Supplementary Information

In silico Approach for the Development of Novel Antiviral Compounds Based on SARS-COV-2 Protease Inhibition

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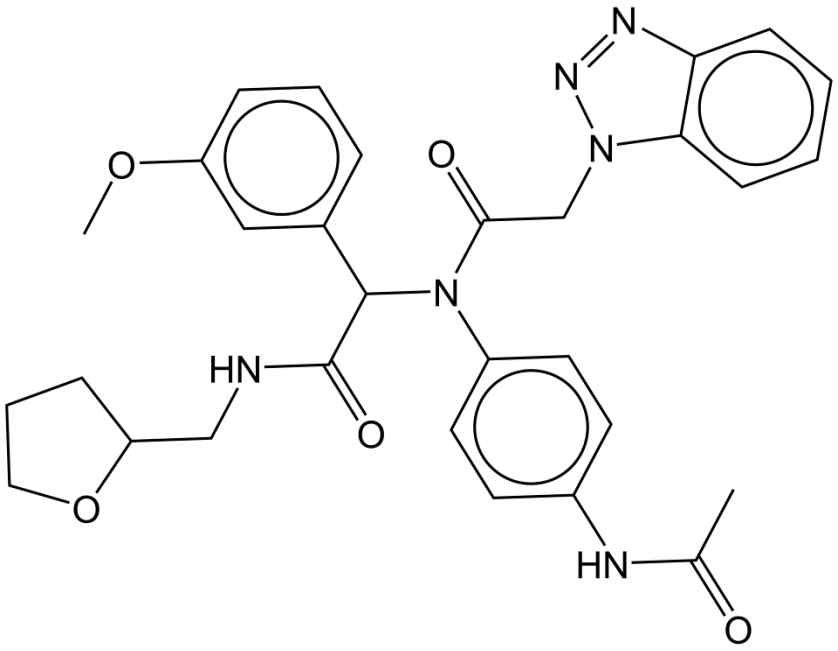
Table S1. The SMILES notation of the studied molecules, calculated values for the DCW, experimental data (Ac) – expr, the values of Ac calculated with the application of CORAL software – calc, the difference between expr and calc – diff for the built QSPR model

			Split 1				Split 2				Split 3			
ID	SMILES	Expr	DCW(1,15)	Calc	Diff	Set	DCW(1,20)	Calc	Diff	Set	DCW(2,20)	Calc	Diff	Set
1	CSc1nc2c(n1C(=O)c1ccc(cc1)OC)cc1c(c2)OCCO1	-3.035	191.0467	-2.9774	-0.0576	Training	142.2804	-2.9829	-0.0521	Training	171.4428	-3.0608	0.0258	Training
2	CCC(c1ccc(cc1)N(C(c1cccnc1)C(=O)NC1CCCC1)C(=O)c1ccco1)C	-3.348	146.9445	-3.4638	0.1158	Training	117.5586	-3.3695	0.0215	Training	131.2709	-3.5282	0.1802	Test
3	ClCC(=O)N1N=C(CC1c1ccc(c(c1)OC)OC)c1cccs1	-3.362	148.4575	-3.4471	0.0851	Training	122.827	-3.2871	-0.0749	Training	139.8657	-3.4282	0.0662	Training
4	ClCC(=O)N1N=C(CC1c1ccc(c(c1)OC)OC(F)F)c1cccs1	-3.447	158.1734	-3.34	-0.107	Training	109.3986	-3.4972	0.0502	Test	148.9344	-3.3227	-0.1243	Training
5	O=C(C(N(c1c(C)cc(cc1C)C)C(=O)Cn1nnc2c1cccc2)c1cscc1)NC(C)(C)C	-3.463	152.7398	-3.3999	-0.0631	Training	104.0824	-3.5803	0.1173	Test	131.2839	-3.5281	0.0651	Training
6	CCc1cc(=O)oc2c1ccc(c2)OC(=O)c1ccco1	-3.472	146.3027	-3.4709	-0.0011	Training	101.5378	-3.6201	0.1481	Training	135.0344	-3.4844	0.0124	Test
7	O=c1cc(C)c2c(o1)cc(cc2)OC(=O)c1ccco1	-3.524	127.8694	-3.6742	0.1502	Test	114.5477	-3.4166	-0.1074	Training	132.291	-3.5163	-0.0077	Test
8	ClCC(=O)N1NC(C(=O)C1c1ccc(cc1)OC)c1c[nH]c2c1cccc2	-3.554	141.2034	-3.5271	-0.0269	Training	103.567	-3.5884	0.0344	Training	132.5728	-3.5131	-0.0409	Training
9	COc1ccccc1OCCNC(=O)c1cc(=O)[nH]c2c1cccc2	-3.603	126.181	-3.6928	0.0898	Test	93.0717	-3.7525	0.1495	Test	120.0341	-3.6589	0.0559	Training
10	Brc1ccc(cc1)C(=O)Cn1nnc2c1cccc2	-3.603	108.5679	-3.8871	0.2841	Test	89.83337	-3.8032	0.2002	Training	93.83819	-3.9637	0.3607	Training
11	ClCC(=O)N1N=C(CC1c1ccc(cc1)C)c1cccs1	-3.622	121.6509	-3.7428	0.1208	Test	95.02927	-3.7219	0.0999	Training	114.1167	-3.7278	0.1058	Training
12	ClCC(=O)N1CCN(CC1)c1nc(CC)nc2c1c1CCC(Cc1s2)C	-3.627	135.6303	-3.5886	-0.0384	Training	98.89386	-3.6615	0.0345	Test	125.4373	-3.5961	-0.0309	Training
13	CCOc1ccc2c(c1)C(=O)C(=O)N2CC1COc2c(O1)cccc2	-3.632	126.3135	-3.6914	0.0594	Training	89.56604	-3.8073	0.1753	Test	110.1557	-3.7739	0.1419	Training
14	ClCC(=O)c1cc(n(c1C)c1cccc(c1)[N+](=O)[O-])C	-3.661	116.8458	-3.7958	0.1348	Training	93.39686	-3.7474	0.0864	Training	108.0849	-3.798	0.137	Training
15	CC(=O)c1cc([nH]c1N1CCCC1)c1ccccc1	-3.666	125.6978	-3.6982	0.0322	Training	93.3048	-3.7489	0.0829	Training	112.3184	-3.7487	0.0827	Training
16	O=C(c1cc(=O)[nH]c2c1cccc2)N1CCN(CC1)S(=O)(=O)c1c(C)c(C)cc(c1C)C	-3.684	119.8414	-3.7628	0.0788	Test	102.9719	-3.5977	-0.0863	Test	122.9421	-3.6251	-0.0589	Training
17	NC(=O)CCn1c(C(=O)c2ccc(cc2)Cl)c2c([n+]1[O-])cccc2	-3.688	116.1138	-3.8039	0.1159	Training	95.3769	-3.7165	0.0285	Training	111.8064	-3.7547	0.0667	Test
18	O=C(c1cc(=O)[nH]c2c1cccc2)N1CCN(CC1)c1cccc(c1)C(F)(F)F	-3.708	108.9754	-3.8826	0.1746	Training	83.97989	-3.8947	0.1867	Test	102.9201	-3.8581	0.1501	Training
19	COc1cc(C=NNC(=O)Cn2nnc3c2cccc3)cc(c1OC)OC	-3.714	115.6903	-3.8085	0.0945	Test	101.4737	-3.6211	-0.0929	Training	120.9777	-3.648	-0.066	Training
20	ClCC(=O)N1N=C(CC1c1ccco1)c1ccc(o1)C	-3.716	122.6417	-3.7319	0.0159	Test	93.52205	-3.7455	0.0295	Test	133.3605	-3.5039	-0.2121	Training
21	O=C(Nc1scc(c1C(=O)O)c1ccccc1)/C=C/c1cccs1	-3.718	117.9579	-3.7835	0.0655	Test	91.53872	-3.7765	0.0585	Test	114.8707	-3.719	0.001	Test
22	Clc1ccc(c(c1)n1c(O)c2c(c1O)CC(CC2)C)OC(=O)c1ccco1	-3.732	112.8091	-3.8403	0.1083	Test	88.54481	-3.8233	0.0913	Test	119.2867	-3.6676	-0.0644	Training
23	CC(c1ccc(cc1)N(C(c1cccnc1)C(=O)NC1CCCC1)C(=O)c1ccco1)C	-3.773	119.4615	-3.767	-0.006	Training	91.32691	-3.7798	0.0068	Training	113.2792	-3.7375	-0.0355	Training
24	CCC(NC(=O)C(c1cccn1C)N(C(=O)Cn1nnc2c1cccc2)c1ccc(cc1)NC(=O)C)(C)C	-3.799	106.6723	-3.908	0.109	Test	92.92627	-3.7548	-0.0442	Training	103.9515	-3.8461	0.0471	Training
25	Clc1ccc(cc1)C(=O)Oc1cccnc1	-3.8	111.7303	-3.8522	0.0522	Training	87.63408	-3.8376	0.0376	Training	101.6611	-3.8727	0.0727	Training
26	CCc1ccc2c(c1)C(NC(=O)C)C(=O)N2CCN1CCOCC1	-3.817	107.4081	-3.8999	0.0829	Test	86.17675	-3.8603	0.0433	Training	97.24054	-3.9241	0.1071	Test
27	O=c1[nH]c2ccccc2c(c1)C(=O)N1CCN(CC1)c1cccc(c1C)C	-3.823	112.6391	-3.8422	0.0192	Training	95.03444	-3.7218	-0.1012	Training	96.72072	-3.9302	0.1072	Test
28	O=C(Nc1nonc1[N+](=O)[O-])CSc1ccccn1	-3.849	114.8528	-3.8178	-0.0312	Training	85.39091	-3.8726	0.0236	Training	112.6714	-3.7446	-0.1044	Test
29	Brc1ccc(c(c1)C(=O)/C=C/c1ccccc1F)OC(=O)c1ccco1	-3.853	114.3391	-3.8235	-0.0295	Training	78.49294	-3.9805	0.1275	Training	94.80878	-3.9524	0.0994	Training
30	O=Cc1cn(nc1c1cccnc1)Cc1ccccc1	-3.858	106.0191	-3.9152	0.0572	Training	85.4899	-3.8711	0.0131	Test	101.1935	-3.8781	0.0201	Test
31	CC(=O)NC1C(=O)N(c2c1cc(Br)cc2)CCN1CCOCC1	-3.88	107.4031	-3.9	0.02	Training	87.3369	-3.8422	-0.0378	Training	115.5746	-3.7108	-0.1692	Training

32	COc1cccc(c1)C(N(C(=O)Cn1nnc2c1cccc2)Cc1ccco1)C(=O)NCc1ccco1	-3.89	103.0469	-3.948	0.058	Training	78.02785	-3.9878	0.0978	Training	89.66435	-4.0123	0.1223	Test
33	COc1ccc(cc1)N(C1(CCCCC1)C(=O)NC1CCCC1)C(=O)Cn1nnc2c1cccc2	-3.897	102.0423	-3.9591	0.0621	Training	80.24485	-3.9531	0.0561	Test	100.7647	-3.8831	-0.0139	Training
34	COc1ccccc1/C=C/C(=O)c1cc(Br)ccc1OC(=O)c1ccco1	-3.951	115.6705	-3.8088	-0.1422	Training	85.82502	-3.8658	-0.0852	Training	99.71205	-3.8954	-0.0556	Test
35	CC(=O)NC1C(=O)N(c2c1cc(F)cc2)CCN1CCOCC1	-3.959	94.73635	-4.0397	0.0807	Training	79.21946	-3.9692	0.0102	Training	85.56653	-4.06	0.101	Training
36	COc1ccc(cc1)C(N(C(=O)Cn1nnc2c1cccc2)c1ccc(cc1)NC(=O)C)C(=O)NCC1CCCO1	-3.971	88.85384	-4.1046	0.1336	Training	72.31236	-4.0772	0.1062	Training	88.76433	-4.0227	0.0517	Training
37	NC(=O)CCn1c(C(=O)c2ccc(cc2)C)c2c([n+]1[O-])cccc2	-3.971	86.25872	-4.1332	0.1622	Training	72.77988	-4.0699	0.0989	Training	83.47973	-4.0842	0.1132	Training
38	O=C1NC(=O)N(C(=O)/C/1=C/C1CNc2c1cccc2)c1ccccc1F	-3.976	100.1775	-3.9797	0.0037	Training	77.57438	-3.9949	0.0189	Training	78.69751	-4.1399	0.1639	Training
39	ClCC(=O)N(c1ccccc1)NC(=O)Nc1ccccc1	-3.984	93.5311	-4.053	0.069	Training	68.47335	-4.1372	0.1532	Test	93.04135	-3.973	-0.011	Training
40	COc1ccc2c(c1)C(=O)C(=O)N2CC1COc2c(O1)cccc2	-3.988	91.2584	-4.078	0.09	Training	76.57903	-4.0104	0.0224	Training	88.98712	-4.0202	0.0322	Test
41	NC(=O)CCn1c(C(=O)c2cc(Cl)c(c(c2)Cl)N)c2c([n+]1[O-])cccc2	-3.992	100.8193	-3.9726	-0.0194	Training	72.62637	-4.0723	0.0803	Test	89.78303	-4.0109	0.0189	Training
42	ClCC(=O)N1CCc2c(C1c1cc(Br)ccc1F)cc(c(c2)OC)OC	-3.995	96.06595	-4.025	0.03	Training	73.22992	-4.0628	0.0678	Training	104.7472	-3.8368	-0.1582	Training
43	Clc1ccc(cc1)C(=O)Cn1nnc2c1cccc2	-3.996	108.2881	-3.8902	-0.1058	Training	80.23363	-3.9533	-0.0427	Training	92.64401	-3.9776	-0.0184	Training
44	O=c1[nH]c2ccccc2c(c1)C(=O)N1CCN(CC1)c1ccccc1	-3.998	106.8171	-3.9064	-0.0916	Training	82.37216	-3.9198	-0.0782	Training	88.74021	-4.023	0.025	Test
45	O=C(N1c2ccccc2Sc2c1cccc2)Sc1nnc(s1)C	-4.019	99.55612	-3.9865	-0.0325	Training	70.72021	-4.1021	0.0831	Training	88.83119	-4.022	0.003	Training
46	COc1cccc(c1)C(N(C(=O)Cn1nnc2c1cccc2)C1CC1)C(=O)Nc1ccc(cc1)F	-4.022	88.29946	-4.1107	0.0887	Training	76.73848	-4.008	-0.014	Training	84.24669	-4.0753	0.0533	Training
47	ClCC(=O)N(c1cn(c2c1cccc2)C(=O)C)c1ccc(cc1)[N+](=O)[O-]	-4.034	99.52477	-3.9869	-0.0471	Training	73.28342	-4.062	0.028	Test	88.37324	-4.0273	-0.0067	Training
48	CC(C12CN(CC(C2=O)(CN(C1)C(=O)c1ccccc1[N+](=O)[O-])C(C)C)C(=O)c1ccccc1[N+](=O)[O-])C	-4.046	89.21029	-4.1006	0.0546	Training	74.482	-4.0432	-0.0028	Training	88.30246	-4.0281	-0.0179	Training
49	O=C1C(=O)c2c(N1C/C=C/c1ccccc1)cccc2	-4.049	82.64793	-4.173	0.124	Test	68.15264	-4.1422	0.0932	Training	73.03257	-4.2058	0.1568	Training
50	COc1cccc(c1)C(N(C(=O)Cn1nnc2c1cccc2)c1ccc(cc1)NC(=O)C)C(=O)NCC1CCCO1	-4.049	97.2821	-4.0116	-0.0374	Training	74.11691	-4.049	0	Training	91.80906	-3.9873	-0.0617	Training
51	Brc1ccc(c(c1)C(=O)/C=C/c1ccc(cc1)C)OC(=O)c1ccco1	-4.049	87.55596	-4.1189	0.0699	Training	82.51209	-3.9177	-0.1313	Training	88.59285	-4.0247	-0.0243	Training
52	Clc1ccc(cc1)C(=O)Nc1ccc2c(c1)ncn2C	-4.056	94.90826	-4.0378	-0.0182	Training	71.36199	-4.092	0.036	Training	83.76051	-4.081	0.025	Test
53	ClCC(=O)Nc1sc(c(c1C(=O)c1ccccc1)C)C	-4.066	99.17473	-3.9907	-0.0753	Test	76.20326	-4.0163	-0.0497	Training	89.65857	-4.0123	-0.0537	Test
54	CCC(NC(=O)C(N(C(=O)Cn1nnc2c1cccc2)c1ccc(cc1)NC(=O)C)c1ccc(cc1)O)(C)C	-4.073	96.13088	-4.0243	-0.0487	Training	71.80961	-4.085	0.012	Training	94.95083	-3.9508	-0.1222	Test
55	O=C(Nc1cccc(c1)S(=O)(=O)N(C)C)CSc1cccc2c1nccc2	-4.081	87.24246	-4.1223	0.0413	Training	71.79017	-4.0853	0.0043	Test	73.63405	-4.1988	0.1178	Training
56	OC(=O)c1ccc2c(c1)scn2	-4.084	94.39792	-4.0434	-0.0406	Training	63.2961	-4.2182	0.1342	Training	78.58027	-4.1412	0.0572	Training
57	Cc1ccc(cc1)C(=O)Oc1ccc2c(c1)ncn2C	-4.106	95.14946	-4.0351	-0.0709	Test	70.46195	-4.1061	0.0001	Test	85.10342	-4.0653	-0.0407	Training
58	O=C(Nc1ccc(c(c1)C)Br)COn1nnc2c1cc(cc2)S(=O)(=O)C	-4.126	92.16972	-4.068	-0.058	Training	68.79412	-4.1322	0.0062	Training	79.88922	-4.126	0	Test
59	ClCC(=O)N(c1ccc(cc1)OC)Cc1cc(=O)[nH]c2c1cccc2	-4.148	99.71531	-3.9848	-0.1632	Test	74.56897	-4.0419	-0.1061	Training	93.67463	-3.9656	-0.1824	Training
60	CC(=O)Nc1ccc(cc1)N(C(c1ccc(c(c1)O)O)C(=O)NC1CCCC1)C(=O)Cn1nnc2c1cccc2	-4.151	91.62113	-4.074	-0.077	Test	65.34174	-4.1862	0.0352	Training	75.67461	-4.175	0.024	Training
61	Brc1cncc(c1)C(=O)NN=Cc1c(O)ccc2c1cccc2	-4.159	88.14523	-4.1124	-0.0466	Training	67.41464	-4.1538	-0.0052	Training	71.3351	-4.2255	0.0665	Training
62	O=C(C(N(C(=O)Cn1nnc2c1cccc2)c1ccc2c(c1)CCC2)c1ccco1)NCc1ccco1	-4.18	94.4661	-4.0427	-0.1373	Training	68.98147	-4.1293	-0.0507	Training	84.33834	-4.0742	-0.1058	Training
63	NC(=O)CCn1[n+]([O-])c2c(c1C(=O)c1cccc(c1)[N+](=O)[O-])cccc2	-4.183	90.15153	-4.0902	-0.0928	Training	72.84963	-4.0688	-0.1142	Training	82.01439	-4.1013	-0.0817	Training
64	O=C(c1cccnc1)OCC(=O)N1c2ccccc2Sc2c1cccc2	-4.207	75.03295	-4.257	0.05	Training	65.31577	-4.1866	-0.0204	Test	69.85804	-4.2427	0.0357	Training
65	ClCC(=O)N(CCc1ccccc1)CCc1ccccc1	-4.212	86.13061	-4.1346	-0.0774	Test	71.32331	-4.0926	-0.1194	Training	75.27312	-4.1797	-0.0323	Training
66	Cc1ccc(cc1C)C(=O)n1cnc2c1cccc2	-4.228	72.84283	-4.2812	0.0532	Test	67.68673	-4.1495	-0.0785	Training	77.97949	-4.1482	-0.0798	Training

67	Clc1ccc(c(c1)n1c(O)ccc1O)OC(=O)c1ccco1	-4.265	80.70575	-4.1944	-0.0706	Training	62.17387	-4.2357	-0.0293	Training	70.5261	-4.2349	-0.0301	Training
68	O=C1C(=O)c2c(N1CCCc1ccccc1)cccc2	-4.268	74.03118	-4.2681	0.0001	Test	57.57805	-4.3076	0.0396	Training	63.79414	-4.3133	0.0453	Test
69	NC(=O)CCn1c(C(=O)c2ccc(cc2)C)c2c([n+]1[O-])cc(cc2)C(F)(F)F	-4.303	93.86246	-4.0493	-0.2537	Training	65.04741	-4.1908	-0.1122	Test	73.57098	-4.1995	-0.1035	Training
70	O=C1C(=O)c2c(N1CC1COc3c(O1)cccc3)cccc2	-4.318	77.54426	-4.2293	-0.0887	Test	64.65189	-4.197	-0.121	Training	79.97669	-4.125	-0.193	Training
71	O=C1c2cccc(c2N(C1=O)CCOc1ccccc1)C	-4.332	72.55486	-4.2843	-0.0477	Training	59.88549	-4.2715	-0.0605	Training	69.85021	-4.2428	-0.0892	Training
72	CCN(C(=O)Cn1cc(c2c1cccc2)C=C1C(=O)NC(=O)N(C1=O)c1ccccc1F)CC	-4.342	66.99827	-4.3456	0.0036	Training	54.32391	-4.3585	0.0165	Training	56.40038	-4.3993	0.0573	Training
73	O=C(Nc1cccnc1)/C=C/c1ccccc1Cl	-4.383	63.25761	-4.3869	0.0039	Test	56.46077	-4.3251	-0.0579	Training	54.0935	-4.4261	0.0431	Test
74	Cc1ccc(cc1)c1n[nH]c(c1)NC(=O)c1ccccc1[N+](=O)[O-]	-4.386	59.29294	-4.4306	0.0446	Training	42.35587	-4.5457	0.1597	Training	60.56534	-4.3508	-0.0352	Test
75	Fc1ccc2c(c1)CCC(N2CC(=O)N1CCC2C(C1)c1cc(C)ccc1N2)C	-4.403	62.79251	-4.392	-0.011	Training	56.69212	-4.3215	-0.0815	Test	54.70272	-4.419	0.016	Training
76	COc1cccc(c1)C=NNC(=S)Nc1cccnc1	-4.41	60.81144	-4.4139	0.0039	Training	51.2253	-4.407	-0.003	Training	52.48002	-4.4449	0.0349	Training
77	O=C(NCc1cccnc1)/C=C/c1ccc(c(c1)[N+](=O)[O-])Cl	-4.444	46.63089	-4.5703	0.1263	Training	52.48817	-4.3872	-0.0568	Training	49.81521	-4.4759	0.0319	Training
78	O=C(C(N(C(=O)c1csnn1)c1ccc(cc1)C(C)C)c1cccnc1)NC1CCCC1	-4.449	67.40309	-4.3412	-0.1078	Training	54.71848	-4.3523	-0.0967	Training	65.94762	-4.2882	-0.1608	Training
79	O=C(Nc1cccnc1)Cc1ccc(c(c1)Cl)Cl	-4.449	56.50075	-4.4614	0.0124	Training	48.92512	-4.4429	-0.0061	Training	38.42962	-4.6084	0.1594	Test
80	COc1ccc2c(c1)ccc(c2)C1(C)NC(=O)N(C1=O)CC(=O)NCc1ccco1	-4.493	52.64497	-4.504	0.011	Training	49.79411	-4.4294	-0.0636	Training	49.93528	-4.4745	-0.0185	Training
81	O=C(N1CCOCC1)Cn1cc(c2c1cccc2)C=C1C(=O)NC(=O)N(C1=O)c1ccccc1F	-4.535	52.017	-4.5109	-0.0241	Training	41.1522	-4.5645	0.0295	Training	54.16679	-4.4253	-0.1097	Training
82	Cc1cc(n(n1)C(=O)c1ccc(c(c1)Br)C)C	-4.543	44.31838	-4.5958	0.0528	Training	47.85184	-4.4597	-0.0833	Test	48.2726	-4.4939	-0.0491	Training
83	O=C(Nc1cccnc1)/C=C/c1c(F)cccc1Cl	-4.566	63.83912	-4.3805	-0.1855	Training	42.75936	-4.5394	-0.0266	Training	48.1481	-4.4953	-0.0707	Training
84	COCN(c1c(CC)cccc1CC)C(=O)Cn1nnc2c1cccc2	-4.608	55.4706	-4.4728	-0.1352	Training	44.65676	-4.5097	-0.0983	Training	42.92453	-4.5561	-0.0519	Training

Table S2. The example of DCW(1,20) calculation.



SMILES notation:
COc1cccc(c1)C(N(C(=O)Cn1nnc2c1cccc2)c1ccc(cc1)NC(=O)C)C(=O)NCC1CCCO1
DCW = 74.11691
Prediction for EndPoint = -4.0490

C.....	0.3306	(.....	-0.9927	c...c.....	0.3214	n...n...c...	0.0856
O.....	-0.7382	C.....	0.3306	c...c.....	0.3214	n...c...2...	-0.0548
c.....	-0.7267	(.....	-0.9927	c...(.....	0.202	c...2...c...	0.3196
1.....	-0.725	=.....	0.298	c...(.....	0.202	2...c...1...	-0.959
c.....	-0.7267	O.....	-0.7382	c...c.....	0.3214	c...1...c...	1.5745
c.....	-0.7267	(.....	-0.9927	c...1.....	0.1033	c...c...1...	0.0646
c.....	-0.7267	N.....	0.0542	1...(.....	-0.682	c...c...c...	0.3652
c.....	-0.7267	C.....	0.3306	N...(.....	-0.8114	c...c...c...	0.3652
(.....	-0.9927	C.....	0.3306	N...C.....	-0.6558	c...c...2...	0.4611
c.....	-0.7267	1.....	-0.725	C...(.....	-0.5067	c...2...(...	-0.6595
1.....	-0.725	C.....	0.3306	=...(.....	-0.2762	c...(...2...	-0.1228
(.....	-0.9927	C.....	0.3306	O...=.....	-0.9352	1...c...(...	0.5233
C.....	0.3306	C.....	0.3306	O...(.....	0.2537	c...1...c...	1.5745
(.....	-0.9927	O.....	-0.7382	C...(.....	-0.5067	c...c...1...	0.0646
N.....	0.0542	1.....	-0.725	C...(.....	-0.5067	c...c...c...	0.3652
(.....	-0.9927	O...C.....	0.0436	C...(.....	-0.5067	c...c...(...	1.6158
C.....	0.3306	c...O.....	0.3363	C...(.....	-0.5067	c...(...c...	0.1717
(.....	-0.9927	c...1.....	0.1033	=...(.....	-0.2762	c...c...(...	1.6158
=.....	0.298	c...1.....	0.1033	O...=.....	-0.9352	c...c...1...	0.0646
O.....	-0.7382	c...c.....	0.3214	O...(.....	0.2537	c...1...(...	0.364
(.....	-0.9927	c...c.....	0.3214	N...(.....	-0.8114	N...(...1...	0.0087
C.....	0.3306	c...c.....	0.3214	N...C.....	-0.6558	C...N...(...	0.1869

n.....	0.3619	c...(.....	0.202	C...C.....	-0.7029	N...C...(...	-0.6811
1.....	-0.725	c...(.....	0.202	C...1.....	0.0167	C...(...=...	0.1504
n.....	0.3619	c...1.....	0.1033	C...1.....	0.0167	O...=...(...	-0.6501
n.....	0.3619	1...(.....	-0.682	C...C.....	-0.7029	=...O...(...	-0.7415
c.....	-0.7267	C...(.....	-0.5067	C...C.....	-0.7029	O...(...C...	0.2791
2.....	0.6779	C...(.....	-0.5067	O...C.....	0.0436	(...C...(...	0.1825
c.....	-0.7267	N...(.....	-0.8114	O...1.....	0.0231	C...(...C...	-0.7918
1.....	-0.725	N...(.....	-0.8114	c...O...C...	-1.2198	(...C...(...	0.1825
c.....	-0.7267	C...(.....	-0.5067	O...c...1...	0.425	C...(...=...	0.1504
c.....	-0.7267	C...(.....	-0.5067	c...1...c...	1.5745	O...=...(...	-0.6501
c.....	-0.7267	=...(.....	-0.2762	c...c...1...	0.0646	=...O...(...	-0.7415
c.....	-0.7267	O...=.....	-0.9352	c...c...c...	0.3652	O...(...N...	0.476
2.....	0.6779	O...(.....	0.2537	c...c...c...	0.3652	C...N...(...	0.1869
(.....	-0.9927	C...(.....	-0.5067	c...c...(...	1.6158	N...C...C...	2.0352
c.....	-0.7267	n...C.....	0.3088	c...(...c...	0.1717	C...C...1...	0.0438
1.....	-0.725	n...1.....	0.3079	1...c...(...	0.5233	C...1...C...	0.6494
c.....	-0.7267	n...1.....	0.3079	c...1...(...	0.364	C...C...1...	0.0438
c.....	-0.7267	n...n.....	-0.0491	C...(...1...	-0.6398	C...C...C...	2.3965
c.....	-0.7267	n...c.....	0.2585	(...C...(...	0.1825	O...C...C...	0.6191
(.....	-0.9927	c...2.....	0.0387	N...(...C...	0.085	C...O...1...	2.0395
c.....	-0.7267	c...2.....	0.0387	(...N...(...	0.3534	Cmax.2.....	0.4289
c.....	-0.7267	c...1.....	0.1033	N...(...C...	0.085	Nmax.3.....	0.3646
1.....	-0.725	c...1.....	0.1033	(...C...(...	0.1825	Omax.5.....	0.1192
(.....	-0.9927	c...c.....	0.3214	C...(...=...	0.1504	Smax.0.....	2.2498
N.....	0.0542	c...c.....	0.3214	O...=...(...	-0.6501	NOSP11000000	-0.3719
C.....	0.3306	c...c.....	0.3214	=...O...(...	-0.7415	HALO00000000	0.233
(.....	-0.9927	c...2.....	0.0387	O...(...C...	0.2791	BOND10000000	7.2238
=.....	0.298	2...(.....	0.0833	n...C...(...	-0.8626	++++N---O===	0.2501
O.....	-0.7382	c...(.....	0.202	C...n...1...	-0.2063	++++O---B2==	2.9152
(.....	-0.9927	c...1.....	0.1033	n...1...n...	0.4243	++++N---B2==	-0.7011
C.....	0.3306	c...1.....	0.1033	n...n...1...	0.1287	10011000000	-0.7302

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

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
10001000000	1.98664	2.27544	1.35382	P3E0N...4-..	0.3584	0.01539	-0.98214	VS3-N...2...	0.26991	1.09438	0.19551
10001000010	-0.72891	0.27326	0.32472	P3E0N...5-..	-0.39881	2.04352	1.15591	VS3-N...18..	2.0281	0.04224	2.05989
10001000100	2.24986	3.43461	0.22897	P3E0N...6-..	-0.67431	1.14733	2.55625	VS3-N...21..	-0.59394	0.26275	0.62548
10001001010	2.94961	2.58351	0.50054	P3E0O...0-..	0.73666	0.00618	0.41387	VS3-N...3...	-0.43072	-0.16403	-0.56379
10011000000	0.39547	-0.61024	-0.73024	P3E0O...1-..	-0.03662	-0.15695	0.36075	VS3-N...4...	-1.06775	0.49606	-0.14748
10011000010	-0.2757	1.79927	-0.26908	P3E0O...2-..	0.47288	0.29205	0.26172	VS3-N...5...	2.34496	0.09555	2.38251
10011000100	2.33604	-0.16396	0.06994	P3E0O...3-..	1.13242	0.39796	-0.41148	VS3-N...6...	0.07346	0.4755	0.08364
10011001000	-0.85671	0.04454	0.3673	P3E0O...4-..	-1.2048	-0.38613	-0.47251	VS3-N...7...	-0.08855	0.08477	0.25709
10011001100	-0.59413	0.42778	-0.98949	P3E0O...5-..	1.15198	1.41134	2.15261	VS3-N...8...	-0.82887	-1.39248	0.16578
10011001110	0.02936	-0.9032	-0.50803	P3E0S...1-..	-0.04159	2.23028	0.05101	VS3-N...9...	-0.61473	2.39244	0.08356
10011100000	0.84864	0.28716	0.5095	P3E0S...2-..	-0.1077	2.26042	0.10082	VS3-O...10..	-0.98442	0.03972	0.41766
10011100010	-1.06951	1.32	-1.49467	P3E0S...4-..	-0.52578	-0.53894	0.49903	VS3-O...11..	-0.12214	0.2286	0.20569
(...(.....	0.15483	0.45292	0.02298	P3E0o...1-..	-0.47041	-0.30238	0.29349	VS3-O...14..	-0.26955	0.28529	0.18478
(..........	0.38036	0.17096	-0.99268	P3E0o...2-..	0.29344	-1.11985	-0.75162	VS3-O...2...	0.16955	1.26025	-0.63129
(...C...(...	0.08002	-0.60754	0.18247	P3E0s...1-..	0.3301	-0.34274	0.48285	VS3-O...3...	0.42146	0.16528	0.2101
(...F...(...	-0.76706	0.06024	0.20595	P3E0s...2-..	2.12958	1.65995	0.30903	VS3-O...4...	0.39112	0.32534	0.26008
(...Br..(...	-1.43206	-2.69818	-0.91521	P3E0s...3-..	1.27117	1.23571	1.16169	VS3-O...5...	0.2209	-0.04264	0.15801
(...Cl..(...	-0.75259	-0.87207	-0.14983	P4E0C...0-..	2.14668	0.5542	0.63333	VS3-O...6...	-0.40468	0.56293	0.2536
(...N...(...	0.15902	0.10763	0.35336	P4E0C...1-..	0.24462	0.72058	0.29022	VS3-O...7...	-0.98741	-1.64867	0.33362
(...O...(...	0.82184	1.78373	-0.54791	P4E0C...10-.	0.22733	0.59035	0.30857	VS3-O...8...	0.45968	-0.05036	0.1238
(...S...(...	0.43688	-0.66548	-0.77689	P4E0C...11-.	0.41199	0.10301	2.08612	VS3-O...9...	0.47931	0.32063	2.21194
(...c...(...	-0.65237	-0.95002	0.34203	P4E0C...12-.	-0.95789	-0.73529	-0.8173	VS3-S...11..	-0.21522	-0.1671	-0.37079
(...n...(...	-0.64142	0.14207	-0.60973	P4E0C...13-.	-2.41886	-1.7157	5.26181	VS3-S...14..	0.67267	-0.01185	0.31715
++++F---B2==	-0.17094	0.03729	0.20343	P4E0C...14-.	0.55185	0.10076	0.71493	VS3-S...5...	-0.38243	-0.89751	-4.11491
++++F---Br==	0.3266	1.92389	-0.55024	P4E0C...16-.	0.45867	-0.79026	0.44333	VS3-S...7...	2.34369	2.06294	0.61945
++++F---Cl==	-0.73956	-0.80405	-4.08009	P4E0C...2-..	0.29135	0.36145	0.38588	VS3-S...9...	0.67812	2.27789	2.12685
++++F---N===	0.38859	-0.50174	0.09985	P4E0C...3-..	0.44616	-0.02099	0.06334	VS3-o...10..	-0.75463	-0.5909	-1.81098
++++F---O===	-0.73131	0.07809	-0.57455	P4E0C...4-..	2.48629	0.03342	-0.55966	VS3-o...11..	1.23415	0.2942	0.48777
++++CL--Br==	-1.05343	-0.87694	2.33182	P4E0C...5-..	0.27404	0.46774	0.35529	VS3-o...6...	-1.03908	-0.72184	0.26856
++++CL--N===	0.23456	2.63313	1.56877	P4E0C...6-..	0.018	-0.74305	0.01379	VS3-o...7...	2.28648	2.2343	-0.37584
++++CL--O===	0.43753	-0.68988	1.80939	P4E0C...7-..	-0.63673	0.10287	-0.79602	VS3-o...8...	2.22533	2.26262	4.13941
++++CL--S===	0.86595	2.43523	2.14529	P4E0C...8-..	-0.96375	-0.64128	0.39617	VS3-s...10..	1.09345	2.62178	0.33592

++++Br--B2==	2.37527	0.25558	-0.21154	P4E0C...9-..	0.32094	1.10507	4.3107	VS3-s...13..	-0.0031	-0.59038	-0.76978
++++Br--N===	2.24884	4.08899	0.96627	P4E0F...1-..	0.96767	0.58998	-0.00761	VS3-s...7...	-0.13915	-1.19964	-1.16915
++++Br--O===	0.11309	-0.01002	0.42973	P4E0F...4-..	0.30015	-0.65315	-0.82981	VS3-s...8...	2.36114	1.21341	0.79226
++++Br--S===	-0.2528	2.36828	-0.18373	P4E0Br..1-..	0.11796	0.66855	1.97096	Smax.0.....	-0.65174	2.38818	2.24985
++++Cl--B2==	0.43461	1.16486	-1.94998	P4E0Br..4-..	0.35058	0.04477	-0.06059	Smax.1.....	-0.96839	0.2477	0.13328
++++N---B2==	0.35841	-0.11485	-0.70113	P4E0Cl..1-..	2.35942	2.341	0.27932	[...(.....	-1.0966	0.01273	-0.71241
++++N---O===	0.44561	0.34154	0.25014	P4E0Cl..3-..	2.41505	-0.08126	2.00445	[...(...1...	1.02952	0.04978	0.40604
++++N---S===	-0.8946	0.38615	0.4292	P4E0Cl..4-..	0.05601	-0.12541	-0.05891	[...(...=...	-0.13429	-0.62889	-0.69586
++++O---B2==	9.81519	3.09597	2.91522	P4E0N...0-..	0.37668	-0.00893	0.3947	[...(...C...	2.39029	0.25082	0.10469
++++O---S===	-1.40068	0.20301	2.36456	P4E0N...1-..	2.48464	-1.06816	5.98355	[...(...Cl..	-0.87323	-1.19139	-0.01575
++++S---B2==	2.19085	0.31217	0.22488	P4E0N...10-.	-4.65723	-6.50824	-0.85931	[...(...O...	-0.48385	0.31666	-0.99257
+.....	1.67286	-1.19767	0.52205	P4E0N...11-.	-0.88866	1.96418	2.19852	[...(...[...	0.4491	-0.76719	0.1567
+...[...(...	-0.60072	0.11373	0.03231	P4E0N...14-.	1.84754	2.20428	-0.21635	[...+.....	0.96181	0.40027	0.77769
-.....	0.44989	-1.03034	0.13861	P4E0N...2-..	-0.6568	0.04832	0.07282	[...+...N...	-0.76928	-0.0702	0.14334
-...[...(...	2.08527	-0.9583	-0.14388	P4E0N...19-.	0.28022	-0.72826	0.10619	[...-.....	0.70303	-1.36904	-0.50062
/...(.....	-0.83823	-0.89966	0.39171	P4E0N...3-..	0.24438	0.12657	0.45724	[...-...O...	-1.26703	0.03843	-0.98681
/.....	0.05502	1.20005	0.27236	P4E0N...4-..	0.20327	0.05081	0.15148	[.....	-0.24726	0.65877	0.02153
/...C...(...	-0.50631	-0.74746	0.03573	P4E0N...6-..	0.47103	0.18681	0.08587	[...1.....	0.24472	-0.13658	2.3841
/...C.../...	3.88792	6.2645	2.21355	P4E0N...7-..	0.10744	1.46848	-0.67494	[...1...[...	0.32922	0.95678	-0.50699
1...(.....	-0.88647	-0.53661	-0.68198	P4E0N...8-..	-0.15703	0.96519	0.30607	[...H.....	2.03667	2.42619	-0.66125
1...(.../...	-0.16259	-3.58134	-0.67786	P4E0O...0-..	0.96558	2.49588	0.48545	[...N...+...	-0.94203	-0.5782	0.15428
1.....	0.07088	-0.61258	-0.725	P4E0O...1-..	0.29668	-0.54945	-0.41648	[...N.....	0.63144	-0.67991	0.10878
1.../.....	-0.32414	2.36942	-0.67848	P4E0O...12-.	0.00505	-1.08059	-1.35653	[...O...-...	0.93335	-1.55038	-0.87615
1...C...(...	-0.85724	0.13669	0.04957	P4E0O...17-.	-0.61753	-0.49958	1.2498	[...O.....	1.87726	-0.41672	-0.30473
1...C.../...	2.76418	5.36876	4.25196	P4E0O...2-..	-2.44741	-1.13395	-2.31766	[...c...(...	0.25737	0.21632	0.02039
1...F...(...	-0.86333	-0.99589	0.17246	P4E0O...3-..	2.46943	2.205	0.05077	[...c...1...	0.47055	0.03045	0.17797
1...N...(...	-0.74858	0.03961	0.02261	P4E0O...4-..	0.26542	2.42858	0.07965	[...c...2...	0.41686	1.75272	0.0331
1...N...1...	2.15266	1.17634	-0.04367	P4E0O...5-..	0.83243	-3.29483	-0.60085	[...n...+...	0.76332	-0.96771	0.46612
1...O...(...	-1.00225	-1.67247	-2.04167	P4E0O...6-..	-0.75685	2.13922	0.66732	[...n...1...	-1.24319	-0.42944	0.45575
1...[...+...	-0.004	0.29724	0.3169	P4E0O...7-..	-0.87706	-0.9081	-0.72617	[...n...H...	1.64934	3.16306	2.22362
1...c...(...	0.16075	-0.67558	0.52334	P4E0S...1-..	-0.71181	-1.17581	-0.02704	c...(.....	0.1953	0.34191	0.20199
1...c.../...	1.40432	-0.88451	1.14304	P4E0S...2-..	-0.51767	0.09598	0.45866	c...(...1...	-0.61214	-0.22007	0.27776
1...c...1...	2.10523	0.36357	0.35747	P4E0S...3-..	2.48051	2.11862	2.57601	c...(...2...	-0.18695	-0.07014	-0.12277
1...n...(...	-0.35428	2.4231	-0.56348	P4E0S...4-..	-1.0458	1.93728	2.05051	c...(...3...	0.04127	-0.82224	-0.56249
1...o...(...	0.31748	2.00136	2.09789	P4E0S...8-..	1.12671	0.65838	0.57188	c...(...=...	0.40026	2.36757	0.2749

1...s...(...	-0.90313	-0.6556	-0.40558	P4E0o...1-..	0.05482	0.13664	-0.67764	c...(...C...	0.12889	0.34374	0.29765
2...(.....	-0.90852	0.31369	0.08333	P4E0o...4-..	-0.80991	0.04825	-1.19725	c...(...F...	-2.52888	-1.61649	-0.67416
2.....	-0.5274	-0.86885	0.67795	P4E0o...6-..	-0.59434	0.69323	0.187	c...(...Br..	0.22694	-0.80887	-0.41667
2...1.....	1.85686	-0.21959	0.27378	P4E0s...1-..	0.97419	2.24934	2.19707	c...(...Cl..	0.7906	0.35256	0.21527
2...C...(...	-0.86324	-0.40351	0.24012	P4E0s...3-..	-0.96283	-0.3138	0.02303	c...(...N...	-0.662	-0.82765	-1.05612
2...N...(...	-1.02514	-0.67422	0.23846	P4E0s...4-..	-0.69027	2.17271	2.3896	c...(...O...	0.2473	0.22204	-0.08639
2...c...(...	0.3773	0.02403	0.18298	P4E0s...7-..	0.13307	2.72173	-0.02907	c...(...[...	0.62566	0.28352	-0.80651
2...c...1...	-0.39253	0.44184	-0.95904	NNC-C...101.	-0.86926	0.46532	0.35302	c...(...c...	-1.22698	-0.18396	0.1717
3...(.....	0.0571	2.03546	0.20848	NNC-C...110.	0.18794	0.3815	0.1367	c.....	0.46657	0.22473	-0.72668
3.....	0.39261	2.49457	-0.96699	NNC-C...202.	-0.1104	2.15913	-1.65686	c.../.....	-0.57584	-0.87437	-0.97905
3...c...(...	-0.285	-1.31759	0.1895	NNC-C...211.	0.29566	0.4687	-0.99337	c.../...C...	0.10627	0.0102	0.48779
3...c...2...	2.19938	2.27641	2.44226	NNC-C...220.	0.34837	-0.60713	-0.98837	c...1...(...	-0.53693	0.34525	0.36396
=...(...(...	0.17916	0.8407	-0.81229	NNC-C...303.	0.10882	-0.74197	-0.07094	c...1.....	-0.89502	-0.2754	0.10332
=...(.....	2.00043	0.22534	-0.27615	NNC-C...312.	-0.83765	-2.0144	-0.62769	c...1.../...	-0.11257	-1.43555	-0.10795
=.....	-0.50529	-0.12566	0.29799	NNC-C...321.	-0.66311	0.23057	-0.07606	c...1...C...	0.18332	-0.54648	0.35952
=...1.....	-0.51219	-0.73271	-0.59614	NNC-C...330.	0.16045	-0.76882	0.40004	c...1...F...	2.0851	0.42901	0.19697
=...1.../...	3.17531	3.11667	0.96217	NNC-C...431.	-0.45392	1.24047	0.86411	c...1...Cl..	-0.78004	0.60495	-0.03166
=...2.....	0.02286	0.1147	0.37688	NNC-C...440.	-0.11586	0.09651	-0.87779	c...1...N...	0.10738	-0.29957	0.44791
=...C...(...	0.18903	-0.83172	0.45762	NNC-F...110.	0.07713	0.38434	-0.09156	c...1...O...	-0.79468	1.39457	1.76251
=...C.../...	0.00465	0.05207	0.10391	NNC-Br..110.	-0.379	0.35119	2.28732	c...1...[...	0.01558	-0.90761	0.30787
=...C...1...	-0.61969	2.17023	-0.70744	NNC-Cl..110.	2.06333	-0.97848	0.47346	c...1...c...	2.50818	-0.40877	1.57451
=...N...1...	2.4587	2.14589	0.13007	NNC-N...110.	0.71814	0.45894	0.47176	c...2...(...	-1.10755	-1.38383	-0.65953
=...O...(...	-0.62459	0.3553	-0.7415	NNC-N...202.	0.00705	-0.66602	0.04196	c...2.....	0.21551	0.24342	0.0387
=...S...(...	-1.79484	-0.75151	0.15707	NNC-N...211.	0.31195	1.13424	1.81994	c...2...N...	0.46157	1.76916	-0.65821
=...c...1...	0.02464	2.29257	2.11159	NNC-N...220.	-0.66974	-0.8078	-0.98823	c...2...S...	-0.16766	0.28641	0.64209
C...(...(...	1.95069	-0.34839	-1.19131	NNC-N...312.	0.19204	-0.79718	0.43308	c...2...c...	0.19636	1.02119	0.31959
C...(.....	0.07378	0.16918	-0.50665	NNC-N...321.	-0.86984	2.30817	0.00336	c...3...(...	0.26843	-0.46684	0.27931
C...(...1...	1.04086	-0.98564	-0.63982	NNC-N...330.	0.30766	-0.59293	-0.51872	c...3.....	0.19527	0.32395	-0.4619
C...(...2...	-0.67466	0.31276	0.42574	NNC-O...101.	0.16806	0.58649	0.03415	c...3...c...	0.23613	0.8947	0.8148
C...(...=...	0.26702	0.05664	0.15041	NNC-O...110.	0.03442	0.38546	0.16771	c...=.....	2.4395	2.00253	0.29406
C...(...C...	-0.90784	-0.88757	-0.79176	NNC-O...211.	-0.68848	2.18022	0.31477	c...=...O...	0.59099	2.04356	0.2964
C.....	-0.34185	0.29935	0.33058	NNC-O...220.	0.40266	0.08823	0.23473	c...C...(...	-0.04656	0.23988	-0.88547
C.../...(...	-0.64642	0.4721	0.41573	NNC-S...110.	-0.76334	-1.53804	-0.51769	c...C.....	-0.89937	-0.625	-1.90407
C.../.....	0.20068	0.16103	0.30284	NNC-S...220.	1.16885	-0.0663	-0.4239	c...C...=...	0.03385	0.18785	2.1896
C.../...1...	2.36295	0.38239	0.42433	NNC-S...422.	-0.19277	-0.58935	-0.64545	c...C...C...	0.17079	0.03768	0.35625

C.../...C...	2.10623	2.0365	2.02892	NNC-o...202.	2.4279	1.94307	2.01394	c...C...N...	-0.86701	-0.53823	0.13051
C...1...(...	-0.97274	0.13768	0.00356	NNC-o...220.	0.1473	0.06279	-0.10031	c...Br.....	0.23751	2.30103	0.32032
C...1.....	-0.75828	-0.51664	0.01672	NNC-s...211.	-2.11884	0.09773	-0.84484	c...Cl.....	1.45553	0.40118	2.05023
C...1...2...	0.08797	-1.12669	-0.76194	NNC-s...220.	0.6417	0.18143	0.06217	c...N...(...	-0.5498	-0.66668	0.00382
C...1...=...	-0.68124	-0.75235	-0.91031	NNE0C...100-	0.43544	0.31653	-0.14967	c...N.....	1.16731	0.89965	0.49555
C...1...C...	-0.7043	-0.50412	0.64943	NNE0C...109-	0.28397	0.25125	0.00228	c...N...C...	2.92353	4.25079	2.60784
C...2...(...	-0.5212	-1.13793	-1.86752	NNE0C...200-	0.20143	0.29759	-3.5796	c...O...(...	0.73589	2.14251	1.54193
C...2.....	0.32483	0.44429	-0.1242	NNE0C...209-	0.09526	0.60817	-0.43311	c...O.....	1.15472	0.2555	0.33635
C...2...1...	1.05468	-0.7895	0.11158	NNE0C...218-	-0.98264	0.36865	0.35168	c...O...C...	0.16313	0.06093	-1.21975
C...2...=...	-0.28275	0.00365	1.0386	NNE0C...300-	0.07878	-2.45935	0.39818	c...S...(...	0.02161	-0.58077	0.84609
C...=.....	0.41209	-0.75252	-0.08592	NNE0C...309-	-0.90927	-1.61	-0.27437	c...S.....	2.26579	1.03023	0.92434
C...=...1...	4.3505	4.34479	2.02303	NNE0C...318-	-0.04826	0.07932	0.201	c...S...2...	0.1431	-0.879	0.06885
C...=...C...	0.39112	-0.77384	0.0655	NNE0C...327-	0.21792	0.13119	0.49386	c...S...C...	-0.14126	2.44354	-0.22904
C...C...(...	2.01924	-0.6994	0.56604	NNE0C...427-	0.20733	-0.38507	-0.96952	c...[.....	1.27242	0.68466	-0.41111
C...C.....	0.20575	0.43321	-0.7029	NNE0C...436-	0.21199	-1.41774	0.24747	c...[...H...	-0.61421	0.77017	0.12073
C...C...1...	0.3154	-0.20764	0.04377	NNE0F...109-	0.18091	0.05785	0.21238	c...c...(...	0.42382	-0.99522	1.6158
C...C...2...	0.55175	-0.43335	0.20573	NNE0Br..109-	2.46206	0.67419	-0.70048	c...c.....	-0.04669	0.23266	0.32142
C...C...C...	1.1372	0.31272	2.39649	NNE0Cl..109-	0.62893	0.41625	2.28584	c...c...1...	0.3507	0.10477	0.06463
C...N...(...	0.21159	0.12956	0.18688	NNE0N...109-	0.0339	-0.02116	0.18898	c...c...2...	-0.54621	-0.49141	0.46109
C...N...1...	0.2874	0.35752	2.17388	NNE0N...200-	0.01366	0.10617	-0.90256	c...c...3...	-0.74216	0.46357	-0.62553
C...O...(...	-5.68116	-6.70564	1.72868	NNE0N...209-	0.00871	0.47824	-2.09162	c...c...c...	0.1058	0.26534	0.36522
C...O...1...	1.93896	0.79554	2.03953	NNE0N...218-	0.28302	0.36865	1.08104	c...n...(...	1.16746	0.39569	-0.18389
C...O...C...	0.29453	0.01557	0.13904	NNE0N...309-	-0.97543	0.09656	-0.7825	c...n...1...	-2.10713	4.28496	1.66834
C...c...1...	-0.7493	-1.53913	-1.27585	NNE0N...318-	-0.12177	0.23342	0.028	c...n...2...	-0.96262	1.04851	3.86992
C...c...2...	-1.02529	-0.62673	1.28328	NNE0N...327-	-0.12648	-0.56638	-0.0378	c...n...c...	-0.72699	-0.66037	0.39434
C...n...1...	1.49629	-0.67762	-0.20629	NNE0O...100-	-0.60127	0.33773	0.25543	c...o...(...	2.25921	-0.40242	1.55161
C...n...2...	2.01962	1.44106	0.03057	NNE0O...109-	-0.98031	-0.95069	0.47431	c...o...1...	2.30479	0.03787	0.12458
C3.....0...	-0.07348	0.34884	0.00428	NNE0O...209-	0.34908	-0.52632	0.11329	c...s...(...	2.59816	0.43682	0.90332
C3.....1...	0.14705	-0.46933	-0.46993	NNE0O...218-	0.46082	1.13791	2.18936	c...s...1...	2.4677	0.66417	-0.0726
C4.....0...	3.602	11.72941	3.09033	NNE0S...109-	0.05449	1.22209	1.14156	e0p2C...10+.	-0.98367	0.33033	0.07837
C5.....0...	-0.82982	-0.29485	0.41935	NNE0S...218-	0.37393	0.03671	0.47469	e0p2C...2+..	0.37127	0.40796	0.29215
C5....H.1...	2.23096	2.39791	0.20912	NNE0S...418-	-0.6873	-0.65093	0.34951	e0p2C...3+..	0.38681	0.00071	0.39758
C5...AH.1...	0.38216	0.99333	2.35586	NNE0o...200-	1.10553	-0.06943	2.378	e0p2C...4+..	0.50348	0.31072	0.03007
C5...AH.2...	-0.93606	2.44025	0.55019	NNE0o...218-	0.11692	0.34336	-0.25037	e0p2C...5+..	0.16947	0.39067	0.35187
C5...AH.3...	0.00653	0.5043	2.65781	NNE0s...209-	-0.59589	-0.66657	-1.07883	e0p2C...6+..	-0.16898	-1.13692	0.25471

C5...AH.4...	0.04788	-1.39568	0.30511	NNE0s...218-	0.50658	1.80583	0.26503	e0p2C...7+..	-0.90503	-0.33459	-0.79651
C6...A..1...	2.4762	1.00333	2.0262	NOSP01000000	2.5344	2.26508	2.09409	e0p2C...8+..	0.35126	0.1937	0.29961
C6...A..2...	0.43189	-0.60394	-0.04285	NOSP11000000	0.14629	-0.00026	-0.37188	e0p2C...9+..	0.47028	-0.74418	-0.56795
C6...A..3...	0.06843	0.1297	0.44534	NOSP11100000	0.54586	-0.03458	0.38508	e0p2F...3+..	-0.87927	-0.8286	0.03548
C6...AH.1...	1.90853	2.45237	-0.08229	S...(.....	-0.62405	0.27505	0.25545	e0p2Br..3+..	-0.00341	2.22515	0.36547
C6...AH.2...	0.22575	2.11604	0.3301	S...(...2...	0.33015	-0.22048	-0.72353	e0p2Cl..2+..	1.01898	0.42033	0.21312
C6...AH.3...	2.29352	3.45933	1.33779	S...(...=...	0.13132	0.38595	0.26522	e0p2Cl..3+..	0.19309	0.36027	0.48552
C6...AH.4...	-0.58423	-0.65674	0.01364	S...(...N...	0.15048	-0.65508	-0.72451	e0p3C...10+.	0.16421	0.29972	0.43544
C7.....0...	-0.85599	-0.56394	0.13595	S.....	1.83762	-0.67406	-0.44233	e0p3C...11+.	-0.75537	0.04986	0.03745
C7...AH.1...	2.05792	2.11567	2.34779	S...2.....	0.45071	-1.08358	0.43058	e0p3C...12+.	-0.24449	-1.17819	0.58026
BOND10000000	8.94516	13.08141	7.22376	S...=...(...	-0.7299	-1.18065	0.08055	e0p3C...2+..	2.09813	-0.20332	0.07296
F...(.....	1.43475	0.44097	-0.60948	S...=.....	-1.21615	-1.23608	1.31501	e0p3C...3+..	-0.79104	-0.90227	-1.93901
F...(...1...	-1.10819	1.00846	1.98984	S...C...(...	-0.0365	-1.0653	0.25882	e0p3C...4+..	0.42671	2.45642	2.32459
F...(...C...	0.47876	0.26678	-0.58958	S...C.....	2.14435	0.46364	-1.04551	e0p3C...5+..	1.4262	-0.8832	0.44245
F.....	0.29933	0.16608	-0.86299	S...c...1...	0.43744	2.03133	0.45472	e0p3C...6+..	0.15693	-0.1278	0.00525
F...1.....	-0.65676	-0.60761	0.39989	S...c...2...	0.43679	0.34424	0.08513	e0p3C...7+..	0.18454	0.40036	-0.80382
EC0-C...1...	1.33343	-0.70168	2.08608	S2E0C...0-..	-0.9488	-0.00354	-1.33226	e0p3C...8+..	0.24701	-1.85041	0.35201
EC0-C...2...	-0.98473	-0.68768	-0.20758	S2E0C...1-..	2.31282	6.23914	2.97568	e0p3C...9+..	-0.76679	0.38658	0.0833
EC0-C...3...	-0.87435	-0.88187	-0.90917	S2E0C...10-.	-5.06072	-5.46312	-0.47685	e0p2N...3+..	0.11205	-0.02944	-0.07326
EC0-C...4...	-0.8675	0.19865	-0.85571	S2E0C...11-.	0.16594	0.29054	-0.12335	e0p2N...4+..	0.39551	0.353	0.32006
EC0-F...1...	0.19472	-0.55014	0.15879	S2E0C...12-.	0.04335	-1.19084	-0.93333	e0p2N...5+..	0.08597	0.05157	-0.50184
EC0-Br..1...	0.20512	-0.26029	-0.72634	S2E0C...2-..	0.42085	-0.31668	2.1276	e0p2N...6+..	-0.68083	0.08408	0.04001
EC0-Cl..1...	-0.32422	0.13405	2.59179	S2E0C...3-..	0.17811	-0.00932	0.0573	e0p2N...7+..	-0.11474	2.53325	-0.2959
EC0-N...1...	0.14209	0.12488	0.43858	S2E0C...4-..	0.13606	0.01125	0.40397	e0p2N...8+..	-0.44746	-0.90497	0.09984
EC0-N...2...	-0.84074	-0.60677	-0.35414	S2E0C...5-..	-0.60074	0.2755	2.29755	e0p2N...9+..	0.07307	-0.23109	0.19375
EC0-N...3...	0.38067	0.60143	0.21184	S2E0C...6-..	-0.9074	0.28149	0.04225	e0p2O...3+..	0.1273	0.22243	0.34022
EC0-O...1...	-0.71622	-0.95598	0.04938	S2E0C...7-..	-0.2164	-0.03672	-0.66301	e0p2O...4+..	-0.69941	0.32864	-1.40181
EC0-O...2...	-0.06109	0.29033	0.00625	S2E0C...8-..	0.96579	1.36538	0.0826	e0p2O...5+..	2.02372	-0.22981	0.60765
EC0-S...1...	0.47602	-1.6274	0.26981	S2E0C...9-..	2.25172	-0.44344	0.11377	e0p2O...6+..	0.33552	2.0109	0.90787
EC0-S...2...	2.0542	-0.08174	-0.98529	S2E0F...3-..	1.08831	0.05615	0.31335	e0p3F...3+..	0.44658	-0.64833	-0.06288
EC0-S...4...	-0.01906	0.41285	-0.19033	S2E0F...4-..	0.26835	0.00349	0.02775	e0p3F...4+..	0.41845	2.14268	-0.21173
EC0-o...2...	2.10864	2.23249	2.45933	S2E0Br..3-..	0.09339	2.26231	0.37357	e0p3Br..3+..	0.11007	0.28505	0.4095
EC0-s...2...	0.13433	2.4597	0.56522	S2E0Br..4-..	-0.25068	-0.20585	0.0372	e0p3Br..4+..	0.29975	0.53297	0.04254
EC2-C...10..	0.3599	-0.63413	-0.76609	S2E0Cl..2-..	0.06502	0.06627	0.06008	e0p2S...3+..	0.46139	-0.04694	0.4675
EC2-C...11..	0.30712	0.03521	-0.28346	S2E0Cl..3-..	0.13676	2.13808	0.32001	e0p2S...4+..	2.07078	0.12752	-0.24984

EC2-C...12..	0.00033	-0.76009	2.12283	S2E0Cl..4-..	-0.70208	1.8671	-0.48406	e0p2S...5+..	2.44121	0.52853	0.89321
EC2-C...13..	0.33338	-0.04111	0.48041	S2E0N...1-..	6.24307	3.78681	3.91207	e0p2S...6+..	-0.24904	0.37784	-0.98852
EC2-C...14..	-0.34939	-0.72404	0.04791	S2E0N...10-.	2.02773	-0.6006	1.98448	e0p3Cl..3+..	0.27937	2.38474	0.11486
EC2-C...15..	0.30144	-0.19674	0.25587	S2E0N...11-.	2.10953	2.25836	2.27513	e0p3Cl..4+..	-0.82964	-0.85447	-0.93016
EC2-C...16..	-0.08983	0.40038	2.07207	S2E0N...2-..	-0.09317	0.24945	-0.84046	e0p4C...10+.	-0.28932	-0.93674	0.30068
EC2-C...17..	0.10856	0.21782	-0.79792	S2E0N...3-..	0.05544	0.37314	0.14471	e0p4C...11+.	0.1568	-0.97157	-0.8397
EC2-C...18..	0.31104	-0.62373	-0.15577	S2E0N...4-..	0.13761	0.2976	-0.35338	e0p4C...12+.	-0.03671	0.09639	0.45011
EC2-C...19..	0.19026	-0.66914	2.34399	S2E0N...5-..	0.16214	0.74659	-0.89861	e0p4C...13+.	-1.00517	0.26568	0.08997
EC2-C...20..	1.09592	2.2709	3.2232	S2E0N...6-..	0.34923	0.30188	1.31896	e0p4C...14+.	0.45916	0.08039	0.43001
EC2-C...21..	0.35105	0.05018	2.03222	S2E0N...7-..	-0.66176	0.22509	0.00713	e0p4C...15+.	1.05147	1.27611	-0.29916
EC2-C...22..	0.43326	-0.77189	-2.29108	S2E0N...8-..	-0.99615	-0.94914	-1.08996	e0p4C...2+..	0.32808	3.36571	2.59167
EC2-C...23..	0.42687	0.31068	2.44792	S2E0N...9-..	-0.76624	-0.51912	-0.44635	e0p4C...16+.	0.19386	2.21319	-0.54969
EC2-C...24..	-0.73815	0.41025	-1.3745	S2E0O...1-..	-1.63806	-3.05344	-1.56584	e0p4C...17+.	0.06058	-0.73189	0.37443
EC2-C...27..	-1.44568	-0.55078	-0.31158	S2E0O...2-..	0.08999	2.48075	0.21804	e0p4C...18+.	0.22288	0.01934	0.04174
EC2-C...3...	-1.10568	0.01758	-0.83064	S2E0O...3-..	1.34389	1.21962	-0.10065	e0p4C...19+.	-1.08278	-0.35982	-0.11231
EC2-C...29..	0.9315	-3.77907	2.61219	S2E0O...4-..	-0.76162	-0.58262	-0.26656	e0p4C...20+.	-0.86387	0.27893	-0.52123
EC2-C...4...	0.42323	0.42259	0.45162	S2E0O...5-..	1.25961	0.24229	-0.96355	e0p4C...21+.	-0.37466	0.52262	1.84969
EC2-C...5...	0.26041	0.47713	0.24698	S2E0O...6-..	0.41921	0.10723	0.04183	e0p4C...3+..	-0.80704	-0.90485	-0.24486
EC2-C...6...	0.28932	0.13851	0.49066	S2E0O...7-..	0.13022	-0.74773	-0.93139	e0p4C...4+..	-0.66889	2.22512	0.10584
EC2-C...7...	0.35682	0.14855	-0.52433	S2E0S...0-..	0.771	-0.22161	-0.04317	e0p4C...5+..	0.46566	-0.05193	1.37894
EC2-C...8...	2.2569	2.05776	2.20267	S2E0S...3-..	0.35104	1.42147	-0.73673	e0p4C...6+..	0.14062	0.72633	0.15469
EC2-C...9...	-0.55987	0.35133	0.43636	S2E0S...5-..	2.21948	2.112	2.42632	e0p4C...7+..	0.43342	0.16473	0.43935
EC2-F...5...	-0.42596	-0.57238	0.98744	S2E0S...6-..	0.31052	0.18841	0.09618	e0p4C...8+..	0.22762	2.22979	-0.18437
EC2-F...6...	-0.51393	0.06646	0.15025	S2E0S...8-..	-0.66793	-1.11753	0.3575	e0p4C...9+..	0.01658	0.12005	0.28689
EC2-Br..5...	-0.48756	1.4495	2.32549	S2E0o...4-..	0.39317	-0.50288	0.22965	e0p3N...10+.	-0.60725	0.03983	-0.27227
EC2-Br..6...	-0.24792	-0.66485	0.08141	S2E0o...5-..	1.19693	-0.53672	0.45496	e0p3N...11+.	2.27325	2.14237	-0.86853
EC2-Cl..4...	0.24725	-0.17781	-0.86642	S2E0o...6-..	2.38456	2.13563	-1.27909	e0p3N...2+..	0.31712	1.07352	0.59467
EC2-Cl..5...	1.50158	0.85005	2.22015	S2E0s...3-..	-0.74884	-0.87493	-0.97014	e0p3N...4+..	0.80155	0.5327	-0.26267
EC2-Cl..6...	-0.95706	0.00598	-0.1373	S2E0s...5-..	-0.25131	3.74403	-0.40257	e0p3N...5+..	0.00814	-1.06205	-0.00042
EC2-N...10..	0.39626	0.07774	0.1163	S2E0s...7-..	-0.73317	2.15717	-0.53475	e0p3N...6+..	0.3688	0.44278	0.08182
EC2-N...11..	0.4828	-0.99913	0.10551	S3E0C...0-..	1.65408	-0.99338	-0.70228	e0p3N...7+..	0.46442	0.39812	0.36069
EC2-N...12..	0.17004	-0.54882	0.41366	S3E0C...1-..	0.00706	-0.69701	0.17743	e0p3N...8+..	0.44597	2.22745	0.36548
EC2-N...13..	0.11085	2.03085	2.09426	S3E0C...10-.	0.03027	2.41532	-0.4291	e0p3N...9+..	0.28095	-0.65854	-0.37134
EC2-N...14..	-0.80067	-0.95777	-0.90678	S3E0C...11-.	0.02106	0.60885	-0.67114	e0p3O...2+..	0.32396	-0.21099	0.43265
EC2-N...15..	2.3234	-0.67061	2.17642	S3E0C...12-.	-0.01538	-0.04595	-0.16313	e0p3O...3+..	-0.14387	-0.36005	0.68422

EC2-N...16..	-0.18898	-2.34796	-2.95272	S3E0C...13-.	0.04631	0.25024	0.21969	e0p3O...4+..	0.21481	-0.27713	-0.65819
EC2-N...17..	-0.53355	0.15998	-0.52331	S3E0C...14-.	0.0049	0.30456	2.18695	e0p3O...5+..	2.41161	2.38951	2.2488
EC2-N...18..	2.26421	0.01972	0.0142	S3E0C...15-.	-1.45349	0.05894	0.0316	e0p3O...6+..	1.53163	0.95085	2.23071
EC2-N...19..	0.17887	-0.93194	0.06661	S3E0C...16-.	2.11956	2.33775	0.39911	e0p3O...7+..	0.43958	0.35097	0.46445
EC2-N...20..	-1.7961	-2.63789	-0.91104	S3E0C...17-.	-1.5826	-0.60645	-0.62827	e0p4F...3+..	-0.57297	-0.95209	0.29743
EC2-N...21..	0.71265	-0.27914	0.58549	S3E0C...2-..	0.27429	2.52373	1.68185	e0p4F...6+..	0.18295	0.49407	0.2457
EC2-N...22..	0.05464	-0.77245	-0.82946	S3E0C...3-..	0.47348	0.35625	0.38625	e0p4Br..3+..	0.36314	0.0541	2.4347
EC2-N...23..	3.37699	1.8545	0.16687	S3E0C...4-..	-0.93473	-0.61452	1.3293	e0p4Br..6+..	0.06727	0.31814	0.0778
EC2-N...4...	-0.03328	0.25868	-0.71803	S3E0C...5-..	0.1353	0.33032	0.40759	e0p3S...3+..	-1.07194	-1.38599	-0.8003
EC2-N...9...	0.13378	-0.83364	-0.58222	S3E0C...6-..	0.1197	0.30557	1.11043	e0p3S...5+..	2.45806	2.25649	-0.33346
EC2-O...10..	-0.97934	0.10397	0.05953	S3E0C...7-..	0.03894	0.43282	0.27864	e0p3S...6+..	-0.90629	0.87647	0.01443
EC2-O...11..	0.22069	2.11239	1.27346	S3E0C...8-..	0.135	-0.57563	0.41162	e0p3S...8+..	-0.87719	0.32612	0.1414
EC2-O...12..	1.02826	2.3615	0.12485	S3E0C...9-..	0.23201	0.49088	0.37742	e0p4Cl..3+..	-0.11666	2.38107	0.18685
EC2-O...13..	0.17976	-1.7382	1.19929	S3E0F...3-..	-0.43814	-0.70003	0.05208	e0p4Cl..5+..	0.85198	0.24658	2.28072
EC2-O...4...	0.19638	-1.44827	0.17604	S3E0F...4-..	-0.2098	-0.89458	0.33557	e0p4Cl..6+..	0.55636	0.49357	-0.71496
EC2-O...5...	-0.50469	-0.73846	0.02202	S3E0F...5-..	2.33545	2.42237	-0.04077	e0p4N...10+.	0.31179	0.06563	0.34973
EC2-O...6...	-0.98201	0.13757	0.14343	S3E0F...6-..	0.48171	-0.69144	1.40917	e0p4N...11+.	3.18838	0.91422	0.30805
EC2-O...7...	1.03562	2.15881	0.17717	S3E0Br..3-..	6.6247	4.51131	2.52368	e0p4N...12+.	0.30572	0.42111	0.26418
EC2-O...8...	-0.42132	-2.60232	-0.90195	S3E0Br..4-..	0.04908	0.4982	0.09559	e0p4N...13+.	1.12347	0.80565	0.10728
EC2-O...9...	5.99516	1.7481	2.04759	S3E0Cl..2-..	0.10799	-0.64032	-0.16994	e0p4N...14+.	-0.36079	1.17982	0.06922
EC2-S...11..	-0.53704	2.26223	0.30132	S3E0Cl..3-..	0.47196	0.33385	0.88396	e0p4N...15+.	2.49267	0.4944	0.13954
EC2-S...12..	2.24782	1.19841	0.23536	S3E0Cl..4-..	-0.75885	-0.25885	0.59294	e0p4N...2+..	0.62504	0.24561	0.26561
EC2-S...14..	1.06539	-0.86593	0.12266	S3E0Cl..5-..	-0.12274	1.43134	-0.30097	e0p4N...16+.	-0.6862	-1.43304	0.25758
EC2-S...20..	1.20331	0.56386	0.49351	S3E0Cl..6-..	-0.00565	-0.61346	0.84022	e0p4N...17+.	0.10851	0.11799	2.33664
EC2-S...5...	-0.26735	-0.78173	-0.42607	S3E0N...0-..	-0.46347	0.07602	-1.02237	e0p4N...18+.	2.1519	0.06572	0.10984
EC2-S...9...	2.40698	1.69205	0.14614	S3E0N...1-..	0.42184	2.07231	0.04992	e0p4N...25+.	-0.71977	-0.92102	-0.64886
EC2-o...10..	-0.56314	0.04727	2.37138	S3E0N...10-.	0.43502	0.14057	0.04204	e0p4N...4+..	0.5507	-0.86947	0.52674
EC2-o...11..	0.21401	-0.83843	2.47561	S3E0N...11-.	-0.96838	0.39442	0.09411	e0p4N...5+..	-1.64714	3.08866	0.12504
EC2-o...12..	2.16656	1.76217	0.14536	S3E0N...12-.	2.73052	2.94486	2.90888	e0p4N...6+..	1.49589	6.30859	2.3778
EC2-s...11..	3.13425	1.63576	0.36096	S3E0N...13-.	0.06766	0.4785	1.03017	e0p4N...7+..	-0.83049	-2.56436	0.34369
EC2-s...13..	-0.90932	-0.84778	0.05746	S3E0N...14-.	-0.2887	0.37037	0.03548	e0p4N...8+..	0.0761	-0.86339	0.33023
EC2-s...9...	-0.55745	-1.26584	1.1121	S3E0N...16-.	0.43087	2.41078	-0.04552	e0p4N...9+..	0.07336	-0.99221	0.54163
EC3-C...10..	2.4474	2.53105	2.31054	S3E0N...2-..	0.37683	-0.18076	-0.01571	e0p4O...10+.	1.38443	1.0253	0.16581
EC3-C...12..	-0.94498	0.33457	-0.4771	S3E0N...18-.	0.03508	0.44157	0.27144	e0p4O...11+.	-2.10859	-2.48132	-2.18511
EC3-C...13..	-1.70415	-4.68511	-2.95646	S3E0N...3-..	-0.48186	-0.97315	-0.6514	e0p4O...14+.	-0.90007	-1.03009	0.30624

EC3-C...14..	1.49585	-0.91963	0.33671	S3E0N...4-..	0.31074	-0.72514	0.35025	e0p4O...2+..	0.16312	-0.49995	2.37527
EC3-C...15..	0.13832	-0.53318	0.06897	S3E0N...5-..	0.26551	-0.47349	-0.05424	e0p4O...19+.	-0.87554	-0.89225	-0.93205
EC3-C...16..	0.07726	-1.12449	0.47937	S3E0N...6-..	0.23023	-3.14669	0.63523	e0p4O...3+..	-0.00123	1.88285	-1.70384
EC3-C...17..	-0.87432	2.44012	0.12829	S3E0N...7-..	-0.58561	0.43824	-0.00674	e0p4O...4+..	-0.18337	0.32261	0.39523
EC3-C...18..	-0.8897	0.07184	0.23995	S3E0N...8-..	-0.02605	0.37439	0.12116	e0p4O...5+..	0.42456	-0.33804	0.23732
EC3-C...19..	0.33637	-0.74043	-0.54066	S3E0N...9-..	-4.35528	0.35463	0.40329	e0p4O...6+..	0.01758	0.23207	0.17172
EC3-C...20..	0.37335	0.22522	2.3851	S3E0O...1-..	-0.93927	-0.88383	-0.85516	e0p4O...7+..	2.26212	-0.96335	0.04421
EC3-C...21..	-0.69938	0.376	0.42	S3E0O...10-.	3.33965	-1.62377	0.79017	e0p4O...8+..	1.59711	0.88501	0.97281
EC3-C...22..	-0.55503	-0.0714	-0.50953	S3E0O...13-.	0.4249	4.54962	-0.968	e0p4O...9+..	0.3092	0.26954	0.42352
EC3-C...24..	0.0914	0.03712	0.00464	S3E0O...2-..	0.32657	2.03247	0.00312	e0p4S...12+.	-0.4626	-0.9911	-0.56462
EC3-C...25..	-0.82089	0.11224	0.48117	S3E0O...3-..	0.23745	0.12772	0.10784	e0p4S...3+..	-2.05418	0.1908	-0.71501
EC3-C...26..	0.74239	0.27776	0.17576	S3E0O...4-..	0.15312	-0.58104	-0.97541	e0p4S...6+..	0.6346	-0.11714	2.61593
EC3-C...27..	-0.9867	0.05339	-0.82894	S3E0O...5-..	2.14415	-0.59562	0.1896	e0p4S...7+..	0.16117	2.33489	1.90844
EC3-C...28..	0.37998	0.45118	-0.24271	S3E0O...6-..	1.01875	-0.3755	-0.56712	e0p4S...8+..	2.0505	0.576	2.08547
EC3-C...29..	0.04328	-0.69267	-0.73137	S3E0O...7-..	0.4677	0.32642	0.17652	e0p2o...4+..	1.36054	1.7411	-0.07647
EC3-C...30..	0.04602	0.26784	0.21028	S3E0O...8-..	0.39449	0.6702	0.37746	e0p2o...5+..	0.09351	2.1934	0.26357
EC3-C...31..	-0.9514	0.10559	0.22256	S3E0O...9-..	1.11464	0.25608	0.15059	e0p2o...6+..	2.13467	0.33404	-0.61251
EC3-C...32..	-0.77263	-0.77954	0.07958	S3E0S...1-..	0.09061	-0.68147	0.13089	e0p2s...4+..	-0.86685	-0.03379	-0.37583
EC3-C...33..	0.24683	0.13255	-0.53008	S3E0S...12-.	-0.62795	-0.9372	0.59073	e0p2s...5+..	-0.10329	0.26961	-0.03742
EC3-C...34..	0.17934	0.1682	2.02238	S3E0S...4-..	-0.72195	0.07725	0.13977	e0p2s...6+..	-4.61479	-8.59535	-2.45103
EC3-C...35..	0.48339	1.34558	0.13676	S3E0S...5-..	1.6353	-0.03023	0.60054	e0p3o...5+..	-0.77796	0.03654	-0.04721
EC3-C...36..	-0.6941	-0.65949	-1.50778	S3E0S...7-..	1.84559	0.34975	2.15261	e0p3o...6+..	0.1694	-0.68075	1.53289
EC3-C...37..	-0.26391	-0.64795	0.46617	S3E0S...9-..	0.42433	2.39654	-0.74903	e0p3s...5+..	-1.02886	0.00084	-0.69737
EC3-C...38..	2.2428	4.36364	-0.95422	S3E0o...4-..	0.37238	0.38624	-0.5716	e0p3s...6+..	2.35228	1.23306	1.43768
EC3-C...39..	-5.62347	-7.59348	-2.6606	S3E0o...5-..	0.28786	2.33248	0.126	e0p3s...7+..	1.89181	1.38677	-0.13585
EC3-C...40..	2.1921	0.07178	0.06025	S3E0o...6-..	-0.05434	2.47749	5.03971	e0p4o...10+.	0.71446	0.98261	0.98515
EC3-C...41..	0.2567	-0.75117	0.49224	S3E0o...8-..	-0.67585	0.15873	-0.82825	e0p4o...5+..	0.43094	-0.55217	0.39512
EC3-C...42..	-0.60069	-0.46004	0.4454	S3E0o...9-..	2.16774	0.06689	1.06924	e0p4o...8+..	-0.60581	-1.38851	-1.29618
EC3-C...43..	0.1404	2.07436	1.94814	S3E0s...11-.	-0.61012	2.14623	0.07428	e0p4s...11+.	0.93326	2.70696	0.23581
EC3-C...44..	-1.01084	-3.91763	-0.70248	S3E0s...5-..	-0.4634	2.45161	-0.0442	e0p4s...5+..	1.91738	0.15689	2.32651
EC3-C...45..	0.4388	0.76331	0.18277	S3E0s...6-..	0.67073	-0.55328	0.23021	e0p4s...7+..	-0.20375	-0.72694	0.89493
EC3-C...46..	0.57992	2.42563	0.39754	S3E0s...8-..	1.29733	-1.28214	2.21231	e0p4s...8+..	0.62484	1.22138	1.60716
EC3-C...47..	-0.41757	0.04282	-0.69944	PT2-C...1...	0.25446	0.0693	0.21564	e0s2C...10+.	0.28363	0.43828	-0.80799
EC3-C...48..	-3.89514	0.49349	-0.85123	PT2-C...2...	0.0104	-0.39062	0.4262	e0s2C...11+.	0.02308	-0.6894	0.14963
EC3-C...49..	1.27036	1.00364	0.25839	PT2-C...3...	0.01511	0.39917	0.16105	e0s2C...12+.	0.0828	-0.50526	0.1099

EC3-C...50..	2.26057	1.11994	2.35375	PT2-C...4...	0.23879	2.11235	0.22635	e0s2C...13+.	2.41737	2.04026	0.03467
EC3-C...51..	3.27844	3.40051	2.72135	PT2-C...5...	0.23234	0.18556	0.18168	e0s2C...14+.	0.79528	-0.21625	0.84063
EC3-C...52..	0.94823	-0.32316	-0.77139	PT2-C...6...	-0.55037	0.27335	-0.7294	e0s2C...15+.	0.41416	0.4388	0.35714
EC3-C...53..	-0.47846	-0.68309	0.06355	PT2-F...2...	-0.7776	-0.83954	-0.82214	e0s2C...16+.	0.2974	-0.0571	-2.99729
EC3-C...54..	0.1198	1.72054	-0.21065	PT2-Br..2...	0.20027	0.42966	0.38518	e0s2C...17+.	1.33291	2.06132	0.44383
EC3-C...55..	3.17958	2.45057	1.26776	PT2-Cl..1...	0.15043	2.20063	0.08925	e0s2C...18+.	-0.04171	0.03733	-0.5432
EC3-C...56..	0.37252	-0.15314	0.28864	PT2-Cl..2...	2.24181	1.83744	0.46165	e0s2C...3+..	0.24648	-0.18343	-1.23651
EC3-C...57..	-0.1084	0.4929	2.09437	PT2-N...2...	0.26891	-0.33348	0.18241	e0s2C...4+..	0.41971	0.0237	0.28022
EC3-C...58..	0.40291	-0.90994	0.49695	PT2-N...3...	0.15725	0.00072	0.46811	e0s2C...5+..	0.14447	0.08648	0.09886
EC3-C...59..	-0.76062	0.25665	0.31197	PT2-N...4...	0.21449	-0.59258	0.22417	e0s2C...6+..	0.02963	-0.01824	2.45376
EC3-C...60..	-0.0621	0.27675	0.22206	PT2-N...5...	-0.61027	-0.45973	0.0295	e0s2C...7+..	0.39783	0.28224	0.25459
EC3-C...61..	-0.50608	2.12337	-0.71404	PT2-N...6...	-0.50659	0.39077	0.22569	e0s2C...8+..	-0.63842	0.3346	0.28393
EC3-C...62..	0.00438	-0.67216	0.25922	PT2-O...1...	-1.19702	-0.05726	-1.06649	e0s2C...9+..	0.19948	0.45233	0.27579
EC3-C...63..	0.02535	-1.21165	-0.59298	PT2-O...2...	-0.70802	-0.8914	0.24298	e0s2F...5+..	0.70054	0.15585	0.28428
EC3-C...64..	-0.31816	0.39804	-0.72302	PT2-O...3...	-0.12735	0.13949	-0.10439	e0s2F...6+..	0.47988	0.13496	-0.44289
EC3-C...67..	1.48643	-1.2821	-0.91509	PT2-O...4...	-0.53032	-1.66095	-0.16213	e0s2Br..5+..	0.1464	0.53521	0.43839
EC3-C...7...	-0.75002	-0.73814	-0.61236	PT2-S...2...	2.29124	2.51706	0.47538	e0s2Br..6+..	-1.28715	-0.50273	-0.96516
EC3-C...73..	-0.3753	-0.80296	0.2259	PT2-S...3...	-0.84643	2.48825	0.05127	e0s2Cl..4+..	-0.20294	0.4522	2.39549
EC3-C...8...	1.07336	0.46577	0.12963	PT2-S...4...	0.64094	0.40579	0.54594	e0s2Cl..5+..	0.30239	0.433	2.25776
EC3-C...9...	0.45059	2.44915	2.3082	PT2-o...2...	2.35903	2.47798	-0.183	e0s2Cl..6+..	-0.65338	-0.94611	-0.82549
EC3-F...13..	-0.73963	0.83686	2.33485	PT2-o...3...	0.13127	-0.34548	0.48992	e0s3C...10+.	0.38811	0.29257	0.00186
EC3-F...14..	0.4848	-0.81918	0.22243	PT2-o...4...	0.34623	1.55267	-0.47855	e0s3C...11+.	-0.60808	0.45674	-0.3519
EC3-F...15..	2.51565	2.31785	2.63999	PT2-s...2...	0.97315	0.5619	-0.53246	e0s3C...12+.	0.32492	0.37926	0.40929
EC3-F...16..	0.50074	-0.45175	0.21048	PT2-s...3...	-0.01151	0.82841	2.4101	e0s3C...13+.	0.14137	-0.8641	0.40859
EC3-Br..13..	6.71455	6.37473	6.26475	PT2-s...4...	-4.45254	-7.84056	-1.28223	e0s3C...14+.	0.12913	-0.03029	0.30409
EC3-Br..14..	0.40119	0.18522	0.3117	PT3-C...1...	-0.56477	-0.89487	-0.43404	e0s3C...15+.	0.31497	2.25519	0.43862
EC3-Cl..13..	0.34969	2.33702	1.17158	PT3-C...2...	1.29018	0.10162	-1.12067	e0s3C...16+.	0.00879	0.47124	-0.58067
EC3-Cl..14..	-0.54865	-1.24617	-1.58419	PT3-C...3...	0.45676	0.47492	0.1986	e0s3C...17+.	0.04038	-0.74657	-0.80964
EC3-Cl..15..	0.48976	0.01094	-0.80727	PT3-C...4...	0.42883	0.03419	0.24097	e0s3C...18+.	-0.20837	2.0331	-0.59389
EC3-Cl..16..	0.43335	-0.66109	-0.08218	PT3-C...5...	-0.148	-0.76297	0.39104	e0s3C...19+.	0.41406	0.23967	0.06251
EC3-Cl..7...	-0.70399	0.04931	0.17964	PT3-C...6...	0.33714	0.24693	0.25203	e0s3C...20+.	0.34982	0.32397	0.33175
EC3-Cl..8...	-0.02058	0.07927	1.08971	PT3-C...7...	0.4629	2.34055	-0.00514	e0s3C...21+.	-0.73794	-0.96287	-0.53926
EC3-N...11..	0.45148	0.49527	1.25913	PT3-C...8...	0.26695	0.39226	2.09375	e0s3C...22+.	-0.96577	0.48336	0.28696
EC3-N...18..	-0.77315	0.03748	-0.00271	PT3-C...9...	-0.53928	0.08078	0.24847	e0s3C...23+.	-1.11596	-0.3977	-0.03093
EC3-N...19..	0.40666	2.44319	0.33478	PT3-F...2...	0.38274	0.41004	0.11768	e0s3C...4+..	1.58612	4.439	1.31169

EC3-N...20..	0.39729	-0.86881	-0.73119	PT3-F...3...	0.49343	-0.96117	-0.79908	e0s3C...5+..	-0.22572	0.22231	0.11931
EC3-N...21..	-1.07487	1.44079	-0.68357	PT3-Br..2...	2.01079	2.23228	0.035	e0s3C...6+..	-0.69696	2.4127	0.23294
EC3-N...22..	-0.77258	0.46284	-0.75409	PT3-Br..3...	-0.621	0.05247	0.11333	e0s3C...7+..	-4.69471	-1.2232	0.54447
EC3-N...23..	4.47468	0.3339	2.19531	PT3-Cl..2...	0.18659	0.29612	0.05552	e0s3C...8+..	0.46252	0.03358	0.423
EC3-N...24..	-0.82288	0.07006	0.18356	PT3-Cl..3...	1.19216	0.51779	-0.52696	e0s3C...9+..	0.55076	-0.95326	0.01796
EC3-N...25..	-0.76112	0.16091	-0.7494	PT3-N...1...	0.26717	-0.60636	-0.53077	e0s2N...10+.	1.37279	0.32675	0.25599
EC3-N...26..	-9.74342	-9.98429	0.20476	PT3-N...2...	0.287	-0.08437	0.06108	e0s2N...11+.	0.17601	0.18085	0.32788
EC3-N...27..	0.23482	-0.01961	0.40325	PT3-N...3...	0.44718	-0.45533	0.32902	e0s2N...12+.	0.66483	2.20169	0.4971
EC3-N...28..	-0.23515	-0.91014	-0.56576	PT3-N...4...	-0.94672	0.43766	0.11704	e0s2N...13+.	0.38183	-0.99152	0.34408
EC3-N...29..	2.07828	1.54962	0.74321	PT3-N...5...	-0.64698	0.10138	1.32398	e0s2N...14+.	-0.72413	-4.49693	-0.93082
EC3-N...30..	0.24997	0.42254	-0.81375	PT3-N...6...	-0.79221	0.24709	0.19353	e0s2N...15+.	-0.68755	-0.58	0.14095
EC3-N...31..	-0.86675	0.22567	0.13594	PT3-N...7...	-0.70767	-0.71245	0.3442	e0s2N...16+.	-0.40794	0.26939	-0.22353
EC3-N...32..	2.64128	2.23265	0.45034	PT3-N...8...	2.21669	2.34135	0.00539	e0s2N...17+.	3.80867	4.03358	2.0866
EC3-N...33..	2.38669	2.14317	0.09121	PT3-O...1...	0.2805	-0.07065	0.11413	e0s2N...4+..	0.46123	0.27832	-0.20141
EC3-N...34..	0.1299	0.4716	-0.79014	PT3-O...2...	0.09109	-0.10368	0.42608	e0s2N...7+..	-1.62868	-0.04157	-0.63087
EC3-N...35..	-0.5526	-0.50295	2.66565	PT3-O...3...	0.24514	-0.69168	0.18021	e0s2N...8+..	0.2621	0.24078	0.31508
EC3-N...36..	0.72725	0.61258	-0.08839	PT3-O...4...	2.41388	1.05345	0.37069	e0s2N...9+..	0.51274	0.20414	0.37486
EC3-N...38..	0.37647	0.40865	0.11955	PT3-O...5...	0.28582	-0.67247	0.44503	e0s2O...10+.	4.22034	1.92666	0.50933
EC3-N...39..	0.63607	0.13864	1.52788	PT3-O...6...	-0.76382	2.67907	-1.03992	e0s2O...11+.	-0.88276	-0.65226	-0.10429
EC3-N...41..	2.46111	2.61004	-0.2276	PT3-S...2...	1.86384	0.1626	-3.30216	e0s2O...4+..	0.4835	-0.43383	1.00819
EC3-N...42..	1.79283	2.187	2.38598	PT3-S...3...	-0.69645	2.44017	-0.11805	e0s2O...5+..	0.07283	1.38092	0.04336
EC3-N...43..	-0.79234	-0.97751	-0.11	PT3-S...4...	2.02275	0.4295	0.43765	e0s2O...6+..	0.21566	0.29905	0.48506
EC3-N...44..	0.4326	0.29253	0.6581	PT3-S...6...	0.26073	-0.74893	1.30128	e0s2O...7+..	0.22443	0.07866	-0.13582
EC3-N...45..	0.09203	-1.31588	-0.64163	PT3-o...3...	0.33135	-0.81257	0.15236	e0s2O...8+..	-1.00423	0.11839	0.52276
EC3-N...47..	-0.96075	-0.69625	-0.8336	PT3-o...4...	0.24298	2.09265	0.00176	e0s2O...9+..	0.00885	0.47217	0.22994
EC3-N...48..	-0.58218	-2.0013	0.20778	PT3-s...3...	-0.72682	-0.67342	-0.82591	e0s3F...5+..	-0.5303	0.4384	-0.91886
EC3-N...50..	-0.14582	-1.89878	-0.92649	PT3-s...4...	2.15052	2.48839	2.11635	e0s3F...6+..	0.10784	-0.43326	0.318
EC3-N...51..	2.19357	2.33966	-0.24405	PT3-s...5...	0.75956	-1.35258	0.34659	e0s3F...7+..	0.30865	2.12979	2.04866
EC3-N...52..	0.20478	0.78068	-1.35822	PT4-C...1...	0.42208	-1.92986	-0.152	e0s3F...8+..	0.11544	-0.86912	0.29264
EC3-N...53..	2.3774	0.25176	1.11935	PT4-C...10..	-0.69424	-0.50114	-0.73166	e0s3Br..5+..	3.53791	6.71238	2.55523
EC3-N...55..	0.49669	0.25994	0.27297	PT4-C...11..	2.03684	0.27353	0.46569	e0s3Br..6+..	0.33988	0.3588	-0.18722
EC3-N...56..	-0.36685	-1.92685	-1.02506	PT4-C...12..	0.47871	0.19061	1.1254	e0s2S...10+.	-0.78877	-0.04126	-0.13743
EC3-N...58..	2.18928	0.46184	1.30542	PT4-C...13..	-0.8079	-1.06188	0.98847	e0s2S...12+.	-0.14245	-1.46549	-0.95956
EC3-N...59..	-1.02558	-4.32443	-1.68341	PT4-C...14..	-0.17964	0.06681	0.25528	e0s2S...5+..	-0.30041	0.28562	-0.10274
EC3-N...60..	0.26085	2.01269	0.19436	PT4-C...15..	-0.44902	-0.70689	-0.25441	e0s2S...7+..	2.45868	1.9517	0.15081

EC3-O...11..	-0.12347	-0.40081	-0.13179	PT4-C...16..	-0.61148	0.50198	0.08761	e0s2S...8+..	-0.56181	1.59458	0.1188
EC3-O...12..	0.45666	-0.27435	0.3635	PT4-C...17..	0.069	0.17921	0.12884	e0s2S...9+..	2.01107	0.1417	1.51467
EC3-O...13..	-0.16318	-0.48587	0.09868	PT4-C...2...	0.1286	0.41307	0.35261	e0s3Cl..4+..	-0.52796	0.17811	1.87768
EC3-O...14..	0.13447	-0.20017	0.20687	PT4-C...18..	0.30303	-0.48782	-0.73343	e0s3Cl..5+..	0.25307	2.7312	1.89931
EC3-O...15..	0.22826	2.00338	0.52951	PT4-C...3...	-0.23984	0.02758	0.41206	e0s3Cl..6+..	0.09765	0.00685	0.28969
EC3-O...16..	-0.91846	2.00704	0.15305	PT4-C...4...	0.23529	0.00657	0.29259	e0s3Cl..7+..	0.00495	-0.88592	0.04749
EC3-O...17..	-0.30323	-0.64254	-0.83154	PT4-C...5...	0.11967	1.30695	2.00534	e0s3Cl..8+..	-1.00134	-0.78537	-0.61551
EC3-O...18..	0.39478	-0.61682	-0.05201	PT4-C...6...	0.18749	0.25961	0.26883	e0s3N...10+.	0.2379	0.07329	-0.10401
EC3-O...19..	2.41916	0.4321	1.37393	PT4-C...7...	1.19135	1.58921	2.40401	e0s3N...11+.	0.63553	0.27717	0.4804
EC3-O...20..	-0.06463	-0.76158	-0.62473	PT4-C...8...	0.46899	0.16917	0.08514	e0s3N...12+.	-0.55731	-1.12994	0.21124
EC3-O...21..	-0.29967	1.14599	0.05506	PT4-C...9...	0.19327	0.28984	0.17753	e0s3N...13+.	-2.52653	-1.96334	-7.15284
EC3-O...22..	-1.05661	1.56339	0.49568	PT4-F...2...	1.24609	-0.5329	0.20058	e0s3N...14+.	-0.45047	-0.86609	0.11029
EC3-O...23..	0.40499	2.45761	-0.66251	PT4-F...5...	0.17607	-0.23447	0.4723	e0s3N...15+.	-0.443	-0.75191	-0.42883
EC3-O...24..	-0.27276	-0.72075	0.65919	PT4-Br..2...	2.39665	2.10155	0.40698	e0s3N...16+.	0.34688	0.42714	-0.05061
EC3-O...25..	-0.77762	-0.77366	-0.4498	PT4-Br..5...	-0.92996	-0.85895	0.06694	e0s3N...17+.	0.26057	0.11198	0.05689
EC3-O...27..	2.49443	2.07676	2.29724	PT4-Cl..2...	-0.15259	2.44971	2.12274	e0s3N...18+.	2.4074	0.24233	0.23138
EC3-O...28..	0.21841	0.72734	1.49079	PT4-Cl..4...	0.22708	-0.97919	-0.87897	e0s3N...19+.	0.31891	0.13577	-0.45152
EC3-O...32..	2.46657	2.74136	2.25542	PT4-Cl..5...	-0.79795	-0.09277	-0.62732	e0s3N...20+.	0.19041	-0.22953	0.24669
EC3-O...33..	2.04924	1.2565	3.98774	PT4-N...1...	0.55799	0.43577	-0.90503	e0s3N...24+.	0.49755	-0.01563	2.34721
EC3-O...35..	-0.82875	-0.76781	-0.60688	PT4-N...10..	-0.58567	-0.31984	-0.48783	e0s3N...3+..	0.48964	0.16283	0.12483
EC3-S...14..	-1.01298	-1.62648	-0.55086	PT4-N...11..	2.42647	0.10145	-0.50982	e0s3N...6+..	0.41391	-0.92941	-0.78327
EC3-S...23..	2.31511	2.15739	1.73124	PT4-N...12..	2.79413	-1.72994	-0.17318	e0s3N...8+..	0.30858	0.2933	0.16018
EC3-S...25..	4.18039	-0.027	2.02285	PT4-N...13..	0.29598	0.06228	2.07408	e0s3N...9+..	1.42636	4.47233	0.59799
EC3-S...35..	-0.63081	-1.31345	-0.41031	PT4-N...14..	2.20713	2.00761	0.41539	e0s3O...10+.	0.11108	0.28091	0.45484
EC3-S...38..	-0.24301	1.08536	0.00896	PT4-N...16..	2.58681	2.30829	-0.27888	e0s3O...11+.	1.22338	0.24157	0.18626
EC3-o...23..	1.71128	1.22366	2.00508	PT4-N...2...	-0.43051	-0.64696	0.29593	e0s3O...12+.	0.3787	-0.27914	-0.91377
EC3-o...24..	-0.82291	0.44509	-0.65129	PT4-N...22..	-0.34746	-0.8065	0.19785	e0s3O...13+.	-0.33451	-0.67679	-0.54797
EC3-o...25..	0.14954	-0.29356	0.57957	PT4-N...3...	-0.96762	0.3798	-0.97567	e0s3O...15+.	-1.08309	-0.75148	0.88993
EC3-o...26..	1.24554	4.14851	2.11004	PT4-N...4...	0.47205	1.41412	0.40732	e0s3O...3+..	0.2392	-0.52028	0.22321
EC3-o...28..	-0.66109	-0.498	-0.87538	PT4-N...5...	-0.30512	-1.10182	-0.96848	e0s3O...4+..	0.24082	0.29293	1.27095
EC3-o...35..	2.09204	2.18342	2.12962	PT4-N...6...	-0.30112	-0.12376	-0.76973	e0s3O...5+..	-0.77087	0.21005	0.34387
EC3-s...20..	-1.08807	0.3158	-1.02984	PT4-N...7...	7.51721	3.25739	-1.60476	e0s3O...6+..	0.01115	0.11899	0.47877
EC3-s...26..	0.00947	0.96908	2.16359	PT4-N...8...	-0.14404	0.36462	1.23865	e0s3O...7+..	0.18614	2.31159	0.32537
EC3-s...28..	1.98136	0.96746	-0.77692	PT4-N...9...	0.38077	-0.89649	0.48502	e0s3O...8+..	-0.83938	0.08941	0.22432
EC3-s...31..	2.62267	-0.98167	1.42922	PT4-O...1...	1.37096	0.01705	-0.04746	e0s3O...9+..	-0.05488	0.16777	-0.54279

EC3-s...37..	0.2403	0.26811	0.21	PT4-O...13..	-1.50701	-1.09625	0.19097	e0s3S...11+.	0.46234	2.16379	2.348
H.....	0.89678	2.97961	0.21829	PT4-O...2...	0.36697	0.20108	-0.70637	e0s3S...13+.	1.31148	0.34806	-0.72935
Br..(.....	-2.31961	-2.79923	-1.4517	PT4-O...18..	0.23504	-0.48254	-0.51993	e0s3S...16+.	0.01112	-0.97941	0.39022
Br..(...C...	-0.59845	0.45082	-0.27149	PT4-O...3...	0.48588	-0.10847	-0.96543	e0s3S...6+..	0.04327	-1.15905	-0.31894
Br.....	0.36912	0.41168	1.14251	PT4-O...4...	0.39082	1.45783	0.45152	e0s3S...9+..	2.63493	10.32733	9.17314
Br..c...1...	0.21202	0.01707	2.02815	PT4-O...5...	0.33873	-0.5392	-0.32683	e0s2o...10+.	0.01986	-0.67877	0.84987
Cl..(.....	-0.95718	0.61057	0.44041	PT4-O...6...	3.45186	0.71846	0.335	e0s2o...8+..	0.09057	0.01514	-0.74567
Cl..(...1...	0.83591	-0.78967	0.30389	PT4-O...7...	-0.52015	-0.90714	3.96309	e0s2o...9+..	0.40876	-0.24864	0.32664
Cl..(...2...	2.18608	0.05885	2.43016	PT4-O...8...	-0.94387	-0.64319	0.81537	e0s2s...11+.	0.49004	-1.11992	0.05659
Cl..(...Cl..	0.14765	-1.88091	0.53108	PT4-O...9...	-0.54838	0.14914	0.23599	e0s2s...7+..	0.09324	0.03739	-0.33584
Cl.....	0.03501	0.52815	-0.86741	PT4-S...10..	0.01948	0.25989	-0.3344	e0s2s...9+..	3.55913	4.50171	1.68066
Cl..1.....	-0.97697	-0.64197	-0.97209	PT4-S...2...	0.5859	-0.54629	-4.22334	e0s3o...10+.	0.29621	1.46135	4.95425
Cl..C.....	2.00104	2.48238	-0.50044	PT4-S...5...	1.28269	2.34703	-0.21107	e0s3o...12+.	-0.75128	-0.43578	-0.24922
Cl..C...C...	0.36561	0.01188	0.12703	PT4-S...6...	1.147	2.07079	1.85755	e0s3o...13+.	1.07271	2.21836	1.31321
Cl..c...1...	4.3243	0.5122	1.25189	PT4-o...3...	0.42921	0.17841	0.16043	e0s3o...8+..	-0.91067	-0.93903	0.58624
Cmax.1.....	-0.80591	1.08364	-0.05379	PT4-o...6...	-1.79995	-2.58895	-2.72761	e0s3o...9+..	2.31314	0.3736	0.48936
Cmax.2.....	-0.70572	-0.48621	0.42893	PT4-o...8...	0.45718	2.35114	0.08014	e0s3s...10+.	-0.35635	0.15468	-0.79801
Cmax.3.....	2.31983	2.26876	-0.72641	PT4-s...3...	1.2109	-0.02519	3.28907	e0s3s...12+.	2.17992	0.6088	2.99656
HALO00000000	0.49841	1.06342	0.23296	PT4-s...5...	-1.28085	0.09922	-0.47482	e0s3s...15+.	-0.84569	0.02836	0.26181
HALO00100000	2.46865	1.2245	-1.33792	PT4-s...6...	0.33047	0.36743	2.43622	e0s3s...9+..	-0.01375	2.22087	-0.60565
HALO01000000	-0.26839	-1.92121	1.97373	PT4-s...9...	0.00905	2.20336	-0.07072	e0nnC...102+	-0.26835	0.46876	0.33394
HALO10000000	-0.19363	-0.52712	0.62303	Nmax.0.....	2.8306	1.38072	2.23903	e0nnC...111+	0.4909	0.03032	0.16418
HALO10100000	2.00342	1.4555	1.22493	Nmax.1.....	0.13778	0.25297	0.38643	e0nnC...204+	0.2135	0.04661	-2.60528
HALO11000000	-0.61618	0.15821	-0.80196	Nmax.2.....	2.40929	0.19397	0.27371	e0nnC...213+	-0.92306	0.40976	0.21202
HALO11100000	-1.46825	-0.96083	-0.39065	Nmax.3.....	0.18661	-1.01225	0.36461	e0nnC...222+	0.08025	-0.66826	-0.53828
N...(.....	0.35248	-0.12537	-0.81142	Nmax.4.....	0.45299	-0.90449	-0.69629	e0nnC...306+	-1.35365	-1.03976	-0.00294
N...(...1...	-0.75675	0.84863	0.00873	Omax.1.....	0.4973	0.0018	-0.64437	e0nnC...315+	0.20669	-3.00856	-0.82151
N...(...C...	-0.21659	0.2758	0.08496	Omax.2.....	3.42136	2.37076	2.25833	e0nnC...324+	0.18926	0.40724	-0.68808
N...+.....	-0.87132	-0.96453	-1.27362	Omax.3.....	0.25608	2.27222	1.97351	e0nnC...333+	-0.61913	0.20436	0.45031
N.....	-0.61072	-0.53831	0.05425	Omax.4.....	-3.13641	-1.05822	-1.83583	e0nnC...435+	-0.68759	0.50274	-0.0533
N...1.....	1.42567	0.09595	0.21592	Omax.5.....	-0.00591	-0.30399	0.11918	e0nnC...444+	0.45785	2.24527	-1.04165
N...1...C...	1.86629	4.64481	-0.00495	Omax.7.....	-0.92579	1.02599	-0.85459	e0nnF...111+	0.3349	0.08334	0.2532
N...1...N...	-0.65	0.17332	0.40911	VS2-C...10..	1.38407	0.72743	0.45669	e0nnBr..111+	-0.04566	2.30613	-0.89873
N...2.....	0.2998	-0.35555	-1.05923	VS2-C...11..	0.42574	-0.57049	0.2984	e0nnCl..111+	0.44556	0.3887	-0.80044
N...2...C...	0.02195	1.39331	-0.61813	VS2-C...12..	0.47504	0.39153	0.05779	e0nnN...111+	-0.01902	0.22348	0.35738

N...=.....	-0.57441	2.61859	-0.11743	VS2-C...13..	0.4547	-0.87171	0.43206	e0nnN...204+	-0.51019	0.07391	0.16291
N...=...C...	2.23926	-0.11195	-0.42279	VS2-C...14..	0.38394	0.4596	0.1299	e0nnN...213+	0.04699	-0.45019	0.80574
N...C...(...	-0.78602	0.11425	-0.68113	VS2-C...15..	-0.84177	-1.94109	1.03908	e0nnN...222+	0.33317	-0.15933	-0.89743
N...C.....	-0.40371	0.22941	-0.65579	VS2-C...2...	-0.89662	-0.4577	0.30536	e0nnN...315+	1.13751	-0.86983	0.68222
N...C...1...	2.12146	0.26976	0.18247	VS2-C...3...	1.23068	0.38735	0.14678	e0nnN...324+	-0.03569	0.16708	0.09088
N...C...2...	1.15511	2.30103	0.10391	VS2-C...4...	0.11794	0.48692	0.41945	e0nnN...333+	0.18758	0.29942	-0.53914
N...C...C...	5.83411	6.81947	2.03521	VS2-C...5...	0.10172	0.60464	-0.93757	e0nnO...102+	-0.18289	0.37783	-0.67987
N...N...(...	-0.97812	-1.10514	0.30803	VS2-C...6...	0.29477	0.63962	-0.55993	e0nnO...111+	0.24563	0.40195	0.14759
N...N.....	2.23962	2.25339	0.13211	VS2-C...7...	-0.69819	-0.06214	0.11691	e0nnO...213+	0.4004	0.5662	2.13864
N...N...=...	0.13933	0.23872	0.28748	VS2-C...8...	0.04004	-0.13492	0.70959	e0nnO...222+	0.44606	-0.47718	0.13313
N...N...C...	-0.60089	-0.1096	0.01787	VS2-C...9...	0.2772	-0.50324	-0.77541	e0nnS...111+	-0.90701	0.18387	-0.76549
N...[...(...	2.24563	-0.17968	-0.82755	VS2-F...4...	-1.61332	-0.70755	0.41691	e0nnS...222+	0.36614	0.10389	-0.4678
N...[...1...	-0.6863	0.08052	0.12762	VS2-F...5...	-0.95116	0.05127	-0.65364	e0nnS...426+	1.00777	1.17979	0.03227
N...c...1...	-0.65653	-0.30374	-0.73751	VS2-Br..4...	2.44327	2.07903	2.37106	e0nno...204+	0.23278	1.9705	2.59109
N...c...2...	4.74282	5.38096	2.43725	VS2-Br..5...	0.33303	-0.69641	-0.5473	e0nno...222+	0.49457	2.33966	0.2871
O...(...(...	-1.34551	0.32495	-0.21474	VS2-Cl..3...	1.25434	-0.28018	0.22487	e0nns...213+	-1.63575	-1.21582	-0.17567
O...(.....	0.10035	0.27528	0.25367	VS2-Cl..4...	2.15842	2.19455	0.47377	e0nns...222+	0.28853	2.18978	0.02666
O...(../...	-0.88041	0.00958	0.12893	VS2-Cl..5...	-0.80908	-0.86913	1.33063	n...(.....	0.09641	0.21663	0.45282
O...(...1...	-0.75834	0.4239	0.35185	VS2-N...10..	0.04925	0.76657	0.61846	n...(...1...	0.35253	0.19676	-0.35001
O...(...2...	-0.15368	2.49441	2.24113	VS2-N...11..	-0.0815	-1.09916	-0.38202	n...(...O...	-0.83423	0.30829	0.02803
O...(...C...	0.24582	0.03808	0.27915	VS2-N...12..	-0.12205	-1.08795	0.05175	n...(...c...	2.05941	1.96844	0.36533
O...(...F...	-0.53035	4.02393	2.23811	VS2-N...13..	0.05173	0.31179	-0.83179	n...+.....	-0.05218	0.49026	0.46647
O...(...N...	-0.04156	-1.81111	0.47604	VS2-N...14..	1.20055	4.1435	2.86398	n...+...[...	1.01381	0.45494	0.26647
O...(...O...	-0.64541	2.36654	-0.75104	VS2-N...3...	0.56818	0.07054	-0.67302	n.....	0.32298	-0.6438	0.36189
O...-.....	1.39401	-0.7654	0.15458	VS2-N...4...	2.96503	2.46034	2.23389	n...1...(...	-0.80894	0.33474	-0.38065
O.....	-0.70025	0.26093	-0.73823	VS2-N...5...	-0.09425	0.47866	-0.13984	n...1.....	0.14668	0.36842	0.30787
O...1...(...	-1.51952	-2.10862	3.18822	VS2-N...6...	0.25234	-0.05388	0.06884	n...1...C...	1.57742	0.21353	0.099
O...1.....	0.54077	2.39146	0.02311	VS2-N...7...	-0.17728	-0.69471	-0.82874	n...1...[...	1.22073	0.02362	0.24116
O...=...(...	-0.55521	0.02474	-0.65005	VS2-N...8...	0.1816	0.47095	0.27634	n...1...c...	-0.21795	0.31245	0.31641
O...=.....	-0.56927	-0.17535	-0.93516	VS2-N...9...	0.07825	-0.29272	0.20383	n...1...n...	0.07161	0.36388	0.42428
O...=...1...	0.33424	-1.33652	0.30233	VS2-O...3...	-0.34438	-0.50391	-0.26518	n...2.....	0.56476	0.00738	-0.20623
O...=...2...	-1.3442	-1.43252	-0.95522	VS2-O...4...	0.26289	0.37849	0.552	n...2...C...	1.40918	1.95453	-0.90256
O...=...C...	-0.04624	-0.72001	0.28246	VS2-O...5...	0.15004	0.09638	0.24372	n...2...n...	1.31646	0.86058	-0.19383
O...C...(...	1.23145	0.05876	0.31019	VS2-O...6...	1.15581	1.8592	1.40649	n...C...(...	0.36029	0.2839	-0.86262
O...C.....	0.44544	2.44785	0.04362	VS2-O...7...	0.3868	0.36399	2.23596	n...C.....	0.05115	0.27151	0.30878

O...C...1...	1.05478	-1.10829	0.9711	VS2-O...8...	0.28238	2.33282	0.92794	n...C...C...	0.20329	-0.20365	0.48976
O...C...C...	2.28312	2.45744	0.61907	VS2-O...9...	0.13822	0.01627	-0.57058	n...H.....	3.48506	1.71904	-0.99867
O...C...N...	-1.69091	-1.9792	-1.0682	VS2-S...10..	0.28901	-1.05848	0.01636	n...H...[...	0.13677	1.53383	-0.77528
O...[...(...	-0.95302	-0.14045	0.17418	VS2-S...4...	0.5139	0.53499	-0.71959	n...O.....	0.14188	-0.66129	2.1398
O...[...1...	-0.70786	-0.6487	0.3735	VS2-S...5...	-0.64596	0.3041	-0.2332	n...O...C...	1.12812	-0.39734	-0.75783
O...c...1...	0.76218	0.30401	0.42498	VS2-S...7...	2.00347	2.09294	0.08534	n...[...(...	0.08031	0.0207	0.3171
O...c...2...	-0.7944	2.13301	1.94981	VS2-S...8...	-0.88182	-0.06688	0.14057	n...[.....	0.6555	2.16689	2.0211
O...c...3...	0.88807	-1.18153	-0.67053	VS2-o...6...	0.46421	0.02409	0.26852	n...[...1...	2.14383	-0.9717	2.21785
O...n...1...	0.15826	-0.2156	-0.05466	VS2-o...7...	0.34192	2.27018	0.23761	n...[...c...	2.2504	0.28929	0.18621
P2E0C...0-..	0.17145	0.38359	0.36592	VS2-o...8...	2.42288	-0.23439	0.04008	n...[...n...	1.34076	0.0399	0.35453
P2E0C...1-..	-0.07334	-0.66504	-0.18458	VS2-s...5...	-0.00427	1.67686	0.30239	n...c...(...	1.21262	0.15215	-0.52035
P2E0C...2-..	0.40136	0.07832	0.02013	VS2-s...7...	0.93305	2.56815	0.20563	n...c.....	0.7922	2.42025	0.25851
P2E0C...3-..	0.05077	-0.78601	-0.64163	VS2-s...9...	0.01198	-0.82854	-0.72734	n...c...1...	0.01573	1.88952	0.44941
P2E0F...1-..	0.10628	0.33401	-0.83658	VS3-C...10..	-0.31273	0.03401	-2.35658	n...c...2...	0.63351	0.07769	-0.05478
P2E0Br..1-..	-0.12523	-0.24204	0.33677	VS3-C...11..	0.2785	0.37974	0.10586	n...c...3...	2.70713	0.34284	0.60643
P2E0Cl..0-..	-0.69339	2.46819	0.15703	VS3-C...12..	1.13457	2.42959	0.32075	n...c...c...	1.41939	-0.61488	0.20197
P2E0Cl..1-..	1.32378	1.5548	0.06117	VS3-C...13..	0.17366	0.46471	2.43279	n...c...n...	-0.82021	-1.08132	2.21471
P2E0N...0-..	0.27787	-0.06264	0.40386	VS3-C...14..	-0.93999	-0.79744	0.43762	n...n.....	-0.63141	-0.93151	-0.04912
P2E0N...1-..	-0.61022	0.54117	0.20841	VS3-C...15..	-0.05628	0.04953	0.18014	n...n...1...	0.32839	0.35192	0.12872
P2E0N...2-..	-0.82469	-0.41497	0.09268	VS3-C...16..	0.03568	0.08532	0.48205	n...n...2...	2.61541	1.48424	-0.16594
P2E0N...3-..	-0.17755	-0.96673	0.39838	VS3-C...17..	0.44917	-0.07569	-0.62708	n...n...c...	0.21464	0.20351	0.08559
P2E0O...0-..	0.1456	0.90496	0.03372	VS3-C...18..	0.01936	0.61583	0.00515	n...o...n...	-0.59246	2.47931	0.18141
P2E0O...1-..	0.26782	0.71819	0.16201	VS3-C...19..	0.46703	0.7137	0.28673	n...s...c...	-1.99768	-0.31588	-0.00748
P2E0O...2-..	2.34567	-0.00752	0.15577	VS3-C...20..	-1.07845	-0.83334	-0.78429	o...(.....	0.42935	0.08798	-0.54202
P2E0S...0-..	0.13766	0.13375	0.24243	VS3-C...3...	-1.23534	0.77184	-2.11194	o...(...O...	2.41601	1.84773	2.01934
P2E0S...1-..	-5.95268	-8.4813	-2.71129	VS3-C...4...	0.15275	0.37931	0.70034	o...(...c...	0.26605	1.34438	0.47774
P2E0S...2-..	-0.50917	-1.23081	0.40607	VS3-C...5...	2.05627	0.36003	0.32778	o.....	2.16368	2.02107	0.22965
P2E0o...0-..	1.89592	0.20062	-0.31327	VS3-C...6...	0.39839	-0.19758	-0.54953	o...1...(...	0.01539	2.03773	0.18066
P2E0o...1-..	1.81868	2.1456	1.20463	VS3-C...7...	0.07255	0.35975	-0.89649	o...1.....	-0.60189	0.70152	-0.06381
P2E0o...2-..	1.187	2.27725	-0.66596	VS3-C...8...	-0.20627	0.67925	0.09984	o...c.....	0.27577	0.10949	2.34833
P2E0s...0-..	-0.53848	-0.6088	-0.9683	VS3-C...9...	0.0257	0.13263	-0.03579	o...c...2...	2.46479	0.04768	-0.86888
P2E0s...1-..	0.92112	2.11073	0.76588	VS3-F...4...	-1.33512	-0.01988	0.11308	o...c...c...	1.46285	0.52824	2.32217
P2E0s...2-..	-3.41614	-4.67095	0.595	VS3-F...5...	-0.91036	-0.64034	-0.23904	o...n.....	1.72087	0.54855	0.01586
P3E0C...0-..	0.20249	0.09081	-0.25602	VS3-F...6...	0.23645	3.37914	0.13481	o...n...1...	-0.14051	1.95855	0.17407
P3E0C...1-..	0.29926	1.13392	0.05996	VS3-F...7...	0.17514	-0.68282	-0.79501	o...n...c...	2.53897	1.06468	0.11088

P3E0C...2-..	-0.67287	0.18632	0.18181	VS3-Br..4...	3.9539	6.75096	6.52499	s...(.....	0.45445	2.22397	-0.3418
P3E0C...3-..	0.72786	0.12766	0.40738	VS3-Br..5...	2.37043	-0.849	0.00788	s...(...1...	0.71452	1.50194	3.06742
P3E0C...4-..	-0.50027	0.15772	0.14163	VS3-Cl..3...	-0.58406	0.90094	-0.16471	s...(...c...	-0.43673	0.11953	0.00222
P3E0C...5-..	0.41334	2.48911	0.01488	VS3-Cl..4...	0.4173	2.31084	0.03566	s.....	2.44393	0.16738	0.09162
P3E0C...6-..	0.05245	-0.88925	-0.21731	VS3-Cl..5...	-0.89772	-0.39305	2.06156	s...1...(...	-0.99382	2.17211	0.15119
P3E0F...1-..	0.48122	-0.95898	0.47254	VS3-Cl..6...	0.33928	0.68634	0.1048	s...1.....	0.08795	2.09146	0.43888
P3E0F...2-..	-0.00605	-0.11568	-0.74316	VS3-Cl..7...	-0.85429	2.30468	0.74727	s...1...c...	1.27604	2.44332	-0.08635
P3E0Br..1-..	0.09744	2.37415	0.06763	VS3-N...10..	-1.33491	-1.05397	-0.0446	s...c...(...	-1.17212	0.37889	0.10349
P3E0Br..2-..	-0.19665	0.83073	0.07061	VS3-N...11..	2.40105	4.69309	2.36349	s...c.....	0.10404	2.14332	2.14193
P3E0Cl..1-..	3.2201	2.04716	0.16756	VS3-N...12..	-1.45613	-4.96898	0.40651	s...c...1...	-0.69194	0.49128	0.05294
P3E0Cl..2-..	0.28472	-1.48493	-1.34618	VS3-N...13..	-0.55273	0.29137	0.05122	s...c...c...	2.40149	0.2165	0.14036
P3E0N...0-..	0.75016	-0.83259	0.08232	VS3-N...14..	2.49151	0.05715	0.10668	s...c...n...	2.89276	-0.19948	1.41667
P3E0N...1-..	0.47784	-0.76137	0.40831	VS3-N...15..	1.48903	1.02278	2.21273	s...n.....	-1.34853	-0.70957	-0.12006
P3E0N...2-..	0.42529	1.24658	0.05676	VS3-N...16..	0.24763	-0.59101	0.48276	s...n...n...	-2.01941	-1.73913	-0.51348
P3E0N...3-..	-0.07838	-0.66316	0.66957	VS3-N...17..	0.0118	-0.35854	0.23863				

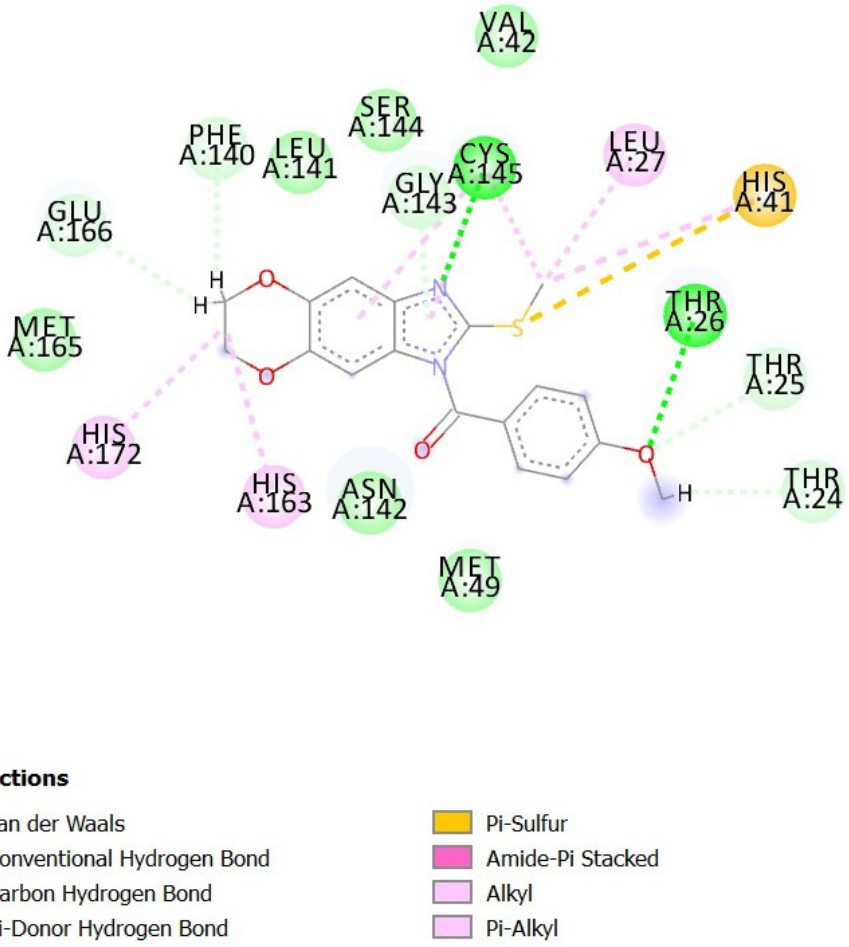


Figure S1. Two-dimensional representation of the interaction between molecule A and amino acids inside 3CLpro binding pocket.

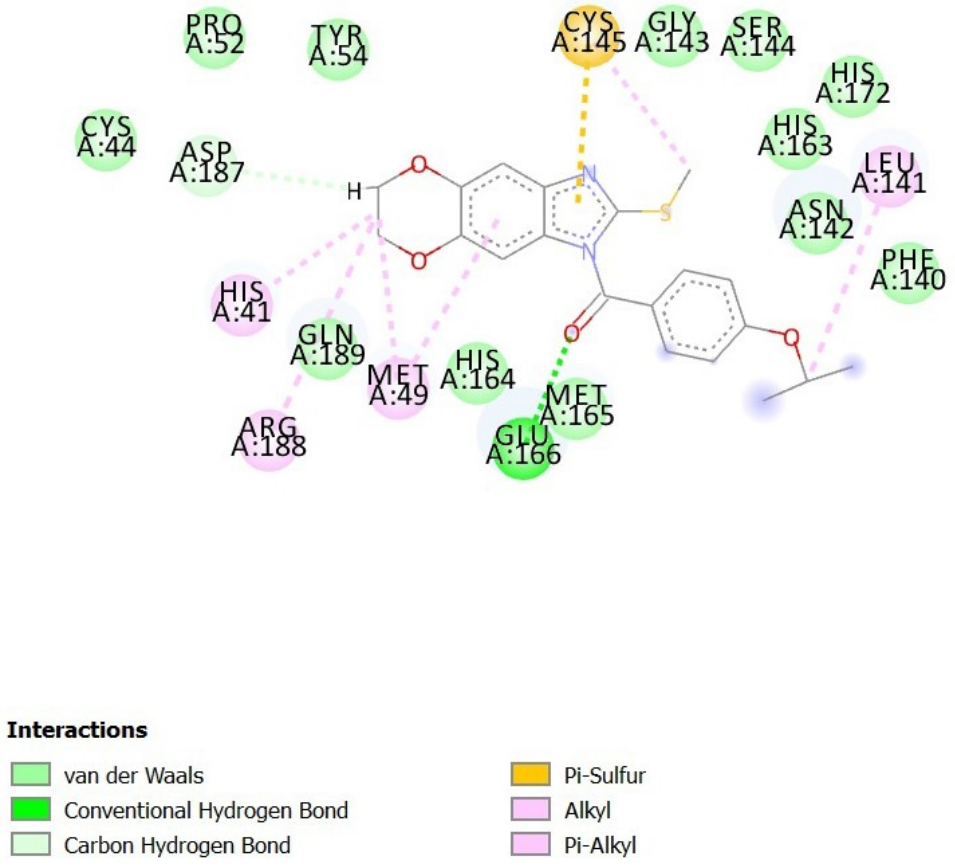


Figure S2. Two-dimensional representation of the interaction between molecule A1 and amino acids inside 3CLpro binding pocket.

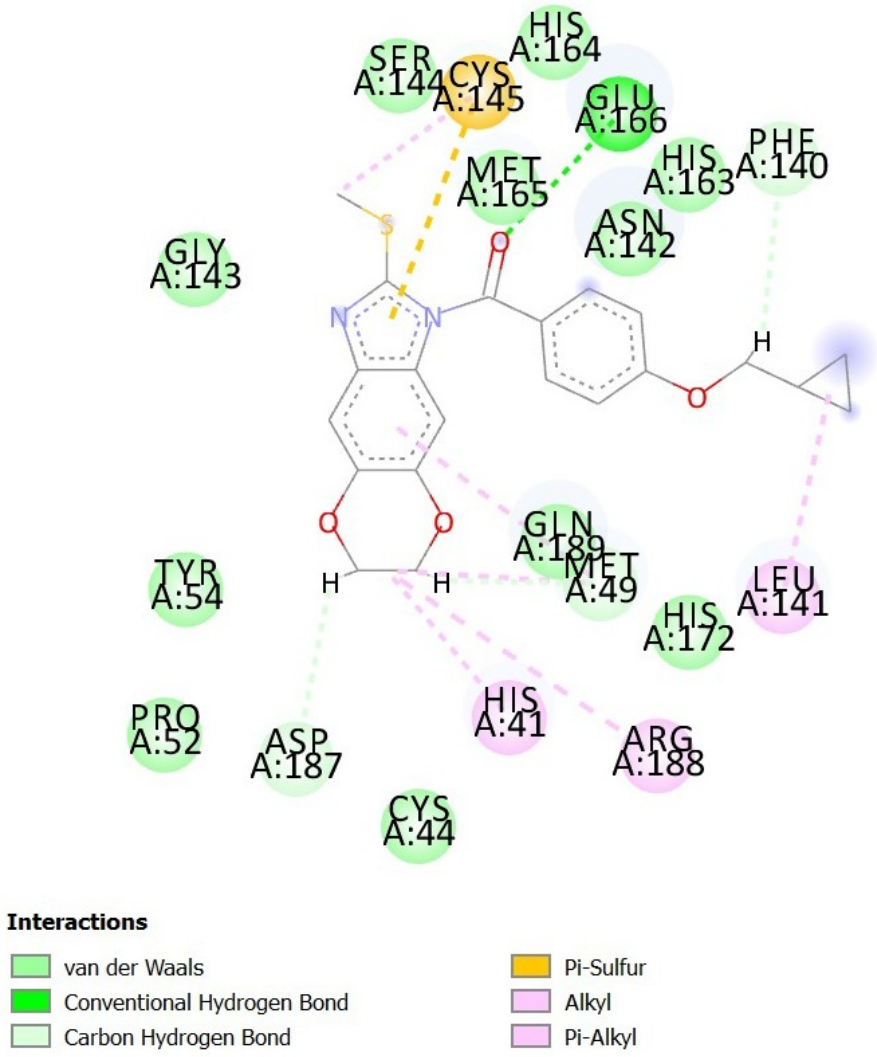


Figure S3. Two-dimensional representation of the interaction between molecule A2 and amino acids inside 3CLpro binding pocket.

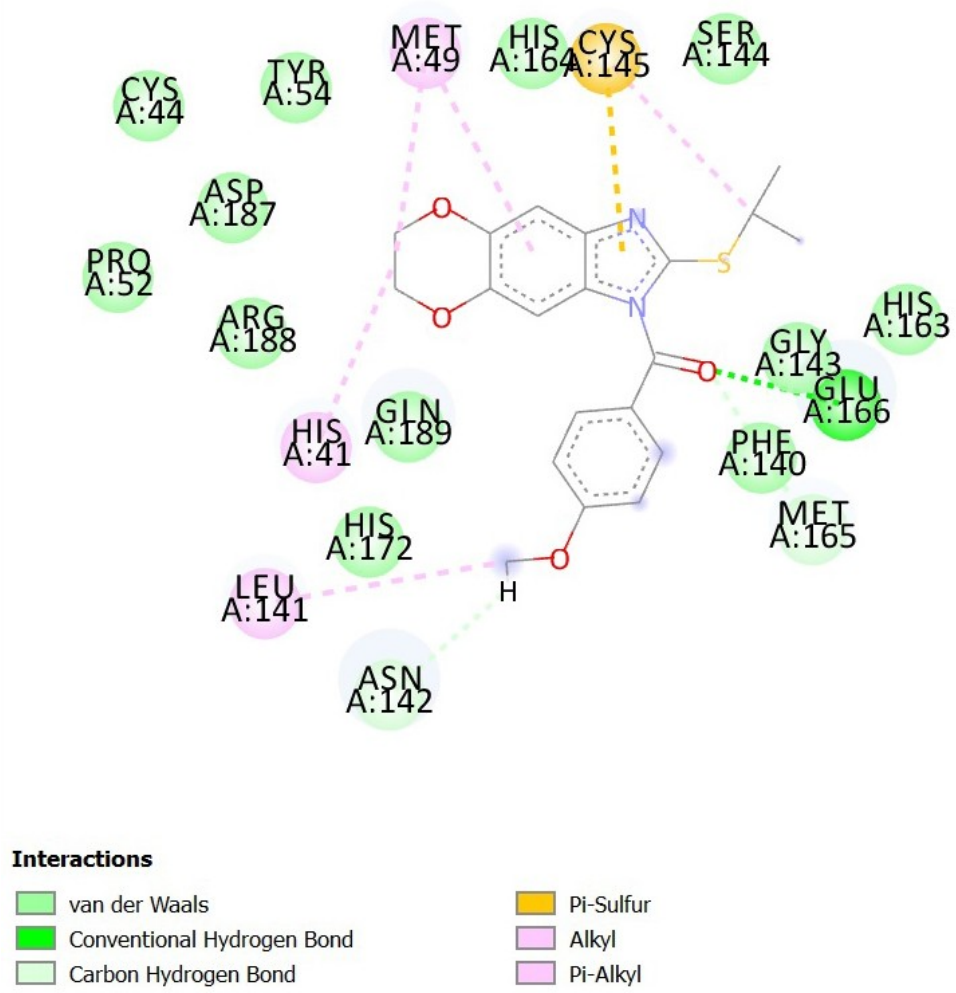


Figure S4. Two-dimensional representation of the interaction between molecule A3 and amino acids inside 3CLpro binding pocket.

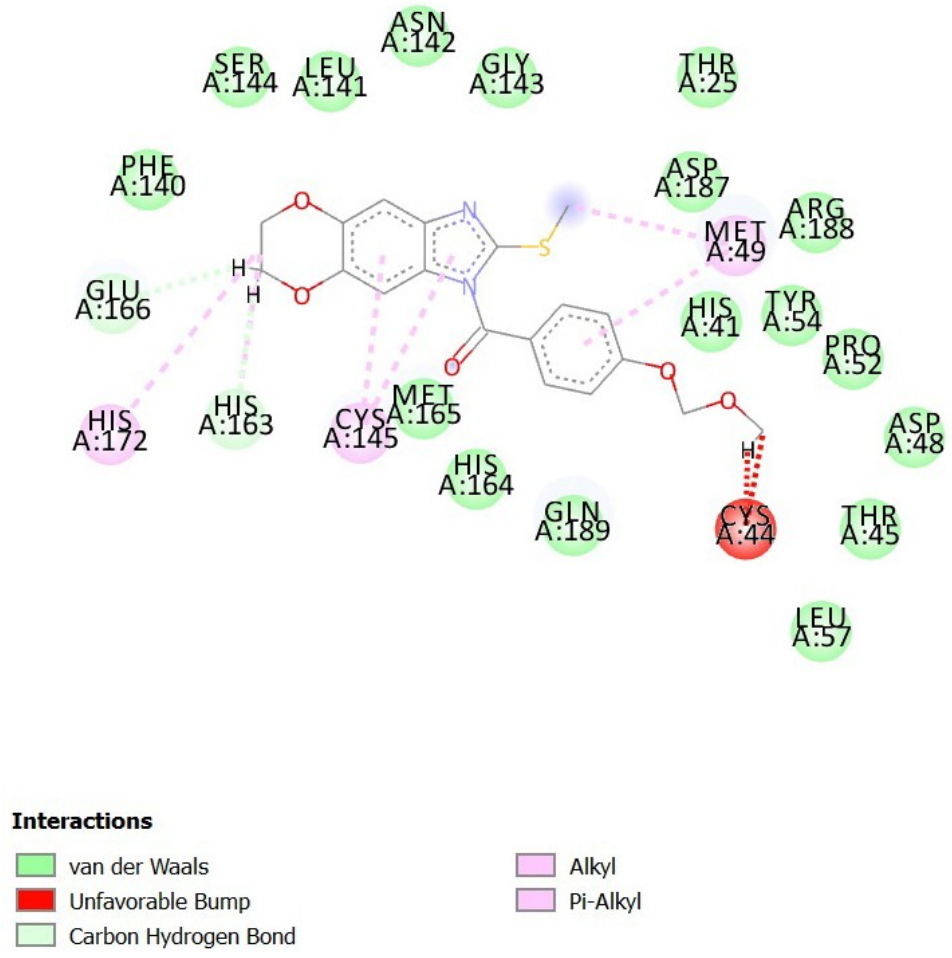


Figure S5. Two-dimensional representation of the interaction between molecule A4 and amino acids inside 3CLpro binding pocket.

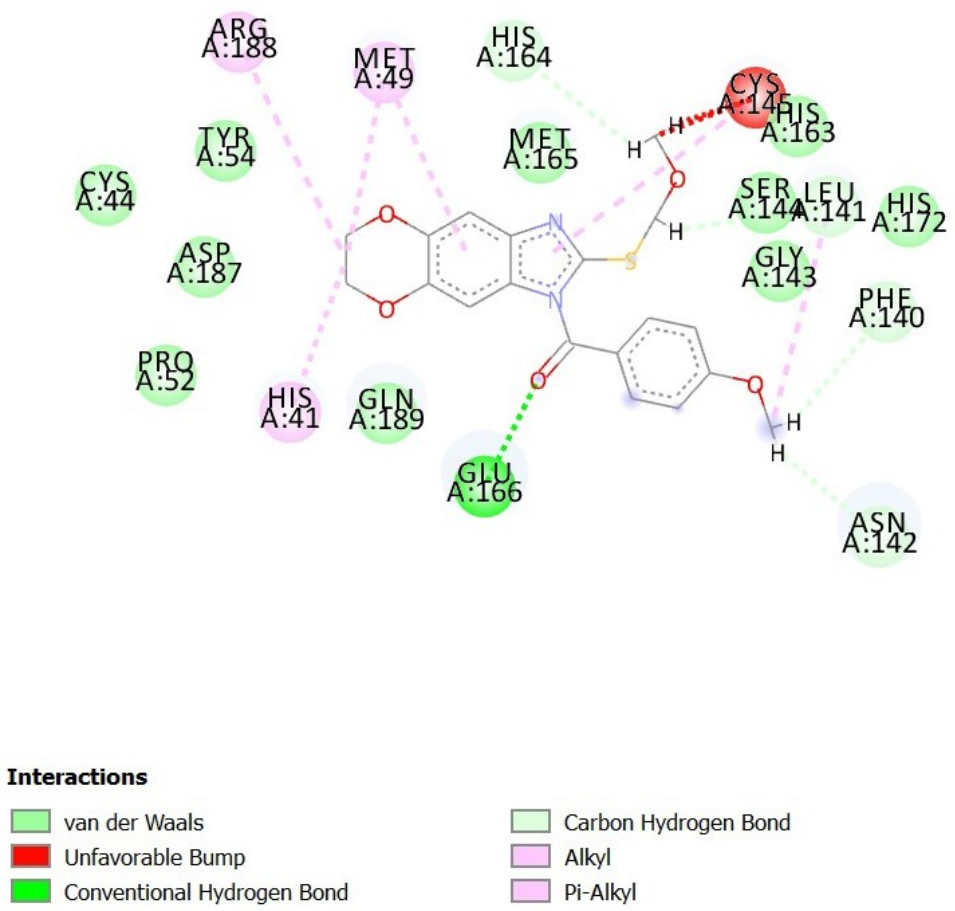


Figure S6. Two-dimensional representation of the interaction between molecule A5 and amino acids inside 3CLpro binding pocket.