Supplementary material

Development of novel analgesics related to TRPV1 antagonism - in silico approach

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Monte Carlo optimization

The molecular descriptors were all computed using the CORAL software (CORrelation and Logic), which can be accessed at http://www.insilico.eu/coral. Once an optimal descriptor is identified through the application of the Monte Carlo method, each descriptor is assigned a numerical value known as the correlation weight (CW). The Monte Carlo method accomplishes this by generating suitable random numbers and observing how this fractional number corresponds to a specific property or properties. The CW value is then randomly assigned to the descriptors based on the SMILES notation for each individual Monte Carlo run and for a specified endpoint.

The optimization process of the Monte Carlo method involves performing numerical calculations to determine the correlation weights that yield the maximum correlation coefficient value between the optimal descriptor and a given endpoint. When utilizing this method for creating a QSAR model, it's essential to consider two key parameters. Threshold is a coefficient used to categorize a range of molecular features, which encompass both SMILES-based indices and SMILES-based molecular fragments. These features are derived from SMILES notation and sorted into two categories: a) active ones (in this case, the modeling process involves the correlation weight); and b) rare ones (in this case, the modeling process omits the correlation weight). The process is executed as follows: If a particular molecular feature (X) extracted from the SMILES notation of molecules in the training set occurs fewer than T times, then the molecule descriptor X is excluded from the model construction. Consequently, the numerical value for this feature (the correlation weight of X, CW(X)) is set to zero, categorizing it as "rare." All other molecular features that occur more frequently are considered "active" and can be employed in the model-building process. N_{epoch}, representing the epoch number in Monte

Carlo optimization, is crucial for achieving the highest statistical quality within the training set. When an unlimited number of epochs is employed, the training set attains the maximum correlation coefficient through the mentioned Monte Carlo optimization. However, it's important to note that the maximum correlation coefficient between the endpoint for the external test set and the optimal descriptor is achieved with a specific, finite number of epochs. The calculations favor this specific epoch number, as it offers excellent predictive potential for the obtained model, provided that the number of epochs reaches this value. However, it's worth noting that an increase in the threshold (T) results in a decrease in the correlation coefficient within the training set. Nonetheless, it is important to highlight that there exists a threshold value that maximizes the correlation coefficient of the test set. From a practical perspective, the mentioned threshold is the preferred choice. Furthermore, defining optimal values for both the threshold (T) and the Monte Carlo optimization epoch number (Nepoch), is essential for constructing a robust QSAR model. This construction involves the utilization of both SMILES notation and optimal descriptors based on the molecular graph, as outlined in reference. Monte Carlo method simulations are carried out using iterative algorithms to uncover the distribution of an unknown probabilistic entity. In the Monte Carlo optimization process, the epoch number is still a part of the equation for a specific target function within the training set. The initial step involves setting the CW (SA) for each SMILES SA attribute, with all CW values commencing at $1 \pm 0.01 \times Rnd$ (where Rnd is a random value generator with a range between 0 and 1). The usual sequential order of attribute numbers is replaced with a random sequence. The subsequent step involves evaluating the initial value of the target function and making further adjustments to the correlation weights. After this, the relevant steps must be reiterated in the Monte Carlo optimization process for all the non-rare attributes, as specified in references.

Table S1. The SMILES notation of the studied molecules, calculated values for the DCW, experimental data (Ac) – Expr, the values of Ac calculated with the application of CORAL software – Calc, the difference between Expr and Calc – Diff for the built QSPR model.

	SMILES notation	Expr	Split 1				Split 2				Split 3			
			DCW	Calc	Diff	Set	DCW	Calc	Diff	Set	DCW	Calc	Diff	Set
1			159.9478	5.905	0.005	Tr	193.0673	6.026	-0.116	Tr	122.6809	6.3569	-0.4469	Ts
2	Fc1c(F)cc(cc1F)C1N=C(NC1c1ccc(cc1)C(F)(F)F)N1CCN(CC1)c1ncccc1C(F)(F)F	8.15	206.2158	7.7455	0.4045	Tr	245.2146	7.5722	0.5778	Ts	154.807	7.4473	0.7027	Tr
3	Fc1cc(F)cc(c1)C1N=C(NC1c1ccc(cc1)C(F)(F)F)N1CCN(CC1)c1ncccc1C(F)(F)F	7.46	197.8163	7.4114	0.0486	Tr	237.611	7.3468	0.1132	Tr	149.5209	7.2679	0.1921	Tr
4	CC1CN(CCN1C1=NC(C(N1)c1ccc(cc1)C(F)(F)F)c1ccccc1)c1ncccc1C(F)(F)F	6.93	188.4242	7.0378	-0.1078	Ts	231.8087	7.1747	-0.2447	Tr	146.442	7.1634	-0.2334	Tr
5	CC1N=C(NC1c1ccc(cc1)C(F)(F)F)N1CCN(CC1)c1ncccc1C(F)(F)F	6.2	171.3771	6.3596	-0.1596	Tr	194.996	6.0832	0.1168	Tr	117.6965	6.1877	0.0123	Tr
6	OCc1cnc(c(c1)Cl)N1CCN(CC1)C1=NC(C(N1)c1ccc(cc1)C(F)(F)F)c1ccccc1	7.05	180.6065	6.7268	0.3232	Tr	234.67	7.2596	-0.2096	Tr	143.8353	7.0749	-0.0249	Tr
7	OCc1cnc(c(c1)Cl)N1CCN(C(C1)C)C1=NC(C(N1)c1ccc(cc1)C(F)(F)F)c1cc(F)c(c(c1)F)F	9	235.8255	8.9234	0.0766	Tr	289.1133	8.8739	0.1261	Tr	183.7053	8.4281	0.5719	Tr
8	ClC1N=C(NC1c1ccc(cc1)C(F)(F)F)N1CCN(CC1)c1ncccc1C(F)(F)F	6.8	170.3861	6.3202	0.4798	Tr	188.7796	5.8989	0.9011	Tr	126.3666	6.482	0.318	Ts
9	COC(=O)C1N=C(NC1c1ccc(cc1)C(F)(F)F)N1CCN(CC1)c1ncccc1C(F)(F)F	5.93	156.534	5.7691	0.1609	Tr	197.0457	6.144	-0.214	Tr	114.0121	6.0627	-0.1327	Tr
10	O=C(C1N=C(NC1c1ccc(cc1)C(F)(F)F)N1CCN(CC1)c1ncccc1C(F)(F)F)N1CCN(CC1)C(C)C	6.15	167.8353	6.2187	-0.0687	Tr	204.6496	6.3694	-0.2194	Tr	117.5254	6.1819	-0.0319	Tr
11	CC(CN1CCCCC1CNC(=O)C1N=C(NC1c1ccc(cc1)C(F)(F)F)N1CCN(CC1)c1ncccc1C(F)(F)F)C	5.72	152.3155	5.6013	0.1187	Tr	182.3677	5.7088	0.0112	Tr	116.2236	6.1377	-0.4177	Ts
12	O=C(C1N=C(NC1c1ccc(cc1)C(F)(F)F)N1CCN(CC1)c1ncccc1C(F)(F)F)NCC1CCCCN1	5.53	161.8959	5.9824	-0.4524	Tr	174.7835	5.4839	0.0461	Tr	112.4514	6.0097	-0.4797	Tr
13	O=N(=O)c1cc(cc2c1nc([nH]2)N1CCN(CC1)c1ncccc1C(F)(F)F)C(F)(F)F	5.78	149.6153	5.4939	0.2861	Tr	200.8737	6.2575	-0.4775	Tr	113.8947	6.0587	-0.2787	Tr
14	Nc1cc(cc2c1nc([nH]2)N1CCN(CC1)c1ncccc1C(F)(F)F)C(F)(F)F	5.47	165.8413	6.1394	-0.6694	Tr	185.7299	5.8085	-0.3385	Tr	100.1663	5.5928	-0.1228	Tr
15	OCc1cnc(c(c1)Cl)N1CCN(C(C1)C)c1nc2c([nH]1)cc(cc2NC(=O)OC(C)(C)C)C(F)(F)F	8.68	216.0934	8.1385	0.5415	Ts	271.7437	8.3589	0.3211	Ts	180.6766	8.3253	0.3547	Tr
16	OCc1cnc(c(c1)Cl)N1CCN(C(C1)C)c1nc2c([nH]1)cc(cc2N(Cc1ccccc1)Cc1ccccc1)C(F)(F)F	8.72	226.4902	8.5521	0.1679	Tr	290.0499	8.9017	-0.1817	Tr	197.2834	8.8889	-0.1689	Ts
17	O=C(N1CCN(CC1)c1ncccc1Cl)Nc1ccc(cc1)C(C)(C)C	9.4	203.1393	7.6232	1.7768	Tr	235.239	7.2765	2.1235	Tr	171.0636	7.999	1.401	Tr
18	FC(c1ccc2c(c1)nc(n2Cc1ccccc1)N1CCN(CC1)c1ncccc1C(F)(F)F)(F)F	5.19	163.1271	6.0314	-0.8414	Ts	197.767	6.1654	-0.9754	Tr	137.8902	6.8731	-1.6831	Tr
19	Brc1cc2nc([nH]c2cc1C(F)(F)F)N1CCN(CC1)c1ncccc1C(F)(F)F	6.78	175.5917	6.5273	0.2527	Tr	196.2194	6.1195	0.6605	Tr	119.7027	6.2558	0.5242	Tr
20	Brc1cc(cc2c1nc([nH]2)N1CCN(CC1)c1ncccc1C(F)(F)F)C(F)(F)F	6.88	170.1255	6.3098	0.5702	Tr	205.2406	6.387	0.493	Tr	110.0926	5.9297	0.9503	Tr
21	Brc1cnc(c(c1)Cl)N1CCN(C(C1)C)c1nc2c([nH]1)cc(cc2c1cc(F)c(c(c1)F)F)C(F)(F)F	8.47	218.5829	8.2375	0.2325	Tr	266.6598	8.2081	0.2619	Tr	180.1892	8.3088	0.1612	Ts
22	CN(c1ccc(cc1)c1cc(cc2c1nc([nH]2)N1CCN(CC1)c1ncccc1C(F)(F)F)C(F)(F)F)C	6.97	167.2008	6.1935	0.7765	Tr	221.9474	6.8823	0.0877	Tr	148.6066	7.2368	-0.2668	Ts
23	FC(c1cc(C=Cc2ccccc2)c2c(c1)[nH]c(n2)N1CCN(CC1)c1ncccc1C(F)(F)F)(F)F	6.73	178.4781	6.6421	0.0879	Ts	204.7599	6.3727	0.3573	Ts	143.9614	7.0792	-0.3492	Tr
24	C=Cc1cnc(c(c1)Cl)N1CCN(C(C1)C)c1[nH]c2c(n1)c(cc(c2)C(F)(F)F)c1cc(F)c(c(c1)F)F	8.89	238.0248	9.0109	-0.1209	Tr	281.5958	8.651	0.239	Tr	189.0847	8.6107	0.2793	Tr
25	FC(c1cc2[nH]c(nc2cc1c1ccc(cc1)C(F)(F)F)N1CCN(CC1)c1ncccc1C(F)(F)F)(F)F	5.08	159.1955	5.875	-0.795	Ts	204.6736	6.3702	-1.2902	Tr	132.1199	6.6773	-1.5973	Tr
26	CC(c1cnc(c(c1)Cl)N1CCN(C(C1)C)c1[nH]c2c(n1)c(cc(c2)C(F)(F)F)c1cc(F)c(c(c1)F)F)O	9.22	227.6433	8.598	0.622	Tr	274.6644	8.4455	0.7745	Ts	194.5069	8.7947	0.4253	Ts
27	CC(c1cnc(c(c1)Cl)N1CCN(C(C1)C)c1[nH]c2c(n1)c(cc(c2)C(F)(F)F)c1cc(F)c(c(c1)F)F)O	8.59	227.6433	8.598	-0.008	Ts	274.6644	8.4455	0.1445	Tr	194.5069	8.7947	-0.2047	Tr
28	Fc1c(F)cc(cc1F)c1cc(cc2c1nc([nH]2)N1CCN(CC1)c1ncccc1C(F)(F)F)C(F)(F)F	7.48	198.4288	7.4358	0.0442	Tr	245.5604	7.5825	-0.1025	Tr	155.8492	7.4826	-0.0026	Tr
29	FC(c1cc2[nH]c(nc2c(c1)c1nccs1)N1CCN(CC1)c1ncccc1C(F)(F)F)(F)F	6.16	175.0246	6.5047	-0.3447	Tr	202.8488	6.316	-0.156	Ts	123.4946	6.3845	-0.2245	Tr

30	Fc1ccc(cc1F)Cc1cc(cc2c1nc([nH]2)N1CCN(CC1)c1ncccc1C(F)(F)F)C(F)(F)F	7.15	183.9545	6.86	0.29	Ts	221.5132	6.8695	0.2805	Tr	146.7246	7.173	-0.023	Tr
31	FC(c1cc2[nH]c(nc2c(c1)c1ccc(cc1)C(F)(F)F)N1CCN(CC1)c1ncccc1C(F)(F)F)(F)F	7.29	192.8662	7.2145	0.0755	Tr	234.6997	7.2605	0.0295	Tr	139.8972	6.9412	0.3488	Ts
32	FC(Oc1cccc(c1)c1cc(cc2c1nc([nH]2)N1CCN(CC1)c1ncccc1C(F)(F)F)C(F)(F)F)(F)F	7.59	194.7435	7.2892	0.3008	Tr	241.3217	7.4568	0.1332	Tr	146.8518	7.1773	0.4127	Tr
33	FC(c1cc(c2ccc(cc2)C(C)(C)C)c2c(c1)[nH]c(n2)N1CCN(CC1)c1ncccc1C(F)(F)F)(F)F	7.89	229.5505	8.6738	-0.7838	Tr	273.8878	8.4224	-0.5324	Tr	164.9201	7.7905	0.0995	Tr
34	FC(c1cc2[nH]c(nc2c(c1)c1cccs1)N1CCN(CC1)c1ncccc1C(F)(F)F)(F)F	6.43	172.9859	6.4236	0.0064	Tr	203.1243	6.3242	0.1058	Tr	121.4334	6.3146	0.1154	Tr
35	FC(c1cc2[nH]c(nc2c(c1)c1nccnc1)N1CCN(CC1)c1ncccc1C(F)(F)F)(F)F	6.89	180.6507	6.7285	0.1615	Tr	216.4241	6.7186	0.1714	Ts	121.621	6.3209	0.5691	Tr
36	COc1ccc(cn1)c1cc(cc2c1nc([nH]2)N1CCN(CC1)c1ncccc1C(F)(F)F)C(F)(F)F	6.95	172.3289	6.3975	0.5525	Tr	230.1028	7.1242	-0.1742	Tr	135.495	6.7918	0.1582	Tr
37	FC(c1cc2[nH]c(nc2c(c1)c1cc2c(s1)cccc2)N1CCN(CC1)c1ncccc1C(F)(F)F)(F)F	7.59	183.1725	6.8289	0.7611	Ts	233.707	7.231	0.359	Tr	142.395	7.026	0.564	Ts
38	Nc1ccc(cc1)c1cc(cc2c1nc([nH]2)N1CCN(CC1)c1ncccc1C(F)(F)F)C(F)(F)F	5.72	168.4988	6.2451	-0.5251	Tr	199.0899	6.2046	-0.4846	Tr	128.2628	6.5464	-0.8264	Tr
39	Clc1ccc2c(c1)[nH]c(n2)N1CCN(CC1)c1ncccc1C(F)(F)F	5.95	159.7835	5.8984	0.0516	Tr	179.6381	5.6278	0.3222	Tr	105.7283	5.7815	0.1685	Tr
40	N#Cc1ccc2c(c1)[nH]c(n2)N1CCN(CC1)c1ncccc1C(F)(F)F	5.48	164.1353	6.0715	-0.5915	Tr	189.1418	5.9096	-0.4296	Ts	102.2801	5.6645	-0.1845	Tr
41	COC(=O)c1ccc2c(c1)[nH]c(n2)N1CCN(CC1)c1ncccc1C(F)(F)F	5.91	157.8609	5.8219	0.0881	Ts	192.3893	6.0059	-0.0959	Tr	101.4245	5.6355	0.2745	Tr
42	FC(c1cc(cc2c1nc([nH]2)N1CCN(CC1)c1ncccc1C(F)(F)F)C(F)(F)F)(F)F	6.49	174.6783	6.4909	-0.0009	Tr	215.4241	6.6889	-0.1989	Tr	120.667	6.2886	0.2014	Ts
43	FC(c1cnc2c(c1)[nH]c(n2)N1CCN(CC1)c1ncccc1C(F)(F)F)(F)F	5.81	171.983	6.3837	-0.5737	Tr	194.9838	6.0828	-0.2728	Ts	114.9414	6.0942	-0.2842	Tr
44	FC(c1ccc2c(n1)[nH]c(n2)N1CCN(CC1)c1ncccc1C(F)(F)F)(F)F	5.96	166.3166	6.1583	-0.1983	Tr	179.6718	5.6288	0.3312	Tr	101.326	5.6321	0.3279	Tr
45	Clc1cccnc1N1CCN(CC1)c1nc2c([nH]1)cc(cc2)C(C)(C)C	7.06	198.4347	7.436	-0.376	Tr	232.566	7.1972	-0.1372	Ts	146.1988	7.1551	-0.0951	Tr
46	CC1CN(CCN1c1nc2c([nH]1)cc(cc2)C(F)(F)F)c1ncccc1C(F)(F)F	7.32	177.2731	6.5942	0.7258	Ts	208.8189	6.4931	0.8269	Ts	119.6924	6.2555	1.0645	Tr
47	CCC1CN(CCN1c1nc2c([nH]1)cc(cc2)C(F)(F)F)c1ncccc1C(F)(F)F	6.19	165.7717	6.1366	0.0534	Tr	193.7599	6.0466	0.1434	Tr	111.6088	5.9811	0.2089	Tr
48	CCCC1CN(CCN1c1nc2c([nH]1)cc(cc2)C(F)(F)F)c1ncccc1C(F)(F)F	5.49	163.6884	6.0538	-0.5638	Ts	183.6835	5.7478	-0.2578	Ts	113.4776	6.0445	-0.5545	Ts
49	CC1CN(CCN1c1nc2c([nH]1)cc(cc2c1cc(F)c(c(c1)F)F)C(F)(F)F)c1ncccc1Br	6.98	208.3055	7.8287	-0.8487	Tr	245.6228	7.5843	-0.6043	Ts	163.0056	7.7255	-0.7455	Tr
50	CC1CN(CCN1c1ncccc1Br)c1nc2c([nH]1)cc(cc2c1cc(F)c(c(c1)F)F)C(F)(F)F	8.37	202.6127	7.6022	0.7678	Tr	242.1295	7.4808	0.8892	Tr	164.848	7.7881	0.5819	Ts
51	CC1CN(CCN1c1ncccc1Br)c1nc2c([nH]1)cc(cc2c1cc(F)c(c(c1)F)F)C(F)(F)F	6.12	202.6127	7.6022	-1.4822	Tr	242.1295	7.4808	-1.3608	Tr	164.848	7.7881	-1.6681	Tr
52	FC(c1ccc(nc1)N1CCN(CC1)c1nc2c([nH]1)cc(cc2)C(F)(F)F)(F)F	4.95	150.1488	5.5151	-0.5651	Tr	181.0066	5.6684	-0.7184	Tr	98.0886	5.5222	-0.5722	Tr
53	FC(c1cccc(n1)N1CCN(CC1)c1nc2c([nH]1)cc(cc2)C(F)(F)F)(F)F	4.4	139.7178	5.1002	-0.7002	Tr	168.5759	5.2998	-0.8998	Ts	88.2945	5.1898	-0.7898	Tr
54	Ic1cccnc1N1CCN(CC1)c1nc2c([nH]1)cc(cc2)C(F)(F)F	6.66	157.628	5.8127	0.8473	Tr	191.8089	5.9887	0.6713	Ts	105.2859	5.7665	0.8935	Tr
55	N#Cc1cccnc1N1CCN(CC1)c1nc2c([nH]1)cc(cc2)C(F)(F)F	5.2	150.074	5.5122	-0.3122	Tr	187.4518	5.8595	-0.6595	Ts	95.9227	5.4487	-0.2487	Tr
56	OCc1cnc(c(c1)Cl)N1CCN(CC1)c1nc2c([nH]1)cc(cc2)C(F)(F)F	7.19	191.9449	7.1778	0.0122	Tr	227.6597	7.0517	0.1383	Ts	122.6853	6.3571	0.8329	Tr
57	Clc1cc(cnc1N1CCN(CC1)c1nc2c([nH]1)cc(cc2)C(F)(F)F)C(=O)N	6.37	154.4372	5.6857	0.6843	Tr	184.0316	5.7581	0.6119	Tr	114.0325	6.0634	0.3066	Ts
58	CNC(=O)c1cnc(c(c1)Cl)N1CCN(CC1)c1nc2c([nH]1)cc(cc2)C(F)(F)F	6.31	165.3069	6.1181	0.1919	Ts	208.6174	6.4871	-0.1771	Tr	118.9308	6.2296	0.0804	Tr
59	FC(c1ccc2c(c1)[nH]c(n2)N1CCN(CC1)c1ccccc1C(F)(F)F)(F)F	5.69	157.1833	5.795	-0.105	Tr	184.446	5.7704	-0.0804	Tr	108.624	5.8798	-0.1898	Tr
60	FC(c1ccc2c(c1)[nH]c(n2)N1CCN(CC1)c1ccncc1C(F)(F)F)(F)F	5.62	161.6682	5.9734	-0.3534	Tr	177.2264	5.5563	0.0637	Tr	98.9495	5.5515	0.0685	Tr
61	Clc1cnccc1N1CCN(CC1)c1nc2c([nH]1)cc(cc2)C(F)(F)F	5.41	155.8348	5.7413	-0.3313	Ts	189.4068	5.9175	-0.5075	Tr	103.1	5.6923	-0.2823	Ts
62	Clc1cccc(c1N1CCN(CC1)c1nc2c([nH]1)cc(cc2)C(F)(F)F)Cl	4.4	144.1792	5.2777	-0.8777	Tr	176.8138	5.5441	-1.1441	Ts	96.7135	5.4756	-1.0756	Tr
63	FC(c1ccc(cc1)c1[nH]c(nc1c1ccc(cc1)C(F)(F)F)N1CCN(CC1)c1ncccc1C(F)(F)F)(F)F	6.24	171.9863	6.3839	-0.1439	Ts	219.1737	6.8001	-0.5601	Ts	140.0446	6.9462	-0.7062	Tr
64	FC(c1ccc(cc1)c1cnc([nH]1)N1CCN(CC1)c1ncccc1C(F)(F)F)(F)F	6.06	163.8154	6.0588	0.0012	Tr	192.085	5.9969	0.0631	Tr	126.1935	6.4761	-0.4161	Ts

65	OCc1cnc(c(c1)C(F)(F)F)N1CCN(C(C1)C)c1nc2c([nH]1)cc(cc2c1cc(F)c(c(c1)F)F)C(F)(F)F	8.85	228.644	8.6378	0.2122	Ts	291.6336	8.9486	-0.0986	Tr	186.2696	8.5151	0.3349	Tr
66	COC(=O)c1cnc(c(c1)C(F)(F)F)N1CCN(C(C1)C)c1nc2c([nH]1)cc(cc2c1cc(F)c(c(c1)F)F)C(F)(F)F~	9.52	217.6246	8.1994	1.3206	Ts	289.2957	8.8793	0.6407	Tr	187.9043	8.5706	0.9494	Tr
67	FC(c1ccc2c(c1)[nH]c(n2)N1CCN(CC1)c1ncccc1C(F)(F)F)(F)F	6.96	168.9536	6.2632	0.6968	Tr	192.8447	6.0194	0.9406	Tr	110.2962	5.9366	1.0234	Tr
68	Brc1ccc2c(c1)[nH]c(n2)N1CCN(CC1)c1ncccc1C(F)(F)F	6.91	160.2622	5.9175	0.9925	Tr	194.9131	6.0807	0.8293	Tr	105.2977	5.7669	1.1431	Tr
69	OCC(=O)Nc1cnc(c(c1)Cl)N1CCN(C(C1)C)c1nc2c([nH]1)cc(cc2c1ccc(cc1)F)C(F)(F)F	7.52	193.1574	7.2261	0.2939	Ts	243.0431	7.5079	0.0121	Tr	161.7263	7.6821	-0.1621	Tr
70	FC(c1cc(N2CCOCC2)c2c(c1)[nH]c(n2)N1CCN(CC1)c1ncccc1C(F)(F)F)(F)F	7.3	197.6195	7.4036	-0.1036	Tr	231.4226	7.1633	0.1367	Tr	127.5966	6.5237	0.7763	Tr
71	FC(c1cc2[nH]c(nc2c(c1)C1CCC(CC1)C(F)(F)F)N1CCN(CC1)c1ncccc1C(F)(F)F)(F)F	8	197.1212	7.3837	0.6163	Ts	237.0996	7.3316	0.6684	Ts	135.5243	6.7928	1.2072	Tr
72	FC(c1cc2[nH]c(nc2c(c1)c1ccccc1)N1CCN(CC1)c1ncccc1C(F)(F)F)(F)F	6.85	181.9953	6.782	0.068	Ts	228.6033	7.0797	-0.2297	Tr	139.4605	6.9264	-0.0764	Tr
73	Fc1ccc2c(c1)[nH]c(n2)N1CCN(CC1)c1ncccc1C(F)(F)F	5.4	154.8323	5.7015	-0.3015	Tr	181.7913	5.6917	-0.2917	Tr	104.1537	5.7281	-0.3281	Tr
74	FC(c1ccc2c(c1)[nH]c(n2)N1CCN(CC1)c1ccccn1)(F)F	5.24	131.2477	4.7632	0.4768	Ts	156.1051	4.93	0.31	Tr	96.538	5.4696	-0.2296	Ts
75	Cc1cccnc1N1CCN(CC1)c1nc2c([nH]1)cc(cc2)C(F)(F)F	6.4	159.6432	5.8928	0.5072	Tr	193.8379	6.0489	0.3511	Tr	109.3539	5.9046	0.4954	Tr
76	Clc1cncc(c1N1CCN(CC1)c1nc2c([nH]1)cc(cc2)C(F)(F)F)Cl	5.86	153.9119	5.6648	0.1952	Tr	180.5419	5.6546	0.2054	Tr	92.6912	5.339	0.521	Tr
77	Clc1cncnc1N1CCN(CC1)c1nc2c([nH]1)cc(cc2)C(F)(F)F	5.68	167.426	6.2024	-0.5224	Ts	191.8381	5.9896	-0.3096	Ts	111.9744	5.9935	-0.3135	Tr
78	FC(c1ccc(cc1)c1[nH]c(nc1c1ccccc1)N1CCN(CC1)c1ncccc1C(F)(F)F)(F)F	6.97	170.2984	6.3167	0.6533	Tr	214.6049	6.6646	0.3054	Ts	141.9397	7.0106	-0.0406	Ts
79	Fc1cc(cc(c1F)F)c1nc([nH]c1c1cc(F)c(c(c1)F)F)N1CCN(CC1)c1ncccc1C(F)(F)F	7.36	214.89	8.0906	-0.7306	Tr	245.5316	7.5816	-0.2216	Tr	170.5824	7.9827	-0.6227	Tr
80	OCc1cnc(c(c1)Cl)N1CCN(C(C1)C)c1[nH]c(c(n1)c1ccccc1)c1ccc(cc1)C(F)(F)F	7.59	214.3719	8.07	-0.48	Tr	262.3428	8.0801	-0.4901	Tr	167.1832	7.8673	-0.2773	Tr
81	CCN1CCCC1CNC(=O)c1nc([nH]c1c1ccc(cc1)C(F)(F)F)N1CCN(CC1)c1ncccc1C(F)(F)F	5.39	165.9789	6.1449	-0.7549	Tr	192.1385	5.9985	-0.6085	Tr	107.5996	5.845	-0.455	Ts
82	Fc1c(F)cc(cc1F)CNc1cc(cc2c1nc([nH]2)N1CCN(CC1)c1ncccc1C(F)(F)F)C(F)(F)F	6.88	200.888	7.5336	-0.6536	Tr	222.7595	6.9064	-0.0264	Ts	151.723	7.3426	-0.4626	Tr
83	OCc1cnc(c(c1)Cl)N1CCN(C(C1)C)c1nc2c([nH]1)cc(cc2NC(=O)C1CCCCC1)C(F)(F)F	8.8	230.0557	8.6939	0.1061	Tr	284.8899	8.7487	0.0513	Ts	175.7987	8.1597	0.6403	Tr
84	OCc1cnc(c(c1)Cl)N1CCN(C(C1)C)c1nc2c([nH]1)cc(cc2NCc1ccccc1)C(F)(F)F	8.15	205.4742	7.716	0.434	Ts	253.9668	7.8318	0.3182	Tr	171.7403	8.022	0.128	Ts
85	Clc1cc(cnc1N1CCN(CC1)c1nc2c([nH]1)cc(cc2)C(F)(F)F)C(=O)C	6.24	165.7232	6.1347	0.1053	Tr	202.271	6.2989	-0.0589	Tr	119.1272	6.2363	0.0037	Tr
86	[O-]C(=O)c1cnc(c(c1)Cl)N1CCN(C(C1)C)c1[nH]c2c(n1)c(cc(c2)C(F)(F)F)c1cc(F)c(c(c1)F)F	7.34	207.0258	7.7778	-0.4378	Tr	265.0893	8.1615	-0.8215	Tr	186.8257	8.534	-1.194	Tr
87	FC(c1ccc2c(c1)n(Cc1ccccc1)c(n2)N1CCN(CC1)c1ncccc1C(F)(F)F)(F)F	6.24	162.4556	6.0047	0.2353	Tr	194.2506	6.0611	0.1789	Tr	128.7072	6.5614	-0.3214	Tr
88	Fc1ccc(cc1F)c1ccc2c(c1)[nH]c(n2)N1CCN(CC1)c1ncccc1C(F)(F)F	5.94	155.899	5.7439	0.1961	Tr	198.7715	6.1952	-0.2552	Tr	120.0723	6.2684	-0.3284	Ts
89	FC(c1cc2[nH]c(nc2cc1NCc1ccc(cc1)C(F)(F)F)N1CCN(CC1)c1ncccc1C(F)(F)F)(F)F	7.03	181.1812	6.7496	0.2804	Tr	229.2688	7.0994	-0.0694	Tr	150.1071	7.2878	-0.2578	Tr
90	Nc1cnc(c(c1)Cl)N1CCN(C(C1)C)c1nc2c([nH]1)cc(cc2c1ccc(cc1)F)C(F)(F)F	7.01	183.7844	6.8532	0.1568	Tr	208.6523	6.4881	0.5219	Tr	150.9309	7.3157	-0.3057	Tr
91	FC(c1cc(N2CCCCC2)c2c(c1)[nH]c(n2)N1CCN(CC1)c1ncccc1C(F)(F)F)(F)F	7.54	197.3591	7.3932	0.1468	Ts	237.5074	7.3437	0.1963	Tr	139.3912	6.9241	0.6159	Tr
92	FC(c1cc2[nH]c(nc2c(c1)c1ccccn1)N1CCN(CC1)c1ncccc1C(F)(F)F)(F)F	6.57	180.4155	6.7192	-0.1492	Tr	222.3756	6.895	-0.325	Tr	138.0458	6.8784	-0.3084	Tr
93	CC(c1ccc2c(c1)[nH]c(n2)N1CCN(CC1)c1ncccc1C(F)(F)F)(C)C	6.74	198.1639	7.4252	-0.6852	Ts	229.0476	7.0929	-0.3529	Tr	130.0747	6.6079	0.1321	Ts
94	Cc1ccc2c(c1)[nH]c(n2)N1CCN(CC1)c1ncccc1C(F)(F)F	5.47	154.1099	5.6727	-0.2027	Tr	178.5811	5.5965	-0.1265	Ts	104.689	5.7463	-0.2763	Ts
95	CC1CN(CCN1c1nc2c([nH]1)cc(cc2c1cc(F)c(c(c1)F)F)C(F)(F)F)c1ncccc1Br	8.17	208.3055	7.8287	0.3413	Tr	245.6228	7.5843	0.5857	Ts	163.0056	7.7255	0.4445	Ts
96	FC(c1ccnc(c1)N1CCN(CC1)c1nc2c([nH]1)cc(cc2)C(F)(F)F)(F)F	5.25	137.4867	5.0114	0.2386	Tr	163.2069	5.1406	0.1094	Tr	102.0183	5.6556	-0.4056	Ts
97	Clc1cccnc1N1CCN(CC1)c1nc2c([nH]1)cc(cc2)C(F)(F)F	6.51	168.4976	6.2451	0.2649	Ts	201.9319	6.2889	0.2211	Tr	124.0505	6.4034	0.1066	Tr
98	CCOC(=O)c1cccnc1N1CCN(CC1)c1nc2c([nH]1)cc(cc2)C(F)(F)F	4.62	143.7833	5.2619	-0.6419	Tr	182.9556	5.7262	-1.1062	Tr	91.4174	5.2958	-0.6758	Tr

Table S2. The list of SAks together with their correlation weights for the three runs of the Monte Carlo optimization.

SAk	CW(SAk)			SAk	CW(SAk)			SAk	CW(SAk)			SAk	CW(SAk)		
	Run 1	Run 2	Run 3		Run 1	Run 2	Run 3		Run 1	Run 2	Run 3		Run 1	Run 2	Run 3
00010001000	-0.1609	-0.6627	-0.0545	P2E0C...1-..	0.1848	0.366	0.3202	PT2-C...5...	-0.1864	0.216	0.373	e0p2C...2+..	-0.1156	-0.6638	-0.4048
00010001010	0.7724	1.2127	0.7918	P2E0C...2-..	-0.3374	0.8085	-0.8085	PT2-C...6...	0.229	0.0848	0.0816	e0p2C...3+..	0.0264	0.3835	-0.0241
00010001100	-0.5396	-0.0192	-0.5549	P2E0C...3-..	-0.0599	1.0463	0.4148	PT2-F...2...	-0.0368	0.0291	0.2877	e0p2C...4+..	0.3107	0.3564	0.1366
00011001000	-0.0745	0.5092	0.1787	P2E0F...1-..	0.0742	0.4737	0.2153	PT2-F...3...	0.4329	0.2422	-0.0094	e0p2C...5+..	0.1177	0.3164	0.0997
10010001000	-0.713	0.9582	0.5583	P2E0F...2-..	-0.4384	-0.079	0.3314	PT2-Br..2...	1.1782	0.0989	0.4911	e0p2C...6+..	0.405	0.0951	0.3443
10011001000	-1.5693	-1.2625	-0.6384	P2E0Br..1-..	0.9921	-0.4102	0.014	PT2-Cl..2...	1.2586	1.2202	0.1811	e0p2C...7+..	0.5246	0.3488	0.1102
10011001100	-0.1998	0.507	0.433	P2E0Cl..1-..	0.3476	1.0843	0.1727	PT2-N...2...	-0.9146	-1.5727	-1.0632	e0p2C...8+..	-0.1429	0.1208	-0.0822
(...(.....	-0.2314	-0.3196	0.2736	P2E0N...0-..	0.2326	0.6087	0.3723	PT2-N...3...	0.0564	0.099	1.46	e0p2C...9+..	0.1508	0.0893	0.2155
(.....	1.2677	1.2733	0.1116	P2E0N...1-..	0.4919	0.449	-0.0534	PT2-N...4...	-0.485	-0.6681	-0.4175	e0p2F...3+..	0.359	-0.0151	1.4659
(...1...(...	0.1573	1.4817	0.1397	P2E0N...2-..	0.1393	0.1977	0.1234	PT2-N...5...	0.331	0.0355	-0.3388	e0p2F...4+..	0.3594	0.0219	-0.0618
(...2...(...	0.2187	0.1395	0.8664	P2E0O...0-..	1.2873	0.3901	0.0855	PT2-O...1...	-0.3979	0.4067	1.156	e0p2Br..3+..	0.1373	0.3135	0.1889
(...C...(...	0.3349	0.3478	0.3527	P2E0O...1-..	-0.2163	-0.4179	-0.0022	PT2-O...2...	-0.3115	0.052	-0.3956	e0p2Cl..3+..	1.3016	0.1787	1.5409
(...F...(...	-0.5499	-0.3192	-0.0813	P3E0C...0-..	0.1253	0.354	0.5576	PT3-C...2...	0.2686	0.5311	0.9989	e0p3C...10+.	0.0675	0.2678	0.0944
(...Cl..(...	0.8314	1.3686	0.5521	P3E0C...1-..	0.2137	0.1774	0.1576	PT3-C...3...	0.2506	0.4709	0.3762	e0p3C...3+..	1.1003	0.9401	1.2462
(...c...(...	0.5333	0.5461	1.3036	P3E0C...2-..	0.0035	-0.2069	-0.5213	PT3-C...4...	0.4519	0.1461	-0.4067	e0p3C...4+..	0.558	0.1648	0.3343
(=..#)..Y.Y.	3.319	3.6448	0.6208	P3E0C...3-..	0.1133	-0.2886	-0.1301	PT3-C...5...	-0.1771	-0.2947	-0.2708	e0p3C...5+..	0.1315	0.0037	0.2903
(F..#)..Y.Y.	5.9292	3.8408	2.5728	P3E0C...4-..	0.2988	0.0229	0.3696	PT3-C...6...	-0.0368	-0.0337	-0.2701	e0p3C...6+..	-0.4059	0.1915	0.4843
(F..=)..Y.Y.	3.4356	2.3918	2.099	P3E0C...5-..	-0.8743	-0.9613	0.7561	PT3-C...7...	0.1611	0.1825	0.3958	e0p3C...7+..	0.1828	-0.0761	0.4696
(F..N)..Y.Y.	3.71	0.2221	4.3984	P3E0C...6-..	0.0509	0.1362	0.5218	PT3-C...8...	-0.3057	1.4412	0.5106	e0p3C...8+..	-0.4722	-0.6366	-0.0013
(F..O)..Y.Y.	6.5283	4.0192	-0.2497	P3E0F...1-..	0.2546	0.161	0.2541	PT3-F...2...	0.0401	0.2804	0.1607	e0p3C...9+..	1.2233	-0.1738	0.1702
(F..P)..Y.Y.	1.6714	1.3009	1.7131	P3E0F...2-..	0.4736	0.3614	-0.2453	PT3-F...3...	-0.0252	0.2358	0.4116	e0p2N...4+..	0.4262	0.0886	0.3887
(F..S)..Y.Y.	5.8266	2.7089	0.5067	P3E0F...3-..	0.0629	0.7103	0.5161	PT3-F...4...	-0.1806	0.5484	1.06	e0p2N...5+..	1.279	0.2678	0.407
(F.Br)..Y.Y.	3.8359	1.7746	1.548	P3E0Br..2-..	0.0403	1.0966	1.2666	PT3-Br..3...	1.298	0.4537	-0.1388	e0p2N...6+..	0.3874	-0.3976	-0.4816
(F.Cl)..Y.Y.	2.7673	4.2881	-0.2524	P3E0Cl..2-..	0.3205	-0.0691	0.3353	PT3-Cl..3...	0.6054	1.0917	0.6691	e0p2N...7+..	-0.6326	-0.9635	-0.0787
(Br.#)..Y.Y.	3.5428	1.3161	1.0405	P3E0N...1-..	-0.894	-1.3108	-0.6083	PT3-N...2...	-0.5925	-1.6777	-2.4417	e0p2N...8+..	1.1423	-0.4857	0.0167
(Br.=)..Y.Y.	2.7748	2.9188	1.8473	P3E0N...2-..	0.5015	-0.2199	0.176	PT3-N...3...	-0.9243	-0.3638	-0.6001	e0p2O...2+..	1.2663	1.2407	0.4707
(Br.N)..Y.Y.	3.4418	1.212	1.6452	P3E0N...3-..	1.4124	1.4464	-0.023	PT3-N...4...	-0.3536	0.1363	0.5976	e0p2O...3+..	0.0952	0.4295	-0.0458
(Br.O)..Y.Y.	4.1949	0.4351	0.7308	P3E0N...4-..	1.409	0.0435	-1.2026	PT3-N...5...	-0.4471	0.2273	0.0296	e0p2O...4+..	0.5341	0.2922	-0.4846
(Br.P)..Y.Y.	2.3177	3.7317	1.6121	P3E0N...5-..	0.1351	0.4694	-0.2136	PT3-N...6...	-0.3579	-0.8139	-0.9949	e0p3F...3+..	0.1884	0.1718	-0.028
(Br.S)..Y.Y.	3.1507	0.2608	1.2263	P3E0O...0-..	0.1376	0.1296	-0.2001	PT3-N...7...	-0.607	-1.0006	-0.357	e0p3F...4+..	-0.4495	1.8481	-0.5697
(Cl.#)..Y.Y.	2.094	2.9823	2.3408	P3E0O...1-..	-0.3639	0.433	0.083	PT3-O...2...	0.4125	0.0401	-0.0018	e0p3F...5+..	0.4519	1.2515	0.1273
(Cl.=)..Y.Y.	1.9312	2.8412	0.4806	P3E0O...2-..	-0.2475	-0.4047	-0.3299	PT3-O...3...	-0.6554	-0.1093	0.0444	e0p3Br..4+..	1.6211	0.2189	-0.2138

(Cl.N)..Y.Y.	4.8056	3.8581	2.3421	P4E0C...0-..	-0.2452	-0.4108	0.2812	PT4-C...10..	1.1359	0.2632	0.7713	e0p3Cl..4+..	-0.5127	-0.151	1.0404
(Cl.O)..Y.Y.	3.5238	1.9214	1.8976	P4E0C...1-..	0.4344	0.3244	0.1819	PT4-C...11..	0.1574	0.2644	-0.9348	e0p4C...10+.	0.1709	0.2865	0.0855
(Cl.P)..Y.Y.	3.0394	1.9907	2.7465	P4E0C...10-.	0.2654	-0.0011	1.07	PT4-C...12..	0.4312	0.1309	0.2727	e0p4C...11+.	0.025	-0.1357	-0.6625
(Cl.S)..Y.Y.	3.0622	3.4892	2.3409	P4E0C...12-.	0.4051	0.4862	0.1427	PT4-C...13..	0.2552	-0.1979	0.6456	e0p4C...12+.	-0.049	-0.7417	0.2506
(ClBr)..Y.Y.	4.7397	2.4395	-0.1596	P4E0C...13-.	0.6074	-0.0518	0.2484	PT4-C...14..	0.4144	0.1467	0.0819	e0p4C...13+.	1.1122	-0.0021	0.1029
(N..=)..Y.Y.	4.9494	2.7508	-0.0304	P4E0C...16-.	0.3034	0.4879	0.2876	PT4-C...15..	0.9095	0.3271	3.4504	e0p4C...14+.	0.1058	0.2954	0.3095
(N..O)..Y.Y.	4.0709	6.4107	1.8855	P4E0C...2-..	-0.5624	-0.0086	0.077	PT4-C...18..	0.2107	1.0037	0.5824	e0p4C...16+.	-0.0932	0.2282	0.395
(N..P)..Y.Y.	3.6039	4.8606	0.9667	P4E0C...3-..	-0.475	0.3719	-0.1911	PT4-C...2...	0.1614	1.0681	-0.2775	e0p4C...17+.	0.3256	0.2197	1.4983
(N..S)..Y.Y.	1.9909	2.8905	1.7575	P4E0C...4-..	0.7803	-0.7416	0.1688	PT4-C...3...	-0.0139	-0.0124	-0.2856	e0p4C...20+.	0.4695	0.1525	0.4394
(O..#)..Y.Y.	2.5459	1.673	1.164	P4E0C...5-..	0.5949	-0.0612	1.0914	PT4-C...4...	0.2894	0.2244	0.1541	e0p4C...4+..	-1.5116	0.8533	-0.6908
(O..=)..Y.Y.	0.5641	4.2211	0.6717	P4E0C...6-..	-1.0086	0.5864	-0.6127	PT4-C...5...	0.1125	0.1389	0.2135	e0p4C...5+..	0.1974	0.6266	0.271
(O..P)..Y.Y.	2.8335	3.4043	3.05	P4E0C...7-..	-0.1463	-0.4168	-0.1649	PT4-C...6...	0.0887	0.2743	1.0358	e0p4C...6+..	0.7734	0.0482	0.4875
(O..S)..Y.Y.	2.7706	2.0306	0.7696	P4E0C...8-..	0.2416	0.2398	0.7581	PT4-C...7...	-0.0175	0.1914	-0.3526	e0p4C...7+..	0.3978	-0.3351	0.4991
(P..#)..Y.Y.	2.6924	2.5496	0.8397	P4E0F...1-..	0.4128	-0.3653	-0.0038	PT4-C...8...	0.0903	-1.0558	0.1094	e0p4C...8+..	0.8138	0.7542	0.4607
(P..=)..Y.Y.	4.2339	1.8912	2.1158	P4E0F...3-..	-0.0373	0.2483	-0.0697	PT4-C...9...	-0.5639	-0.7645	-0.1795	e0p4C...9+..	-0.014	0.2147	0.385
(S..#)..Y.Y.	4.1107	4.4123	0.5819	P4E0F...4-..	0.482	0.4735	0.4581	PT4-F...2...	0.0749	-0.4928	-0.2573	e0p3N...3+..	-1.095	-1.0125	-1.1841
(S..=)..Y.Y.	1.9898	2.7489	1.2851	P4E0F...7-..	0.3922	0.0944	0.5473	PT4-F...4...	-0.0471	-0.2241	0.1929	e0p3N...5+..	1.2328	-0.6928	-1.7959
(S..P)..Y.Y.	2.8034	2.4544	2.9565	P4E0Br..4-..	0.1382	1.3363	-0.0563	PT4-F...5...	-0.6795	0.4975	-0.3683	e0p3N...6+..	-0.1971	-0.4859	-0.1365
1...(.....	0.5757	0.1284	0.8061	P4E0Cl..4-..	0.0054	0.8058	1.0318	PT4-F...8...	-0.2592	0.415	0.1318	e0p3N...7+..	0.0009	0.4964	0.01
1.....	-0.1256	-0.4939	0.2906	P4E0N...1-..	-4.5763	-3.8117	-2.1063	PT4-Br..5...	-0.3468	0.494	0.4084	e0p3N...8+..	0.2907	-0.2405	0.0677
1...C...(...	0.0622	-0.0048	0.4098	P4E0N...10-.	1.2165	0.4742	1.1514	PT4-Cl..5...	0.3735	1.4054	0.9467	e0p3N...9+..	1.2437	0.5624	-0.4604
1...F...(...	0.3249	1.4599	0.1348	P4E0N...11-.	-0.4461	0.0624	-0.1235	PT4-N...10..	0.1549	0.1225	0.1531	e0p3O...3+..	1.4129	0.4147	0.0275
1...N...(...	1.2509	0.4699	0.1976	P4E0N...3-..	0.8524	1.2036	-0.3647	PT4-N...12..	0.1561	0.3038	0.2621	e0p3O...4+..	0.2352	0.101	-0.0407
1...N...1...	0.533	-0.5761	-0.0877	P4E0N...4-..	1.0527	0.0108	0.8875	PT4-N...13..	-0.6149	-0.5687	-0.5318	e0p4F...3+..	-0.0741	1.1546	0.2711
1...c...(...	0.0432	1.1277	-0.3129	P4E0N...7-..	0.5364	-0.1863	0.0179	PT4-N...4...	0.3693	-0.5119	-0.3331	e0p4F...5+..	0.3885	0.3955	0.1342
1...c...1...	-0.475	-0.011	-0.0862	P4E0N...8-..	-0.0325	-0.4429	-0.0849	PT4-N...5...	-1.5675	-1.8344	-1.5685	e0p4F...6+..	0.9583	0.4921	-0.2762
1...n...(...	-0.9885	-0.448	0.3334	P4E0O...2-..	0.405	-0.354	1.0356	PT4-N...6...	2.1293	1.9359	1.8485	e0p4F...9+..	1.5777	0.5027	-0.0221
2...(.....	-0.0489	0.1177	0.3586	P4E0O...3-..	0.4658	0.64	0.3865	PT4-N...7...	0.0155	0.1546	-0.0479	e0p4Br..6+..	0.2968	1.2285	-0.3182
2.....	0.438	1.3567	0.4303	P4E0O...4-..	-0.6786	-1.0276	-0.2842	PT4-N...9...	1.4387	0.2541	0.903	e0p4Cl..6+..	0.6453	0.2103	-0.1238
2...c...(...	1.4234	1.3006	0.5707	NNC-C...101.	-0.8581	0.8491	1.165	PT4-O...2...	-0.4803	-0.3428	0.5383	e0p4N...10+.	-0.3872	-0.904	0.3609
2...c...1...	-0.5547	-0.5361	-0.6572	NNC-C...110.	0.8467	0.3865	-0.0527	PT4-O...4...	0.7815	-0.0477	-0.1056	e0p4N...11+.	0.3352	0.0666	1.0302
2...n...(...	-0.3948	-0.0118	0.0887	NNC-C...211.	-1.7854	-0.8466	-1.1837	PT4-O...5...	0.4878	0.344	0.2945	e0p4N...12+.	-0.4738	0.0603	-0.5187
<#>..0000...	-0.1432	-0.0203	0.7084	NNC-C...220.	0.2785	0.4385	0.4341	VS2-C...10..	-0.1353	-0.0649	-0.2587	e0p4N...13+.	-1.5426	-0.6746	-0.7026
=...(.....	-2.1722	-2.4914	-1.5713	NNC-C...303.	0.7741	1.1982	1.5808	VS2-C...11..	0.0573	-0.1431	0.3371	e0p4N...14+.	1.2727	0.3001	1.0798
=.....	0.7456	0.3414	0.0478	NNC-C...312.	-0.2174	-0.0489	0.4524	VS2-C...12..	-0.0847	0.2794	0.7783	e0p4N...15+.	0.6248	-0.2588	0.4816

=...C...(...	1.4309	0.3532	0.7989	NNC-C...321.	0.1673	0.2263	0.3512	VS2-C...3...	-0.9296	-0.1637	-0.6369	e0p4N...17+.	-0.2331	0.0951	0.2279
=...N...1...	7.587	4.4806	4.2316	NNC-C...330.	-0.0599	0.1134	0.0798	VS2-C...4...	0.2247	0.2871	-0.2478	e0p4N...5+..	-0.9429	-0.8872	-0.2054
=...O...(...	-1.0767	-0.2423	-0.5443	NNC-C...413.	0.4039	0.2455	-0.1323	VS2-C...5...	0.8021	0.4926	-0.1185	e0p4N...7+..	-0.7481	-0.1816	-0.2649
<=>..0000...	0.3171	1.1845	0.1804	NNC-F...110.	0.2596	0.082	0.0186	VS2-C...6...	-0.6153	-0.8796	-0.4372	e0p4N...8+..	1.1332	0.7476	1.1248
<=>..0001...	1.0312	0.5686	0.4734	NNC-Br..110.	0.1703	0.3368	1.2441	VS2-C...7...	0.0748	0.3908	0.2709	e0p4O...5+..	-0.1523	0.255	0.7562
<=>..0002...	-0.7007	-2.6979	-1.0513	NNC-Cl..110.	0.202	0.5881	0.8674	VS2-C...8...	-0.3926	0.0868	-0.2259	e0p4O...6+..	0.0209	0.6749	0.1667
<F>..0003...	3.1853	0.2532	0.3219	NNC-N...110.	-0.911	0.5265	0.107	VS2-C...9...	0.2289	-0.0176	1.2534	e0s2C...10+.	0.3227	-0.3651	0.4999
<F>..0006...	-0.1767	1.364	0.0051	NNC-N...211.	1.1797	0.5936	0.1953	VS2-F...4...	0.3274	-0.0628	0.2833	e0s2C...11+.	0.1939	0.4981	0.9454
<F>..0007...	-0.1282	-0.386	0.3494	NNC-N...220.	0.0976	-0.3737	-0.2473	VS2-F...5...	-0.2607	0.2011	0.0663	e0s2C...12+.	0.2981	-0.2257	0.1564
<F>..0009...	0.2728	0.2965	0.3268	NNC-N...330.	-0.0924	-0.215	-0.3043	VS2-F...6...	0.3057	0.3065	0.5407	e0s2C...13+.	-0.3174	-0.2526	-0.3033
<F>..0010...	0.1541	0.0076	0.454	NNC-O...110.	0.1648	-0.0123	0.1781	VS2-Br..5...	1.398	0.3952	0.9008	e0s2C...14+.	0.1338	0.1591	1.2884
 .0002...	-0.8909	-1.6613	-0.6454	NNC-O...220.	-0.4241	-0.148	1.3278	VS2-Cl..5...	-0.0892	0.7981	0.9572	e0s2C...15+.	0.2734	0.5937	0.1371
 .0003...	0.1383	0.2072	-0.0554	NNE0C...100-	-0.3166	1.4699	1.6234	VS2-N...10..	-1.2867	-1.8766	-0.9245	e0s2C...4+..	-0.8087	-0.8729	-0.4148
 .0004...	0.745	-0.3299	0.2508	NNE0C...109-	0.5031	0.0636	0.3688	VS2-N...11..	-1.3415	-0.7586	-1.5474	e0s2C...5+..	0.4469	0.1157	1.8792
<Cl>.0002...	-0.2912	-0.5924	-0.5501	NNE0C...209-	-1.3615	-1.4169	-1.3021	VS2-N...5...	0.144	1.0987	-0.2325	e0s2C...6+..	0.2844	0.0091	1.3519
<Cl>.0003...	1.4548	1.1176	0.7027	NNE0C...218-	0.1423	-0.1247	-0.1669	VS2-N...7...	-0.1813	0.5791	-0.0939	e0s2C...7+..	-0.2097	-0.2622	0.6156
<Cl>.0004...	0.4367	0.5208	-0.1305	NNE0C...300-	0.1245	0.5997	2.3633	VS2-N...8...	-0.326	-0.1025	-0.2084	e0s2C...8+..	0.2814	0.2026	-0.4709
<N>..0002...	-0.8141	-0.5503	-1.8745	NNE0C...309-	-0.1197	-0.1862	1.1612	VS2-N...9...	2.9413	3.8478	1.9212	e0s2C...9+..	0.7233	1.2228	0.5511
<N>..0003...	1.069	1.0603	1.1971	NNE0C...318-	0.2724	0.4299	0.447	VS2-O...3...	0.7871	0.5021	0.6547	e0s2F...5+..	0.3748	0.463	0.6353
<N>..0004...	0.2123	1.9569	-0.5681	NNE0C...327-	-0.0838	-0.0269	0.3945	VS2-O...4...	0.2308	0.1344	0.1251	e0s2F...6+..	0.6024	-0.4039	-0.575
<O>..0000...	0.1234	0.0408	0.196	NNE0C...409-	0.944	0.2063	0.7587	VS2-O...5...	0.394	0.1692	-0.4139	e0s2F...7+..	0.292	0.6375	-0.1194
<O>..0001...	1.0533	0.067	-0.4008	NNE0F...109-	0.1853	-0.1011	-0.0537	VS3-C...10..	0.3755	0.2323	-0.2641	e0s2Br..6+..	-0.0159	0.4714	1.3905
<O>..0002...	0.3881	-0.0259	-0.087	NNE0Br..109-	0.8621	0.5325	1.0438	VS3-C...11..	0.0965	-0.1699	-0.4152	e0s2Cl..6+..	0.6799	-0.1166	-0.1072
<S>..0000...	2.7745	3.2977	0.8746	NNE0Cl..109-	0.1828	1.2862	1.516	VS3-C...12..	0.526	-0.3102	0.7087	e0s3C...10+.	0.7604	0.0809	0.2445
C...(...(...	2.2966	1.1045	1.7781	NNE0N...109-	0.521	-0.3194	0.7871	VS3-C...13..	-0.3209	0.0214	0.0146	e0s3C...11+.	0.5763	-0.1946	1.5172
C...(.....	0.0599	0.2396	0.4633	NNE0N...209-	0.0573	0.0333	-0.1527	VS3-C...14..	-1.0893	-0.7264	-0.0936	e0s3C...12+.	-1.7662	-0.0241	-0.6083
C...(...1...	2.0751	2.0849	1.1594	NNE0N...218-	-0.0422	0.1274	0.4977	VS3-C...15..	0.3633	0.0134	0.2601	e0s3C...13+.	-0.1657	-0.014	-0.0095
C...(...2...	-0.3796	-0.072	0.5047	NNE0N...327-	-0.179	-0.1607	-0.1031	VS3-C...16..	0.1569	0.0926	0.1722	e0s3C...14+.	0.2421	0.2848	0.1592
C...(...=...	-0.7601	-0.8882	-0.8839	NNE0O...109-	0.4452	0.3096	0.504	VS3-C...17..	0.5307	0.3957	0.1191	e0s3C...15+.	0.2516	0.0138	0.0487
C...(...C...	1.393	0.0329	0.8787	NNE0O...218-	-0.0909	0.0351	-0.4577	VS3-C...18..	1.6852	1.0931	1.5057	e0s3C...16+.	0.2893	-0.3005	0.3439
C.....	-0.4623	-0.3247	-0.3361	NOSP10000000	0.3164	0.2903	0.6488	VS3-C...19..	-0.1668	1.0558	0.1489	e0s3C...17+.	-0.183	0.2778	0.2752
C...1...(...	-0.1337	0.7075	0.1533	NOSP11000000	0.3707	0.4187	0.2429	VS3-C...4...	1.0956	2.2122	1.2232	e0s3C...18+.	-0.7595	-0.4356	0.0981
C...1.....	0.4435	0.4048	-0.5409	S2E0C...0-..	-0.2438	0.0309	0.0072	VS3-C...5...	0.0933	0.3522	0.8929	e0s3C...19+.	0.0995	0.4765	0.3255
C...1...C...	-0.4157	0.2542	-0.3459	S2E0C...1-..	-0.3858	-0.4872	0.0097	VS3-C...6...	0.715	0.0178	1.2767	e0s3C...20+.	1.1683	0.0787	0.1715
C...=.....	0.5335	0.2167	0.6122	S2E0C...10-.	-0.0802	0.0195	1.4483	VS3-C...7...	0.2824	0.6974	0.3105	e0s3C...21+.	2.1381	0.172	1.6017

C...C...(...	-0.358	-0.1833	0.0764	S2E0C...2-..	0.2445	0.062	0.1828	VS3-C...8...	0.0537	0.8924	0.1471	e0s3C...22+.	0.2906	0.468	0.1587
C...C.....	0.3596	-0.0918	-0.4259	S2E0C...3-..	0.1686	0.4547	-0.0564	VS3-C...9...	0.2401	0.0471	-0.3653	e0s3C...5+..	2.4481	1.4178	0.4044
C...C...1...	-1.1616	-0.7212	-0.11	S2E0C...4-..	0.3168	0.0543	0.0111	VS3-F...4...	-0.5621	0.2544	0.1497	e0s3C...7+..	0.9754	0.5053	0.4099
C...C...C...	-0.1669	0.3479	-0.0908	S2E0C...5-..	-0.2846	0.1017	-0.0756	VS3-F...5...	0.2426	0.2175	0.0611	e0s3C...8+..	0.2832	0.4072	0.0844
C...N...(...	-0.4017	-0.5693	-0.1388	S2E0C...6-..	-0.2806	0.0127	-0.2199	VS3-F...6...	0.1781	0.345	0.6542	e0s3C...9+..	0.4496	-0.5264	1.6543
C...N...1...	0.4418	0.416	0.1723	S2E0C...7-..	0.1123	0.2053	0.0636	VS3-F...7...	0.6193	1.0759	0.3915	e0s2N...10+.	1.0588	1.5858	0.2024
C...O...C...	-0.3707	-0.5182	0.6817	S2E0C...8-..	-1.6139	-0.2947	-0.588	VS3-Cl..7...	3.8854	3.2303	1.2916	e0s2N...11+.	0.129	0.519	-0.0492
C...c...1...	0.0938	1.1633	0.8964	S2E0C...9-..	0.2529	0.4343	0.4877	VS3-Cl..8...	0.4611	1.0046	-0.7515	e0s2N...12+.	0.1205	-0.2651	-0.1123
BOND00000000	0.3744	0.2283	0.1922	S2E0F...3-..	-0.4284	0.3837	1.5605	VS3-N...10..	0.0558	0.2168	0.2504	e0s2N...13+.	-0.7607	-0.8813	-0.7802
BOND10000000	0.3635	-0.1431	0.5601	S2E0F...4-..	0.3324	0.1006	-0.0999	VS3-N...11..	2.2127	2.2903	2.4849	e0s2N...9+..	-0.6973	-0.6519	-0.1125
F...(...(...	0.4632	-0.1075	0.3315	S2E0F...5-..	0.3418	0.2214	0.2616	VS3-N...12..	0.1477	-0.2224	0.0624	e0s2O...4+..	0.8693	0.4938	1.0008
F...(.....	0.2182	0.1022	0.0918	S2E0Br..4-..	0.6528	1.1933	0.9528	VS3-N...13..	-0.1287	0.2351	0.2093	e0s2O...5+..	-0.2222	0.2511	1.513
F...(...1...	-2.1056	-0.1212	0.0813	S2E0Cl..4-..	-0.0097	0.7084	0.4147	VS3-N...14..	-3.8404	-2.7575	-1.3585	e0s2O...6+..	-0.42	0.1181	-0.3968
F...(...C...	1.0575	0.5935	1.0121	S2E0N...2-..	1.891	0.0911	0.3147	VS3-N...15..	1.2338	0.3483	-0.2275	e0s3F...5+..	-0.3119	0.4308	-0.7865
F...(...F...	-1.4607	-0.4615	0.0196	S2E0N...3-..	-1.4932	0.6319	-0.2893	VS3-N...16..	0.1547	0.3092	-0.3092	e0s3F...6+..	-0.0075	0.3656	0.4209
F.....	0.0071	0.3546	0.3709	S2E0N...4-..	-0.238	-0.5393	-1.0262	VS3-N...8...	1.0619	1.9005	0.0041	e0s3F...7+..	0.4657	1.2567	0.8423
F...1.....	1.3108	-0.183	0.2135	S2E0N...5-..	-0.0381	-0.2288	-0.4019	VS3-N...9...	1.3635	1.1629	0.5467	e0s3F...8+..	0.3038	0.5835	0.1525
F...C...(...	0.0489	0.3559	0.3045	S2E0N...6-..	0.2502	1.4247	0.2846	VS3-O...4...	1.2671	0.0219	0.199	e0s3Cl..8+..	3.0555	3.7714	2.4072
F...C.....	-0.8274	-0.2404	0.4288	S2E0N...7-..	0.3113	0.3157	0.4635	VS3-O...5...	0.1492	0.134	-0.2411	e0s3Cl..9+..	-1.37	-0.2699	-0.4749
F...c...1...	-0.4877	-0.1123	0.4904	S2E0N...8-..	-1.0901	-1.3214	-1.616	VS3-O...7...	-0.4948	-0.9889	-0.405	e0s3N...11+.	0.1284	0.0121	0.0355
EC0-C...1...	0.0787	0.7205	0.9103	S2E0N...9-..	0.3703	-0.2282	-0.0439	[AA7].....	-0.5286	-0.4535	-0.0588	e0s3N...12+.	1.2153	0.4111	1.2216
EC0-C...2...	0.0394	0.2752	0.414	S2E0O...2-..	0.3295	0.385	0.6192	[AA8].....	0.3814	0.4001	0.7044	e0s3N...13+.	0.0223	0.0427	0.062
EC0-C...3...	-0.2664	-0.0335	-0.7607	S2E0O...3-..	-0.2964	1.685	-0.1497	[nH].....	0.7513	-0.4346	-0.1057	e0s3N...14+.	-0.1423	0.4896	0.3292
EC0-C...4...	-0.0287	-0.0089	-0.173	S2E0O...4-..	-0.2412	0.5107	0.0914	c...(.....	-1.0207	0.1039	0.1999	e0s3N...15+.	-0.2272	0.2426	0.534
EC0-F...1...	0.2106	-0.1536	0.3526	S3E0C...0-..	2.1294	0.6991	0.5189	c...(...1...	0.2999	0.4308	0.3637	e0s3N...16+.	-0.2996	-0.3817	-0.0011
EC0-Br..1...	1.2157	-0.138	0.0551	S3E0C...1-..	-0.5584	-1.0472	-0.7503	c...(...2...	0.0036	-0.1287	-0.1131	e0s3N...17+.	-0.3124	0.1111	-0.5107
EC0-Cl..1...	0.4803	-0.1188	0.9454	S3E0C...10-.	0.1805	0.2807	0.368	c...(...C...	0.3427	0.3725	1.405	e0s3N...18+.	1.0155	0.1432	-0.2568
EC0-N...1...	-0.1478	-0.7791	-0.5174	S3E0C...11-.	0.4111	0.222	-0.4098	c...(...F...	0.2151	0.3137	0.8251	e0s3N...19+.	-0.0983	-1.0361	-1.6185
EC0-N...2...	-1.5547	-0.416	-0.974	S3E0C...12-.	-1.1972	-1.9273	-0.6203	c...(...O...	-0.58	-0.6375	-0.4721	e0s3N...9+..	-0.1019	-0.5463	-0.4234
EC0-N...3...	-0.2897	-1.0239	-0.2728	S3E0C...13-.	0.1319	0.283	-0.2408	c...(...c...	0.7183	0.3909	0.2654	e0s3O...5+..	0.9833	1.3084	0.208
EC0-O...1...	0.0134	0.0306	0.5873	S3E0C...14-.	0.8671	0.5412	-0.072	c.....	0.3778	0.3603	0.0465	e0s3O...6+..	-0.1774	-0.1754	0.3929
EC0-O...2...	-0.0489	-0.2923	0.0545	S3E0C...15-.	2.1275	1.541	0.2574	c...1...(...	0.7465	1.2073	0.2406	e0s3O...8+..	0.7837	1.9416	0.3576
Br.....	0.7117	0.3525	1.0822	S3E0C...16-.	-0.274	0.3042	0.2808	c...1.....	0.2163	0.0273	0.0952	e0nnC...102+	2.3037	2.3725	1.1327
Cl..(.....	0.3793	-0.1155	-0.2131	S3E0C...2-..	0.2617	0.0697	-0.2123	c...1...C...	-0.1846	0.0078	0.2782	e0nnC...111+	-0.0749	0.3406	0.8425
Cl..(...1...	0.449	0.1921	0.4992	S3E0C...3-..	1.5138	1.4024	0.0895	c...1...F...	-0.5098	-0.4047	1.6875	e0nnC...213+	-1.264	-1.8913	-1.2618

Cl.....	0.1891	0.8898	0.5926	S3E0C...4-..	0.2772	0.1816	0.3841	c...1...N...	0.3918	-0.0116	-0.424	e0nnC...222+	0.3349	0.2277	0.4882
Cl..c...1...	1.6426	0.8325	0.6114	S3E0C...5-..	1.2196	0.4043	0.1529	c...1...c...	-0.3096	-0.6672	0.7524	e0nnC...306+	-0.2993	0.5691	0.3694
HALO10000000	-1.4463	-1.0855	-0.6764	S3E0C...6-..	0.453	0.2986	0.3117	c...2...(...	0.8616	-0.8595	0.2418	e0nnC...315+	0.932	1.2264	0.6644
HALO10100000	1.2849	0.1211	1.7282	S3E0C...7-..	0.5204	0.4945	-0.2583	c...2.....	-0.2718	0.2435	0.0583	e0nnC...324+	0.9501	0.1769	-0.3685
HALO11000000	1.2268	1.3882	0.7425	S3E0C...8-..	-0.5148	-0.2155	0.374	c...2...c...	0.3023	0.0003	0.1318	e0nnC...333+	0.4169	0.0866	0.0584
N...(.....	2.2029	0.6325	1.8556	S3E0C...9-..	0.1953	0.376	0.1361	c...C.....	0.3852	0.0307	-1.2665	e0nnC...417+	1.3076	0.7646	0.3138
N...(...1...	-0.335	-0.1561	-0.4995	S3E0F...3-..	0.2521	0.1865	0.0332	c...C...O...	1.8316	1.8624	1.4041	e0nnF...111+	0.2683	-0.3738	0.2886
N...(...2...	1.2411	0.7094	0.6523	S3E0F...4-..	0.7129	0.3035	0.371	c...F.....	0.0276	0.2868	-0.4313	e0nnBr..111+	1.1479	-0.5498	0.1861
N...(...C...	0.3388	1.6976	1.6575	S3E0F...5-..	0.5849	0.3219	0.2478	c...Cl.....	1.8713	0.6267	-0.026	e0nnCl..111+	1.4231	1.182	0.6668
N...(...F...	-0.3763	-0.0173	-0.3993	S3E0F...6-..	-0.1968	0.5845	0.354	c...N.....	0.0543	0.5912	0.1804	e0nnN...111+	-0.8107	0.2194	-0.262
N...(...Cl..	1.3792	0.9904	0.3156	S3E0Cl..6-..	3.5271	2.7863	2.6457	c...c...(...	-0.5561	0.5906	0.1144	e0nnN...213+	1.0887	0.4461	-0.2564
N.....	-0.5832	-0.0039	-0.1445	S3E0Cl..7-..	-0.0023	-1.3405	1.7365	c...c.....	-0.446	0.2399	0.1336	e0nnN...222+	0.0691	-0.3652	-0.2271
N...1.....	-1.4179	-1.0107	-0.7082	S3E0N...10-.	0.5715	0.3546	-0.137	c...c...1...	0.8172	0.5666	-0.1625	e0nnN...333+	-0.2184	-0.0427	-0.1709
N...1...C...	0.2821	-0.1165	-0.0284	S3E0N...11-.	-0.5764	-0.3881	-0.778	c...c...2...	-1.1999	-1.6347	-2.6721	e0nnO...111+	0.4011	0.1783	0.2319
N...2.....	1.1754	1.458	0.5679	S3E0N...12-.	2.2533	1.7564	0.6653	c...c...c...	-0.2415	-0.0578	0.1654	e0nnO...222+	1.4443	0.0121	0.2816
N...=.....	1.5971	1.7668	0.1295	S3E0N...13-.	-0.048	0.3884	1.2346	c...n...(...	-0.0612	-0.7385	0.3766	n...(.....	0.1845	0.3663	0.1902
N...=...C...	5.9903	6.2982	3.2634	S3E0N...14-.	-0.5342	-1.2476	-0.9175	c...n...1...	0.0683	-0.0329	0.0845	n...(...c...	0.1265	-0.1749	0.0169
N...C...(...	-0.0752	-0.3603	-0.2294	S3E0N...15-.	0.17	-0.2484	0.2153	c...n...c...	0.8703	0.74	0.1709	n.....	0.0809	0.3635	0.2927
N...C.....	0.3744	0.1831	-0.1215	S3E0N...4-..	0.3588	1.1083	-0.0313	[xyx#].....	0.3094	0.5213	0.6203	n...1...(...	-0.1585	0.345	-0.2577
N...C...1...	-0.0161	0.3493	-0.0931	S3E0N...7-..	0.2544	0.2211	0.1644	[xyx10].....	0.48	0.4755	0.2831	n...1.....	-0.5831	-0.9384	-0.5053
N...C...C...	-4.8593	-3.5119	-2.8109	S3E0N...8-..	-0.0086	0.5807	0.1263	[xyx4].....	2.7515	2.5476	2.3877	n...1...c...	-0.3552	-0.1631	0.1866
N...c...1...	0.1003	0.0217	0.4924	S3E0N...9-..	0.3652	0.9045	-0.2315	[xyx6].....	0.129	0.3907	0.1764	n...2...(...	0.427	1.2518	0.6257
O...(.....	0.869	0.755	0.4135	S3E0O...2-..	-0.2659	0.636	0.2404	[xyx7].....	-0.2148	-0.5452	-0.6527	n...2.....	1.0431	0.6374	-0.6087
O...(...C...	1.0591	0.1644	1.308	S3E0O...3-..	0.036	0.2923	0.1315	[xyx8].....	0.8432	0.447	0.6329	n...c...(...	-1.4168	-0.5151	0.3674
O.....	0.0831	0.0257	0.4964	S3E0O...4-..	0.145	0.5457	0.0094	[xyyx0].....	-0.1128	-0.1695	0.3581	n...c.....	0.5292	1.1185	0.7165
O...=...(...	-0.5894	-0.4562	-1.3163	S3E0O...6-..	-1.2053	-0.223	-0.8336	[xyyx1].....	0.444	0.0913	0.3917	n...c...1...	0.0932	1.305	1.2119
O...=.....	0.0971	0.3697	0.322	PT2-C...1...	-2.1536	-1.4821	-1.3868	[xyzyx0]....	0.4959	0.1709	0.2996	n...c...2...	-0.2265	-0.4736	-0.0489
O...C...(...	0.0776	0.3492	0.4008	PT2-C...2...	0.2908	0.4681	0.0268	[xyzyx1]....	0.2273	-0.7294	0.4074	n...c...c...	1.2842	1.1049	2.3328
O...C.....	0.1807	0.215	0.0126	PT2-C...3...	-0.0622	0.0667	0.0015	[xyzyx2]....	-1.4101	-0.7549	0.0968				
P2E0C...0-..	0.068	1.0467	-0.2934	PT2-C...4...	0.4602	0.4184	0.0318	[xyzyx3]....	0.3643	0.3725	1.1756				