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SUPPLEMENTARY MATERIAL TO

Monte Carlo optimization based QSAR modeling of the cytotoxicity of acrylic acid-based dental monomers

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

	SMILES notation	Expr	Split 1				Split 2				Split 3			
			DCW	Calc	Diff.	Set	DCW	Calc	Diff.	Set	DCW	Calc	Diff.	Set
1	OC(COC(=O)C(=C)C)COc1ccc(cc1)C(c1ccc(cc1)OCC(COC(=O)C(=C)C)O)(C)C	4.523	153.6227	4.6717	-0.1487	Tr	131.3798	4.5272	-0.0042	Tr	101.8029	4.6189	-0.0959	Tr
2	O=C(OCCOC(=O)C(=C)C)NCCCCCCNC(=O)OC(C(OC(=O)C(=C)C)(C)C)C	4.046	135.7561	4.1632	-0.1172	Tr	120.7312	4.0288	0.0172	Tr	93.9162	4.1786	-0.1326	Tr
3	CCCCCCCCCCCCCOC(=O)C=C	4	127.3104	3.9229	0.0771	Tr	119.513	3.9718	0.0282	Tr	96.78843	4.339	-0.339	Tr
4	OCCOC(=O)C=C	3.721	85.8679	2.7434	0.9776	Tr	103.3123	3.2134	0.5076	Ts	75.13836	3.1303	0.5907	Tr
5	CCC(COC(=O)C(=C)C)CC	3.481	98.29383	3.097	0.384	Tr	102.7258	3.186	0.295	Tr	68.51583	2.7605	0.7205	Tr
6	CC(=C)C(=O)OCC1CO1	3.432	80.86003	2.6008	0.8312	Tr	101.5913	3.1329	0.2991	Tr	73.62916	3.046	0.386	Tr
7	O=C(C(=C)C)OCCOc1ccccc1	3.319	107.3223	3.354	-0.035	Tr	101.8979	3.1472	0.1718	Tr	78.05005	3.2928	0.0262	Tr
8	CC(COC(=O)C=C)O	3.237	99.58373	3.1337	0.1033	Ts	107.8482	3.4257	-0.1887	Tr	72.10373	2.9608	0.2762	Tr
9	O=C(C(=C)C)OCc1ccccc1	3.194	93.18357	2.9516	0.2424	Tr	101.2897	3.1187	0.0753	Tr	77.69698	3.2731	-0.0791	Ts
10	O=C(C(=C)C)OCC(COC(=O)C(=C)C)(C)C	3.187	106.4787	3.33	-0.143	Tr	102.3464	3.1682	0.0188	Tr	82.20556	3.5248	-0.3378	Tr
11	CCCCCCCCCCCCCOC(=O)C(=C)C	3.174	97.531	3.0753	0.0987	Ts	99.81803	3.0499	0.1241	Tr	73.98246	3.0657	0.1083	Tr
12	CCCCOCCOC(=O)C(=C)C	3.125	92.20183	2.9236	0.2014	Ts	101.7043	3.1381	-0.0131	Tr	71.97876	2.9539	0.1711	Tr
13	O=C(C(=C)C)OCCOC(=O)C(=C)C	2.975	75.04993	2.4355	0.5395	Tr	94.44037	2.7981	0.1769	Ts	60.70989	2.3247	0.6503	Tr
14	CCCCOC(=O)C=C	2.955	104.3175	3.2685	-0.3135	Tr	106.9926	3.3857	-0.4307	Ts	80.88324	3.451	-0.496	Tr
15	O=C(C(=C)C)OCCOCCOC(=O)C(=C)C	2.873	87.5084	2.7901	0.0829	Tr	95.66482	2.8554	0.0176	Tr	68.07138	2.7357	0.1373	Ts
16	C=CC(=O)OCC(C)C	2.87	106.2149	3.3225	-0.4525	Tr	94.80212	2.8151	0.0549	Tr	72.58719	2.9878	-0.1178	Ts
17	OC(COC(=O)C(=C)C)COC(=O)C(=C)C	2.827	80.71603	2.5967	0.2303	Tr	98.43524	2.9851	-0.1581	Ts	67.13854	2.6836	0.1434	Tr
18	O=C(C(=C)C)OCCOCCOCCOC(=O)C(=C)C	2.824	84.61243	2.7076	0.1164	Tr	95.2272	2.835	-0.011	Tr	67.82279	2.7218	0.1022	Tr
19	O=C(C(=C)C)OCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOC(=O)C(=C)C	2.788	81.14627	2.609	0.179	Ts	92.60148	2.7121	0.0759	Tr	66.32961	2.6385	0.1495	Tr
20	O=C(C(=C)C)OCCOCCOCCOCCOCCOCCOCCOCCOCCOC COCCOCCOCCOCCOCCOC(=O)C(=C)C	2.772	78.2578	2.5268	0.2452	Tr	90.41339	2.6096	0.1624	Tr	65.08669	2.5691	0.2029	Tr
21	CC(OC(=O)C(=C)C)CCOC(=O)C(=C)C	2.77	73.47979	2.3908	0.3792	Tr	92.54971	2.7096	0.0604	Tr	68.52136	2.7608	0.0092	Tr
22	CCCOC(=O)C=C	2.759	81.24828	2.6119	0.1471	Ts	100.0274	3.0597	-0.3007	Tr	67.80606	2.7209	0.0381	Tr
23	O=C(C(=C)C)OCCOCCOCCOCCOC(=O)C(=C)C	2.706	83.50628	2.6762	0.0298	Tr	94.78958	2.8145	-0.1085	Tr	67.57421	2.708	-0.002	Ts
24	COC(=O)C=C	2.6	67.60376	2.2236	0.3764	Ts	90.17226	2.5983	0.0017	Ts	64.39926	2.5307	0.0693	Ts
25	CCCCOC(=O)C(=C)C	2.567	83.64036	2.68	-0.113	Tr	88.79469	2.5339	0.0331	Tr	63.37059	2.4733	0.0937	Tr
26	CCOCCOC(=O)C(=C)C	2.565	75.55814	2.4499	0.1151	Ts	86.2699	2.4157	0.1493	Tr	61.63122	2.3762	0.1888	Tr

	SMILES notation	Expr	Split 1				Split 2				Split 3			
			DCW	Calc	Diff.	Set	DCW	Calc	Diff.	Set	DCW	Calc	Diff.	Set
27	CC(COC(=O)C(=C)C)C	2.532	77.15368	2.4954	0.0366	Tr	82.63017	2.2453	0.2867	Tr	62.84333	2.4438	0.0882	Ts
28	O=C(C(=C)C)OCCCCCCOC(=O)C(=C)C	2.442	88.26477	2.8116	-0.3696	Tr	97.62552	2.9472	-0.5052	Ts	69.70968	2.8272	-0.3852	Tr
29	CCOC(=O)C=C	2.432	82.57289	2.6496	-0.2176	Tr	85.66366	2.3873	0.0447	Tr	60.85801	2.333	0.099	Ts
30	CC(=C)C(=O)OCC1CCCO1	2.328	92.03577	2.9189	-0.5909	Tr	98.05556	2.9674	-0.6394	Tr	65.66598	2.6014	-0.2734	Tr
31	CC(=C)C(=O)OCCOC(=O)c1ccc2c(c1)C(=O)OC2=O	2.292	63.64959	2.111	0.181	Tr	84.57794	2.3365	-0.0445	Ts	60.12902	2.2923	-0.0003	Ts
32	CC(COC(=O)C(=C)C)O	2.062	73.87312	2.402	-0.34	Tr	87.70105	2.4827	-0.4207	Tr	61.46598	2.367	-0.305	Ts
33	COCCOC(=O)C(=C)C	2.056	71.08387	2.3226	-0.2666	Ts	83.33848	2.2785	-0.2225	Ts	57.44907	2.1427	-0.0867	Ts
34	CC(=C)C(=O)OCCO	1.997	70.67814	2.3111	-0.3141	Tr	73.44776	1.8155	0.1815	Tr	60.12424	2.292	-0.295	Tr
35	CCCOC(=O)C(=C)C	1.991	63.77341	2.1145	-0.1235	Ts	71.94311	1.7451	0.2459	Ts	53.48796	1.9215	0.0695	Tr
36	O=C(C(=C)C)OCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCO CCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOC(=O)C(=C)C	1.988	72.21267	2.3547	-0.3667	Tr	84.96481	2.3546	-0.3666	Tr	62.12272	2.4036	-0.4156	Tr
37	CCOC(=O)C(=C)C	1.534	48.05303	1.6671	-0.1331	Ts	65.31183	1.4347	0.0993	Tr	55.24573	2.0197	-0.4857	Tr
38	CN(CCOC(=O)C(=C)C)C	1.057	38.04694	1.3823	-0.3253	Tr	58.02168	1.0934	-0.0364	Ts	41.67586	1.2621	-0.2051	Tr
39	COC(=O)C(=C)C	1.046	44.01846	1.5523	-0.5063	Tr	60.05954	1.1888	-0.1428	Tr	46.13592	1.5111	-0.4651	Tr

Table S-II. The statistical quality of QSAR models developed with the Monte Carlo optimization method for predicting the cytotoxicity of acrylic acid-based dental monomers

	Run	Training set							Test set						
		r^2	CCC	IIC	q^2	RMSE	MAE	F	r^2	CCC	IIC	q^2	RMSE	MAE	F
Split 1	1	0.6442	0.7836	0.5665	0.5936	0.468	0.354	49	0.8815	0.9387	0.5747	0.8203	0.206	0.159	59
	2	0.6663	0.7997	0.5762	0.6137	0.453	0.340	54	0.8936	0.9282	0.5775	0.8419	0.245	0.190	67
	3	0.6439	0.7834	0.7489	0.5879	0.468	0.337	49	0.8815	0.9253	0.6957	0.8285	0.246	0.196	60
	Av	0.6515	0.7889	0.6305	0.5984	0.463	0.344	51	0.8855	0.9307	0.6160	0.8302	0.232	0.182	62
Split 2	1	0.8855	0.9393	0.8646	0.8751	0.247	0.180	209	0.8069	0.8819	0.8977	0.7072	0.272	0.215	33
	2	0.8686	0.9297	0.8698	0.8554	0.265	0.193	178	0.8038	0.8834	0.8964	0.7483	0.278	0.227	33
	3	0.8671	0.9288	0.8691	0.8512	0.267	0.202	176	0.8023	0.8806	0.8957	0.7041	0.278	0.230	32
	Av	0.8737	0.9326	0.8678	0.8606	0.260	0.192	188	0.8043	0.8820	0.8966	0.7199	0.276	0.224	33
Split 3	1	0.8102	0.8952	0.7314	0.7852	0.301	0.227	115	0.8027	0.7968	0.8958	0.6967	0.437	0.374	33
	2	0.7998	0.8888	0.7465	0.7753	0.309	0.235	108	0.7880	0.8098	0.8877	0.6682	0.424	0.336	30
	3	0.7985	0.8880	0.7260	0.7685	0.310	0.227	107	0.7831	0.7920	0.8847	0.6676	0.426	0.336	29
	Av	0.8028	0.8907	0.7346	0.7763	0.301	0.229	110	0.7913	0.7995	0.8894	0.6775	0.429	0.349	31

r^2 – Correlation coefficient; CCC – Concordance correlation coefficient IIC – Index of ideality of correlation q^2 – Cross-validated correlation coefficient RMSE – Root-mean-square deviation; MAE – Mean absolute error F – Fischer ratio; Av – Average value for statistical parameters obtained from three independent Monte Carlo optimization runs

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

	Split 1		Split 2		Split 3	
Run	Training	Test	Training	Test	Training	Test
0	0.7779	0.9025	0.9222	0.8107	0.8481	0.856
1	0.0004	0.1169	0.0824	0.0308	0	0.1555
2	0.0002	0.0035	0.021	0.0536	0.0401	0.0423
3	0.0005	0.3662	0.0008	0.0552	0.0113	0.0533
4	0.014	0.1484	0.0412	0.177	0.0079	0.0129
5	0.0001	0.0024	0.0376	0.1078	0.0511	0.0294
6	0.0279	0.0496	0.0001	0.0006	0.0581	0.008
7	0	0.0748	0.0376	0.0631	0.0018	0.0511
8	0.0162	0.1267	0.2047	0.0599	0.033	0.0068
9	0.0367	0.2484	0.0032	0.3614	0.0026	0.2574
10	0.0159	0.2321	0.0114	0.0379	0.009	0.0733
R_r^2	0.0112	0.1369	0.044	0.0947	0.0215	0.069
$^cR_p^2$	0.7723	0.8312	0.9	0.7619	0.8373	0.8208
$^CR_p^2 = R \times (R^2 - R_r^2)^{1/2}$ should be > 0.5						

Table S-IV. The list of SAks together with their correlation weights for the three runs of the Monte Carlo optimization obtained from QSAR model for cytotoxicity of acrylic acid-based dental monomers

SA_k(CW)	CW			SA_k(CW)	CW			SA_k(CW)	CW			SA_k(CW)	CW		
	Run 1	Run 2	Run 3		Run 1	Run 2	Run 3		Run 1	Run 2	Run 3		Run 1	Run 2	Run 3
10001000000	2.04072	1.64329	2.17548	EC0-C...2...	-0.57805	2.13528	0.26973	P4E0C...0-..	0.19057	-0.42875	-0.64271	S2E0O...6-..	2.64238	1.68778	-0.65004
10011000000	-0.68648	-0.89667	-1.64588	EC0-C...3...	0.60777	-0.64754	0.09522	P4E0C...1-..	1.15094	0.14607	0.35132	S2E0O...7-..	2.59459	-1.3961	0.82873
(...(.....	1.86481	2.36047	1.83992	EC0-C...4...	-1.08495	2.88662	4.42322	P4E0C...10-.	-0.30488	-0.88076	2.07319	S3E0C...0-..	2.6031	2.80396	3.19456
(..........	2.38315	0.01164	0.48356	EC0-N...2...	0.71245	1.41515	-0.46103	P4E0C...11-.	0.78769	0.2757	0.1774	S3E0C...1-..	3.26508	1.7543	2.38114
(...C...(...	0.59231	0.23821	0.75957	EC0-N...3...	-0.05248	-0.67878	-0.79341	P4E0C...12-.	2.09153	-0.41509	-0.75097	S3E0C...10-.	1.41755	-0.98002	1.14167
(...O...(...	-1.76475	-0.02351	3.13201	EC0-O...1...	-0.73709	2.01317	-0.78123	P4E0C...2-..	1.45036	1.456	-0.17449	S3E0C...11-.	-1.11642	1.76198	0.61019
++++N---B2==	-0.66841	-0.9578	-0.02689	EC0-O...2...	0.43285	-0.67693	-0.95118	P4E0C...3-..	-0.93113	-0.42538	0.24947	S3E0C...2-..	0.02929	-0.50083	0.31047
++++N---O===	-0.0466	-0.51999	-0.59267	Cmax.0.....	0.07451	-0.90299	-0.78808	P4E0C...4-..	0.08828	0.17332	0.85628	S3E0C...3-..	0.63614	2.14929	-0.42529
++++O---B2==	2.93892	2.29353	4.26808	Cmax.1.....	0.62707	-0.98917	-0.35355	P4E0C...6-..	-0.90566	-0.64323	-0.86677	S3E0C...4-..	-0.86744	2.18077	0.12449
1...(.....	-0.55378	-1.23046	-0.99908	Cmax.2.....	2.15876	2.21378	1.33399	P4E0C...7-..	-0.20717	0.38263	-0.73385	S3E0C...5-..	-0.57557	1.25306	2.41236
1..........	1.72756	3.4168	1.46401	HALO00000000	3.10012	5.12254	0.67608	P4E0C...9-..	1.99289	0.80198	3.80959	S3E0C...6-..	1.32358	-1.46925	-1.79261
1...c...(...	2.01002	-0.86826	-0.95821	N...(.....	-1.54125	-0.74101	-0.71144	P4E0N...0-..	1.63655	2.41321	-0.63807	S3E0C...7-..	-0.86923	3.47435	-0.01045
2..........	-0.69637	2.4027	-0.58136	N...(...C...	-1.47049	-0.96695	-0.76188	P4E0N...2-..	-0.52122	1.13736	-0.98008	S3E0C...8-..	0.09488	3.10096	-1.50905
2...c...(...	0.47004	1.4202	-0.47823	N..........	-1.12924	-1.38708	-0.81376	P4E0O...0-..	-0.30012	0.0685	-0.65479	S3E0C...9-..	-0.48167	-1.05033	-0.85821
=...(.....	-0.73963	-1.82271	-0.56441	N...C...(...	2.89675	-0.07344	-0.63735	P4E0O...1-..	3.0397	1.28555	2.0656	S3E0N...1-..	-0.67174	-1.14393	-0.65369
=..........	-0.0911	-0.84168	0.02385	N...C.....	-0.66218	-1.12418	-1.09708	P4E0O...11-.	-0.55104	1.60997	-0.09848	S3E0N...2-..	0.32892	-1.68074	0.33572
=...2.....	-0.07831	-0.53642	0.64225	N...C...C...	0.35577	1.32927	0.17781	P4E0O...2-..	-4.96228	-5.71882	-2.52658	S3E0N...3-..	-1.91307	1.03169	1.05043
=...C...(...	2.12334	-0.15232	1.48761	O...(...(...	-1.60948	-0.33487	-1.10797	P4E0O...3-..	-0.50319	0.47694	-0.31965	S3E0O...0-..	2.70025	-0.53862	-0.69574
=...O...(...	-0.47436	-0.7329	0.07426	O...(.....	-0.67315	-0.21132	-0.69041	P4E0O...4-..	-0.63363	-0.88632	-1.97634	S3E0O...1-..	0.27918	2.34591	0.23796
C...(...(...	-4.48737	-2.88755	-1.87188	O...(...1...	-1.55361	2.71448	3.41292	P4E0O...6-..	0.84905	2.26782	1.14724	S3E0O...2-..	0.55713	-0.98591	-0.81886
C...(.....	0.85977	0.7236	0.43071	O...(...C...	2.11584	4.06705	2.38901	P4E0O...8-..	2.70512	0.55054	-0.38219	S3E0O...3-..	-1.37363	-1.83098	0.23636
C...(...1...	-0.43911	-1.79311	-0.79008	O...(...O...	-2.33768	-1.1146	-0.78522	NNE0C...100-	-0.49194	-1.60235	-0.5722	S3E0O...4-..	4.46801	4.21327	2.10524
C...(...=...	-0.91602	-0.83295	-0.25098	O..........	-0.53045	-0.64042	-0.79137	NNE0C...109-	0.23401	2.63775	2.20755	S3E0O...5-..	-1.4588	0.24585	0.0096
C...(...C...	-1.41874	-0.16738	-0.75001	O...1.....	2.28796	4.46072	-0.75215	NNE0C...209-	0.12554	0.46501	0.33865	S3E0O...7-..	2.32898	-0.69626	2.68917
C..........	-0.85829	-0.91601	-0.30648	O...=...(...	-0.55988	-1.18035	-0.17877	NNE0C...218-	1.18373	-0.25966	-1.31109	S3E0O...8-..	0.51323	-0.7615	2.23785
C...1.....	2.36179	1.07117	2.38854	O...=.....	-0.96694	-0.80896	-0.23906	NNE0C...300-	1.71752	1.90165	2.03515	Nmax.0.....	1.8318	1.89273	-0.1544
C...1...C...	2.03818	2.30487	0.44927	O...=...2...	4.11841	2.14122	-0.83664	NNE0C...309-	-1.12492	-0.98457	-0.38732	Nmax.1.....	-0.27836	-0.67618	-0.66019
C...2.....	-0.11522	4.24878	0.45511	O...=...C...	2.40021	0.9572	2.39268	NNE0C...318-	-0.73448	-1.45937	0.39744	Nmax.2.....	-1.79641	1.64042	-1.95179

SA_k(CW)	CW			SA_k(CW)	CW			SA_k(CW)	CW			SA_k(CW)	CW		
	Run 1	Run 2	Run 3		Run 1	Run 2	Run 3		Run 1	Run 2	Run 3		Run 1	Run 2	Run 3
C...2...=...	1.27096	-0.6899	0.82935	O...C...(...	1.09343	1.18595	-0.74038	NNE0C...327-	0.2283	0.95106	-0.58411	Omax.1.....	1.38989	1.37447	2.17207
C...=...(...	-0.95726	-0.11894	-0.48055	O...C.....	0.92199	0.50283	0.05931	NNE0C...427-	2.96874	-0.50624	-0.17058	Omax.2.....	-1.51955	-1.87402	-1.92046
C...=.....	4.22321	1.85861	2.46372	O...C...1...	3.25323	3.99833	4.43099	NNE0C...436-	-2.10898	0.76726	1.8355	Omax.3.....	4.26554	2.09267	2.37161
C...=...C...	2.8012	3.20602	1.43809	O...C...2...	-1.1112	0.87075	1.79825	NNE0N...218-	-1.15669	-1.42372	-0.98128	Omax.4.....	0.72815	4.33725	-1.10246
C...C...(...	1.33519	0.6716	0.91631	O...C...C...	0.31427	0.27734	0.32731	NNE0N...327-	0.41046	-0.85664	-0.70549	Omax.6.....	2.46839	2.34804	2.34852
C...C.....	1.22831	0.44223	2.02694	O...c...1...	4.08137	-1.50835	0.20516	NNE0O...109-	-0.20716	1.50682	2.11827	Omax.7.....	2.66992	2.6593	2.31455
C...C...1...	-1.92915	1.26609	-1.55957	P2E0C...0-..	0.24879	0.46539	0.2662	NNE0O...218-	0.58391	0.00576	-0.91952	Omax.8.....	-0.85145	1.52513	-0.63281
C...C...=...	0.76893	0.77539	0.81123	P2E0C...1-..	0.4909	-0.23989	0.30203	NOSP01000000	1.99412	1.31782	2.3857	Smax.0.....	2.35774	4.91929	1.30464
C...C...C...	0.82138	0.9339	0.92997	P2E0C...2-..	0.69635	-1.18758	0.05557	NOSP11000000	-0.38648	-0.62676	-0.51823	c...(.....	-1.1569	-0.55175	-0.60163
C...N...(...	-1.03468	-0.9504	-0.73638	P2E0N...1-..	-0.00182	3.08929	1.52438	S2E0C...0-..	0.52342	0.00279	1.01559	c...(...C...	-0.77989	-0.45582	-0.09065
C...N...C...	1.91526	1.30654	1.68492	P2E0N...2-..	-1.82858	1.14379	2.27136	S2E0C...1-..	0.25801	1.20806	0.81339	c...(...O...	2.23292	-0.89815	-0.58278
C...O...(...	-0.85745	-1.81488	-0.68961	P2E0O...0-..	0.47633	-0.73191	1.03036	S2E0C...2-..	0.04606	0.00094	0.20543	c...(...c...	-1.12445	3.08107	1.33856
C...O...1...	-1.0489	1.51674	2.21203	P2E0O...1-..	-0.36896	-0.74227	0.00983	S2E0C...3-..	-0.52242	-0.0755	-0.65247	c.....	0.13081	1.0173	0.06026
C...O...C...	-0.65933	0.6882	-0.72869	P2E0O...2-..	-0.97739	-0.65778	-0.59931	S2E0C...4-..	0.74275	-2.71042	-0.52924	c...1...(...	-0.55346	-0.71309	-1.28325
C...c...1...	0.34836	-1.96338	2.04929	P2E0O...3-..	-1.65077	-1.82568	-1.67783	S2E0C...5-..	2.17321	-0.2486	0.30416	c...1.....	-0.47171	-0.95229	1.79985
C3.....0...	-0.72705	-1.88642	-0.59877	P3E0C...0-..	-0.07245	0.22551	-0.20371	S2E0C...6-..	-0.89218	-1.31795	0.42055	c...1...c...	1.32654	1.66162	0.07356
C3....H.1...	2.99293	2.31551	2.51151	P3E0C...1-..	1.06332	1.94457	-0.66478	S2E0C...7-..	-0.68778	0.39354	2.26095	c...2.....	-0.77289	4.49669	2.04563
C4.....0...	0.67212	-1.22272	2.18393	P3E0C...2-..	1.44811	0.01957	0.46843	S2E0C...8-..	2.30477	4.43347	-1.74675	c...2...c...	0.60447	3.31636	-0.54616
C5.....0...	4.3235	4.16548	4.3648	P3E0C...3-..	-1.5109	-1.56784	-1.43801	S2E0C...9-..	-0.74215	-0.64691	0.90498	c...C.....	1.89214	0.8456	1.92529
C5....H.1...	-1.78297	-4.67514	-1.47067	P3E0C...4-..	0.49952	0.42785	-0.53465	S2E0N...1-..	-1.03619	-0.66219	-0.68997	c...C...O...	2.35666	1.88731	0.22163
C5...AH.1...	1.35155	-0.46432	-0.52543	P3E0C...5-..	2.3124	3.31191	0.02562	S2E0N...3-..	-0.66226	2.2539	1.04249	c...O.....	0.53269	0.01469	2.60098
C6.....0...	2.27699	1.28413	-0.68345	P3E0N...0-..	1.12737	-1.34512	2.37152	S2E0O...0-..	-0.01955	-0.84339	1.13238	c...O...C...	1.50841	-2.82109	-1.96518
C6...A..1...	0.78966	-0.22067	1.00799	P3E0N...2-..	-0.95411	-0.74931	-0.96078	S2E0O...1-..	2.26042	4.4307	2.44092	c...c...(...	-0.42576	0.9723	-0.59307
C6...A..2...	3.48234	0.93083	-1.05247	P3E0O...0-..	0.64866	-0.92118	0.26571	S2E0O...2-..	0.19888	0.74327	-0.03641	c...c.....	2.06053	0.31807	1.86427
C7.....0...	0.69561	4.4304	2.06093	P3E0O...1-..	2.01562	-0.73381	0.74247	S2E0O...3-..	2.25665	3.43735	1.17877	c...c...1...	-0.83299	-0.7083	-0.116
BOND10000000	1.41096	0.83037	0.01221	P3E0O...2-..	-0.63439	-1.50608	0.57711	S2E0O...4-..	-0.52118	0.29808	-0.89888	c...c...2...	-0.42429	2.28212	0.83626
EC0-C...1...	-0.60445	-1.14516	-0.42115	P3E0O...3-..	-1.90308	0.5397	0.75782	S2E0O...5-..	2.41122	2.44651	2.32521	c...c...c...	-0.05854	2.36627	0.60061