

Supplementary material

QSAR modeling of sphingomyelin synthase 2 inhibitors as potential anti-atherosclerotic agents

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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	<chem>O=C(c1cccc1OCc1cccc1)NCc1cccc1</chem>	4.466	212.8467	5.0057	-0.5397	Ts	161.7	4.8622	-0.3962	Tr	192.0838	5.0245	-0.5585	Ts
2	<chem>O=C(c1cccc1OCc1cccc1)NCc1ccco1</chem>	4.31	194.9352	4.4864	-0.1764	Tr	151.761	4.4647	-0.1547	Ts	181.0138	4.6273	-0.3173	Tr
3	<chem>O=C(c1cccc1OCc1cccc1)NC1CCCCC1</chem>	4.363	199.9763	4.6325	-0.2695	Ts	141.3195	4.0472	0.3158	Tr	173.6847	4.3643	-0.0013	Ts
4	<chem>O=C(c1cccc1OCc1cccc1)Nc1cccn1</chem>	4.932	221.6138	5.2598	-0.3278	Ts	166.0163	5.0348	-0.1028	Tr	199.6628	5.2964	-0.3644	Tr
5	<chem>O=C(c1cccc1OCc1cccc1)Nc1ccnc1</chem>	5.495	213.4823	5.0241	0.4709	Tr	168.1532	5.1202	0.3748	Tr	197.1759	5.2072	0.2878	Tr
6	<chem>O=C(c1cccc1OCc1cccc1F)Nc1cccn1</chem>	5.456	235.6016	5.6654	-0.2094	Ts	177.1477	5.4799	-0.0239	Tr	217.3225	5.9301	-0.4741	Tr
7	<chem>O=C(c1cccc1OCc1cccc1Cl)Nc1cccn1</chem>	5.959	239.7461	5.7855	0.1735	Tr	181.9187	5.6707	0.2883	Tr	218.3012	5.9652	-0.0062	Tr
8	<chem>O=C(c1cccc1OCc1cccc1C)Nc1cccn1</chem>	5.824	229.8703	5.4992	0.3248	Tr	175.3043	5.4062	0.4178	Tr	208.8883	5.6275	0.1965	Tr
9	<chem>CCc1cccc1COc1cccc1C(=O)Nc1cccn1</chem>	6.056	232.763	5.5831	0.4729	Tr	169.3155	5.1667	0.8893	Ts	208.8661	5.6267	0.4293	Tr
10	<chem>O=C(c1cccc1OCc1cccc1C(F)F)Nc1cccn1</chem>	5.678	243.6948	5.9	-0.222	Tr	177.3891	5.4896	0.1884	Tr	206.0323	5.525	0.153	Ts
11	<chem>N#Cc1cccc1COc1cccc1C(=O)Nc1cccn1</chem>	4.498	211.8075	4.9755	-0.4775	Tr	157.6853	4.7016	-0.2036	Tr	202.7553	5.4074	-0.9094	Tr
12	<chem>Fc1ccc(c1)COc1cccc1C(=O)Nc1cccn1</chem>	5.796	232.4921	5.5752	0.2208	Tr	178.8054	5.5462	0.2498	Tr	205.6458	5.5111	0.2849	Tr
13	<chem>Clc1ccc(c1)COc1cccc1C(=O)Nc1cccn1</chem>	5.854	232.3901	5.5723	0.2817	Tr	179.3452	5.5678	0.2862	Tr	202.76	5.4076	0.4464	Tr
14	<chem>N#Cc1ccc(c1)COc1cccc1C(=O)Nc1cccn1</chem>	4.217	213.6209	5.0281	-0.8111	Tr	160.1027	4.7983	-0.5813	Tr	195.2391	5.1377	-0.9207	Ts
15	<chem>Fc1ccc(c1)COc1cccc1C(=O)Nc1cccn1)Cl</chem>	6.131	251.492	6.1261	0.0049	Tr	193.814	6.1464	-0.0154	Tr	207.7397	5.5862	0.5448	Ts
16	<chem>O=C(c1cccc1OCc1c(F)ccc1Cl)Nc1cccn1</chem>	5.824	246.5124	5.9817	-0.1577	Tr	190.0362	5.9953	-0.1713	Tr	218.4873	5.9719	-0.1479	Tr
17	<chem>Clc1ccc(c1)COc1cccc1C(=O)Nc1cccn1)Cl</chem>	6.004	246.0622	5.9687	0.0353	Tr	192.1312	6.0791	-0.0751	Tr	206.1415	5.5289	0.4751	Ts
18	<chem>O=C(c1cccc1OCc1ccc(c1F)Cl)Nc1cccn1</chem>	6.161	246.8233	5.9907	0.1703	Tr	186.4696	5.8527	0.3083	Ts	203.7446	5.4429	0.7181	Tr
19	<chem>O=C(c1cccc1OCc1ccc(c1F)Cl)Nc1cccn1</chem>	5.509	246.8233	5.9907	-0.4817	Tr	186.4696	5.8527	-0.3437	Tr	203.7446	5.4429	0.0661	Ts
20	<chem>Fc1ccc(c1)COc1cccc1C(=O)Nc1cccn1)C</chem>	6.131	237.8394	5.7303	0.4007	Tr	185.211	5.8024	0.3286	Ts	208.7563	5.6227	0.5083	Tr
21	<chem>Clc1ccc(c1)COc1cccc1C(=O)Nc1cccn1)C</chem>	5.959	237.7374	5.7273	0.2317	Ts	185.7508	5.824	0.135	Ts	205.8705	5.5192	0.4398	Tr
22	<chem>O=C(c1cccc1OCc1ccc(c1C)Cl)Nc1cccn1</chem>	5.42	241.382	5.833	-0.413	Tr	180.915	5.6306	-0.2106	Tr	202.8838	5.412	0.008	Tr
23	<chem>O=C(c1cccc1OCc1c(C)ccc1C)Nc1cccn1</chem>	6.051	235.9443	5.6753	0.3757	Tr	181.9791	5.6731	0.3779	Tr	212.1697	5.7452	0.3058	Tr
24	<chem>COc1ccc(c1)COc1cccc1C(=O)Nc1cccn1)OC</chem>	5.553	219.8874	5.2098	0.3432	Tr	173.8078	5.3464	0.2066	Ts	197.2829	5.211	0.342	Tr
25	<chem>COc1cc(Cl)ccc1COc1cccc1C(=O)Nc1cccn1</chem>	6.174	235.6224	5.666	0.508	Tr	177.209	5.4824	0.6916	Tr	210.887	5.6992	0.4748	Tr
26	<chem>COCCOc1cc(Cl)ccc1COc1cccc1C(=O)Nc1cccn1</chem>	4.936	228.9288	5.4719	-0.5359	Tr	180.1408	5.5996	-0.6636	Tr	203.5242	5.435	-0.499	Ts
27	<chem>COCCCOc1cc(Cl)ccc1COc1cccc1C(=O)Nc1cccn1</chem>	5.387	236.0212	5.6775	-0.2905	Tr	184.4724	5.7728	-0.3858	Tr	204.9817	5.4873	-0.1003	Tr
28	<chem>ClCCCCOc1cccc1COc1cccc1C(=O)Nc1cccn1</chem>	5.886	245.0568	5.9395	-0.0535	Tr	191.6615	6.0603	-0.1743	Tr	228.3855	6.327	-0.441	Tr
29	<chem>ClCCCCCOc1cccc1COc1cccc1C(=O)Nc1cccn1</chem>	6.174	254.6737	6.2183	-0.0443	Tr	193.1781	6.121	0.053	Tr	232.4665	6.4735	-0.2995	Tr
30	<chem>ClCCCCCOc1cccc1COc1cccc1C(=O)Nc1cccn1</chem>	6.328	259.18	6.349	-0.021	Ts	195.4234	6.2108	0.1172	Ts	235.9646	6.599	-0.271	Tr

31	CCCCCOC1ccc(cc1COc1cccc1C(=O)Nc1cccn1)Cl	6.284	260.5714	6.3893	-0.1053	Tr	195.6212	6.2187	0.0653	Tr	227.7255	6.3034	-0.0194	Tr
32	CCCCCOC1ccc(cc1COc1cccc1C(=O)Nc1cccn1)Cl	6.367	265.0777	6.52	-0.153	Tr	197.8665	6.3085	0.0585	Tr	231.2237	6.4289	-0.0619	Tr
33	N#CC(c1cccc1OCc1cccc1)Nc1cccc1	4.87	193.2597	4.4378	0.4322	Tr	158.8082	4.7465	0.1235	Tr	187.965	4.8767	-0.0067	Ts
34	O=C(c1cccc1OCc1cccc1)Nc1cccc1	4.873	225.5428	5.3738	-0.5008	Ts	164.6764	4.9812	-0.1082	Tr	195.7141	5.1547	-0.2817	Tr
35	CN(C(=O)c1c(OCc2cccc2)c2cccc2n(c1=O)C)Cc1cc(cc(c1)C(F)(F)F)C(F)(F)F	3.215	156.9518	3.3851	-0.1701	Tr	130.2064	3.6028	-0.3878	Ts	142.2004	3.2346	-0.0196	Ts
36	CN(C(=O)c1c(N2CCCC2)c2cccc2n(c1=O)C)Cc1cc(cc(c1)C(F)(F)F)C(F)(F)F	3.022	122.3235	2.3812	0.6408	Tr	99.66351	2.3814	0.6406	Tr	129.6891	2.7857	0.2363	Tr
37	CN(C(=O)c1c(N2CCCC2)c2cccc2n(c1=O)C)Cc1cc(cc(c1)C(F)(F)F)C(F)(F)F	1.959	128.8538	2.5705	-0.6115	Tr	105.3381	2.6083	-0.6493	Tr	128.741	2.7516	-0.7926	Tr
38	CN(C(=O)c1c(OCOCc2cccc2)c2cccc2n(c1=O)C)Cc1cc(cc(c1)C(F)(F)F)C(F)(F)F	3.42	162.9241	3.5583	-0.1383	Tr	130.8248	3.6275	-0.2075	Tr	152.9288	3.6195	-0.1995	Tr
39	CCCOc1c(C(=O)N(Cc2cc(cc(c2)C(F)(F)F)C(F)(F)F)C)c(=O)n(c2c1cccc2)C	2.678	146.8754	3.093	-0.415	Tr	117.2821	3.0859	-0.4079	Tr	122.607	2.5316	0.1464	Ts
40	CC(CCOc1c(C(=O)N(Cc2cc(cc(c2)C(F)(F)F)C(F)(F)F)C)c(=O)n(c2c1cccc2)C)C	3.456	145.7841	3.0613	0.3947	Tr	120.2264	3.2037	0.2523	Tr	135.2871	2.9865	0.4695	Tr
41	CN(C(=O)c1c(OC(CCC(F)(F)F)c2cccc2n(c1=O)C)Cc1cc(cc(c1)C(F)(F)F)C(F)(F)F	3.921	158.0671	3.4175	0.5035	Ts	133.2855	3.7259	0.1951	Ts	136.4274	3.0274	0.8936	Tr
42	CN(C(=O)c1c(OC(CCCc2cccc2)c2cccc2n(c1=O)C)Cc1cc(cc(c1)C(F)(F)F)C(F)(F)F	3.678	173.2918	3.8589	-0.1809	Tr	131.5643	3.6571	0.0209	Tr	160.4345	3.8889	-0.2109	Ts
43	CN(C(=O)c1c(OC(CCC2CCCC2)c2cccc2n(c1=O)C)Cc1cc(cc(c1)C(F)(F)F)C(F)(F)F	3.319	170.7423	3.7849	-0.4659	Ts	130.6205	3.6193	-0.3003	Tr	148.3493	3.4552	-0.1362	Tr
44	O=C(N1CCC(CC1)CCCOc1c(C(=O)N(Cc2cc(cc(c2)C(F)(F)F)C(F)(F)F)C)c(=O)n(c2c1cccc2)C)OC(C)(C)C	4.523	188.6545	4.3043	0.2187	Ts	140.3706	4.0092	0.5138	Tr	175.0577	4.4136	0.1094	Tr
45	COc1cc(cc(c1)OC)CN(C(=O)c1c(OC(CCC2CCN(CC2)C(=O)OC(C)(C)C)c2cccc2n(c1=O)C)C	4.041	167.8367	3.7007	0.3403	Ts	132.7577	3.7048	0.3362	Tr	158.7649	3.8289	0.2121	Tr
46	CCOc1cc(cc(c1)OCC)CN(C(=O)c1c(OC(CCC2CCN(CC2)C(=O)OC(C)(C)C)c2cccc2n(c1=O)C)C	3.42	166.1029	3.6504	-0.2304	Ts	136.2401	3.8441	-0.4241	Ts	155.945	3.7278	-0.3078	Tr
47	COc1cc(cc(c1)OC)CN(C(=O)c1c(OC(CCC2CCN(CC2)C(=O)OC(C)(C)C)c2cccc2n(c1=O)C)C	2.796	148.6235	3.1437	-0.3477	Ts	125.605	3.4188	-0.6228	Ts	158.068	3.8039	-1.0079	Tr
48	COc1cc(cc(c1)OC)CN(C(=O)c1c(OC(CCC2CCN(CC2)C(=O)OC(C)(C)C)c2cccc2n(c1=O)C)C	3.886	165.0164	3.6189	0.2671	Tr	139.0239	3.9554	-0.0694	Tr	160.5884	3.8944	-0.0084	Tr
49	COc1cc(cc(c1)OC)CN(C(=O)c1c(OC(CCC2CCN(CC2)C(=O)OC2(C)CC2)c2cccc2n(c1=O)C)C	3.523	171.7291	3.8136	-0.2906	Tr	135.1535	3.8006	-0.2776	Ts	150.2536	3.5236	-0.0006	Ts
50	O=C(N1CCC(CC1)CCCOc1c(C(=O)N(Cc2cc(cc(c2)C(F)(F)F)C(F)(F)F)C)c(=O)n(c2c1cccn2)C)OC1(C)CC1	4.328	193.4988	4.4447	-0.1167	Tr	152.4437	4.492	-0.164	Tr	182.4142	4.6775	-0.3495	Tr
51	COc1cc(CN(C(=O)c2c(OC(CCC3CCN(CC3)C(=O)OC3(C)CC3)c3cccn3n(c2=O)C)C)cc(c1)C(F)(F)F	4.347	178.8292	4.0194	0.3276	Tr	148.8595	4.3487	-0.0017	Ts	169.498	4.2141	0.1329	Tr

Table S2. Y-randomization of the best conformational-independent QSAR model (best optimization run) for three independent splits

0	0.9087	0.8907	0.9098	0.9496	0.8706	0.8622
1	0.0041	0.069	0.0531	0.0326	0.112	0.2024
2	0.0012	0.0003	0.0209	0.0043	0.0035	0.1849
3	0.0887	0.1878	0.0233	0.1523	0.1154	0.045
4	0.0034	0.0005	0.0113	0.0038	0.0936	0.0177
5	0.0127	0.0307	0.0783	0.1507	0.0321	0.2207
6	0.0013	0.0365	0.0011	0.0001	0.109	0.0009
7	0.0084	0.0312	0.0061	0.0714	0.0061	0
8	0.0428	0.1349	0.0028	0.1472	0.1238	0.069
9	0.002	0.1988	0.0534	0.087	0.0359	0.4832
10	0.0519	0.0372	0.0433	0.4174	0.0303	0.0966
R_r^2	0.0216	0.0727	0.0294	0.1067	0.0662	0.1321
$^C R_p^2$	0.8979	0.8536	0.895	0.8946	0.8369	0.7935
$^C R_p^2 = R \times (R^2 - R_r^2)^{1/2}$ should be > 0.5						

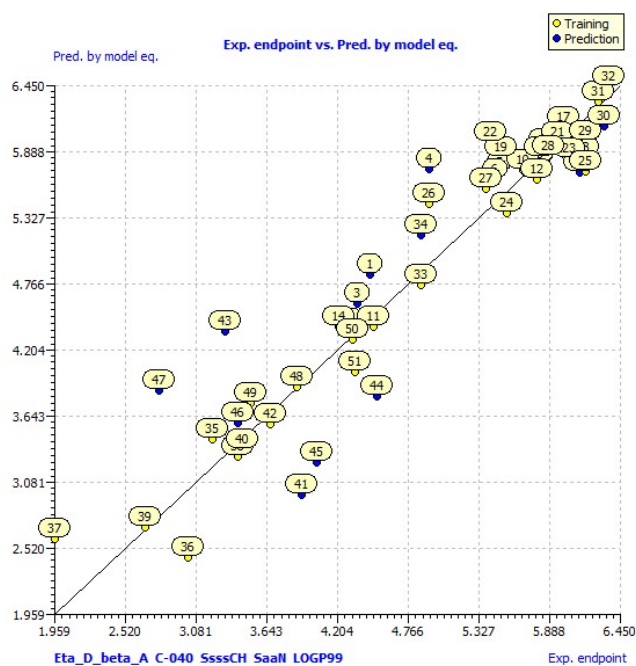


Figure S2. Graphical representation of developed QSAR model with GA-MLR method.

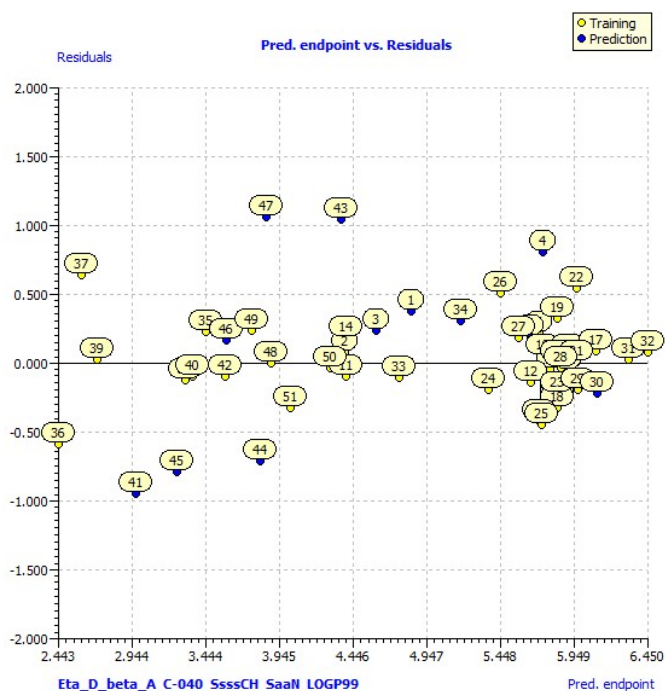


Figure S3. Difference between experimental and calculated pIC50 values.

Table S3. The list of SAKs together with their correlation weights for the three runs of the Monte Carlo optimization

SA(CW)	CW			SA(CW)	CW			SA(CW)	CW		
	Run 1	Run 2	Run 3		Run 1	Run 2	Run 3		Run 1	Run 2	Run 3
10011000000	0.35132	-0.53063	0.36493	P3E0N...2-..	0.28165	-0.33181	-0.90029	PT3-F...2...	0.31793	0.06637	0.37476
10011000100	0.43689	0.13129	2.33622	P3E0N...3-..	-1.14751	2.86331	-5.78355	PT3-Cl...2...	0.3596	-1.54317	2.17869
10011001000	0.35024	-0.48188	-0.89997	P3E0O...1-..	-0.09428	-4.56238	-3.84769	PT3-Cl...3...	0.15549	0.28409	-0.00629
(... (.....	-0.85382	-0.59507	-0.51747	P3E0O...2-..	2.44893	1.1044	0.26047	PT3-N...3...	0.14772	0.20373	0.22428
(.....	-0.91955	-0.99136	-0.28377	P3E0O...3-..	-0.62513	0.71983	0.13964	PT3-N...4...	0.32228	-1.79676	-1.44134
(...C...(...	0.3128	0.21298	0.96189	P4E0C...0-..	2.11915	0.01107	-0.86892	PT3-N...5...	0.17947	-0.5012	-0.35453
(...F...(...	-0.49576	-0.61689	-0.39806	P4E0C...1-..	2.13154	2.00758	0.20218	PT3-O...3...	0.32894	0.22456	2.40429
(...Cl...(...	-1.14238	-2.40972	-2.99893	P4E0C...10-	3.06733	3.12176	-0.49618	PT3-O...4...	0.33371	0.3691	0.38232
(...N...(...	-0.91325	-0.85094	0.03513	P4E0C...11-	0.14867	-0.98707	-0.99622	PT3-O...5...	1.26921	0.76419	-0.36066
(...c...(...	5.34982	4.74388	3.56112	P4E0C...2-..	0.37596	0.11956	0.03574	PT4-C...1...	0.10137	-0.583	2.16399
(...n...(...	0.33984	0.36141	-0.93303	P4E0C...18-	0.1022	-0.86029	0.52663	PT4-C...10..	0.23816	0.17242	-0.27638
++++F---B2==	0.05707	2.66614	0.95542	P4E0C...3-..	0.21667	2.24515	1.42956	PT4-C...11..	0.48528	-0.92975	-0.58432
++++F---N===	0.25757	0.29639	2.05544	P4E0C...4-..	2.06452	0.35076	0.13021	PT4-C...12..	-0.07233	1.00027	1.05317
++++F---O===	2.35589	2.1542	2.03234	P4E0C...5-..	0.47676	-0.80111	2.29863	PT4-C...13..	0.19454	0.3228	0.2866
++++CL--N==	0.52361	0.07011	2.0375	P4E0C...6-..	-0.49367	0.2564	2.33052	PT4-C...14..	0.11245	-1.11815	0.11671
++++CL--O==	2.16621	2.29707	0.16695	P4E0C...7-..	0.13744	0.44349	0.3253	PT4-C...2...	-0.98973	-0.76165	0.25507
++++Cl--B2==	0.23507	0.70088	2.3659	P4E0C...8-..	0.41597	0.10706	0.19891	PT4-C...20..	-0.14083	-0.09172	0.18789
++++N---B2==	0.57232	3.69819	2.41296	P4E0C...9-..	0.29242	0.33301	0.38108	PT4-C...3...	0.45292	-1.28786	2.36927
++++N---O===	4.44369	6.20738	3.25608	P4E0F...3-..	0.39353	0.05479	0.06085	PT4-C...4...	0.03048	-0.59268	0.12405
++++O---B2==	-0.59366	-0.57871	-1.83575	P4E0Cl...1-..	0.22096	0.13773	2.31049	PT4-C...5...	0.4749	0.37534	0.03835
1...(.....	0.15311	-0.61785	0.13718	P4E0Cl...4-..	-0.07315	0.59908	-0.1126	PT4-C...6...	2.15388	0.23881	0.45972
1.....	0.3326	0.20497	0.35164	P4E0N...0-..	0.52801	0.34168	0.31685	PT4-C...7...	0.00933	0.26345	0.40663
1...C...(...	3.5827	4.06599	2.59849	P4E0N...1-..	-0.07626	1.96231	0.35296	PT4-C...8...	0.45885	0.17906	-1.28272
1...c...(...	0.25077	0.28605	0.06738	P4E0N...3-..	-2.8845	-1.05364	-3.28372	PT4-C...9...	0.33908	0.1894	0.13291
2...(.....	-3.78507	-2.046	-4.08832	P4E0N...4-..	0.09752	0.42415	2.11226	PT4-F...4...	0.43273	0.37875	0.19593
2.....	-0.23116	-0.11825	-0.76376	P4E0N...5-..	0.04726	0.36135	-0.182	PT4-Cl...2...	-0.10789	2.22614	-0.35639
2...c...(...	-0.70066	-0.62944	0.29603	P4E0N...6-..	0.2261	0.33013	0.24528	PT4-Cl...5...	1.99865	1.94757	2.41766
2...c...1...	-0.78579	0.2971	0.38896	P4E0N...7-..	-0.82718	-0.89458	-2.22099	PT4-N...3...	0.293	0.27156	0.2699
2...n...(...	0.32936	1.24236	0.72954	P4E0O...4-..	0.28447	0.59324	0.47821	PT4-N...6...	2.36206	2.37483	0.16846
=...(.....	0.2346	-0.78541	0.66703	P4E0O...7-..	0.20703	0.41445	0.08065	PT4-N...8...	-0.65798	0.18712	0.09342

=.....	0.62749	0.25644	0.49554	NNC-C...101.	0.25366	-0.88205	0.21427	PT4-N...9...	0.2811	0.3817	0.49519
=...1.....	0.47364	0.7299	0.40172	NNC-C...110.	0.35646	2.31553	0.49037	PT4-O...5...	0.07169	0.46877	0.18672
=...C...(...	-0.18122	2.10975	-0.11371	NNC-C...211.	0.35731	0.48699	0.19772	PT4-O...6...	2.24962	0.43487	-0.38815
=...O...(...	-0.11764	0.29381	0.40165	NNC-C...220.	0.13162	0.17743	0.44051	PT4-O...8...	0.13636	0.21895	0.0233
C...(.....	-0.67097	-0.21356	-0.56477	NNC-C...303.	0.08668	0.20689	0.23306	PT4-O...9...	-2.91294	-1.63669	-1.28586
C...(1...	0.48283	0.63363	0.41409	NNC-C...312.	0.04781	0.67628	-0.51448	Nmax.1.....	3.3281	4.28418	2.20762
C...(2...	5.70197	1.83618	2.11199	NNC-C...321.	0.15618	0.16022	0.94006	Nmax.2.....	-0.16608	-1.64458	-0.9317
C...(=...	0.45223	-0.76475	-0.88741	NNC-C...330.	-0.43751	0.24811	-0.78764	Omax.2.....	0.13659	2.21818	0.26553
C...(C...	0.08301	0.01918	0.0284	NNC-C...413.	0.40933	0.09537	0.38471	Omax.3.....	4.6229	0.84214	6.87131
C.....	0.55689	0.35424	0.00429	NNC-C...431.	-1.1658	-0.52655	0.47087	VS2-C...10..	0.41708	0.26239	0.62377
C...1.....	0.5866	0.35406	0.35851	NNC-F...110.	0.4174	0.49661	0.31958	VS2-C...11..	-0.77306	0.232	-0.99776
C...2...(...	-0.55104	0.15233	-0.78314	NNC-Cl.110.	0.3297	1.14466	1.12987	VS2-C...12..	-0.59704	-0.59841	0.24861
C...2.....	0.13996	0.02678	-0.85506	NNC-N...220.	-0.49095	1.14604	1.98376	VS2-C...13..	0.22012	0.51584	0.13299
C...=.....	0.31465	0.10198	0.12618	NNC-N...330.	-0.98072	0.64823	-0.09079	VS2-C...2...	0.14974	-0.44496	0.27197
C...C...(...	0.11312	0.70294	-0.77315	NNC-O...110.	0.27198	0.29501	0.49705	VS2-C...3...	0.16647	0.49369	0.41659
C...C.....	0.12441	0.25942	0.45159	NNC-O...220.	0.36197	0.42799	-0.78649	VS2-C...4...	0.42262	0.02988	0.03415
C...C...2...	0.32665	0.20542	-0.57192	NNE0C...100-	0.03174	0.00051	0.08664	VS2-C...5...	0.1274	0.26495	0.00065
C...C...C...	-2.2028	-2.41462	-2.87674	NNE0C...109-	0.4163	0.47983	-0.92245	VS2-C...6...	-0.77538	0.2868	-1.61257
C...N...(...	0.00951	0.31119	-0.99215	NNE0C...209-	0.44492	0.38059	0.13689	VS2-C...7...	0.35792	0.30515	0.36543
C...O...(...	0.36144	0.29603	-0.70007	NNE0C...218-	0.4055	0.24372	0.49568	VS2-C...8...	0.00021	0.45431	0.06731
C...O...1...	2.2816	0.4385	0.41734	NNE0C...300-	0.33885	0.02294	2.23269	VS2-C...9...	-0.1913	1.49124	-1.78279
C...c...1...	0.35172	-0.21506	0.31097	NNE0C...309-	0.05478	0.1494	0.30902	VS2-F...5...	0.09995	0.02811	0.29709
C...c...2...	0.18149	-0.70124	0.27057	NNE0C...318-	2.40746	0.2618	0.38787	VS2-Cl.4...	0.30292	0.10539	2.30113
C3.....0...	-0.87545	2.36833	0.04388	NNE0C...327-	1.25754	0.00561	1.471	VS2-Cl.5...	2.58929	-0.57985	0.61727
C4.....0...	6.66574	8.25992	8.30711	NNE0C...409-	-0.51028	-0.90343	0.01237	VS2-N...6...	-0.09799	2.16477	0.40202
C5.....0...	2.53991	-1.05146	0.42654	NNE0C...427-	0.38125	0.48452	0.23916	VS2-N...7...	0.08149	-0.89424	0.0336
C6...A.3...	-0.06321	0.35113	0.21385	NNE0F...109-	0.49965	0.16101	-0.03046	VS2-N...8...	-0.39503	1.8919	1.43179
C6...AH.3...	2.06027	0.45318	-0.05845	NNE0Cl.109-	0.17099	2.08262	2.26174	VS2-N...9...	0.35392	-0.63484	0.5639
C6...AH.4...	-0.11078	0.02183	0.16353	NNE0N...218-	1.84156	-0.37092	-0.42026	VS2-O...5...	0.36394	0.2744	0.29156
C7.....0...	6.94193	10.18229	7.03508	NNE0N...327-	-0.10887	0.34695	-0.51325	VS2-O...6...	-0.32129	0.29987	-0.73184
BOND10000000	0.48182	1.01452	2.2636	NNE0O...109-	0.41941	0.36691	0.34815	VS2-O...7...	-2.38115	-3.52993	-2.01936
F...(...(...	0.14069	0.3093	-0.85837	NNE0O...218-	0.15192	0.00144	0.19944	VS2-O...8...	-2.34747	-0.40437	-0.90734
F...(.....	0.30444	0.20869	0.13225	NOSP11000000	7.4841	4.88942	6.3387	VS3-C...10..	0.42851	0.07917	0.46528
F...(C...	0.223	-0.61651	-0.8886	S2E0C...0-..	0.2889	0.44013	0.43948	VS3-C...11..	0.25017	0.44602	-0.64864

F...(F...	-0.80932	-0.52904	-0.75423	S2E0C...1-..	0.38415	0.08518	0.13456	VS3-C...12..	-0.94017	0.06329	0.33608
F.....	0.45554	0.35025	0.08991	S2E0C...10-	-0.95739	0.35571	0.11073	VS3-C...13..	-0.91122	-2.46147	0.20877
EC0-C...1...	0.20352	0.21342	0.26174	S2E0C...2-..	0.29029	0.58628	-0.5805	VS3-C...14..	0.24391	0.16266	-0.7949
EC0-C...2...	0.26499	0.44877	-0.73832	S2E0C...3-..	0.19394	0.13079	0.00375	VS3-C...16..	-0.80694	-1.1465	0.14956
EC0-C...3...	-0.62062	-0.86192	-0.48149	S2E0C...4-..	2.04651	0.25985	2.34736	VS3-C...17..	0.48761	0.42605	-0.4846
EC0-C...4...	5.76528	8.40464	7.51174	S2E0C...5-..	0.29618	0.18196	0.31988	VS3-C...2...	0.28381	0.28338	0.28669
EC0-F...1...	0.20719	0.47034	-0.71782	S2E0C...6-..	-0.5773	0.14657	0.16813	VS3-C...3...	0.11888	0.39285	0.0325
EC0-Cl..1...	0.05837	-0.8368	0.09077	S2E0C...7-..	0.20178	-0.96646	0.09063	VS3-C...4...	0.47065	-0.64669	0.30205
EC0-N...2...	4.77885	4.374	0.0434	S2E0C...8-..	0.1528	0.60035	0.00045	VS3-C...5...	0.3067	2.03688	0.08535
EC0-N...3...	0.46731	0.3483	-0.52763	S2E0C...9-..	0.12705	0.77809	0.2597	VS3-C...6...	0.22896	0.08899	0.32917
EC0-O...1...	2.37434	-0.15103	-0.50388	S2E0F...4-..	0.30625	0.24038	0.02466	VS3-C...7...	1.24589	1.1226	3.05816
EC0-O...2...	0.2266	0.4672	0.17118	S2E0Cl..3-..	0.39582	-0.69176	0.16946	VS3-C...8...	0.0687	0.4149	0.13092
Cl..(.....	0.22279	0.29289	0.39372	S2E0Cl..4-..	0.14029	0.08879	0.0532	VS3-C...9...	0.34934	-0.08224	2.16423
Cl..(...1...	0.38325	1.98023	0.10069	S2E0N...4-..	0.39894	2.01373	0.09904	VS3-F...4...	0.2493	-0.01776	0.20951
Cl.....	0.45386	-0.80571	0.3261	S2E0N...6-..	0.03278	0.28516	0.26498	VS3-Cl..5...	0.25443	2.13702	0.24758
Cmax.1.....	2.26986	1.74942	2.17134	S2E0O...4-..	0.02695	0.02249	0.181	VS3-Cl..6...	0.34067	-0.56024	0.74975
Cmax.2.....	-0.8456	-2.2848	-1.70205	S2E0O...5-..	0.28585	0.20489	0.41692	VS3-N...10..	-0.0725	0.94327	0.46067
HALO00000000	1.48967	0.09514	1.01317	S2E0O...6-..	-1.12412	-3.57099	-2.92146	VS3-N...13..	0.49177	0.14032	0.36733
HALO01000000	2.18075	2.29873	0.22731	S3E0C...0-..	0.2494	2.45629	0.2997	VS3-N...7...	0.21601	1.04691	2.28284
HALO10000000	0.35196	0.22623	-0.74191	S3E0C...1-..	0.26936	0.06787	0.43269	VS3-N...9...	-11.0698	-5.80905	-11.7237
N...(.....	-0.14158	-0.26323	-0.55475	S3E0C...10-	0.4538	0.43666	-0.82123	VS3-O...10..	-0.01415	0.36843	1.23614
N...(1...	-0.65358	-1.31473	0.16721	S3E0C...11-	-0.95997	0.21353	0.40615	VS3-O...11..	0.05807	0.5546	0.17534
N...(C...	1.35148	-0.77895	0.15651	S3E0C...13-	-0.25426	-1.00102	-0.51735	VS3-O...12..	0.05472	0.58514	1.93138
N...(Cl..	0.27234	1.67778	-2.20781	S3E0C...14-	0.43471	-0.19779	0.19424	VS3-O...13..	0.4224	0.14298	-0.62694
N.....	-1.44847	-3.28645	-0.7298	S3E0C...2-..	0.4194	0.0822	0.04975	VS3-O...8...	0.28251	0.2078	-0.01541
N...C.....	0.45405	0.12049	0.23797	S3E0C...3-..	0.35648	0.31233	2.13129	VS3-O...9...	-0.81417	-0.97055	-1.04872
N...c...1...	0.12963	0.16834	2.32537	S3E0C...4-..	-0.53961	0.44737	0.12453	Smax.0.....	6.85306	7.15935	4.2841
O...(.....	-0.70409	-0.50139	-0.99128	S3E0C...5-..	0.3848	0.67394	0.39418	c...(.....	0.09917	0.01242	0.17214
O...(C...	0.42618	-0.80817	0.675	S3E0C...6-..	-0.56859	-0.73059	-0.55425	c...(2...	-4.01859	-7.00115	-4.09992
O...(N...	0.33435	2.46296	2.35716	S3E0C...7-..	0.23294	0.72699	0.32427	c...(=...	0.06764	0.4608	-0.05844
O.....	0.11857	0.11923	0.12129	S3E0C...8-..	0.0344	-0.0881	0.45731	c...(C...	0.611	0.52413	0.31217
O...1.....	0.00039	0.25203	2.46952	S3E0C...9-..	0.35251	0.35533	0.03876	c...(O...	0.36407	-0.58613	0.10711
O...=...(	2.035	-0.89185	-0.6294	S3E0F...3-..	-0.54639	0.05675	0.38697	c...(C...	0.28141	0.54169	0.4344
O...=.....	-0.01674	-0.98955	-0.85337	S3E0Cl..4-..	0.31646	0.23869	-1.8954	c.....	0.45699	0.35851	0.02755

O...=...1...	0.46703	0.18269	0.01531	S3E0Cl..5-..	2.22982	1.30908	1.74259	c...1...(...	0.36935	0.62324	0.24452
O...=...C...	0.44036	-0.27559	0.44	S3E0N...10-	0.34155	-0.45242	-0.53074	c...1.....	2.00241	0.29108	0.19197
O...C...(...	0.30113	0.19605	1.91215	S3E0N...5-..	2.05082	-0.2887	0.04163	c...1...=...	-0.50183	0.32569	-0.87581
O...C.....	0.44431	0.41247	0.39379	S3E0N...7-..	0.21604	-0.69848	-0.84728	c...1...C...	-1.6814	0.59882	3.17056
O...C...1...	-2.0191	-1.20036	-0.10551	S3E0O...10-	0.19815	1.23117	-0.40701	c...1...O...	0.47391	2.18535	2.40521
O...C...C...	0.44577	-0.23038	0.32506	S3E0O...11-	0.57145	0.3745	-0.82642	c...1...c...	0.48248	0.00117	0.30668
O...c...1...	0.26001	0.15182	0.1124	S3E0O...6-..	-0.04386	0.59571	2.38848	c...2...(...	-0.78998	0.30755	0.47188
P2E0C...0-..	0.39996	-0.30419	0.46467	S3E0O...7-..	-1.44472	-3.81264	0.40831	c...2.....	-1.80902	-1.32139	-2.66333
P2E0C...1-..	0.41985	-0.64346	0.28216	S3E0O...8-..	-0.89539	-0.51681	0.67878	c...2...c...	-1.43832	-3.19473	-1.78033
P2E0C...2-..	0.31437	0.41617	0.29173	S3E0O...9-..	-0.53755	-0.89417	-1.51694	c...C...(...	0.49797	-0.63283	-0.08752
P2E0C...3-..	0.55877	-0.86504	0.09322	PT2-C...1...	0.15065	0.11112	0.11524	c...C.....	-0.87451	-1.12223	0.17022
P2E0F...1-..	2.93207	3.61423	2.35199	PT2-C...2...	0.3559	0.28169	0.02183	c...C...O...	0.25414	-0.79804	0.48982
P2E0F...2-..	0.27021	-0.90303	0.15234	PT2-C...3...	0.08686	0.1095	0.2654	c...N...(...	2.18214	0.03726	0.19175
P2E0Cl..1-..	0.59336	0.00139	0.12974	PT2-C...4...	0.43562	0.23425	0.88921	c...N.....	2.23488	2.17202	0.35976
P2E0N...0-..	0.3112	-0.57844	0.18914	PT2-C...5...	0.35792	-0.50041	0.69804	c...O.....	0.30282	-0.71818	0.2398
P2E0N...1-..	0.43642	-0.8145	0.01936	PT2-C...6...	-2.30187	-1.72203	0.90361	c...O...C...	0.03072	0.3956	0.46718
P2E0N...2-..	0.35706	0.27356	1.91663	PT2-F...2...	2.19069	3.37273	3.05057	c...C...(...	-0.72043	-0.6551	0.47854
P2E0O...0-..	0.11425	-0.78917	1.20364	PT2-F...3...	0.25588	-0.93961	0.14426	c...C.....	0.11774	0.49318	0.07046
P2E0O...1-..	0.49753	0.40146	-0.50312	PT2-Cl..2...	0.29794	2.14518	0.07897	c...C...1...	0.49676	0.42535	0.09025
P2E0O...3-..	0.00857	0.24879	0.11916	PT2-N...3...	0.41906	0.05291	-0.9444	c...C...2...	-2.74389	-1.24652	-1.40343
P3E0C...0-..	0.20148	1.93565	0.31974	PT2-N...4...	-0.20701	-0.96343	-0.81344	c...C...C...	0.29513	0.15729	0.11491
P3E0C...1-..	0.45648	2.27052	2.36794	PT2-O...2...	0.22775	0.34433	0.20854	c...n...1...	0.54795	-0.12275	0.49855
P3E0C...2-..	-0.97015	-0.56721	0.11965	PT2-O...3...	0.34289	2.30374	0.08972	n...(.....	-0.04507	0.96037	0.64009
P3E0C...3-..	-0.86332	0.26181	0.27612	PT2-O...5...	0.02133	0.64401	0.38215	n...(...O...	-0.85256	0.33401	-0.61849
P3E0C...4-..	0.26931	0.4233	-0.7295	PT3-C...1...	0.22587	-0.95643	0.21164	n...(...C...	0.45825	-0.92213	0.02448
P3E0C...5-..	-1.07435	-0.92234	-0.66481	PT3-C...2...	0.38871	0.31896	0.31336	n.....	2.45621	0.43652	0.00834
P3E0C...6-..	0.40256	0.15825	0.1915	PT3-C...3...	0.12471	-0.02628	0.04452	n...1...(...	2.43435	0.00052	0.38251
P3E0F...1-..	0.29361	0.48325	0.28635	PT3-C...4...	0.30584	0.37162	0.48096	n...1.....	0.09596	2.12819	2.78766
P3E0Cl..1-..	2.03765	1.77364	0.24402	PT3-C...5...	0.03566	2.09321	0.03	n...2.....	0.1809	0.01428	-0.24631
P3E0Cl..2-..	0.23405	1.91922	0.96799	PT3-C...6...	0.42346	-0.04635	-0.4275	n...2...c...	0.13544	-0.6059	-0.84693
P3E0N...0-..	0.74408	0.69427	0.30255	PT3-C...7...	0.1565	0.6075	0.108	n...C.....	0.14349	2.36674	0.29109
P3E0N...1-..	-1.13557	-2.9896	0.77996	PT3-C...8...	-0.86523	-0.70349	0.07258	n...C...c...	0.13244	0.00876	0.50161