3552	0.0607
102	-14.3073	0.5266	0.0798	-	0.7193	-
103	-10.5747	0.5433	0.0833	1	0.8398	-0.1602
104	-17.938	0.5633	0.0824	-	1.1949	-
105*	-14.3653	0.5767	0.0861	1.6866	1.4579	-0.2287
106	-15.9715	0.5702	0.082	1.143	1.0936	-0.0494
107	-12.9632	0.5156	0.0828	1.2175	1.1755	-0.042
108	-15.359	0.5679	0.0695	1.4362	1.4345	-0.0017
109	-11.4662	0.5916	0.0724	1.6848	1.6754	-0.0094
110*	-19.2371	0.6226	0.092	1.2323	1.4902	0.2579

111	-15.6234	0.6195	0.0794	1.8488	2.0456	0.1968
112	-18.9335	0.5471	0.0819	1.2923	1.1892	-0.1031
113	-15.4543	0.5666	0.0805	1.3838	1.4409	0.0571
114	-19.2813	0.576	0.0805	1.1335	1.1759	0.0424
115	-15.1627	0.6818	0.0787	1.8041	1.7153	-0.0888
116*	-21.2839	0.5665	0.0793	1	0.912	-0.088
117	-17.4899	0.601	0.079	1	1.1077	0.1077
118	-24.1402	0.5548	0.0838	1	1.1532	0.1532

Table S52. Descriptors, experimental and predicted pIC_{50} values and their residuals for compounds in scaffold based QSAR model against S5.

No.	RNCl	RNCSz	FNSA2Q	Exp.	Pred.	Res.
119	0.0182	6.8224	-3.6672	-	1.1874	-
120	0.0196	4.2424	-3.6026	1.8451	1.7286	-0.1165
121	0.0185	3.2996	-3.551	1.8451	1.824	-0.0211
122	0.0175	3.0427	-3.3659	1.6532	1.6032	-0.05
123*	0.0192	3.5808	-3.4257	1.6021	1.6315	0.0294
124*	0.0167	3.0447	-3.365	3	1.5653	-1.4347
125	0.0172	2.804	-3.5996	2.0792	1.9419	-0.1373
126	0.0182	3.4277	-3.6575	1.699	1.9183	0.2193
127	0.0364	6.6788	-3.4183	1.5441	1.6518	0.1077
128	0.0351	2.6574	-3.0568	2.1761	2.0171	-0.159
129	0.0333	2.6083	-3.0736	1.699	1.9768	0.2778
130	0.0345	2.2085	-3.2882	2.0791	2.3864	0.3073
131*	0.0364	6.6788	-3.4309	2.4472	1.6679	-0.7793
132*	0.0392	4.0722	-3.4268	2.6021	2.3513	-0.2508
133*	0.037	2.8263	-3.4555	2.699	2.5708	-0.1282

134	0.0351	2.7152	-3.2287	2.4771	2.2243	-0.2528
135	0.0385	2.7587	-3.3291	2.301	2.4828	0.1818
136	0.0333	2.665	-3.2331	2.3222	2.1685	-0.1537
137	0.0345	2.5483	-3.3246	2.3222	2.3587	0.0365
138	0.0364	2.9284	-3.4966	2.6812	2.5732	-0.108
139	0.037	5.7423	-3.3415	1.8451	1.7865	-0.0586
140*	0.0392	3.9452	-3.3629	2.6021	2.2973	-0.3048
141*	0.037	2.9971	-3.3548	2.0414	2.4046	0.3632
142	0.0351	2.5876	-3.3182	2.415	2.3668	-0.0482
143	0.0385	2.8708	-3.266	2.301	2.3775	0.0765
144	0.0333	2.5975	-3.1552	2.0792	2.0835	0.0043
145	0.0345	2.7183	-3.3662	2.3222	2.3747	0.0525
146	0.0364	3.1053	-3.4127	2.699	2.4271	-0.2719
147	0.0208	3.6257	-3.6216	1.8451	1.9386	0.0935
148*	0.0196	3.3864	-3.5762	-	1.8822	-
149	0.0204	3.5213	-3.5843	1.9542	1.8962	-0.058
150	0.0192	3.3917	-3.6665	1.9031	1.9811	0.078

Table S53. Descriptors, experimental and predicted pIC_{50} values and their residuals for compounds in scaffold based QSAR model against S6.

No.	EMiNACC	$PNSA2_Q$	$EHBCA_Q$	Exp.	Pred.	Res.
151	-0.4884	-462.484	37.9029	1.6232	**1.4075**	-0.2157
152	-0.4338	-485.623	29.6297	1.9605	1.8434	-0.1171
153	-0.5317	-756.608	73.0075	1.8692	1.9351	0.0659
154*	-0.4202	-585.458	60.6669	2.0943	1.8645	-0.2298
155	-0.4216	-512.505	44.9903	1.5717	1.7838	0.2121
156	-0.556	-580.691	44.2396	1.3483	1.5259	0.1776
157	-0.4282	-531.224	42.0627	1.9309	1.8754	-0.0555
158	-0.3829	-587.773	80.5014	1.8062	1.7425	-0.0637
159	-0.3933	-512.98	43.3637	1.8451	1.9244	0.0793
160*	-0.4783	-544.722	46.2851	1.5527	1.6661	0.1134
161	-0.5628	-487.301	35.5833	1.1367	1.239	0.1023
162	-0.5696	-606.877	35.3034	1.8014	1.7056	-0.0958
163	-0.5897	-632.378	39.7817	1.9175	1.6642	-0.2533
164	-0.5649	-662.908	35.3944	1.8531	1.9532	0.1001
165	-0.5244	-587.248	40.5516	1.6656	1.7344	0.0688

166	-0.5221	-551.904	29.7145	1.7657	1.7538	-0.0119
167	-0.7004	-476.613	29.9382	0.7243	0.7147	-0.0096
168*	-0.4932	-488.099	42.0487	1.7218	1.4337	-0.2881
169	-0.434	-444.514	34.6632	1.4425	1.602	0.1595
170	-0.4184	-439.827	26.3991	1.7324	1.7646	0.0322
171	-0.6323	-479.106	20.299	1.1038	1.1405	0.0367
172*	-0.5457	-760.596	75.7041	1.4265	1.8558	0.4293
173*	-0.4778	-433.597	24.3326	1.7427	1.5263	-0.2164

Table S54. Descriptors, experimental and predicted pIC_{50} values and their residuals for compounds in scaffold based QSAR model against S7.

No.	PMIB	$EHDSA_Q$	EMaNACC	Exp.	Pred.	Res.
174*	0.0194	103.06	0.0157	1.5798	1.4567	-0.1231
175*	0.0172	102.5828	-0.0614	1.2553	1.158	-0.0973
176	0.019	99.2429	0.0656	0.301	0.1523	-0.1487
177	0.0157	96.3801	0.1469	0.4771	0.6611	0.184
178	9.55E-03	114.0339	0.2122	1.2304	0.9864	-0.244
179	0.014	100.1972	0.138	1.3979	1.5251	0.1272
180	8.44E-03	127.3936	0.1052	1.0792	0.8249	-0.2543
181	9.67E-03	129.3021	0.1316	-	0.5169	-
182	9.51E-03	93.5174	0.162	1.2553	1.328	0.0727
183	0.0117	114.5111	0.1648	0.6021	0.6959	0.0938
184	0.0162	41.0331	0.2018	0.699	0.4631	-0.2359
185*	0.0178	108.7855	0.1153	1.3424	1.1544	-0.188
186	0.0156	102.1057	0.0217	0.301	0.3336	0.0326
187	0.0168	104.9685	0.246	0.699	0.5584	-0.1406
188	0.0151	101.1514	0.2554	0.699	0.8103	0.1113

189	8.17E-03	132.1649	0.2157	0.301	0.5455	0.2445
190*	0.0119	108.3084	0.1981	1.699	1.8632	0.1642
191	7.12E-03	138.3675	0.1812	0.4771	0.6539	0.1768
192	8.07E-03	130.7335	0.2433	-	0.8325	-
193	8.12E-03	102.5828	0.2112	1.5798	1.3556	-0.2242
194	0.01	122.1451	0.2851	-	0.9009	-
195	0.014	69.6609	0.3249	1.6021	1.6883	0.0862

Table S55. Descriptors, experimental and predicted pIC_{50} values and their residuals for compounds in scaffold based QSAR model against S8.

No.	MaPCH	TE/#A-T	MiERIC	Exp.	Pred.	Res.
196*	0.0864	3.7014	8.10E-08	-1.4559	-1.2319	0.224
197*	0.0546	3.5865	1.06E-07	-1.4559	-1.616	-0.1601
198	0.0546	3.5655	3.45E-08	-1.3098	-1.1505	0.1593
199	0.0546	3.4543	2.33E-07	-0.3767	-0.3503	0.0264
200	0.0546	3.3614	1.59E-07	-0.2549	-0.3126	-0.0577
201	0.0546	3.7042	9.93E-08	-1.3979	-1.3296	0.0683
202	0.0546	3.7399	5.74E-08	-1.5528	-1.5292	0.0236
203	0.0546	3.5946	5.28E-08	-1.4089	-1.1759	0.233
204	0.0546	3.7082	2.44E-08	-1.6198	-1.5356	0.0842
205	0.0597	3.721	7.07E-08	-1.1938	-1.2087	-0.0149
206	0.0546	3.5566	2.32E-09	-1.0458	-1.2125	-0.1667
207*	0.084	3.6204	5.81E-08	-0.5186	-0.3614	0.1572
208*	0.0546	3.6085	7.09E-09	-0.2314	-0.3305	-0.0991
209	0.0546	3.7111	2.46E-08	-1.3468	-1.5423	-0.1955
210	0.0552	3.7188	1.65E-07	-1.0506	-1.1638	-0.1132

211	0.0989	3.729	5.71E-08	0.5848	0.5881	0.0033
212	0.0546	3.468	4.60E-09	-0.9335	-0.9837	-0.0502
213	0.0546	3.3038	2.31E-09	-1.0044	-1.3771	-0.3727

Table S56. Descriptors, experimental and predicted pIC_{50} values and their residuals for compounds in scaffold based QSAR model against S9.

No.	MiERIN	MaREHN	ABOC	Exp.	Pred.	Res.
214	6.34E-05	13.63	1.1068	0.4771	0.7132	0.2361
215	3.93E-05	13.64	1.0807	1.2041	0.9636	-0.2405
216	6.96E-05	13.691	1.1189	0.4771	0.8092	0.3321
217*	4.36E-05	13.649	1.1257	1.2553	1.5407	0.2854
218	4.87E-05	13.634	1.1335	0.4771	0.4197	-0.0574
219	5.01E-05	13.629	1.1026	0.4771	0.724	0.2469
220	7.32E-06	13.645	1.1058	0.8451	0.6535	-0.1916
221	4.72E-05	13.646	1.1218	0.4771	0.5778	0.1007
222*	1.62E-04	13.639	1.1253	0.301	0.4642	0.1632
223	8.73E-05	13.646	1.1026	0.7782	0.862	0.0838
224	1.94E-04	13.65	1.1393	0.301	0.7265	0.4255
225	8.00E-05	13.656	1.1496	0.8451	0.3961	-0.449
226	7.25E-05	13.639	1.1331	0.7782	0.4921	-0.2861
227*	6.95E-05	13.635	1.1255	0.4771	0.5508	0.0737

228	5.62E-06	13.65	1.1293	0.4771	0.4247	-0.0524
229	1.27E-04	13.653	1.1476	0.4771	0.5076	0.0305
230	1.30E-04	13.597	1.1257	0.4771	0.5496	0.0725
231*	1.29E-04	13.627	1.1026	1.3222	1.5871	0.2649
232	2.48E-04	13.609	1.1069	-	1.0389	-
233	1.70E-04	13.623	1.0808	1.3222	1.186	-0.1362
234	5.73E-04	13.775	1.1066	2.7324	2.3057	-0.4267
235	5.95E-04	13.798	1.0797	2.6232	2.7081	0.0849
236*	5.82E-04	13.746	1.0854	1.2553	1.4442	0.1889
237	3.46E-04	13.767	1.0569	2	2.3015	0.3015
238	7.89E-07	13.974	1.1195	1.2788	1.6186	0.3398
239	1.62E-06	13.97	1.0934	2.0569	1.8759	-0.181
240*	1.43E-03	13.636	1.0641	4	4.1063	0.1063
241	1.46E-03	13.624	1.0754	4	4.0236	0.0236
242	3.56E-05	13.859	1.0673	2.0969	1.8399	-0.257
243	2.72E-06	13.881	1.0774	2.749	1.7398	-1.0092

Table S57. Descriptors, experimental and predicted pIC_{50} values and their residuals for compounds in scaffold based QSAR model against S10.

No.	MaenACH	HNMV	MaPPBO	Exp.	Pred.	Res.
244	69.487	3.19E+03	0.8969	0.699	0.3821	-0.3169
245	69.484	3.20E+03	0.8978	0.4771	0.4541	-0.023
246	69.583	3.19E+03	0.8939	-0.1249	0.1175	0.2424
247	69.597	3.15E+03	0.895	-0.1249	-0.3058	-0.1809
248*	69.073	3.19E+03	0.8976	0.4771	0.3745	-0.1026
249	68.058	3.20E+03	0.8983	-1.1249	-0.8061	0.3188
250	69.099	3.15E+03	0.8975	0.4771	0.3646	-0.1125
251	67.13	3.14E+03	0.8983	-1.1249	-1.2882	-0.1633
252*	69.025	3.18E+03	0.8985	-1.1249	-1.2174	-0.0925
253	67.139	3.18E+03	0.8993	-1.6021	-1.4114	0.1907
254	69.327	3.41E+03	0.8928	-1.4559	-1.6442	-0.1883
255	69.313	3.41E+03	0.8941	-1.6021	-1.5133	0.0888
256	69.077	3.20E+03	0.8937	-0.5229	-0.4424	0.0805
257*	68.778	3.19E+03	0.8947	-1.301	-1.5119	-0.2109
258	69.4	3.20E+03	0.8935	0.301	0.1998	-0.1012

259	67.191	3.17E+03	0.8957	-1.699	-1.7202	-0.0212
260	69.207	3.25E+03	0.9001	0.0607	0.1553	0.0946
244	69.487	3.19E+03	0.8969	0.699	0.3821	-0.3169
245	69.484	3.20E+03	0.8978	0.4771	0.4541	-0.023
246	69.583	3.19E+03	0.8939	-0.1249	0.1175	0.2424
247	69.597	3.15E+03	0.895	-0.1249	-0.3058	-0.1809
248	69.073	3.19E+03	0.8976	0.4771	0.3745	-0.1026
249	68.058	3.20E+03	0.8983	-1.1249	-0.8061	0.3188
250	69.099	3.15E+03	0.8975	0.4771	0.3646	-0.1125
251	67.13	3.14E+03	0.8983	-1.1249	-1.2882	-0.1633
252	69.025	3.18E+03	0.8985	-1.1249	-1.2174	-0.0925
253	67.139	3.18E+03	0.8993	-1.6021	-1.4114	0.1907
254	69.327	3.41E+03	0.8928	-1.4559	-1.6442	-0.1883
255	69.313	3.41E+03	0.8941	-1.6021	-1.5133	0.0888
256	69.077	3.20E+03	0.8937	-0.5229	-0.4424	0.0805
257	68.778	3.19E+03	0.8947	-1.301	-1.5119	-0.2109
258	69.4	3.20E+03	0.8935	0.301	0.1998	-0.1012

259	67.191	3.17E+03	0.8957	-1.699	-1.7202	-0.0212
260	69.207	3.25E+03	0.9001	0.0607	0.1553	0.0946

Table S58. Descriptors, experimental and predicted pIC_{50} values and their residuals for compounds in scaffold based QSAR model against S11.

No.	1XGP	DPSA2z	EHDSAQ	Exp.	Pred.	Res.
261	2.22E+05	2.22E+05	178.9235	0.5999	0.5817	-0.0182
262	2.15E+05	2.15E+05	166.041	0.5809	0.5168	-0.0641
263	2.43E+05	2.43E+05	151.25	0.5809	0.096	-0.4849
264	2.35E+05	2.35E+05	115.9424	0.179	0.1894	0.0104
265	2.55E+05	2.55E+05	180.832	-0.4949	-0.4727	0.0222
266*	2.47E+05	2.47E+05	115.4653	-0.9208	-0.7716	0.1492
267	2.29E+05	2.29E+05	160.3155	0.1818	0.3766	0.1948
268	2.24E+05	2.24E+05	146.4787	0.143	0.1199	-0.0231
269	2.46E+05	2.46E+05	176.5379	0.4265	0.3316	-0.0949
270*	2.41E+05	2.41E+05	172.2437	0.4048	0.312	-0.0928
271	2.21E+05	2.21E+05	207.0742	0.6464	0.6742	0.0278
272	2.18E+05	2.18E+05	164.6096	0.6138	0.6247	0.0109
273	2.44E+05	2.44E+05	168.9038	0.4942	0.286	-0.2082
274*	2.39E+05	2.39E+05	141.2303	0.3324	0.1129	-0.2195
275	2.58E+05	2.58E+05	151.7271	0.0492	0.0175	-0.0317

276	2.51E+05	2.51E+05	143.616	-0.3665	-0.2848	0.0817
277*	2.31E+05	2.31E+05	183.2177	0.4579	0.5424	0.0845
278	2.27E+05	2.27E+05	172.7208	0.2253	0.1897	-0.0356
279	2.47E+05	2.47E+05	190.8518	0.4786	0.6066	0.128
280*	2.44E+05	2.44E+05	197.5316	0.4014	0.2328	-0.1686

Table S59. Descriptors, experimental and predicted pIC_{50} values and their residuals for compounds in scaffold based QSAR model against S12.

No.	HLEG	MaeeRN	KSI3	Exp.	Pred.	Res.
281	8.451	133.04	2.9118	0.0086	0.1317	0.1231
282	8.492	132.658	2.6827	0.1553	0.1454	-0.0099
283	8.452	135.636	3.1276	0.7782	0.4742	-0.304
284	8.348	141.181	2.8381	-0.1739	0.6646	0.8385
285*	8.257	130.875	3.2351	1	-0.5812	-1.5812
286*	8.273	130.911	3.467	1	-0.4604	-1.4604
287	8.304	143.542	3.4065	1	0.9528	-0.0472
288	8.336	140.98	3.7004	1	0.8646	-0.1354
289	8.92	133.1	2.5318	1	1.4267	0.4267
290	8.453	141.715	2.4625	1	0.923	-0.077
291*	8.358	141.189	2.6962	1	0.653	-0.347
292*	8.686	133.075	2.9118	1	0.8379	-0.1621
293	8.659	132.986	3.3104	1	0.8667	-0.1333
294	8.476	141.701	3.2351	1	1.2207	0.2207
295	8.598	133.018	2.8041	1	0.5366	-0.4634

296	8.297	140.336	5.0738	1	1.0895	0.0895
297	8.227	141.245	4.9822	1	0.9493	-0.0507
298*	8.131	141.421	2.6827	1	1.02E+00	0.022
299*	8.128	141.281	2.6104	1	-0.0504	-1.0504
300	8.632	132.973	4.0131	1	0.9942	-0.0058
301	8.345	141.547	3.9284	1	1.0197	0.0197
302	8.35	141.193	2.6104	1	0.6039	-0.3961
303	7.759	141.236	2.9825	-1.0458	-1.0472	-0.0014
304	8.392	133.026	2.9939	-1	-0.0217	0.9783
305	8.309	141.153	2.9218	-0.9208	0.57	1.4908
306*	8.376	141.347	3.1348	0.6128	0.8544	0.2416
307	8.485	133.1	3.5215	1	0.4216	-0.5784
308	8.393	141.461	3.4487	1	1.0109	0.0109
309	8.764	132.939	2.4451	1	0.9174	-0.0826
310	8.454	141.423	2.3743	1	0.8687	-0.1313
311	8.77	133.003	2.4451	1	0.9421	-0.0579
312*	8.597	141.599	2.3743	1	1.3148	0.3148

313*	8.319	140.884	3.205	-0.6198	0.6559	1.2757
314	8.329	141.233	3.5063	1	0.8126	-0.1874
315	8.34	141.15	3.6113	1	0.868	-0.132
316	8.31	141.142	3.6113	1	0.7775	-0.2225
317	8.333	141.185	4.0173	1	0.9719	-0.0281
318	8.335	141.18	3.9074	1	0.9446	-0.0554
319*	3.977	141.236	4.0173	1	2.0441	1.0441
320*	8.327	141.147	4.3468	1	1.0483	0.0483
321	8.332	141.164	4.4614	1	1.0992	0.0992
322	8.382	141.401	3.4066	1	0.9591	-0.0409
323	8.378	141.294	4.5439	1	1.2751	0.2751
324	8.327	141.162	4.377	1	1.0589	0.0589
325	8.324	140.872	5.7688	1	1.4344	0.4344

Table S60. Descriptors, experimental and predicted pIC_{50} values and their residuals for compounds in scaffold based QSAR model against S13.

No.	MiERIN	MiAOEP	MiBON(0.1)	Exp.	Pred.	Res.
326	1.47E-03	0.7383	0.1318	1.1761	1.6396	0.4635
327	1.88E-03	0.7393	0.1319	2	1.7877	-0.2123
328	2.57E-03	0.7414	0.1314	2	1.9652	-0.0348
329	1.43E-03	0.7377	0.1315	2	1.6068	-0.3932
330	1.11E-03	0.7367	0.1343	1.7782	1.8008	0.0226
331	1.06E-03	0.7401	0.1305	-0.0969	1.251	1.3479
332*	1.98E-04	0.7439	0.1273	1.1761	0.3766	-0.7995
333*	6.45E-04	0.7363	0.135	0.699	1.6838	0.9848
334	1.02E-03	0.7406	0.1311	2	1.2774	-0.7226
335	1.63E-03	0.7389	0.1334	2	1.8591	-0.1409
336	1.49E-03	0.7379	0.1321	1.7782	1.6907	-0.0875
337	1.15E-03	0.74	0.1312	2	1.3616	-0.6384
338	2.13E-04	0.7396	0.1321	1	1.0622	0.0622
339	2.03E-04	0.7368	0.1331	1.2672	1.2693	0.0021
340	2.03E-04	0.7368	0.1331	1	1.2684	0.2684

341*	1.75E-04	0.7378	0.1327	-0.0458	0.1767	0.2225
342*	3.58E-09	0.7397	0.1319	0.9031	0.9389	0.0358
343	4.16E-04	0.703	0.1271	2	1.9379	-0.0621
344	3.09E-03	0.7522	0.1315	2	1.8152	-0.1848
345	2.95E-03	0.7519	0.1314	0.9031	1.7608	0.8577
346	3.08E-03	0.7523	0.1315	2	1.8114	-0.1886
347	3.22E-03	0.7521	0.1314	2	1.87	-0.13
348	1.97E-03	0.7519	0.1321	1.6021	1.3936	-0.2085
349	2.01E-03	0.7519	0.1321	1.4771	1.4119	-0.0652
350*	1.98E-03	0.7519	0.1321	1.6021	1.3977	-0.2044
351*	2.54E-07	0.7514	0.1322	1.9777	1.5442	-0.4335
352	1.83E-03	0.7311	0.1322	1.9542	2.1046	0.1504
353	2.79E-06	0.7521	0.1322	0.699	0.5201	-0.1789
354	3.02E-06	0.752	0.1321	0.301	0.5184	0.2174
355	3.20E-06	0.7521	0.1322	0.301	0.5183	0.2173
356	2.49E-07	0.7521	0.1322	0.7782	0.5229	-0.2553
357	2.23E-06	0.7487	0.1279	0.8751	0.1765	-0.6986

358	1.88E-06	0.7487	0.1279	-0.3979	0.1758	0.5737
359	3.23E-04	0.7489	0.128	0.301	0.3195	0.0185
360*	7.32E-08	0.7509	0.1309	0.301	0.4231	0.1221
361*	1.10E-06	0.7509	0.1309	0.3979	0.4264	0.0285

Table S61. Descriptors, experimental and predicted pIC_{50} values and their residuals for compounds in scaffold based QSAR model against S14.

No.	MaTICC	$EPNSA3_Q$	MiTICN	Exp.	Pred.	Res.
362*	20.371	-44.604	15.879	1.2404	0.6936	-0.5468
363	20.332	-39.5719	15.938	1.7853	1.1331	-0.6522
364	20.306	-30.1436	15.972	1.7482	2.2686	0.5204
365	20.458	-35.0332	15.924	0	0.1572	0.1572
366	20.241	-35.7454	15.99	1.8451	2.2207	0.3756
367*	20.205	-42.8067	15.95	2.0414	2.3144	0.273
368	20.375	-39.9787	15.887	1.4472	1.1292	-0.318
369	20.337	-36.9676	15.947	1.9243	1.2844	-0.6399
370	20.314	-27.62	15.986	2.1584	2.3057	0.1473
371	20.248	-32.2708	16.006	0	2.3679	2.3679
372	20.212	-43.0682	15.959	1.9956	2.0721	0.0765
373	20.345	-38.7766	15.96	0	0.7806	0.7806
374	20.321	-27.3557	15.997	2.0043	2.1056	0.1013
375	20.256	-33.2291	16.02	2	1.9603	-0.0397
376*	20.124	-44.3707	15.938	1.8513	1.3777	-0.4736

377	20.363	-39.793	15.959	0	0.4161	0.4161
378	20.342	-30.165	16	1.9823	1.4207	-0.5616
379	20.274	-35.6463	16.019	2	1.4169	-0.5831
380*	20.213	-51.631	15.924	1.9345	1.4032	-0.5313
381	20.351	-45.8202	15.929	0	0.1869	0.1869
382	20.329	-33.0434	15.967	1.6128	1.645	0.0322
383*	20.263	-40.5619	15.985	0	0.366	0.366

Table S62. Descriptors, experimental and predicted pIC_{50} values and their residuals for compounds in scaffold based QSAR model against S15.

No.	RNN	MiERIC	MIA	Exp.	Pred.	Res.
384	0.12	1.52E-04	0.0343	1.5966	1.8569	0.2603
385	0.1304	3.10E-03	0.0224	0.8129	0.7358	-0.0771
386	0.1304	2.95E-03	0.0301	1.0043	0.8658	-0.1385
387*	0.1304	3.02E-03	0.0112	0.8573	0.6652	-0.1921
388	0.1111	5.41E-06	0.0172	1.5763	1.6074	0.0311
389	0.1304	1.49E-03	0.0368	1.9053	1.5161	-0.3892
390	0.1304	2.90E-03	6.93E-03	0.6721	0.6737	0.0016
391*	0.1739	2.07E-03	0.0932	2.3191	2.5443	0.2252
392	0.1333	5.28E-05	0.0768	2.6496	2.5123	-0.1373
393	0.1852	2.32E-05	0.0166	2.9141	2.8633	-0.0508
394	0.1667	3.41E-04	0.0365	2.6013	2.5995	-0.0018
395*	0.1154	1.35E-07	0.0481	2.5668	2.1642	-0.4026
396	0.1154	3.31E-05	0.097	2.5006	2.3972	-0.1034
397	0.1	1.82E-05	0.0251	1.4786	1.4841	0.0055
398	0.1111	3.45E-05	0.0734	1.7796	2.1085	0.3289

399*	0.0968	3.40E-05	0.0318	1.9609	1.4831	-0.4778
400	0.0833	2.94E-07	0.0516	1.6821	1.4473	-0.2348
401	0.0938	7.12E-04	0.0571	1.6304	1.388	-0.2424
402	0.125	1.66E-04	0.0662	2.1166	2.227	0.1104
403*	0.1379	2.43E-06	0.0543	2.975	2.4066	-0.5684
404	0.12	3.17E-03	0.0531	0.4314	0.8093	0.3779
405	0.1905	2.36E-03	0.1092	2.7832	2.8545	0.0713
406	0.1667	1.65E-05	0.0638	2.9499	2.9792	0.0293
407*	0.1905	1.23E-03	0.0599	1.0253	1.8592	0.8339
408	0.1538	3.90E-04	0.0634	2.6782	2.6054	-0.0728
409	0.1111	3.50E-05	0.0185	1.4502	1.6069	0.1567
410	0.0833	1.26E-05	0.021	1.5079	1.1633	-0.3446
411*	0.1154	2.44E-03	0.0281	2.2512	1.795	-0.4562
412	0.0811	2.84E-06	0.0138	0.6435	1.0633	0.4198
413*	0.0882	1.10E-04	0.0135	0.7324	1.1398	0.4074

Table S63. Descriptors, experimental and predicted pIC_{50} values and their residuals for compounds in scaffold based QSAR model against S16.

No.	IOKSE	$EFHBSA_Q$	RNN	Exp.	Pred.	Res.
414	261.423	261.423	2.7607	0.3424	0.8127	0.4703
415	261.316	261.316	2.7607	0.1139	0.7507	0.6368
416*	261.343	261.343	2.7607	0.0414	0.7091	0.6677
417	261.274	261.274	2.7607	0.9868	0.8766	-0.1102
418	260.658	260.658	3.1799	0.7076	0.9237	0.2161
419*	260.848	260.848	3.0054	0.2304	0.7142	0.4838
420	260.808	260.808	3.2284	0.9031	1.0717	0.1686
421	260.817	260.817	3.2284	0.0414	0.3235	0.2821
422*	261.397	261.397	3.0258	1.1523	0.8689	-0.2834
423	261.317	261.317	3.0258	1.1367	0.9202	-0.2165
424	261.139	261.139	3.0364	1.3979	0.6764	-0.7215
425*	261.208	261.208	3.1143	1.3979	0.9356	-0.4623
426	261.217	261.217	2.9501	0.6128	0.4997	-0.1131
427	261.267	261.267	2.9893	1.1038	0.7968	-0.307
428	261.27	261.27	3.0949	0.2304	0.8859	0.6555
429	260.822	260.822	2.7607	0.0719	1.0639	0.992
430	260.835	260.835	2.7607	0.9912	1.1171	0.1259

431*	260.66	260.66	2.7607	1.0864	1.0566	-0.0298
432	260.734	260.734	2.9571	1.3979	1.3412	-0.0567
433	260.871	260.871	2.7486	1.3979	1.1834	-0.2145
434*	260.786	260.786	2.9768	1.3979	1.3857	-0.0122
435	260.875	260.875	2.9768	0.8109	0.7219	-0.089
436	260.777	260.777	3.0258	1.3979	1.2255	-0.1724
437*	260.515	260.515	3.0258	1.3979	1.3442	-0.0537
438	260.667	260.667	3.1143	1.3979	1.2913	-0.1066
439	260.783	260.783	2.9501	0.7853	0.7884	0.0031
440*	260.693	260.693	2.9893	1.3979	1.205	-0.1929
441	260.835	260.835	3.0949	0.9868	0.9889	0.0021
442	260.923	260.923	2.6543	1.3979	1.4505	0.0526
443*	260.765	260.765	2.7486	1.3979	1.1874	-0.2105
444	260.83	260.83	2.7259	1.3979	0.9224	-0.4755
445	260.488	260.488	2.8936	1.0969	1.1467	0.0498
446*	260.777	260.777	2.8936	1.3979	1.0192	-0.3787
447	260.457	260.457	2.8936	1.3979	1.1341	-0.2638
448	260.676	260.676	2.7486	1.3979	1.1989	-0.199
449*	260.387	260.387	2.7486	1.3979	1.1444	-0.2535

450	260.835	260.835	2.7607	1.3979	1.0674	-0.3305
451	260.816	260.816	3.1143	0.4624	0.8586	0.3962
452	257.672	257.672	2.6635	0.2553	1.2586	1.0033
453	257.838	257.838	2.6635	1.0682	1.2031	0.1349
454	257.888	257.888	2.6635	1.1 303	1.1357	0.0054
455*	256.761	256.761	2.6801	1.3979	1.4007	0.0028
456	255.789	255.789	2.9295	1.3979	1.5643	0.1664
457	256.828	256.828	2.9295	1.0864	1.3804	0.294
458	258.192	258.192	3.1443	1.3979	0.9449	-0.453
459	257.628	257.628	2.8351	0.9191	0.9603	0.0412
460	258.004	258.004	2.903	1.3979	1.1866	-0.2113
461	256.752	256.752	2.9903	1.2788	1.2424	-0.0364
462*	256.902	256.902	2.6361	1.3979	1.5287	0.1308
463	257.018	257.018	2.6801	1.3979	1.3179	-0.08
464	255.721	255.721	2.6108	1.3979	1.4681	0.0702
465*	258.002	258.002	2.5343	1.3979	1.1108	-0.2871
466	256.06	256.06	2.5343	1.3979	1.3725	-0.0254
467	257.935	257.935	3.0259	1.0874	0.9527	-0.1347
468*	259.016	259.016	3.0581	1.1483	1.1664	0.0181

469	255.919	255.919	2.9877	1.3979	1.4389	0.041
470	257.42	257.42	3.0581	1.3979	1.3883	-0.0096
471*	259.076	259.076	3.0875	0.9552	1.265	0.3098
472	257.415	257.415	3.0875	1.3979	1.5148	0.1169
473	256.256	256.256	2.8921	1.3979	1.345	-0.0529
474	258.892	258.892	2.9071	0.2788	1.0341	0.7553
475	256.539	256.539	2.8411	1.3979	1.2036	-0.1943
476	257.503	257.503	2.9071	0.9191	1.1551	0.236
477*	258.914	258.914	2.9361	0.7566	1.1867	0.4301
478	257.514	257.514	2.9361	1.3979	1.2717	-0.1262
479	256.451	256.451	2.7515	1.3979	1.1442	-0.2537

Table S64: Analysis of Inter-correlation of the descriptors along with correlation of activity for the developed models.

No.	R2 Pred	D1	D2	D3		D1	D2	D3
M1	0.71	MannRCN	ASCI1	RNCSz	D1	1.0000	0.1592	-0.516
					D2	0.1592	1.0000	0.3773
					D3	-0.516	0.3773	1.0000
M2	0.56	MaenCC	$PNSA1_Q$	PNSA2z	D1	1.0000	0.3145	-0.3721
					D2	0.3145	1.0000	-0.5748
					D3	-0.3721	-0.5748	1.0000
M3	0.67	MiNRIO	$HACA1_Q$	RPCSz	D1	1.0000	-0.4274	-0.3208
					D2	-0.4274	1.0000	0.5562
					D3	-0.3208	0.5562	1.0000
M4	0.97	FPSA3z	WNSA2z	BI	D1	1.0000	-0.0271	0.6226
					D2	-0.0271	1.0000	-0.5360
					D3	0.6226	-0.5360	1.0000
M5	0.69	YZS	RI0	MiERIC	D1	1.0000	0.5719	-0.2289
					D2	0.5719	1.0000	-0.2302
					D3	-0.2289	-0.2302	1.0000
M6	0.94	$WPSA1_Q$	MiTICS	MiNACN	D1	1.0000	-0.7752	0.2853
					D2	-0.7752	1.0000	-0.6026
					D3	0.2853	-0.6026	1.0000
M7	0.72	XYZ/XYR	MiERIC	RNO	D1	1.0000	0.3075	0.3379
					D2	0.3075	1.0000	0.3478
					D3	0.3379	0.3478	1.0000

M8	0.58	HLEG	$WNSA3_Q$	MiERIN	D1	1.0000	0.4272	0.5521
					D2	0.4272	1.0000	0.5910
					D3	0.5521	0.5910	1.0000
M9	0.92	A1ERIC	SIC1	YZS	D1	1.0000	0.0016	0.4347
					D2	0.0016	1.0000	0.3792
					D3	0.4347	0.3792	1.0000
M10	0.43	MiTICN	PNSA1z	CHaSz	D1	1.0000	0.5573	0.3216
					D2	0.5573	1.0000	0.4297
					D3	0.3216	0.4297	1.0000
M11	0.93	FNSA2z	$ERPCG_Q$	MienACH	D1	1.0000	-0.3213	0.3888
					D2	-0.3213	1.0000	-0.1387
					D3	0.3888	-0.1387	1.0000
M12	0.73	MiPCC	MiBOC(0.1)	THCMD	D1	1.0000	0.0368	-0.0331
					D2	0.0368	1.0000	0.1072
					D3	-0.0331	0.1072	1.0000
M13	0.58	RE/T	LNMVF	ACIC1	D1	1.0000	-0.7513	0.2404
					D2	-0.7513	1.0000	-0.3645
					D3	0.2404	-0.3645	1.0000
M14	0.75	MaBON	MienACN	NN	D1	1.0000	-0.2096	0.4859
					D2	-0.2096	1.0000	0.4268
					D3	0.4859	0.4268	1.0000
M15	0.30	$FNSA2_Q$	PP/SD	MaenAC	D1	1.0000	0.2841	-0.2431
					D2	0.2841	1.0000	-0.5342
					D3	-0.2431	-0.5342	1.0000

					D1	1.0000	0.0999	0.0693
M16	0.86	EMaNACH	$HDSA2_Q$	MaeeRC	D2	0.0999	1.0000	0.2707
					D3	0.0693	0.2707	1.0000
					D1	1.0000	-0.1970	0.2484
M17	0.90	$HDCA2_Q$	WNSA2z	MienANN	D2	-0.1970	1.0000	-0.2012
					D3	0.2484	-0.2012	1.0000
					D1	1.0000	0.0354	0.0386
M18	0.83	ZXS/ZXR	$ERNCS_Q$	MiBOC(0.1)	D2	0.0354	1.0000	-0.1702
					D3	0.0386	-0.1702	1.0000
					D1	1.0000	0.0133	0.5859
M19	0.80	NN	RNBr	Mi1ERIC	D2	0.0133	1.0000	0.2480
					D3	0.5859	0.2480	1.0000
					D1	1.0000	0.2011	0.0412
M20	0.46	MaeeRC	$ERPCS_Q$	ASIC1	D2	0.2011	1.0000	0.1757
					D3	0.0412	0.1757	1.0000
					D1	1.0000	0.1782	-0.4228
M21	0.48	$EFPSA1_Q$	ANRIO	$EHDSA_Q$	D2	0.1782	1.0000	-0.1934
					D3	-0.4228	-0.1934	1.0000
					D1	1.0000	0.5730	-0.6428
M22	0.58	MiPC(QMin)	Ma1ERIC	MaenACO	D2	0.5730	1.0000	-0.7131
					D3	-0.6428	-0.7131	1.0000
					D1	1.0000	0.0478	-0.0578
M23	0.81	WPSA1z	MiTICN	$HDCA1_Q$	D2	0.0478	1.0000	-0.0388
					D3	-0.0578	-0.0388	1.0000

					D1	1.0000	-0.1759	0.0643
M24	0.87	SIC2	LNMVF	$FPSA3_Q$	D2	-0.1759	1.0000	0.1966
					D3	0.0643	0.1866	1.0000
					D1	1.0000	-0.0902	0.2359
M25	0.74	ABOC	$ERNCS_Q$	EMaNAC	D2	-0.0902	1.0000	-0.2830
					D3	0.2359	-0.2830	1.0000
					D1	1.0000	-0.0413	0.0358
M26	0.77	CIC2	AVN	MiRECN	D2	-0.0413	1.0000	0.0849
					D3	0.0358	0.0849	1.0000
					D1	1.0000	0.4230	0.0197
M27	0.50	HOMO1	MaTICH	$EFHDSA_Q$	D2	0.4230	1.0000	0.2469
					D3	0.0197	0.2469	1.0000
					D1	1.0000	0.1628	0.0289
M28	0.76	MiPCN	EE+eeR-CC	$EFHDCA_Q$	D2	0.1628	1.0000	0.3119
					D3	0.0289	0.3119	1.0000
					D1	1.0000	0.1331	0.0886
M29	0.69	MaASEN	RNCl	$HDSA_Q$	D2	0.1331	1.0000	0.0404
					D3	0.0886	0.0404	1.0000
					D1	1.0000	0.6236	0.4451
M30	0.76	IOKSE	$EFHBSA_Q$	RNN	D2	0.6236	1.0000	0.2009
					D3	0.4451	0.2009	1.0000
					D1	1.0000	0.7753	-0.2104
S1	0.75	VE/T	$WPSA3_Q$	LNMVF	D2	0.7753	1.0000	0.0295
					D3	-0.2104	0.0295	1.0000

					D1	1.0000	-0.0384	-0.1120
S2	0.69	RNB	MaenAC	PMIA	D2	-0.0384	1.0000	0.2100
					D3	-0.1120	0.2100	1.0000
					D1	1.0000	-0.0271	0.6226
S3	0.98	FPSA3z	WNSA2z	BI	D2	-0.0271	1.0000	-0.5360
					D3	0.6226	-0.5360	1.0000
					D1	1.0000	-0.0801	-0.4736
S4	0.88	PPSA3z	ZXS/ZXR	$RNCG_Q$	D2	-0.0801	1.0000	0.0405
					D3	-0.4736	0.0405	1.0000
					D1	1.0000	-0.2003	0.7441
S5	0.77	RNCl	RNCSz	$FNSA2_Q$	D2	-0.2003	1.0000	-0.4205
					D3	0.7441	-0.4205	1.0000
					D1	1.0000	0.1854	0.3458
S6	0.88	EMiNACC	$PNSA2_Q$	$EHBCA_Q$	D2	0.1854	1.0000	-0.6048
					D3	0.3458	-0.6048	1.0000
					D1	1.0000	-0.5798	-0.2870
S7	0.89	PMIB	$EHDSA_Q$	EMaNACC	D2	-0.5798	1.0000	-0.0984
					D3	-0.2870	-0.0984	1.0000
					D1	1.0000	0.2947	-0..0774
S8	0.96	MaPCHz	TE/#A-T	MiERIC	D2	0.2947	1.0000	-0.3023
					D3	-0.0774	-0.3023	1.0000
					D1	1.0000	-0.0733	-0.3830
S9	0.93	MiERIN	MaREHN	ABOC	D2	-0.0733	1.0000	-0.2993
					D3	-0.3830	-0.2993	1.0000

					D1	1.0000	0.3997	-0.2799
S10	0.96	MaenACH	HNMVF	MaPPBO	D2	0.3997	1.0000	-0.5168
					D3	-0.2799	-0.5168	1.0000
					D1	1.0000	0.2876	0.1911
S11	0.93	1XGP	DPSA2z	$EHDSA_Q$	D2	0.2876	1.0000	0.6387
					D3	0.1911	0.6387	1.0000
					D1	1.0000	-0.6706	-0.3939
S12	0.69	HLEG	MaeeRN	KSI3	D2	-0.6706	1.0000	0.3975
					D3	-0.3939	0.3975	1.0000
					D1	1.0000	0.1681	0.2068
S13	0.65	MiERIN	MiAOEP	MiBON(0.1)	D2	0.1681	1.0000	0.1897
					D3	0.2068	0.1897	1.0000
					D1	1.0000	-0.0236	-0.5988
S14	0.74	MaTICC	$EPNSA3_Q$	MiTICN	D2	-0.0236	1.0000	0.5868
					D3	-0.5988	0.5868	1.0000
					D1	1.0000	0.2278	0.2923
S15	0.92	RNN	MiERIC	MIA	D2	0.2278	1.0000	-0.0604
					D3	0.2923	-0.0604	1.0000
					D1	1.0000	0.4120	0.2262
S16	0.48	MaenACC	$FNSA1_Q$	AIC1	D2	0.4120	1.0000	0.3896
					D3	0.2262	0.3896	1.0000

Table S65a: Cell line with type of cancer in parenthesis, scaffolds involved, regression summary (regression equation, correlation coefficient R^2, cross validation coefficient R_{cv}^2 & average residual AE) and number of compounds (training set TR and test set TS) in various cell lines based QSAR models.

No	Cell line (Type)	Scf	Regression equation	R^2	R_{cv}^2	AE	F	S^2	# of comp.	
									TR	TS
M1	A498 (renal)	**S13**	=-3.3738* MannRCN+-1.2453* ASIC1 - 1.0807* RNCSz+4.6355	0.71	0.56	0.62	14.87	0.239	31	5
M2	A549 (Lung)	**S16**	=-1.3066* MaenACC +1.1275* PNSA1Q - 7.9011* PNSA2z +3.3541	0.56	0.49	0.27	18.41	0.094	56	10
M3	A2780 (Ovarian)	**S2**	=5.3016* MiNRIO +6.1285* HACA1Q- 1.222* RPCSz -3.6341	0.68	0.54	0.22	13.89	0.043	30	5
M4	ACHN (Renal)	**S3**	=7.4622*FPSA3z -7.8674* WNSA2z- 1.0224* BI+1.8722	0.96	0.95	0.05	105.93	0.001	16	3
M5	A431 (Skin)	**S2**	=-7.2276* YZS +1.0111*RI0* +7.4112.* MiERIC +2.5462	0.69	0.59	0.14	13.43	0.036	30	5
M6	B16-F10 (Melanoma)	**S11**	=-1.0251* WPSA1Q -1.7686* MiTICS +1.6039* MiNACN +2.7567	0.94	0.89	0.11	62.56	0.015	17	3
M7	BE2-C (Neuronal)	**S2**	=-5.0255* XYS/XYR +1.4971* MiERIC - 6.7892* RNO +5.2368	0.72	0.63	0.16	16.67	0.030	29	7
M8	BEL-7402 (Heptocellular)	**S12**	=2.6386* HLEG -6.0993* WNSA2Q- 4.8693* MiERIN-2.2423	0.58	0.44	0.31	12.34	0.177	35	10
M9	Calu1 (Lung)	**S3**	=2.2933* A1ERIC -2.3063*SIC1 - 3.0798*YZS +5.2315	0.93	0.80	0.12	41.25	0.023	16	3
M10	DU145	**S3, S13**	=7.0109* MiTICN-7.8249* PNSA1z -	0.43	0.32	0.45	11.60	0.307	57	15

	(Prostate)		2.7692* CHaSz -6.9257							
M11	H69 (Lung)	**S8**	=-1.1403* FNSA2z -5.8440* ERPCGQ - 5.2628* MienACH +3.4678	0.93	0.81	0.13	44.62	0.033	15	3
M12	H522 (lung)	**S1**3	=1.4711*MiPCCz* +2.3775* MiBOC(0.1) +8.7939* THCMD-2.1601	0.73	0.63	0.24	18.26	0.201	28	8
M13	HCT116 (Colon)	**S3, S5, S6**	=2.7531* RE/T+3.3081* LNMVF+64.6887* ACIC1 -1.0055	0.59	0.49	0.29	24.10	0.119	60	14
M14	Hela (Cervical)	**S7, S9, S10**	=-6.4020*MaBON -9.5518*MienACN +7.3732NN +3.7878	0.76	0.71	0.40	43.55	0.377	55	13
M15	HT29 (Colon)	**S2, S16**	=-6.4490*FNSA2Q+ 1.3955*PP/SD +9.1032*MaenAC-1. 6224	0.30	0.22	0.27	9.54	0.098	81	20
M16	JLc (Leukemia)	**S1**	=-7.0103*EMaNACH + 1.5761*HDSA2Q - 1.0051* MaeeRC + 1.0507	0.86	0.82	0.33	44.61	0.069	32	9
M17	L120 (Leukemia)	**S15**	=-4.8986*HDCA2Q + 1.7065 *WNSA2z – 1.4993 *MienANN + 6.9159	0.90	0.84	0.17	43.50	0.066	25	6
M18	LLc (Lung)	**S1**	=- 1.5310 * ZXS/ZXR + 2.7870 *ERNCSQ- 6.4016* MiBOC(0.1)+ 7.9845	0.83	0.78	0.38	36.82	0.155	32	9
M19	M14 (Melanoma)	**S13**	=-8.1796*NN -5.0035*RNBr +1.1723* MiERIC+4.9692	0.81	0.70	0.25	28.09	0.156	30	6
M20	MCF7 (Breast)	**S2, S4, S5, S9, S10, S11, S13, S14, S16**	=6.4410*MaeeRC-3.4532* ERPCSQ - 1.7867*ASIC1 -2.7106	0.46	0.44	0.55	52.87	0.663	231	49
M21	MLM (glioblastoma)	**S16**	=-8.2245*EFPSA1Q + 1.1671* ANRIO - 4.4003*EHDSAQ	0.48	0.40	0.28	14.37	0.124	53	13

M22	H460 (Lung)	**S2, S3, S14**	=-1.3004* MiPC +6.3227* Ma1ERIC+ 2.4755*MaenACO	0.59	0.49	0.41	19.82	0.152	60	16
M23	P388 (Leukemia)	**S1**	=-3.4460*WPSA1z + 6.8634*MiTICN + 8.1021*HDCA1Q – 9.9755	0.81	0.73	0.31	31.74	0.0751	32	9
M24	Panc1 (Pancreatic)	**S3**	=1.8296*SIC2+ 3.3629*LNMVF -1.7681* FPSA3Q-3.0118	0.87	0.73	0.11	21.63	0.016	16	3
M25	SF-468 (CNS)	**S14**	=2.4189*ABOC-3.9606* ERNCSQ +2.4054*EMaNAC -2.3761	0.74	0.56	0.27	9.38	0.171	18	4
M26	SJ-G2 (Brain)	**S2**	=5.1327*CIC2 +1.5429*AVN +2.0716* MiRECN -7.3156	0.77	0.60	0.13	18.67	0.034	26	9
M27	SKMEL-5 (Melanoma)	**S16**	=-1.2423*HOMO1+4.6277*MaTICH – 2.3144*EFHDSA -6.8356	0.51	0.45	0.22	15.52	0.111	51	15
M28	SKOV3 (Ovarian)	**S13**	=2.7606* MiPCNz -3.5240*EE+eeRCC +1.3856*EFHDCAQ +5.0366	0.76	0.66	0.28	20.69	0.141	29	7
M29	SW480 (Colon)	**S2**	=7.0573*MaASEN - 605367* RNCl - 1.1217*HDSAQ+1.3202	0.69	0.	0.27	32.20	0.130	50	15
M30	U251 (CNS)	**S13**	=-1.1620*IOKSE + 5.3498*EFHBSAQ – 1.5086*RNN+7.2762	0.76	0.69	0.31	24.27	0.154	29	7

Table S65b: Cell line with type of cancer in parenthesis, scaffolds involved, regression summary (regression equation, correlation coefficient R^2, cross validation coefficient R_{cv}^2 and average residual) and number of compounds (training set TR and test set TS) in various scaffolds based QSAR models.

No.	Cell lines (Type)	Regression equation	R^2	R_{CV}^2	AE	F	S2	# Comp	
								TR	TE
S1	P388 (Leukemia)	=-6.2155*VE/T + 2.3164* WPSA3Q + 3.3250*LNMVF + 1.5252	0.75	0.67	0.35	26.74	0.145	31	9
S2	HT29 (Colon)	=1.8444* RNB – 3.3083* MaenAC + .13180* PMIA + 6.1097	0.69	0.55	0.12	15.36	0.033	27	8
S3	ACHN (Renal)	=7.4622 * FPSA3z – 7.8674*WNSA2z – 1.0224* BI + 1.8722	0.98	0.95	0.05	105.92	0.001	15	4
S4	MCF7 (Breast)	= -2.0431 * PPSA3z + 2.7466 * ZXS/ZXR- 2.0527 * RNCGQ + 3.5395	0.89	0.73	0.09	29.10	0.009	17	5
S5	HCT116 (Colon)	=4.1330* RNCl – 2.1896 *RNCSz – 1.2796 * FNSA2Q - 2.7626	0.77	0.66	0.21	21.31	0.028	23	8
S6	HCT116 (Colon)	=4.0785* EMiNACC -4.1004 * PNSA2Q- 1.4298 EHBCAQ + 2.0450	0.88	0.82	0.14	31.98	0.018	18	5
S7	HeLa (Cervical)	=-9.3376*PMIB – 2.0744* EHDSAQ + 1.7527 * EMaNACC + 3.8717	0.85	0.75	0.14	19.85	0.036	15	4
S8	H69 (Lung)	= 4.7221* MaPCHz – 2.5135 * TE/#A-T + 2.6179 * MiERIC	0.96	0.93	0.12	76.93	0.019	14	4
S9	HeLa (cervical)	=2.1519 *MiERIN + 3.4050* MaREHN - 1.0293 *	0.93	0.90	0.12	84.32	0.074	22	6

		ABOC – 3.4442							
S10	HeLa (Cervical)	=9.0910* MaenACH -6.2862 * HNMVF + 1.2038 * MaPPBO -1.5070	0.96	0.90	0.15	50.38	0.051	14	3
S11	B16-F10 (Melanoma)	=-2.7430 *1XGP + 5.4109 * DPSA2z- 6.9408* EHDSAQ + 3.9304	0.93	0.88	0.11	41.90	0.012	15	5
S12	BEL-7402 (Melanoma)	= 2.98993 * HLEG + 1.0598* MaeeRN + 2.9834 * KSI3-4.0099	0.70	0.60	0.35	20.86	0.106	32	11
S13	M14 (Melanoma)	=4.4562* MiERIN – 3.6455 * MiAOEP + 1.0863 * MiBON (0.1) + 1.3577	0.65	0.56	0.31	15.05	0.215	28	8
S14	SF-268 (CNS)	=-1.3737 * MaTICC + 1.2771* EPNSA3Q-1.2524*MiTICN + 4.8510	0.74	0.59	0.46	11.22	0.240	17	5
S15	L120 (Leukemia)	= 1.712 *RNN – 4.0400* MiERIC + 9.1240* MIA – 4.5014	0.92	0.89	0.24	71.94	0.055	22	8
S16	A549 (Lung)	=-1.2148* MaenACC + 5.4537 * FNSA1Q – 6.7738* AIC1	0.48	0.38	0.24	12.46	0.087	49	17

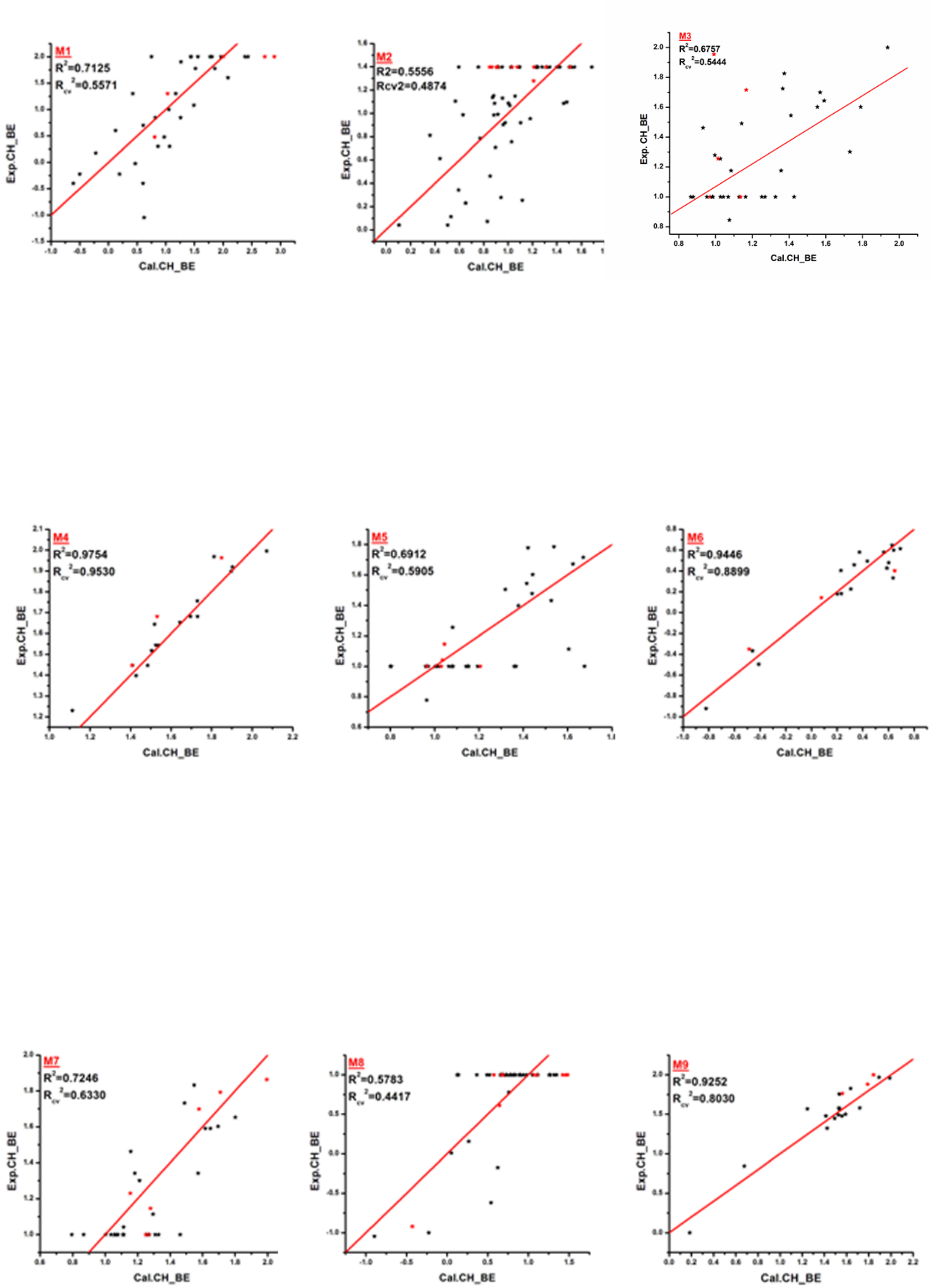
Table S66: Comparative statistical significance (correlation coefficient R^2 and cross validation coefficient R_{cv}^2) of various type of cancer involved in the cell line based QSAR study.

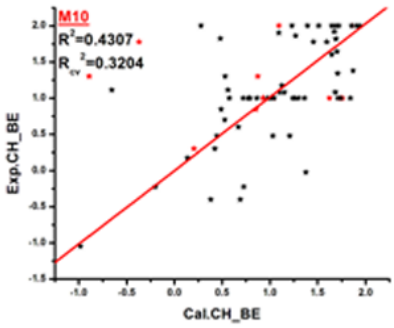
Cancer type	a		b		c		d		e		f		Average	
	R^2	R_{CV}^2	R^2	R_{CV}^2	R^2	R_{CV}^2	R^2	R_{CV}^2	R^2	R_{CV}^2	R^2	R_{CV}^2	R^2	R_{CV}^2
Leukemia[1]	0.81	0.73	0.86	0.82	0.90	0.84	-	-	-	-	-	-	0.86	0.80
Lung[2]	0.83	0.78	0.59	0.49	0.56	0.49	0.73	0.63	0.93	0.80	0.94	0.81	0.76	0.67
Colon[3]	0.31	0.22	0.69	0.60	0.59	0.49	-	-	-	-	-	-	0.53	0.44
Breast[4]	0.46	0.44	-	-	-	-	-	-	-	-	-	-	0.46	0.44
Ovarian[5]	0.66	0.54	0.76	0.66	-	-	-	-	-	-	-	-	0.71	0.6
Skin[6]	0.69	0.59	-	-	-	-	-	-	-	-	-	-	0.69	0.59
Prostate[7]	0.43	0.32	-	-	-	-	-	-	-	-	-	-	0.43	0.32
Neuronal[8]	0.72	0.63	-	-	-	-	-	-	-	-	-	-	0.72	0.63
Brain[9]	0.77	0.60	-	-	-	-	-	-	-	-	-	-	0.77	0.6
Melanoma[10]	0.51	0.45	0.48	0.40	0.94	0.89	0.81	0.70	-	-	-	-	0.69	0.61
Cervical[11]	0.77	0.71	-	-	-	-	-	-	-	-	-	-	0.77	0.71
Heptocellular[12]	0.58	0.44	-	-	-	-	-	-	-	-	-	-	0.58	0.44
CNS[13]	0.74	0.56	0.76	0.69	-	-	-	-	-	-	-	-	0.75	0.63

Renal[14]	0.71	0.56	0.98	0.95	-	-	-	-	-	-	-	-	0.85	0.76
Pancreatic[15]	0.87	0.73	-	-	-	-	-	-	-	-	-	-	0.87	0.73

1 a=P388, b=JLc, c=L120; 2 a=LLc, b=H460, c=A549, d=H522, e=Calu1, f=H69; 3 a=HT29, b=SW480, c=HCT116; 4 a=MCF7; 5 a=A2780, b=SKOV3; 6 a=A431;
7 a=DU145; 8 a=BE2-C; 9 a=SJ-G2; 10 a=SKMEL-5, b=MLM, c=B16-F10, d=M14; 11 a=HeLa; 12 a=BEL-7402; 13 a=SF-268, b=U251; 14 a=A498, b=ACHN;15 a=Panc1.

Figure S1a: Plot between experimental and predicted IC_{50} values for cell line based QSAR models with correlation coefficient and cross validation coefficient.

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Rcv2=0.3204
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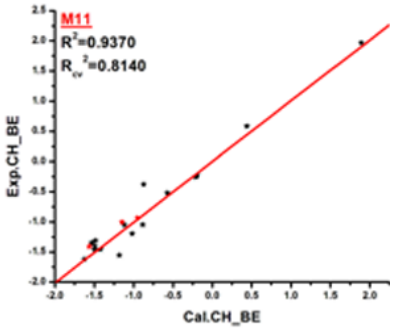
Cal.CH_BE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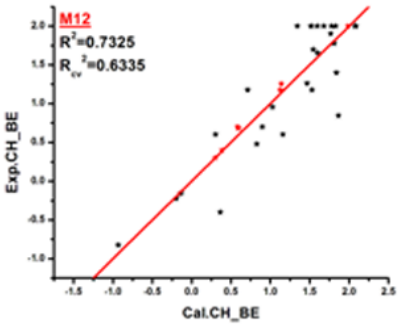
Cal.CH_BE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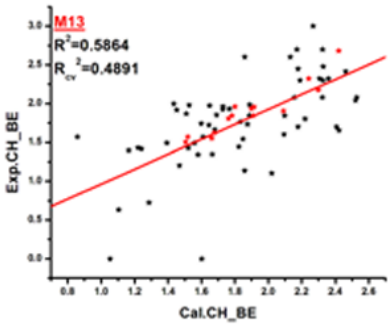
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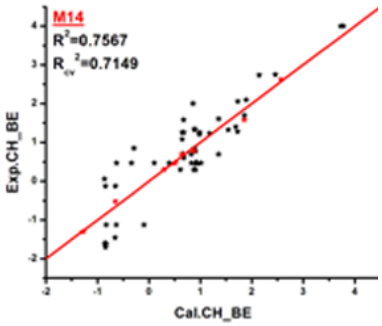
R_cv²=0.4891
Exp.CH_BE
Cal.CH_BE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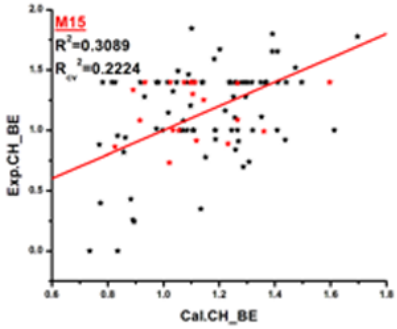
R²=0.7567
R_cv²=0.7149
Exp.CH_BE
Cal.CH_BE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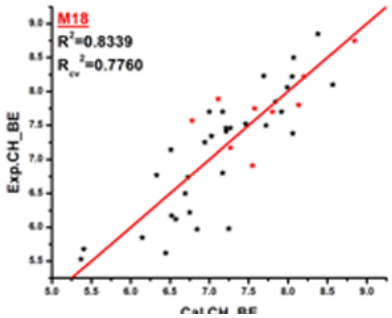
Cal.CH_BE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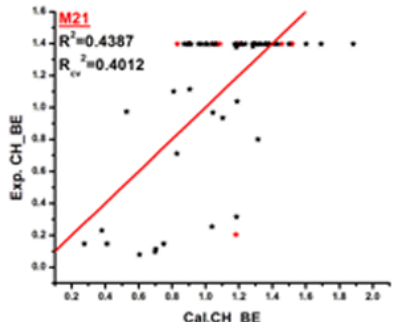
R_cv²=0.7760
Exp.CH_BE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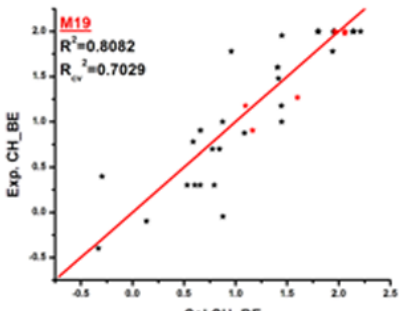
Exp. CH_BE
Cal.CH_BE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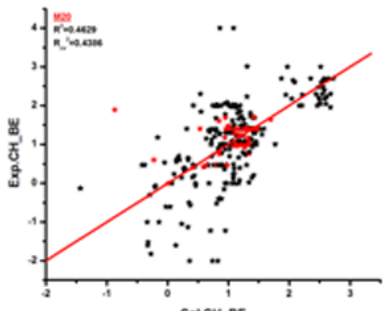
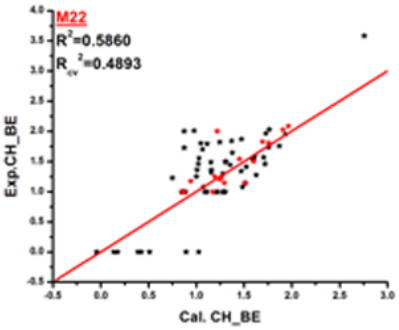
Exp. CH_BE


M20
Exp.CH_BE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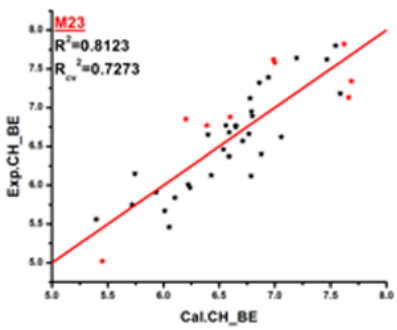
Exp.CH_BE
Cal. CH_BE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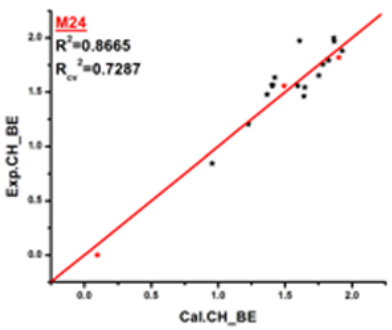
Cal.CH_BE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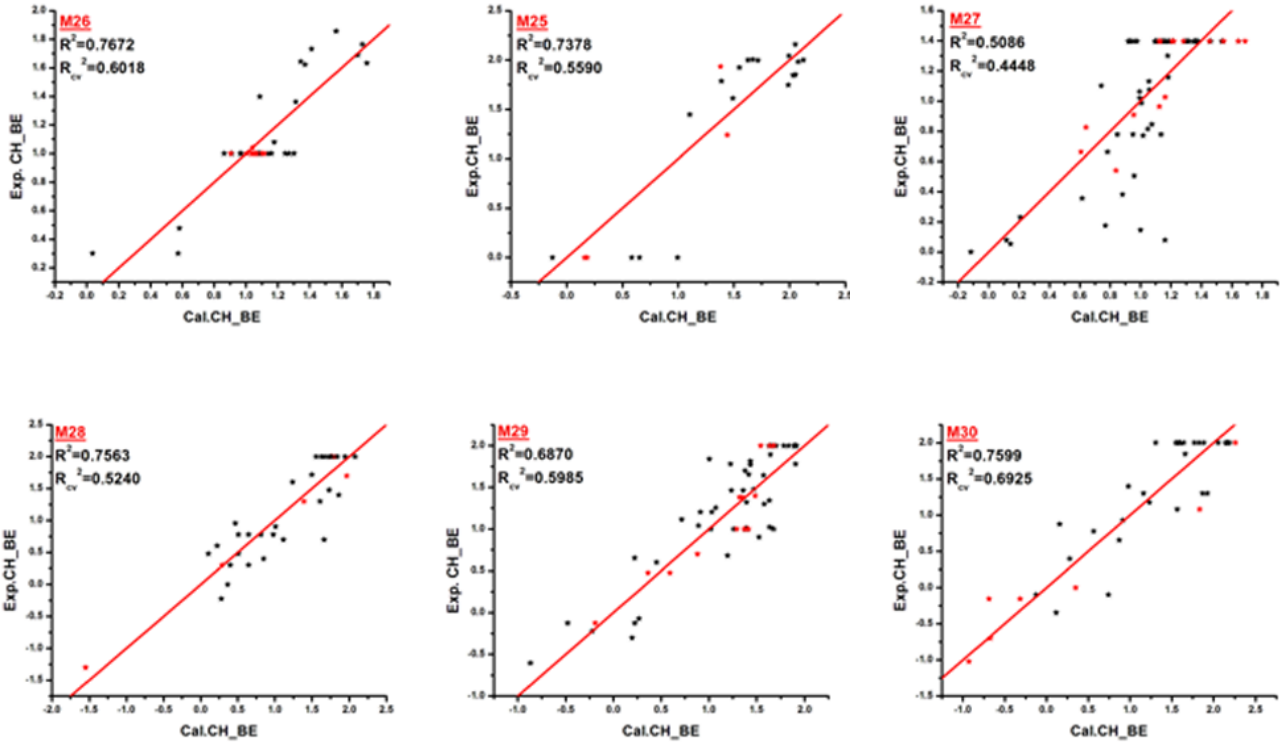
Cal.CH_BE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Exp. CH_BE
Cal.CH_BE
M25
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Rcv2=0.5590
Exp.CH_BE
Cal.CH_BE
M27
R2=0.5086
Rcv2=0.4448
Exp.CH_BE
Cal.CH_BE
M28
R2=0.7563
Rcv2=0.5240
Exp.CH_BE
Cal.CH_BE
M29
R2=0.6870
Rcv2=0.5985
Exp. CH_BE
Cal.CH_BE
M30
R2=0.7599
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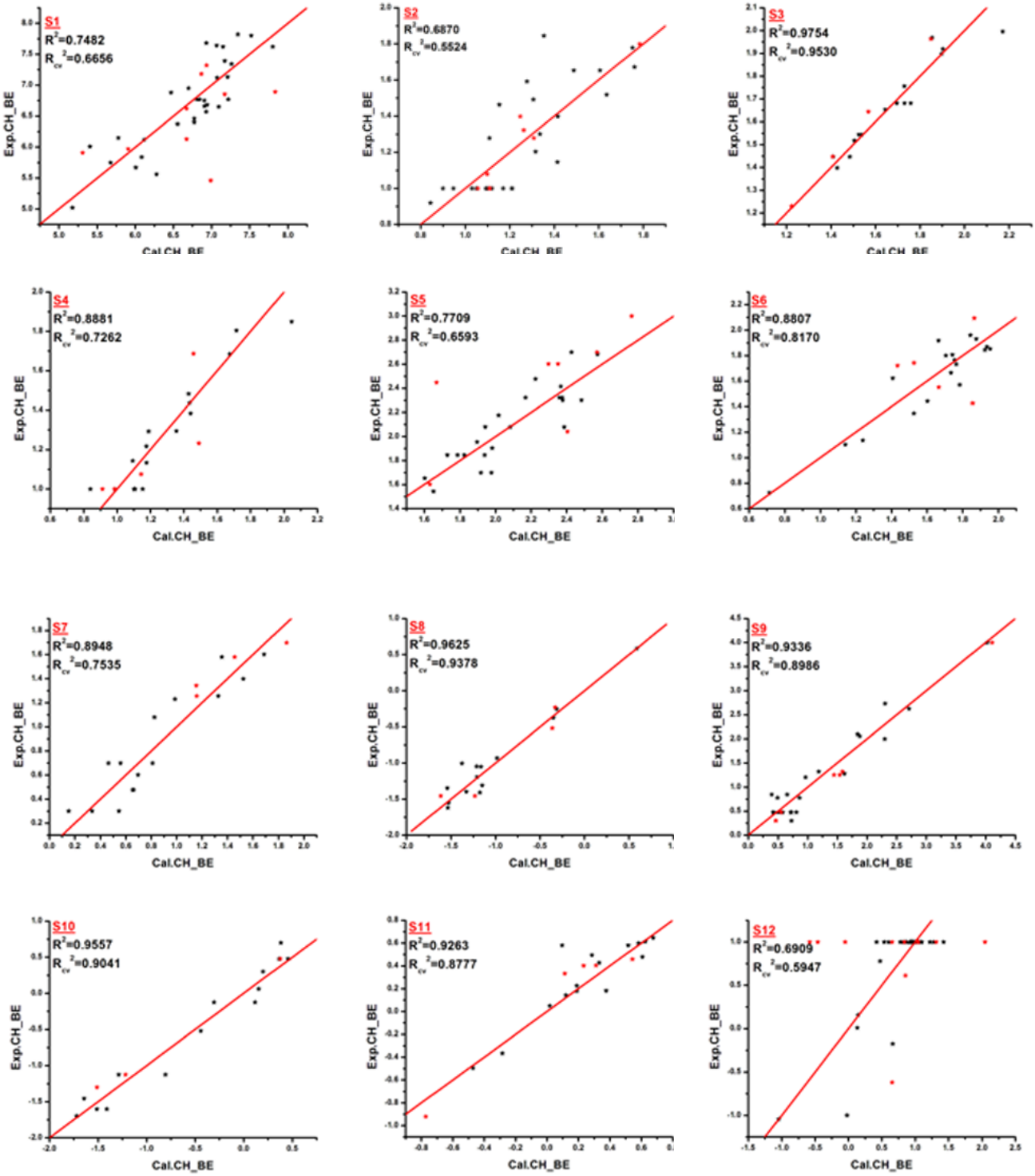
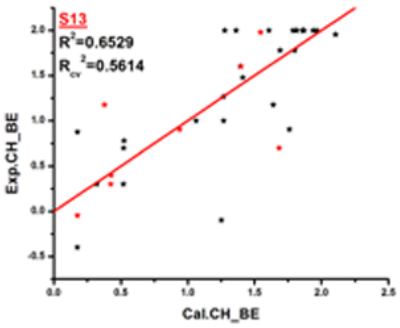
Cal.CH_BE

Figure S1b- Plot between experimental and predicted IC_{50} values for scaffold based QSAR models with correlation coefficient and cross validation coefficient.

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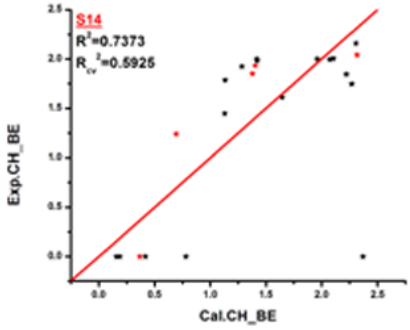
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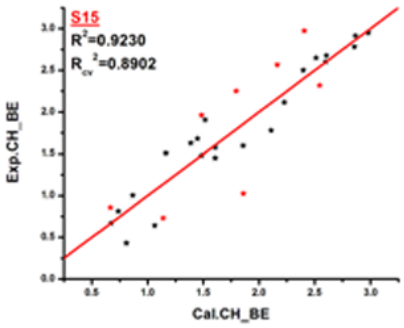
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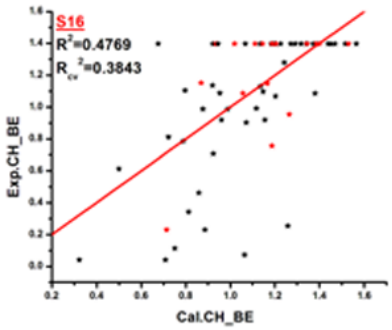
Cal.CH_BE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