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Supporting Information to

Molecular Modeling on Structure-Function Analysis of Human Progesterone Receptor Modulators

Ria PAL, Md Ataul ISLAM, Tabassum HOSSAIN, Achintya SAHA

Published in Sci Pharm. 2011; 79: 461–477 doi:10.3797/scipharm.1105-03

Available from: http://dx.doi.org/10.3797/scipharm.1105-03

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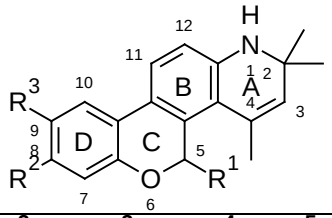
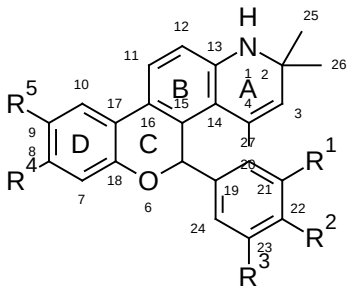
Tab. S1. Structural features and binding affinity (K_i) of hPR-A modulators



Cpd no.	R^1	R^2	R^3	R^4	R^5	R^6	R^7	R^8	K_i (nM)
1	H	H	H	–	–	–	–	–	84.00
2	CH_3	H	H	–	–	–	–	–	3.30
3	$(CH_2)_3CH_3$	H	H	–	–	–	–	–	0.95
4	$(CH_2)_5CH_3$	H	H	–	–	–	–	–	23.00
5	$(CH_2)_4Cl$	H	H	–	–	–	–	–	3.20
6	$CH_2CH=CH_2$	H	H	–	–	–	–	–	4.80
7	H	H	F	–	–	–	–	–	6.10
8	CH_3	H	F	–	–	–	–	–	1.10
9	$(CH_2)_3CH_3$	H	F	–	–	–	–	–	2.90
10	H	H	Cl	–	–	–	–	–	3.60
11	$(CH_2)_3CH_3$	H	Cl	–	–	–	–	–	0.87
12	H	H	CH_3	–	–	–	–	–	50.20
13	$(CH_2)_3CH_3$	H	CH_3	–	–	–	–	–	1.20
14	$(CH_2)_3CH_3$	H	OCH_3	–	–	–	–	–	3.50
15	$(CH_2)_3CH_3$	F	H	–	–	–	–	–	26.50
16	$O(CH_2)_2CH_3$	H	H	–	–	–	–	–	64.00
17	OCH_3	H	F	–	–	–	–	–	38.40
18	$O(CH_2)_2CH_3$	H	F	–	–	–	–	–	6.00
19	OCH_3	H	Cl	–	–	–	–	–	16.40
20	$O(CH_2)_2CH_3$	H	Cl	–	–	–	–	–	1.50
21	OCH_3	F	H	–	–	–	–	–	80.50
22	$S(CH_2)_2CH_3$	H	H	–	–	–	–	–	24.30
23	$S(CH_2)_2CH_3$	H	F	–	–	–	–	–	6.60

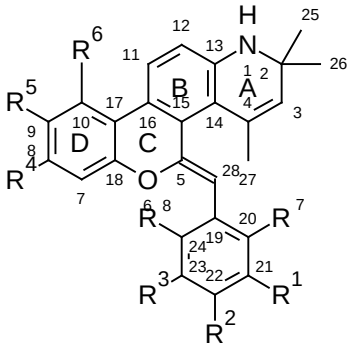


Cpd no.	R^1	R^2	R^3	R^4	R^5	R^6	R^7	R^8	K_i (nM)
24	H	Cl	H	H	H	–	–	–	0.70
25	H	Cl	H	H	F	–	–	–	0.32
26	H	Cl	H	F	H	–	–	–	2.70
27	H	Cl	H	H	Cl	–	–	–	0.59
28	H	Cl	H	H	OCH_3	–	–	–	2.40
29	H	H	H	H	F	–	–	–	2.20
30	H	H	Cl	H	F	–	–	–	0.32

Tab. S1. (Cont.)

Cpd no.	R^1	R^2	R^3	R^4	R^5	R^6	R^7	R^8	K_i (nM)
31	H	Cl	CH_3	H	F	–	–	–	0.49
32	H	OCH_3	H	H	F	–	–	–	2.70
33	H	H	CH_3	H	F	–	–	–	0.37
34	H	H	CF_3	H	F	–	–	–	0.78
35	H	F	CH_3	H	F	–	–	–	1.30
36	H	H	H	H	Cl	–	–	–	0.74
37	H	Br	H	H	Cl	–	–	–	0.59
38	H	OCH_3	H	H	Cl	–	–	–	0.93
39	H	H	Cl	H	Cl	–	–	–	0.48
40	H	H	CH_3	H	Cl	–	–	–	0.55
41	H	H	CF_3	H	Cl	–	–	–	1.10
42	H	H	F	H	Cl	–	–	–	0.34
43	H	Cl	CH_3	H	Cl	–	–	–	0.50
44	H	F	CH_3	H	Cl	–	–	–	1.30
45	H	H	H	H	H	–	–	–	3.60
46	H	F	H	H	H	–	–	–	5.30
47	H	Br	H	H	H	–	–	–	0.55
48	H	H	F	H	H	–	–	–	0.69
49	H	H	Cl	H	H	–	–	–	0.43
50	H	H	Br	H	H	–	–	–	1.10
51	H	CF_3	H	H	H	–	–	–	10.80
52	H	$COCH_3$	H	H	H	–	–	–	8.80
53	H	CH_3	H	H	H	–	–	–	2.30
54	H	OCH_3	H	H	H	–	–	–	13.30
55	H	H	CF_3	H	H	–	–	–	2.60
56	H	Cl	Cl	H	H	–	–	–	3.40
57	H	Cl	F	H	H	–	–	–	0.41
58	H	Cl	CH_3	H	H	–	–	–	1.20
59	H	F	CF_3	H	H	–	–	–	6.80
60	H	CH_3	F	H	H	–	–	–	1.80
61	Cl	H	Cl	H	H	–	–	–	1.70
62	F	H	Br	H	H	–	–	–	2.40
63	CH_3	H	Br	H	H	–	–	–	0.87
64[a]	H	Br	H	H	H	–	–	–	3.90
65[b]	H	H	Br	H	H	–	–	–	13.80
66[c,d]	H	Cl	H	H	H	–	–	–	11.60
67[d]	H	Cl	H	H	H	–	–	–	10.10
68[d,e]	H	Cl	H	H	H	–	–	–	24.60
69[f]	H	H	H	H	H	–	–	–	80.00
70[d,g]	H	Cl	H	H	H	–	–	–	1.30
71[d,g]	H	H	H	H	H	–	–	–	28.60
72[d,g]	H	H	H	H	H	–	–	–	6.60
73[d,g]	H	H	F	H	H	–	–	–	2.60
74[d,g]	H	H	CF_3	H	H	–	–	–	16.60
75[d,g,h]	H	Cl	H	H	H	–	–	–	5.30

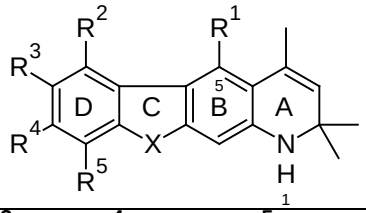
Tab. S1. (Cont.)



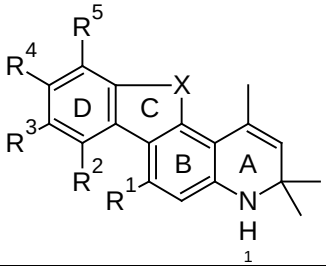
Cpd no.	R^1	R^2	R^3	R^4	R^5	R^6	R^7	R^8	K_i (nM)
76	H	H	H	H	H	H	CH_3	H	0.66
77	H	H	H	H	H	F	H	H	0.61
78	F	H	H	H	H	F	H	H	5.50
79	H	F	H	H	H	F	H	H	0.71
80	H	H	H	H	H	F	CH_3	H	1.50
81	H	H	H	F	H	H	H	H	0.62
82	H	H	H	F	H	H	CH_3	H	0.55
83	H	H	H	F	H	H	CH_2CH_3	H	2.30
84	H	H	H	F	H	H	$CH_2CH_2CH_3$	H	1.60
85	H	H	H	F	H	H	$CH(CH_3)_2$	H	1.90
86	H	H	H	F	H	H	OCH_3	H	3.80
87	H	H	H	F	H	H	SCH_3	H	0.59
88	H	H	H	F	H	H	F	H	0.62
89	H	H	H	F	H	H	Cl	H	22.40
90	H	H	H	F	H	H	Br	H	16.40
91	H	H	H	F	H	H	CHO	H	2.60
92	H	H	H	F	H	H	OCF_3	H	6.40
93[i]	H	H	H	F	H	H	H	H	1.50
94[i]	H	H	H	F	H	H	CH_3	H	1.40
95[j]	H	H	H	F	H	H	H	H	9.20
96[j]	H	H	H	F	H	H	H	CH_3	0.42
97	H	H	H	F	H	H	$N(CH_3)_2$	H	1.20
98	F	H	H	H	H	H	H	H	0.83
99[d]	F	H	H	H	H	H	H	H	6.30
100[d,g]	F	H	H	H	H	H	H	H	3.50
101[d,g]	H	H	H	H	H	H	H	H	4.90
102[k]	H	H	H	H	H	H	H	H	2.10
103	H	H	H	H	H	H	H	H	4.90
104	H	H	H	H	H	H	F	H	5.60
105	H	F	H	H	H	H	H	H	3.50
106	H	H	H	H	H	H	Br	H	5.50
107	H	Br	H	H	H	H	H	H	8.70
108	H	H	H	H	H	H	Cl	H	1.30
109	H	Cl	H	H	H	H	H	H	60.00
110	H	F	H	H	H	H	F	H	3.20

Tab. S1. (Cont.)

Cpd no.	R^1	R^2	R^3	R^4	R^5	R^6	R^7	R^8	K_i (nM)
111	H	H	F	H	H	H	F	H	1.50
112	H	H	H	H	H	H	F	F	31.30
113	F	F	H	H	H	H	H	H	3.60
114	F	H	F	H	H	H	H	H	12.60



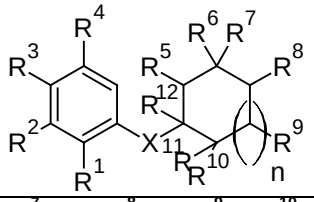
Cpd no.	R^1	R^2	R^3	R^4	R^5	X	K_i (nM)
115	H	H	H	H	H	–	133.00
116	H	H	H	H	H	CH_2	14.00
117	H	H	H	H	CH_2OH	CH_2	12.40
118	H	H	H	$COCH_3$	H	CH_2	176.00
119	H	H	H	Br	H	CH_2	24.00
120	H	H	H	Cl	H	CH_2	29.00
121	H	F	H	H	H	CH_2	11.20
122	H	H	H	H	H	O	184.00
123	H	H	H	H	H	NH	113.00
124	H	H	H	H	H	C=O	3553.00
125	H	F	H	H	H	C=O	29.10
126[l]	H	H	H	H	H	CH_2	87.00
127	H	H	H	H	H	C(H)OH	483.00
128	H	H	H	Br	H	C(H)OH	1858.00
129	H	H	H	F	H	C(H)OH	101.00
130	H	F	H	H	H	C(H)OH	449.00
131	Cl	H	H	H	H	C(H)OH	53.10
132	H	H	F	H	F	C(H)OH	202.00
133	F	H	H	F	H	$C(H)OCOCF_3$	62.50

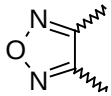


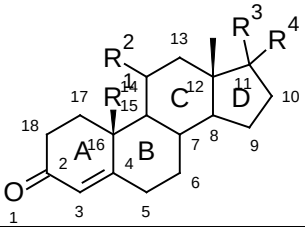
Cpd no.	R^1	R^2	R^3	R^4	R^5	X	K_i (nM)
134	H	H	H	H	H	CH_2	13.00
135	H	H	H	NO_2	H	CH_2	57.00
136	H	H	H	Br	H	CH_2	200.00
137	H	H	H	H	F	CH_2	15.50

Tab. S1. (Cont.)

Cpd no.	R^1	R^2	R^3	R^4	R^5	X	K_i (nM)
138	H	H	F	NO_2	H	CH_2	97.00
139	F	H	H	F	H	CH_2	20.90
140	H	H	H	H	H	O	77.00
141	H	H	H	H	H	$NCH_2CH_2CH_2CH_3$	77.00



Cpd.	R^1	R^2	R^3	R^4	R^5	R^6	R^7	R^8	R^9	R^{10}	R^{11}	$R^1{}_2$	X	n	K_i (nM)
142	OH	H	Br	OCH_3	$=CH_2$	H	H	H	$-Br^m$	$-CH_3{}^n$	$-CH_3{}^m$	H	CH_2(R)	1	490.00
143	OH	H	Br	OCH_3	$=CH_2$	H	H	H	$-Br^m$	$-CH_3{}^n$	$-CH_3{}^m$	H	CH_2(S)	1	343.00
144	OH	H	Br	OCH_3	$=CH_2$	H^o		H	H	$-CH_3{}^n$	$-CH_3{}^m$	H	CH_2	1	77.00
145	OH	H	Br	OCH_3	$=CH_2$	H^p		H	H	$-CH_3{}^n$	$-CH_3{}^m$	H	CH_2	1	156.00
146	OH	H	Br	OCH_3	$=CH_2$	H^o		CH_3	H	$-CH_3{}^n$	$-CH_3{}^m$	H	CH_2	1	31.00
147	OH	H	Br	OCH_3	$=CH_2$	H^o		H	-	$-CH_3{}^n$	$-CH_3{}^m$	H	CH_2	0	441.00
148	OH	H	Br	OCH_3	$=CH_2$	H	H	$-CH_3{}^n$	H	$-CH_3{}^n$	$-CH_3{}^m$	H	$-CH_2{}^n$	1	22.00
149	OH	H	Br	OCH_3	$=CH_2$	H	H	$-CH_2OH^n$	H	$-CH_3{}^n$	$-CH_3{}^m$	H	$-CH_2{}^n$	1	3247.00
150	$OCOCH_3$	H	Br	OCH_3	$=CH_2$	H^p		CH_3	H	$-CH_3{}^n$	$-CH_3{}^m$	H	CH_2	1	59.60
151	$OCOCH_3$	H	Br	OCH_3	Δ	H^p		CH_3	H	$-CH_3{}^n$	$-CH_3{}^m$	H	CH_2	1	98.00
152	OH	H	Br	OCH_3	$CH_3{}^p$	H		$=CH_2$	H	$-CH_3{}^n$	$-CH_3{}^m$	H	CH_2	1	109.00
153	OH	H	Br	OCH_3	$=CH_2$	H^p		CH_3	H	$-CH_3{}^n$	$-CH_3{}^m$	H	-CH=CH-CH_2	1	84.00
154	H	H	NO_2	CH_3	$=CH_2$	H^p		CH_3	H	$-CH_3{}^n$	$-CH_3{}^m$	H	CH_2	1	28.80
155	H	H	NO_2	H	$=CH_2$	H^p		CH_3	H	$-CH_3{}^n$	$-CH_3{}^m$	H	CH_2	1	53.50
156	H	H	NO_2	H	$=CH_2$	H^p		CH_3	H	$-CH_3{}^n$	$-CH_3{}^m$	H	S	1	119.00
157	H	H	NO_2	H	$=CH_2$	H^p		CH_3	H	$-CH_3{}^n$	$-CH_3{}^m$	OH	CH_2	1	243.00
158	H			H	$=CH_2$	H^p		CH_3	H	$-CH_3{}^n$	$-CH_3{}^m$	H	CH_2	1	88.00
159	OH	H	Br	OCH_3	$=CH_2$	H	H	H	H	$-CH_3{}^n$	$-CH_3{}^m$	H	CH_2(R)	1	218.00
160	OH	H	Br	OCH_3	$=CH_2$	H	H	H	H	$-CH_3{}^n$	$-CH_3{}^m$	H	CH_2(S)	1	34.00
161	OH	H	Br	OCH_3	$=CH_2$	$-CH_3{}^n$	$-OH^n$	H	H	$-CH_3{}^n$	$-CH_3{}^m$	H	$-CH_2{}^n$	1	275.00
162	$OCOCH_3$	H	Br	OCH_3	$=CH_2$	$CH_3{}^p$		H	H	$-CH_3{}^n$	$-CH_3{}^m$	H	$-CH_2{}^n$	1	455.00
163	OH	H	Br	OCH_3	$=CH_2$	H	H	H	H	$=CH_3{}^q$		H	CH_2(R)	1	71.00
164	OH	H	Br	OCH_3	$=CH_2$	H	H	H	H	$=CH_3{}^q$		H	CH_2(R)	1	69.00
165	$OCOCH_3$	H	Br	OCH_3	$=CH_2$	H^p		CH_3	H	$-CH_3{}^m$		H	$-CH_2{}^n$	1	21.00
166	OH	H	Br	OCH_3	$=CH_2$	H^p		CH_3	H	$-CH_3{}^m$		H	$-CH_2{}^n$	1	84.00



Cpd. No.	R^1	R^2	R^3	R^4	K_i (nM)
167	$-CH_3$	-H	-H	$-COCH_3$	3.50
168	$-CH_3$	-H	$-OCOCH_3$	$-COCH_3$	0.34
169	-H	$-C_6H_5N(CH_3)_2$	-OH	$-CCCH_3$	1.10
170	-H	-H	-OH	-CCH	1.87

Tab. S1. (Cont.)

[a] N at 21, [b] N at 24, [c] =CH_2 at 4, [d] saturation at 3, [e] =O at 4, [f] O at 5, not 6, [g] O at 3, [h] extra methyl at 4, [i] N at 22, [j] N at 20, [k] saturation at 28, [l] indicates absence of double bond, [m] asymmetric bold bonds, [n] asymmetric hashed bonds, [o] asymmetric dashed bonds, [p] double bond at neighbouring C, [q] wavy double bond. Compd. No. 1–23 [56]; Compd. No. 24–44, 69, 167, 168, 170 [57]; Compd. No. 45–65 [58]; Compd. No. 66–68, 70–75, 98–101 [59]; Compd. No. 76–97 [60]; Compd. No. 102–114 [61]; Compd. No. 115–141, 169 [62]; Compd. No. 142–166 [63].

Tab. S2. Observed and predicted activities (pK_i) of compounds

Cpd no.	Activity (pKi)			Cpd no.	Activity (pKi)		
	Observed	Predicted			Observed	Predicted	
		QSAR	Pharmacoph.			QSAR	Pharmacoph.
1[^,≠]	2.076	2.436	1.721	33[#,≠]	4.432	3.958	4.409
2[#,≠]	3.481	2.871	3.292	34[#,≠]	4.108	3.816	4.367
3[#,*]	4.022	3.290	4.260	35[#,ψ]	3.886	4.032	4.347
4[#,≠]	2.638	2.351	3.678	36[^,ψ]	4.131	3.616	4.155
5[^,ψ]	3.495	3.355	4.201	37[^,≠]	4.229	3.943	3.569
6[#,≠]	3.319	3.119	3.252	38[^,≠]	4.032	3.616	3.180
7[#,≠]	3.215	3.083	2.959	39[#,ψ]	4.319	4.092	4.398
8[$,≠]	3.959	3.083	3.509	40[#,*]	4.260	4.093	4.076
9[#,ψ]	3.538	3.042	4.137	41[^,ψ]	3.959	4.113	4.377
10[#,≠]	3.444	3.281	3.553	42[#,ψ]	4.469	4.072	4.538
11[#,ψ]	4.060	3.174	3.699	43[#,ψ]	4.301	4.047	4.125
12[#,ψ]	2.299	2.931	2.046	44[#,≠]	3.886	4.211	4.387
13[^,≠]	3.921	3.494	3.770	45[^,ψ]	3.444	3.227	2.824
14[#,≠]	3.456	3.136	3.328	46[$,ψ]	3.276	3.698	3.770
15[#,ψ]	2.577	2.891	2.536	47[#,≠]	4.260	3.692	4.004
16[#,≠]	2.194	2.845	2.222	48[#,ψ]	4.161	3.770	3.409
17[$,ψ]	2.416	2.885	1.824	49[$,≠]	4.367	3.724	4.409
18[$,ψ]	3.222	3.061	4.076	50[^,*]	3.959	3.839	4.337
19[#,≠]	2.785	2.875	1.824	51[#,*]	2.967	3.329	3.155
20[#,≠]	3.824	3.053	3.495	52[#,*]	3.056	3.351	3.086
21[#,*]	2.094	2.729	1.824	53[#,≠]	3.638	3.298	3.721
22[$,ψ]	2.614	2.913	2.688	54[#,≠]	2.876	3.314	3.097
23[#,≠]	3.180	3.177	4.046	55[#,ψ]	3.585	3.532	4.328
24[^,≠]	4.155	3.623	4.046	56[#,ψ]	3.469	3.921	4.357
25[#,*]	4.495	3.826	3.770	57[$,ψ]	4.387	3.937	3.658
26[$,ψ]	3.569	3.704	3.824	58[#,≠]	3.921	3.971	4.337
27[$,ψ]	4.229	3.641	3.796	59[^,ψ]	3.167	3.196	4.347
28[^,ψ]	3.620	3.462	3.387	60[$,≠]	3.745	3.805	3.125
29[$,*]	3.658	3.616	2.886	61[#,ψ]	3.770	3.379	4.387
30[#,*]	4.495	4.033	4.398	62[#,≠]	3.620	3.686	4.367
31[$,≠]	4.310	4.139	4.377	63[#,*]	4.060	3.544	4.387
32[^,≠]	3.569	3.475	3.337	64[#,≠]	3.409	3.860	3.886

Tab. S2. (Cont.)

Cpd no.	Activity (pKi)			Cpd no.	Activity (pKi)		
	Obser-ved	Predicted			Obser-ved	Predicted	
		QSAR	Pharmacoph.			QSAR	Pharmacoph.
65[#,≠]	2.860	3.201	4.201	106[#,≠]	3.260	2.955	4.347
66[#,≠]	2.936	3.667	3.357	107[#,≠]	3.060	2.935	3.721
67[#,ψ]	2.996	3.451	3.420	108[$,1]	3.886	3.332	4.276
68[#,≠]	2.609	3.236	3.420	109[#,ψ]	2.222	2.702	2.252
69[#,ψ]	2.097	1.970	2.432	110[^,*]	3.495	3.516	3.959
70[#,≠]	3.886	3.393	3.585	111[^,≠]	3.824	3.754	4.000
71[#,≠]	2.544	3.157	3.252	112[#,ψ]	2.504	2.461	2.602
72[$,ψ]	3.180	3.050	3.244	113[$,≠]	3.444	3.652	4.125
73[^,≠]	3.585	3.567	3.081	114[^,≠]	2.900	3.296	4.155
74[#,≠]	2.780	3.432	2.893	115[^,≠]	1.876	1.836	1.699
75[^,*]	3.276	3.340	3.319	116[#,≠]	2.854	2.422	1.602
76[^,≠]	4.180	3.367	4.229	117[^,≠]	2.907	2.773	2.854
77[^,≠]	4.215	3.294	3.824	118[#,≠]	1.754	2.496	1.721
78[#,≠]	3.260	3.637	3.886	119[#,≠]	2.620	2.626	1.745
79[$,*]	4.149	3.341	4.000	120[#,ψ]	2.538	2.179	1.745
80[#,≠]	3.824	3.766	4.268	121[^,≠]	2.951	2.646	2.398
81[^,*]	4.208	3.297	3.770	122[^,ψ]	1.735	2.283	1.602
82[$,≠]	4.260	3.693	4.201	123[#,≠]	1.947	2.457	1.620
83[#,ψ]	3.638	3.833	4.114	124[#,*]	0.449	2.099	1.602
84[$,ψ]	3.796	3.976	4.367	125[$,≠]	2.536	2.274	1.620
85[^,ψ]	3.721	3.779	4.420	126[$,ψ]	2.060	2.485	1.770
86[^,ψ]	3.420	3.556	4.319	127[#,≠]	1.316	1.674	1.602
87[#,≠]	4.229	3.606	4.004	128[#,≠]	0.731	1.576	1.699
88[^,ψ]	4.208	3.518	3.959	129[#,ψ]	1.996	1.526	1.745
89[#,ψ]	2.650	3.478	2.688	130[#,ψ]	1.348	1.887	1.620
90[^,ψ]	2.785	3.425	2.924	131[^,≠]	2.275	1.612	1.770
91[#,≠]	3.585	3.466	4.081	132[#,*]	1.695	1.884	1.678
92[#,≠]	3.194	3.762	4.237	133[#,*]	2.204	2.472	2.041
93[$,≠]	3.824	3.475	3.337	134[$,ψ]	2.886	2.540	1.602
94[^,ψ]	3.854	3.792	4.260	135[#,ψ]	2.244	2.569	1.959
95[#,ψ]	3.036	3.853	3.886	136[$,≠]	1.699	2.567	1.959
96[#,*]	4.377	3.059	4.292	137[#,≠]	2.810	2.521	2.004
97[#,≠]	3.921	3.479	4.444	138[#,ψ]	2.013	2.788	1.854
98[#,ψ]	4.081	3.453	3.886	139[#,ψ]	2.680	2.526	2.921
99[$,ψ]	3.201	3.623	4.000	140[#,≠]	2.114	2.233	1.538
100[#,ψ]	3.456	3.304	4.000	141[^,≠]	2.114	2.906	2.155
101[#,*]	3.310	3.052	3.886	142[#,ψ]	1.310	1.736	2.027
102[$,ψ]	3.678	3.154	4.194	143[#,ψ]	1.465	1.716	1.959
103[#,ψ]	3.310	2.935	3.770	144[#,ψ]	2.114	1.796	1.569
104[^,ψ]	3.252	3.407	3.959	145[#,≠]	1.807	1.962	1.585
105[#,≠]	3.456	3.106	4.056	146[$,≠]	2.509	1.945	1.921

Tab. S2. (Cont.)

Cpd no.	Activity (pKi)			Cpd no.	Activity (pKi)		
	Obser-ved	Predicted			Obser-ved	Predicted	
		QSAR	Pharmacoph.			QSAR	Pharmacoph.
147[$,*]	1.356	1.534	1.367	159[#,≠]	1.662	2.617	1.569
148[#,≠]	2.658	2.027	2.013	160[^,≠]	2.469	1.800	1.699
149[^,*]	0.489	2.087	1.481	161[^,ψ]	1.561	1.719	1.337
150[#,≠]	2.225	2.105	2.004	162[^,≠]	1.342	1.996	2.018
151[#,*]	2.009	2.227	2.022	163[#,*]	2.149	2.957	1.745
152[#,*]	1.963	1.874	1.959	164[$,ψ]	2.161	2.158	1.658
153[#,ψ]	2.076	1.864	2.027	165[^,*]	2.678	2.377	2.022
154[$,≠]	2.541	2.230	2.004	166[$,≠]	2.076	1.968	1.959
155[#,*]	2.272	1.803	1.959	167[^,≠]	3.456	3.189	3.387
156[^,≠]	1.924	1.565	2.022	168[#,≠]	4.469	3.474	4.495
157[#,≠]	1.614	1.807	2.000	169[#,≠]	3.959	2.770	3.678
158[#,≠]	2.056	2.485	2.027	170[#,≠]	3.728	3.251	3.824

[#] QSAR Tr; [$] QSAR Ts; [^] QSAR Vs; [*] Pharmacophore Tr; [ψ] Pharmacophore Ts; [≠] PharmacophoreVs

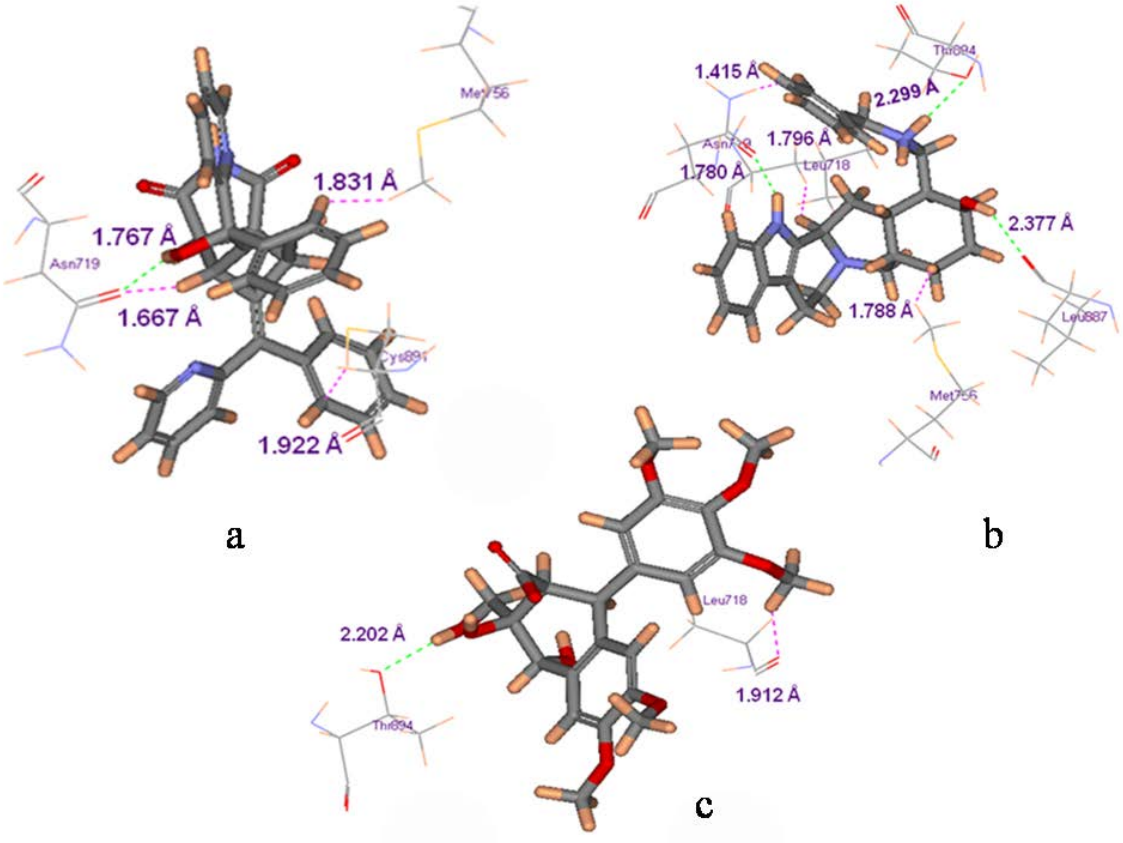


Fig. S1. Hit ligands at the binding site of 2OVH [64]. Catalytic residues are labeled.
(a) NCI0101316
(b) NCI0023681
(c) NCI0050131

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