

Article

Hits discovery on the Androgen receptor: *in silico* approaches to identify agonists compounds

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Supplementary Information

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Table S1. Unambiguous Tox21 agonist molecules considered in the study

Molecules screened by one of the 18 pharmacophore models generated are highlighted in green.

PUBCHEM_RESULT_TAG	PUBCHEM_SID	PUBCHEM_CID	PUBCHEM_ACTIVITY_OUTCOME	PUBCHEM_ACTIVITY_SCORE	Activity Summary	Ratio Activity	Ratio Potency (uM)	Ratio Efficacy (%)
72	144205785	3033968	Active	56	active agonist	active agonist	0.000648625	44.7551
124	144206952	10631	Active	75	active agonist	active agonist	0.000785827	119.711
156	144209642	980	Active	80	active agonist	active agonist	0.001	143.371
220	144212910	9878	Active	68	active agonist	active agonist	0.001	92.3037
227	144213960	13109	Active	55	active agonist	active agonist	0.001	41.2919
195	144211847	6238	Active	63	active agonist	active agonist	0.00128805	75.9148
138	144207887	6013	Active	88	active agonist	active agonist	0.0014244	179.06
145	144208410	9904	Active	71	active agonist	active agonist	0.00165644	111.574
218	144212744	6230	Active	58	active agonist	active agonist	0.00223835	58.7889
194	144211772	9782	Active	64	active agonist	active agonist	0.00227281	82.5659
14	144204071	443935	Active	61	active agonist	active agonist	0.00256454	71.6766
60	144205410	68947	Active	78	active agonist	active agonist	0.00258222	145.444
81	144206014	27812	Active	59	active agonist	active agonist	0.00268325	63.4127
77	144205996	66359	Active	71	active agonist	active agonist	0.00301065	117.705
137	144207737	25015	Active	67	active agonist	active agonist	0.00325022	102.331
142	144208185	10635	Active	69	active agonist	active agonist	0.00329688	110.444
7	144203910	6231	Active	60	active agonist	active agonist	0.0036225	71.5271
73	144205803	444008	Active	64	active agonist	active agonist	0.00379019	88.2847
94	144206325	14708	Active	63	active agonist	active agonist	0.00393847	84.2886
24	144204418	440707	Active	67	active agonist	active agonist	0.00393847	102.973

133	144207161	5284587	Active	59	active agonist	active agonist	0.00495824	67.7005
228	144214019	6010	Active	75	active agonist	active agonist	0.00504666	141.776
116	144206781	3034658	Active	75	active agonist	active agonist	0.00578088	145.211
211	144212605	16533	Active	63	active agonist	active agonist	0.00640565	87.5693
55	144205191	9677	Active	71	active agonist	active agonist	0.00700369	127.15
87	144206191	6917715	Active	58	active agonist	active agonist	0.0072777	67.3898
15	144204077	247839	Active	71	active agonist	active agonist	0.00842704	130.459
104	144206667	14743	Active	84	active agonist	active agonist	0.00870756	197.859
209	144212587	5995	Active	82	active agonist	active agonist	0.00977052	188.113
139	144208013	5754	Active	64	active agonist	active agonist	0.0102642	95.6772
118	144206893	229455	Active	77	active agonist	active agonist	0.01028	163.422
90	144206222	231084	Active	78	active agonist	active agonist	0.0106822	169.661
69	144205669	20469	Active	63	active agonist	active agonist	0.0119856	96.191
26	144204426	71414	Active	61	active agonist	active agonist	0.0145209	85.9625
10	144203988	224246	Active	67	active agonist	active agonist	0.0149856	117.168
200	144212257	28417	Active	57	active agonist	active agonist	0.0160903	67.3858
120	144206895	31378	Active	70	active agonist	active agonist	0.0162927	133.941
92	144206313	68952	Active	71	active agonist	active agonist	0.0162927	137.702
206	144212471	5833	Active	59	active agonist	active agonist	0.0184045	76.5593
203	144212335	6741	Active	62	active agonist	active agonist	0.0194938	96.7905
196	144211864	439501	Active	52	active agonist	active agonist	0.022421	40.2118
98	144206491	636398	Active	64	active agonist	active agonist	0.0230141	106.309
106	144206694	5876	Active	67	active agonist	active agonist	0.0239145	122.796
208	144212586	441207	Active	53	active agonist	active agonist	0.0247039	47.8229
128	144207031	5745	Active	58	active agonist	active agonist	0.0253315	75.5809
61	144205416	155143	Active	71	active agonist	active agonist	0.0258222	146.503
59	144205275	5877	Active	58	active agonist	active agonist	0.0278822	76.7288

222	144213304	5755	Active	62	active agonist	active agonist	0.029736	101.938
27	144204427	5952	Active	74	active agonist	active agonist	0.0301065	165.61
70	144205769	68873	Active	73	active agonist	active agonist	0.0301065	163.515
84	144206153	248271	Active	57	active agonist	active agonist	0.0325083	72.4677
113	144206719	21700	Active	64	active agonist	active agonist	0.0337801	110.851
86	144206181	443936	Active	60	active agonist	active agonist	0.0351016	87.6863
100	144206581	71470	Active	62	active agonist	active agonist	0.0379019	101.342
102	144206625	5702068	Active	62	active agonist	active agonist	0.0379019	104.942
13	144204069	16490	Active	62	active agonist	active agonist	0.0391149	101.479
132	144207117	63049	Active	62	active agonist	active agonist	0.0425266	103.592
46	144204950	26133	Active	59	active agonist	active agonist	0.0495824	86.7531
126	144206973	65359	Active	61	active agonist	active agonist	0.0578088	99.9483
129	144207048	16158	Active	61	active agonist	active agonist	0.0648625	100.613
96	144206477	9270	Active	54	active agonist	active agonist	0.0756242	59.7639
193	144211757	222786	Active	63	active agonist	active agonist	0.0776062	121.639
135	144207269	5281034	Active	57	active agonist	active agonist	0.0814027	83.6766
140	144208052	6446	Active	67	active agonist	active agonist	0.0843204	144.894
95	144206364	6540478	Active	57	active agonist	active agonist	0.0848517	84.0618
201	144212286	5284486	Active	53	active agonist	active agonist	0.0870756	57.1597
215	144212719	6166	Active	71	active agonist	active agonist	0.0904822	172.962
19	144204238	6714002	Active	51	active agonist	active agonist	0.0909931	42.8088
23	144204404	5282494	Active	58	active agonist	active agonist	0.0952052	85.9906
184	144210627	5994	Active	70	active agonist	active agonist	0.0977004	166.694
35	144204576	2724385	Active	49	active agonist	active agonist	0.1028	28.8159
97	144206482	91670	Active	68	active agonist	active agonist	0.124545	162.83
182	144210516	5865	Active	59	active agonist	active agonist	0.13281	102.808
89	144206221	111332	Active	58	active agonist	active agonist	0.15089	97.138

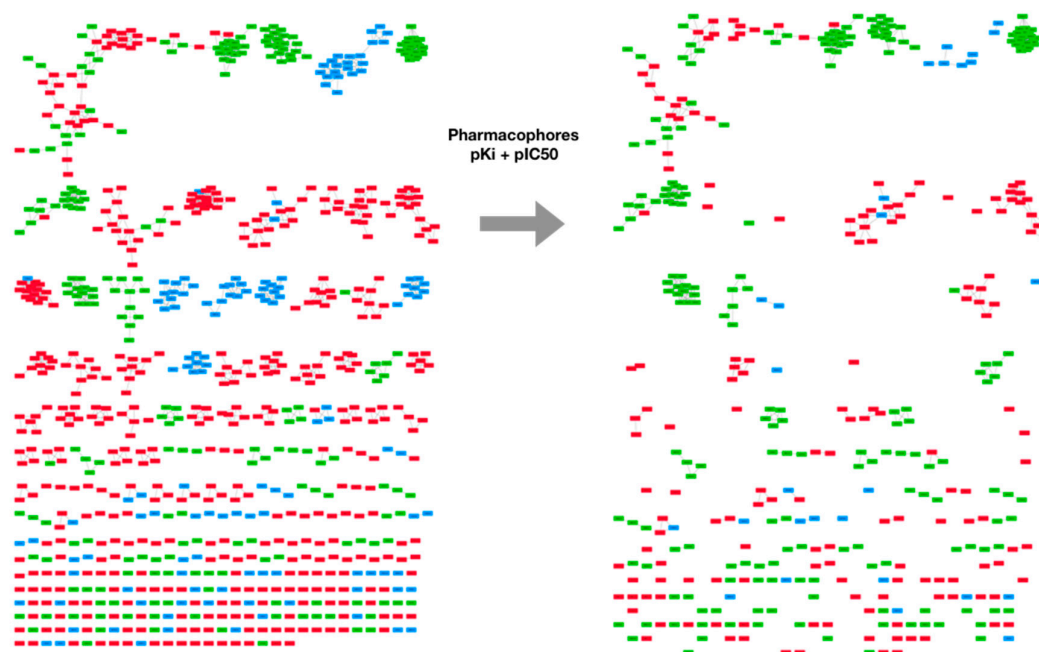
17	144204183	5282493	Active	60	active agonist	active agonist	0.15089	107.657
53	144205152	11876263	Active	62	active agonist	active agonist	0.162927	126.768
21	144204277	636374	Active	55	active agonist	active agonist	0.188658	75.499
44	144204881	5834	Active	58	active agonist	active agonist	0.197391	100.959
99	144206578	229295	Active	53	active agonist	active agonist	0.197391	61.2609
105	144206681	60196346	Active	56	active agonist	active agonist	0.213138	87.5614
56	144205200	6300	Active	66	active agonist	active agonist	0.239145	166.106
78	144206006	40973	Active	48	active agonist	active agonist	0.239145	28.7062
216	144212723	656583	Active	50	active agonist	active agonist	0.26499	42.7332
226	144213947	5753	Active	61	active agonist	active agonist	0.291709	125.972
71	144205772	444025	Active	49	active agonist	active agonist	0.364749	38.888
186	144210896	6128	Active	67	active agonist	active agonist	0.388952	190.293
210	144212603	11273	Active	61	active agonist	active agonist	0.419981	135.259
88	144206200	9568628	Active	59	active agonist	active agonist	0.425266	122.034
136	144207339	6279	Active	55	active agonist	active agonist	0.436145	89.2318
9	144203980	9051	Active	54	active agonist	active agonist	0.438876	80.8287
125	144206954	656804	Active	56	active agonist	active agonist	0.441903	100.412
213	144212641	5284557	Active	60	active agonist	active agonist	0.528725	133.415
144	144208409	68289	Active	56	active agonist	active agonist	0.577411	103.833
49	144205052	60198	Active	68	active agonist	active agonist	0.600704	215.297
198	144212039	108956	Active	48	active agonist	active agonist	0.609064	30.0663
48	144205004	13789	Active	59	active agonist	active agonist	0.700369	135.682
121	144206907	10041070	Active	59	active agonist	active agonist	0.916208	145.051
31	144204447	30323	Active	59	active agonist	active agonist	0.952052	145.996
80	144206008	6918178	Active	52	active agonist	active agonist	0.952052	74.1174
224	144213522	26041	Active	52	active agonist	active agonist	0.989298	71.7675

Table S2. PDB structures used for docking

PDB	Protein	Exp	Resolution	Chain	Profile	Smiles
1T5Z	AR	X-ray	2.30	A	agonist	<chem>C[C@]12CC[C@H]3[C@@H](CC[C@H]4CC(=O)CC[C@]34C)[C@@H]1CC[C@@H]2O</chem>
1T63	AR	X-ray	2.07	A	agonist	<chem>C[C@]12CC[C@H]3[C@@H](CC[C@H]4CC(=O)CC[C@]34C)[C@@H]1CC[C@@H]2O</chem>
1T65	AR	X-ray	1.66	A	agonist	<chem>C[C@]12CC[C@H]3[C@@H](CC[C@H]4CC(=O)CC[C@]34C)[C@@H]1CC[C@@H]2O</chem>
1XJ7	AR	X-ray	2.70	A	agonist	<chem>C[C@]12CC[C@H]3[C@@H](CC[C@H]4CC(=O)CC[C@]34C)[C@@H]1CC[C@@H]2O</chem>
1XOW	AR	X-ray	1.80	A	agonist	<chem>C[C@]1(O)CC[C@H]2[C@@H]3CCC4=CC(=O)CCC4=C3C=C[C@]12C</chem>
1XQ3	AR	X-ray	2.25	A	agonist	<chem>C[C@]1(O)CC[C@H]2[C@@H]3CCC4=CC(=O)CCC4=C3C=C[C@]12C</chem>
2AM9	AR	X-ray	1.64	A	agonist	<chem>C[C@]12CC[C@H]3[C@@H](CCC4=CC(=O)CC[C@]34C)[C@@H]1CC[C@@H]2O</chem>
2AMA	AR	X-ray	1.90	A	agonist	<chem>C[C@]12CC[C@H]3[C@@H](CC[C@H]4CC(=O)CC[C@]34C)[C@@H]1CC[C@@H]2O</chem>
2AMB	AR	X-ray	1.75	A	agonist	<chem>CC[C@]1(O)CC[C@H]2[C@@H]3CCC4=CC(=O)CCC4=C3C=C[C@]12CC</chem>
2AO6	AR	X-ray	1.89	A	agonist	<chem>C[C@]1(O)CC[C@H]2[C@@H]3CCC4=CC(=O)CCC4=C3C=C[C@]12C</chem>
2AX9	AR	X-ray	1.65	A	agonist	<chem>C[C@](O)(CBr)C(=O)Nc1ccc(c(c1)C(F)(F)F)[N+](O-)=O</chem>
2AXA	AR	X-ray	1.80	A	agonist	<chem>C[C@](O)(COc1ccc(F)cc1)C(=O)Nc1ccc(c(c1)C(F)(F)F)[N+](O-)=O</chem>
2PIO	AR	X-ray	2.03	A	agonist	<chem>C[C@]12CC[C@H]3[C@@H](CC[C@H]4CC(=O)CC[C@]34C)[C@@H]1CC[C@@H]2O</chem>
2PIP	AR	X-ray	1.80	L	agonist	<chem>C[C@]12CC[C@H]3[C@@H](CC[C@H]4CC(=O)CC[C@]34C)[C@@H]1CC[C@@H]2O</chem>
2PIQ	AR	X-ray	2.40	A	agonist	<chem>C[C@]12CC[C@H]3[C@@H](CC[C@H]4CC(=O)CC[C@]34C)[C@@H]1CC[C@@H]2O</chem>
2PIR	AR	X-ray	2.10	A	agonist	<chem>C[C@]12CC[C@H]3[C@@H](CC[C@H]4CC(=O)CC[C@]34C)[C@@H]1CC[C@@H]2O</chem>
2PIT	AR	X-ray	1.76	A	agonist	<chem>C[C@]12CC[C@H]3[C@@H](CC[C@H]4CC(=O)CC[C@]34C)[C@@H]1CC[C@@H]2O</chem>
2PIU	AR	X-ray	2.12	A	agonist	<chem>C[C@]12CC[C@H]3[C@@H](CC[C@H]4CC(=O)CC[C@]34C)[C@@H]1CC[C@@H]2O</chem>
2PIV	AR	X-ray	1.95	A	agonist	<chem>C[C@]12CC[C@H]3[C@@H](CC[C@H]4CC(=O)CC[C@]34C)[C@@H]1CC[C@@H]2O</chem>
2PIW	AR	X-ray	2.58	A	agonist	<chem>C[C@]12CC[C@H]3[C@@H](CC[C@H]4CC(=O)CC[C@]34C)[C@@H]1CC[C@@H]2O</chem>
2PIX	AR	X-ray	2.40	A	agonist	<chem>C[C@]12CC[C@H]3[C@@H](CC[C@H]4CC(=O)CC[C@]34C)[C@@H]1CC[C@@H]2O</chem>
2PKL	AR	X-ray	2.49	A	agonist	<chem>C[C@]12CC[C@H]3[C@@H](CC[C@H]4CC(=O)CC[C@]34C)[C@@H]1CC[C@@H]2O</chem>
2PNU	AR	X-ray	1.65	A	agonist	<chem>C[C@]12CCC(=O)C[C@@H]1CC[C@H]1[C@@H]3CC[C@H](O)[C@@]3(CCOc3cc(F)cc(F)c3)CC[C@H]21</chem>
2Q7I	AR	X-ray	1.87	A	agonist	<chem>C[C@]12CC[C@H]3[C@@H](CCC4=CC(=O)CC[C@]34C)[C@@H]1CC[C@@H]2O</chem>

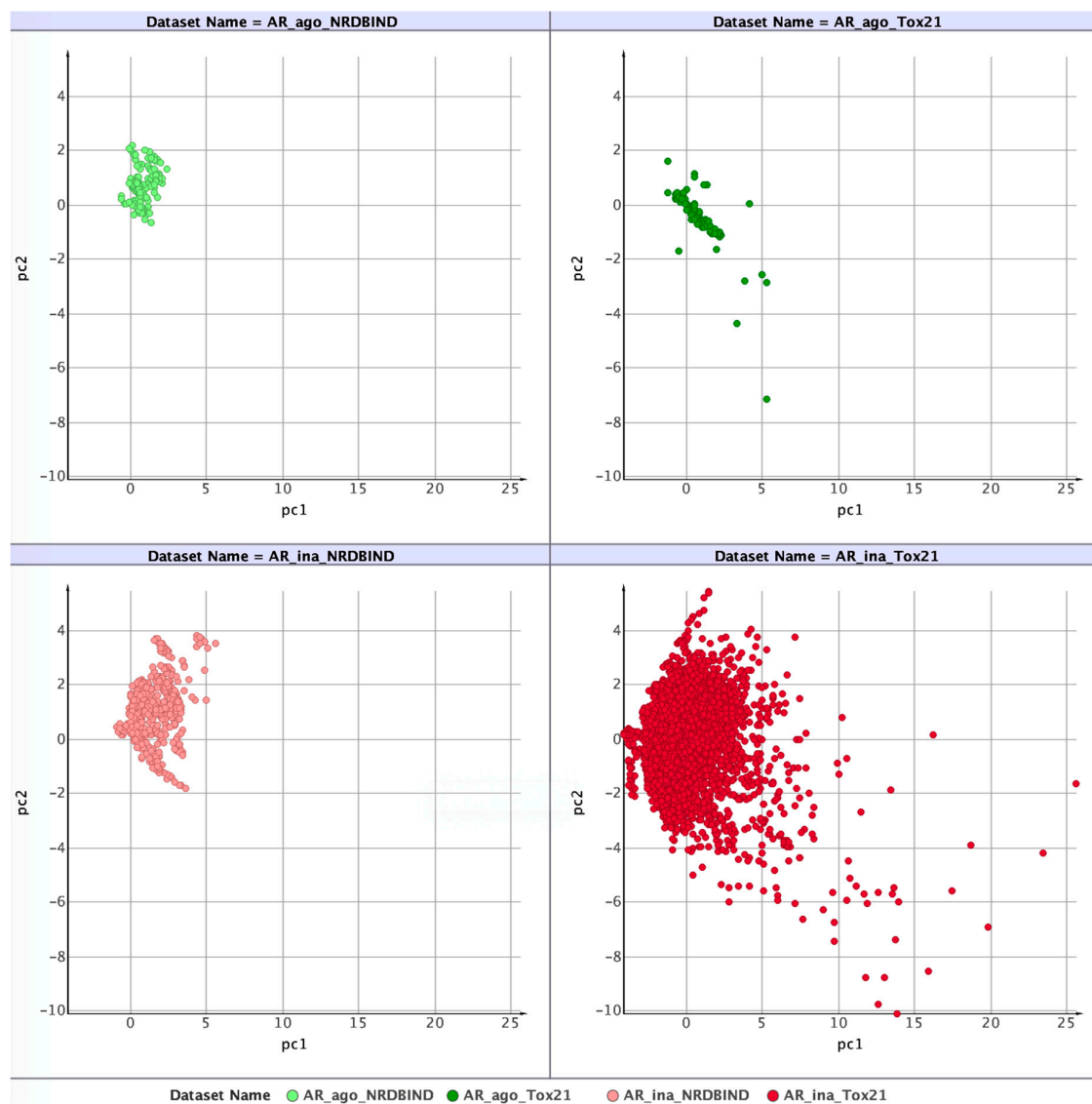
2Q7J	AR	X-ray	1.90	A	agonist	C[C@]12CC[C@H]3[C@@H](CCC4=CC(=O)CC[C@]34C)[C@@H]1CC[C@@H]2O
2Z4J	AR	X-ray	2.60	A	agonist	C[C@]12CC[C@H]3[C@@H](CC[C@H]4CC(=O)CC[C@]34C)[C@@H]1CC[C@@H]2O
3L3X	AR	X-ray	1.55	A	agonist	C[C@]12CC[C@H]3[C@@H](CC[C@H]4CC(=O)CC[C@]34C)[C@@H]1CC[C@@H]2O
3L3Z	AR	X-ray	2.00	A	agonist	C[C@]12CC[C@H]3[C@@H](CC[C@H]4CC(=O)CC[C@]34C)[C@@H]1CC[C@@H]2O
5JJM	AR	X-ray	2.15	A, B, C, D	agonist	C[C@]12CC[C@H]3[C@@H](CC[C@H]4CC(=O)CC[C@]34C)[C@@H]1CC[C@@H]2O

Figure S1. Structural Network Analysis



Molecular networks of molecules sharing structural similarity. Colored rounded rectangles represent molecules (green: agonist, red: antagonist, blue: non binder). Each edge connects two molecules with a $T_c \geq 0.90$. The right panel highlights the compounds that have been screened with the ensemble of pKi and pIC50 pharmacophore models.

Figure S2. Chemical Space Analysis (PCA) of the NR-DBIND and Tox21 datasets



Principal component analysis of the NR-DBIND (left) and Tox21 (right) datasets used for the study. Classical descriptors (molecular weight, cLogP, number of H-bond donor, number of H-bond acceptor, total surface area, total polar surface area, MolFlex, MolComplex, number of rotatable bonds, number of aromatic rings, number of aromatic atoms) were computed with DataWarrior for each molecules, and used to perform the principal component analysis with DataWarrior. The agonist (green) and non-agonist (red) compounds are plotted on the 2 first PCA axes covering respectively 41% and 21% of the variance. Agonist and non-agonist molecules of the NR-DBIND are overlapping. Agonist compounds from the Tox21 do not significantly cover the chemical space of agonist compounds from the NR-DBIND.

Table S3. Pharmacophore model coordinates

AR_agonist_pIC50_1.xyz	exclusion -10.135822 1.0116034 6.197093 1.5 1.0
type x y z tolerance weight additional_flag	exclusion 1.8641777 -6.4883966 -5.802907 1.5 1.0
H -2.9198 -2.233 1.7059 1.9499999 1.0	exclusion 6.3641777 -0.48839664 -2.802907 1.5 1.0
H -1.548751 0.485183 2.418983 1.65 1.0	exclusion 4.8641777 -6.4883966 4.697093 1.5 1.0
H 0.026497 -2.481257 -1.100548 1.8 1.0	exclusion -4.1358223 1.0116034 10.697093 1.5 1.0
H -5.340819 1.037824 -4.330588 1.5 1.0 optional	exclusion 7.2814 -1.6627 3.3877 1.0 1.0
AR -1.3839295 -0.03724755 2.523065 1.3499999 1.0 optional	exclusion -7.773383 4.8079166 -5.028417 1.15 1.0
HBA -0.7136 -0.302 -3.2851 1.0 1.0 optional	exclusion -2.6358223 1.0116034 -8.802907 1.5 1.0
HBA -4.6358213 -0.08600117 5.9669733 1.2 1.0	exclusion -5.6437 3.9592 -7.0959 1.0 1.0
HBA -2.9672925 0.33049953 4.7568355 1.5 0.6 optional	exclusion 6.3641777 -1.9883966 6.197093 1.5 1.0
exclusion -5.293088 -2.0412688 -0.61673087 0.70000005 1.0	exclusion 0.3641777 -1.9883966 -8.802907 1.5 1.0
exclusion -3.3181 2.4367 1.9151 0.5500001 1.0	exclusion 6.3641777 -4.9883966 -2.802907 1.5 1.0
exclusion -3.1410472 2.2917879 -0.39625537 0.5500001 1.0	exclusion -4.1358223 -4.9883966 10.697093 1.5 1.0
exclusion -4.4484153 -4.604938 1.77696 0.70000005 1.0	exclusion -7.1358223 5.5116034 7.697093 1.5 1.0
exclusion -6.4796 -0.5423 0.6502 1.0 1.0	exclusion 7.8641777 1.0116034 1.697093 1.5 1.0
exclusion -2.1395998 -5.3094363 0.73701465 1.0 1.0	exclusion -8.1142845 0.6358953 -8.090595 1.0 1.0
exclusion -4.627818 -4.460462 -0.685709 1.0 1.0	exclusion 7.8641777 -4.9883966 1.697093 1.5 1.0
exclusion -0.998721 -0.6687772 5.442823 0.5500001 1.0	exclusion -10.135822 -1.9883966 9.197093 1.5 1.0
exclusion -5.6358223 2.5116034 0.19709301 1.5 1.0	exclusion -8.635822 2.5116034 10.697093 1.5 1.0
exclusion -2.7919 -5.9426 2.8556 1.0 1.0	exclusion -7.1358223 -1.9883966 12.197093 1.5 1.0
exclusion 0.5452 0.014 4.9244 1.0 1.0	
exclusion 0.3641777 -3.4883966 4.697093 1.5 1.0	AR_agonist_pIC50_2.xyz
exclusion -6.46607 -2.786647 -1.8006656 0.70000005 1.0	type x y z tolerance weight additional_flag
exclusion -3.4191852 -2.6506124 -3.9097943 1.0 1.0	H -4.878049 -1.9267721 1.5680003 1.5 1.0
exclusion -5.7515216 -1.5225985 5.3207 0.3 1.0	H 3.3174267 -2.1993847 2.1833172 1.5 1.0
exclusion 1.4587915 -4.8365192 -0.11959292 0.70000005 1.0	HBA 1.4906029 -1.342783 1.9695095 1.5 0.6 optional
exclusion -7.945017 -1.5594493 3.594639 1.0 1.0	HBA 1.3689609 -2.528245 0.25184643 1.5 1.0
exclusion -0.1099 3.287 -1.9868 1.0 1.0	HBA -0.58239555 -1.8389704 -1.7128992 1.8 1.0
exclusion -4.6001 -3.1043 6.4186 1.0 1.0	HBA 3.2769208 -1.4075683 0.72404313 1.5 0.8 optional
exclusion -1.3476417 2.5284102 5.7501097 1.0 1.0	HBA -4.481324 -0.027195176 5.8645244 1.5 1.0
exclusion -2.2901 4.2627 4.1325 1.0 1.0	exclusion 0.12195206 -3.528245 5.865656 1.5 1.0
exclusion 2.6846204 -1.6315789 -2.5315604 0.70000005 1.0	exclusion -2.878048 -8.028245 1.3656559 1.5 1.0
exclusion -7.07831 -3.0160356 5.300307 1.0 1.0	exclusion 0.12195206 -8.028245 4.365656 1.5 1.0
exclusion 1.7265 3.5619 0.194 0.70000005 1.0	exclusion -7.378048 2.471755 2.865656 1.5 1.0
exclusion -2.6358223 4.0116034 -2.802907 1.5 1.0	exclusion 1.621952 -8.028245 -0.1343441 1.5 1.0
exclusion -3.8742 3.3511 5.5871 0.85 1.0	exclusion 0.12195206 5.471755 1.3656559 1.5 1.0
exclusion 0.8228 -2.8134 -4.4829 1.0 1.0	exclusion -2.878048 -6.528245 7.365656 1.5 1.0
exclusion 3.8653 -2.7423 2.7422 1.0 1.0	exclusion -4.378048 5.471755 2.865656 1.5 1.0
exclusion 3.8862178 -0.63308275 -1.0083754 1.0 1.0	exclusion 1.621952 3.971755 5.865656 1.5 1.0
exclusion 3.4406161 -1.4336029 4.3236413 1.0 1.0	exclusion -7.378048 2.471755 -1.6343441 1.5 1.0
exclusion -4.1358223 -7.9883966 1.697093 1.5 1.0	exclusion 4.621952 0.971755 5.865656 1.5 1.0
exclusion 2.705726 -4.5239234 -2.7431297 1.0 1.0	exclusion 1.621952 -0.528245 8.865656 1.5 1.0
exclusion -1.1358223 -7.9883966 -1.302907 1.5 1.0	exclusion -4.378048 2.471755 -4.634344 1.5 1.0
exclusion -4.1358223 5.5116034 3.197093 1.5 1.0	exclusion -5.878048 -8.028245 4.365656 1.5 1.0
exclusion -2.6358223 -6.4883966 6.197093 1.5 1.0	exclusion -2.878048 3.971755 7.365656 1.5 1.0
exclusion 0.3641777 5.5116034 0.19709301 1.5 1.0	exclusion -7.378048 -5.028245 -3.134344 1.5 1.0
exclusion 0.3641777 -7.9883966 3.197093 1.5 1.0	exclusion -4.378048 -8.028245 -3.134344 1.5 1.0
exclusion -10.135822 -0.48839664 1.697093 1.5 1.0	exclusion 3.121952 -5.028245 -4.634344 1.5 1.0
exclusion 1.8641777 4.0116034 4.697093 1.5 1.0	exclusion -7.378048 -0.528245 -4.634344 1.5 1.0
exclusion 3.3641777 2.5116034 -2.802907 1.5 1.0	exclusion -1.378048 5.471755 -3.134344 1.5 1.0
exclusion -7.1358223 -4.9883966 -4.302907 1.5 1.0	exclusion 4.621952 3.971755 -0.1343441 1.5 1.0
exclusion 1.8641777 1.0116034 7.697093 1.5 1.0	exclusion -7.378048 -8.028245 -0.1343441 1.5 1.0
exclusion -1.1358223 -1.9883966 9.197093 1.5 1.0	exclusion -7.378048 -5.028245 7.365656 1.5 1.0
exclusion -10.135822 -3.4883966 -1.302907 1.5 1.0	exclusion 3.121952 -6.528245 7.365656 1.5 1.0
exclusion -8.635822 4.0116034 3.197093 1.5 1.0	exclusion -4.378048 -5.028245 -6.134344 1.5 1.0
exclusion 0.3641777 2.5116034 -5.802907 1.5 1.0	exclusion -10.378048 -0.528245 2.865656 1.5 1.0
exclusion -2.6358223 4.0116034 7.697093 1.5 1.0	exclusion 3.121952 2.471755 -4.634344 1.5 1.0
exclusion -7.1358223 -7.9883966 -1.302907 1.5 1.0	exclusion -1.378048 -3.528245 10.365656 1.5 1.0
exclusion -10.135822 -3.4883966 4.697093 1.5 1.0	exclusion 4.621952 -8.028245 2.865656 1.5 1.0
exclusion -4.1358223 -7.9883966 -4.302907 1.5 1.0	exclusion 0.12195206 -8.028245 -4.634344 1.5 1.0
exclusion -7.1358223 -4.9883966 7.697093 1.5 1.0	exclusion -2.878048 0.971755 10.365656 1.5 1.0
exclusion -7.1358223 -7.9883966 4.697093 1.5 1.0	exclusion -10.378048 -0.528245 -1.6343441 1.5 1.0
exclusion -5.6358223 -1.9883966 -7.302907 1.5 1.0	exclusion 7.621952 -2.028245 -0.1343441 1.5 1.0
exclusion 4.8641777 4.0116034 1.697093 1.5 1.0	exclusion -2.878048 -0.528245 -7.634344 1.5 1.0
exclusion 3.3641777 -1.9883966 -5.802907 1.5 1.0	exclusion -10.378048 -5.028245 -0.1343441 1.5 1.0
exclusion -2.6358223 -4.9883966 -7.302907 1.5 1.0	exclusion -5.878048 -2.028245 10.365656 1.5 1.0
exclusion 3.3641777 -7.9883966 -1.302907 1.5 1.0	exclusion 6.121952 -6.528245 -1.6343441 1.5 1.0
exclusion -10.135822 -6.4883966 1.697093 1.5 1.0	exclusion -10.378048 -5.028245 4.365656 1.5 1.0

exclusion 6.121952 -3.528245 7.365656 1.5 1.0
exclusion 7.621952 -5.028245 2.865656 1.5 1.0
exclusion 6.121952 -2.028245 -4.634344 1.5 1.0
exclusion 0.12195206 -5.028245 -7.634344 1.5 1.0
exclusion -7.378048 5.471755 5.865656 1.5 1.0
exclusion 7.621952 2.471755 2.865656 1.5 1.0
exclusion 0.12195206 2.471755 -7.634344 1.5 1.0
exclusion 3.121952 -2.028245 -7.634344 1.5 1.0
exclusion -10.378048 -2.028245 7.365656 1.5 1.0
exclusion -10.378048 2.471755 5.865656 1.5 1.0
exclusion 7.621952 2.471755 -3.134344 1.5 1.0
exclusion -5.878048 3.971755 10.365656 1.5 1.0
exclusion -8.878048 0.971755 10.365656 1.5 1.0

AR_agonist_plC50_3.xyz
type x y z tolerance weight additional_flag
H -0.105062515 -1.179263 0.1378745 1.5 1.0
H -4.878049 -1.9267721 1.5680003 1.5 1.0
H -1.3866 0.6644 -1.7227 1.5 1.0 optional
H 3.3174267 -2.1993847 2.1833172 1.5 1.0 optional
HBA 1.4906029 -1.342783 1.9695095 1.5 0.6 optional
HBA 1.3689609 -2.528245 0.25184643 1.5 1.0 optional
HBA 0.0746 -2.4358 -2.1944 1.3 1.0
HBA 3.2769208 -1.4075683 0.72404313 1.5 0.8 optional
HBA -4.481324 -0.027195176 5.8645244 1.5 1.0
HBD 0.0746 -2.4358 -2.1944 1.3 1.0
exclusion 1.0568539 1.9167469 0.9933936 1.0 1.0
exclusion -0.2763 2.6214 -0.1839 0.85 1.0
exclusion -4.3077 2.7755 -0.6619 1.0 1.0
exclusion 0.12195206 -3.528245 5.865656 1.5 1.0
exclusion -6.4468 -4.2524 3.7042 0.70000005 1.0
exclusion -7.8602 -3.1071 3.032 1.0 1.0
exclusion -7.7428 -0.8222 4.0929 0.40000007 1.0
exclusion -2.878048 -8.028245 1.3656559 1.5 1.0
exclusion -7.378048 2.471755 2.865656 1.5 1.0
exclusion 2.9774487 -0.8933885 -3.9466786 1.0 1.0
exclusion -0.42314953 0.7521222 -5.308382 1.0 1.0
exclusion -7.6394 0.8035 4.5971 0.70000005 1.0
exclusion 0.12195206 5.471755 1.3656559 1.5 1.0
exclusion 1.3474331 -0.95326644 -5.4101567 0.70000005 1.0
exclusion -7.378048 2.471755 -1.6343441 1.5 1.0
exclusion 0.12195206 -8.028245 4.365656 1.5 1.0
exclusion 1.621952 -8.028245 -0.1343441 1.5 1.0
exclusion -4.378048 5.471755 2.865656 1.5 1.0
exclusion -4.378048 2.471755 -4.634344 1.5 1.0
exclusion 1.621952 3.971755 5.865656 1.5 1.0
exclusion -2.878048 -6.528245 7.365656 1.5 1.0
exclusion -7.378048 -5.028245 -3.134344 1.5 1.0
exclusion 4.621952 5.471755 5.865656 1.5 1.0
exclusion -2.878048 3.971755 7.365656 1.5 1.0
exclusion -7.378048 -0.528245 -4.634344 1.5 1.0
exclusion -1.378048 5.471755 -3.134344 1.5 1.0
exclusion 1.621952 -0.528245 8.865656 1.5 1.0
exclusion -5.878048 -8.028245 4.365656 1.5 1.0
exclusion -4.378048 -8.028245 -3.134344 1.5 1.0
exclusion 3.121952 -5.028245 -4.634344 1.5 1.0
exclusion 4.621952 3.971755 -0.1343441 1.5 1.0
exclusion 3.121952 2.471755 -4.634344 1.5 1.0
exclusion -4.378048 -5.028245 -6.134344 1.5 1.0
exclusion -7.378048 -8.028245 -0.1343441 1.5 1.0
exclusion -10.378048 -0.528245 2.865656 1.5 1.0
exclusion -7.378048 -5.028245 7.365656 1.5 1.0
exclusion -2.878048 -0.528245 -7.634344 1.5 1.0
exclusion 0.12195206 -8.028245 -4.634344 1.5 1.0
exclusion -10.378048 -0.528245 -1.6343441 1.5 1.0
exclusion 3.121952 -6.528245 7.365656 1.5 1.0
exclusion 4.621952 -8.028245 2.865656 1.5 1.0
exclusion -1.378048 -3.528245 10.365656 1.5 1.0
exclusion -10.378048 -5.028245 -0.1343441 1.5 1.0
exclusion -2.878048 0.971755 10.365656 1.5 1.0
exclusion 7.621952 -2.028245 -0.1343441 1.5 1.0

exclusion 0.12195206 -5.028245 -7.634344 1.5 1.0
exclusion 6.121952 -6.528245 -1.6343441 1.5 1.0
exclusion -10.378048 -5.028245 4.365656 1.5 1.0
exclusion 6.121952 -2.028245 -4.634344 1.5 1.0
exclusion 0.12195206 2.471755 -7.634344 1.5 1.0
exclusion -5.878048 -2.028245 10.365656 1.5 1.0
exclusion -7.378048 5.471755 5.865656 1.5 1.0
exclusion 6.121952 -3.528245 7.365656 1.5 1.0
exclusion 7.621952 -5.028245 2.865656 1.5 1.0
exclusion 3.121952 -2.028245 -7.634344 1.5 1.0
exclusion 7.621952 2.471755 2.865656 1.5 1.0
exclusion -10.378048 2.471755 5.865656 1.5 1.0
exclusion -10.378048 -2.028245 7.365656 1.5 1.0
exclusion 7.621952 2.471755 -3.134344 1.5 1.0
exclusion -5.878048 3.971755 10.365656 1.5 1.0
exclusion -8.878048 0.971755 10.365656 1.5 1.0

AR_agonist_plC50_4.xyz
type x y z tolerance weight additional_flag
H -1.1157844 -3.1968117 -1.8414524 1.5 0.9
H -4.878049 -1.9267721 1.5680003 1.65 1.0
H 3.3174267 -2.1993847 2.1833172 1.65 1.0 optional
H 3.982065 -4.637866 1.084596 1.65 1.0 optional
HBA 1.3689609 -2.528245 0.25184643 1.5 1.0 optional
HBA 0.0746 -2.4358 -2.1944 1.5999999 1.0
HBA -4.481324 -0.027195176 5.8645244 1.5 1.0
HBA 4.0726 -5.7427 2.1088 1.4499999 1.0 optional
HBD 0.0746 -2.4358 -2.1944 1.5999999 1.0
exclusion 0.6718311 -5.879855 0.38533354 0.5500001 1.0
exclusion 0.07695001 -5.49255 -1.0778999 0.3 1.0
exclusion 1.0568539 1.9167469 0.9933936 1.0 1.0
exclusion 2.3925571 0.061763123 3.8795493 1.0 1.0
exclusion -0.2763 2.6214 -0.1839 0.85 1.0
exclusion 0.12195206 -3.528245 5.865656 1.5 1.0
exclusion 2.0722547 -4.384985 -2.4863462 0.475 1.0
exclusion -4.3077 2.7755 -0.6619 1.0 1.0
exclusion 0.6475 2.3914 -2.7504 1.0 1.0
exclusion -2.878048 -8.028245 1.3656559 1.5 1.0
exclusion -6.4468 -4.2524 3.7042 0.5500001 1.0
exclusion 4.506343 -2.4397821 4.837199 0.9250001 1.0
exclusion 2.9774487 -0.8933885 -3.9466786 1.0 1.0
exclusion 1.621952 -8.028245 -0.1343441 1.5 1.0
exclusion -6.6974 -2.2391 5.163 0.70000005 1.0
exclusion 0.12195206 -8.028245 4.365656 1.5 1.0
exclusion -7.8602 -3.1071 3.032 1.0 1.0
exclusion -0.42314953 0.7521222 -5.308382 1.0 1.0
exclusion 1.3474331 -0.95326644 -5.4101567 0.70000005 1.0
exclusion -7.7428 -0.8222 4.0929 0.40000007 1.0
exclusion 0.12195206 5.471755 1.3656559 1.5 1.0
exclusion -2.878048 -6.528245 7.365656 1.5 1.0
exclusion 4.621952 0.971755 5.865656 1.5 1.0
exclusion 3.121952 -5.028245 -4.634344 1.5 1.0
exclusion -7.6394 0.8035 4.5971 0.70000005 1.0
exclusion -7.378048 2.471755 2.865656 1.5 1.0
exclusion 1.621952 3.971755 5.865656 1.5 1.0
exclusion -2.1342 -6.4166 -5.3384 1.0 1.0
exclusion 1.621952 -0.528245 8.865656 1.5 1.0
exclusion -4.378048 2.471755 -4.634344 1.5 1.0
exclusion -4.378048 -8.028245 -3.134344 1.2 1.0
exclusion -7.378048 2.471755 -1.6343441 1.5 1.0
exclusion -4.378048 5.471755 2.865656 1.5 1.0
exclusion 4.621952 3.971755 -0.1343441 1.5 1.0
exclusion -5.878048 -8.028245 4.365656 1.5 1.0
exclusion -7.378048 -5.028245 -3.134344 1.5 1.0
exclusion 3.121952 2.471755 -4.634344 1.5 1.0
exclusion 0.12195206 -8.028245 -4.634344 1.5 1.0
exclusion -2.878048 3.971755 7.365656 1.5 1.0
exclusion -1.378048 5.471755 -3.134344 1.5 1.0
exclusion -4.378048 -5.028245 -6.134344 1.2 1.0
exclusion 7.621952 -2.028245 -0.1343441 1.5 1.0
exclusion -7.378048 -0.528245 -4.634344 1.5 1.0

exclusion -7.378048 -8.028245 -0.1343441 1.2 1.0
exclusion 6.121952 -6.528245 -1.6343441 0.60000014 1.0
exclusion -1.378048 -3.528245 10.365656 1.5 1.0
exclusion -2.878048 -0.528245 -7.634344 1.5 1.0
exclusion -7.378048 -5.028245 7.365656 1.5 1.0
exclusion 6.121952 -2.028245 -4.634344 1.5 1.0
exclusion 0.12195206 -5.028245 -7.634344 1.5 1.0
exclusion -10.378048 -0.528245 2.865656 1.5 1.0
exclusion -2.878048 0.971755 10.365656 1.5 1.0
exclusion 7.621952 2.471755 2.865656 1.5 1.0
exclusion 3.121952 -2.028245 -7.634344 1.5 1.0
exclusion -10.378048 -0.528245 -1.6343441 1.5 1.0
exclusion -10.378048 -5.028245 -0.1343441 1.5 1.0
exclusion 0.12195206 2.471755 -7.634344 1.5 1.0
exclusion -5.878048 -2.028245 10.365656 1.5 1.0
exclusion -10.378048 -5.028245 4.365656 1.5 1.0
exclusion 7.621952 2.471755 -3.134344 1.5 1.0
exclusion -7.378048 5.471755 5.865656 1.5 1.0
exclusion -10.378048 -2.028245 7.365656 1.5 1.0
exclusion -10.378048 2.471755 5.865656 1.5 1.0
exclusion -5.878048 3.971755 10.365656 1.5 1.0
exclusion 8.944 -5.7368 6.6717 1.0 1.0
exclusion 5.8225 -11.667 3.364 1.4499999 1.0
exclusion -8.878048 0.971755 10.365656 1.5 1.0
exclusion 8.6164 -9.6329 5.2445 1.0 1.0
exclusion 11.4354 -6.9268 3.2255 1.4499999 1.0

AR_agonist_plc50_5.xyz
type x y z tolerance weight additional_flag
H -2.4656188 0.21610793 3.6876354 1.5 1.0
H 2.8281 -0.2638 0.6191 1.5 1.0
AR -2.116787 0.025461506 2.5768085 0.8999999 1.0 optional
HBA -5.090538 -2.683052 1.8703 1.5 1.0
HBA -5.090538 -2.683052 1.8703 1.5 1.0
HBA 1.5376356 0.7359357 -1.6168168 1.55 1.0
HBA 2.51505 3.2198 -0.5912 1.0 1.0
HBD -3.8525 -2.3115 1.0883 1.0 1.0 optional
HBD 2.4431 1.143 -1.2819 1.15 1.0
exclusion -3.5980172 2.7061825 -0.13935457 0.85 1.0
exclusion -4.590538 0.81694794 -1.0984335 1.5 1.0
exclusion -5.163 3.5522 -2.3772 1.0 1.0
exclusion 0.5048 -3.5662 -2.7694 1.0 1.0
exclusion -4.956978 -1.6838886 5.7322807 0.5500001 1.0
exclusion 2.909462 -3.683052 1.9015665 1.5 1.0
exclusion -6.090538 5.316948 1.9015665 1.5 1.0
exclusion -4.590538 0.81694794 -5.5984335 1.5 1.0
exclusion -0.090538025 -5.183052 4.9015665 1.5 1.0
exclusion -0.090538025 -6.683052 0.4015665 1.5 1.0
exclusion -3.090538 -5.183052 -4.0984335 1.5 1.0
exclusion -7.590538 2.316948 4.9015665 1.5 1.0
exclusion -9.090538 2.316948 0.4015665 1.5 1.0
exclusion 1.409462 5.316948 4.9015665 1.5 1.0
exclusion -7.590538 -2.183052 -4.0984335 1.5 1.0
exclusion -0.090538025 2.316948 7.9015665 1.5 1.0
exclusion -0.090538025 -2.183052 7.9015665 1.5 1.0
exclusion 1.409462 -5.183052 -4.0984335 1.5 1.0
exclusion 4.409462 2.316948 4.9015665 1.5 1.0
exclusion -4.590538 5.316948 6.4015665 1.5 1.0
exclusion -1.590538 -2.183052 -7.0984335 1.5 1.0
exclusion 5.909462 -0.68305206 1.9015665 1.5 1.0
exclusion -7.590538 5.316948 -2.5984335 1.5 1.0
exclusion 1.409462 0.81694794 -7.0984335 1.5 1.0
exclusion -1.590538 3.816948 -7.0984335 1.5 1.0
exclusion -1.590538 8.316948 3.4015665 1.5 1.0
exclusion -4.590538 -8.183052 0.4015665 1.5 1.0
exclusion 5.909462 3.816948 0.4015665 1.5 1.0
exclusion -10.590538 -0.68305206 3.4015665 1.5 1.0
exclusion 4.409462 -2.183052 6.4015665 1.5 1.0
exclusion -10.590538 -2.183052 -1.0984335 1.5 1.0
exclusion -3.090538 -5.183052 7.9015665 1.5 1.0
exclusion -4.590538 0.81694794 9.4015665 1.5 1.0

exclusion 4.409462 -2.183052 -5.5984335 1.5 1.0
exclusion -7.590538 -6.683052 -2.5984335 1.5 1.0
exclusion -3.090538 -8.183052 4.9015665 1.5 1.0
exclusion 2.909462 8.316948 1.9015665 1.5 1.0
exclusion -4.590538 8.316948 -4.0984335 1.5 1.0
exclusion -4.590538 9.816948 0.4015665 1.5 1.0
exclusion -0.090538025 9.816948 -1.0984335 1.5 1.0
exclusion 7.409462 -0.68305206 -2.5984335 1.5 1.0
exclusion -7.590538 -8.183052 3.4015665 1.5 1.0
exclusion 5.909462 2.316948 -5.5984335 1.5 1.0
exclusion -0.090538025 8.316948 -5.5984335 1.5 1.0
exclusion -7.590538 -5.183052 7.9015665 1.5 1.0
exclusion -10.590538 -5.183052 4.9015665 1.5 1.0
exclusion -10.590538 -6.683052 0.4015665 1.5 1.0
exclusion 4.409462 8.316948 -2.5984335 1.5 1.0

AR_agonist_plc50_6.xyz
type x y z tolerance weight additional_flag
H -3.4514 1.0771 4.3852 1.5 1.0
H 0.88327503 3.391725 -1.04795 1.65 0.9
H -1.738301 5.508399 0.86265 1.65 0.6999999
HBA -3.2635 -1.6899 0.8343 1.0 1.0 optional
HBA -5.090538 -2.683052 1.8703 1.35 1.0
HBA -2.08235 4.4583 -0.8103 1.0 1.0
HBD -3.9624 -2.519 0.7145 1.0 1.0 optional
HBD 0.49741682 0.80437005 -1.3490461 1.5 0.85
exclusion -4.590538 0.81694794 -1.0984335 1.5 1.0
exclusion 0.908126 0.3742931 1.742094 0.5500001 1.0
exclusion -0.9783 -3.1359 -2.4056 1.0 1.0
exclusion -2.9913013 -2.1621735 -3.3311615 1.0 1.0
exclusion 1.3774 -2.6022 -0.8725 1.0 1.0
exclusion -3.3620198 3.9151378 3.3372664 0.5500001 1.0
exclusion 0.0695 2.7309 4.7602 0.70000005 1.0
exclusion -1.9325 -1.7055 5.8282 0.5500001 1.0
exclusion -3.0908 -5.4261 0.9536 1.0 1.0
exclusion -4.1167383 -2.7405355 5.364767 1.0 1.0
exclusion 1.1681994 -2.1687124 -3.782334 1.0 1.0
exclusion -4.882004 -5.041749 -0.8730904 1.0 1.0
exclusion -6.2331 -2.037 4.4856 1.0 1.0
exclusion -4.6728 -0.4352 6.0685 1.0 1.0
exclusion -7.2728615 -0.43441314 3.83522 1.0 1.0
exclusion -3.243 -5.2722 3.3972 1.0 1.0
exclusion 2.44447 1.9878845 -3.2491229 0.40000007 1.0
exclusion -7.0552 -3.8986 1.5993 0.3 1.0
exclusion 2.3505034 0.17919168 -3.9458914 1.0 1.0
exclusion -8.361377 -1.7143651 0.9787548 1.0 1.0
exclusion -7.1968517 -2.9113777 3.3724964 0.70000005 1.0
exclusion 2.909462 -3.683052 1.9015665 1.5 1.0
exclusion -5.5444 -3.9963 4.3798 1.0 1.0
exclusion -4.590538 0.81694794 -5.5984335 1.5 1.0
exclusion -0.7887 -6.0242 -1.8328 1.0 1.0
exclusion -0.090538025 -6.683052 0.4015665 1.5 1.0
exclusion -3.090538 -5.183052 -4.0984335 1.5 1.0
exclusion -0.090538025 -5.183052 4.9015665 1.5 1.0
exclusion -9.090538 2.316948 0.4015665 1.5 1.0
exclusion -7.590538 2.316948 4.9015665 1.5 1.0
exclusion -7.590538 -2.183052 -4.0984335 1.5 1.0
exclusion 1.409462 5.316948 4.9015665 1.5 1.0
exclusion -0.090538025 2.316948 7.9015665 1.5 1.0
exclusion 1.409462 -5.183052 -4.0984335 1.5 1.0
exclusion -0.090538025 -2.183052 -7.9015665 1.5 1.0
exclusion -1.590538 -2.183052 -7.0984335 1.5 1.0
exclusion 2.92025 3.11535 -4.8966 1.0 1.0
exclusion -4.590538 5.316948 6.4015665 1.5 1.0
exclusion 4.409462 2.316948 4.9015665 1.5 1.0
exclusion 5.909462 -0.68305206 1.9015665 1.5 1.0
exclusion 1.409462 0.81694794 -7.0984335 1.5 1.0
exclusion -1.590538 3.816948 -7.0984335 1.5 1.0
exclusion -1.8454 5.8052 6.9856 1.0 1.0
exclusion -4.590538 -8.183052 0.4015665 1.5 1.0
exclusion -1.590538 8.316948 3.4015665 1.5 1.0

exclusion -10.590538 -2.183052 -1.0984335 1.5 1.0
exclusion -10.590538 -0.68305206 3.4015665 1.5 1.0
exclusion 5.909462 3.816948 0.4015665 1.5 1.0
exclusion -3.090538 -5.183052 7.9015665 1.5 1.0
exclusion 4.409462 -2.183052 6.4015665 1.5 1.0
exclusion -4.590538 0.81694794 9.4015665 1.5 1.0
exclusion 1.6654 6.4936 -4.8499 1.0 1.0
exclusion -7.590538 -6.683052 -2.5984335 1.5 1.0
exclusion 4.409462 -2.183052 -5.5984335 1.5 1.0
exclusion -3.090538 -8.183052 4.9015665 1.5 1.0
exclusion 4.352683 5.7230835 -3.2380333 1.0 1.0
exclusion 2.909462 8.316948 1.9015665 1.5 1.0
exclusion -1.4862 6.5713 -6.8669 1.0 1.0
exclusion -0.090538025 9.816948 -1.0984335 1.5 1.0
exclusion 7.409462 -0.68305206 -2.5984335 1.5 1.0
exclusion -0.0642 6.4304 -7.2351 1.0 1.0
exclusion -7.590538 -8.183052 3.4015665 1.5 1.0
exclusion 5.909462 2.316948 -5.5984335 1.5 1.0
exclusion -0.090538025 8.316948 -5.5984335 1.5 1.0
exclusion -7.590538 -5.183052 7.9015665 1.5 1.0
exclusion -10.590538 -6.683052 0.4015665 1.5 1.0
exclusion -10.590538 -5.183052 4.9015665 1.5 1.0
exclusion 4.409462 8.316948 -2.5984335 1.5 1.0

AR_agonist_pIC50_7.xyz
type x y z tolerance weight additional_flag
H -2.256744 -0.8094 0.843231 1.5 1.0
H -2.1117377 0.29971588 2.8835704 1.5 1.0
H 1.14125 1.487675 -0.18205 1.5 1.0 optional
H -1.2755611 4.4307227 -0.011332989 1.5 1.0 optional
AR -2.1329167 -0.6932333 0.79718333 0.9 1.0
AR -2.1329167 -0.6932333 0.79718333 0.9 1.0
AR -2.4868333 0.51523334 2.91135 0.9 1.0
AR -2.4868333 0.51523334 2.91135 0.9 1.0
HBA 1.1029867 2.375317 -1.9777594 1.0 1.0 optional
HBA -5.090538 -2.683052 1.8703 1.0500001 1.0
HBA -5.090538 -2.683052 1.8703 1.0500001 1.0
HBD 1.131 1.4799 -2.4577 1.0 1.0 optional
exclusion -0.3118732 0.38481152 -2.378739 0.40000007 1.0
exclusion 1.354037 -0.55367494 0.64744127 0.3 1.0
exclusion -4.590538 0.81694794 -1.0984335 1.5 1.0
exclusion -2.5508 -1.51265 -2.06995 0.40000007 1.0
exclusion 1.6315 -2.1866 -0.4448 0.70000005 1.0
exclusion 2.7142124 -0.075254664 -0.28047994 0.3 1.0
exclusion -3.9739 4.7248 -1.5559 0.70000005 1.0
exclusion 2.5749 3.2659 2.4316 1.0 1.0
exclusion -2.7073 4.9305 3.6776 1.0 1.0
exclusion 0.3205947 1.1527587 -4.700446 1.0 1.0
exclusion 1.5958765 5.1410017 -0.19463223 0.40000007 1.0
exclusion -4.6587 -2.2232 4.1097 0.3 1.0
exclusion 0.4529 3.9473 -3.8352 0.5500001 1.0
exclusion -2.3359709 6.4811664 1.0484855 0.5500001 1.0
exclusion -0.40982127 5.9751835 2.7868388 1.0 1.0
exclusion -1.2962675 6.741718 0.23532347 0.40000007 1.0
exclusion 4.4618335 1.2397462 -0.55274975 1.0 1.0
exclusion 2.0213642 5.615441 1.0691017 0.5500001 1.0
exclusion 3.3894 -2.9429 -0.9735 0.70000005 1.0
exclusion -2.6712818 3.2471917 -5.1903167 0.70000005 1.0
exclusion 2.909462 -3.683052 1.9015665 1.5 1.0
exclusion 2.3692777 -0.86607534 -4.3872204 1.0 1.0
exclusion -6.090538 5.316948 1.9015665 1.5 1.0
exclusion -4.590538 0.81694794 -5.5984335 1.5 1.0
exclusion -4.5479 -4.0711 4.68125 1.0 1.0
exclusion 4.3122 0.15155001 -3.4522 1.0 1.0
exclusion 4.751 2.0201 -2.4523 1.0 1.0
exclusion 1.409462 5.316948 4.9015665 1.5 1.0
exclusion 2.8857 5.653 -1.9198 1.0 1.0
exclusion -6.494 -0.0094 5.5781 1.0 1.0
exclusion -7.134 -4.203 -0.215 1.0 1.0
exclusion -0.090538025 -5.183052 4.9015665 1.5 1.0
exclusion -0.090538025 -6.683052 0.4015665 1.5 1.0

exclusion -3.090538 -5.183052 -4.0984335 1.5 1.0
exclusion 4.409462 2.316948 4.9015665 1.5 1.0
exclusion -7.590538 2.316948 4.9015665 1.5 1.0
exclusion 5.909462 -0.68305206 1.9015665 1.5 1.0
exclusion -9.090538 2.316948 0.4015665 1.5 1.0
exclusion -0.090538025 2.316948 7.9015665 1.5 1.0
exclusion -5.2368 -2.2749 6.7124 1.0 1.0
exclusion 1.409462 -5.183052 -4.0984335 1.5 1.0
exclusion -1.590538 -2.183052 -7.0984335 1.5 1.0
exclusion -7.590538 -2.183052 -4.0984335 1.5 1.0
exclusion -0.090538025 -2.183052 7.9015665 1.5 1.0
exclusion 5.909462 3.816948 0.4015665 1.5 1.0
exclusion 1.409462 0.81694794 -7.0984335 1.5 1.0
exclusion -4.590538 5.316948 6.4015665 1.5 1.0
exclusion -1.590538 3.816948 -7.0984335 1.5 1.0
exclusion -1.590538 8.316948 3.4015665 1.5 1.0
exclusion -7.590538 5.316948 -2.5984335 1.5 1.0
exclusion 4.409462 -2.183052 6.4015665 1.5 1.0
exclusion 4.409462 -2.183052 -5.5984335 1.5 1.0
exclusion 2.909462 8.316948 1.9015665 1.5 1.0
exclusion -4.590538 -8.183052 0.4015665 1.5 1.0
exclusion -0.090538025 9.816948 -1.0984335 1.5 1.0
exclusion -4.590538 8.316948 -4.0984335 1.5 1.0
exclusion -4.590538 0.81694794 9.4015665 1.5 1.0
exclusion 7.409462 -0.68305206 -2.5984335 1.5 1.0
exclusion -3.090538 -5.183052 7.9015665 1.5 1.0
exclusion -10.590538 -0.68305206 3.4015665 1.5 1.0
exclusion -10.590538 -2.183052 -1.0984335 1.5 1.0
exclusion -4.590538 9.816948 0.4015665 1.5 1.0
exclusion 5.909462 2.316948 -5.5984335 1.5 1.0
exclusion -0.090538025 8.316948 -5.5984335 1.5 1.0
exclusion -7.590538 -6.683052 -2.5984335 1.5 1.0
exclusion -3.090538 -8.183052 4.9015665 1.5 1.0
exclusion 4.409462 8.316948 -2.5984335 1.5 1.0
exclusion -7.590538 -8.183052 3.4015665 1.5 1.0
exclusion -7.590538 -5.183052 7.9015665 1.5 1.0
exclusion -10.590538 -5.183052 4.9015665 1.5 1.0
exclusion -10.590538 -6.683052 0.4015665 1.5 1.0

AR_agonist_pIC50_8.xyz
type x y z tolerance weight additional_flag
H -3.3344 0.936 3.1501 1.5 1.0
AR -1.3079333 -0.40653336 0.68436664 0.9 1.0
AR -3.4715667 -1.311 1.3516166 0.9 1.0
HBA -3.322144 -2.355218 0.249044 1.0 1.0 optional
HBA -5.3487 -3.1598 0.977 1.0 1.0
HBA -5.3487 -3.1598 0.977 1.0 1.0
HBD 0.9492 -0.5764 -0.9835 1.0 1.0
exclusion 0.041781068 1.4559435 -1.6739007 0.3 1.0
exclusion -0.6880145 -0.4216839 -2.91756 0.70000005 1.0
exclusion -4.590538 0.81694794 -1.0984335 1.5 1.0
exclusion -0.6529544 2.152721 -3.176307 0.5500001 1.0
exclusion 1.6709759 -2.5583906 -1.7021456 0.40000007 1.0
exclusion 3.5809526 -1.3432535 0.8431765 0.70000005 1.0
exclusion 1.1612061 3.1900568 -3.9661293 1.0 1.0
exclusion 2.1822643 1.5171382 -4.2002077 0.40000007 1.0
exclusion 0.71207047 -1.4328523 -5.1807055 0.70000005 1.0
exclusion 2.909462 -3.683052 1.9015665 1.5 1.0
exclusion -4.590538 0.81694794 -5.5984335 1.5 1.0
exclusion 3.120185 4.6482716 -1.8489956 0.5500001 1.0
exclusion -3.090538 -5.183052 -4.0984335 1.5 1.0
exclusion -0.090538025 -6.683052 0.4015665 1.5 1.0
exclusion 4.4388714 2.7927876 -2.4253163 0.70000005 1.0
exclusion 5.1919003 0.63335 -1.84235 0.3 1.0
exclusion -6.090538 5.316948 1.9015665 1.5 1.0
exclusion -0.090538025 -5.183052 4.9015665 1.5 1.0
exclusion 1.409462 -5.183052 -4.0984335 1.5 1.0
exclusion -1.590538 -2.183052 -7.0984335 1.5 1.0
exclusion 1.409462 5.316948 4.9015665 1.5 1.0
exclusion -7.590538 -2.183052 -4.0984335 1.5 1.0
exclusion 5.909462 -0.68305206 1.9015665 1.5 1.0

exclusion -9.090538 2.316948 0.4015665 1.5 1.0
exclusion 1.409462 0.81694794 -7.0984335 1.5 1.0
exclusion 4.409462 2.316948 4.9015665 1.5 1.0
exclusion -7.590538 2.316948 4.9015665 1.5 1.0
exclusion -1.590538 3.816948 -7.0984335 1.5 1.0
exclusion -0.090538025 2.316948 7.9015665 1.5 1.0
exclusion -0.090538025 -2.183052 7.9015665 1.5 1.0
exclusion 5.909462 3.816948 0.4015665 1.5 1.0
exclusion -7.590538 5.316948 -2.5984335 1.5 1.0
exclusion 4.409462 -2.183052 -5.5984335 1.5 1.0
exclusion -4.590538 5.316948 6.4015665 1.5 1.0
exclusion -1.590538 8.316948 3.4015665 1.5 1.0
exclusion -4.590538 -8.183052 0.4015665 1.5 1.0
exclusion 4.409462 -2.183052 6.4015665 1.5 1.0
exclusion -10.590538 -2.183052 -1.0984335 1.5 1.0
exclusion 7.409462 -0.68305206 -2.5984335 1.5 1.0
exclusion 2.909462 8.316948 1.9015665 1.5 1.0
exclusion -7.590538 -6.683052 -2.5984335 1.5 1.0
exclusion -3.090538 -5.183052 7.9015665 1.5 1.0
exclusion -10.590538 -0.68305206 3.4015665 1.5 1.0
exclusion -4.590538 8.316948 -4.0984335 1.5 1.0
exclusion 5.909462 2.316948 -5.5984335 1.5 1.0
exclusion -3.090538 -8.183052 4.9015665 1.5 1.0
exclusion -4.590538 0.81694794 9.4015665 1.5 1.0
exclusion -0.090538025 9.816948 -1.0984335 1.5 1.0
exclusion -0.090538025 8.316948 -5.5984335 1.5 1.0
exclusion -4.590538 9.816948 0.4015665 1.5 1.0
exclusion 4.409462 8.316948 -2.5984335 1.5 1.0
exclusion -7.590538 -8.183052 3.4015665 1.5 1.0
exclusion -7.590538 -5.183052 7.9015665 1.5 1.0
exclusion -10.590538 -6.683052 0.4015665 1.5 1.0
exclusion -10.590538 -5.183052 4.9015665 1.5 1.0

AR_agonist_pIC50_9.xyz

type x y z tolerance weight additional_flag
H -2.256744 -0.8094 0.843231 1.5 1.0
H -2.1117377 0.29971588 2.8835704 1.5 1.0
H 1.14125 1.487675 -0.18205 1.5 1.0 optional
H -1.2755611 4.4307227 -0.011332989 1.5 1.0 optional
AR -2.1329167 -0.6932333 0.79718333 0.9 1.0
AR -2.1329167 -0.6932333 0.79718333 0.9 1.0
AR -2.4868333 0.51523334 2.91135 0.9 1.0
AR -2.4868333 0.51523334 2.91135 0.9 1.0
HBA 1.1029867 2.375317 -1.9777594 1.0 1.0 optional
HBA -5.090538 -2.683052 1.8703 1.0500001 1.0
HBA -5.090538 -2.683052 1.8703 1.0500001 1.0
HBD 1.131 1.4799 -2.4577 1.0 1.0 optional
exclusion -4.590538 0.81694794 -1.0984335 1.5 1.0
exclusion -2.5508 -1.51265 -2.06995 0.40000007 1.0
exclusion -1.8326857 1.6538229 -3.7507627 0.40000007 1.0
exclusion 1.6315 -2.1866 -0.4448 0.70000005 1.0
exclusion 2.7142124 -0.075254664 -0.28047994 0.3 1.0
exclusion -3.9739 4.7248 -1.5559 0.40000007 1.0
exclusion 2.5749 3.2659 2.4316 1.0 1.0
exclusion -2.7073 4.9305 3.6776 1.0 1.0
exclusion 0.3205947 1.1527587 -4.700446 1.0 1.0
exclusion 1.5958765 5.1410017 -0.19463223 0.40000007 1.0
exclusion -4.6587 -2.2232 4.1097 0.3 1.0
exclusion 0.4529 3.9473 -3.8352 0.3 1.0
exclusion -2.3359709 6.4811664 1.0484855 0.5500001 1.0
exclusion -0.40982127 5.9751835 2.7868388 1.0 1.0
exclusion -1.2962675 6.741718 0.23532347 0.40000007 1.0
exclusion 2.0213642 5.615441 1.0691017 0.5500001 1.0
exclusion 4.4618335 1.2397462 -0.55274975 1.0 1.0
exclusion -2.6712818 3.2471917 -5.1903167 0.70000005 1.0
exclusion 3.3894 -2.9429 -0.9735 0.70000005 1.0
exclusion 2.3692777 -0.86607534 -4.3872204 1.0 1.0
exclusion 2.909462 -3.683052 1.9015665 1.5 1.0
exclusion -4.577157 -1.787242 5.637041 1.0 1.0
exclusion -6.090538 5.316948 1.9015665 1.5 1.0
exclusion -4.590538 0.81694794 -5.5984335 1.5 1.0

exclusion -4.5479 -4.0711 4.68125 1.0 1.0
exclusion 4.3122 0.15155001 -3.4522 1.0 1.0
exclusion 2.8857 5.653 -1.9198 1.0 1.0
exclusion 4.751 2.0201 -2.4523 1.0 1.0
exclusion 1.409462 5.316948 4.9015665 1.5 1.0
exclusion -6.494 -0.0094 5.5781 1.0 1.0
exclusion -7.134 -4.203 -0.215 1.0 1.0
exclusion -0.090538025 -6.683052 0.4015665 1.5 1.0
exclusion -0.090538025 -5.183052 4.9015665 1.5 1.0
exclusion -3.090538 -5.183052 -4.0984335 1.5 1.0
exclusion 4.409462 2.316948 4.9015665 1.5 1.0
exclusion -7.590538 2.316948 4.9015665 1.5 1.0
exclusion -9.090538 2.316948 0.4015665 1.5 1.0
exclusion 5.909462 -0.68305206 1.9015665 1.5 1.0
exclusion -0.090538025 2.316948 7.9015665 1.5 1.0
exclusion 1.409462 -5.183052 -4.0984335 1.5 1.0
exclusion -7.590538 -2.183052 -4.0984335 1.5 1.0
exclusion -1.590538 -2.183052 -7.0984335 1.5 1.0
exclusion 1.409462 0.81694794 -7.0984335 1.5 1.0
exclusion 5.909462 3.816948 0.4015665 1.5 1.0
exclusion -4.590538 5.316948 6.4015665 1.5 1.0
exclusion -0.090538025 -2.183052 7.9015665 1.5 1.0
exclusion -1.590538 3.816948 -7.0984335 1.5 1.0
exclusion -7.590538 5.316948 -2.5984335 1.5 1.0
exclusion -1.590538 8.316948 3.4015665 1.5 1.0
exclusion 4.409462 -2.183052 6.4015665 1.5 1.0
exclusion 4.409462 -2.183052 -5.5984335 1.5 1.0
exclusion 2.909462 8.316948 1.9015665 1.5 1.0
exclusion -4.590538 -8.183052 0.4015665 1.5 1.0
exclusion -4.590538 8.316948 -4.0984335 1.5 1.0
exclusion -0.090538025 9.816948 -1.0984335 1.5 1.0
exclusion -4.590538 0.81694794 9.4015665 1.5 1.0
exclusion -10.590538 -2.183052 -1.0984335 1.5 1.0
exclusion -10.590538 -0.68305206 3.4015665 1.5 1.0
exclusion 7.409462 -0.68305206 -2.5984335 1.5 1.0
exclusion -4.590538 9.816948 0.4015665 1.5 1.0
exclusion -3.090538 -5.183052 7.9015665 1.5 1.0
exclusion 5.909462 2.316948 -5.5984335 1.5 1.0
exclusion -0.090538025 8.316948 -5.5984335 1.5 1.0
exclusion -7.590538 -6.683052 -2.5984335 1.5 1.0
exclusion -3.090538 -8.183052 4.9015665 1.5 1.0
exclusion 4.409462 8.316948 -2.5984335 1.5 1.0
exclusion -7.590538 -8.183052 3.4015665 1.5 1.0
exclusion -7.590538 -5.183052 7.9015665 1.5 1.0
exclusion -10.590538 -6.683052 0.4015665 1.5 1.0
exclusion -10.590538 -5.183052 4.9015665 1.5 1.0

AR_agonist_pKi_1.xyz

type x y z tolerance weight additional_flag
H -1.7001194 0.27979022 -0.51461804 1.5 1.0
H 1.0111487 -0.6803593 -3.6627116 1.5 1.0
H 2.1654782 1.5565534 -0.24641228 1.35 1.0
H -1.877025 0.056724504 4.4903493 1.5 1.0 optional
AR -1.2215242 0.060515195 -1.8829569 0.8999999 1.0
HBA 1.3659799 -5.551115E-17 1.110223E-16 1.5 1.0 optional
HBA -0.7545196 -1.0558171 1.9792697 1.5 1.0
HBA -2.517291 0.6468353 -5.0968246 1.5 1.0
HBA -2.517291 0.6468353 -5.0968246 1.5 1.0
HBA -4.2668376 0.2590977 -3.9114542 1.5 1.0 optional
HBD -4.3518734 0.27820322 -3.8643675 1.5 0.8 optional
exclusion -3.93295 -2.48975 -0.36124998 0.70000005 1.0
exclusion -3.5485935 1.7570832 1.4885219 1.0 1.0
exclusion -0.117598325 2.6081965 2.4300706 0.5500001 1.0
exclusion -5.0400305 3.5107024 -0.20309341 1.0 1.0
exclusion -3.6702645 -2.0525813 2.893721 1.0 1.0
exclusion -0.8518734 5.4441833 -0.096824646 1.5 1.0
exclusion -3.0468028 -2.9509373 -5.4920006 1.0 1.0
exclusion -6.6333 -0.4417 -2.5402 1.0 1.0
exclusion -1.1009195 2.6516218 4.0896034 0.5500001 1.0
exclusion 4.3660417 2.4529862 -2.2251582 1.0 1.0
exclusion 1.3061 2.9907 3.4449 1.0 1.0

exclusion 2.1481266 3.9441833 -4.5968246 1.5 1.0
exclusion -4.4413 2.2664 3.2445 1.0 1.0
exclusion -0.35395026 -0.16883606 -7.2620335 1.0 1.0
exclusion 2.6739 -1.3559 -6.0772 1.0 1.0
exclusion -3.8518734 5.4441833 -3.0968246 1.5 1.0
exclusion 3.8511586 2.0754263 2.1752548 0.70000005 1.0
exclusion -7.2236166 1.6773332 -2.5415668 1.0 1.0
exclusion 5.1481266 -2.0558167 -1.5968246 1.5 1.0
exclusion -0.8518734 -6.5558167 -1.5968246 1.5 1.0
exclusion -2.5424 2.5023 -7.8933 1.0 1.0
exclusion -6.578859 1.615443 -5.644575 1.0 1.0
exclusion -5.3518734 5.4441833 1.4031754 1.5 1.0
exclusion -3.8518734 -6.5558167 1.4031754 1.5 1.0
exclusion -0.8518734 5.4441833 4.4031754 1.5 1.0
exclusion 1.705 -3.7667 4.9132 1.0 1.0
exclusion -6.8518734 -5.0558167 -1.5968246 1.5 1.0
exclusion 6.879114 0.5669891 -1.1772339 1.0 1.0
exclusion -3.8518734 -6.5558167 -4.5968246 1.5 1.0
exclusion -6.8518734 -3.5558167 2.9031754 1.5 1.0
exclusion 0.6481266 -6.5558167 2.9031754 1.5 1.0
exclusion -8.351873 2.4441833 1.4031754 1.5 1.0
exclusion 5.1481266 5.4441833 -1.5968246 1.5 1.0
exclusion 3.6481266 5.4441833 2.9031754 1.5 1.0
exclusion -0.8518734 6.9441833 -6.0968246 1.5 1.0
exclusion -5.3518734 -0.55581665 5.9031754 1.5 1.0
exclusion 3.6481266 -6.5558167 -3.0968246 1.5 1.0
exclusion 0.6481266 -6.5558167 -6.0968246 1.5 1.0
exclusion 6.6481266 2.4441833 1.4031754 1.5 1.0
exclusion 5.1481266 -5.0558167 1.4031754 1.5 1.0
exclusion 3.6481266 -3.5558167 -7.5968246 1.5 1.0
exclusion -9.851873 -0.55581665 -1.5968246 1.5 1.0
exclusion 5.1481266 0.94418335 -7.5968246 1.5 1.0
exclusion -0.8518734 -2.0558167 7.4031754 1.5 1.0
exclusion 2.1481266 8.444183 -0.096824646 1.5 1.0
exclusion -8.351873 5.4441833 -1.5968246 1.5 1.0
exclusion -2.3518734 2.4441833 7.4031754 1.5 1.0
exclusion -6.8518734 5.4441833 -6.0968246 1.5 1.0
exclusion -3.8518734 -5.0558167 5.9031754 1.5 1.0
exclusion 2.1481266 3.9441833 -9.096825 1.5 1.0
exclusion 2.7676 0.6804 7.2234 1.0 1.0
exclusion 8.148127 0.94418335 -3.0968246 1.5 1.0
exclusion 5.657113 -0.29750106 5.3446264 1.0 1.0
exclusion -2.3518734 0.94418335 -10.596825 1.5 1.0
exclusion -2.3518734 2.4441833 -9.096825 1.5 1.0
exclusion 6.9096 -2.6437 3.436 1.0 1.0
exclusion -9.851873 2.4441833 -4.5968246 1.5 1.0
exclusion 5.1481266 2.4441833 5.9031754 1.5 1.0
exclusion 0.6481266 -2.0558167 -10.596825 1.5 1.0
exclusion -3.8518734 5.4441833 -9.096825 1.5 1.0
exclusion -6.8518734 2.4441833 -9.096825 1.5 1.0
exclusion -6.8518734 -5.0558167 -7.5968246 1.5 1.0
exclusion -9.851873 -3.5558167 -4.5968246 1.5 1.0
exclusion 3.9393 -3.7184 6.8784 1.0 1.0
exclusion -5.3518734 -2.0558167 -10.596825 1.5 1.0
exclusion -9.851873 -0.55581665 -7.5968246 1.5 1.0
exclusion 8.7841 -0.3911 5.0917 1.0 1.0

AR_agonist_pKi_2.xyz
type x y z tolerance weight additional_flag
H -1.7001194 0.27979022 -0.51461804 1.5 1.0
H 1.0111487 -0.6803593 -3.6627116 1.5 1.0
H 2.1654782 1.5565534 -0.24641228 1.35 1.0 optional
H -1.877025 0.056724504 4.4903493 1.5 1.0 optional
AR -1.2215242 0.060515195 -1.8829569 0.8999999 1.0 optional
HBA 1.3659799 -5.551115E-17 1.110223E-16 1.5 1.0 optional
HBA -0.7545196 -1.0558171 1.9792697 1.5 1.0
HBA -2.517291 0.6468353 -5.0968246 1.5 1.0
HBA -2.517291 0.6468353 -5.0968246 1.5 1.0
HBA -4.2668376 0.2590977 -3.9114542 1.5 1.0 optional
HBD -4.3518734 0.27820322 -3.8643675 1.5 0.8 optional
HBD 2.7931 -0.6282 5.0386 1.0 1.0

exclusion -3.93295 -2.48975 -0.36124998 0.70000005 1.0
exclusion -3.5485935 1.7570832 1.4885219 1.0 1.0
exclusion -0.117598325 2.6081965 2.4300706 0.5500001 1.0
exclusion -5.0400305 3.5107024 -0.20309341 1.0 1.0
exclusion -3.6702645 -2.0525813 2.893721 1.0 1.0
exclusion -0.8518734 5.4441833 -0.096824646 1.5 1.0
exclusion -3.0468028 -2.9509373 -5.4920006 1.0 1.0
exclusion -6.6333 -0.4417 -2.5402 1.0 1.0
exclusion -1.1009195 2.6516218 4.0896034 0.5500001 1.0
exclusion 4.3660417 2.4529862 -2.2251582 1.0 1.0
exclusion 1.3061 2.9907 3.4449 1.0 1.0
exclusion 2.1481266 3.9441833 -4.5968246 1.5 1.0
exclusion -4.4413 2.2664 3.2445 1.0 1.0
exclusion -0.35395026 -0.16883606 -7.2620335 1.0 1.0
exclusion 2.6739 -1.3559 -6.0772 1.0 1.0
exclusion -3.8518734 5.4441833 -3.0968246 1.5 1.0
exclusion 3.8511586 2.0754263 2.1752548 0.70000005 1.0
exclusion -7.2236166 1.6773332 -2.5415668 1.0 1.0
exclusion 5.1481266 -2.0558167 -1.5968246 1.5 1.0
exclusion -0.8518734 -6.5558167 -1.5968246 1.5 1.0
exclusion -2.5424 2.5023 -7.8933 1.0 1.0
exclusion -6.578859 1.615443 -5.644575 1.0 1.0
exclusion -5.3518734 5.4441833 1.4031754 1.5 1.0
exclusion -3.8518734 -6.5558167 1.4031754 1.5 1.0
exclusion -0.8518734 5.4441833 4.4031754 1.5 1.0
exclusion 1.705 -3.7667 4.9132 1.0 1.0
exclusion -6.8518734 -5.0558167 -1.5968246 1.5 1.0
exclusion 6.879114 0.5669891 -1.1772339 1.0 1.0
exclusion -3.8518734 -6.5558167 -4.5968246 1.5 1.0
exclusion -6.8518734 -3.5558167 2.9031754 1.5 1.0
exclusion 0.6481266 -6.5558167 2.9031754 1.5 1.0
exclusion -8.351873 2.4441833 1.4031754 1.5 1.0
exclusion 5.1481266 5.4441833 -1.5968246 1.5 1.0
exclusion 3.6481266 5.4441833 2.9031754 1.5 1.0
exclusion -0.8518734 6.9441833 -6.0968246 1.5 1.0
exclusion -5.3518734 -0.55581665 5.9031754 1.5 1.0
exclusion 3.6481266 -6.5558167 -3.0968246 1.5 1.0
exclusion 0.6481266 -6.5558167 -6.0968246 1.5 1.0
exclusion 6.6481266 2.4441833 1.4031754 1.5 1.0
exclusion 5.1481266 -5.0558167 1.4031754 1.5 1.0
exclusion 3.6481266 -3.5558167 -7.5968246 1.5 1.0
exclusion -9.851873 -0.55581665 -1.5968246 1.5 1.0
exclusion 5.1481266 0.94418335 -7.5968246 1.5 1.0
exclusion -0.8518734 -2.0558167 7.4031754 1.5 1.0
exclusion 2.1481266 8.444183 -0.096824646 1.5 1.0
exclusion -8.351873 5.4441833 -1.5968246 1.5 1.0
exclusion -2.3518734 2.4441833 7.4031754 1.5 1.0
exclusion -6.8518734 5.4441833 -6.0968246 1.5 1.0
exclusion -3.8518734 -5.0558167 5.9031754 1.5 1.0
exclusion 2.1481266 3.9441833 -9.096825 1.5 1.0
exclusion 2.7676 0.6804 7.2234 1.0 1.0
exclusion 8.148127 0.94418335 -3.0968246 1.5 1.0
exclusion 5.657113 -0.29750106 5.3446264 1.0 1.0
exclusion -2.3518734 0.94418335 -10.596825 1.5 1.0
exclusion -2.3518734 -5.0558167 -9.096825 1.5 1.0
exclusion 6.9096 -2.6437 3.436 1.0 1.0
exclusion -9.851873 2.4441833 -4.5968246 1.5 1.0
exclusion 5.1481266 2.4441833 5.9031754 1.5 1.0
exclusion 0.6481266 -2.0558167 -10.596825 1.5 1.0
exclusion -3.8518734 5.4441833 -9.096825 1.5 1.0
exclusion -6.8518734 2.4441833 -9.096825 1.5 1.0
exclusion -6.8518734 -5.0558167 -7.5968246 1.5 1.0
exclusion -9.851873 -3.5558167 -4.5968246 1.5 1.0
exclusion 3.9393 -3.7184 6.8784 1.0 1.0
exclusion -5.3518734 -2.0558167 -10.596825 1.5 1.0
exclusion -9.851873 -0.55581665 -7.5968246 1.5 1.0
exclusion 8.7841 -0.3911 5.0917 1.0 1.0

AR_agonist_pKi_3.xyz
type x y z tolerance weight additional_flag
H -1.7001194 0.27979022 -0.51461804 1.5 1.0

H 1.0111487 -0.6803593 -3.6627116 1.5 1.0
H 2.1654782 1.5565534 -0.24641228 1.35 1.0 optional
H -1.877025 0.056724504 4.4903493 1.5 1.0 optional
AR -1.2215242 0.060515195 -1.8829569 0.8999999 1.0 optional
HBA 1.3659799 -5.551115E-17 1.110223E-16 1.5 1.0 optional
HBA -0.7545196 -1.0558171 1.9792697 1.5 1.0
HBA -2.517291 0.6468353 -5.0968246 1.5 1.0
HBA -2.517291 0.6468353 -5.0968246 1.5 1.0
HBA -4.2668376 0.2590977 -3.9114542 1.5 1.0 optional
HBD -4.3518734 0.27820322 -3.8643675 1.5 0.8 optional
HBD 4.5331 -1.1992 2.9795 1.0 1.0
exclusion -3.93295 -2.48975 -0.36124998 0.70000005 1.0
exclusion -3.5485935 1.7570832 1.4885219 1.0 1.0
exclusion -0.117598325 2.6081965 2.4300706 0.5500001 1.0
exclusion -5.0400305 3.5107024 -0.20309341 1.0 1.0
exclusion -3.6702645 -2.0525813 2.893721 1.0 1.0
exclusion -0.8518734 5.4441833 -0.096824646 1.5 1.0
exclusion -3.0468028 -2.9509373 -5.4920006 1.0 1.0
exclusion -6.6333 -0.4417 -2.5402 1.0 1.0
exclusion -1.1009195 2.6516218 4.0896034 0.5500001 1.0
exclusion 4.3660417 2.4529862 -2.2251582 1.0 1.0
exclusion 1.3061 2.9907 3.4449 1.0 1.0
exclusion 2.1481266 3.9441833 -4.5968246 1.5 1.0
exclusion -4.4413 2.2664 3.2445 1.0 1.0
exclusion -0.35395026 -0.16883606 -7.2620335 1.0 1.0
exclusion 2.6739 -1.3559 -6.0772 1.0 1.0
exclusion -3.8518734 5.4441833 -3.0968246 1.5 1.0
exclusion 3.8511586 2.0754263 2.1752548 0.70000005 1.0
exclusion -7.2236166 1.6773332 -2.5415668 1.0 1.0
exclusion 5.1481266 -2.0558167 -1.5968246 1.5 1.0
exclusion -0.8518734 -6.5558167 -1.5968246 1.5 1.0
exclusion -2.5424 2.5023 -7.8933 1.0 1.0
exclusion -6.578859 1.615443 -5.644575 1.0 1.0
exclusion -5.3518734 5.4441833 1.4031754 1.5 1.0
exclusion -3.8518734 -6.5558167 1.4031754 1.5 1.0
exclusion -0.8518734 5.4441833 4.4031754 1.5 1.0
exclusion 1.705 -3.7667 4.9132 1.0 1.0
exclusion -6.8518734 -5.0558167 -1.5968246 1.5 1.0
exclusion 6.879114 0.5669891 -1.1772339 1.0 1.0
exclusion -3.8518734 -6.5558167 -4.5968246 1.5 1.0
exclusion -6.8518734 -3.5558167 2.9031754 1.5 1.0
exclusion 0.6481266 -6.5558167 2.9031754 1.5 1.0
exclusion -8.351873 2.4441833 1.4031754 1.5 1.0
exclusion 5.1481266 5.4441833 -1.5968246 1.5 1.0
exclusion 3.6481266 5.4441833 2.9031754 1.5 1.0
exclusion -0.8518734 6.9441833 -6.0968246 1.5 1.0
exclusion -5.3518734 -0.55581665 5.9031754 1.5 1.0
exclusion 3.6481266 -6.5558167 -3.0968246 1.5 1.0
exclusion 0.6481266 -6.5558167 -6.0968246 1.5 1.0
exclusion 6.6481266 2.4441833 1.4031754 1.5 1.0
exclusion 5.1481266 -5.0558167 1.4031754 1.5 1.0
exclusion 3.6481266 -3.5558167 -7.5968246 1.5 1.0
exclusion -9.851873 -0.55581665 -1.5968246 1.5 1.0
exclusion 5.1481266 0.94418335 -7.5968246 1.5 1.0
exclusion -0.8518734 -2.0558167 7.4031754 1.5 1.0
exclusion 2.1481266 8.444183 -0.096824646 1.5 1.0
exclusion -8.351873 5.4441833 -1.5968246 1.5 1.0
exclusion -2.3518734 2.4441833 7.4031754 1.5 1.0
exclusion -6.8518734 5.4441833 -6.0968246 1.5 1.0
exclusion -3.8518734 -5.0558167 5.9031754 1.5 1.0
exclusion 2.1481266 3.9441833 -9.096825 1.5 1.0
exclusion 2.7676 0.6804 7.2234 1.0 1.0
exclusion 8.148127 0.94418335 -3.0968246 1.5 1.0
exclusion 5.657113 -0.29750106 5.3446264 1.0 1.0
exclusion -2.3518734 0.94418335 -10.596825 1.5 1.0
exclusion -2.3518734 -5.0558167 -9.096825 1.5 1.0
exclusion 6.9096 -2.6437 3.436 1.0 1.0
exclusion -9.851873 2.4441833 -4.5968246 1.5 1.0
exclusion 5.1481266 2.4441833 5.9031754 1.5 1.0
exclusion 0.6481266 -2.0558167 -10.596825 1.5 1.0
exclusion -3.8518734 5.4441833 -9.096825 1.5 1.0

exclusion -6.8518734 2.4441833 -9.096825 1.5 1.0
exclusion -6.8518734 -5.0558167 -7.5968246 1.5 1.0
exclusion -9.851873 -3.5558167 -4.5968246 1.5 1.0
exclusion 3.9393 -3.7184 6.8784 1.0 1.0
exclusion -5.3518734 -2.0558167 -10.596825 1.5 1.0
exclusion -9.851873 -0.55581665 -7.5968246 1.5 1.0
exclusion 8.7841 -0.3911 5.0917 1.0 1.0

AR_agonist_pKi_4.xyz
type x y z tolerance weight additional_flag
H 3.2584445 -0.5966948 0.18658751 1.5 1.0
H 0.219393 2.086963 -3.724195 1.5 1.0
H 6.2643 2.9099 -1.3666 1.5 1.0
H -1.6543 2.3695 0.878 1.5 1.0 optional
AR 3.3452833 0.36258334 -0.74438334 0.9 1.0
HBA -0.10538763 -0.2157634 -0.6887795 1.15 1.0
HBA 3.0264 2.0808 -4.0087 1.0 1.0
HBA 6.9772263 0.13540444 0.8755529 1.5 1.0
HBA 6.9772263 0.13540444 0.8755529 1.5 1.0
HBD 5.1685 -0.6734 1.0433 1.0 1.0 optional
exclusion 0.6752064 -1.70805 -2.244657 0.3 1.0
exclusion 0.8221855 -2.3757172 1.8267413 0.5500001 1.0
exclusion 3.4293 -2.4079 2.9143 0.70000005 1.0
exclusion 1.1876 4.2405 1.1905 1.0 1.0
exclusion 1.5131068 -0.12550813 3.8889604 1.0 1.0
exclusion 1.279 -2.1889 -4.7712 1.0 1.0
exclusion 5.956312 -3.096695 -2.221096 1.5 1.0
exclusion 0.4609 -4.4358 -0.9249 1.0 1.0
exclusion -2.2735 -2.6673 -1.9683 0.85 1.0
exclusion 6.8406496 0.8041644 -4.534912 1.0 1.0
exclusion 2.9563122 5.903305 -0.72109604 1.5 1.0
exclusion 0.546826 -1.4462416 -6.034606 0.70000005 1.0
exclusion 7.4595 -2.6503 0.8169 0.70000005 1.0
exclusion 7.5084 -0.6356 -3.8889 0.70000005 1.0
exclusion 7.4179 -2.0806 2.1303 0.70000005 1.0
exclusion 2.9563122 4.403305 3.778904 1.5 1.0
exclusion 2.9563122 -6.096695 0.77890396 1.5 1.0
exclusion 6.5004 -3.8586 2.3992 1.0 1.0
exclusion -0.42999417 -5.4383593 -2.572224 1.0 1.0
exclusion -3.8693948 -1.5261428 0.6058817 0.70000005 1.0
exclusion 9.2478 -0.812 -0.8059 1.0 1.0
exclusion -0.5141 -3.4554 -5.6902 0.5500001 1.0
exclusion 7.4945655 -0.99537516 3.8891528 1.0 1.0
exclusion 2.9563122 -6.096695 -3.721096 1.5 1.0
exclusion -1.5436878 -4.596695 2.278904 1.5 1.0
exclusion 4.456312 -3.096695 -6.721096 1.5 1.0
exclusion -2.2919235 1.2855067 -5.817031 0.5500001 1.0
exclusion -1.5436878 -0.09669495 5.278904 1.5 1.0
exclusion 5.956312 5.903305 -3.721096 1.5 1.0
exclusion -3.7634 4.1692 -0.8317 1.0 1.0
exclusion -4.350715 -0.082826495 2.2720928 0.70000005 1.0
exclusion 2.9563122 -0.09669495 6.778904 1.5 1.0
exclusion 9.2695 2.72 1.6221 1.0 1.0
exclusion 9.9252 1.9595 -0.1488 1.0 1.0
exclusion 1.4563122 -4.596695 5.278904 1.5 1.0
exclusion 4.456312 1.403305 -8.221096 1.5 1.0
exclusion -0.04368782 -1.596695 -8.221096 1.5 1.0
exclusion -5.5488 -1.0231 -0.8747 1.0 1.0
exclusion -4.3876 -2.6105 -4.2275 0.5500001 1.0
exclusion -0.04368782 7.403305 -3.721096 1.5 1.0
exclusion -0.04368782 7.403305 2.278904 1.5 1.0
exclusion 2.9563122 5.903305 -6.721096 1.5 1.0
exclusion -3.0436878 4.403305 -5.221096 1.5 1.0
exclusion -0.04368782 2.903305 -8.221096 1.5 1.0
exclusion -1.5436878 4.403305 5.278904 1.5 1.0
exclusion 5.956312 -6.096695 3.778904 1.5 1.0
exclusion 8.956312 -3.096695 -5.221096 1.5 1.0
exclusion -4.543688 -4.596695 -0.72109604 1.5 1.0
exclusion -4.543688 4.403305 2.278904 1.5 1.0
exclusion 8.956312 1.403305 -6.721096 1.5 1.0
exclusion 7.456312 4.403305 5.278904 1.5 1.0

exclusion 7.456312 7.403305 0.77890396 1.5 1.0
exclusion 8.956312 -6.096695 -0.72109604 1.5 1.0
exclusion -6.043688 -0.09669495 -3.721096 1.5 1.0
exclusion -3.0436878 7.403305 -0.72109604 1.5 1.0
exclusion 10.456312 4.403305 -3.721096 1.5 1.0
exclusion -6.043688 4.403305 -2.221096 1.5 1.0
exclusion -6.043688 -0.09669495 3.778904 1.5 1.0
exclusion 11.956312 -3.096695 -2.221096 1.5 1.0
exclusion 11.956312 -3.096695 2.278904 1.5 1.0
exclusion 10.456312 1.403305 6.778904 1.5 1.0
AR_agonist_pKi_5.xyz
type x y z tolerance weight additional_flag
H -1.34128 0.27870655 0.17449707 1.65 0.79999995
H -0.92364997 -1.12815 3.2632499 1.475 0.79999995
H -4.5511 -1.7566 1.1545 1.5 1.0
HBA -0.019875329 3.286779 2.2467232 1.5 0.9
HBA -1.3355 -1.0864 3.7493 1.15 0.79999995 optional
HBA 2.2645416 0.55866444 6.335511 1.5 1.0 optional
HBA -3.4634752 -0.85143393 -3.0877333 1.5 1.0
HBD 2.7018173 0.16188556 6.386695 1.0250001 0.8
exclusion -1.4634752 5.6485662 -2.5877333 1.5 1.0
exclusion -5.963475 4.1485662 4.9122667 1.5 1.0
exclusion -7.463475 -0.35143375 3.4122667 1.5 1.0
exclusion -7.463475 2.6485662 0.41226673 1.5 1.0
exclusion -4.463475 -0.35143375 7.9122667 1.5 1.0
exclusion -4.463475 7.1485662 1.9122667 1.5 1.0
exclusion -2.9634752 4.1485662 7.9122667 1.5 1.0
exclusion 6.036525 -1.8514338 1.9122667 1.5 1.0
exclusion 3.0365248 -4.8514338 -1.0877333 1.5 1.0
exclusion 3.0365248 5.6485662 -2.5877333 1.5 1.0
exclusion 6.036525 2.6485662 -1.0877333 1.5 1.0
exclusion 6.036525 4.1485662 3.4122667 1.5 1.0
exclusion -2.9634752 2.6485662 -5.5877333 1.5 1.0
exclusion 0.036524773 8.648566 0.41226673 1.5 1.0
exclusion -5.963475 5.6485662 -2.5877333 1.5 1.0
exclusion -1.4634752 8.648566 4.9122667 1.5 1.0
exclusion -1.4634752 -3.3514338 9.412267 1.5 1.0
exclusion 3.0365248 8.648566 3.4122667 1.5 1.0
exclusion 1.5365248 7.1485662 7.9122667 1.5 1.0
exclusion -1.4634752 1.1485662 10.912267 1.5 1.0
exclusion 3.1463 -1.3839 9.7072 1.15 1.0
exclusion -8.963475 -3.3514338 0.41226673 1.5 1.0
exclusion 3.0365248 -4.8514338 7.9122667 1.5 1.0
exclusion -8.963475 -0.35143375 -2.5877333 1.5 1.0
exclusion 6.036525 -4.8514338 4.9122667 1.5 1.0
exclusion 6.036525 -1.8514338 7.9122667 1.5 1.0
exclusion 6.036525 4.1485662 7.9122667 1.5 1.0
exclusion 1.5365248 4.1485662 10.912267 1.5 1.0
exclusion 1.5365248 -3.3514338 -7.0877333 1.5 1.0
exclusion -1.4634752 -6.3514338 -5.5877333 1.5 1.0
exclusion 0.036524773 1.1485662 -8.587733 1.5 1.0
exclusion 9.036525 -0.35143375 4.9122667 1.5 1.0
exclusion 4.536525 1.1485662 10.912267 1.5 1.0
exclusion -2.9634752 -1.8514338 -8.587733 1.5 1.0
exclusion -8.963475 2.6485662 -5.5877333 1.5 1.0
exclusion 1.5365248 -1.8514338 12.412267 1.5 1.0
exclusion -8.963475 -4.8514338 -4.0877333 1.5 1.0
exclusion -5.963475 1.1485662 -8.587733 1.5 1.0
exclusion -5.963475 -4.8514338 -7.0877333 1.5 1.0
exclusion -8.963475 -1.8514338 -7.0877333 1.5 1.0
AR_agonist_pKi_6.xyz
type x y z tolerance weight additional_flag
H 3.2584445 -0.5966948 0.18658751 1.5 1.0
H 5.538154 1.4239805 -1.9566746 1.5 0.8888889
H 1.0291 2.1836 -3.4243 1.5 1.0
H -1.6543 2.3695 0.878 1.5 1.0 optional
AR 3.2405105 -0.18585388 -0.3379436 0.8999999 1.0 optional
AR 3.6529207 1.414057 -2.1158662 0.8999999 0.5555556
optional
HBA -1.29125 0.081 -0.8679 1.3 1.0
HBA 6.9772263 0.13540444 0.8755529 1.5 1.0

HBA 6.9772263 0.13540444 0.8755529 1.5 1.0
HBD 5.1685 -0.6734 1.0433 1.0 1.0 optional
exclusion 0.6752064 -1.70805 -2.244657 0.3 1.0
exclusion 0.8221855 -2.3757172 1.8267413 0.5500001 1.0
exclusion 3.4293 -2.4079 2.9143 0.70000005 1.0
exclusion 1.1876 4.2405 1.1905 1.0 1.0
exclusion 1.5131068 -0.12550813 3.8889604 1.0 1.0
exclusion 1.279 -2.1889 -4.7712 1.0 1.0
exclusion 5.956312 -3.096695 -2.221096 1.5 1.0
exclusion 0.4609 -4.4358 -0.9249 1.0 1.0
exclusion -2.2735 -2.6673 -1.9683 1.0 1.0
exclusion 6.8406496 0.8041644 -4.534912 1.0 1.0
exclusion 2.9563122 5.903305 -0.72109604 1.5 1.0
exclusion 0.546826 -1.4462416 -6.034606 0.70000005 1.0
exclusion 7.4595 -2.6503 0.8169 0.70000005 1.0
exclusion 7.5084 -0.6356 -3.8889 0.70000005 1.0
exclusion 7.4179 -2.0806 2.1303 0.70000005 1.0
exclusion 2.9563122 4.403305 3.778904 1.5 1.0
exclusion 2.9563122 -6.096695 0.77890396 1.5 1.0
exclusion 6.5004 -3.8586 2.3992 1.0 1.0
exclusion -0.42999417 -5.4383593 -2.572224 1.0 1.0
exclusion -3.8693948 -1.5261428 0.6058817 0.70000005 1.0
exclusion 9.2478 -0.812 -0.8059 1.0 1.0
exclusion -0.5141 -3.4554 -5.6902 0.5500001 1.0
exclusion 7.4945655 -0.99537516 3.8891528 1.0 1.0
exclusion 2.9563122 -6.096695 -3.721096 1.5 1.0
exclusion -1.5436878 -4.596695 2.278904 1.5 1.0
exclusion 4.456312 -3.096695 -6.721096 1.5 1.0
exclusion -2.2919235 1.2855067 -5.817031 0.5500001 1.0
exclusion -1.5436878 -0.09669495 5.278904 1.5 1.0
exclusion 5.956312 5.903305 -3.721096 1.5 1.0
exclusion -3.7634 4.1692 -0.8317 1.0 1.0
exclusion -4.350715 -0.082826495 2.2720928 0.70000005 1.0
exclusion 2.9563122 -0.09669495 6.778904 1.5 1.0
exclusion 9.2695 2.72 1.6221 1.0 1.0
exclusion 9.9252 1.9595 -0.1488 1.0 1.0
exclusion 1.4563122 -4.596695 5.278904 1.5 1.0
exclusion 4.456312 1.403305 -8.221096 1.5 1.0
exclusion -0.04368782 -1.596695 -8.221096 1.5 1.0
exclusion -5.5488 -1.0231 -0.8747 1.0 1.0
exclusion -4.3876 -2.6105 -4.2275 0.5500001 1.0
exclusion -0.04368782 7.403305 -3.721096 1.5 1.0
exclusion -0.04368782 7.403305 2.278904 1.5 1.0
exclusion -3.0436878 4.403305 -5.221096 1.5 1.0
exclusion 2.9563122 5.903305 -6.721096 1.5 1.0
exclusion -0.04368782 2.903305 -8.221096 1.5 1.0
exclusion 5.956312 -6.096695 3.778904 1.5 1.0
exclusion -1.5436878 4.403305 5.278904 1.5 1.0
exclusion 8.956312 -3.096695 -5.221096 1.5 1.0
exclusion -4.543688 -4.596695 -0.72109604 1.5 1.0
exclusion -4.543688 4.403305 2.278904 1.5 1.0
exclusion 8.956312 1.403305 -6.721096 1.5 1.0
exclusion 7.456312 4.403305 5.278904 1.5 1.0
exclusion 7.456312 7.403305 0.77890396 1.5 1.0
exclusion 8.956312 -6.096695 -0.72109604 1.5 1.0
exclusion -6.043688 -0.09669495 -3.721096 1.5 1.0
exclusion -3.0436878 7.403305 -0.72109604 1.5 1.0
exclusion 10.456312 4.403305 -3.721096 1.5 1.0
exclusion -6.043688 4.403305 -2.221096 1.5 1.0
exclusion -6.043688 -0.09669495 3.778904 1.5 1.0
exclusion 11.956312 -3.096695 -2.221096 1.5 1.0
exclusion 11.956312 -3.096695 2.278904 1.5 1.0
exclusion 10.456312 1.403305 6.778904 1.5 1.0
AR_agonist_pKi_7.xyz
type x y z tolerance weight additional_flag
H 3.2584445 -0.5966948 0.18658751 1.5 1.0
H 0.49229652 2.4328814 -3.0908976 1.5 1.0
H 6.2643 2.9099 -1.3666 1.5 1.0
H -1.6543 2.3695 0.878 1.5 1.0 optional
AR 3.3452833 0.36258334 -0.74438334 0.9 1.0
AR 5.6331334 0.5085833 0.14336668 0.9 1.0

HBA 0.13455619 -0.5106817 -0.40198973 1.075 1.0
HBA 6.9772263 0.13540444 0.8755529 1.5 1.0
HBA 6.9772263 0.13540444 0.8755529 1.5 1.0
HBD 5.1685 -0.6734 1.0433 1.0 1.0 optional
exclusion 0.6752064 -1.70805 -2.244657 0.3 1.0
exclusion 0.8221855 -2.3757172 1.8267413 0.5500001 1.0
exclusion 3.4293 -2.4079 2.9143 0.70000005 1.0
exclusion 1.5131068 -0.12550813 3.8889604 1.0 1.0
exclusion 1.1876 4.2405 1.1905 1.0 1.0
exclusion 5.956312 -3.096695 -2.221096 1.5 1.0
exclusion 2.5624974 4.9280396 -1.4910501 0.75 1.0
exclusion 1.279 -2.1889 -4.7712 1.0 1.0
exclusion 0.4609 -4.4358 -0.9249 1.0 1.0
exclusion 5.4564 2.2894 -5.137 0.70000005 1.0
exclusion 6.8406496 0.8041644 -4.534912 1.0 1.0
exclusion 7.4595 -2.6503 0.8169 0.70000005 1.0
exclusion -2.2735 -2.6673 -1.9683 0.85 1.0
exclusion 7.5084 -0.6356 -3.8889 0.70000005 1.0
exclusion 7.4179 -2.0806 2.1303 0.70000005 1.0
exclusion 0.546826 -1.4462416 -6.034606 0.70000005 1.0
exclusion 2.9563122 4.403305 3.778904 1.5 1.0
exclusion 6.5004 -3.8586 2.3992 1.0 1.0
exclusion 2.9563122 -6.096695 0.77890396 1.5 1.0
exclusion 9.2478 -0.812 -0.8059 1.0 1.0
exclusion -0.42999417 -5.4383593 -2.572224 1.0 1.0
exclusion 7.4945655 -0.99537516 3.8891528 1.0 1.0
exclusion -3.8693948 -1.5261428 0.6058817 0.70000005 1.0
exclusion -0.5141 -3.4554 -5.6902 0.5500001 1.0
exclusion 2.9563122 -6.096695 -3.721096 1.5 1.0
exclusion -1.5436878 -4.596695 2.278904 1.5 1.0
exclusion 4.456312 -3.096695 -6.721096 1.5 1.0
exclusion 5.956312 5.903305 -3.721096 1.5 1.0
exclusion -1.5436878 -0.09669495 5.278904 1.5 1.0
exclusion 9.2695 2.72 1.6221 1.0 1.0
exclusion 2.9563122 -0.09669495 6.778904 1.5 1.0
exclusion 9.9252 1.9595 -0.1488 1.0 1.0
exclusion -3.7634 4.1692 -0.8317 1.0 1.0
exclusion -4.350715 -0.082826495 2.2720928 0.70000005 1.0
exclusion 1.4563122 -4.596695 5.278904 1.5 1.0
exclusion 4.456312 1.403305 -8.221096 1.5 1.0
exclusion -0.04368782 -1.596695 -8.221096 1.5 1.0
exclusion -5.5488 -1.0231 -0.8747 1.0 1.0
exclusion -0.04368782 7.403305 2.278904 1.5 1.0
exclusion -0.04368782 7.403305 -3.721096 1.5 1.0
exclusion 2.9563122 5.903305 -6.721096 1.5 1.0
exclusion 5.956312 -6.096695 3.778904 1.5 1.0
exclusion -4.3876 -2.6105 -4.2275 0.5500001 1.0
exclusion 8.956312 -3.096695 -5.221096 1.5 1.0
exclusion -3.0436878 4.403305 -5.221096 1.5 1.0
exclusion -0.04368782 2.903305 -8.221096 1.5 1.0
exclusion -1.5436878 4.403305 5.278904 1.5 1.0
exclusion -4.543688 -4.596695 -0.72109604 1.5 1.0
exclusion 7.456312 4.403305 5.278904 1.5 1.0
exclusion 8.956312 1.403305 -6.721096 1.5 1.0
exclusion 7.456312 7.403305 0.77890396 1.5 1.0
exclusion 8.956312 -6.096695 -0.72109604 1.5 1.0
exclusion -4.543688 4.403305 2.278904 1.5 1.0
exclusion -6.043688 -0.09669495 -3.721096 1.5 1.0
exclusion -3.0436878 7.403305 -0.72109604 1.5 1.0
exclusion 10.456312 4.403305 -3.721096 1.5 1.0
exclusion -6.043688 -0.09669495 3.778904 1.5 1.0
exclusion -6.043688 4.403305 -2.221096 1.5 1.0
exclusion 11.956312 -3.096695 -2.221096 1.5 1.0
exclusion 11.956312 -3.096695 2.278904 1.5 1.0
exclusion 10.456312 1.403305 6.778904 1.5 1.0

AR_agonist_pKi_8.xyz

type x y z tolerance weight additional_flag

H 0.8132 2.6514 -2.9695 1.65 1.0 optional

H -1.2100599 -0.96596044 -3.6484063 1.2 1.0 optional

H 6.2643 2.9099 -1.3666 1.5 1.0

H -2.6573 0.5737 -1.1608 0.9000001 1.0 optional
AR 3.1588833 0.4086 -0.89596665 0.9 1.0
AR 5.6331334 0.5085833 0.14336668 0.9 1.0
HBA 6.9772263 0.13540444 0.8755529 1.5 1.0
HBA 6.9772263 0.13540444 0.8755529 1.5 1.0
HBD 0.3618781 -0.60609084 -0.26339486 1.0375 1.0
HBD 5.1685 -0.6734 1.0433 1.0 1.0 optional
exclusion 2.7049987 -2.8022203 0.3382277 0.5500001 1.0
exclusion 1.5776782 -2.0284271 1.3728259 0.40000007 1.0
exclusion 0.26070845 -3.1098564 -0.31139922 0.79999995 1.0
exclusion 1.411428 -1.6956403 -4.138379 0.3 1.0
exclusion 0.3116014 -2.7836537 -2.4785357 0.3 1.0
exclusion -0.866022 -2.2690651 -1.4176152 0.3 1.0
exclusion -0.83237815 1.1296759 1.2017852 0.40000007 1.0
exclusion 5.095967 -2.5869017 0.9038878 0.5500001 1.0
exclusion 1.5779581 3.9840655 -0.16736549 0.40000007 1.0
exclusion -1.4812236 -0.38520342 0.81282264 0.3 1.0
exclusion -1.6794137 -1.1599922 -0.034049213 0.3 1.0
exclusion 2.141247 4.300698 -1.762455 0.33750004 1.0
exclusion 3.4293 -2.4079 2.9143 0.40000007 1.0
exclusion -2.068098 -1.2382709 -0.6885412 0.3 1.0
exclusion 1.5131068 -0.12550813 3.8889604 1.0 1.0
exclusion 5.956312 -3.096695 -2.221096 1.5 1.0
exclusion 0.912913 -1.8175708 -5.402903 0.3 1.0
exclusion 5.4564 2.2894 -5.137 0.70000005 1.0
exclusion 6.8406496 0.8041644 -4.534912 1.0 1.0
exclusion -2.1504378 -2.5071254 -3.7297456 0.3 1.0
exclusion 7.4595 -2.6503 0.8169 0.70000005 1.0
exclusion 1.2861247 2.5475392 -6.150199 0.475 1.0
exclusion 7.5084 -0.6356 -3.8889 0.70000005 1.0
exclusion 7.4179 -2.0806 2.1303 0.70000005 1.0
exclusion 0.3703595 2.9288347 -6.056521 0.40000007 1.0
exclusion 2.9563122 -6.096695 0.77890396 1.5 1.0
exclusion -3.9054086 -0.69276834 -0.9777765 0.3 1.0
exclusion -0.42999417 -5.4383593 -2.572224 1.0 1.0
exclusion 2.9563122 4.403305 3.778904 1.5 1.0
exclusion 6.5004 -3.8586 2.3992 0.85 1.0
exclusion -0.5141 -3.4554 -5.6902 0.5500001 1.0
exclusion -3.8693948 -1.5261428 0.6058817 0.40000007 1.0
exclusion 2.9563122 -6.096695 -3.721096 1.5 1.0
exclusion -1.5436878 -4.596695 2.278904 1.5 1.0
exclusion 9.2478 -0.812 -0.8059 1.0 1.0
exclusion 4.456312 -3.096695 -6.721096 1.5 1.0
exclusion 7.4945655 -0.99537516 3.8891528 1.0 1.0
exclusion -1.5436878 -0.09669495 5.278904 1.5 1.0
exclusion -4.350715 -0.082826495 2.2720928 0.70000005 1.0
exclusion 5.956312 5.903305 -3.721096 1.5 1.0
exclusion 2.9563122 -0.09669495 6.778904 1.5 1.0
exclusion 1.4563122 -4.596695 5.278904 1.5 1.0
exclusion 4.456312 1.403305 -8.221096 1.5 1.0
exclusion 9.2695 2.72 1.6221 1.0 1.0
exclusion 9.9252 1.9595 -0.1488 1.0 1.0
exclusion -0.04368782 -1.596695 -8.221096 1.5 1.0
exclusion -4.3876 -2.6105 -4.2275 0.85 1.0
exclusion -5.5488 -1.0231 -0.8747 1.0 1.0
exclusion -3.0436878 4.403305 -5.221096 0.60000014 1.0
exclusion -0.04368782 2.903305 -8.221096 1.5 1.0
exclusion -4.543688 -4.596695 -0.72109604 1.5 1.0
exclusion -0.04368782 7.403305 -3.721096 1.0500001 1.0
exclusion 2.9563122 5.903305 -6.721096 1.5 1.0
exclusion -0.04368782 7.403305 2.278904 1.5 1.0
exclusion 5.956312 -6.096695 3.778904 1.5 1.0
exclusion 8.956312 -3.096695 -5.221096 1.5 1.0
exclusion -1.5436878 4.403305 5.278904 1.5 1.0
exclusion -4.543688 4.403305 2.278904 1.5 1.0
exclusion -6.043688 -0.09669495 -3.721096 1.5 1.0
exclusion 8.956312 1.403305 -6.721096 1.5 1.0
exclusion 8.956312 -6.096695 -0.72109604 1.5 1.0
exclusion 7.456312 4.403305 5.278904 1.5 1.0
exclusion 7.456312 7.403305 0.77890396 1.5 1.0
exclusion -3.0436878 7.403305 -0.72109604 1.5 1.0

exclusion -6.043688 4.403305 -2.221096 1.5 1.0
exclusion -6.043688 -0.09669495 3.778904 1.5 1.0
exclusion 10.456312 4.403305 -3.721096 1.5 1.0
exclusion 11.956312 -3.096695 -2.221096 1.5 1.0
exclusion 11.956312 -3.096695 2.278904 1.5 1.0
exclusion 10.456312 1.403305 6.778904 1.5 1.0

AR_agonist_pKi_9.xyz

type x y z tolerance weight additional_flag

H 0.7821676 0.54710287 -3.9959369 1.5 1.0
H -3.0296412 -0.47392425 -6.5054703 1.5 1.0
H -1.6239414 0.74701 0.26291734 1.5 1.0
AR 0.33102262 0.51067054 -4.1728907 0.8999999 1.0
AR 0.04975804 0.35514832 -6.612386 0.8999999 1.0
AR -1.3876553 0.67787683 -0.21738094 0.8999999 0.9411765
HBA 1.177459 0.5631988 -9.026758 1.5 1.0
HBA 1.4155989 0.5353879 -6.7443023 1.5 1.0
exclusion -4.240395 -1.8740256 -3.7364535 1.0 1.0
exclusion -3.309 -2.0721 -1.2725 1.0 1.0
exclusion -1.0296412 4.3582516 -5.526758 1.5 1.0
exclusion -1.0296412 -6.1417484 -4.026758 1.5 1.0
exclusion 3.4703588 -3.1417484 -7.026758 1.5 1.0
exclusion 4.970359 -1.6417484 -2.5267582 1.5 1.0
exclusion -4.029641 5.8582516 -2.5267582 1.5 1.0
exclusion -2.5296412 -6.1417484 -8.526758 1.5 1.0
exclusion -5.529641 -6.1417484 -4.026758 1.5 1.0
exclusion -8.529641 -1.6417484 -4.026758 1.5 1.0
exclusion -5.529641 2.8582516 -10.026758 1.5 1.0
exclusion 4.970359 4.3582516 -5.526758 1.5 1.0
exclusion 1.9703588 5.8582516 -8.526758 1.5 1.0
exclusion -8.529641 1.3582516 -7.026758 1.5 1.0
exclusion 3.4703588 -6.1417484 -2.5267582 1.5 1.0
exclusion 1.9703588 7.3582516 -4.026758 1.5 1.0
exclusion -5.529641 -4.6417484 0.4732418 1.5 1.0
exclusion 0.47035885 -6.1417484 0.4732418 1.5 1.0
exclusion 6.470359 -0.14174843 -7.026758 1.5 1.0
exclusion -8.529641 2.8582516 -2.5267582 1.5 1.0
exclusion -2.5296412 5.8582516 -10.026758 1.5 1.0
exclusion -7.029641 5.8582516 -5.526758 1.5 1.0
exclusion 4.970359 2.8582516 -10.026758 1.5 1.0
exclusion 1.9703588 -6.1417484 -10.026758 1.5 1.0
exclusion -8.529641 -0.14174843 0.4732418 1.5 1.0
exclusion -1.0296412 7.3582516 0.4732418 1.5 1.0
exclusion -8.529641 -4.6417484 -7.026758 1.5 1.0
exclusion -2.5296412 2.8582516 -13.026758 1.5 1.0
exclusion -5.529641 -1.6417484 3.4732418 1.5 1.0
exclusion -2.5296412 -4.6417484 3.4732418 1.5 1.0
exclusion -8.529641 -1.6417484 -10.026758 1.5 1.0
exclusion -5.529641 -4.6417484 -11.526758 1.5 1.0
exclusion -5.529641 -0.14174843 -13.026758 1.5 1.0
exclusion -7.029641 5.8582516 0.4732418 1.5 1.0
exclusion -1.0296412 -4.6417484 -13.026758 1.5 1.0
exclusion 6.470359 -3.1417484 -10.026758 1.5 1.0
exclusion 6.470359 -0.14174843 1.9732418 1.5 1.0
exclusion 0.47035885 2.8582516 4.973242 1.5 1.0
exclusion 4.970359 -4.6417484 1.9732418 1.5 1.0
exclusion 0.47035885 -0.14174843 -14.526758 1.5 1.0
exclusion 3.4703588 -3.1417484 -13.026758 1.5 1.0
exclusion -7.029641 2.8582516 3.4732418 1.5 1.0
exclusion -4.029641 5.8582516 3.4732418 1.5 1.0
exclusion 0.47035885 5.8582516 -13.026758 1.5 1.0
exclusion 3.4703588 -0.14174843 4.973242 1.5 1.0
exclusion 1.9703588 -4.6417484 4.973242 1.5 1.0
exclusion -1.0296412 -1.6417484 6.473242 1.5 1.0
exclusion -4.029641 1.3582516 6.473242 1.5 1.0
exclusion 3.4703588 2.8582516 -14.526758 1.5 1.0
exclusion 6.470359 -0.14174843 -13.026758 1.5 1.0