

## SUPPORTING INFORMATION

### Structure-based discovery of ABCG2 inhibitors: a homology protein-based pharmacophore modeling and molecular docking approach

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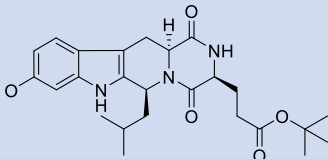
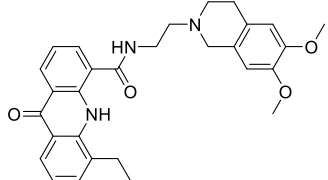
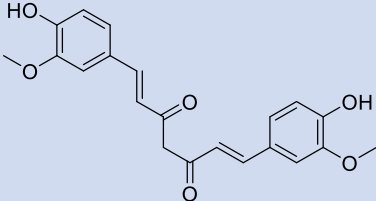
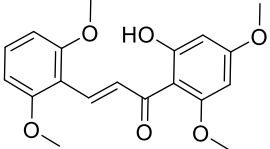
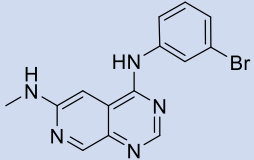
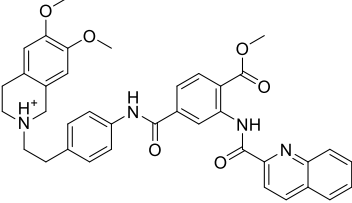
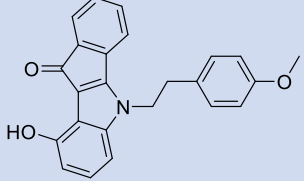
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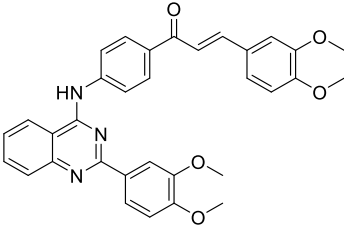
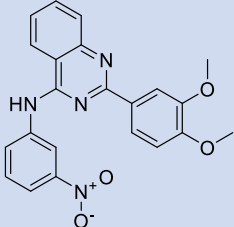
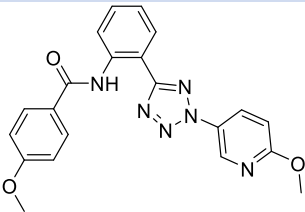
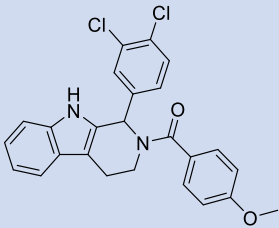
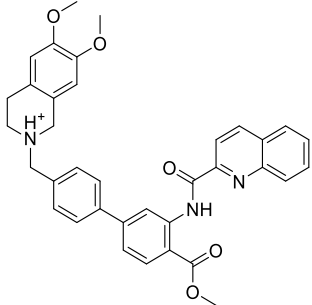
**Table S1.** ABCG2 strong inhibitors in the training set

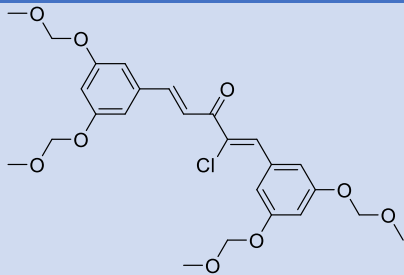
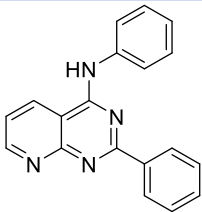
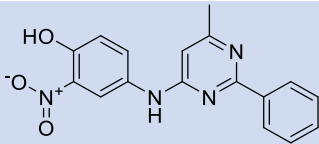
**Table S2.** Docking scores of ABCG2 inhibitors in test set of the pharmacophore model

**Figure S1.** The amino acid sequence of the ABCG2 protein

**Table S1.** ABCG2 strong inhibitors in the training set

No	Substance name/ structure group	Structure	IC <sub>50</sub> (nM)
1	JMC_2009_52_1190_Ko143 Derivative of fumitremorgin C		225
2	JMC_2009_52_1191_Elacridar Acridone derivative		250
3	DMD_2017_45_1166_Curcumin Curcumin group		650
4	BMC_2012_20_346_25 Chalcone derivative		530
5	CMC_2012_7_650_PD158780 pyrido[3,4,d]pyrimidine derivative		360
6	JMC_2009_52_1190_6 Tariquidar derivative		60
7	DDDT_2015_9_3481_5j Indeno[1,2-b]indol derivative		200

No	Substance name/ structure group	Structure	IC <sub>50</sub> (nM)
8	JMC_2016_117_212_35 Chalcone derivative combines with quinazoline		190
9	BMC_2013_21_7858_31 Quinazoline derivative		76
10	JMC_2018_146_483_43 Tariquidar derivative		61.6
11	JMC_2016_59_6121_51 tetrahydro-β-carboline derivative		233
12	ACSMCL_2013_4_393_22a biphenyl benzanilide derivative		591

No	Substance name/ structure group	Structure	IC <sub>50</sub> (nM)
13	DMD_2017_45_1166_GOY168 Curcumin derivative		250
14	JMC_2018_61_3382_15 Pyridopyrimidine derivative		149
15	JMC_2017_60_4474_47 Pyrimidine derivative		98.8

**Table S2.** Docking scores of ABCG2 inhibitors in test set of the pharmacophore model

No.	Name	Pharmacophore model	Docking score	pIC <sub>50</sub>
1	CMC_2015_10_742_14	1	-28.34	5.79
2	BMC_2013_21_7858_53	1	-28.25	6.48
3	CMC_2013_8_125_9	0	-27.56	5.07
4	JMC_2018_146_483_27	1	-27.20	6.57
5	JMC_2018_146_483_37	1	-27.03	6.72
6	JMC_2018_146_483_33	1	-26.99	6.13
7	JMC_2018_146_483_36	1	-26.87	6.59
8	JMC_2018_146_483_30	1	-26.86	6.75
9	CMC_2012_7_650_nilotinib	0	-26.41	6.17
10	JMC_2018_61_7952_49	1	-26.28	5.94
11	JMC_2018_61_7952_24	1	-25.91	7.1
12	CMC_2013_8_125_26	0	-25.90	4.67
13	CMC_2013_8_125_8	0	-25.76	5.41
14	JMC_2018_61_7952_36	1	-25.66	7.18
15	CMC_2013_8_125_7	0	-25.62	5.16
16	JMC_2018_61_3389_22	1	-25.35	5.28
17	JMC_2018_146_483_31	1	-25.28	6.54

No.	Name	Pharmacophore model	Docking score	pIC <sub>50</sub>
18	JMC_2018_61_7952_39	1	-25.20	7.35
19	JMC_2018_61_7952_16	1	-25.13	6.92
20	JMC_2018_61_7952_57	1	-25.05	6.56
21	JMC_2018_61_3389_34	1	-24.96	5.19
22	BMC_2013_21_7858_22	1	-24.94	5.61
23	CMC_2015_10_742_32	0	-24.89	5.21
24	JMC_2015_58_3910_7	1	-24.63	7
25	CMC_2013_8_125_10	0	-24.53	5.57
26	JMC_2015_58_3910_9	1	-24.46	6.58
27	BMC_2017_22_6766_12	1	-24.44	6.92
28	JMC_2018_61_3389_26	1	-24.33	6.13
29	JMC_2018_61_3389_45	1	-24.12	4.77
30	CMC_2013_8_125_18	0	-24.00	5.09
31	JMC_2018_61_3389_11	1	-23.91	6.28
32	JMC_2018_61_7952_15	1	-23.91	7.19
33	CMC_2015_10_742_7	0	-23.88	5.45
34	JMC_2018_61_7952_25	1	-23.86	6.04
35	CMC_2015_10_742_27	0	-23.81	6.25
36	JMC_2018_61_7952_51	1	-23.68	5.98
37	BMC_2013_21_7858_11	1	-23.66	6.24
38	JMC_2018_146_483_28	1	-23.61	6.37
39	CMC_2013_8_125_16	0	-23.57	5.88
40	BMC_2013_21_7858_26	1	-23.56	6.82
41	JMC_2018_61_7952_41	1	-23.55	7.63
42	JMC_2018_146_483_11	1	-23.54	5.63
43	BMC_2013_21_7858_20	1	-23.51	6.89
44	JMC_2018_61_3389_20	1	-23.42	5.91
45	CMC_2015_10_742_8	0	-23.37	5.75
46	JMC_2018_61_3389_12	1	-23.37	6.28
47	JMC_2018_61_7952_56	1	-23.35	7.1
48	JMC_2018_61_7952_21	1	-23.31	7.29
49	JMC_2015_58_3910_25	1	-23.30	7.1
50	CMC_2015_10_742_21	0	-23.20	5.68
51	JMC_2018_61_3389_44	1	-23.19	5.91
52	BMC_2013_21_7858_14	1	-23.12	5.78
53	JMC_2015_58_3910_11	1	-23.08	6.93
54	JMC_2018_61_7952_37	1	-23.07	7.21
55	JMC_2018_61_3389_30	1	-23.02	6.02
56	JMC_2015_58_3910_10	1	-22.99	7.1
57	JMC_2018_146_483_8	1	-22.94	6.36
58	CMC_2013_8_125_12	0	-22.93	5.59

No.	Name	Pharmacophore model	Docking score	pIC <sub>50</sub>
59	JMC_2018_61_7952_46	1	-22.89	6.1
60	CMC_2015_10_742_33	0	-22.87	5.47
61	JMC_2018_61_3389_24	1	-22.84	6.79
62	JMC_2018_61_7952_50	0	-22.83	5.79
63	JMC_2018_61_7952_55	1	-22.82	6.45
64	JMC_2018_61_7952_22	1	-22.80	7.31
65	JMC_2018_61_3389_39	1	-22.76	6.21
66	BMC_2013_21_7858_13	1	-22.75	5.71
67	JMC_2018_61_3389_25	1	-22.73	6.34
68	JMC_2018_61_7952_14	1	-22.69	6.97
69	JMC_2018_61_3389_37	1	-22.61	6.79
70	JMC_2015_58_3910_19	1	-22.54	6.57
71	JMC_2018_61_3389_41	1	-22.49	5.82
72	JMC_2018_61_3389_23	1	-22.49	6.75
73	JMC_2015_58_3910_20	1	-22.48	6.7
74	JMC_2018_61_7952_26	1	-22.48	7.33
75	CMC_2013_8_125_11	0	-22.45	5.39
76	JMC_2018_61_3389_40	1	-22.29	6.2
77	JMC_2015_58_3910_22	1	-22.20	7.14
78	BMC_2013_21_7858_24	1	-22.19	6.6
79	JMC_2018_61_7952_31	1	-22.13	7.56
80	JMC_2018_61_3389_46	1	-22.13	6.05
81	JMC_2018_61_3389_10	1	-22.11	6.83
82	JMC_2018_61_7952_30	1	-22.09	7.22
83	JMC_2018_146_483_43	1	-22.06	7.21
84	CMC_2013_8_125_21	0	-22.01	5.46
85	JMC_2018_61_7952_35	1	-22.00	7.35
86	CMC_2015_10_742_24	0	-21.98	5.54
87	JMC_2015_58_3910_23	1	-21.98	6.74
88	JMC_2018_61_3389_38	1	-21.98	6.27
89	JMC_2018_61_7952_58	1	-21.88	5.2
90	JMC_2018_146_483_40	1	-21.83	6.89
91	JMC_2015_58_3910_5	1	-21.82	6.74
92	CMC_2015_10_742_19	1	-21.82	4.64
93	JMC_2018_61_7952_23	1	-21.81	7.43
94	JMC_2018_146_483_12	1	-21.75	4.82
95	CMC_2012_7_650_imatinib	1	-21.73	5.03
96	BMC_2013_21_7858_40	0	-21.68	5.95
97	JMC_2018_61_7952_17	1	-21.67	7.48
98	JMC_2018_61_3389_27	1	-21.64	5.9
99	JMC_2018_61_7952_45	1	-21.59	6.14

No.	Name	Pharmacophore model	Docking score	pIC <sub>50</sub>
100	JMC_2015_58_3910_14	1	-21.48	6.86
101	JMC_2018_61_3389_21	1	-21.34	5.69
102	CMC_2015_10_742_11	0	-21.32	4.87
103	JMC_2015_58_3910_24	1	-21.30	7.19
104	JMC_2018_146_483_32	1	-21.30	6.35
105	JMC_2015_58_3910_21	1	-21.26	6.93
106	BMC_2013_21_7858_31	1	-21.25	7.12
107	BMC_2013_21_7858_30	1	-21.21	6.19
108	JMC_2018_61_7952_43	1	-21.20	6.43
109	CMC_2015_10_742_20	0	-21.16	5.75
110	CMC_2013_8_125_4	1	-21.16	5.8
111	BMC_2013_21_7858_36	1	-21.12	6.85
112	CMC_2015_10_742_9	0	-21.07	6.03
113	BMC_2012_22_6766_11	1	-21.04	5.23
114	BMC_2013_21_7858_10	1	-21.01	5.43
115	BMC_2013_21_7858_28	1	-20.98	6.54
116	JMC_2018_146_483_10	1	-20.98	6.12
117	JMC_2018_61_3389_35	1	-20.98	6.58
118	CMC_2015_10_742_18	1	-20.97	5.08
119	JMC_2018_146_483_9	0	-20.97	6.95
120	JMC_2018_61_7952_42	1	-20.88	7.24
121	BMC_2013_21_7858_33	1	-20.88	6.52
122	JMC_2018_61_3389_19	1	-20.84	6.69
123	JMC_2018_61_7952_34	1	-20.84	7
124	BMC_2013_21_7858_12	1	-20.82	5.17
125	JMC_2018_146_483_35	1	-20.80	6.57
126	BMC_2013_21_7858_50	1	-20.78	6.17
127	JMC_2018_146_483_24	1	-20.61	5.97
128	JMC_2018_61_7952_32	1	-20.60	7.23
129	CMC_2015_10_742_5	0	-20.54	5.91
130	JMC_2015_58_3910_17	1	-20.51	4.95
131	JMC_2018_61_3389_13	1	-20.48	4.71
132	JMC_2018_61_7952_44	1	-20.44	6.19
133	JMC_2018_61_7952_38	1	-20.41	7.48
134	BMC_2013_21_7858_27	1	-20.41	5.7
135	JMC_2018_146_483_23	1	-20.36	6.54
136	CMC_2015_10_742_17	1	-20.34	5.94
137	CMC_2013_8_125_28	0	-20.29	5.34
138	JMC_2018_61_3389_16	1	-20.28	6.82
139	JMC_2018_61_3389_50	1	-20.24	5.88
140	JMC_2018_61_3389_53	1	-20.18	6.69

No.	Name	Pharmacophore model	Docking score	pIC <sub>50</sub>
141	JMC_2018_146_483_26	1	-20.14	6.29
142	BMC_2013_21_7858_35	1	-20.14	6.59
143	JMC_2015_58_3910_16	1	-20.13	6.35
144	BMC_2013_21_7858_21	1	-20.00	6.01
145	BMC_2013_21_7858_32	1	-19.98	6.52
146	JMC_2018_61_3389_31	1	-19.86	5.89
147	JMC_2018_61_7952_18	1	-19.82	7.43
148	CMC_2013_8_125_25	0	-19.79	5.94
149	JMC_2016_59_6121_45	0	-19.68	5.88
150	CMC_2013_8_125_13	0	-19.64	5.51
151	JMC_2018_61_7952_48	1	-19.63	5.27
152	JMC_2018_146_483_34	1	-19.63	6.45
153	JMC_2018_146_483_44	1	-19.59	6.99
154	CMC_2015_10_742_16	1	-19.43	5.48
155	JMC_2018_146_483_7	0	-19.40	7.05
156	CMC_2013_8_125_27	0	-19.30	5.44
157	JMC_2018_61_7952_28	1	-19.27	7.12
158	JMC_2016_59_6121_29	0	-19.12	5.11
159	JMC_2018_61_7952_47	1	-19.11	6.08
160	JMC_2018_146_483_25	1	-19.08	6.09
161	JMC_2015_58_3910_18	1	-19.06	6.97
162	JMC_2016_59_6121_40	0	-19.02	5.9
163	BMC_2013_21_7858_47	1	-19.02	6.09
164	JMC_2018_146_483_22	1	-18.95	6.25
165	BMC_2012_20_346_32	0	-18.86	5.01
166	BMC_2013_21_7858_37	1	-18.83	6.33
167	JMC_2016_59_6121_33	0	-18.76	5.96
168	BMC_2012_22_6766_23	1	-18.55	5.1
169	JMC_2018_61_3389_18	1	-18.54	6.46
170	CMC_2013_8_125_17	0	-18.48	5.06
171	JMC_2018_61_3389_52	1	-18.45	6.82
172	JMC_2018_146_483_13	1	-18.42	4.73
173	BMC_2013_21_7858_15	1	-18.42	5.65
174	CMC_2012_7_650_PD158780	0	-18.39	6.44
175	BMC_2012_20_346_20	1	-18.28	5.99
176	BMC_2013_21_7858_17	1	-18.27	5.71
177	BMC_2013_21_7858_51	1	-18.25	6.1
178	JMC_2018_146_483_21	1	-18.19	5.16
179	BMC_2012_20_346_9	0	-18.16	5.71
180	BMC_2013_21_7858_25	1	-18.14	5.82
181	JMC_2018_61_3389_36	1	-18.13	6.37



No.	Name	Pharmacophore model	Docking score	pIC <sub>50</sub>
182	JMC_2018_146_483_42	1	-18.10	6.89
183	BMC_2012_20_346_37	0	-18.08	4.65
184	CMC_2015_10_742_6	0	-18.06	5.88
185	CMC_2015_10_742_29	0	-18.04	5.74
186	JMC_2018_61_7952_33	1	-18.02	7.52
187	BMC_2012_20_346_34	0	-18.01	5.25
188	BMC_2013_21_7858_38	0	-17.98	5.97
189	JMC_2016_59_6121_41	0	-17.93	5.75
190	JMC_2018_146_483_20	1	-17.91	5.49
191	BMC_2013_21_7858_48	0	-17.84	5.53
192	BMC_2012_20_346_40	1	-17.81	6.14
193	BMC_2013_21_7858_41	0	-17.79	6.03
194	JMC_2018_61_3389_17	1	-17.74	6.62
195	BMC_2013_21_7858_29	1	-17.74	6.38
196	CMC_2013_8_125_23	0	-17.72	4.89
197	JMC_2018_61_3389_32	1	-17.71	6.24
198	JMC_2016_59_6121_35	0	-17.70	6.16
199	JMC_2018_61_3389_33	1	-17.65	6.04
200	BMC_2012_20_346_22	0	-17.42	5.95
201	JMC_2016_59_6121_49	1	-17.39	6.09
202	JMC_2016_59_6121_23	1	-17.39	5.72
203	BMC_2012_22_6766_22	1	-17.23	5.05
204	JMC_2018_146_483_29	1	-17.23	6.64
205	JMC_2016_59_6121_47	1	-17.23	5.84
206	JMC_2018_146_483_41	1	-17.23	7.11
207	JMC_2016_59_6121_31	0	-17.21	5.35
208	JMC_2016_59_6121_26	0	-17.14	5.84
209	BMC_2012_22_6766_24	1	-17.10	5.03
210	CMC_2015_10_742_28	0	-16.94	5.29
211	JMC_2016_59_6121_52	1	-16.87	6.62
212	JMC_2016_59_6121_39	0	-16.77	6.48
213	BMC_2012_20_346_44	0	-16.76	5.14
214	JMC_2016_59_6121_42	0	-16.75	5.99
215	JMC_2016_59_6121_38	0	-16.67	6.13
216	BMC_2013_21_7858_43	1	-16.58	5.76
217	CMC_2012_7_650_AG1428	1	-16.57	5.26
218	BMC_2013_21_7858_46	1	-16.56	5.42
219	JMC_2012_55_966_6i	1	-16.46	6.8
220	JMC_2016_59_6121_32	0	-16.45	5.72
221	BMC_2012_20_346_13	0	-16.43	5.66
222	BMC_2012_20_346_42	0	-16.34	5.25

No.	Name	Pharmacophore model	Docking score	pIC <sub>50</sub>
223	JMC_2016_59_6121_22	0	-16.31	5.56
224	BMC_2013_21_7858_42	0	-16.09	5.32
225	JMC_2016_59_6121_51	1	-16.08	6.63
226	BMC_2012_20_346_10	0	-16.07	5.48
227	JMC_2016_59_6121_43	1	-16.06	6.16
228	BMC_2012_20_346_41	0	-16.03	5.71
229	BMC_2012_22_6766_19	1	-15.93	5.29
230	BMC_2013_21_7858_44	1	-15.91	5.62
231	CMC_2013_8_125_20	0	-15.84	5.51
232	JMC_2016_59_6121_24	0	-15.78	5.66
233	JMC_2016_59_6121_46	1	-15.72	5.76
234	BMC_2012_22_6766_20	1	-15.71	5.23
235	CMC_2013_8_125_22	0	-15.70	5.66
236	JMC_2018_146_483_19	1	-15.66	5.08
237	JMC_2016_59_6121_53	0	-15.65	6.42
238	BMC_2012_22_6766_21	1	-15.64	5.09
239	JMC_2016_59_6121_37	0	-15.57	6.06
240	JMC_2013_67_115_19	0	-15.44	5.16
241	JMC_2016_59_6121_44	1	-15.42	5.96
242	BMC_2012_20_346_33	1	-15.39	5.71
243	BMC_2012_20_346_31	0	-15.26	5.03
244	JMC_2012_55_966_6f	1	-15.23	6.74
245	CMC_2013_8_125_24	1	-15.21	5.53
246	BMC_2012_20_346_39	0	-15.16	5.54
247	JMC_2012_55_966_6h	1	-15.16	6.7
248	JMC_2013_67_115_21	0	-15.15	4.65
249	BMC_2012_20_346_16	1	-15.11	5.48
250	JMC_2016_59_6121_50	1	-15.03	6.05
251	JMC_2016_59_6121_48	1	-14.99	5.91
252	BMC_2012_22_6766_18	1	-14.98	5.05
253	BMC_2012_20_346_38	0	-14.86	5.59
254	BMC_2012_20_346_5	1	-14.78	5.3
255	JMC_2018_146_483_17	1	-14.76	4.8
256	JMC_2013_67_115_20	0	-14.54	6.14
257	JMC_2016_59_6121_25	1	-14.18	5.44
258	CMC_2012_7_650_gefitinib	0	-13.84	5.49
259	BMC_2012_20_346_14	1	-13.80	5.97
260	BMC_2012_20_346_12	0	-13.77	4.51
261	JMC_2013_67_115_29	0	-13.61	4.96
262	JMC_2016_59_6121_21	0	-13.48	5.63
263	JMC_2016_59_6121_55	0	-13.45	4.98

No.	Name	Pharmacophore model	Docking score	pIC <sub>50</sub>
264	JMC_2018_146_483_14	0	-13.26	4.4
265	JMC_2013_67_115_17	0	-13.21	6.28
266	JMC_2018_146_483_18	1	-13.17	5.12
267	BMC_2012_20_346_15	0	-13.01	5.83
268	BMC_2013_21_7858_49	1	-12.97	5.86
269	JMC_2013_67_115_16	1	-12.86	5.91
270	JMC_2013_67_115_32	0	-12.84	4.95
271	JMC_2009_52_1191_Elacridar	0	-12.84	6.6
272	JMC_2013_67_115_8	1	-12.82	5.93
273	JMC_2013_67_115_18	0	-12.81	5.54
274	JMC_2012_55_966_6e	1	-12.72	6.33
275	BMC_2012_20_346_21	0	-12.55	5.58
276	BMC_2012_20_346_7	0	-12.55	4.92
277	JMC_2013_67_115_25	0	-12.51	5.61
278	BMC_2013_21_7858_54	1	-12.50	5.76
279	JMC_2012_55_966_6g	1	-12.48	6.96
280	BMC_2012_20_346_11	0	-12.41	5.2
281	JMC_2013_67_115_15	0	-12.40	5.89
282	JMC_2012_55_966_6a	1	-12.37	6.77
283	JMC_2013_67_115_30	0	-12.26	5.05
284	BMC_2012_20_346_30	1	-12.14	5.76
285	BMC_2012_20_346_26	1	-12.11	5.55
286	BMC_2012_20_346_27	1	-12.06	5.94
287	JMC_2013_67_115_26	0	-12.04	5.08
288	JMC_2013_67_115_22	0	-11.90	5.57
289	BMC_2012_20_346_24	1	-11.85	5.52
290	JMC_2013_67_115_24	1	-11.84	6.37
291	JMC_2013_67_115_14	0	-11.83	5.88
292	JMC_2013_67_115_4	0	-11.73	6
293	JMC_2013_67_115_6	0	-11.58	5.92
294	JMC_2013_67_115_27	0	-11.58	5.61
295	JMC_2013_67_115_31	0	-11.57	5.21
296	JMC_2013_67_115_33	1	-11.24	5.51
297	JMC_2013_67_115_28	1	-11.17	6.23
298	JMC_2013_67_115_9	1	-11.07	5.93
299	BMC_2012_20_346_17	0	-10.87	4.97
300	JMC_2013_67_115_23	0	-10.52	5.97
301	BMC_2012_20_346_8	1	-10.36	6.07
302	BMC_2012_20_346_29	1	-10.28	5.11
303	JMC_2013_67_115_7	1	-10.23	5.11
304	JMC_2013_67_115_34	1	-10.00	5.37

No.	Name	Pharmacophore model	Docking score	pIC <sub>50</sub>
305	BMC_2012_20_346_25	1	-9.99	6.28
306	JMC_2009_52_1191_Tariquidar	1	-9.89	6.04
307	BMC_2012_20_346_28	1	-9.75	5.42
308	JMC_2013_67_115_5	0	-9.67	4.91
309	JMC_2009_52_1191_11	0	-9.35	5.99
310	JMC_2013_67_115_12	1	-9.27	6.27
311	JMC_2009_52_1191_10	0	-8.86	6.2
312	BMC_2012_20_346_19	0	-8.73	5.72
313	JMC_2009_52_1191_14	1	-8.20	6.01
314	JMC_2009_52_1191_15	0	-8.16	5.7
315	JMC_2013_67_115_13	1	-8.13	5.49
316	JMC_2013_67_115_10	1	-7.44	6.09
317	JMC_2009_52_1191_12	0	-6.81	6.5
318	JMC_2013_67_115_11	1	-6.73	5.22
319	JMC_2009_52_1191_5	0	-6.63	6.92
320	JMC_2009_52_1191_9	0	-6.27	6.26
321	JMC_2009_52_1191_8	1	-6.22	6.75
322	JMC_2009_52_1190_Ko143	1	-6.22	6.65
323	JMC_2009_52_1191_7	0	-6.21	6.74
324	JMC_2009_52_1191_6	0	-6.20	7.22
325	JMC_2009_52_1191_13	0	-4.12	6.07

>sp|Q9UNQ0|ABCG2\_HUMAN ATP-binding cassette sub-family G member 2  
OS=Homo sapiens OX=9606 GN=ABCG2 PE=1 SV=3

MSSSNVEVFIPVSQGNTNGFPATASNDLKAFTEGAVLSFHNICYRVKLKSGF  
LPCRKPVEKEILSNINGIMKPGLNAILGPTGGGKSSLLDVLAARKDPSGLSG  
DVLINGAPRPANFKCNSGYVVQDDVVMGTLTVRENLQFSAALRLATTMTN  
HEKNERINRVIQELGLDKVADSKVGTQFIRGVSGGERKRTSIGMELITDPSIL  
FLDEPTTGLDSSTANAVLLLLKRMSKQGRTIIFSIHQPRYSIFKLFDSTLLAS  
GRLMFHGP AQEALGYFESAGYHCEAYNNPADFFLDIINGDSTAV ALNREED  
FKATEIIEPSKQDKPLIEKLA EIYVNSSFYKETKAELHQLSGGEKKKKITVFK  
EISYTTSFCHQLRWVSKRSFKNLLGNPQASIAQIIVTVVLGLVIGAIYFGLKN  
DSTGIQNRAGVLFFLT TNQCFSSVSAVELFVVEKKLFIHEYISGY YRVSSYFL  
GKLLSDLLPMRMLPSIIFTCIVYFMLGLKPKADAFFVMMFTLMMVAYSASS  
MALAIAAGQSVVSVATLLMTICFVFM MIFSGLLVNLT TIASWLSWLQYFSIP  
RYGFTALQHNEFLGQNFCPGLNATGNNPCNYATCTGEEYLVKQGIDLSPW  
GLWKNHVALACMIVIFLTIA YLKLLFLKKYS

**Figure S1:** The amino acid sequence of the ABCG2 protein