

Supplementary material

Development of novel therapeutics for glaucoma filtration surgery based on transforming growth factor- β receptor 1 inhibition

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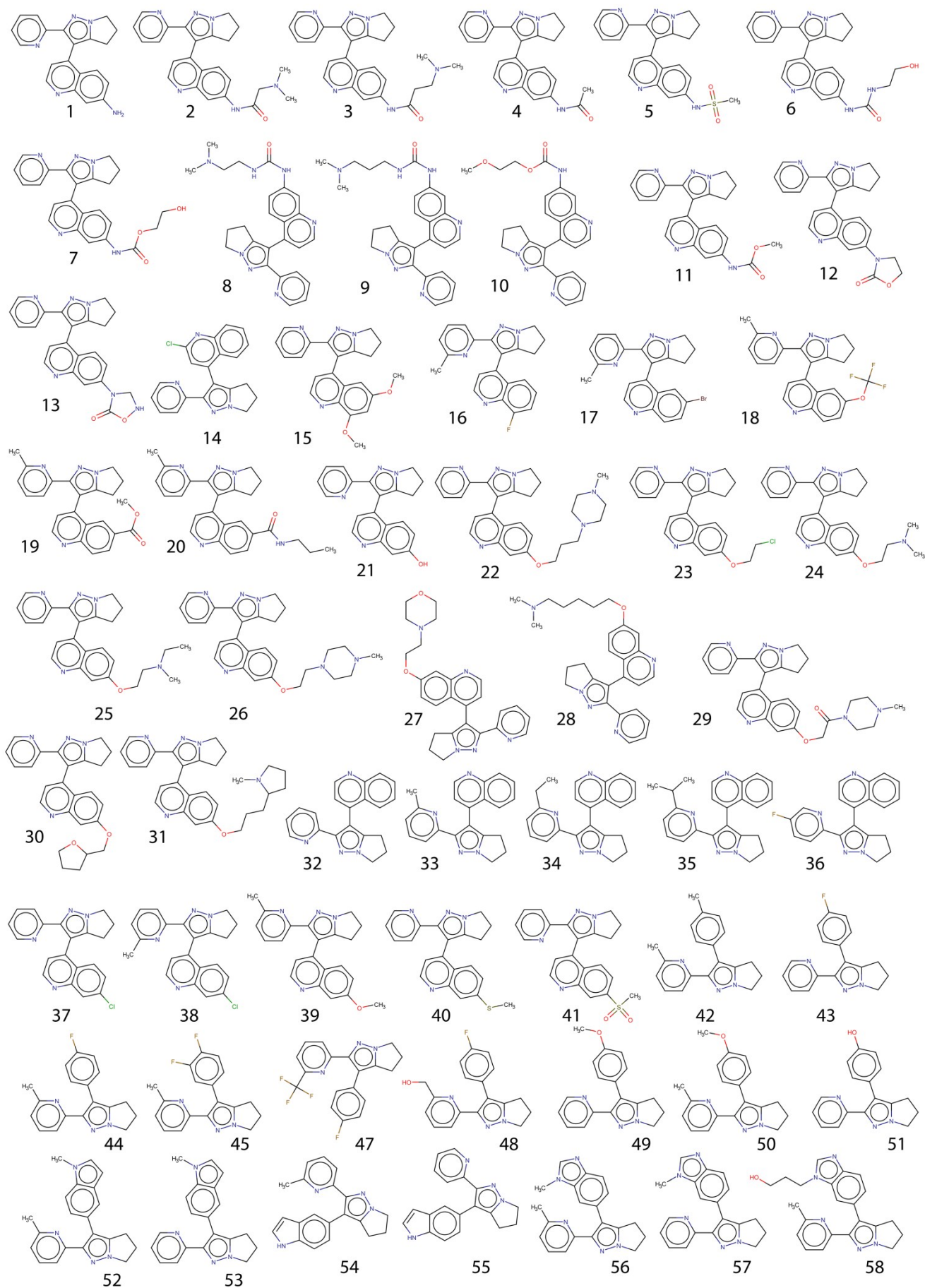
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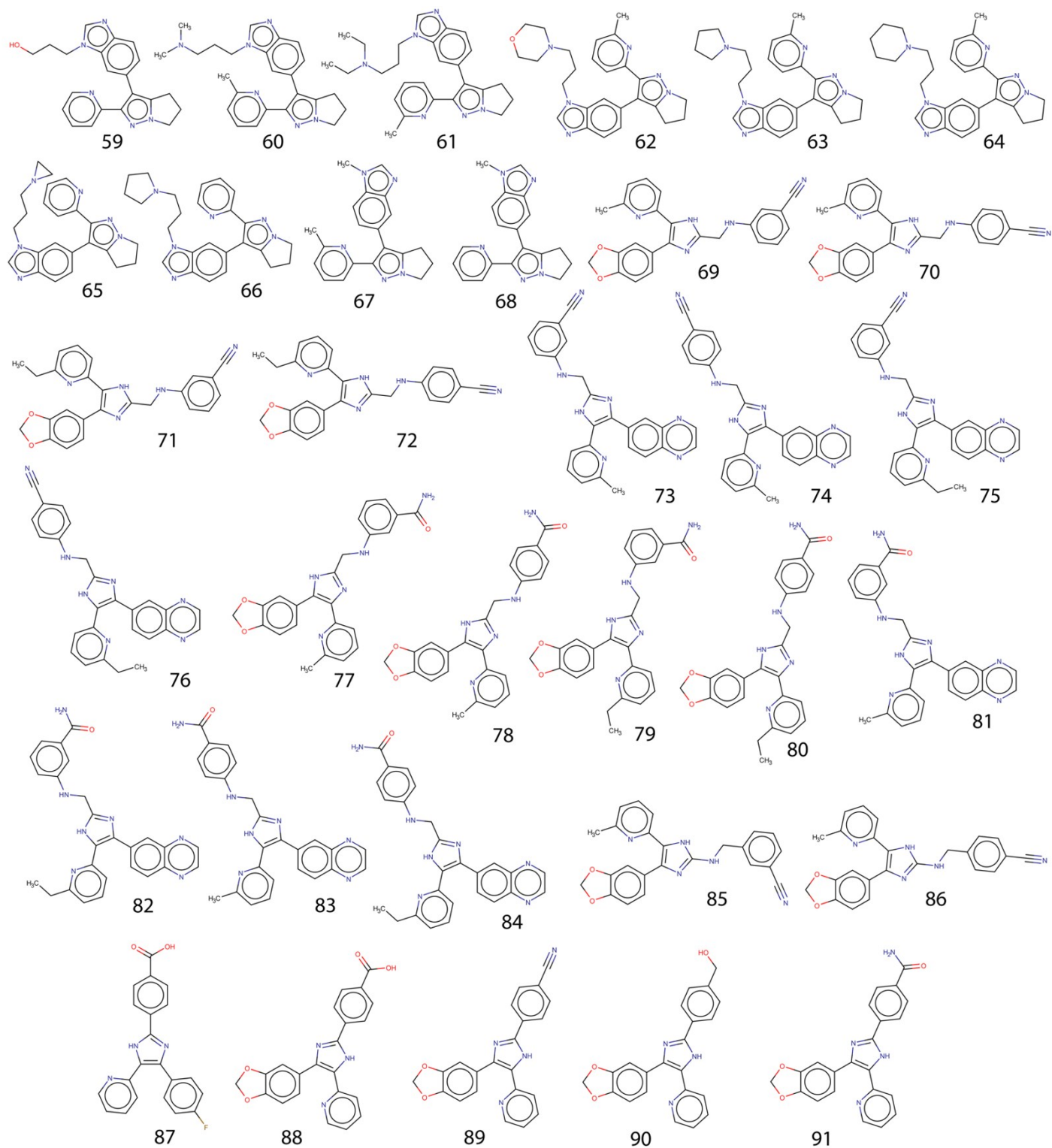


Figure S1. Structures of molecules used for QSAR modeling.

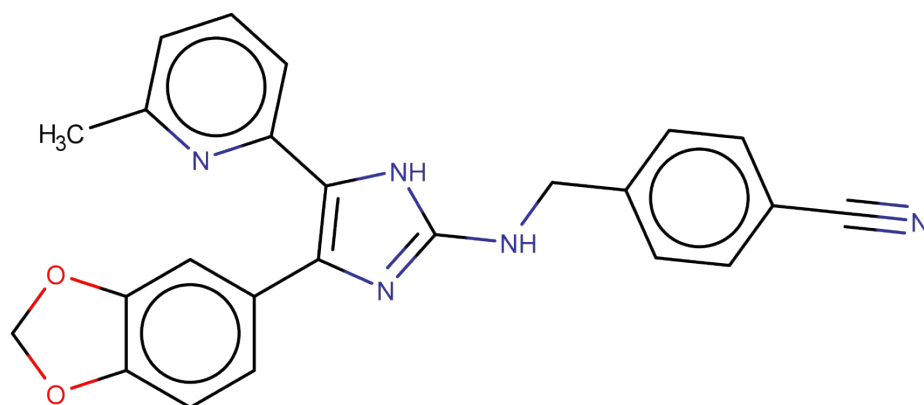
Table S1. The SMILES notation of the studied molecules, calculated values for the DCW, experimental data (Ac) – expr, the values of Ac calculated with the application of CORAL software – calc, the difference between expr and calc – diff for the built QSPR model

			Split 1				Split 2				Split 3			
	SMILES notation	Ac(expr.)	DCW	Ac(calc.)	Diff	Set	DCW	Ac(calc.)	Diff	Set	DCW	Ac(calc.)	Diff	Set
1	<chem>Nc1ccc2c(c1)nc2c1c2CCc2nc1c1ccccn1</chem>	7.23	54.27022	7.1619	0.0681	Test	60.77331	6.9124	0.3176	Test	100.0573	7.2015	0.0285	Training
2	<chem>CN(C)CC(=O)Nc1ccc2c(c1)nc2c1c2CCc2nc1c1ccccn1</chem>	7.19	54.92311	7.208	-0.018	Training	62.9254	7.0978	0.0922	Test	105.8558	7.5903	-0.4003	Training
3	<chem>CN(C)CCC(=O)Nc1ccc2c(c1)nc2c1c2CCc2nc1c1ccccn1</chem>	7.6	56.74242	7.3363	0.2637	Training	64.18276	7.2062	0.3938	Training	99.37462	7.1557	0.4443	Test
4	<chem>CC(=O)Nc1ccc2c(c1)nc2c1c2CCc2nc1c1ccccn1</chem>	7.06	50.47183	6.894	0.166	Training	58.20813	6.6914	0.3686	Training	93.43269	6.7573	0.3027	Training
5	<chem>CS(=O)(=O)Nc1ccc2c(c1)nc2c1c2CCc2nc1c1ccccn1</chem>	5.63	37.50249	5.9791	-0.3491	Test	47.93039	5.8058	-0.1758	Training	81.2949	5.9433	-0.3133	Training
6	<chem>OCCNC(=O)Nc1ccc2c(c1)nc2c1c2CCc2nc1c1ccccn1</chem>	7.49	53.84829	7.1322	0.3578	Training	70.95019	7.7893	-0.2993	Training	103.6804	7.4445	0.0455	Training
7	<chem>O=C(OCCO)Nc1ccc2c(c1)nc2c1c2CCc2nc1c1ccccn1</chem>	7.1	59.33267	7.519	-0.419	Training	67.32721	7.4771	-0.3771	Training	103.7158	7.4468	-0.3468	Training
8	<chem>CN(C)CCNC(=O)Nc1ccc2c(c1)nc2c1c2CCc2nc1c1ccccn1</chem>	6.59	53.17825	7.0849	-0.4949	Training	60.12014	6.8561	-0.2661	Training	92.24675	6.6777	-0.0877	Test
9	<chem>CN(C)CCNC(=O)Nc1ccc2c(c1)nc2c1c2CCc2nc1c1ccccn1</chem>	7.74	54.8824	7.2051	0.5349	Test	68.38887	7.5686	0.1714	Test	103.31	7.4196	0.3204	Training
10	<chem>O=C(OCCOC)Nc1ccc2c(c1)nc2c1c2CCc2nc1c1ccccn1</chem>	7.47	53.27165	7.0915	0.3785	Test	64.82409	7.2615	0.2085	Training	101.6855	7.3107	0.1593	Training
11	<chem>O=C(OC)Nc1ccc2c(c1)nc2c1c2CCc2nc1c1ccccn1</chem>	7.4	58.22994	7.4413	-0.0413	Training	64.44668	7.2289	0.1711	Test	103.4673	7.4302	-0.0302	Training
12	<chem>O=C1OCCN1c1ccc2c(c1)nc2c1c2CCc2nc1c1ccccn1</chem>	7.37	56.18812	7.2972	0.0728	Training	66.28959	7.3877	-0.0177	Test	101.4661	7.296	0.074	Test
13	<chem>O=C1ONCN1c1ccc2c(c1)nc2c1c2CCc2nc1c1ccccn1</chem>	7.55	61.68603	7.6851	-0.1351	Training	67.17704	7.4642	0.0858	Training	101.0823	7.2702	0.2798	Training
14	<chem>Clc1nc2ccccc2c(c1)c1c2CCc2nc1c1ccccn1</chem>	4.869	37.27188	5.9628	-1.0938	Test	45.26969	5.5765	-0.7075	Training	75.15706	5.5317	-0.6627	Training
15	<chem>COc1cc2c(nc2c2c3CCc3nc2c2cccc2)c(OC)c1</chem>	5.36	36.41958	5.9027	-0.5427	Test	44.24599	5.4883	-0.1283	Training	68.26187	5.0694	0.2906	Training
16	<chem>Fc1cccc2c1nc2c1c2CCc2nc1c1cccc(C)n1</chem>	6.03	40.46132	6.1878	-0.1578	Training	49.10721	5.9072	0.1228	Training	84.16304	6.1357	-0.1057	Training
17	<chem>Brclcc2c(cc1)nc2c1c2CCc2nc1c1cccc(C)n1</chem>	7.05	49.00173	6.7903	0.2597	Test	56.73262	6.5642	0.4858	Training	95.67829	6.9079	0.1421	Training
18	<chem>FC(F)(F)Oc1cc2c(cc1)nc2c1c2CCc2nc1c1cccc(C)n1</chem>	6.85	47.77345	6.7036	0.1464	Training	60.62404	6.8995	-0.0495	Training	96.71776	6.9776	-0.1276	Training
19	<chem>O=C(OC)c1cc2c(cc1)nc2c1c2CCc2nc1c1cccc(C)n1</chem>	6.28	46.17977	6.5912	-0.3112	Training	59.17873	6.775	-0.495	Training	89.95154	6.5238	-0.2438	Test
20	<chem>CCCN(C(=O)c1cc2c(cc1)nc2c1c2CCc2nc1c1cccc(C)n1</chem>	6.71	46.02743	6.5805	0.1295	Training	60.57505	6.8953	-0.1853	Test	92.43678	6.6905	0.0195	Training
21	<chem>Oc1ccc2c(c1)nc2c1c2CCc2nc1c1ccccn1</chem>	6.8	55.88635	7.2759	-0.4759	Training	66.14944	7.3757	-0.5757	Training	99.03612	7.133	-0.333	Training
22	<chem>CN1CCN(CC1)CCCOc1ccc2c(c1)nc2c1c2CCc2nc1c1ccccn1</chem>	7.13	51.15221	6.942	0.188	Training	61.97072	7.0156	0.1144	Test	93.13835	6.7375	0.3925	Training
23	<chem>C1CCOc1ccc2c(c1)nc2c1c2CCc2nc1c1ccccn1</chem>	7.48	53.18733	7.0855	0.3945	Test	65.84048	7.349	0.131	Training	105.1569	7.5435	-0.0635	Training
24	<chem>CN(C)CCOc1ccc2c(c1)nc2c1c2CCc2nc1c1ccccn1</chem>	7.62	57.78975	7.4102	0.2098	Training	69.981	7.7058	-0.0858	Training	111.0671	7.9398	-0.3198	Training
25	<chem>CCN(C)CCOc1ccc2c(c1)nc2c1c2CCc2nc1c1ccccn1</chem>	7.07	59.35148	7.5204	-0.4504	Training	61.99656	7.0178	0.0522	Training	101.996	7.3315	-0.2615	Training
26	<chem>CN1CCN(CC1)CCOc1ccc2c(c1)nc2c1c2CCc2nc1c1ccccn1</chem>	7	56.35698	7.3091	-0.3091	Training	66.03271	7.3656	-0.3656	Training	100.354	7.2214	-0.2214	Training
27	<chem>O(CCN1CCOCC1)c1cc2nccc(c3c4CCc4nc3c3cccn3)c2cc1</chem>	7.16	49.87602	6.8519	0.3081	Training	58.07465	6.6799	0.4801	Training	94.49598	6.8286	0.3314	Test

28	CN(C)CCCCOe1ccc2c(c1)ccc2c1c2CCn2nc1c1cccn1	7.33	53.41521	7.1016	0.2284	Training	62.99132	7.1035	0.2265	Test	95.66343	6.9069	0.4231	Training
29	CN1CCN(CC1)C(=O)COe1ccc2c(c1)ccc2c1c2CCn2nc1c1cccn1	7.31	55.14877	7.2239	0.0861	Training	69.07247	7.6275	-0.3175	Test	101.0094	7.2654	0.0446	Test
30	c1cc2c(cc1OCC1CCCO1)ccc2c1c2CCn2nc1c1cccn1	6.89	54.22619	7.1588	-0.2688	Training	60.76836	6.912	-0.022	Training	94.34748	6.8186	0.0714	Training
31	CN1CCCC1CCCOe1ccc2c(c1)ccc2c1c2CCn2nc1c1cccn1	7.14	56.74465	7.3365	-0.1965	Training	70.05499	7.7122	-0.5722	Test	101.1047	7.2717	-0.1317	Test
32	C1CCe2c(c(nn12)c1cccn1)c1cnc2ccccc21	6.98	50.78892	6.9163	0.0637	Training	59.12177	6.7701	0.2099	Training	91.88298	6.6533	0.3267	Training
33	Cc1cccc(n1)c1nn2CCc2c1c1cnc2ccccc21	7.11	51.28279	6.9512	0.1588	Training	62.89804	7.0955	0.0145	Training	97.84675	7.0533	0.0567	Test
34	CCc1cccc(n1)c1nn2CCc2c1c1cnc2ccccc21	7.15	47.7479	6.7018	0.4482	Test	57.13289	6.5987	0.5513	Training	94.79465	6.8486	0.3014	Test
35	CC(C)c1cccc(n1)c1nn2CCc2c1c1cnc2ccccc21	5.89	37.51089	5.9797	-0.0897	Training	53.38746	6.276	-0.386	Training	83.91465	6.119	-0.229	Training
36	Fc1ccc(nc1)c1nn2CCc2c1c1cnc2ccccc21	6.82	51.63924	6.9763	-0.1563	Training	64.89067	7.2672	-0.4472	Training	97.38009	7.022	-0.202	Test
37	Clc1ccc2c(c1)ccc2c1c2CCn2nc1c1cccn1	7.27	50.34181	6.8848	0.3852	Training	62.59793	7.0696	0.2004	Training	94.64133	6.8383	0.4317	Training
38	Clc1ccc2c(c1)ccc2c1c2CCn2nc1c1cccc(C)n1	7.32	53.30182	7.0936	0.2264	Test	67.33	7.4774	-0.1574	Training	99.62176	7.1723	0.1477	Training
39	COc1ccc2c(c1)ccc2c1c2CCn2nc1c1cccc(C)n1	7.06	51.36141	6.9567	0.1033	Training	64.39838	7.2248	-0.1648	Training	99.83993	7.1869	-0.1269	Training
40	CSc1ccc2c(c1)ccc2c1c2CCn2nc1c1cccn1	6.96	46.14403	6.5887	0.3713	Training	51.53091	6.116	0.844	Training	89.32914	6.4821	0.4779	Training
41	CS(=O)(=O)c1ccc2c(c1)ccc2c1c2CCn2nc1c1cccn1	5.03	24.3017	5.0479	-0.0179	Training	43.32561	5.409	-0.379	Test	69.95764	5.1831	-0.1531	Training
42	Cc1ccc(cc1)c1c2CCn2nc1c1cccc(C)n1	5.4	41.35246	6.2507	-0.8507	Training	50.70464	6.0448	-0.6448	Training	79.28582	5.8086	-0.4086	Training
43	Fc1ccc(cc1)c1c2CCn2nc1c1cccn1	5.88	39.75046	6.1377	-0.2577	Test	51.2483	6.0917	-0.2117	Test	83.19686	6.0709	-0.1909	Training
44	Fc1ccc(cc1)c1c2CCn2nc1c1cccc(C)n1	6.76	44.82529	6.4957	0.2643	Training	55.34704	6.4449	0.3151	Training	87.38565	6.3518	0.4082	Training
45	Fc1ccc(cc1F)c1c2CCn2nc1c1cccc(C)n1	6.47	45.76258	6.5618	-0.0918	Training	51.47419	6.1111	0.3589	Training	83.12785	6.0662	0.4038	Training
46	FC(F)(F)c1ccc(n1)c1nn2CCc2c1c1ccc(F)cc1	6.06	39.8774	6.1466	-0.0866	Training	49.89185	5.9748	0.0852	Training	89.04755	6.4632	-0.4032	Test
47	Fc1ccc(cc1)c1c2CCn2nc1c1cccc(CO)n1	5.58	37.35541	5.9687	-0.3887	Test	49.67771	5.9563	-0.3763	Training	82.55212	6.0276	-0.4476	Training
48	CS(=O)(=O)c1ccc(cc1)c1c2CCn2nc1c1cccc(C)n1	4.71	18.9284	4.6688	0.0412	Training	39.65403	5.0926	-0.3826	Test	72.08596	5.3258	-0.6158	Test
49	COc1ccc(cc1)c1c2CCn2nc1c1cccn1	6.19	41.4701	6.259	-0.069	Training	51.63783	6.1252	0.0648	Training	89.19257	6.4729	-0.2829	Training
50	COc1ccc(cc1)c1c2CCn2nc1c1cccc(C)n1	6.92	46.54494	6.617	0.303	Training	55.73658	6.4784	0.4416	Training	93.38136	6.7538	0.1662	Training
51	Oc1ccc(cc1)c1c2CCn2nc1c1cccn1	7.3	47.45042	6.6808	0.6192	Test	57.83242	6.659	0.641	Test	89.6404	6.503	0.797	Training
52	Cn1ccc2ccc(cc12)c1c2CCn2nc1c1cccc(C)n1	5.39	33.00348	5.6617	-0.2717	Test	44.88233	5.5432	-0.1532	Test	71.65439	5.2969	0.0931	Training
53	Cn1ccc2cc(ccc12)c1c2CCn2nc1c1cccn1	4.91	27.92864	5.3037	-0.3937	Training	40.78358	5.19	-0.28	Training	67.4656	5.016	-0.106	Training
54	Cc1cccc(n1)c1nn2CCc2c1c1ccc2[NH]ccc2c1	7.33	58.65726	7.4714	-0.1414	Training	63.11406	7.1141	0.2159	Test	103.2785	7.4175	-0.0875	Training
55	C1CCc2c(c(nn12)c1cccn1)c1ccc2[NH]ccc2c1	7.17	56.04856	7.2874	-0.1174	Test	59.97111	6.8433	0.3267	Training	98.10641	7.0707	0.0993	Training
56	Cn1cnc2ccc(cc21)c1c2CCn2nc1c1cccc(C)n1	7.66	56.88556	7.3464	0.3136	Training	68.80807	7.6047	0.0553	Training	102.025	7.3335	0.3265	Training
57	Cn1cnc2ccc(cc21)c1c2CCn2nc1c1cccn1	7.12	51.81072	6.9884	0.1316	Training	64.70933	7.2516	-0.1316	Training	97.83618	7.0526	0.0674	Training
58	OCCN1cnc2ccc(cc21)c1c2CCn2nc1c1cccc(C)n1	7.39	58.2358	7.4417	-0.0517	Training	63.78272	7.1717	0.2183	Training	98.11433	7.0712	0.3188	Test
59	OCCN1cnc2ccc(cc21)c1c2CCn2nc1c1cccn1	7.1	53.16097	7.0837	0.0163	Training	59.68397	6.8185	0.2815	Training	93.92554	6.7903	0.3097	Training
60	CN(C)CCN1cnc2ccc(cc21)c1c2CCn2nc1c1cccc(C)n1	7.07	52.62273	7.0457	0.0243	Training	65.92258	7.3561	-0.2861	Training	98.79957	7.1172	-0.0472	Test
61	CCN(CC)CCN1cnc2ccc(cc21)c1c2CCn2nc1c1cccc(C)n1	6.91	53.26882	7.0913	-0.1813	Training	58.88074	6.7493	0.1607	Test	94.33525	6.8178	0.0922	Training

62	Cc1cccc(n1)c1nn2CCc2c1c1ccc2nen(CCCN3CCOCC3)c2c1	7.16	54.32615	7.1659	-0.0059	Training	66.52695	7.4082	-0.2482	Training	103.1296	7.4075	-0.2475	Training
63	Cc1cccc(n1)c1nn2CCc2c1c1ccc2nen(CCCN3CCCC3)c2c1	7.13	49.08419	6.7961	0.3339	Test	59.31153	6.7865	0.3435	Test	97.81819	7.0514	0.0786	Training
64	Cc1cccc(n1)c1nn2CCc2c1c1ccc2nen(CCCN3CCCC3)c2c1	6.81	50.46533	6.8935	-0.0835	Training	58.61854	6.7267	0.0833	Training	95.24086	6.8785	-0.0685	Training
65	C1CCc2c(c(nn12)c1cccn1)c1ccc2nen(CCCN3CC3)c2c1	6.41	42.52988	6.3337	0.0763	Training	56.0177	6.5026	-0.0926	Training	92.17376	6.6728	-0.2628	Training
66	C1CCc2c(c(nn12)c1cccn1)c1ccc2nen(CCCN3CCCC3)c2c1	6.61	46.47549	6.6121	-0.0021	Test	56.16858	6.5156	0.0944	Training	92.64606	6.7045	-0.0945	Training
67	Cn1cnc2cc(ccc12)c1c2CCn2nc1c1cccc(C)n1	5.77	33.16483	5.6731	0.0969	Training	50.33734	6.0132	-0.2432	Training	77.53787	5.6914	0.0786	Training
68	Cn1cnc2cc(ccc12)c1c2CCn2nc1c1cccn1	5.32	28.09	5.3151	0.0049	Training	46.23859	5.66	-0.34	Test	73.34908	5.4105	-0.0905	Training
69	Cc1cccc(n1)c1[NH]c(CNc2cc(C#N)ccc2)nc1c1ccc2OCOc2c1	7.337	56.08334	7.2898	0.0472	Training	65.5257	7.3219	0.0151	Training	105.1131	7.5405	-0.2035	Training
70	Cc1cccc(n1)c1[NH]c(CNc2ccc(C#N)cc2)nc1c1ccc2OCOc2c1	6.767	46.47397	6.612	0.155	Training	59.14174	6.7718	-0.0048	Test	94.64751	6.8387	-0.0717	Training
71	CCc1cccc(n1)c1[NH]c(CNc2cc(C#N)ccc2)nc1c1ccc2OCOc2c1	7.137	51.91165	6.9955	0.1415	Test	60.65122	6.9019	0.2351	Training	99.46739	7.1619	-0.0249	Training
72	CCc1cccc(n1)c1[NH]c(CNc2ccc(C#N)cc2)nc1c1ccc2OCOc2c1	6.444	42.30228	6.3177	0.1263	Training	54.26725	6.3518	0.0922	Training	89.00177	6.4601	-0.0161	Test
73	Cc1cccc(n1)c1[NH]c(CNc2cccc(C#N)c2)nc1c1cc2ncnc2cc1	7.921	65.7789	7.9738	-0.0528	Training	72.50425	7.9232	-0.0022	Training	109.2634	7.8188	0.1022	Test
74	Cc1cccc(n1)c1[NH]c(CNc2ccc(C#N)cc2)nc1c1cc2ncnc2cc1	7.377	56.45866	7.3163	0.0607	Training	64.33268	7.2191	0.1579	Training	98.40702	7.0908	0.2862	Training
75	CCc1cccc(n1)c1[NH]c(CNc2cccc(C#N)c2)nc1c1cc2ncnc2cc1	6.924	61.60721	7.6795	-0.7555	Training	67.62976	7.5032	-0.5792	Training	103.6177	7.4403	-0.5163	Training
76	CCc1cccc(n1)c1[NH]c(CNc2ccc(C#N)cc2)nc1c1cc2ncnc2cc1	7.328	52.28697	7.022	0.306	Training	59.45819	6.7991	0.5289	Training	92.76127	6.7122	0.6158	Test
77	NC(=O)c1ccc(cc1)NCc1[NH]c(c2cccc(C)n2)c(n1)c1ccc2OCOc2c1	7.678	57.40977	7.3834	0.2946	Training	65.62262	7.3303	0.3477	Training	103.6294	7.441	0.237	Test
78	NC(=O)c1ccc(cc1)NCc1[NH]c(c2cccc(C)n2)c(n1)c1ccc2OCOc2c1	6.582	55.65852	7.2599	-0.6779	Test	62.67112	7.0759	-0.4939	Training	96.23487	6.9452	-0.3632	Training
79	NC(=O)c1ccc(cc1)NCc1[NH]c(c2cccc(CC)n2)c(n1)c1ccc2OCOc2c1	7.337	50.97331	6.9294	0.4076	Training	61.70002	6.9923	0.3447	Training	97.29776	7.0165	0.3205	Training
80	NC(=O)c1ccc(cc1)NCc1[NH]c(c2cccc(CC)n2)c(n1)c1ccc2OCOc2c1	6.415	49.22206	6.8058	-0.3908	Training	58.74853	6.7379	-0.3229	Test	89.90326	6.5206	-0.1056	Test
81	NC(=O)c1ccc(cc1)NCc1cc(c([NH]1)c1nc(C)ccc1)c1cc2ncnc2cc1	8	63.49328	7.8125	0.1875	Training	70.85123	7.7808	0.2192	Training	110.4515	7.8985	0.1015	Training
82	NC(=O)c1ccc(cc1)NCc1nc(c([NH]1)c1cccc(CC)n1)c1cc2ncnc2cc1	7.125	54.25232	7.1607	-0.0357	Test	67.10439	7.4579	-0.3329	Training	106.4497	7.6302	-0.5052	Training
83	NC(=O)c1ccc(cc1)NCc1nc(c([NH]1)c1cccc(C)n1)c1cc2ncnc2cc1	7.824	58.93753	7.4912	0.3328	Test	68.07548	7.5416	0.2824	Training	105.3868	7.5589	0.2651	Training
84	NC(=O)c1ccc(cc1)NCc1nc(c([NH]1)c1cccc(CC)n1)c1cc2ncnc2cc1	7.036	52.50107	7.0371	-0.0011	Test	64.15289	7.2036	-0.1676	Training	99.05516	7.1343	-0.0983	Training
85	Cc1cccc(n1)c1[NH]c(NCc2cccc(C#N)c2)nc1c1ccc2OCOc2c1	7.62	58.27523	7.4444	0.1756	Training	69.65691	7.6779	-0.0579	Test	104.8989	7.5262	0.0938	Training
86	Cc1cccc(n1)c1[NH]c(NCc2ccc(C#N)cc2)nc1c1ccc2OCOc2c1	6.815	49.70565	6.8399	-0.0249	Training	61.46628	6.9721	-0.1571	Training	94.47942	6.8275	-0.0125	Training
87	O=C(O)c1ccc(cc1)c1nc(c([NH]1)c1cccn1)c1ccc(F)cc1	5.824	36.19547	5.8869	-0.0629	Training	49.18075	5.9135	-0.0895	Training	83.50064	6.0912	-0.2672	Test
88	O=C(O)c1ccc(cc1)c1[NH]c(c2cccn2)c(n1)c1ccc2OCOc2c1	6.77	46.72515	6.6297	0.1403	Training	53.83504	6.3146	0.4554	Training	93.21321	6.7426	0.0274	Training
89	N#Cc1ccc(cc1)c1[NH]c(c2cccn2)c(n1)c1ccc2OCOc2c1	5.53	34.70447	5.7817	-0.2517	Training	49.81341	5.968	-0.438	Training	84.45175	6.155	-0.625	Test
90	OCc1ccc(cc1)c1[NH]c(c2cccn2)c(n1)c1ccc2OCOc2c1	6.585	41.07418	6.231	0.354	Training	57.34144	6.6167	-0.0317	Training	92.31259	6.6822	-0.0972	Training
91	NC(=O)c1ccc(cc1)c1[NH]c(c2cccn2)c(n1)c1ccc2OCOc2c1	7.027	48.53041	6.757	0.27	Training	60.40937	6.8811	0.1459	Training	94.19115	6.8081	0.2189	Test

Table S2. The example of DCW(3,11) calculation



SMILES notation : Cc1cccc(n1)c1[NH]c(NCc2ccc(C#N)cc2)nc1c1ccc2OCOc2c1

DCW = 61.46628

Calculated activity: 6.9721

SA _k	CW(SA _k)	SA _k	CW(SA _k)	SA _k	CW(SA _k)	SA _k	CW(SA _k)	SA _k	CW(SA _k)	SA _k	CW(SA _k)	SA _k	CW(SA _k)	SA _k	CW(SA _k)	SA _k	CW(SA _k)
EC0-C...1...	0.087	PT3-C...2...	-0.6913	VS2-C...4...	-0.1364	NNC-C...110.	-0.7502	P3E0C...1-..	0.2263	S2E0C...3-..	-0.8282	NNE0C...109-	-1.5202	C.....	0.4084	c...c.....	0.0813
EC0-C...3...	0.3802	PT3-C...3...	0.0842	VS2-C...5...	0.705	NNC-C...321.	0.2888	P3E0C...0-..	0.0379	S2E0C...2-..	0.0425	NNE0C...318-	0.2369	#.....	0.1897	c...c.....	0.0813
EC0-C...2...	-0.4664	PT3-C...2...	-0.6913	VS2-C...5...	0.705	NNC-C...220.	-0.4258	P3E0C...0-..	0.0379	S2E0C...3-..	-0.8282	NNE0C...218-	0.373	N.....	-0.1868	c...2.....	0.3602
EC0-C...2...	-0.4664	PT3-C...4...	-0.4793	VS2-C...6...	0.0122	NNC-C...220.	-0.4258	P3E0C...2-..	0.039	S2E0C...4-..	0.214	NNE0C...218-	0.373	(.....	0.2143	O...2.....	-0.9232
EC0-C...2...	-0.4664	PT3-C...4...	-0.4793	VS2-C...7...	-0.0902	NNC-C...220.	-0.4258	P3E0C...2-..	0.039	S2E0C...5-..	-0.3761	NNE0C...218-	0.373	c.....	0.2294	O...C.....	0.195
EC0-C...3...	0.3802	PT3-C...6...	-0.1108	VS2-C...10..	0.609	NNC-C...321.	0.2888	P3E0C...3-..	0.022	S2E0C...7-..	-0.1153	NNE0C...318-	0.2369	c.....	0.2294	O...C.....	0.195
EC0-N...2...	0.019	PT3-N...4...	0.7578	VS2-N...8...	-0.0817	NNC-N...220.	0.1073	P3E0N...2-..	0.9034	S2E0N...6-..	0.4818	NNE0N...218-	0.3005	2.....	-0.7381	c...O.....	2.2407
EC0-C...3...	0.3802	PT3-C...6...	-0.1108	VS2-C...11..	-0.3232	NNC-C...321.	0.2888	P3E0C...3-..	0.022	S2E0C...8-..	-0.8678	NNE0C...318-	0.2369	(.....	0.2143	c...2.....	0.3602
EC0-N...2...	0.019	PT3-N...6...	0.0686	VS2-N...9...	-0.5407	NNC-N...211.	0.3484	P3E0N...4-..	0.0683	S2E0N...7-..	0.0177	NNE0N...209-	0.1226	n.....	-1.0496	c...2.....	0.3602
EC0-N...2...	0.019	PT3-N...4...	0.7578	VS2-N...7...	0.5221	NNC-N...211.	0.3484	P3E0N...2-..	0.9034	S2E0N...5-..	-0.1149	NNE0N...209-	0.1226	c.....	0.2294	c...1.....	1.3554
EC0-C...3...	0.3802	PT3-C...4...	-0.4793	VS2-C...7...	-0.0902	NNC-C...303.	2.275	P3E0C...1-..	0.2263	S2E0C...4-..	0.214	NNE0C...300-	-0.2122	1.....	0.3401	C...c...1...	-0.1122
EC0-N...2...	0.019	PT3-N...4...	0.7578	VS2-N...7...	0.5221	NNC-N...220.	0.1073	P3E0N...2-..	0.9034	S2E0N...5-..	-0.1149	NNE0N...218-	0.3005	c.....	0.2294	c...1...c...	0.2601
EC0-C...2...	-0.4664	PT3-C...4...	-0.4793	VS2-C...7...	-0.0902	NNC-C...211.	-0.01	P3E0C...2-..	0.039	S2E0C...5-..	-0.3761	NNE0C...209-	-0.2373	1.....	0.3401	c...c...1...	0.2999
EC0-C...3...	0.3802	PT3-C...3...	0.0842	VS2-C...6...	0.0122	NNC-C...330.	-1.8889	P3E0C...0-..	0.0379	S2E0C...3-..	-0.8282	NNE0C...327-	-1.1314	c.....	0.2294	c...c...c...	0.1041
EC0-C...2...	-0.4664	PT3-C...4...	-0.4793	VS2-C...7...	-0.0902	NNC-C...220.	-0.4258	P3E0C...2-..	0.039	S2E0C...5-..	-0.3761	NNE0C...218-	0.373	c.....	0.2294	c...c...c...	0.1041
EC0-C...2...	-0.4664	PT3-C...4...	-0.4793	VS2-C...7...	-0.0902	NNC-C...220.	-0.4258	P3E0C...2-..	0.039	S2E0C...5-..	-0.3761	NNE0C...218-	0.373	c.....	0.2294	c...c...(...	0.0806
EC0-C...3...	0.3802	PT3-C...2...	-0.6913	VS2-C...5...	0.705	NNC-C...330.	-1.8889	P3E0C...1-..	0.2263	S2E0C...2-..	0.0425	NNE0C...327-	-1.1314	2.....	-0.7381	n...(c...	0.5913
EC0-C...2...	-0.4664	PT3-C...2...	-0.6913	VS2-C...4...	-0.1364	NNC-C...211.	-0.01	P3E0C...0-..	0.0379	S2E0C...2-..	0.0425	NNE0C...209-	-0.2373	O.....	-0.9209	1...n...(...	0.1949
EC0-N...1...	0.8887	PT3-N...2...	-0.2785	VS2-N...3...	-0.7022	NNC-N...110.	0.3893	P3E0N...1-..	0.0987	S2E0N...2-..	-0.7067	NNE0N...109-	2.3585	C.....	0.4084	n...1...(...	0.3894

EC0-C...2...	-0.4664	PT3-C...4...	-0.4793	VS2-C...7...	-0.0902	NNC-C...220.	-0.4258	P3E0C...2-..	0.039	S2E0C...5-..	-0.3761	NNE0C...218-	0.373	O.....	-0.9209	c...(1...	0.0926
EC0-C...2...	-0.4664	PT3-C...4...	-0.4793	VS2-C...7...	-0.0902	NNC-C...220.	-0.4258	P3E0C...2-..	0.039	S2E0C...5-..	-0.3761	NNE0C...218-	0.373	c.....	0.2294	1...c...(	-0.5524
EC0-N...2...	0.019	PT3-N...6...	0.0686	VS2-N...10..	0.4394	NNC-N...220.	0.1073	P3E0N...4-..	0.0683	S2E0N...8-..	0.4823	NNE0N...218-	0.3005	2.....	-0.7381	c...1...[...	0.1876
EC0-C...3...	0.3802	PT3-C...7...	-0.5429	VS2-C...12..	0.1411	NNC-C...321.	0.2888	P3E0C...4-..	0.3926	S2E0C...9-..	-0.7178	NNE0C...318-	0.2369	c.....	0.2294	N...[...1...	0.9603
EC0-C...3...	0.3802	PT3-C...6...	-0.1108	VS2-C...10..	0.609	NNC-C...330.	-1.8889	P3E0C...3-..	0.022	S2E0C...7-..	-0.1153	NNE0C...327-	-1.1314	1.....	0.3401	[...N...H...	0.7052
EC0-C...2...	-0.4664	PT3-C...5...	0.1503	VS2-C...8...	0.5495	NNC-C...220.	-0.4258	P3E0C...3-..	0.022	S2E0C...6-..	-0.0194	NNE0C...218-	0.373	c...C.....	1.3509	[...H...N...	0.0609
EC0-C...2...	-0.4664	PT3-C...5...	0.1503	VS2-C...8...	0.5495	NNC-C...220.	-0.4258	P3E0C...3-..	0.022	S2E0C...6-..	-0.0194	NNE0C...218-	0.373	c...1.....	1.3554	c...[...H...	0.4157
EC0-C...3...	0.3802	PT3-C...4...	-0.4793	VS2-C...8...	0.5495	NNC-C...321.	0.2888	P3E0C...1-..	0.2263	S2E0C...5-..	-0.3761	NNE0C...318-	0.2369	c...1.....	1.3554	[...c...(	0.1079
EC0-O...2...	-0.963	PT3-O...4...	0.554	VS2-O...7...	0.4523	NNC-O...220.	0.3285	P3E0O...2-..	0.6972	S2E0O...5-..	-0.5788	NNE0O...218-	-0.0306	c...c.....	0.0813	c...(N...	1.2931
EC0-C...2...	-0.4664	PT3-C...4...	-0.4793	VS2-C...6...	0.0122	NNC-C...202.	0.7804	P3E0C...2-..	0.039	S2E0C...4-..	0.214	NNE0C...200-	0.2976	c...c.....	0.0813	C...N...(	-0.1249
EC0-O...2...	-0.963	PT3-O...4...	0.554	VS2-O...7...	0.4523	NNC-O...220.	0.3285	P3E0O...2-..	0.6972	S2E0O...5-..	-0.5788	NNE0O...218-	-0.0306	c...c.....	0.0813	c...C...N...	2.4029
EC0-C...3...	0.3802	PT3-C...5...	0.1503	VS2-C...9...	-0.7609	NNC-C...321.	0.2888	P3E0C...2-..	0.039	S2E0C...6-..	-0.0194	NNE0C...318-	0.2369	c...(.....	0.4671	C...c...2...	1.2258
EC0-C...2...	-0.4664	PT3-C...6...	-0.1108	VS2-C...10..	0.609	NNC-C...220.	-0.4258	P3E0C...4-..	0.3926	S2E0C...8-..	-0.8678	NNE0C...218-	0.373	n...(.....	-0.2635	c...2...c...	-0.8229
PT2-C...2...	0.1617	PT4-C...2...	0.0075	VS3-C...5...	0.0543	P2E0C...1-..	0.2956	P4E0C...1-..	0.3492	S3E0C...4-..	0.2228	C7.....0...	3.5925	n...1.....	-1.1894	c...c...2...	0.0329
PT2-C...2...	0.1617	PT4-C...5...	0.0054	VS3-C...7...	0.4176	P2E0C...1-..	0.2956	P4E0C...2-..	0.568	S3E0C...4-..	0.2228	C6...AH.4...	-1.1191	1...(.....	0.2493	c...c...c...	0.1041
PT2-C...3...	-0.3219	PT4-C...2...	0.0075	VS3-C...6...	0.0878	P2E0C...1-..	0.2956	P4E0C...0-..	0.3918	S3E0C...4-..	0.2228	C5...AH.1...	0.3538	c...(.....	0.4671	c...c...(	0.0806
PT2-C...2...	0.1617	PT4-C...8...	2.063	VS3-C...8...	0.3966	P2E0C...0-..	-0.4811	P4E0C...6-..	2.3163	S3E0C...6-..	0.0196	C4.....0...	4.2159	c...1.....	1.3554	c...(C...	0.2545
PT2-C...3...	-0.3219	PT4-C...6...	-0.4106	VS3-C...11..	1.0273	P2E0C...1-..	0.2956	P4E0C...4-..	-0.0394	S3E0C...9-..	0.1222	C3.....0...	2.4535	[...1.....	0.2592	(...C...#...	1.2927
PT2-C...4...	0.1341	PT4-C...10..	-0.4909	VS3-C...12..	-0.2348	P2E0C...1-..	0.2956	P4E0C...7-..	-0.1215	S3E0C...9-..	0.1222	C.....	0.4084	[...N.....	0.0775	N...#...C...	-0.5478
PT2-N...4...	-0.907	PT4-N...6...	0.3703	VS3-N...9...	-0.0447	P2E0N...2-..	-0.9875	P4E0N...4-..	0.6107	S3E0N...7-..	0.3718	c.....	0.2294	N...H.....	0.2324	(...N...#...	-0.0278
PT2-C...5...	-0.8296	PT4-C...8...	2.063	VS3-C...15..	-0.1041	P2E0C...2-..	0.3581	P4E0C...5-..	-0.2974	S3E0C...12-	-0.4691	1.....	0.3401	[...H.....	-0.871	c...(N...	1.2931
PT2-N...3...	0.1256	PT4-N...12..	0.0424	VS3-N...13..	0.2489	P2E0N...1-..	0.3354	P4E0N...10-	0.3293	S3E0N...11-	0.1055	c.....	0.2294	c...[.....	2.2348	c...c...(	0.0806
PT2-N...3...	0.1256	PT4-N...6...	0.3703	VS3-N...11..	0.252	P2E0N...1-..	0.3354	P4E0N...4-..	0.6107	S3E0N...9-..	2.2167	c.....	0.2294	c...(.....	0.4671	c...c...2...	0.0329
PT2-C...3...	-0.3219	PT4-C...6...	-0.4106	VS3-C...12..	-0.2348	P2E0C...0-..	-0.4811	P4E0C...3-..	0.1814	S3E0C...9-..	0.1222	c.....	0.2294	N...(.....	0.3609	c...2...(	0.5056
PT2-N...3...	0.1256	PT4-N...6...	0.3703	VS3-N...9...	-0.0447	P2E0N...1-..	0.3354	P4E0N...4-..	0.6107	S3E0N...7-..	0.3718	c.....	0.2294	N...C.....	0.2402	n...(2...	0.4232
PT2-C...3...	-0.3219	PT4-C...6...	-0.4106	VS3-C...8...	0.3966	P2E0C...1-..	0.2956	P4E0C...4-..	-0.0394	S3E0C...6-..	0.0196	(.....	0.2143	c...C.....	1.3509	c...n...(	0.4935
PT2-C...3...	-0.3219	PT4-C...3...	-0.1022	VS3-C...9...	0.0969	P2E0C...0-..	-0.4811	P4E0C...0-..	0.3918	S3E0C...6-..	0.0196	n.....	-1.0496	c...2.....	0.3602	n...c...1...	2.2423
PT2-C...3...	-0.3219	PT4-C...6...	-0.4106	VS3-C...8...	0.3966	P2E0C...1-..	0.2956	P4E0C...4-..	-0.0394	S3E0C...6-..	0.0196	1.....	0.3401	c...2.....	0.3602	c...1...c...	0.2601
PT2-C...3...	-0.3219	PT4-C...6...	-0.4106	VS3-C...7...	0.4176	P2E0C...1-..	0.2956	P4E0C...4-..	-0.0394	S3E0C...5-..	0.1471	(.....	0.2143	c...c.....	0.0813	1...c...1...	1.1892
PT2-C...3...	-0.3219	PT4-C...2...	0.0075	VS3-C...6...	0.0878	P2E0C...0-..	-0.4811	P4E0C...1-..	0.3492	S3E0C...3-..	-0.7497	c.....	0.2294	c...c.....	0.0813	c...1...c...	0.2601
PT2-C...2...	0.1617	PT4-C...2...	0.0075	VS3-C...4...	2.6522	P2E0C...0-..	-0.4811	P4E0C...0-..	0.3918	S3E0C...2-..	0.5873	1.....	0.3401	c...(.....	0.4671	c...c...1...	0.2999
PT2-N...1...	0.5242	PT4-N...4...	0.0881	VS3-N...4...	0.421	P2E0N...0-..	0.3959	P4E0N...3-..	0.2529	S3E0N...3-..	-1.8147	[.....	0.2671	C...(.....	-0.6301	c...c...c...	0.1041
PT2-C...3...	-0.3219	PT4-C...6...	-0.4106	VS3-C...7...	0.4176	P2E0C...1-..	0.2956	P4E0C...4-..	-0.0394	S3E0C...5-..	0.1471	N.....	-0.1868	C...#.....	0.2637	c...c...2...	0.0329
PT2-C...3...	-0.3219	PT4-C...6...	-0.4106	VS3-C...8...	0.3966	P2E0C...1-..	0.2956	P4E0C...4-..	-0.0394	S3E0C...6-..	0.0196	H.....	0.058	N...#.....	-0.6239	c...2...O...	-1.1093
PT2-N...4...	-0.907	PT4-N...10..	-0.7417	VS3-N...13..	0.2489	P2E0N...2-..	-0.9875	P4E0N...8-..	-0.0089	S3E0N...11-	0.1055	[.....	0.2671	N...(.....	0.3609	C...O...2...	0.7068

PT2-C...5...	-0.8296	PT4-C...11..	-0.5703	VS3-C...15..	-0.1041	P2E0C...2-..	0.3581	P4E0C...8-..	-0.3828	S3E0C...12-.	-0.4691	c.....	0.2294	c...(.....	0.4671	O...C...O...	0.2346
PT2-C...4...	0.1341	PT4-C...10..	-0.4909	VS3-C...16..	1.2504	P2E0C...1-..	0.2956	P4E0C...7-..	-0.1215	S3E0C...13-.	-0.813	(.....	0.2143	c...c.....	0.0813	c...O...C...	0.1709
PT2-C...3...	-0.3219	PT4-C...9...	0.3126	VS3-C...13..	-0.3861	P2E0C...1-..	0.2956	P4E0C...7-..	-0.1215	S3E0C...11-.	0.2922	N.....	-0.1868	c...2.....	0.3602	O...c...2...	-0.4928
PT2-C...3...	-0.3219	PT4-C...9...	0.3126	VS3-C...11..	1.0273	P2E0C...1-..	0.2956	P4E0C...7-..	-0.1215	S3E0C...9-..	0.1222	C.....	0.4084	2...(.....	-0.4737	c...2...c...	-0.8229
PT2-C...4...	0.1341	PT4-C...4...	-0.7278	VS3-C...10..	-0.6522	P2E0C...1-..	0.2956	P4E0C...1-..	0.3492	S3E0C...7-..	0.0564	c.....	0.2294	n...(.....	-0.2635	2...c...1...	-0.8138
PT2-O...3...	-0.3424	PT4-O...6...	0.2332	VS3-O...9...	-0.3406	P2E0O...1-..	-0.9362	P4E0O...4-..	0.247	S3E0O...7-..	3.3267	2.....	-0.7381	n...c.....	0.2698	Cmax.2.....	0.7144
PT2-C...2...	0.1617	PT4-C...8...	2.063	VS3-C...10..	-0.6522	P2E0C...0-..	-0.4811	P4E0C...6-..	2.3163	S3E0C...8-..	0.2241	c.....	0.2294	c...1.....	1.3554	Nmax.3.....	-0.7059
PT2-O...3...	-0.3424	PT4-O...6...	0.2332	VS3-O...10..	0.1186	P2E0O...1-..	-0.9362	P4E0O...4-..	0.247	S3E0O...8-..	-0.2408	c.....	0.2294	c...1.....	1.3554	Omax.2.....	0.1172
PT2-C...4...	0.1341	PT4-C...7...	0.4845	VS3-C...11..	1.0273	P2E0C...1-..	0.2956	P4E0C...4-..	-0.0394	S3E0C...8-..	0.2241	c.....	0.2294	c...1.....	1.3554	Smax.0.....	0.8812
PT2-C...4...	0.1341	PT4-C...10..	-0.4909	VS3-C...13..	-0.3861	P2E0C...2-..	0.3581	P4E0C...8-..	-0.3828	S3E0C...11-.	0.2922	(.....	0.2143	c...1.....	1.3554	BOND01000000	-0.8028

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

SA_k	$CW(SA_k)$			SA_k	$CW(SA_k)$			SA_k	$CW(SA_k)$		
	Run 1	Run 2	Run 3		Run 1	Run 2	Run 3		Run 1	Run 2	Run 3
#.....	0.18968	-0.94226	-0.86424	P4E0N...2-..	0.25844	1.24218	-0.81994	PT4-N...6...	0.37031	2.19039	0.69661
\$0	0.31567	-0.16769	0.08727	P4E0N...3-..	0.25286	-1.82286	-0.56358	PT4-N...7...	0.83912	-0.14867	0.46214
\$100	0.1271	0.09402	0.18017	P4E0N...4-..	0.61068	0.40731	1.01692	PT4-N...9...	0.36309	-0.54541	0.43952
\$1,000	0.68398	2.07425	0.7911	P4E0N...5-..	0.18028	0.48648	-0.86083	PT4-O...1...	1.93296	0.34036	0.70963
\$1,000,000	0.28001	2.01562	1.47232	P4E0N...7-..	0.04015	-0.07536	-1.2497	PT4-O...2...	2.2834	2.0522	1.62306
\$10,000,000	-0.66548	-0.51067	-0.08105	P4E0N...8-..	-0.00889	-0.15949	0.05951	PT4-O...3...	0.19647	0.40333	2.20165
\$11,000,000	2.46729	1.06341	0.77973	P4E0O...0-..	0.0187	0.04735	0.48857	PT4-O...4...	-0.06848	-0.65098	-1.31602
\$1,010,000,000	-0.20937	2.30862	0.64217	P4E0O...1-..	0.20377	0.20154	0.40524	PT4-O...5...	0.1025	-0.62004	0.25047
\$1,011,000,000	-0.01207	-0.72264	-0.1285	P4E0O...3-..	-1.70226	-0.78081	-0.56534	PT4-O...6...	0.23318	0.06697	0.63778
\$10,011,000,000	-0.20089	2.19402	0.29874	P4E0O...4-..	0.247	0.18915	1.104	Nmax.0.....	0.04702	-0.22673	-0.29502
(...C.....	-0.29005	-0.68923	-0.99218	NNC-C...101.	0.1915	0.02738	-0.19792	Nmax.1.....	0.10544	0.00606	-0.22892
(.....	0.21432	0.31708	0.01381	NNC-C...110.	-0.75018	-0.51246	0.55329	Nmax.2.....	1.06709	-0.01462	0.44813
(...C...#...	1.29267	-1.12133	0.88937	NNC-C...202.	0.78044	0.37309	-0.21599	Nmax.3.....	-0.70593	0.09024	-0.1846
(...C...(...	-0.9243	-0.47406	-1.67213	NNC-C...211.	-0.00997	0.34259	0.01793	Omax.0.....	0.15323	2.4995	2.37385
(...F...(...	-0.9904	-0.31466	-0.12081	NNC-C...220.	-0.42584	0.41585	0.37148	Omax.1.....	0.00264	0.53613	0.39384
(...N...#...	-0.02779	-0.206	0.16144	NNC-C...303.	2.27502	2.68617	0.1167	Omax.2.....	0.11716	0.03041	-0.6374
(...c...(...	0.07297	-0.3734	0.33975	NNC-C...312.	0.19758	-0.92085	0.27014	Omax.3.....	2.2492	1.24346	0.19347
1...(.....	0.24929	0.36131	2.14529	NNC-C...321.	0.28885	0.27804	0.12438	VS2-C...10..	0.60903	-0.12334	-0.66379
1.....	0.3401	0.39388	0.40026	NNC-C...330.	-1.88887	-0.94833	-1.27344	VS2-C...11..	-0.3232	-0.16073	0.15624
1...2...(...	-0.95822	-1.44103	-0.00918	NNC-F...110.	-0.51939	-0.49345	-0.14122	VS2-C...12..	0.14113	-2.00713	-0.57861
1...c...(...	-0.55243	0.16771	0.29997	NNC-CI...110.	0.3274	2.04521	1.07485	VS2-C...13..	-0.11828	0.63097	0.09725
1...c...1...	1.1892	0.35409	2.04314	NNC-N...110.	0.38928	-0.11288	-0.31654	VS2-C...14..	-0.30539	0.07692	0.42235
1...n...(...	0.19488	0.00517	0.21077	NNC-N...211.	0.34843	0.60897	0.5846	VS2-C...15..	2.25892	1.14782	0.057
2...(.....	-0.47373	0.28051	-0.04138	NNC-N...220.	0.10726	0.25218	1.47533	VS2-C...2...	-0.98771	-0.75185	-2.20267
2.....	-0.7381	-0.04335	-0.43532	NNC-N...321.	0.17657	0.32952	0.42369	VS2-C...3...	-0.29235	0.33974	1.24922
2...1...(...	2.67974	2.74303	2.03859	NNC-N...330.	0.0166	0.23911	0.1801	VS2-C...4...	-0.13639	-0.58877	-0.55315
2...1.....	2.33999	2.44307	-0.36749	NNC-O...110.	1.9562	0.95116	0.07235	VS2-C...5...	0.70498	-0.19209	-0.04448

2...c...(...	1.7971	0.07248	0.04866	NNC-O...220.	0.32854	-0.12962	0.49517	VS2-C...6...	0.01221	-0.19889	-0.36111
2...c...1...	-0.81379	2.1554	0.38225	NNE0C...100-	0.16556	0.13528	-0.88285	VS2-C...7...	-0.09019	-0.68412	-0.20354
2...n...(...	-0.74161	1.60294	0.65925	NNE0C...109-	-1.52021	1.9109	-0.38085	VS2-C...8...	0.54955	0.02597	1.03263
3...(.....	0.1285	-0.96244	0.02376	NNE0C...200-	0.29758	0.33571	2.12778	VS2-C...9...	-0.76092	0.19684	0.2465
3.....	0.46348	-0.68591	0.17822	NNE0C...209-	-0.23734	0.32298	0.05283	VS2-F...4...	2.25372	0.09928	0.47749
=...(.....	-0.72951	0.3541	0.06175	NNE0C...218-	0.37296	-0.79455	-0.62722	VS2-F...5...	-0.80334	0.20713	-0.76385
=.....	-0.67346	-0.1246	0.02578	NNE0C...300-	-0.21223	0.57654	-0.04759	VS2-Cl...4...	-0.69884	-1.13694	0.41799
=...C...(...	-0.94053	-1.16292	0.22703	NNE0C...309-	0.44045	-0.60202	0.49926	VS2-N...10..	0.43937	0.06862	-0.26118
=...O...(...	0.04258	0.1089	-0.64883	NNE0C...318-	0.23691	0.0803	-0.09222	VS2-N...11..	-0.73343	0.42783	0.12224
C...#.....	0.26366	0.22975	-0.60977	NNE0C...327-	-1.13138	-1.02046	-0.98895	VS2-N...2...	1.92859	0.33416	1.90505
C...(.....	-0.63008	-0.53133	-0.00575	NNE0F...109-	0.49454	-0.96476	-0.11693	VS2-N...3...	-0.70223	-0.1823	1.63001
C...(=...	-0.52476	1.24289	0.06596	NNE0Cl...109-	2.38713	2.1135	0.1207	VS2-N...4...	0.32258	-0.11527	0.43858
C...(C...	-0.57462	-0.61339	-0.08148	NNE0N...109-	2.35851	0.0911	1.29019	VS2-N...5...	2.17811	1.06251	1.4124
C.....	0.40844	-0.81741	0.24987	NNE0N...209-	0.12256	0.57605	0.48544	VS2-N...6...	-0.00331	-0.60571	1.06292
C...1.....	0.82793	-0.20003	0.30092	NNE0N...218-	0.30047	-0.82388	0.4933	VS2-N...7...	0.52215	0.65224	-0.30132
C...1...C...	1.93727	1.81611	0.23313	NNE0N...318-	1.37007	0.44067	0.17248	VS2-N...8...	-0.08166	0.21134	0.21016
C...2.....	-0.15682	0.8351	0.33669	NNE0N...327-	-0.93049	2.04743	0.29578	VS2-N...9...	-0.5407	-0.21305	-0.97242
C...3...(...	-0.62578	-0.58708	0.56537	NNE0O...109-	0.76613	0.54718	-0.19059	VS2-O...2...	0.01945	-0.0334	0.1981
C...3.....	0.19807	0.42221	-0.98065	NNE0O...218-	-0.03055	1.24852	-1.22646	VS2-O...3...	1.58693	4.24312	5.28506
C...=.....	0.4949	-1.23883	1.18907	S2E0C...0-.	1.29163	2.36038	0.00794	VS2-O...4...	0.44864	0.5762	0.48647
C...C...(...	0.23905	0.06729	-0.52234	S2E0C...1-.	-0.72497	0.14772	-0.6872	VS2-O...5...	0.28135	-0.08833	0.05383
C...C.....	0.32079	-0.79148	0.09332	S2E0C...10-.	0.07556	2.28238	0.48943	VS2-O...6...	0.32858	-0.17953	0.22975
C...C...1...	-0.83932	0.0449	0.10603	S2E0C...11-.	0.39523	0.37376	-0.07378	VS2-O...7...	0.4523	-0.6723	0.3173
C...C...2...	-0.00205	2.43056	0.02423	S2E0C...12-.	0.04027	0.28374	1.18517	VS3-C...10..	-0.65223	0.25804	-0.69201
C...C...3...	0.03162	0.36006	0.46703	S2E0C...2-.	0.04253	0.16163	0.1165	VS3-C...11..	1.02732	1.43719	2.23839
C...C...C...	0.42785	0.49871	-0.38128	S2E0C...3-.	-0.82816	-1.37006	-0.75313	VS3-C...12..	-0.23476	-0.09185	0.83194
C...N...(...	-0.12485	-0.08591	-0.33512	S2E0C...4-.	0.21405	0.19061	1.15403	VS3-C...13..	-0.38608	-0.7813	-0.70834
C...N...1...	0.27212	0.15247	-0.06586	S2E0C...5-.	-0.37611	-0.51094	-0.47224	VS3-C...14..	0.45255	0.45879	0.38834
C...N...3...	-0.33836	0.62397	0.37377	S2E0C...6-.	-0.01944	0.26463	0.02123	VS3-C...15..	-0.10407	-0.51307	-1.07343
C...O...(...	-0.33652	-2.25549	-1.44135	S2E0C...7-.	-0.11532	0.1459	2.38052	VS3-C...16..	1.25044	0.23515	-0.29977
C...O...2...	0.7068	0.32121	-0.0723	S2E0C...8-.	-0.86778	0.23668	-0.22591	VS3-C...17..	0.03574	0.23147	0.21925

C...O...C...	0.70025	-0.06179	0.39535	S2E0C...9-..	-0.71778	-1.08661	0.14283	VS3-C...18..	0.22228	0.25772	0.03477
C...c...1...	-0.11221	0.51911	0.37653	S2E0F...3-..	0.54943	0.32647	-0.65524	VS3-C...2...	0.19451	0.12746	0.70365
C...c...2...	1.22583	0.29634	2.35224	S2E0F...4-..	0.09289	-0.24845	-0.49524	VS3-C...19..	0.01406	0.34275	-0.54084
C...n...1...	-0.2834	-1.25679	-0.61606	S2E0Cl...3-..	0.02494	-0.69237	-1.24858	VS3-C...20..	-0.3583	1.59588	0.90737
C...n...2...	0.26961	-0.89389	0.02276	S2E0N...1-..	0.39643	-0.63849	-0.75608	VS3-C...3...	1.34241	0.14425	0.04283
C3.....0...	2.45345	2.06987	1.11455	S2E0N...2-..	-0.70667	-0.87905	-0.51462	VS3-C...4...	2.65224	0.52846	-0.22475
C4.....0...	4.21593	1.50586	1.27149	S2E0N...3-..	1.22763	1.40163	-0.11285	VS3-C...5...	0.05426	0.09198	0.27147
C5.....0...	0.32856	0.47224	-0.12051	S2E0N...4-..	0.42259	-0.20044	-0.8304	VS3-C...6...	0.08777	0.40497	-0.5475
C5...AH.1...	0.35383	0.11444	-0.20819	S2E0N...5-..	-0.11494	0.23273	0.39351	VS3-C...7...	0.41755	0.22749	0.22645
C5...AH.2...	0.44955	0.10984	0.41517	S2E0N...6-..	0.48181	-0.26107	-0.32113	VS3-C...8...	0.39656	0.14736	0.1351
C5...AH.3...	-0.63437	-0.5904	0.6714	S2E0N...7-..	0.01773	1.41943	-0.98986	VS3-C...9...	0.09694	0.37943	0.28586
C6...AH.2...	0.14608	-0.14009	-0.79417	S2E0N...8-..	0.48231	0.42815	-0.31608	VS3-F...4...	0.49208	-1.01783	1.00488
C6...AH.3...	0.31469	-0.16705	0.16748	S2E0N...9-..	0.24047	0.40281	-0.97961	VS3-N...10..	-0.22618	0.4355	0.27114
C6...AH.4...	-1.11912	-0.94378	0.89299	S2E0O...1-..	0.6419	1.34099	0.62526	VS3-N...11..	0.252	0.31938	0.32881
C6...AH.5...	0.25854	2.46533	0.29396	S2E0O...2-..	1.10079	0.10697	0.00596	VS3-N...12..	-1.83204	-0.08838	-0.95687
C7.....0...	3.59248	5.71432	7.0148	S2E0O...3-..	-0.99374	0.06744	0.32571	VS3-N...13..	0.24888	0.14358	0.14143
BOND00000000	1.24574	1.42741	2.33865	S2E0O...4-..	0.31272	0.17408	0.24495	VS3-N...14..	0.27907	0.18582	-0.11417
BOND01000000	-0.80278	-0.79246	-1.4203	S2E0O...5-..	-0.57881	1.30333	1.41809	VS3-N...15..	0.29324	0.25603	-0.67605
BOND10000000	0.34432	-0.56883	-0.6649	S3E0C...0-..	-2.78714	-4.46546	-2.40036	VS3-N...16..	-0.82836	2.08396	0.46064
F...(.....	0.33752	0.10304	0.09737	S3E0C...1-..	0.32296	2.42356	0.44353	VS3-N...17..	0.18969	2.05996	0.11887
F.....	0.3686	2.17427	0.09856	S3E0C...10-..	-0.15379	0.42312	0.25357	VS3-N...2...	0.2629	-0.6664	0.58844
F...c...1...	0.63007	0.31582	0.07028	S3E0C...11-..	0.29216	0.02803	0.27587	VS3-N...4...	0.42101	0.01658	-0.40664
EC0-C...1...	0.08698	-0.60855	-0.79107	S3E0C...12-..	-0.46912	0.10309	0.94891	VS3-N...5...	0.23973	-0.71096	-1.10075
EC0-C...2...	-0.46639	0.03278	-0.33358	S3E0C...13-..	-0.81302	0.49267	0.04326	VS3-N...6...	-0.35248	0.47564	0.46004
EC0-C...3...	0.38019	-0.15473	-0.4669	S3E0C...14-..	0.36875	0.61049	-0.09888	VS3-N...7...	-0.41514	-0.49385	0.81027
EC0-F...1...	-0.99499	0.47194	0.61956	S3E0C...15-..	0.47701	0.38884	0.39007	VS3-N...8...	0.24239	0.09956	0.29817
EC0-Cl...1...	0.07066	-0.07251	0.56317	S3E0C...16-..	-0.23092	-0.43755	0.14198	VS3-N...9...	-0.04467	0.76951	0.94317
EC0-N...1...	0.88865	-0.4593	0.13261	S3E0C...17-..	-0.14138	-0.05333	-0.49041	VS3-O...10..	0.11859	0.58302	-0.1168
EC0-N...2...	0.01896	0.47086	0.29201	S3E0C...2-..	0.5873	0.1068	-1.02903	VS3-O...2...	0.28834	2.15438	0.38342
EC0-N...3...	0.2415	-0.66073	0.42829	S3E0C...3-..	-0.74972	-0.81915	-0.59441	VS3-O...4...	0.28953	1.29095	0.01862
EC0-O...1...	0.24072	-0.99672	0.11499	S3E0C...4-..	0.22278	2.18385	-0.08914	VS3-O...5...	0.00812	0.20193	0.04994

EC0-O...2...	-0.96304	1.14881	0.2561	S3E0C...5-..	0.14707	0.03283	0.09601	VS3-O...6...	0.2713	-0.54629	1.2193
H.....	0.05796	-0.36545	0.4511	S3E0C...6-..	0.01959	0.07594	0.30708	VS3-O...8...	0.45238	1.10665	2.06706
H...[...1...	0.12015	2.38008	0.26693	S3E0C...7-..	0.0564	0.2985	0.0594	VS3-O...9...	-0.34062	-0.12065	-0.70114
Cl.....	0.68451	-0.1529	2.02226	S3E0C...8-..	0.22409	0.15062	0.03213	Smax.0.....	0.88122	-0.67542	0.24035
Cl..c...1...	0.66462	0.46999	-0.83328	S3E0C...9-..	0.12215	2.12036	0.30792	[...(.....	1.93485	0.40322	0.70964
Cmax.2.....	0.71439	2.25606	2.02372	S3E0F...3-..	-0.16023	0.74994	0.19043	[.....	0.26709	0.44933	0.46755
Cmax.3.....	-1.31848	-0.76039	-0.00826	S3E0N...1-..	-0.84616	-0.34541	2.29713	[...1...(...	0.24247	-0.41632	-1.08072
N...#.....	-0.62395	-0.59834	-0.93129	S3E0N...10-	-0.68132	-1.27191	-0.85045	[...1.....	0.25923	0.43175	-0.82976
N...#...C...	-0.54784	0.08111	-0.23249	S3E0N...11-	0.10554	-0.29883	0.18895	[...H.....	-0.87101	0.19195	0.64506
N...(.....	0.36089	0.12157	0.48944	S3E0N...12-	0.3639	-0.90565	0.96151	[...H...N...	0.06089	1.27769	-0.05486
N...(..1...	0.30827	0.48288	-0.04521	S3E0N...13-	0.18138	-0.30225	0.18065	[...N.....	0.07755	-0.07349	0.38626
N...(..C...	0.10198	0.26274	-0.19318	S3E0N...15-	0.21177	0.2288	0.30069	[...N...H...	0.70519	0.20521	0.20275
N.....	-0.18677	-0.08756	0.01649	S3E0N...3-..	-1.81472	-1.53289	-1.54583	[...c...(...	0.10794	0.05939	-0.18092
N...1.....	0.15124	-0.89173	0.37143	S3E0N...5-..	-0.64402	-0.54612	-1.3965	c...(.....	0.46705	0.32668	0.00307
N...3.....	-2.045	0.67901	1.27005	S3E0N...6-..	0.3666	0.26152	-0.11755	c...(..1...	0.09256	0.21991	0.15104
N...3...C...	-1.12913	-1.47714	-0.94495	S3E0N...7-..	0.37179	2.16307	0.97108	c...(..2...	0.00727	-0.89191	-0.4704
N...C...(...	-0.3527	0.47847	-0.32177	S3E0N...8-..	0.17943	-0.04367	-0.54009	c...(..3...	-0.68867	0.68444	-0.9535
N...C.....	0.24025	1.09215	0.31106	S3E0N...9-..	2.21669	2.41455	0.61047	c...(..C...	0.25446	-0.0939	0.26211
N...C...C...	0.09966	-0.76527	0.31741	S3E0O...1-..	-0.81416	-1.39967	1.79727	c...(..F...	-0.58232	-0.87846	0.32915
N...H.....	0.23244	0.30292	-0.24719	S3E0O...2-..	-0.98608	-0.1089	0.24838	c...(..N...	1.2931	2.74031	0.67384
N...[...(...	0.47039	0.43448	0.23019	S3E0O...3-..	-0.91732	0.15843	-0.76698	c...(..O...	-0.06892	-0.75796	1.29622
N...[...1...	0.96026	2.0125	0.2491	S3E0O...4-..	0.26841	-0.76791	2.19952	c...(..[...	0.53863	0.31591	-0.47359
N...c...1...	0.23102	-0.97753	0.43352	S3E0O...6-..	0.96986	0.06033	-1.9284	c...(..c...	0.02615	0.63948	1.32461
N...c...2...	0.10048	2.36491	0.15484	S3E0O...7-..	3.32665	1.73932	-1.86736	c.....	0.22944	0.20561	0.307
O...(.....	-0.99964	-1.10171	-1.23123	S3E0O...8-..	-0.24083	0.67834	0.36928	c...1...(...	0.31589	0.04162	1.18174
O...(..C...	1.58142	2.0174	-0.98058	PT2-C...1...	0.06055	0.36107	0.25035	c...1.....	1.35541	0.37247	0.31579
O...(..N...	-1.51935	-1.7051	-4.66639	PT2-C...2...	0.16171	-0.30937	0.2913	c...1...[...	0.18761	0.59047	0.28212
O.....	-0.92094	0.3985	0.45882	PT2-C...3...	-0.3219	0.34681	0.39866	c...1...c...	0.26009	2.64649	0.44348
O...2.....	-0.92321	2.44263	0.95293	PT2-C...4...	0.13408	0.58873	0.39301	c...2...(...	0.50555	1.19482	1.37332
O...=...(...	0.10896	-0.96743	-0.05638	PT2-C...5...	-0.82957	-0.87727	0.19268	c...2.....	0.3602	-1.26656	-0.01657
O...=.....	0.65589	0.04788	-0.52047	PT2-C...6...	0.04043	0.3048	0.39311	c...2...1...	2.23283	0.1561	2.08007

O...=...C...	-0.17767	0.22217	-0.93525	PT2-F...2...	-0.66441	0.07578	0.1122	c...2...C...	0.34376	0.26858	0.36101
O...C...(...	-1.54772	-1.68947	-1.16432	PT2-Cl...2...	0.59128	-0.77956	-0.34074	c...2...O...	-1.10926	0.56942	0.04127
O...C.....	0.19499	0.12985	0.09099	PT2-N...1...	0.52422	0.04417	0.18617	c...2...c...	-0.82292	-0.57597	-1.16657
O...C...C...	0.47272	-1.42482	-1.26495	PT2-N...2...	0.12612	0.69791	0.89465	c...C.....	1.35092	0.81113	0.64275
O...C...O...	0.23461	1.31706	1.05203	PT2-N...3...	0.12563	0.4913	-0.21626	c...C...C...	0.45051	0.37209	0.46556
O...c...1...	2.42717	2.27833	0.74307	PT2-N...4...	-0.90704	0.31142	2.08637	c...C...N...	2.40294	-0.86085	-0.04031
O...c...2...	-0.49279	-0.34894	1.42459	PT2-O...1...	0.28315	0.44072	-0.77809	c...F.....	0.03616	-0.04071	0.97713
P2E0C...0-...	-0.48113	0.26805	0.05319	PT2-O...2...	1.79932	2.1469	1.37909	c...Cl.....	0.05097	0.08862	-0.82691
P2E0C...1-...	0.29564	-0.84298	0.04131	PT2-O...3...	-0.3424	-1.00999	-0.57695	c...N...(...	0.45524	0.32332	-0.37352
P2E0C...2-...	0.35812	0.11537	-0.82191	PT3-C...1...	0.04383	0.4697	0.44644	c...N.....	0.23693	0.30552	0.31036
P2E0C...3-...	2.01307	-0.26496	-0.85501	PT3-C...2...	-0.69127	0.0865	0.18764	c...N...C...	2.43491	0.11464	1.45681
P2E0F...1-...	-0.24168	0.39491	0.21062	PT3-C...3...	0.08425	0.29418	0.08577	c...O.....	2.2407	0.83125	0.09941
P2E0Cl...1-...	0.15445	0.34974	-0.00023	PT3-C...4...	-0.47925	-0.8772	-0.31995	c...O...C...	0.1709	0.00671	0.23786
P2E0N...0-...	0.39586	0.40336	0.25922	PT3-C...5...	0.1503	1.17504	0.17616	c...[.....	2.23481	0.6442	0.22864
P2E0N...1-...	0.33544	0.30751	0.61111	PT3-C...6...	-0.11079	-0.67189	-0.88311	c...[...H...	0.41566	0.73976	1.18825
P2E0N...2-...	-0.98751	0.18706	-1.97017	PT3-C...7...	-0.54293	-0.45905	0.08135	c...c...(...	0.08064	0.05232	0.17971
P2E0O...0-...	0.30003	-0.01141	0.003	PT3-C...8...	-0.06302	1.04735	0.45704	c...c.....	0.08128	-0.81208	-0.60797
P2E0O...1-...	-0.93624	0.37081	0.53685	PT3-C...9...	-0.21444	-0.6897	-0.51417	c...c...1...	0.29987	0.03854	0.29289
P3E0C...0-...	0.03786	0.29298	0.36868	PT3-F...2...	-0.85531	0.33433	-0.92755	c...c...2...	0.03292	2.16623	0.31465
P3E0C...1-...	0.22627	0.0967	-0.65988	PT3-Cl...2...	-0.25858	0.04381	-0.13249	c...c...c...	0.10406	0.05925	-0.03131
P3E0C...2-...	0.03898	-0.53248	-0.33726	PT3-N...1...	0.31007	0.728	-0.94169	c...n...(...	0.49349	-0.47023	0.35001
P3E0C...3-...	0.02201	-0.49257	-0.86891	PT3-N...2...	-0.27846	-0.82397	-0.24229	c...n...1...	-0.4728	0.29871	-1.08398
P3E0C...4-...	0.39263	0.2723	0.48906	PT3-N...3...	0.15551	0.37663	0.08399	c...n...2...	-0.72885	-0.89354	-0.71636
P3E0C...5-...	0.31788	0.44121	0.31464	PT3-N...4...	0.75779	0.38374	0.18565	c...n...c...	-0.11253	-0.19224	0.35
P3E0C...6-...	-1.07567	-0.62408	-0.32388	PT3-N...5...	-0.05201	0.24096	0.46711	n...(.....	-0.26346	0.04443	0.23366
P3E0F...1-...	0.70367	-0.00273	0.15281	PT3-N...6...	0.06865	1.99033	0.17991	n...(...1...	1.37663	0.29913	0.54349
P3E0Cl...1-...	0.25191	0.07247	0.08368	PT3-N...7...	0.07891	-0.51512	0.29797	n...(...2...	0.42321	0.42525	-0.78596
P3E0N...0-...	-0.31862	0.45008	-0.5853	PT3-O...1...	0.3091	-0.14694	-0.44736	n...(...C...	1.16823	0.36918	0.19491
P3E0N...1-...	0.09866	0.17794	1.03938	PT3-O...2...	-0.47425	-0.831	0.33618	n...(...c...	0.59134	0.27192	0.39215
P3E0N...2-...	0.90338	-0.22628	0.63802	PT3-O...3...	0.10545	0.79449	0.65302	n.....	-1.04963	-0.23634	-1.43454
P3E0N...3-...	0.33917	0.64867	0.1863	PT3-O...4...	0.55401	0.24991	-0.60484	n...1...(...	0.38943	0.74054	-0.58188

P3E0N...4-..	0.06827	0.11103	-0.01161	PT4-C...1...	0.07516	0.26767	0.2677	n...1.....	-1.18941	-0.85808	0.03529
P3E0N...5-..	0.02335	0.33994	-1.11644	PT4-C...10..	-0.49086	-0.07456	-0.28213	n...1...2...	0.51525	1.80433	0.30515
P3E0O...0-..	0.30647	-0.98302	2.32994	PT4-C...11..	-0.57026	-1.69343	-1.07684	n...1...c...	0.47303	-0.20861	-0.89945
P3E0O...1-..	0.20439	0.01207	0.11772	PT4-C...12..	0.12723	0.45983	0.06532	n...2...(...	0.11481	-0.5715	-0.50211
P3E0O...2-..	0.69723	0.1629	1.17498	PT4-C...13..	2.19859	2.31977	0.09291	n...2.....	0.68304	-0.52441	0.29868
P4E0C...0-..	0.39176	0.37092	-0.11777	PT4-C...14..	0.66324	0.2771	0.41562	n...2...C...	-0.22902	-0.44252	0.84806
P4E0C...1-..	0.34918	0.11875	0.35186	PT4-C...15..	-0.01084	0.44867	0.17831	n...2...c...	0.20368	2.38522	0.32141
P4E0C...10-.	0.35301	0.47892	2.44407	PT4-C...2...	0.00746	0.3543	0.16426	n...2...n...	0.12745	0.46956	0.18337
P4E0C...11-.	0.59677	0.14712	0.2725	PT4-C...3...	-0.10216	1.15673	-0.07871	n...C.....	-0.77338	0.16373	0.02866
P4E0C...12-.	0.06572	-0.38315	0.30024	PT4-C...4...	-0.72775	-0.79405	-0.78131	n...C...C...	0.32333	0.12306	0.19192
P4E0C...2-..	0.56804	0.91201	0.63752	PT4-C...5...	0.00538	0.18779	0.14278	n...c...(...	0.24649	0.35213	0.15833
P4E0C...3-..	0.18135	-0.60836	-0.42943	PT4-C...6...	-0.41065	1.03115	-0.00796	n...c.....	0.26977	0.31496	2.07667
P4E0C...4-..	-0.03935	0.36424	0.40907	PT4-C...7...	0.48452	1.24902	0.44583	n...c...1...	2.24228	2.25099	0.07502
P4E0C...5-..	-0.29742	-0.02453	0.1065	PT4-C...8...	2.063	2.23208	0.11626	n...c...2...	0.28738	2.38844	0.34873
P4E0C...6-..	2.31631	0.12465	0.15289	PT4-C...9...	0.31258	0.44186	-0.07932	n...c...c...	0.52486	0.69982	0.21079
P4E0C...7-..	-0.12146	0.25483	0.27447	PT4-F...2...	-0.60501	-0.1986	0.53445	n...c...n...	-1.14177	-0.73328	-0.74182
P4E0C...8-..	-0.38281	-0.57681	-0.07261	PT4-Cl...2...	1.14512	-0.65914	-0.89725	n...n...(...	2.38649	2.33077	1.55333
P4E0C...9-..	1.14108	0.66799	0.35043	PT4-N...1...	0.16403	0.11146	1.37815	n...n.....	0.55246	0.46462	2.32423
P4E0F...1-..	-0.00847	-0.21264	0.07963	PT4-N...10..	-0.7417	-0.91297	-0.44095	n...n...1...	2.58772	2.26299	0.42512
P4E0Cl...1-..	0.57704	0.49345	0.09517	PT4-N...12..	0.0424	0.08764	0.36176	n...n...2...	1.20187	1.33594	0.99951
P4E0N...0-..	0.33148	-0.64032	-0.96733	PT4-N...13..	-0.25202	-0.88438	0.13999				
P4E0N...1-..	-0.32758	0.22344	0.10098	PT4-N...2...	-0.7796	-0.66595	-0.49443				
P4E0N...10-.	0.32935	1.38104	0.02885	PT4-N...3...	0.14541	0.42813	0.62913				
P4E0N...11-.	1.42866	0.73226	0.23004	PT4-N...4...	0.08806	0.87356	1.31079				