

Supporting information for:

Why an integrated approach between search algorithms and chemical intuition is necessary?

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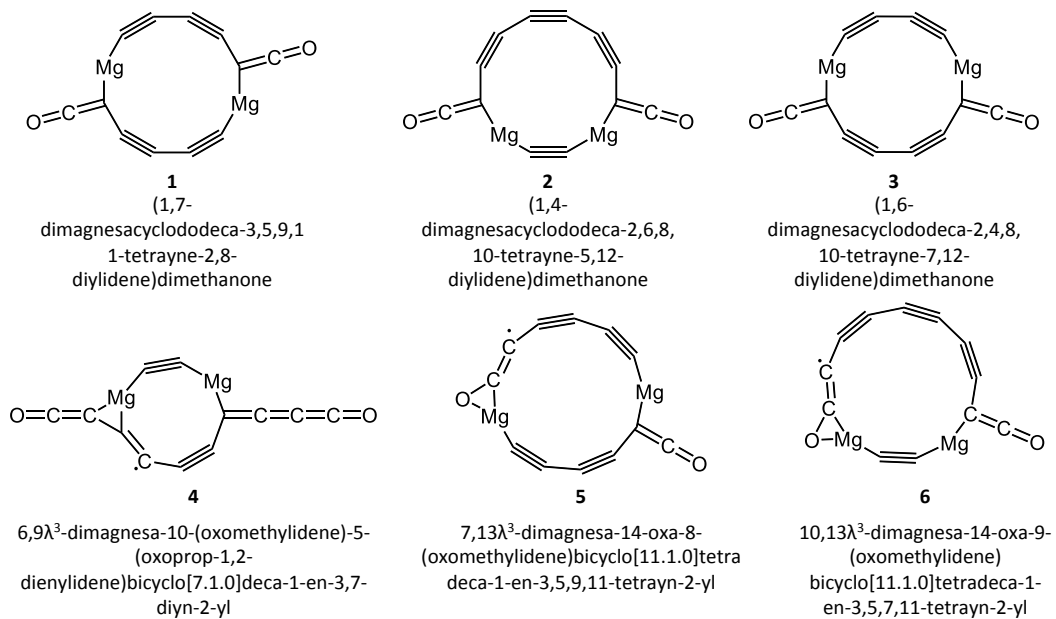


Figure S1: Valence structures and IUPAC names of isomers **1** to **6** of $C_{12}O_2Mg_2$.

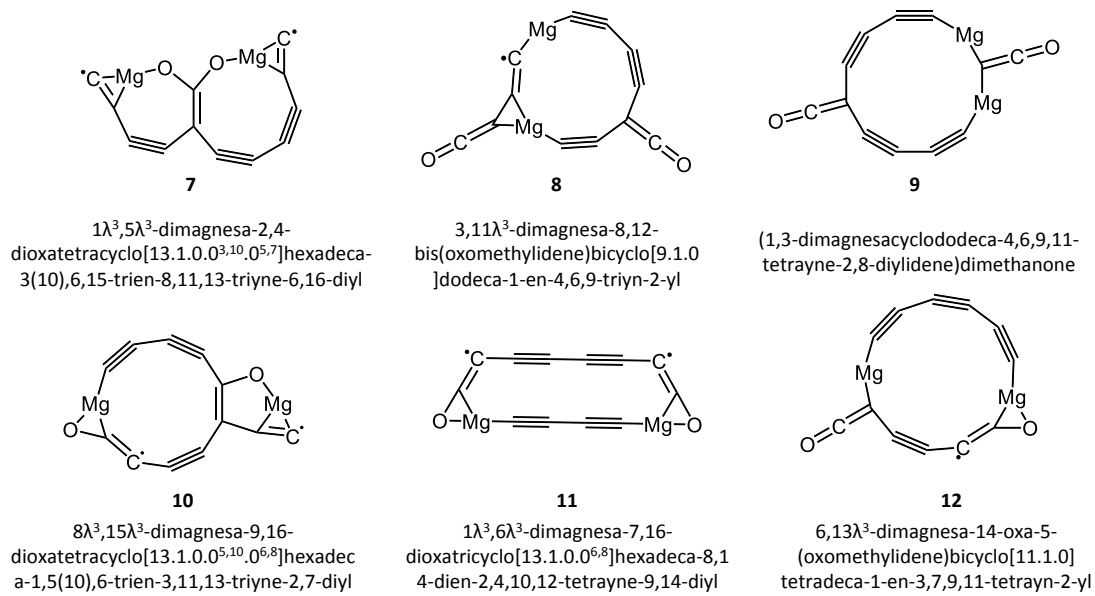


Figure S2: Valence structures and IUPAC names of isomers **7** to **12** of $C_{12}O_2Mg_2$.

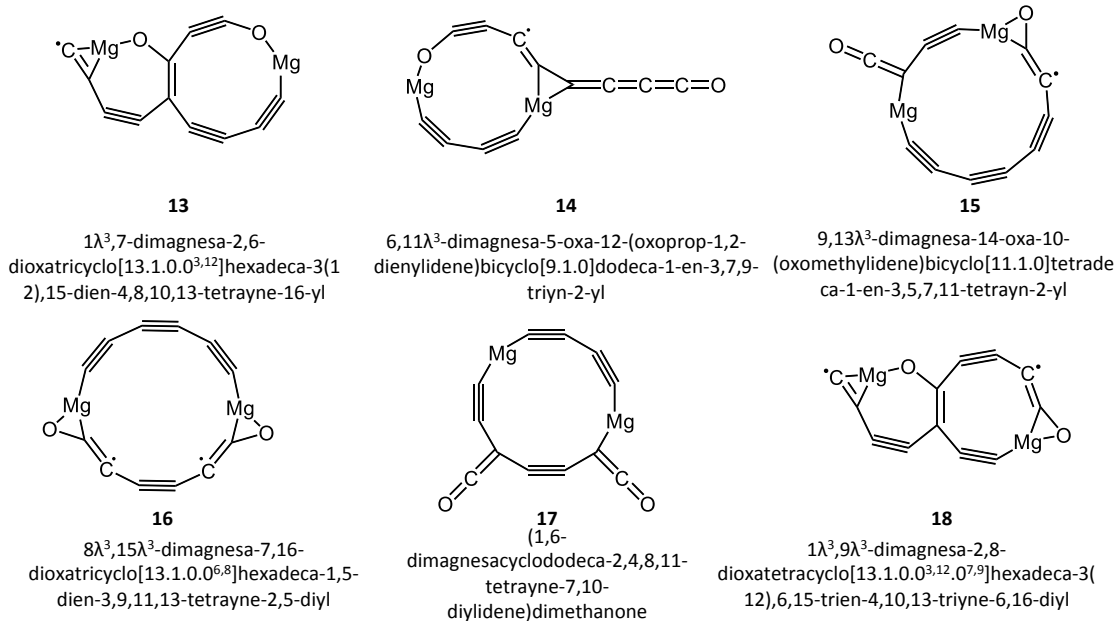
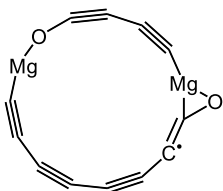
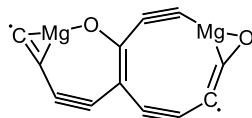


Figure S3: Valence structures and IUPAC names of isomers **13** to **18** of $C_{12}O_2Mg_2$.



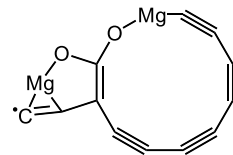
19

9,15 λ^3 -dimagnesa-10,16-dioxabicyclo[13.1.0]hexadeca-1-en-3,5,7,11,13-pentayn-2-yl



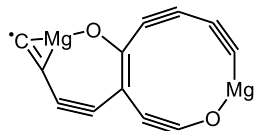
20

1 λ^3 ,6 λ^3 -dimagnesa-2,7-dioxatetracyclo[13.1.0.0^{3,12},0^{6,8}]hexadeca-3(12),8,15-trien-4,10,13-triyn-9,16-diyl



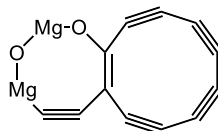
21

1 λ^3 ,5-dimagnesa-2,4-dioxatricyclo[13.1.0.0^{3,14}]hexadeca-3(14),15-dien-6,8,10,12-tetrayne-16-yl



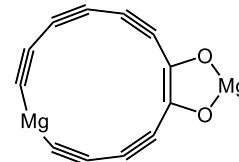
22

1 λ^3 ,8-dimagnesa-2,9-dioxatricyclo[13.1.0.0^{3,12}]hexadeca-3(12),15-dien-4,6,10,13-tetrayne-16-yl



23

12,14-dimagnesa-11,13-dioxabicyclo[8.6.0]hexadeca-2,4,6,8,15-pentayn-1(10)-ene



24

6,15-dimagnesa-14,16-dioxabicyclo[11.3.0]hexadeca-2,4,7,9,11-pentayn-1(13)-ene

Figure S4: Valence structures and IUPAC names of isomers **19** to **24** of $C_{12}O_2Mg_2$.

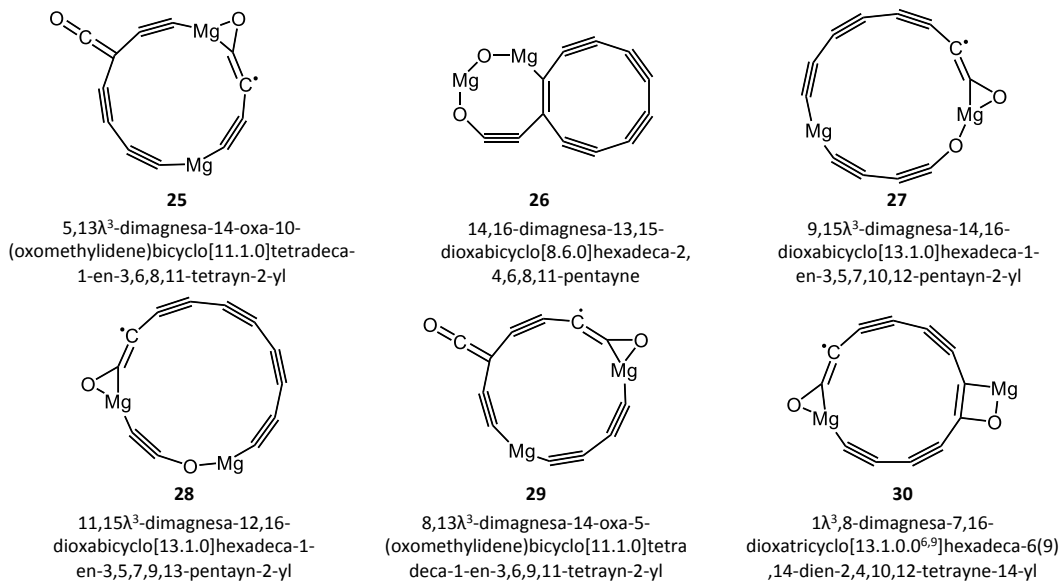


Figure S5: Valence structures and IUPAC names of isomers **25** to **30** of $C_{12}O_2Mg_2$.

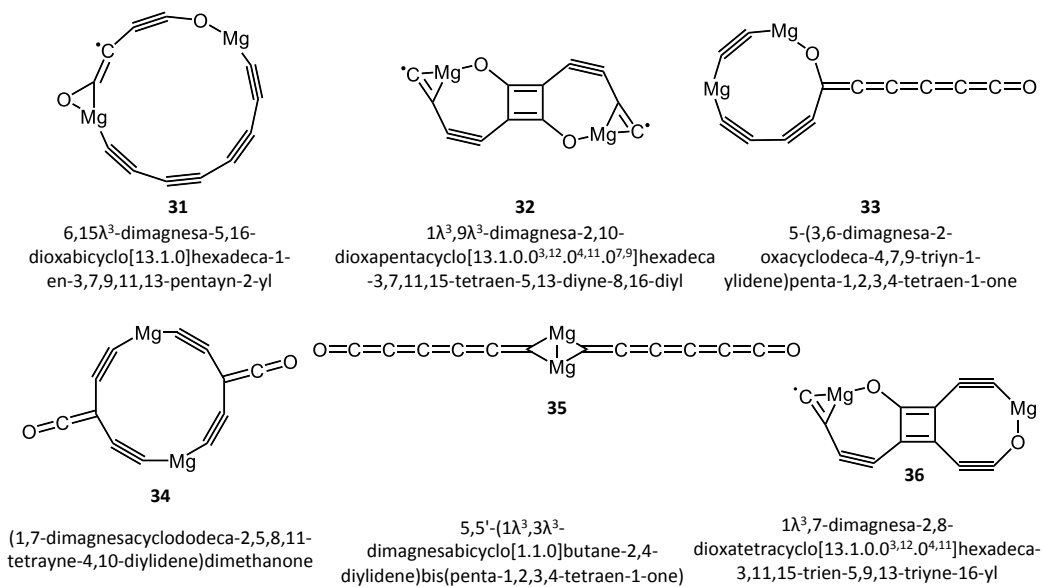


Figure S6: Valence structures and IUPAC names of isomers **31** to **36** of $C_{12}O_2Mg_2$.

Table S1: Total energy (E), zero-point vibrational energy ($ZPVE$), $ZPVE$ -corrected total energy ($E+ZPVE$), thermal correction to Gibbs free energy (G), sum of electronic and thermal Free energies ($E + G$), net dipole moment (μ), relative energy without $ZPVE$ -correction (ΔE_e), $ZPVE$ -corrected relative energy (ΔE_0), and number of imaginary frequencies of $C_{12}O_2Mg_2$ isomers (**1-36**) in their respective singlet ground electronic states calculated at the PBE0-D3/def2-TZVP level of theory.

Isomer	E	$ZPVE$	$E+ZPVE$	G	$E + G$	μ	ΔE_e	ΔE_0	ΔG	NImag
	a.u					Debye	kcal mol ⁻¹			
1	-1006.958624	0.067910	-1006.890715	0.021570	-1006.937054	0.02	0.00	0.00	0.00	0
2	-1006.955368	0.067265	-1006.888103	0.020714	-1006.934654	1.62	2.04	1.64	1.51	0
3	-1006.950734	0.067518	-1006.883216	0.020106	-1006.930628	1.03	4.95	4.71	4.03	0
4	-1006.943620	0.066778	-1006.876842	0.019104	-1006.924516	3.91	9.42	8.70	7.87	0
5	-1006.939033	0.067417	-1006.871616	0.021172	-1006.917861	2.27	12.29	11.98	12.04	0
6	-1006.934599	0.066874	-1006.867725	0.021026	-1006.913573	3.11	15.08	14.43	14.73	0
7	-1006.929617	0.069054	-1006.860563	0.026048	-1006.903569	1.76	18.20	18.92	21.01	0
8	-1006.928290	0.067860	-1006.860430	0.021252	-1006.907038	0.19	19.03	19.00	18.84	0
9	-1006.928271	0.068145	-1006.860126	0.020832	-1006.907439	0.75	19.05	19.19	18.58	0
10	-1006.928890	0.069810	-1006.859079	0.027351	-1006.901539	5.88	18.66	19.85	22.29	0
11	-1006.926160	0.067137	-1006.859023	0.021903	-1006.904257	2.77	20.37	19.89	20.58	0
12	-1006.925604	0.066895	-1006.858710	0.018242	-1006.907362	0.58	20.72	20.08	18.63	0
13	-1006.927838	0.069822	-1006.858015	0.027492	-1006.900346	6.01	19.32	20.52	23.03	0
14	-1006.924885	0.066875	-1006.858010	0.019457	-1006.905428	6.86	21.17	20.52	19.85	0
15	-1006.925134	0.067186	-1006.857948	0.020446	-1006.904688	2.49	21.02	20.56	20.31	0
16	-1006.921186	0.066793	-1006.854393	0.019878	-1006.901308	0.25	23.49	22.79	22.43	0
17	-1006.921702	0.067410	-1006.854292	0.019267	-1006.902435	2.23	23.17	22.86	21.72	0
18	-1006.923853	0.069692	-1006.854161	0.027368	-1006.896485	3.06	21.82	22.94	25.46	0
19	-1006.919851	0.067075	-1006.852775	0.020496	-1006.899355	1.67	24.33	23.81	23.66	0
20	-1006.921028	0.069597	-1006.851430	0.027413	-1006.893615	4.57	23.59	24.65	27.26	0
21	-1006.919053	0.069476	-1006.849577	0.026097	-1006.892956	9.20	24.83	25.81	27.67	0
22	-1006.917899	0.069362	-1006.848537	0.026732	-1006.891167	2.65	25.56	26.47	28.79	0
23	-1006.918011	0.069680	-1006.848331	0.028095	-1006.889916	9.57	25.49	26.60	29.58	0
24	-1006.917084	0.069120	-1006.847964	0.026449	-1006.890635	8.62	26.07	26.83	29.13	0
25	-1006.911137	0.067377	-1006.843760	0.020944	-1006.890193	1.30	29.80	29.46	29.41	0
26	-1006.915333	0.069231	-1006.846102	0.027298	-1006.888035	11.75	27.17	27.99	30.76	0
27	-1006.912947	0.067030	-1006.845917	0.020952	-1006.891995	4.04	28.66	28.11	28.27	0
28	-1006.910815	0.066970	-1006.843845	0.020502	-1006.890313	3.53	30.00	29.41	29.33	0
29	-1006.910852	0.067260	-1006.843592	0.020512	-1006.890340	0.56	29.98	29.57	29.31	0
30	-1006.911179	0.068971	-1006.842208	0.026116	-1006.885063	6.66	29.77	30.44	32.62	0
31	-1006.904427	0.066789	-1006.837638	0.020661	-1006.883766	1.70	34.01	33.31	33.44	0
32	-1006.906485	0.069327	-1006.837158	0.027007	-1006.879478	0.00	32.72	33.61	36.13	0
33	-1006.901879	0.066370	-1006.835509	0.019374	-1006.882505	3.53	35.61	34.64	34.23	0
34	-1006.901132	0.067518	-1006.833614	0.018921	-1006.882211	0.00	36.08	35.83	34.41	0
35	-1006.899786	0.067750	-1006.832036	0.017442	-1006.882344	0.01	36.92	36.82	34.33	0
36	-1006.896847	0.069595	-1006.827252	0.027287	-1006.869560	4.75	38.77	39.82	42.35	0

Table S2: Total energy (E), zero-point vibrational energy ($ZPVE$), $ZPVE$ -corrected total energy ($E+ZPVE$), thermal correction to Gibbs free energy (G), sum of electronic and thermal Free energies ($E + G$), net dipole moment (μ), relative energy without $ZPVE$ -correction (ΔE_e), $ZPVE$ -corrected relative energy (ΔE_0), number of imaginary frequencies, and $\langle S^2 \rangle$ values of $C_{12}O_2Mg_2$ isomers (**1-36**) in their respective triplet ground electronic states calculated at the PBE0-D3/def2-TZVP level of theory.

Isomer	E	$ZPVE$	$E+ZPVE$	G	$E + G$	μ	ΔE_e	ΔE_0	ΔG	NImag	$\langle S^2 \rangle$
	a.u.					Debye	kcal mol ⁻¹				
1	-1006.883654	0.065661	-1006.817993	0.018199	-1006.865455	1.85	24.97	22.89	20.73	0	2.032921
2	-1006.898275	0.064325	-1006.833950	0.016328	-1006.881947	0.55	15.80	12.88	10.38	0	2.057857
3	-1006.889563	0.065777	-1006.823786	0.018063	-1006.871500	3.47	21.27	19.26	16.94	0	2.021401
4	-1006.890796	0.063946	-1006.826850	0.015777	-1006.875019	3.54	20.49	17.34	14.73	0	2.065170
5	-1006.880576	0.064921	-1006.815655	0.017047	-1006.863529	1.24	26.91	24.36	21.94	0	2.054023
6	-1006.877117	0.063916	-1006.813202	0.017035	-1006.860082	2.69	29.08	25.90	24.10	0	2.063486
7	-1006.887976	0.067435	-1006.820540	0.024316	-1006.863660	5.79	22.26	21.30	21.86	0	2.056077
8	-1006.877275	0.065634	-1006.811641	0.017925	-1006.859350	4.18	28.98	26.88	24.56	0	2.041428
9	-1006.879589	0.065835	-1006.813755	0.017538	-1006.862051	5.43	27.53	25.55	22.87	0	2.051841
10	-1006.888186	0.068158	-1006.820028	0.023381	-1006.864805	8.36	22.13	21.62	21.14	0	2.020079
11	-1006.873802	0.064607	-1006.809195	0.018132	-1006.855670	2.45	31.16	28.42	26.87	0	2.059230
12	-1006.871304	0.065096	-1006.806208	0.018223	-1006.853081	4.11	32.72	30.29	28.50	0	2.029518
13	-1006.877620	0.067940	-1006.809679	0.022969	-1006.854651	5.60	28.76	28.11	27.51	0	2.042444
14	-1006.864381	0.064330	-1006.800051	0.015951	-1006.848430	7.63	37.07	34.15	31.42	0	2.040736
15	-1006.872430	0.064734	-1006.807696	0.016758	-1006.855672	2.17	32.02	29.36	26.87	0	2.058280
16	-1006.835602	0.064267	-1006.771335	0.016533	-1006.819069	0.20	55.13	52.17	49.84	0	2.047893
17	-1006.877934	0.065614	-1006.812319	0.017919	-1006.860015	1.90	28.56	26.45	24.15	0	2.029866
18	-1006.865625	0.065892	-1006.799734	0.022941	-1006.842684	1.56	36.29	34.35	35.02	1	2.064198
19	-1006.864317	0.064125	-1006.800192	0.016664	-1006.847653	0.83	37.11	34.06	31.90	0	2.076429
20	-1006.865778	0.066551	-1006.799227	0.023622	-1006.842156	4.52	36.19	34.67	35.35	1	2.055704
21	-1006.888911	0.067492	-1006.821419	0.022335	-1006.866576	4.56	21.68	20.74	20.03	0	2.067834
22	-1006.871713	0.066812	-1006.804901	0.022464	-1006.849249	3.66	32.47	31.11	30.90	0	2.057749
23	-1006.885390	0.067942	-1006.817448	0.025436	-1006.859954	8.90	23.89	23.24	24.18	0	2.097674
24	-1006.923454	0.068976	-1006.854478	0.024959	-1006.898495	3.20	0.00	0.00	0.00	0	2.025295
25	-1006.860490	0.065077	-1006.795413	0.017611	-1006.842879	4.00	39.51	37.06	34.90	0	2.043746
26	-1006.870568	0.067049	-1006.803519	0.023726	-1006.846842	10.96	33.19	31.98	32.41	0	2.109208
27	-1006.868009	0.064765	-1006.803245	0.017721	-1006.850288	1.65	34.79	32.15	30.25	0	2.063849
28	-1006.856046	0.063873	-1006.792172	0.016148	-1006.839898	1.84	42.30	39.10	36.77	0	2.091083
29	-1006.863183	0.065162	-1006.798021	0.017397	-1006.845786	4.63	37.82	35.43	33.08	0	2.036084
30	-1006.898970	0.067735	-1006.831235	0.023139	-1006.875831	3.79	15.36	14.59	14.22	0	2.042510
31	-1006.831678	0.063794	-1006.767883	0.015227	-1006.816451	2.07	57.59	54.34	51.48	0	2.044141
32	-1006.873299	0.068051	-1006.805248	0.023488	-1006.849811	7.74	31.47	30.89	30.55	0	2.053382
33	-1006.883379	0.064667	-1006.818711	0.016212	-1006.867167	6.31	25.15	22.44	19.66	0	2.046610
34	-1006.849211	0.065501	-1006.783711	0.016129	-1006.833082	3.55	46.59	44.41	41.05	0	2.031833
35	-1006.861653	0.065459	-1006.796194	0.013309	-1006.848344	4.95	38.78	36.57	31.47	0	2.037372
36	-1006.877779	0.067716	-1006.810063	0.024170	-1006.853609	2.99	28.66	27.87	28.17	0	2.041732

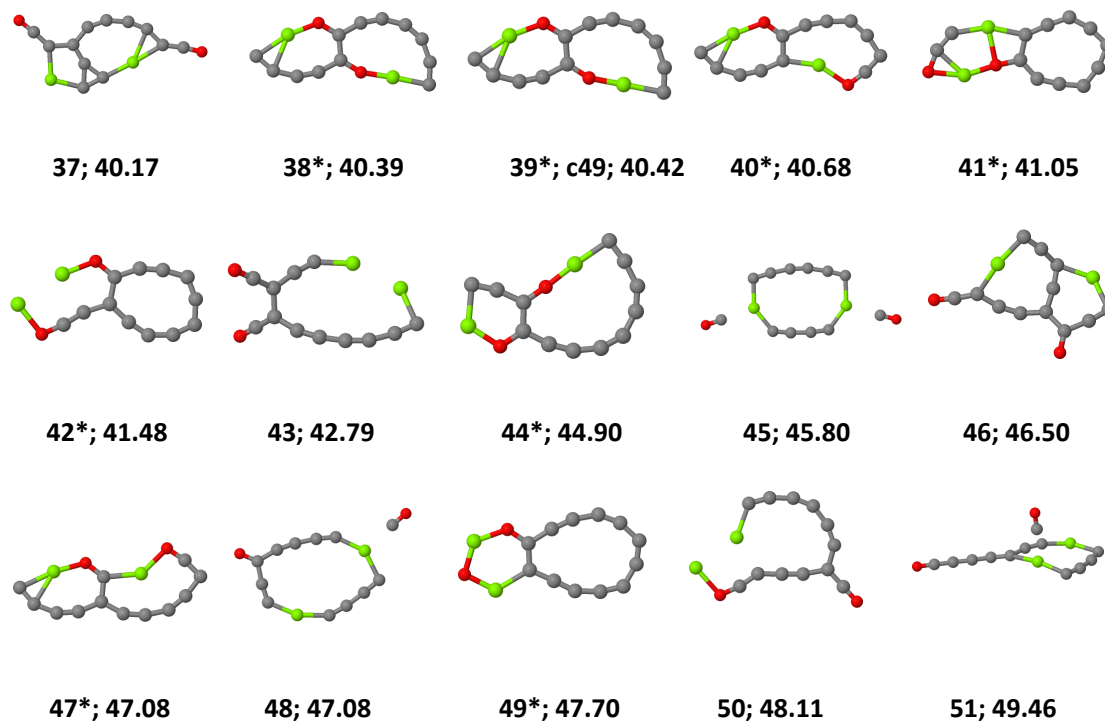


Figure S7: Isomers **37-51** of $C_{12}O_2Mg_2$ considered on the singlet PES. Relative energies including ZPVE corrections (in kcal mol^{-1}) are calculated at the PBE0-D3/def2-TZVP level. Isomers identified by chemical intuition are marked with an asterisk whereas unmarked ones are from AUTOMATON.

Table S3: Total energy (E), zero-point vibrational energy ($ZPVE$), $ZPVE$ -corrected total energy ($E+ZPVE$), thermal correction to Gibbs free energy (G), sum of electronic and thermal Free energies ($E+G$), net dipole moment (μ), relative energy without $ZPVE$ -correction (ΔE_e), $ZPVE$ -corrected relative energy (ΔE_0), and number of imaginary frequencies of $C_{12}O_2Mg_2$ isomers (**37-51**) in their respective singlet ground electronic states calculated at the PBE0-D3/def2-TZVP level of theory.

Isomer	E	$ZPVE$	$E+ZPVE$	G	$E+G$	μ	ΔE_e	ΔE_0	ΔG	NImag
	a.u					Debye	kcal mol ⁻¹			
37	-1006.895684	0.068987	-1006.826697	0.024818	-1006.870866	8.18	39.50	40.17	41.53	0
38	-1006.894807	0.068450	-1006.826357	0.025596	-1006.869211	1.98	40.05	40.38	42.57	0
39	-1006.894788	0.068491	-1006.826297	0.025710	-1006.869078	1.81	40.06	40.42	42.66	0
40	-1006.894739	0.068853	-1006.825886	0.024697	-1006.870042	0.87	40.09	40.68	42.05	0
41	-1006.894277	0.068977	-1006.825300	0.026170	-1006.868107	4.30	40.38	41.05	43.26	0
42	-1006.894583	0.069969	-1006.824613	0.027655	-1006.866928	11.20	40.19	41.48	44.00	0
43	-1006.891292	0.068764	-1006.822528	0.022539	-1006.868753	3.85	42.25	42.79	42.86	0
44	-1006.887884	0.068722	-1006.819163	0.025491	-1006.862393	7.58	44.39	44.90	46.85	0
45	-1006.879066	0.061338	-1006.817728	0.006014	-1006.873052	2.94	49.92	45.80	40.16	0
46	-1006.884964	0.068356	-1006.816608	0.024044	-1006.860920	6.51	46.22	46.50	47.77	0
47	-1006.883999	0.068307	-1006.815692	0.025564	-1006.858435	3.95	46.83	47.08	49.33	0
48	-1006.87976	0.064079	-1006.815682	0.012855	-1006.866905	6.44	49.49	47.08	44.02	0
49	-1006.883878	0.069181	-1006.814697	0.026407	-1006.857471	10.27	46.90	47.70	49.94	0
50	-1006.882119	0.068075	-1006.814044	0.021702	-1006.860417	6.54	48.01	48.11	48.09	0
51	-1006.875557	0.063654	-1006.811903	0.013370	-1006.862187	4.73	52.13	49.45	46.98	0

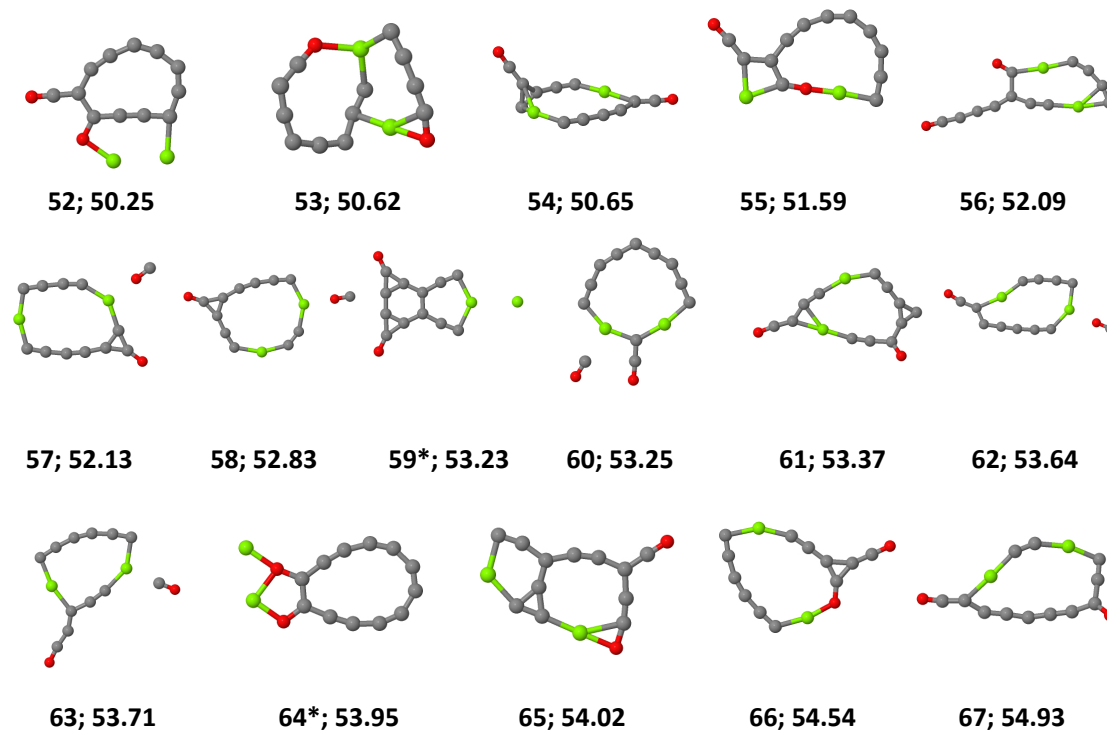


Figure S8: Isomers **52-67** of $C_{12}O_2Mg_2$ considered on the singlet PES. Relative energies including ZPVE corrections (in kcal mol^{-1}) are calculated at the PBE0-D3/def2-TZVP level. Isomers identified by chemical intuition are marked with an asterisk whereas unmarked ones are from AUTOMATON.

Table S4: Total energy (E), zero-point vibrational energy ($ZPVE$), $ZPVE$ -corrected total energy ($E+ZPVE$), thermal correction to Gibbs free energy (G), sum of electronic and thermal Free energies ($E+G$), net dipole moment (μ), relative energy without $ZPVE$ -correction (ΔE_e), $ZPVE$ -corrected relative energy (ΔE_0), and number of imaginary frequencies of $C_{12}O_2Mg_2$ isomers (**52-67**) in their respective singlet ground electronic states calculated at the PBE0-D3/def2-TZVP level of theory.

Isomer	E	$ZPVE$	$E+ZPVE$	G	$E+G$	μ	ΔE_e	ΔE_0	ΔG	NImag
	a.u					Debye	kcal mol ⁻¹			
52	-1006.880455	0.069814	-1006.810641	0.028387	-1006.852068	8.39	49.05	50.25	53.33	1
53	-1006.877254	0.067205	-1006.810050	0.022803	-1006.854451	3.96	51.06	50.61	51.83	0
54	-1006.876231	0.066235	-1006.809997	0.020060	-1006.856171	1.17	51.70	50.65	50.75	0
55	-1006.876763	0.068263	-1006.808500	0.023885	-1006.852878	8.41	51.37	51.59	52.82	0
56	-1006.872803	0.065093	-1006.807710	0.016572	-1006.856231	2.01	53.85	52.09	50.72	0
57	-1006.871180	0.063543	-1006.807637	0.012721	-1006.858459	5.40	54.87	52.13	49.32	0
58	-1006.869810	0.063286	-1006.806525	0.011760	-1006.858050	9.22	55.73	52.83	49.58	0
59	-1006.877152	0.071258	-1006.805894	0.025757	-1006.851395	12.70	51.12	53.23	53.75	0
60	-1006.868346	0.062491	-1006.805855	0.011822	-1006.856524	4.66	56.65	53.25	50.53	0
61	-1006.872586	0.066918	-1006.805668	0.020251	-1006.852335	6.50	53.99	53.37	53.16	0
62	-1006.867229	0.061987	-1006.805242	0.011493	-1006.855736	4.06	57.35	53.63	51.03	0
63	-1006.868556	0.063427	-1006.805129	0.012112	-1006.856444	4.38	56.52	53.71	50.58	0
64	-1006.874625	0.069878	-1006.804746	0.027353	-1006.847272	8.04	52.71	53.95	56.34	0
65	-1006.873991	0.069368	-1006.804624	0.025756	-1006.848235	8.03	53.11	54.02	55.73	0
66	-1006.870165	0.066358	-1006.803807	0.018807	-1006.851358	3.25	55.51	54.54	53.78	0
67	-1006.867689	0.064509	-1006.803180	0.017059	-1006.850630	7.01	57.06	54.93	54.23	0

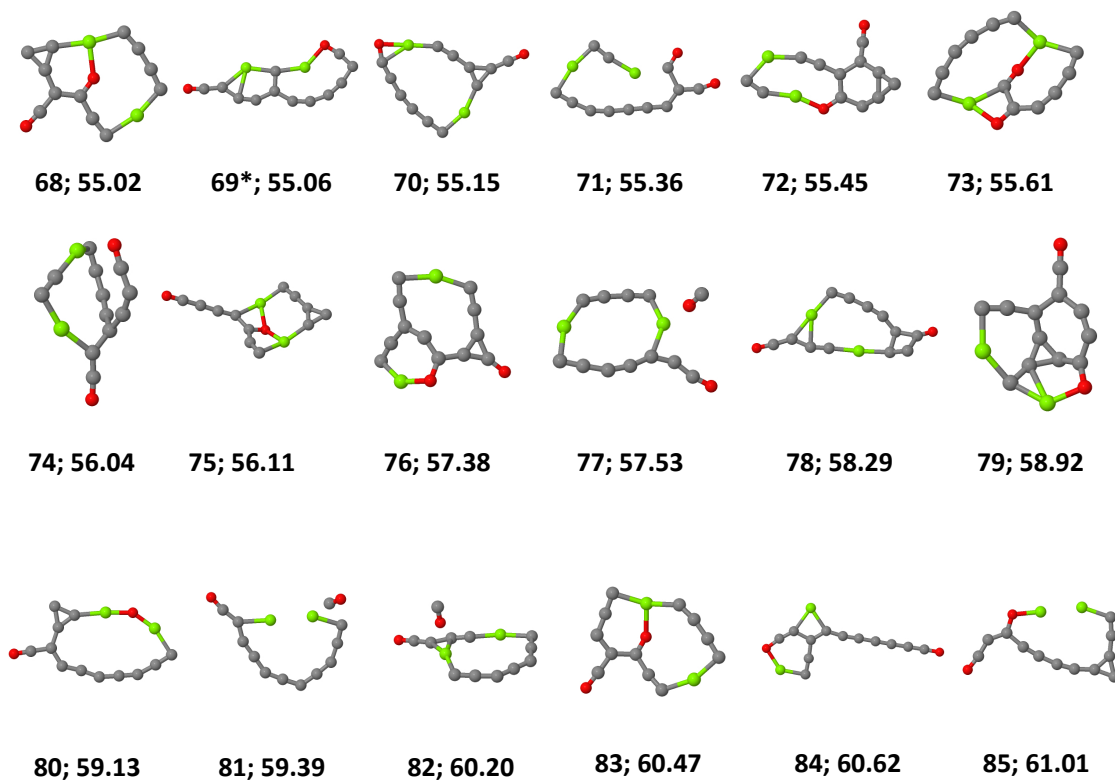


Figure S9: Isomers **68-85** of $C_{12}O_2Mg_2$ considered on the singlet PES. Relative energies including ZPVE corrections (in kcal mol^{-1}) are calculated at the PBE0-D3/def2-TZVP level. Isomers identified by chemical intuition are marked with an asterisk whereas unmarked ones are from AUTOMATON.

Table S5: Total energy (E), zero-point vibrational energy ($ZPVE$), $ZPVE$ -corrected total energy ($E+ZPVE$), thermal correction to Gibbs free energy (G), sum of electronic and thermal Free energies ($E+G$), net dipole moment (μ), relative energy without $ZPVE$ -correction (ΔE_e), $ZPVE$ -corrected relative energy (ΔE_0), and number of imaginary frequencies of $C_{12}O_2Mg_2$ isomers (**68-85**) in their respective singlet ground electronic states calculated at the PBE0-D3/def2-TZVP level of theory.

Isomer	E	$ZPVE$	$E + ZPVE$	G	$E + G$	μ	ΔE_e	ΔE_0	ΔG	NImag
	a.u					Debye	kcal mol ⁻¹			
68	-1006.869833	0.066799	-1006.803034	0.020038	-1006.849795	5.59	55.72	55.02	54.76	0
69	-1006.871664	0.068695	-1006.802969	0.024709	-1006.846955	4.63	54.57	55.06	56.54	0
70	-1006.868957	0.066123	-1006.802835	0.019339	-1006.849618	2.71	56.27	55.15	54.87	0
71	-1006.865711	0.063210	-1006.802501	0.016888	-1006.848823	1.85	58.30	55.35	55.37	0
72	-1006.870286	0.067932	-1006.802354	0.025629	-1006.844657	5.97	55.43	55.45	57.98	0
73	-1006.868071	0.065969	-1006.802102	0.022588	-1006.845483	5.18	56.82	55.60	57.46	0
74	-1006.867786	0.066384	-1006.801402	0.020744	-1006.847042	2.39	57.00	56.04	56.48	0
75	-1006.867971	0.066677	-1006.801294	0.021862	-1006.846109	7.64	56.89	56.11	57.07	0
76	-1006.868379	0.069108	-1006.799271	0.026349	-1006.842030	3.92	56.63	57.38	59.63	0
77	-1006.861050	0.062016	-1006.799034	0.010967	-1006.850083	2.35	61.23	57.53	54.58	0
78	-1006.863716	0.065896	-1006.797821	0.019202	-1006.844514	3.30	59.56	58.29	58.07	0
79	-1006.868108	0.071286	-1006.796823	0.031508	-1006.836600	6.64	56.80	58.92	63.04	0
80	-1006.861551	0.065059	-1006.796492	0.019321	-1006.842230	2.01	60.91	59.13	59.50	0
81	-1006.859372	0.063300	-1006.796072	0.013070	-1006.846302	5.53	62.28	59.39	56.95	0
82	-1006.856419	0.061646	-1006.794773	0.011077	-1006.845342	3.25	64.13	60.20	57.55	0
83	-1006.860241	0.065896	-1006.794346	0.020233	-1006.840008	6.25	61.74	60.47	60.90	0
84	-1006.861854	0.067735	-1006.794118	0.021436	-1006.840418	17.15	60.72	60.62	60.64	0
85	-1006.861350	0.067868	-1006.793482	0.021686	-1006.839664	5.99	61.04	61.01	61.11	0

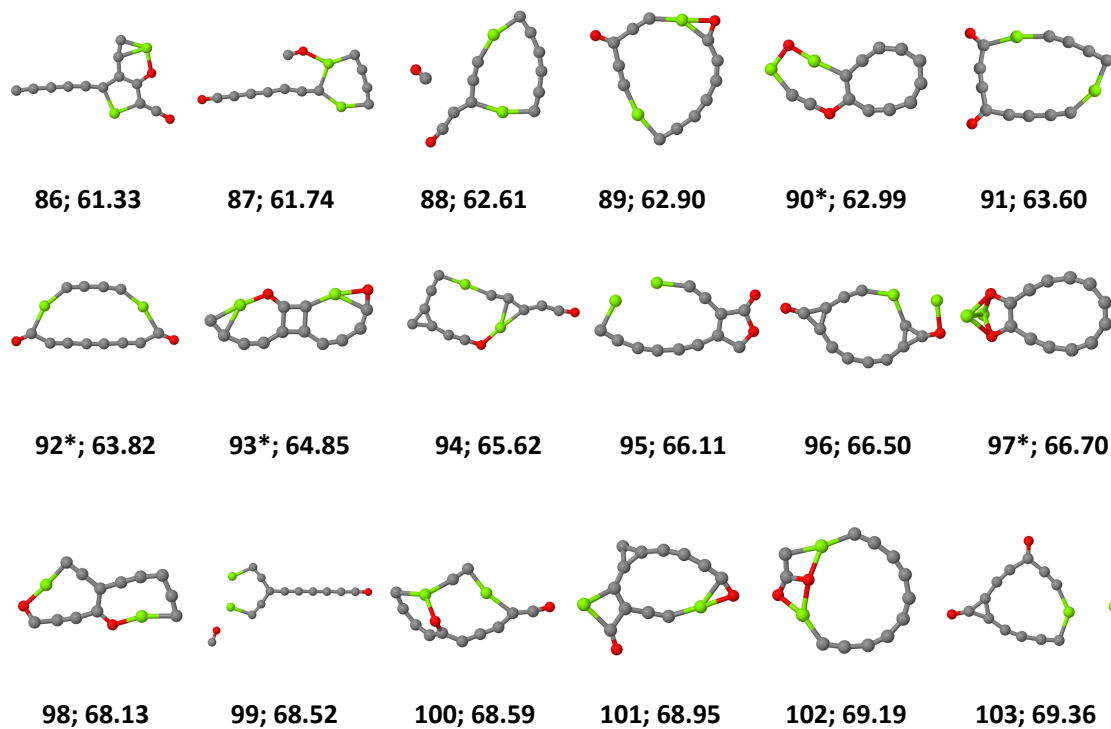


Figure S10: Isomers **86-103** of $C_{12}O_2Mg_2$ considered on the singlet PES. Relative energies including ZPVE corrections (in kcal mol^{-1}) are calculated at the PBE0-D3/def2-TZVP level. Isomers identified by chemical intuition are marked with an asterisk whereas unmarked ones are from AUTOMATON.

Table S6: Total energy (E), zero-point vibrational energy ($ZPVE$), $ZPVE$ -corrected total energy ($E+ZPVE$), thermal correction to Gibbs free energy (G), sum of electronic and thermal Free energies ($E + G$), net dipole moment (μ), relative energy without $ZPVE$ -correction (ΔE_e), $ZPVE$ -corrected relative energy (ΔE_0), and number of imaginary frequencies of $C_{12}O_2Mg_2$ isomers (**86-103**) in their respective singlet ground electronic states calculated at the PBE0-D3/def2-TZVP level of theory.

Isomer	E	$ZPVE$	$E+ZPVE$	G	$E + G$	μ	ΔE_e	ΔE_0	ΔG	NImag
	a.u					Debye	kcal mol ⁻¹			
86	-1006.861254	0.068267	-1006.792987	0.022832	-1006.838422	15.76	61.10	61.33	61.89	0
87	-1006.855629	0.063303	-1006.792326	0.014431	-1006.841198	2.21	64.63	61.74	60.15	0
88	-1006.853201	0.062261	-1006.790940	0.008195	-1006.845006	1.44	66.15	62.61	57.76	0
89	-1006.855489	0.065008	-1006.790481	0.018143	-1006.837346	2.26	64.71	62.90	62.57	0
90	-1006.859746	0.069412	-1006.790334	0.027866	-1006.831880	9.73	62.05	62.99	66.00	0
91	-1006.855231	0.065864	-1006.789367	0.017837	-1006.837394	4.95	64.88	63.60	62.54	0
92	-1006.853064	0.064047	-1006.789017	0.014460	-1006.838604	2.82	66.24	63.82	61.78	0
93	-1006.855959	0.068587	-1006.787372	0.025847	-1006.830112	6.04	64.42	64.85	67.11	0
94	-1006.852069	0.065920	-1006.786149	0.019492	-1006.832577	5.07	66.86	65.62	65.56	0
95	-1006.854255	0.068890	-1006.785365	0.024970	-1006.829285	8.24	65.49	66.11	67.63	0
96	-1006.853823	0.069090	-1006.784733	0.025479	-1006.828344	7.79	65.76	66.50	68.22	0
97	-1006.853770	0.069354	-1006.784415	0.027199	-1006.826571	3.26	65.80	66.70	69.33	0
98	-1006.847379	0.065230	-1006.782150	0.022254	-1006.825125	5.08	69.81	68.13	70.24	0
99	-1006.845821	0.064292	-1006.781529	0.010953	-1006.834868	12.83	70.78	68.52	64.13	0
100	-1006.846742	0.065331	-1006.781411	0.020164	-1006.826578	5.92	70.21	68.59	69.32	0
101	-1006.848428	0.067583	-1006.780844	0.024231	-1006.824197	4.12	69.15	68.95	70.82	0
102	-1006.845929	0.065472	-1006.780458	0.020503	-1006.825426	3.49	70.72	69.19	70.05	0
103	-1006.848326	0.068145	-1006.780181	0.019353	-1006.828973	12.60	69.21	69.36	67.82	0

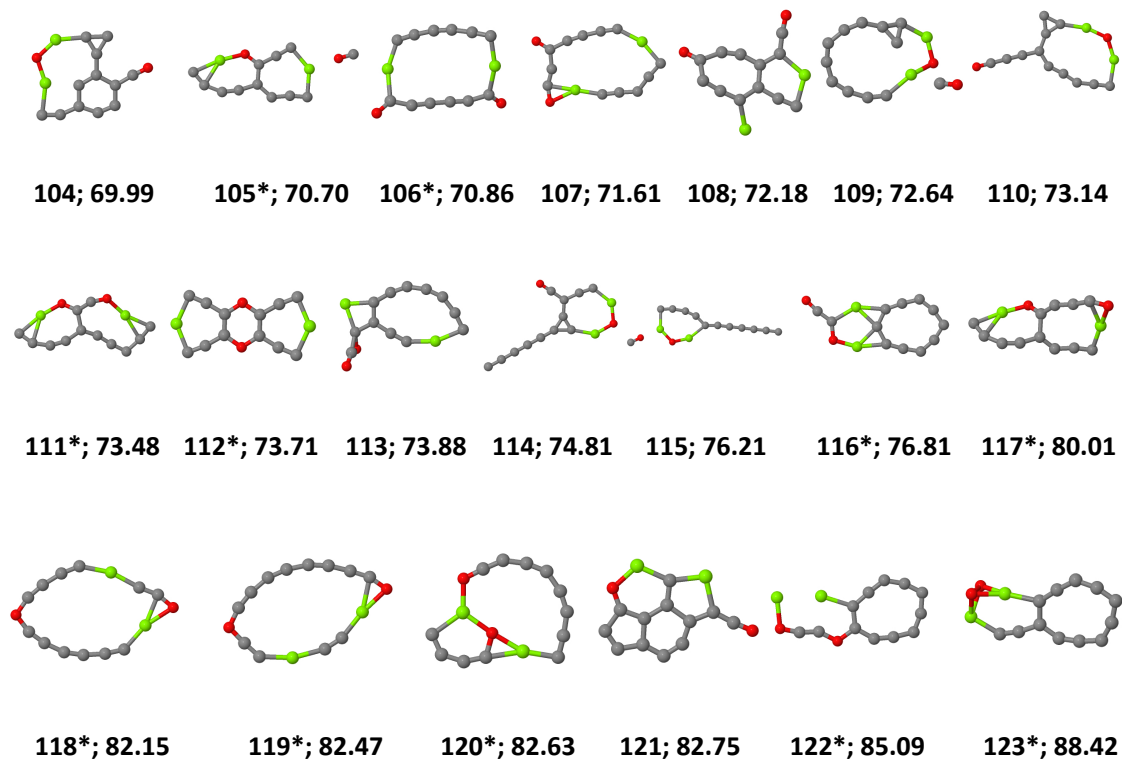


Figure S11: Isomers **104-123** of $C_{12}O_2Mg_2$ considered on the singlet PES. Relative energies including ZPVE corrections (in kcal mol^{-1}) are calculated at the PBE0-D3/def2-TZVP level. Isomers identified by chemical intuition are marked with an asterisk whereas unmarked ones are from AUTOMATON.

Table S7: Total energy (E), zero-point vibrational energy ($ZPVE$), $ZPVE$ -corrected total energy ($E+ZPVE$), thermal correction to Gibbs free energy (G), sum of electronic and thermal Free energies ($E + G$), net dipole moment (μ), relative energy without $ZPVE$ -correction (ΔE_e), $ZPVE$ -corrected relative energy (ΔE_0), and number of imaginary frequencies of $C_{12}O_2Mg_2$ isomers (**104-123**) in their respective singlet ground electronic states calculated at the PBE0-D3/def2-TZVP level of theory.

Isomer	E	$ZPVE$	$E+ZPVE$	G	$E + G$	μ	ΔE_e	ΔE_0	ΔG	NImag
	a.u					Debye	kcal mol ⁻¹			
104	-1006.847384	0.068206	-1006.779178	0.026340	-1006.821044	2.97	69.80	69.99	72.80	0
105	-1006.842496	0.064455	-1006.778041	0.017031	-1006.825465	7.54	72.87	70.70	70.02	0
106	-1006.842243	0.064448	-1006.777796	0.015570	-1006.826673	1.26	73.03	70.86	69.27	0
107	-1006.841494	0.064891	-1006.776604	0.017577	-1006.823917	2.40	73.50	71.61	70.99	0
108	-1006.845141	0.069450	-1006.775691	0.026374	-1006.818767	11.25	71.21	72.18	74.23	0
109	-1006.839222	0.064273	-1006.774949	0.018129	-1006.821093	5.27	74.93	72.64	72.77	0
110	-1006.839335	0.065174	-1006.774162	0.017773	-1006.821562	2.03	74.85	73.14	72.47	0
111	-1006.840201	0.066576	-1006.773625	0.024032	-1006.816169	7.42	74.31	73.48	75.86	0
112	-1006.844604	0.071358	-1006.773246	0.029582	-1006.815022	0.002	71.55	73.71	76.58	0
113	-1006.841411	0.068432	-1006.772980	0.025598	-1006.815813	8.08	73.55	73.88	76.08	0
114	-1006.837907	0.066415	-1006.771492	0.019766	-1006.818141	16.06	75.75	74.81	74.62	0
115	-1006.831120	0.061849	-1006.769272	0.011047	-1006.820073	15.91	80.01	76.21	73.41	0
116	-1006.835096	0.066779	-1006.768316	0.023144	-1006.811952	3.44	77.51	76.81	78.50	0
117	-1006.829229	0.066011	-1006.763218	0.023274	-1006.805955	5.27	81.20	80.01	82.27	0
118	-1006.826873	0.067078	-1006.759795	0.021373	-1006.805500	2.52	82.68	82.15	82.55	0
119	-1006.825602	0.066308	-1006.759294	0.020215	-1006.805387	3.76	83.47	82.47	82.62	0
120	-1006.823105	0.064062	-1006.759043	0.017186	-1006.805919	6.53	85.04	82.63	82.29	0
121	-1006.829159	0.070312	-1006.758847	0.029143	-1006.800016	12.32	81.24	82.75	85.99	0
122	-1006.824480	0.069365	-1006.755115	0.026870	-1006.797610	10.86	84.18	85.09	87.50	0
123	-1006.817738	0.067925	-1006.749813	0.026707	-1006.791031	9.35	88.41	88.42	91.63	0

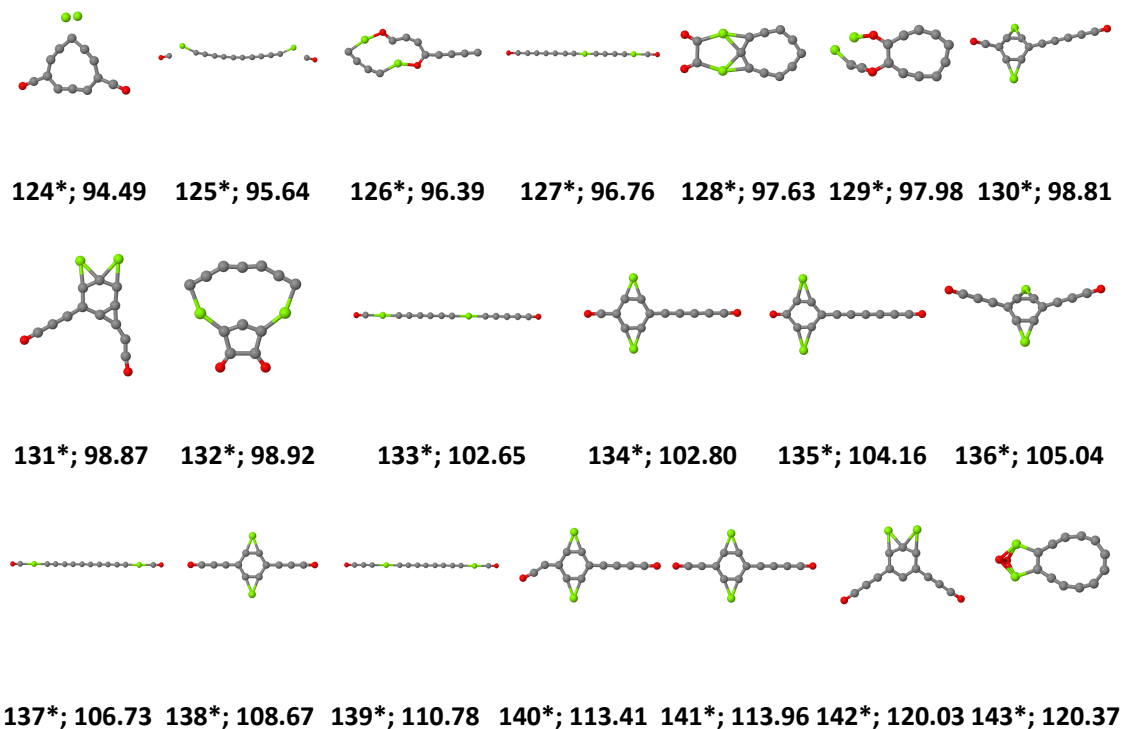


Figure S12: Isomers **124-143** of $C_{12}O_2Mg_2$ considered on the singlet PES. Relative energies including ZPVE corrections (in kcal mol^{-1}) are calculated at the PBE0-D3/def2-TZVP level. Isomers identified by chemical intuition are marked with an asterisk whereas unmarked ones are from AUTOMATON.

Table S8: Total energy (E), zero-point vibrational energy ($ZPVE$), $ZPVE$ -corrected total energy ($E+ZPVE$), thermal correction to Gibbs free energy (G), sum of electronic and thermal Free energies ($E + G$), net dipole moment (μ), relative energy without $ZPVE$ -correction (ΔE_e), $ZPVE$ -corrected relative energy (ΔE_0), and number of imaginary frequencies of $C_{12}O_2Mg_2$ isomers (**124-143**) in their respective singlet ground electronic states calculated at the PBE0-D3/def2-TZVP level of theory.

Isomer	E	$ZPVE$	$E+ZPVE$	G	$E + G$	μ	ΔE_e	ΔE_0	ΔG	NImag
	a.u					Debye	kcal mol ⁻¹			
124	-1006.808350	0.068211	-1006.740139	0.022830	-1006.785520	4.12	94.30	94.49	95.09	0
125	-1006.799876	0.061580	-1006.738296	0.006552	-1006.793324	2.30	99.62	95.64	90.19	0
126	-1006.801339	0.064233	-1006.737106	0.017200	-1006.784139	11.90	98.70	96.39	95.96	0
127	-1006.799195	0.062677	-1006.736518	0.012516	-1006.786679	14.08	100.04	96.76	94.36	1
128	-1006.799877	0.064744	-1006.735133	0.022030	-1006.777847	1.51	99.62	97.63	99.90	1
129	-1006.803856	0.069281	-1006.734575	0.026960	-1006.776896	6.34	97.12	97.98	100.50	0
130	-1006.802264	0.069011	-1006.733253	0.023816	-1006.778448	6.15	98.12	98.81	99.53	0
131	-1006.802528	0.069380	-1006.733148	0.023984	-1006.778544	8.83	97.95	98.87	99.47	0
132	-1006.796707	0.063626	-1006.733081	0.016699	-1006.780008	1.30	101.60	98.92	98.55	0
133	-1006.789876	0.062745	-1006.727131	0.012583	-1006.777293	10.61	105.89	102.65	100.25	1
134	-1006.795659	0.068770	-1006.726889	0.025577	-1006.770082	7.41	102.26	102.80	104.78	1
135	-1006.790896	0.066165	-1006.724730	0.019247	-1006.771649	6.61	105.25	104.16	103.79	0
136	-1006.792235	0.068917	-1006.723318	0.023972	-1006.768263	4.56	104.41	105.04	105.92	0
137	-1006.782855	0.062220	-1006.720635	0.014131	-1006.768724	0.00	110.30	106.73	105.63	2
138	-1006.786303	0.068758	-1006.717545	0.026085	-1006.760218	0.00	108.13	108.67	110.97	1
139	-1006.776749	0.062579	-1006.714170	0.012574	-1006.764175	6.01	114.13	110.78	108.48	1
140	-1006.779149	0.069165	-1006.709984	0.022592	-1006.756557	2.75	112.62	113.41	113.26	0
141	-1006.778172	0.069064	-1006.709108	0.024647	-1006.753525	2.11	113.24	113.96	115.17	1
142	-1006.766677	0.067248	-1006.699428	0.022287	-1006.744390	2.66	120.45	120.03	120.90	1
143	-1006.765560	0.066672	-1006.698888	0.023984	-1006.741576	7.74	121.15	120.37	122.66	0

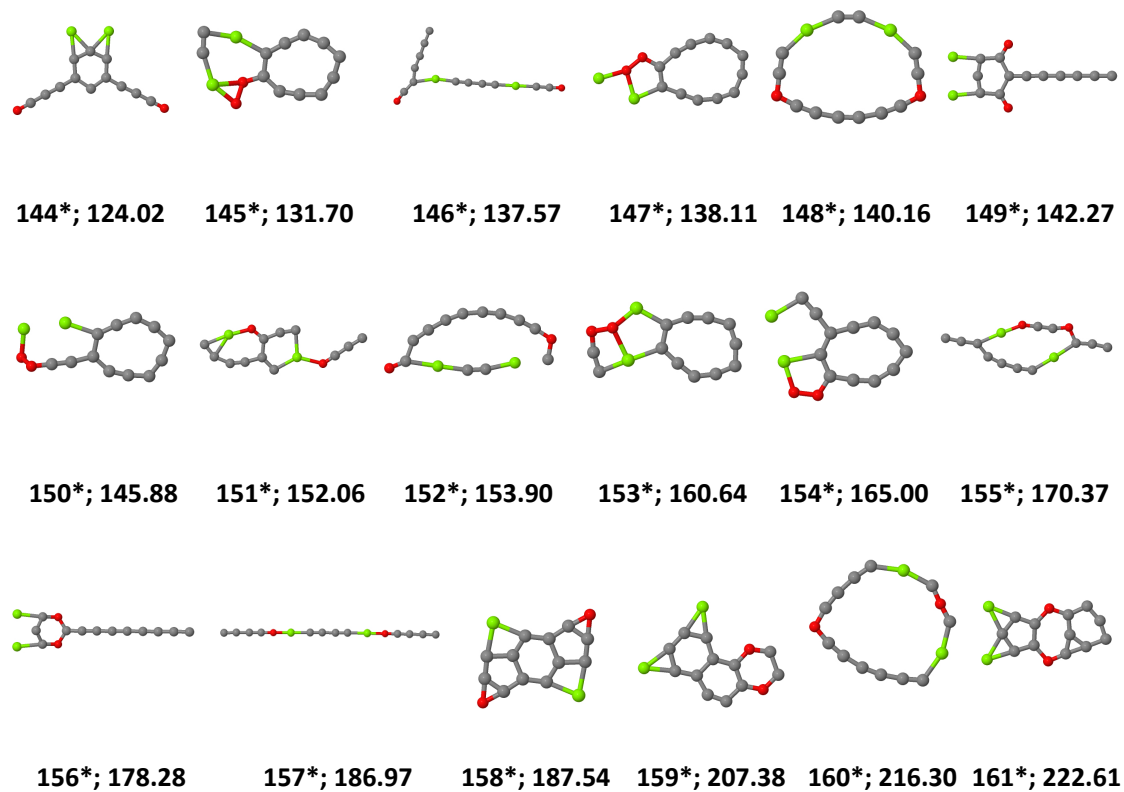


Figure S13: Isomers **144-161** of $C_{12}O_2Mg_2$ considered on the singlet PES. Relative energies including ZPVE corrections (in kcal mol^{-1}) are calculated at the PBE0-D3/def2-TZVP level. Isomers identified by chemical intuition are marked with an asterisk whereas unmarked ones are from AUTOMATON.

Table S9: Total energy (E), zero-point vibrational energy ($ZPVE$), $ZPVE$ -corrected total energy ($E+ZPVE$), thermal correction to Gibbs free energy (G), sum of electronic and thermal Free energies ($E + G$), net dipole moment (μ), relative energy without $ZPVE$ -correction (ΔE_e), $ZPVE$ -corrected relative energy (ΔE_0), and number of imaginary frequencies of $C_{12}O_2Mg_2$ isomers (**144-161**) in their respective singlet ground electronic states calculated at the PBE0-D3/def2-TZVP level of theory.

Isomer	E	$ZPVE$	$E+ZPVE$	G	$E + G$	μ	ΔE_e	ΔE_0	ΔG	NImag
	a.u					Debye	kcal mol ⁻¹			
144	-1006.759914	0.066842	-1006.693072	0.022598	-1006.737316	1.34	124.69	124.02	125.34	2
145	-1006.747521	0.066691	-1006.680830	0.023679	-1006.723842	4.85	132.47	131.70	133.79	0
146	-1006.734059	0.062572	-1006.671486	0.009391	-1006.724668	6.09	140.92	137.57	133.27	0
147	-1006.739512	0.068888	-1006.670624	0.026036	-1006.713476	9.73	137.49	138.11	140.30	0
148	-1006.733468	0.066105	-1006.667363	0.019202	-1006.714266	3.15	141.29	140.15	139.80	0
149	-1006.729833	0.065836	-1006.663996	0.022787	-1006.707046	18.23	143.57	142.27	144.33	2
150	-1006.725950	0.067707	-1006.658243	0.024804	-1006.701146	8.70	146.01	145.88	148.03	0
151	-1006.711524	0.063137	-1006.648388	0.016219	-1006.695305	1.76	155.06	152.06	151.70	1
152	-1006.707712	0.062252	-1006.645460	0.016346	-1006.691366	1.57	157.45	153.90	154.17	0
153	-1006.700389	0.065679	-1006.634711	0.022475	-1006.677914	6.73	162.04	160.64	162.61	0
154	-1006.695426	0.067663	-1006.627763	0.025377	-1006.670049	2.07	165.16	165.00	167.55	0
155	-1006.681623	0.062410	-1006.619212	0.015379	-1006.666244	2.41	173.82	170.37	169.94	0
156	-1006.673615	0.067007	-1006.606608	0.021023	-1006.652592	16.60	178.85	178.28	178.50	0
157	-1006.653705	0.060943	-1006.592763	0.010172	-1006.643533	0.28	191.34	186.97	184.19	0
158	-1006.663171	0.071320	-1006.591851	0.032624	-1006.630547	0.01	185.40	187.54	192.34	0
159	-1006.629674	0.069447	-1006.560226	0.030443	-1006.599231	14.30	206.42	207.38	211.99	1
160	-1006.612046	0.066021	-1006.546025	0.019005	-1006.593041	2.69	217.48	216.30	215.87	0
161	-1006.607174	0.071217	-1006.535957	0.034411	-1006.572763	19.95	220.54	222.61	228.60	3

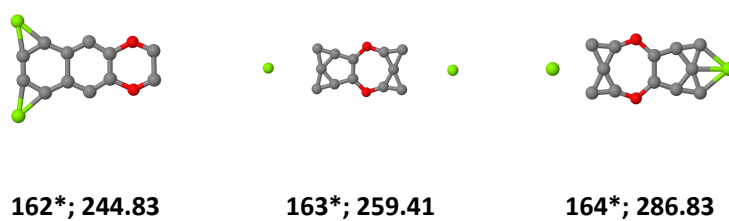


Figure S14: Isomers **162-164** of $C_{12}O_2Mg_2$ considered on the singlet PES. Relative energies including ZPVE corrections (in kcal mol^{-1}) are calculated at the PBE0-D3/def2-TZVP level. Isomers identified by chemical intuition are marked with an asterisk whereas unmarked ones are from AUTOMATON.

Table S10: Total energy (E), zero-point vibrational energy ($ZPVE$), $ZPVE$ -corrected total energy ($E+ZPVE$), thermal correction to Gibbs free energy (G), sum of electronic and thermal Free energies ($E + G$), net dipole moment (μ), relative energy without ZPVE-correction (ΔE_e), ZPVE-corrected relative energy (ΔE_0), and number of imaginary frequencies of $C_{12}O_2Mg_2$ isomers (**162-164**) in their respective singlet ground electronic states calculated at the PBE0-D3/def2-TZVP level of theory.

Isomer	E	$ZPVE$	$E+ZPVE$	G	$E + G$	μ	ΔE_e	ΔE_0	ΔG	NImag
	a.u					Debye	kcal mol ⁻¹			
162	-1006.565175	0.064619	-1006.500556	0.025458	-1006.539717	14.42	246.89	244.83	249.33	1
163	-1006.542967	0.065647	-1006.477320	0.021244	-1006.521723	0.18	260.83	259.41	260.62	2
164	-1006.497508	0.063881	-1006.433627	0.028279	-1006.469229	6.86	289.35	286.83	293.56	5

Optimized geometries of C12O2Mg2 (singlets) obtained at the PBE0-D3/def2-TZVP level

16

isomer 1 (t21) scf done: -1006.958624

C	-1.981691	-1.330069	-0.191075
O	6.528782	-0.241915	-0.124704
C	-4.118835	0.071464	0.075825
C	5.381922	-0.070529	-0.079291
C	-3.117189	-0.862228	-0.095463
C	1.953469	1.385161	0.216538
O	-6.556916	0.298427	0.142910
C	3.089424	0.918190	0.121266
C	-5.409912	0.127225	0.100585
C	0.668018	1.808600	0.307158
Mg	-2.363090	1.209029	0.247252
C	4.090947	-0.014937	-0.052807
C	-0.696141	-1.753569	-0.280980
C	-0.538227	2.033374	0.362574
C	0.510214	-1.977861	-0.336485
Mg	2.334725	-1.153100	-0.217730

16

isomer 2 (c79) scf done: -1006.955368

C	-3.083469	0.632674	-0.055606
Mg	-1.528399	2.078458	-0.033417
C	0.086169	3.266131	0.000962
C	1.305841	3.433577	0.020905
Mg	3.179211	2.720637	0.042534
C	5.063761	1.742747	0.064495
C	4.163874	0.707038	0.044273
C	3.072201	0.128830	0.024375
C	1.817369	-0.348256	0.003326
C	0.604137	-0.513659	-0.014466
C	-0.732698	-0.389861	-0.031880
C	-1.939358	-0.124663	-0.044861
C	-4.368520	0.497144	-0.069489
O	-5.528900	0.499084	-0.082150
C	6.338239	1.955397	0.085558
O	7.455844	2.267224	0.104887

16

isomer 3 (t3) scf done: -1006.950734

O	-5.613861	-2.288338	-0.025087
O	5.218324	-1.856399	0.100513
C	-4.547018	-1.829441	-0.019312
C	4.168069	-1.364687	0.081031
C	-3.419218	-1.199105	-0.015767
Mg	-2.575898	0.702754	-0.038499
C	2.259109	3.264726	-0.012193
C	-2.065621	-1.477176	0.006249
C	3.055472	-0.693634	0.058572
C	-1.453243	2.364986	-0.048614
Mg	2.881542	1.366072	0.025885
C	-0.842878	-1.321282	0.019062
C	1.717127	-1.058125	0.047330
C	-0.304319	2.789605	-0.040041
C	1.034136	3.069409	-0.025815

C	0.502880	-1.197593	0.034340
16			
isomer 4 (t7) scf done: -1006.943620			
O	7.259255	-0.604520	0.023239
O	-6.425611	-1.171750	0.010559
C	6.095150	-0.570971	0.021075
C	-5.285937	-0.956415	0.009916
C	-4.047325	-0.582808	0.007825
C	4.823469	-0.529798	0.018820
Mg	-2.783452	1.093918	-0.008447
C	2.269021	-0.430544	0.012757
C	-2.784447	-1.131244	0.015402
C	1.024188	-0.968824	0.017706
C	-1.167606	2.315880	-0.023028
C	3.544679	-0.539321	0.016551
C	-0.111106	2.976081	-0.032521
C	-0.205647	-1.111831	0.018112
C	-1.548516	-1.166070	0.017342
Mg	1.003417	1.306845	-0.011879

16			
isomer 5 (t2) scf done: -1006.939033			
C	3.680828	-0.769768	-0.001411
C	1.301792	2.541582	0.001434
C	1.202562	-1.496164	0.000053
O	-5.168471	-0.518894	0.004190
C	-4.524571	0.561685	0.004681
C	-1.363902	-1.778213	0.001557
Mg	-3.249866	-1.123749	0.002825
C	2.421412	-1.332658	-0.000698
Mg	2.527663	0.964041	-0.000323
C	-1.276066	2.458760	0.003664
C	0.071515	2.588248	0.002504
C	4.913717	-1.160308	-0.002996
C	-3.572433	1.344497	0.004523
O	6.050428	-1.391614	-0.004463
C	-2.432039	2.071021	0.003938
C	-0.140041	-1.686583	0.000802

16			
isomer 6 (c77) scf done: -1006.934599			
O	-3.787765	-1.616831	-0.134945
C	-3.926527	-0.371023	-0.108842
C	-3.668996	0.834752	-0.098301
C	-3.148623	2.078272	-0.097032
C	-2.383101	3.032632	-0.109907
C	-1.262929	3.767134	-0.139810
C	-0.098070	4.144709	-0.177182
C	1.243146	4.189074	-0.226795
C	2.473274	4.071591	-0.274809
C	3.694538	3.450296	-0.331119
C	4.956006	3.725134	-0.373496
O	6.109570	3.847636	-0.414457
Mg	2.293316	1.847227	-0.306451
C	1.050919	0.258185	-0.288441
C	0.059556	-0.469703	-0.259403
Mg	-1.876217	-0.958991	-0.195604

16
 isomer 7 (c26) scf done: -1006.929617

C	-0.786235	2.673546	0.001216
C	-1.185218	1.346430	0.002730
C	-1.202386	0.119937	0.003349
C	-0.705416	-1.134896	0.002950
C	0.230864	-1.932383	0.001447
C	1.587845	-2.126347	-0.001194
C	2.765638	-1.703976	-0.003775
Mg	1.586564	0.084533	-0.002331
O	1.471755	1.947145	-0.003068
C	0.637305	2.915207	-0.001874
O	1.097459	4.119098	-0.003409
Mg	0.166062	5.744185	-0.002308
C	-1.188145	7.363325	-0.000341
C	-1.892271	6.331052	0.001635
C	-2.029191	4.957619	0.002628
C	-1.608609	3.808019	0.002345

16
 isomer 8 (t63) scf done: -1006.928290

O	-5.918093	-1.196313	-0.335854
C	2.771959	3.178741	1.157035
C	-4.757213	-1.153369	-0.374336
C	2.147340	2.087768	0.708647
C	-3.479281	-0.990021	-0.365137
O	3.299873	4.120981	1.544933
C	-2.324023	-1.656405	-0.717624
C	2.841916	0.974022	0.181149
C	-1.114352	-1.888775	-0.880860
C	3.067274	-0.111827	-0.309713
Mg	0.804507	-2.413626	-1.210131
C	3.009454	-1.359873	-0.857734
Mg	-1.854355	0.291013	0.119742
C	0.728714	1.967326	0.729190
C	-0.439074	1.622998	0.638523
C	2.811941	-2.484792	-1.344064

16
 isomer 9 (c82) scf done: -1006.928271

C	-1.178070	-2.658227	-0.443156
O	5.680409	-0.426263	-0.143641
C	-3.677533	0.320316	0.112462
C	4.537546	-0.335009	-0.112285
Mg	-2.773469	-1.456481	-0.211149
C	1.619002	1.777922	0.297184
O	-6.133781	0.515746	0.179554
C	2.542473	1.003502	0.149087
C	-4.965507	0.422842	0.147651
C	0.440245	2.440561	0.429138
Mg	-2.487077	1.929926	0.378765
C	3.205666	-0.228892	-0.075808
C	0.029084	-2.424404	-0.418281
C	-0.711340	2.862905	0.518594
C	1.303310	-1.957384	-0.353455
C	2.344540	-1.339799	-0.259086

16

isomer 10 (t4) scf done: -1006.928890

O	3.034757	1.406220	-0.019342
O	-4.483109	-1.507478	0.006181
C	0.675994	1.497839	-0.013304
C	-3.252263	-1.793669	0.003889
C	1.884735	0.762608	-0.014651
C	-0.674707	-1.554089	-0.002708
C	-0.465538	1.912141	-0.011368
C	-2.025883	-1.692038	0.000733
Mg	4.527883	0.274625	-0.023474
C	0.497761	-1.236286	-0.006272
C	1.767582	-0.634177	-0.011022
C	4.194776	-1.698664	-0.016065
C	-1.812088	2.107384	-0.007993
C	3.002903	-1.343676	-0.013204
C	-3.048286	2.196815	-0.004923
Mg	-3.660288	0.294290	0.000485

16

isomer 11 (c73) scf done: -1006.926160

C	-1.136466	2.040868	0.001149
C	-2.262586	1.567288	0.001678
C	-3.374720	0.800833	0.003172
C	-4.354937	0.052387	-0.002441
Mg	-3.188175	-1.721525	-0.000721
C	-1.382140	-2.568473	-0.000592
C	-0.164691	-2.425255	-0.000691
C	1.166401	-2.133355	-0.000417
C	2.332057	-1.753986	0.000191
Mg	3.618851	-0.229809	-0.000979
C	3.931309	1.870872	0.003620
O	5.002301	1.209116	0.007029
C	2.727655	2.139266	-0.003648
C	1.396814	2.369676	-0.001248
C	0.175861	2.328570	-0.000495
O	-5.049287	-0.997631	-0.005605

16

isomer 12 (c60) scf done: -1006.925604

C	2.136272	1.423520	-0.022044
Mg	3.580316	0.047576	-0.026636
C	5.658897	-0.559638	-0.040608
O	4.778809	-1.472296	-0.028246
C	2.560529	2.583042	-0.033643
C	3.138999	3.808015	-0.046894
C	3.855763	4.791503	-0.059714
C	4.850968	5.713600	-0.074268
C	5.815272	6.491792	-0.087536
Mg	7.407420	5.271943	-0.090924
C	9.974938	3.824853	-0.098475
O	11.104977	4.093263	-0.107671
C	8.685153	3.659554	-0.088895
C	7.893161	2.509797	-0.075864
C	7.110265	1.576862	-0.064346
C	6.262116	0.511861	-0.051461

16

isomer 13 (c28) scf done: -1006.927838

C	-0.653385	2.555082	-0.001126
C	-1.093245	1.227254	-0.007916
C	-1.245579	0.019948	-0.012995
C	-1.001630	-1.322518	-0.016869
C	-0.604485	-2.506146	-0.019375
Mg	1.258005	-1.788973	-0.008637
O	2.658380	-0.521360	0.002192
C	2.159408	0.638515	0.004318
C	1.640548	1.739583	0.006029
C	0.742053	2.822974	0.005967
O	1.202610	4.041736	0.012468
Mg	0.254163	5.649144	0.014170
C	-1.135382	7.248498	0.013890
C	-1.816375	6.201022	0.007055
C	-1.928457	4.825351	0.001536
C	-1.490612	3.682383	-0.000707

16

isomer 14 (t6) scf done: -1006.924885

C	3.615184	0.330725	-0.007767
Mg	-4.507837	0.254381	0.008202
C	4.883833	0.145709	-0.013955
O	-3.798922	1.995115	0.022683
C	2.337472	0.391652	-0.001882
C	-4.729132	-1.719720	-0.002783
Mg	0.752403	-1.013105	-0.001509
C	-2.536597	1.905638	0.019325
C	6.147061	0.011336	-0.019449
C	-3.509787	-1.962510	-0.005477
O	7.307090	-0.117030	-0.024549
C	-1.325358	1.760212	0.015638
C	1.188191	1.142270	0.005213
C	-2.155800	-2.160953	-0.007634
C	-0.931834	-2.125256	-0.008460
C	-0.016162	1.427260	0.010525

16

isomer 15 (t5) scf done: -1006.925134

Mg	-2.311915	1.750340	-0.011428
C	2.804176	1.443194	0.000824
Mg	1.408949	-2.344058	0.019427
C	-3.939904	-0.688798	0.018385
C	3.541756	-2.225338	0.018846
C	-2.703750	-0.282096	0.009770
C	3.319977	0.335031	0.006064
C	-0.449484	3.442833	-0.011143
O	3.140380	-3.409161	0.024688
C	3.552457	-0.992088	0.012991
O	-5.074009	-0.937203	0.025102
C	-0.423626	-1.583409	0.015744
C	1.886690	2.422622	-0.004424
C	-1.515332	-1.024982	0.013337
C	-1.673963	3.659493	-0.012522
C	0.858166	3.080916	-0.008310

16

isomer 16 (c46) scf done: -1006.921186

C	2.307128	1.614980	-0.019187
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C	2.751396	2.896164	-0.028954
C	3.282196	4.007420	-0.039212
O	3.479208	5.255410	-0.046541
Mg	1.523070	5.240126	-0.026557
C	-0.458381	5.444765	-0.007547
C	-1.236518	4.489706	0.003026
C	-1.975415	3.355842	0.014163
C	-2.433197	2.227355	0.022683
C	-2.693197	0.899188	0.030411
C	-2.799722	-0.328103	0.036320
Mg	-1.238256	-1.565091	0.028619
O	0.152414	-2.941519	0.021481
C	0.881439	-1.909628	0.009764
C	1.275031	-0.742639	0.000994
C	1.849135	0.485881	-0.009881

16

isomer 17 (t12)	scf done: -1006.921702		
C	4.136557	-1.324779	-0.026904
C	-2.126339	-2.384680	0.018775
C	2.903454	-0.944920	-0.022387
O	1.087537	4.484316	-0.034380
C	2.194196	0.246842	-0.016314
C	-2.253531	1.560628	0.036462
O	5.209959	-1.770112	-0.031850
C	1.294803	1.076869	-0.010204
C	-4.609994	-1.592775	0.053432
C	-0.902555	-2.431499	0.003264
C	-3.455714	-2.056475	0.036803
Mg	0.953204	-1.657824	-0.011338
C	0.327577	2.118254	-0.003765
C	0.739491	3.389281	-0.020596
C	-1.070149	1.861083	0.018210
Mg	-3.785748	0.260613	0.050905

16

isomer 18 (c30)	scf done: -1006.923853		
C	-0.735247	2.660870	0.003503
C	-1.274302	1.351401	0.007888
C	-1.694694	0.197986	0.011392
Mg	-0.626041	-1.465388	0.006647
O	0.709075	-2.987223	0.000054
C	1.443653	-1.968695	-0.005211
C	1.816230	-0.796494	-0.008457
C	1.803414	0.557897	-0.009627
C	1.471031	1.728252	-0.008746
C	0.655438	2.882858	-0.004987
O	1.193741	4.072506	-0.009222
Mg	0.324888	5.722953	-0.005508
C	-0.999580	7.377458	0.000836
C	-1.723476	6.359254	0.006034
C	-1.899439	4.990923	0.008303
C	-1.518669	3.827934	0.007100

16

isomer 19 (c43)	scf done: -1006.919851		
C	2.017588	0.892245	0.053694
C	1.067373	-0.053246	0.024698

C	0.084626	-0.777913	-0.004743
C	-1.155114	-1.324651	-0.040702
C	-2.311293	-1.780793	-0.073918
Mg	-3.386954	-0.111501	-0.099436
O	-4.122417	1.603383	-0.115240
C	-3.245839	2.520537	-0.088794
C	-2.374646	3.369301	-0.062588
C	-1.317070	4.221673	-0.031121
C	-0.331120	4.953662	-0.001813
Mg	1.615138	5.266248	0.053368
O	3.583700	5.582621	0.110336
C	3.570277	4.329548	0.106654
C	3.215398	3.150948	0.093401
C	2.689272	1.912989	0.075270

16

isomer 20 (c37) scf done: -1006.921028

Mg	1.803352	-1.110671	-0.001881
O	1.086786	-3.001737	-0.004044
C	0.055833	-2.270973	-0.003984
C	-0.640936	-1.257443	-0.003425
C	-1.041245	0.043708	-0.002515
C	-1.045715	1.258781	-0.001406
C	-0.628399	2.603618	0.000059
C	-1.472424	3.729766	0.000561
C	-1.902648	4.874366	0.001317
C	-1.792747	6.249485	0.002603
C	-1.121424	7.302830	0.003924
Mg	0.288269	5.721630	0.003375
O	1.227478	4.110700	0.002497
C	0.745935	2.895734	0.001180
C	1.658548	1.799036	0.000635
C	2.378259	0.806219	0.000170

16

isomer 21 (t1) scf done: -1006.919053

C	3.852200	1.085037	-0.000397
C	-4.294319	1.291500	-0.001830
C	2.994319	2.118903	0.000668
C	-3.051661	1.222271	-0.001073
C	1.806380	2.436876	0.000609
Mg	-4.137489	-0.689019	-0.002075
C	4.193388	-0.092793	-0.000140
C	-1.681602	0.836387	-0.000464
C	3.299524	-2.537886	-0.000062
O	-0.226594	-1.027522	-0.000363
C	3.827290	-1.406411	-0.001368
Mg	1.445521	-1.737204	-0.000638
C	0.475675	2.288691	0.000628
C	-1.428019	-0.568669	-0.000712
C	-0.602742	1.708092	0.000184
O	-2.402230	-1.429777	-0.001485

16

isomer 22 (c39) scf done: -1006.917899

C	2.198470	-0.839268	-0.002331
C	2.104047	-2.081903	-0.002087
Mg	0.100135	-1.876472	-0.002044

O	-1.681435	-1.272474	-0.002438
C	-1.444507	-0.014770	-0.001741
C	-1.114911	1.154396	-0.001187
C	-0.604141	2.473254	-0.000480
C	-1.427093	3.617531	0.000725
C	-1.851421	4.764553	0.001633
C	-1.728441	6.138141	0.004227
C	-1.051720	7.188176	0.005765
Mg	0.349687	5.594490	0.003465
O	1.269970	3.980058	0.000210
C	0.766375	2.766123	-0.000416
C	1.624927	1.643229	-0.001422
C	2.088977	0.519986	-0.002811

16

isomer 23 (c8) scf done: -1006.918010

C	-0.599476	2.474140	0.000888
C	-1.112366	1.200050	0.002746
C	-1.373922	-0.008717	0.004017
C	-0.861832	-1.228661	0.003364
C	0.054917	-2.083589	0.001950
C	1.320288	-1.650517	-0.001234
C	2.230205	-0.799257	-0.003361
C	2.105886	0.542105	-0.003779
C	1.731010	1.713281	-0.003162
C	0.819587	2.766299	-0.001887
O	1.204238	4.003112	-0.003450
Mg	0.113977	5.538892	-0.002117
O	-0.664275	7.206837	-0.001530
Mg	-2.370350	6.645152	0.002228
C	-2.177098	4.602534	0.003064
C	-1.474771	3.590831	0.002262

16

isomer 24 (t38) scf done: -1006.917084

O	3.635422	0.541453	0.448251
C	-3.598892	1.963285	0.222471
C	2.106033	-1.231150	0.080104
C	-2.261909	2.161188	0.363905
C	-0.415225	-1.855873	-0.249756
C	-4.790602	1.632355	0.072213
C	0.776014	-1.644791	-0.116711
C	-1.050755	2.012166	0.424439
C	-1.766427	-1.904728	-0.369148
C	0.229704	1.605257	0.449984
C	-2.992840	-1.840809	-0.455892
Mg	-4.259903	-0.296929	-0.261594
C	2.374339	0.119940	0.354256
C	1.294575	1.011293	0.417486
Mg	4.577856	-0.920070	-0.238529
O	3.116366	-2.079785	-0.084244

16

isomer 25 (t85) scf done: -1006.911137

O	2.486985	3.781371	0.139965
Mg	1.958400	-2.931431	-0.195487
C	2.913024	2.597301	0.071197
C	2.987707	-1.215722	-0.127251

Mg	0.800392	2.729730	0.115312
C	0.342132	-4.122796	-0.226142
C	-1.051746	1.985943	0.109879
O	-5.232883	0.294246	0.096037
C	2.933998	1.366701	0.007276
C	-4.095270	0.148139	0.068613
C	-1.909709	1.119422	0.080220
C	-0.569573	-3.286407	-0.168086
C	3.027204	0.008754	-0.064687
C	-2.199438	-1.304997	-0.038465
C	-2.768904	-0.013023	0.037353
C	-1.506625	-2.297405	-0.101386

16

isomer 26 (c12) scf done: -1006.915333

C	-0.678044	2.418972	-0.001905
C	-1.333390	1.203306	-0.010887
C	-1.309308	-0.037374	-0.014399
C	-1.040902	-1.344536	-0.016502
C	0.119100	-1.843077	-0.009747
C	1.435139	-1.960327	0.000213
C	2.039247	-0.831922	0.008604
C	2.299295	0.441017	0.014467
C	1.582946	1.488291	0.012551
C	0.750364	2.509105	0.009208
Mg	0.836338	4.609522	0.012974
O	0.817142	6.439747	0.011800
Mg	-0.861699	7.037450	0.001900
O	-2.412095	5.937960	-0.008496
C	-1.922139	4.768842	-0.006155
C	-1.375976	3.675516	-0.003628

16

isomer 27 (t10) scf done: -1006.912947

Mg	-3.913345	-1.381784	0.021711
C	2.227328	2.112101	0.012295
C	-2.272049	-2.505335	0.013405
C	3.461380	2.006348	0.008736
C	-1.044051	-2.456100	0.007043
O	4.588823	1.456644	0.003159
C	-3.988428	1.090376	0.031255
C	0.894949	2.339980	0.017689
C	-2.817343	1.775999	0.029520
Mg	3.312388	-0.082862	-0.002923
C	-1.653866	2.144324	0.026152
C	-0.325412	2.339952	0.022094
C	0.312668	-2.342235	0.000964
O	2.746752	-1.832398	-0.009746
C	-4.984327	0.346685	0.033107
C	1.503757	-2.107811	-0.004255

16

isomer 28 (t24) scf done: -1006.910815

C	-2.970133	1.814193	-0.015658
C	4.635918	-1.641954	0.039148
C	-3.881770	0.988899	-0.032255
C	4.262763	-0.453603	0.044454
O	-4.605810	-0.031411	-0.048412

C	3.748337	0.801665	0.049465
C	-1.813480	2.494805	0.002657
C	-1.253098	-2.090963	-0.029667
C	-0.650092	2.877953	0.018519
Mg	2.810222	-2.459720	0.012492
Mg	-2.873131	-0.998023	-0.037216
C	2.949256	1.727911	0.048968
C	0.686867	2.847397	0.033008
C	-0.108318	-2.535878	-0.019803
C	1.867213	2.516805	0.043009
O	1.064988	-3.007303	-0.010144

16

isomer 29 (t11) scf done: -1006.910852

C	0.709226	2.538450	-0.020776
C	2.523622	-1.877137	-0.018305
C	-1.608844	1.431469	-0.018001
C	1.821897	3.065205	-0.022002
C	3.001361	-0.749842	-0.019790
C	-3.965756	1.041881	-0.016573
Mg	2.914658	1.245343	-0.021455
C	1.157334	-4.094297	-0.014996
C	-2.511681	-0.851245	-0.014555
C	-0.545574	2.013572	-0.019323
C	-2.721960	0.555914	-0.016300
O	3.072842	3.221484	-0.023181
C	1.835705	-3.058445	-0.016600
Mg	-0.722062	-3.389511	-0.014444
O	-5.038010	1.454738	-0.016751
C	-2.191872	-2.029939	-0.012930

16

isomer 30 (t8) scf done: -1006.911179

C	-4.285270	1.066298	0.001034
C	2.966631	0.737494	-0.014101
C	3.056752	-0.655846	-0.011928
C	-0.653014	-1.989162	-0.001968
C	1.842555	-1.387335	-0.008045
Mg	4.982472	0.482537	-0.018454
C	-3.163494	1.579502	-0.002100
Mg	-3.483446	-0.888311	0.002332
C	-0.662407	2.097871	-0.008678
O	4.227962	-1.273709	-0.013343
O	-5.181527	0.176131	0.004612
C	0.664895	1.908866	-0.011174
C	0.684578	-1.756802	-0.004947
C	1.796553	1.432729	-0.012764
C	-1.878387	-2.077747	0.000800
C	-1.884009	2.016488	-0.005758

16

isomer 31 (c7) scf done: -1006.904427

C	-2.051376	-0.833565	-0.063883
Mg	-3.425111	0.636807	-0.098801
O	-4.998244	1.793818	-0.140072
C	-4.050064	2.645131	-0.112192
C	-2.914181	3.125857	-0.079841
C	-1.761555	3.861513	-0.045930

C	-0.707829	4.461603	-0.014101
C	-0.821971	-0.808263	-0.029361
C	0.499303	-0.536447	0.008289
C	1.607887	-0.025643	0.040557
C	2.624407	0.848981	0.071014
C	3.359633	1.823762	0.094038
C	3.816576	3.102209	0.110149
C	4.113340	4.311811	0.122852
Mg	2.196110	4.903598	0.070221
O	0.386036	5.099427	0.019682

16

isomer 32 (c41) scf done: -1006.906485

C	1.912460	-0.819839	-0.000867
C	1.599294	-2.158280	-0.002642
C	0.782122	-3.106885	-0.004520
Mg	-0.412328	-1.395282	-0.004049
O	-1.345838	0.279506	-0.003238
C	-0.658855	1.343472	-0.001421
C	-0.874007	2.740190	-0.000268
C	-1.702798	3.833557	-0.000137
C	-1.962611	5.039207	0.000730
C	-1.649709	6.377731	0.002397
C	-0.832520	7.326326	0.004210
Mg	0.361633	5.614323	0.003859
O	1.296012	3.939942	0.003217
C	0.609027	2.875974	0.001445
C	0.824145	1.479254	0.000306
C	1.652891	0.385849	0.000046

16

isomer 33 (t15) scf done: -1006.901879

C	-5.335525	1.099415	0.173681
O	7.874564	-0.596402	-0.202947
C	-4.105040	1.287385	0.229210
C	6.727587	-0.409537	-0.160867
Mg	-5.004794	-0.819852	-0.302298
C	5.466835	-0.204313	-0.114424
C	-1.492863	-1.180903	-0.374895
C	4.212183	0.000330	-0.067473
C	-2.651142	-1.873775	-0.555543
C	2.947949	0.205625	-0.020066
C	-0.508953	-0.472666	-0.198852
C	1.703603	0.407865	0.026617
C	-3.771468	-2.383106	-0.684370
C	0.380574	0.602466	0.071270
O	-0.223552	1.756842	0.356797
Mg	-2.073246	1.409643	0.266035

16

isomer 34 (c83) scf done: -1006.901132

C	-0.810439	-0.000000	0.967125
C	0.522798	-0.000000	0.969221
C	-1.534728	-0.000000	2.191769
C	-1.530916	-0.000000	-0.259777
C	-2.281776	-0.000000	3.159398
C	-2.274773	-0.000000	-1.229886
Mg	-4.227288	0.000000	3.623981

Mg	-4.219792	-0.000000	-1.696213
C	-6.172459	0.000000	3.158303
C	-6.165454	0.000000	-1.232296
C	-6.915612	0.000000	2.187637
C	-6.911811	0.000000	-0.264115
C	-7.635917	0.000000	0.960637
C	-8.969166	0.000000	0.958547
O	1.672059	-0.000000	0.970946
O	-10.118423	0.000000	0.956728

16

isomer 35 (t65) scf done: -1006.899786

Mg	0.059889	0.752566	0.981949
C	1.659670	-0.131860	0.015721
O	-9.081130	-0.309174	0.116779
C	2.933796	-0.110614	0.004894
C	-7.912832	-0.289651	0.105532
C	5.491014	-0.068024	-0.016689
C	-6.644030	-0.268535	0.093407
C	4.230787	-0.088883	-0.006171
C	-5.358225	-0.247796	0.081481
C	6.776815	-0.046677	-0.027551
C	-4.098001	-0.227443	0.069718
O	9.213962	-0.006885	-0.047482
C	-2.801010	-0.206269	0.057422
C	8.045639	-0.025853	-0.038035
C	-1.526887	-0.185517	0.045336
Mg	0.072889	-1.069897	-0.920718

16

isomer 36 (c38) scf done: -1006.896847

C	2.746290	-0.525510	-0.008958
Mg	1.275853	-1.832304	-0.002801
O	-0.589334	-2.475091	0.004604
C	-0.883151	-1.255511	0.005138
C	-1.009290	-0.031354	0.004813
C	-0.454967	1.235018	0.002106
C	-0.749789	2.578357	0.002389
C	-1.650999	3.610272	0.005080
C	-1.962684	4.803564	0.005528
C	-1.717131	6.152403	0.003832
C	-0.978424	7.164373	0.000546
Mg	0.361046	5.566522	-0.003430
O	1.372125	3.959679	-0.006173
C	0.772524	2.835888	-0.003318
C	1.048165	1.482741	-0.003588
C	2.018683	0.485999	-0.006702

16

37 (t29) scf done: -1006.895684

C	3.743150	0.284719	0.015028
O	-5.143115	1.800756	0.032489
C	5.024299	0.131829	0.009039
C	-4.224361	1.078412	0.021519
O	6.159282	-0.127291	0.002396

C	-3.268086	0.208299	0.007924
Mg	1.909579	-0.771478	0.002547
Mg	-3.159268	-1.838069	-0.024273
C	0.051790	-1.696286	-0.016721
C	-1.794865	0.301719	0.011526
C	2.772109	1.270633	0.029987
C	-0.884306	1.381808	0.030003
C	0.266108	1.805610	0.037395
C	-1.162381	-2.319737	-0.028308
C	-1.099325	-0.870464	-0.005546
C	1.615955	1.705761	0.038191

16

38 (c42) scf done:	-1006.894807		
C	1.927990	-0.688085	-0.002529
C	1.289833	-1.735648	-0.003539
C	0.075583	-2.361766	-0.004291
C	-1.166512	-2.508439	-0.004587
Mg	-1.064830	-0.427495	-0.002633
O	-1.067037	1.385567	-0.000999
C	-0.559935	2.601043	0.000292
C	-1.406073	3.735774	0.001292
C	-1.831695	4.882994	0.002435
C	-1.722485	6.254964	0.003775
C	-1.064735	7.317317	0.004894
Mg	0.378885	5.760706	0.003500
O	1.289754	4.157681	0.002049
C	0.803965	2.921882	0.000799
C	1.657534	1.806587	-0.000200
C	2.058677	0.651965	-0.001192

16

39 (c49) scf done:	-1006.894788		
C	-0.601367	2.642389	-0.006248
O	-1.099977	1.423111	-0.017527
Mg	-1.135740	-0.387543	-0.026547
C	-1.172926	-2.463593	-0.039053
C	0.066163	-2.299098	-0.014343
C	1.281176	-1.675914	0.011579
C	1.915250	-0.626555	0.027800
C	2.035594	0.714205	0.035208
C	1.623250	1.864586	0.031476
C	0.759739	2.972155	0.018841
O	1.235589	4.211720	0.030155
Mg	0.314240	5.808529	0.017447
C	-1.140806	7.355027	-0.005633
C	-1.789780	6.287490	-0.019631
C	-1.889595	4.914875	-0.024445
C	-1.454790	3.771108	-0.019080

16

40 (c32) scf done:	-1006.894739		
C	-0.771099	2.823477	-0.008709
Mg	-0.728479	0.779144	-0.012228
O	-1.601197	-1.027748	-0.029002
C	-0.740785	-1.896224	-0.018065
C	0.290133	-2.620110	-0.004347
C	1.310223	-1.703723	0.012352

C	1.986461	-0.668039	0.024254
C	1.777171	0.675394	0.023627
C	1.401029	1.845631	0.020223
C	0.609890	3.045232	0.011554
O	1.219750	4.207066	0.022468
Mg	0.319008	5.850460	0.012770
C	-0.981490	7.534403	-0.002481
C	-1.709359	6.517510	-0.014856
C	-1.924285	5.154141	-0.020601
C	-1.510950	3.995879	-0.016961

16

41 (c15) scf done: -1006.894277

C	-0.505319	2.322886	0.000822
C	-1.256406	1.173819	0.003031
C	-1.225501	-0.073982	0.003695
C	-0.998200	-1.381138	0.003863
C	0.147967	-1.917354	0.001710
C	1.455050	-2.085726	-0.000973
C	2.108377	-0.985931	-0.002852
C	2.411133	0.277964	-0.004075
C	1.724959	1.343332	-0.003166
C	0.909913	2.378748	-0.002088
Mg	0.804621	4.482214	-0.003208
C	0.004091	6.342001	-0.002811
C	-1.109288	6.903583	-0.000580
O	-2.374710	7.068770	0.002576
Mg	-2.059014	5.103980	0.002669
O	-1.091655	3.559328	0.001386

16

42 (c10) scf done: -1006.894583

C	-0.342864	2.649645	0.000298
C	-0.989086	1.440033	0.002074
C	-1.393248	0.268976	0.003286
C	-1.017454	-0.997249	0.003073
C	-0.212241	-1.961878	0.002016
C	1.091000	-1.670714	-0.000471
C	2.103817	-0.940038	-0.002637
C	2.121994	0.406611	-0.003224
C	1.877014	1.612983	-0.003293
C	1.094512	2.760872	-0.002363
O	1.631376	3.955011	-0.003923
Mg	0.515472	5.458302	-0.002571
Mg	-1.614128	7.286133	0.000519
O	-2.795003	5.675674	0.003480
C	-2.011617	4.709051	0.002515
C	-1.113527	3.859079	0.001220

16

43 (t17) scf done: -1006.891292

C	-1.279900	1.570956	-0.286954
C	3.886562	-1.559041	0.483569
C	-2.362218	0.756113	0.118841
C	1.354069	-1.930626	0.459914
O	-4.235437	-1.758842	-1.308726
C	-0.251577	2.140605	-0.630859
C	-1.126036	-1.416205	0.127488

C	-3.330581	-1.286150	-0.779237
C	5.025112	-1.063566	0.393734
C	-2.314041	-0.719690	-0.133413
O	-4.213963	1.641499	1.509730
C	2.572860	-1.899774	0.530685
Mg	1.782501	2.060439	-0.661921
C	-3.342635	1.234161	0.875643
C	0.024093	-1.752432	0.339224
Mg	4.246849	0.744918	-0.239150

16

44 (c2) scf done: -1006.887884

C	4.026982	1.220214	-0.013052
C	-4.033588	1.291545	-0.076492
C	3.410349	2.434726	-0.067004
C	-2.816487	1.033940	-0.056852
C	2.660528	3.429376	-0.112946
Mg	-4.202917	-0.712087	0.003871
C	3.953550	-0.001431	0.036042
C	-1.516910	0.437191	-0.022745
C	2.241851	-1.765202	0.095026
C	-0.271565	-1.587156	0.069254
C	3.326103	-1.189835	0.079637
C	0.908010	-1.906229	0.090877
Mg	0.982871	2.289025	-0.079236
C	-1.524281	-0.957328	0.034084
O	-0.434364	1.185146	-0.045067
O	-2.640491	-1.703418	0.056085

16

45 (t87) scf done: -1006.879066

Mg	3.134316	0.340129	0.151932
O	-6.217637	-2.197028	-0.216042
C	2.813282	2.344159	0.059528
O	6.593538	-0.151424	0.346188
C	-0.973526	2.313289	-0.138509
C	-1.608012	-2.018553	-0.007599
C	-3.383830	1.360492	-0.229289
C	-5.212200	-1.712602	-0.194624
C	1.583747	2.477902	-0.009992
C	-0.381063	-1.964728	0.054951
C	0.964643	-1.750399	0.117514
C	0.228623	2.504236	-0.082081
C	2.148109	-1.420077	0.166897
C	5.487938	-0.010031	0.285450
C	-2.254919	1.868699	-0.189013
Mg	-3.081525	-0.646291	-0.136841

16

46 t39 scf done: -1006.884964

C	1.719052	-2.037204	0.290242
O	-5.445033	-0.359998	-0.554892
C	4.148675	-0.889425	-0.015824
C	-4.298770	-0.270549	-0.403787
C	3.072949	-1.477896	0.144409
C	-3.043986	-0.041930	-0.168521
Mg	3.356873	0.867423	-0.614824
Mg	-1.895209	1.574723	0.479611

O	1.463902	-3.174808	0.595065
C	-0.499084	3.007427	0.800173
C	0.730417	-1.005832	-0.106057
C	-1.846498	-0.729339	-0.308372
C	0.463668	2.380674	0.331358
C	1.137502	0.264218	-0.243050
C	-0.671960	-1.077693	-0.278470
C	1.358208	1.535507	-0.374954

16

47 c34	scf done:	-1006.883999	
C	2.374085	-1.400311	-0.002874
C	1.650923	-2.436650	-0.003702
C	0.400439	-1.847649	-0.002623
C	-0.558532	-1.067564	-0.001989
C	-1.119577	0.170270	-0.000727
C	-1.303956	1.384707	0.000360
C	-0.907560	2.742116	0.001092
C	-1.715295	3.893752	0.001805
C	-2.034392	5.075431	0.002465
C	-1.824238	6.439490	0.002753
C	-1.080157	7.442609	0.002755
Mg	0.210256	5.762300	0.001272
O	1.058149	4.087406	0.000797
C	0.500030	2.913076	0.000583
Mg	1.114825	0.865366	-0.000850
O	2.833918	-0.269299	-0.002050

16

48 t37	scf done:	-1006.879760	
C	1.614238	-2.170769	-0.889001
C	-2.756417	1.272475	-0.123952
C	0.617480	-2.556019	-1.489233
C	-0.411240	1.561685	0.879066
C	2.630986	-1.611637	-0.166884
C	-1.670972	1.471247	0.383120
C	3.501221	-1.046876	0.508632
C	0.755470	1.521607	1.256278
Mg	-1.309407	-2.318555	-1.996371
O	-4.996520	1.316562	-0.869983
C	-3.124847	-1.458030	-2.056724
C	-3.910423	0.786406	-0.844635
O	4.940129	2.260172	3.179106
C	4.148187	1.755894	2.576083
Mg	2.560108	0.576036	1.255322
C	-3.556424	-0.439449	-1.532567

16

49 c4	scf done:	-1006.883878	
C	1.343879	-1.708779	-0.001579
C	0.211573	-1.224882	-0.001877
C	-1.081524	-0.714894	-0.002281
Mg	-2.832658	-1.853412	-0.003355
O	-4.494469	-1.109262	-0.002569
Mg	-4.067394	0.637502	-0.001387
O	-2.349107	1.334051	-0.002035
C	-1.216913	0.664553	-0.001797
C	-0.020759	1.469800	-0.001098

C	1.064355	2.015835	-0.000434
C	2.392106	2.327572	0.000021
C	3.553255	1.946088	0.000580
C	4.600296	1.067922	0.000698
C	4.511201	-0.163772	0.000195
C	3.874935	-1.352495	-0.000340
C	2.684417	-1.684173	-0.001191

16

50 t18 scf done: -1006.882119

C	1.517320	-1.143875	0.032873
O	-3.225462	-2.330105	0.019114
C	2.914599	-0.875565	0.036398
C	-1.075992	-1.123273	0.027842
Mg	-4.625855	-0.783575	0.023039
C	-2.115501	-1.831872	0.023208
Mg	-2.277717	0.937496	0.032697
C	2.089976	2.719235	0.046298
O	4.588460	-2.712060	0.033215
C	2.910789	1.651671	0.044798
C	0.950169	3.161918	0.046871
C	3.814531	-1.863392	0.034677
C	0.304822	-1.142623	0.030584
C	-1.594566	2.863070	0.040839
C	3.288712	0.492512	0.041654
C	-0.400931	3.176911	0.043591

16

51 t73 scf done: -1006.875557

Mg	-2.885221	2.268545	-0.674070
C	5.976456	-1.017574	-0.261632
C	-4.663220	2.317614	0.293791
C	4.732393	-0.753946	-0.220715
C	-4.193903	1.422304	1.020901
O	7.119683	-1.259164	-0.300638
C	0.038054	0.847932	-0.596647
C	3.473254	-0.493561	-0.174066
C	-3.461901	0.451224	1.659126
C	-1.457556	-2.028674	-0.805233
C	0.945155	-0.040609	-0.029264
C	2.239494	-0.209815	-0.156161
C	-1.056856	1.393832	-0.817212
Mg	-0.935040	-0.546806	0.908357
C	-2.615828	-0.357679	2.046268
O	-1.621848	-2.694413	-1.688717

16

52 t90 scf done: -1006.880455

C	3.178652	-1.500334	0.025834
O	-3.703022	-2.629952	0.000808
Mg	0.989407	3.534763	-0.025841
C	-2.660703	-2.144569	-0.002983
C	3.732740	-0.262634	0.011323
O	-2.431102	0.605931	-0.031596
C	3.164765	0.833085	-0.006541
Mg	-1.576718	2.371145	-0.033382
C	0.990727	1.055068	-0.035277
C	2.310066	-2.370910	0.030061

C	2.128981	1.756917	-0.027359
C	0.958029	-2.499927	0.021285
C	-0.254464	-2.364607	0.011373
C	-0.121154	0.460983	-0.036434
C	-1.444246	-1.594316	-0.006494
C	-1.350134	-0.124941	-0.026410
16			
53	t43	scf done:	-1006.877254
C	-3.040278	-1.504452	0.768035
C	2.027713	2.639251	0.285738
C	-2.034566	-1.942092	0.036010
C	2.415832	1.492578	0.557299
C	-3.195210	-0.251398	0.864222
C	2.735002	0.173361	0.743488
C	-0.982701	-2.076691	-0.669350
Mg	0.405684	2.038662	-0.768548
Mg	1.240981	-1.636113	-0.324966
C	-3.158841	1.062643	0.829579
C	2.961591	-1.033766	0.758243
C	-0.503075	-0.915869	-1.298909
O	2.865332	-2.283952	0.581234
C	-2.321206	1.848285	0.317606
C	0.173260	0.091296	-1.572443
O	-1.505653	2.561721	-0.191846
16			
54	t59	scf done:	-1006.876231
C	-2.831444	0.887254	0.188281
C	3.038274	-0.102155	-1.595093
C	-1.762654	1.487470	0.071080
C	2.278797	-0.888027	-0.865175
Mg	-1.929872	-1.136094	-0.110691
C	1.058847	-1.529527	-0.689012
C	-0.552502	2.088763	-0.067631
C	-0.090803	-1.880538	-0.461849
C	0.596462	2.503157	-0.211118
C	3.261760	-0.232946	0.071840
C	-3.739091	-0.153044	0.244760
O	-6.123683	-0.610444	0.569638
O	5.047371	-0.916963	1.612926
C	-5.007002	-0.330737	0.422254
C	4.233332	-0.671465	0.829313
Mg	2.377359	1.618239	-0.515527
16			
55	t16	scf done:	-1006.876763
C	2.537247	2.380381	-0.029623
C	-1.117721	-1.252896	0.022003
C	-3.193479	0.111572	0.022578
C	4.229371	0.513494	-0.021986
C	3.942851	-2.074344	0.002242
C	1.307924	2.373859	-0.022475
C	3.612563	1.572497	-0.027833
C	4.187861	-0.850520	-0.009303
Mg	1.949330	-1.701023	0.009294
Mg	-3.078904	-1.921041	0.039515
C	-0.875285	1.120154	-0.000005

C	0.045060	1.927153	-0.012812
C	-4.006156	1.111472	0.018194
O	0.149278	-1.491855	0.016473
O	-4.813766	1.957744	0.015348
C	-1.723974	0.012926	0.014570

16

56 t58 scf done: -1006.872803

C	-0.159931	-0.647291	-0.045939
C	1.033751	0.090153	-0.022420
O	1.548115	2.466628	0.031671
C	2.278996	-0.346422	-0.023804
C	-3.565628	1.533849	0.020413
C	-5.408380	-1.682206	-0.050918
C	6.087740	-0.634281	-0.003880
C	0.656621	1.679696	0.012968
C	-1.348911	-0.974508	-0.061488
O	7.249525	-0.697406	0.002286
C	-4.502902	0.733782	0.006166
C	3.544294	-0.424441	-0.016664
Mg	-1.510640	1.525569	0.007449
C	-5.203226	-0.450715	-0.019937
C	4.811402	-0.616261	-0.011703
Mg	-3.327403	-1.538414	-0.063326

16

57 t40 scf done: -1006.871180

C	2.851311	-2.103011	0.093996
C	-1.124500	-2.313828	-0.054838
C	-0.107523	2.198438	0.044003
Mg	-4.206707	-0.060132	-0.139475
C	1.435969	-1.928847	0.044735
O	3.400555	2.555105	0.159150
C	0.087744	-2.211651	-0.008915
C	-1.332114	2.234291	-0.003520
C	2.255780	-0.814320	0.086731
C	-3.913789	1.918757	-0.107188
C	-2.475302	-2.194723	-0.103934
O	3.808794	-2.825731	0.120144
C	-3.695987	-2.007010	-0.146004
C	4.287526	3.253931	0.193396
C	-2.691430	2.101423	-0.057648
Mg	1.614711	1.149368	0.090536

16

58 t36 scf done: -1006.869810

C	-3.417188	-0.330233	0.027352
C	-3.001434	0.973543	0.010981
C	-4.407524	0.700378	0.024785
C	6.244155	1.062715	-0.084481
C	-2.181444	-2.628604	0.038707
C	-1.800141	1.649645	-0.005121
C	-0.647325	2.038738	-0.018251
O	5.129165	0.887232	-0.066570
C	0.692919	2.244465	-0.030605
Mg	-0.185721	-2.947742	0.023681
C	1.749177	-2.449818	0.003164
Mg	2.874714	0.509368	-0.032284

C	2.499212	-1.470977	-0.009177
O	-5.544666	1.065728	0.030027
C	1.926158	2.303192	-0.040636
C	-2.827888	-1.585392	0.035193
16			
59	c22	scf done:	-1006.877153
Mg	0.000000	-4.313119	4.664593
Mg	0.000000	-2.260168	2.357335
O	-3.197008	1.935953	-2.354744
O	3.197008	1.935953	-2.354744
C	-2.139462	1.576988	-1.951604
C	2.139462	1.576988	-1.951604
C	-0.702426	1.596057	-1.972988
C	0.702426	1.596057	-1.972988
C	-1.842708	-1.653977	1.676688
C	1.842708	-1.653977	1.676688
C	-1.382926	-0.889821	0.818533
C	1.382926	-0.889821	0.818533
C	-0.710989	-0.063870	-0.108979
C	0.710989	-0.063870	-0.108979
C	1.327909	0.783195	-1.060166
C	-1.327909	0.783195	-1.060166
16			
60	t100	scf done:	-1006.868346
O	-1.677667	3.298833	3.726675
C	-0.567082	-3.525218	-1.112255
C	-2.086472	-0.209244	2.222589
C	1.975219	2.095684	-0.604505
C	-1.197033	2.700560	2.916582
C	-1.217145	-0.342764	1.277536
C	0.368923	-3.126375	-1.837372
C	1.374559	-2.651757	-2.591301
C	2.650810	1.510389	-1.604325
C	2.890969	-0.623119	-3.011097
C	1.303497	2.569736	0.331173
Mg	-1.045918	-2.029233	0.187278
C	2.793244	0.484276	-2.307959
O	-2.862822	-0.041062	3.093121
C	2.128351	-1.677676	-2.818810
Mg	-0.163380	1.412439	1.175951
16			
61	t47	scf done:	-1006.872586
O	-6.034771	-1.105587	-0.216756
O	3.501714	-2.627679	0.728171
C	-4.955223	-0.686927	-0.139757
C	1.792872	2.808541	0.170683
Mg	-1.671306	-0.925282	-0.118036
C	2.620323	1.915884	-0.003874
C	-3.714168	-0.340250	-0.070871
C	3.465162	0.856954	-0.268082
C	0.276499	-1.504701	-0.107218
C	3.592938	-0.475998	-0.219524
C	-2.945855	0.792282	0.102310
C	2.908684	-1.716239	0.205171
C	-1.919970	1.484652	0.216885

C	4.643544	0.247876	-0.803392
C	1.480843	-1.661226	0.010191
Mg	-0.184931	2.490054	0.317781

16

62 t51 scf done: -1006.867229

O	6.237969	0.599831	0.329873
C	-6.327592	-1.150401	-0.403081
C	5.220803	0.066262	0.222864
O	-5.258817	-0.798067	-0.314640
C	3.965915	-0.319862	0.124149
C	-1.851520	-1.527561	-0.261302
C	3.306733	-1.517558	-0.049488
Mg	-3.148812	0.039836	-0.121948
Mg	2.086461	0.635030	0.164796
C	-3.269386	2.044150	0.120515
C	1.962615	-1.616258	-0.116568
C	-0.621719	-1.652995	-0.226662
C	0.540887	1.937941	0.262438
C	-2.033522	2.160204	0.185011
C	0.718497	-1.682810	-0.175594
C	-0.665138	2.156576	0.240256

16

63 t88 scf done: -1006.868556

C	-0.875431	-1.991203	-2.585457
C	4.786568	0.155559	-0.007996
C	1.095669	0.325480	0.381593
O	5.957225	0.224120	0.029690
C	0.230060	-2.307650	-3.050751
Mg	-2.015231	0.837162	1.193821
Mg	1.476904	-1.318940	-1.802625
C	-2.253005	2.258232	3.077102
C	3.510218	0.189828	0.094509
O	-2.409399	2.923121	3.959453
C	-3.508240	-0.349453	-0.305340
C	-3.929630	0.348743	0.633800
C	-2.860824	-1.058144	-1.268264
C	2.262624	-0.120721	-0.258585
C	-2.016500	-1.570606	-1.980953
C	-0.035484	0.595385	0.787763

16

64 c3 scf done: -1006.874625

Mg	-4.266476	2.188660	-0.112920
Mg	-3.893752	-0.488147	-0.004336
O	-2.338195	-1.563635	0.051086
C	-1.288067	-0.768053	0.027058
C	0.031652	-1.318410	0.059708
C	1.195198	-1.673369	0.083474
C	2.550264	-1.659159	0.093030
C	3.663279	-1.150342	0.081518
C	4.372411	0.003674	0.040446
C	4.243998	1.222951	-0.010077
C	3.265843	2.160030	-0.055399
C	2.066129	2.407454	-0.075454
C	0.754443	2.078522	-0.072388
C	-0.292918	1.450599	-0.055308

C	-1.413160	0.601316	-0.029559
O	-2.685038	1.105525	-0.060245
16			
65	t66	scf done:	-1006.873992
C	-3.669112	2.425533	0.015294
O	2.130415	-3.110999	-0.000113
C	-2.489431	2.026738	0.011754
C	2.497585	-1.885908	0.001681
Mg	-4.181182	0.483851	0.010451
Mg	0.357241	-2.362172	-0.000350
O	4.646572	2.114552	0.001621
C	2.617164	-0.673812	0.003174
C	-2.781658	-1.036359	-0.000361
C	1.266015	1.325388	0.005726
C	3.679458	1.484848	0.002609
C	-1.325815	1.188624	0.005833
C	-1.513873	-1.534222	-0.003885
C	-1.676638	-0.125515	0.001072
C	2.567978	0.754857	0.004100
C	0.062604	1.459851	0.006708
16			
66	t33	scf done:	-1006.870165
C	-4.125621	0.924518	-0.043200
O	5.500950	1.499251	0.008851
C	-4.313282	2.152856	-0.061344
C	4.432580	1.013513	0.010088
C	-3.744765	-0.380184	-0.022838
C	3.259380	0.484879	0.012302
C	-3.138166	-1.436180	-0.004168
C	1.742115	0.595491	0.001776
Mg	-2.321443	2.566205	-0.051966
C	0.642393	1.420318	-0.016850
C	-2.238336	-2.448230	0.015865
C	2.317486	-0.593394	0.021843
C	-1.327793	-3.278806	0.033618
C	-0.377833	2.104326	-0.033324
Mg	0.589183	-2.759287	0.039139
O	2.217504	-1.875056	0.038461
16			
67	t30	scf done:	-1006.867689
C	3.762616	-0.902014	0.215534
O	-6.135466	-0.734712	-0.089611
C	3.950994	0.423678	-0.355155
C	-4.988691	-0.847429	-0.083406
C	4.055157	1.582683	-0.765569
C	-3.686647	-0.785523	0.065571
Mg	2.242364	2.336384	-0.328954
C	-2.583071	-1.492135	-0.270780
C	2.466700	-1.401944	-0.083379
Mg	-2.189742	0.637856	0.508654
C	1.241373	-1.575622	-0.178066
C	-1.299442	-1.580649	-0.247459
C	-0.038816	-1.782053	-0.342612
C	-0.804830	2.069898	0.489608
C	0.312163	2.500131	0.204085

O	4.571349	-1.471792	0.922790
16			
68	t55	scf done:	-1006.869833
C	3.964045	-0.328593	-0.007000
C	-3.548533	1.742410	0.071204
C	1.884670	2.868531	0.086591
C	-2.857420	-1.598190	-0.022563
Mg	-0.075447	2.315810	0.075651
C	0.110905	-1.975912	-0.043386
C	2.699587	1.944677	0.059100
C	0.900700	-2.924822	-0.071123
C	-2.562098	0.756134	0.040650
C	3.414167	0.778406	0.025051
O	0.168346	0.283612	0.016855
O	-3.652373	-2.411971	-0.041693
Mg	2.632242	-1.803701	-0.044909
C	-1.998397	-0.560748	0.002441
C	-2.155287	2.058124	0.075258
C	-0.569541	-0.719710	-0.007310
16			
69	c35	scf done:	-1006.871664
C	2.252239	-1.800197	-0.032517
C	1.458454	-2.787124	-0.014797
C	0.255320	-2.108388	0.006233
C	-0.656731	-1.273352	0.020549
C	-1.208895	-0.033577	0.027926
C	-1.299633	1.189880	0.026339
C	-0.727720	2.506060	0.012203
C	-1.458300	3.747175	0.022407
C	-1.439953	4.976554	0.018745
C	-0.780270	6.192653	0.002905
C	-1.006950	7.464211	0.004375
O	-1.085056	8.624470	0.003190
Mg	0.734609	4.664575	-0.021319
C	0.655209	2.567384	-0.013877
Mg	1.114531	0.535903	-0.017489
O	2.792064	-0.711179	-0.045807
16			
70	t42	scf done:	-1006.868957
C	-2.014921	-2.235368	-0.016449
O	5.592370	1.502872	0.012799
C	-0.960394	-3.091924	-0.015396
C	-0.287237	2.030996	0.001825
C	-2.799039	-1.302345	-0.015898
C	4.517745	1.026171	0.009843
C	0.046654	-3.816811	-0.014104
C	0.759588	1.395084	0.002753
C	-3.487082	-0.139137	-0.014515
C	3.344696	0.510879	-0.002550
C	-4.061453	0.950410	-0.013053
Mg	-2.277527	2.115768	-0.004610
C	2.392504	-0.624645	0.004390
C	1.889860	0.601330	0.003446
O	-4.267950	2.190459	-0.010035
Mg	1.537636	-2.481495	-0.003969

16
71 t54 scf done: -1006.865711
Mg -3.956350 1.091799 -0.001088
O 3.075340 2.000210 -0.016414
C 2.446751 0.995383 -0.010866
C 2.371128 -1.572565 0.000788
C -2.745773 -1.854817 0.009414
C -1.532980 1.678446 -0.006767
C -2.507652 2.452093 -0.007668
C -1.507051 -1.895788 0.007748
C -0.197374 -1.783055 0.005596
C 1.064317 -1.655343 0.003115
C 4.515270 -0.411638 -0.007847
C 3.169577 -0.470159 -0.005381
C -3.973378 -1.308702 0.009205
C -5.051943 -0.671766 0.008633
Mg 0.238403 0.636740 -0.005414
O 5.596648 -0.044288 -0.011551

16
72 t68 scf done: -1006.870286
C 3.249206 -0.056874 0.426328
O 2.503000 3.129531 -0.574373
C -4.969108 -0.034063 0.114166
C 0.830619 -1.355947 -0.224894
C -3.983474 -0.795775 0.013731
C 2.355881 2.017767 -0.329891
C -0.367575 0.708119 0.108738
C 3.131962 -1.543865 0.204306
C 2.157401 0.751972 0.045393
Mg -3.544874 1.382218 0.255161
Mg -1.957466 -1.147204 -0.071614
C 2.110864 -1.961316 -0.440418
C -1.501119 1.200778 0.190230
C 4.151313 -0.869455 0.953164
C 0.860386 0.048423 0.001745
O -0.281083 -2.001325 -0.280358

16
73 t19 scf done: -1006.868071
C 3.939654 1.136241 -0.048993
C -3.956376 -1.090913 -0.074908
C 3.498769 0.009916 0.263383
C -3.496789 0.038527 0.180207
C 2.712967 -1.059889 0.481249
Mg -2.044525 -1.681080 -0.492611
C 1.763467 -1.843399 0.551272
C -2.781741 1.181133 0.374287
Mg 1.919126 1.735245 -0.404091
C -1.873906 1.995937 0.419031
C 0.466442 3.034428 0.180851
C -0.072067 -0.734330 -0.781678
C 0.438106 -1.925394 0.156291
C -0.696126 2.659124 0.346475
O -0.473576 -2.734666 0.384523
O 0.678985 0.184260 -1.028128

16

74 t44 scf done: -1006.867786

Mg	1.324741	1.610214	-0.604394
O	-2.758810	-0.869302	-1.421698
C	3.741253	-0.120895	0.295220
C	-1.628151	-1.181061	-1.547257
O	4.868314	-0.112057	0.571263
C	-1.808334	-0.573280	2.127320
C	2.503187	-0.024295	-0.078142
C	-0.506065	-0.901754	1.909017
C	-0.307268	2.641752	-1.070009
C	-2.998655	-0.219516	2.047794
C	-1.212002	1.928003	-0.604164
C	0.586214	-1.409787	-0.800425
C	1.381449	-0.933947	0.154092
C	-0.422409	-1.603796	-1.585129
C	0.561796	-0.988452	1.320835
Mg	-2.649471	0.714905	0.229812

16

75 t71 scf done: -1006.867971

C	1.542363	-2.953146	0.403626
Mg	2.126448	1.559413	-0.208563
C	-0.131869	2.085433	-0.176672
C	-1.403899	-0.037043	0.498236
O	-6.235694	0.229913	-0.745780
C	-5.119791	0.171734	-0.458647
C	3.350374	-1.243258	-0.437796
C	-0.320451	0.832915	0.455692
Mg	0.169996	-1.541407	0.872794
C	0.552124	2.957742	-0.741985
C	-3.882083	0.102507	-0.134845
O	0.819130	0.375196	0.937597
C	-2.651197	0.090341	0.151997
C	2.414369	-2.171976	-0.016320
C	3.540030	0.100862	-0.608352
C	4.598321	-0.786120	-0.916445

16

76 t56 scf done: -1006.868379

C	2.281038	0.053057	-0.226751
C	2.127111	1.430256	-0.310258
O	-0.277785	-2.367428	1.048331
C	1.902367	2.641223	-0.338431
C	-2.485647	-0.416906	-0.782883
O	3.801072	-1.983820	-0.467408
Mg	0.009841	3.247499	0.037815
Mg	-1.886909	-2.478962	0.046477
C	0.160793	-1.203185	0.596935
C	-1.989997	3.113915	0.322421
C	2.870759	-1.265637	-0.261211
C	-1.680080	0.493776	-0.003942
C	-3.073479	-1.424767	-1.210908
C	-1.943427	1.881661	0.212613
C	-0.596531	-0.088250	0.518387
C	1.527038	-1.018562	0.135182

16

77 t86 scf done: -1006.861050

C	0.830759	0.351643	1.525932
C	-2.670644	2.293243	-0.708626
C	0.915152	-0.730355	0.741649
C	-2.444326	1.212390	-1.245681
C	0.524786	1.415490	2.084047
Mg	-1.970489	3.336348	0.855545
C	1.413367	-1.976073	0.652383
C	-2.064432	-0.006132	-1.738187
O	1.674827	-1.324705	-2.599218
C	-1.651627	-1.111992	-2.108042
C	2.420357	-1.204937	-3.437562
C	-0.766659	3.636469	2.469139
C	-0.113621	2.582857	2.297986
Mg	0.012536	-1.451110	-1.019179
C	2.122438	-2.987423	1.056957
O	2.688808	-3.987775	1.224814

16

78	t84	scf done:	-1006.863716	
O	-6.172173	-1.055962	-0.147085	
C	3.930311	-1.209124	0.849177	
C	-2.534760	-0.999821	-0.069931	
C	4.629080	-0.237906	-0.118506	
C	-5.034779	-0.826035	-0.108507	
O	5.716052	0.040367	-0.483210	
C	-1.295399	-1.067723	-0.049660	
C	2.324009	1.083115	-0.064370	
Mg	0.709366	-1.252809	0.018870	
C	1.292138	1.731238	0.037161	
C	-3.802415	-0.447050	-0.057966	
C	3.208287	0.021273	-0.315953	
C	0.063926	2.302020	0.132763	
Mg	-2.450025	1.164988	0.082335	
C	-1.111238	2.669456	0.210242	
C	2.783949	-1.333402	0.126954	

16

79	t61	scf done:	-1006.868108	
Mg	3.109270	-0.617742	-0.075042	
O	-4.616060	-0.394650	-0.015662	
C	2.340442	1.267624	0.211546	
C	-3.470673	-0.509815	-0.022946	
Mg	0.978855	2.724321	-0.318096	
C	-2.148979	-0.611418	-0.031961	
O	2.163670	-2.290293	-0.468248	
C	-1.414220	-1.754726	-0.438430	
C	1.376129	0.484757	0.741187	
C	-1.212877	0.482869	0.383981	
C	1.013060	-1.961456	0.007493	
C	-0.284668	-2.230863	-0.504506	
C	0.921675	-0.935744	0.978627	
C	-1.042013	2.990676	-0.472455	
C	-0.018574	0.122528	0.919406	
C	-1.234671	1.820892	-0.102414	

16

80	t27	scf done:	-1006.861551	
C	-2.814155	2.383251	0.000283	

C	4.942219	-0.793686	0.000064
C	-1.498208	1.811022	0.000389
C	3.875545	-1.454884	0.000177
C	-2.580488	1.006492	0.000275
C	0.140416	-2.246162	0.000160
O	-5.518602	-0.738353	0.000088
Mg	3.816332	0.932774	0.000209
C	-4.396394	-0.566323	-0.000021
C	2.687339	-2.083105	0.000266
C	-3.045933	-0.354461	0.000119
C	1.444874	-2.169705	0.000274
Mg	0.567223	1.983707	0.000440
C	-1.058267	-1.825972	0.000042
C	-2.313938	-1.531427	0.000000
O	2.357253	1.971375	0.000364

16

81	t96	scf done:	-1006.859372	
C	2.944950	-2.287447	-1.438636	
C	-0.032739	3.020721	0.577840	
C	3.417781	-1.076397	1.250255	
C	1.173264	3.260727	0.980182	
O	3.765146	-2.598623	-2.133232	
C	-1.210158	2.720840	0.207837	
Mg	1.552354	-1.397465	0.358302	
C	2.140076	2.380716	1.179544	
C	3.264288	0.166094	1.307539	
C	-2.032244	1.749303	-0.128216	
C	-3.267800	-0.414947	-0.694920	
C	2.988941	1.485785	1.361178	
C	-4.330701	-1.074933	-1.046986	
C	-2.843260	0.843547	-0.443810	
O	-5.176085	-1.805451	-1.348890	
Mg	-1.193570	-0.791868	-0.171301	

16

82	t97	scf done:	-1006.856419	
Mg	-1.287047	0.641348	0.632965	
C	-2.476416	-1.136201	0.699571	
O	-1.960270	1.303958	-1.473635	
O	-4.692238	-1.988936	1.291714	
C	-2.283380	1.622992	-2.505943	
C	3.073123	1.593785	0.265157	
C	-0.067304	-1.426794	-0.180190	
C	-0.377826	2.386177	1.213201	
C	3.870794	-1.611491	-1.089967	
C	-1.245755	-1.503733	0.209970	
Mg	1.859160	-1.728544	-0.691673	
C	2.163235	2.349606	0.726298	
C	3.939281	-0.426603	-0.664909	
C	4.013228	0.841435	-0.207326	
C	0.853095	2.381211	0.989076	
C	-3.623777	-1.639663	0.994642	

16

83	t81	scf done:	-1006.860241	
C	-0.082406	-1.734411	-0.505745	
C	4.208228	-0.848916	0.219801	

C	-2.993477	0.654505	0.317298
C	0.733986	-2.641008	-0.365307
Mg	-0.042339	2.439710	-0.135515
O	-0.252480	0.522971	-0.814336
C	2.824202	1.364611	0.247172
C	-2.983390	-1.544224	0.265791
C	-2.001566	3.071040	0.293920
C	3.578485	0.222192	0.241676
Mg	2.686911	-2.083173	-0.121614
C	1.972992	2.247825	0.196514
C	-2.206863	-0.455168	-0.012164
C	-0.831958	-0.518991	-0.489082
C	-2.474784	1.900640	0.269315
O	-3.661824	-2.423030	0.503472

16

84	t31	scf done:	-1006.861854	
O	8.058430	0.755906	0.002835	
Mg	-4.223377	1.912966	0.005402	
C	6.905884	0.544602	0.002375	
C	-2.287318	2.294613	0.005697	
C	5.658567	0.315461	0.001864	
O	-5.263121	0.238470	0.002825	
C	4.389922	0.082797	0.001502	
C	-2.007158	1.080605	0.003555	
C	3.151497	-0.146304	0.001165	
C	-4.252380	-0.487328	0.001397	
C	1.876517	-0.388519	0.000801	
C	-3.128819	-1.038820	0.000115	
Mg	-1.785576	-2.799987	-0.003120	
C	-1.825823	-0.335714	0.001162	
C	0.641853	-0.609324	0.000494	
C	-0.622162	-1.008511	-0.000110	

16

85	t26	scf done:	-1006.861350	
C	4.408410	-2.433616	-0.003954	
O	-5.530490	-1.972857	0.001055	
C	4.092293	-1.050097	-0.001586	
C	-4.803012	-1.064148	0.000367	
C	4.225158	0.321128	-0.001100	
C	-4.145613	0.041361	-0.000504	
C	3.079003	-1.951368	-0.000409	
C	-2.873360	0.485932	-0.000218	
C	4.167990	1.555982	-0.000904	
O	-2.490393	1.730036	-0.001181	
C	1.708087	-1.907173	0.001310	
C	-1.760897	-0.434864	0.000543	
Mg	2.219037	2.212462	-0.000238	
Mg	-0.585484	1.907574	-0.000109	
C	0.529579	-1.596302	0.001533	
C	-0.697448	-1.035041	0.001165	

16

86	t23	scf done:	-1006.861254	
C	-0.701151	-0.220564	0.002217	
Mg	2.510708	2.677596	-0.002440	
C	-1.978445	-0.114072	0.002088	

O	2.858168	0.831589	0.000558
C	-3.272745	-0.149546	0.002186
C	0.595074	3.238967	-0.003283
Mg	0.137517	-2.102568	0.005126
C	0.418380	2.007110	-0.001364
C	1.799165	0.050915	0.001851
C	-4.526455	-0.219121	0.002489
C	0.490139	0.583771	0.000947
C	-5.828850	-0.313866	0.002729
O	4.215301	-2.519461	0.006116
C	2.033405	-1.384847	0.004068
C	3.209096	-1.944275	0.005000
C	-7.092224	-0.439344	0.002895

16

87	t83	scf done:	-1006.855629	
C	-2.572056	0.238069	-0.009180	
O	0.963666	2.202851	0.058198	
C	-0.151533	-0.579714	-0.015734	
C	-5.057409	0.824041	-0.008142	
C	-1.304889	0.028807	-0.007392	
O	-7.430983	1.398837	-0.008871	
C	4.490603	-1.972264	-0.025258	
C	4.179703	-3.174673	-0.056120	
C	-0.182854	2.328092	0.055192	
C	1.066608	-0.965403	-0.018426	
C	-3.804584	0.550346	-0.008623	
C	4.592275	-0.600416	0.008129	
C	-6.294459	1.128977	-0.008483	
C	4.454898	0.630301	0.037730	
Mg	2.219064	-2.674632	-0.053784	
Mg	2.424022	0.684674	0.028445	

16

88	t93	scf done:	-1006.853201	
C	-3.177188	-2.690195	-0.392201	
C	-1.098529	-1.214461	-0.294338	
C	3.571877	0.174807	0.251903	
C	-0.317126	1.285747	-0.466720	
O	-4.074175	-3.443989	-0.417410	
C	3.220192	-1.132624	0.347115	
C	-2.320836	-1.736196	-0.395800	
C	2.733344	3.795305	-0.286755	
C	-0.787750	0.150079	-0.408581	
Mg	0.926766	2.873974	-0.456620	
C	2.764673	-2.282709	0.408558	
O	-4.261821	1.406186	0.445828	
C	3.255267	2.683899	-0.081173	
C	3.610065	1.385523	0.120340	
Mg	0.779470	-2.091252	0.089364	
C	-3.695229	0.838168	1.232846	

16

89	t22	scf done:	-1006.855489	
C	3.212217	-0.834229	0.017232	
O	-4.268044	1.933457	-0.006301	
C	3.290793	0.402499	0.014351	
C	-3.136142	1.503133	-0.002568	

C	-0.286500	-4.426450	0.016798
C	-1.954664	2.339629	-0.001281
C	2.616277	-2.024690	0.018389
C	-2.822358	0.087420	0.001211
C	0.782918	-3.790122	0.017738
C	-0.914391	2.979093	-0.000089
Mg	-1.631574	-2.913106	0.010341
C	-2.507977	-1.091119	0.004126
C	2.717624	1.651702	0.010146
Mg	1.096524	2.892860	0.004079
C	1.889412	-3.013793	0.018476
O	3.138879	2.839818	0.010203

16

90	c18	scf done:	-1006.852644	
C	-1.195662	2.225868	0.006985	
C	-1.678217	0.951141	0.010143	
C	-1.429444	-0.271952	0.007757	
C	-0.824428	-1.447027	0.004580	
C	0.360816	-1.869762	-0.003128	
C	1.658465	-1.610035	-0.011515	
C	2.172481	-0.451348	-0.015103	
C	2.058457	0.853661	-0.014671	
C	1.184968	1.763747	-0.009486	
C	0.149653	2.606771	-0.002140	
Mg	0.734799	4.654667	-0.006668	
O	1.447737	6.365827	-0.009768	
Mg	-0.137088	7.242834	0.004129	
C	-1.484832	5.705693	0.011486	
C	-1.851535	4.523984	0.012923	
O	-2.220154	3.268424	0.014473	

16

91	t76	scf done:	-1006.855231	
C	2.573512	1.766835	0.117988	
C	-4.697457	-1.155991	-0.113157	
C	-2.164060	1.706659	-0.167655	
C	-3.947530	-0.167347	-0.140547	
C	2.957714	0.624970	-0.024698	
C	-1.312612	-3.117171	0.062715	
Mg	-0.330173	2.547422	-0.061498	
Mg	-3.245175	-2.529838	0.001823	
C	-3.067991	0.880224	-0.162153	
C	-0.147110	-2.737437	0.036864	
C	3.315562	-0.770989	-0.202934	
C	1.097087	-2.200601	-0.016208	
C	1.762621	2.974162	0.230471	
C	2.163172	-1.623428	-0.080278	
O	2.221314	4.058075	0.524954	
O	4.434819	-1.153935	-0.449900	

16

92	c72	scf done:	-1006.853064	
C	-2.190840	0.000000	-0.797508	
C	-1.048709	0.000000	-0.350055	
C	0.163130	0.000000	0.269838	
C	1.189045	0.000000	0.940730	
Mg	2.088868	-0.000000	2.732205	

C	2.289179	-0.000000	4.866477
C	0.826019	-0.000000	4.933826
C	-0.283279	-0.000000	4.392259
C	-1.519125	-0.000000	3.865962
C	-2.623468	-0.000000	3.341830
C	-3.813531	0.000000	2.718879
C	-4.922057	0.000000	2.182495
C	-5.811608	0.000000	1.023733
O	-7.014697	0.000000	1.027243
Mg	-4.137273	0.000000	-0.323985
O	3.070027	-0.000000	5.778874

16

93	c36	scf done:	-1006.855959	
O	2.753192	-2.000774	0.059383	
C	1.521432	-2.176173	0.047198	
C	0.297918	-2.002125	0.032612	
C	-0.648576	-1.032620	0.015411	
C	-1.107095	0.107991	0.002285	
C	-0.589605	1.402039	-0.001271	
C	-0.893961	2.732714	-0.013947	
C	-1.791778	3.767784	-0.030940	
C	-2.105295	4.961393	-0.042746	
C	-1.851580	6.308765	-0.049516	
C	-1.109249	7.318334	-0.048639	
Mg	0.214290	5.696979	-0.022909	
O	1.239719	4.110035	-0.000624	
C	0.646566	2.972985	0.000996	
C	0.946275	1.630783	0.013772	
Mg	2.076665	-0.043061	0.038003	

16

94	t78	scf done:	-1006.852069	
O	-0.152644	-2.419648	-0.012392	
O	6.620785	-0.072100	0.001199	
C	0.574059	1.165650	0.001331	
Mg	-1.316301	1.952997	0.002522	
C	2.936820	0.117885	-0.000822	
C	-3.728155	-1.039687	-0.011973	
C	5.461628	0.062281	0.000796	
Mg	1.239447	-1.159369	-0.006588	
C	-3.763842	1.506719	-0.002221	
C	-1.347366	-2.036929	-0.012485	
C	-2.513057	-1.679064	-0.012703	
C	-4.247422	0.209792	-0.007854	
C	4.222857	0.418304	0.001136	
C	1.800824	0.943804	0.001343	
C	-3.213690	2.621005	0.002932	
C	-5.140008	-0.886471	-0.013083	

16

95	t53	scf done:	-1006.854255	
O	4.463909	1.496689	-0.006999	
C	-4.124192	-1.338834	-0.034774	
C	0.363017	2.034012	0.001770	
C	-2.859810	-1.826384	-0.039525	
C	1.342407	1.295537	-0.007159	
C	-5.201550	-0.715352	-0.025464	

C	3.791454	0.531699	-0.017103
C	-1.646283	-1.970754	-0.041005
Mg	-1.678321	2.250247	0.005563
C	-0.304459	-1.901897	-0.041264
C	2.327261	0.312938	-0.018643
C	0.883519	-1.629654	-0.038974
C	3.472416	-1.747437	-0.041816
Mg	-4.267971	1.127640	-0.004377
C	2.140570	-1.039856	-0.033307
O	4.369443	-0.792440	-0.031868

16

96	t70	scf done:	-1006.853823	
O	-5.524447	0.886989	0.334226	
O	4.276600	-0.683323	0.445477	
C	-4.377386	0.575183	0.224875	
C	3.193246	-0.873773	-0.153684	
C	-2.995814	0.899296	0.016374	
C	2.009041	-1.536775	-0.392000	
C	-1.818881	1.600537	-0.184229	
C	0.920332	-2.373442	-0.218199	
C	-3.350283	-0.417758	0.181829	
C	-0.273079	-2.531335	-0.021159	
C	-0.685480	2.033322	-0.366019	
C	2.164587	-0.225844	-0.862767	
C	-2.582671	-1.566279	0.204112	
C	-1.585959	-2.262216	0.114212	
Mg	4.033601	1.348154	0.742009	
Mg	1.364588	1.753031	-0.473264	

16

97	c1	scf done:	-1006.853770	
C	1.104272	-1.833452	0.131196	
C	-0.058042	-1.473230	0.093274	
C	-1.336281	-0.866456	0.037927	
C	-1.486869	0.494989	-0.053664	
C	-0.372255	1.367209	-0.097888	
C	0.682878	1.973923	-0.125373	
C	2.004769	2.272978	-0.129302	
C	3.198397	2.007425	-0.097405	
C	4.153504	1.047556	-0.022433	
C	4.288051	-0.168170	0.059581	
C	3.566026	-1.314197	0.126665	
C	2.459459	-1.835129	0.147715	
O	-2.491947	-1.576581	0.070935	
Mg	-3.623740	-0.518289	-1.314056	
Mg	-3.654930	-0.347299	1.277289	
O	-2.769497	0.934609	-0.098101	

16

98	t74	scf done:	-1006.847379	
Mg	2.810695	0.805811	0.058823	
C	-1.295287	1.300276	0.025427	
C	0.099836	-0.681430	-0.074542	
C	-1.090177	-1.460681	-0.053004	
C	3.865118	-1.850398	-0.078369	
C	-3.852765	1.790752	-0.322779	
O	1.022464	1.517297	0.138841	

C	4.527939	-0.649645	-0.027047
C	1.372965	-1.197368	-0.107525
Mg	-3.385501	-0.559606	0.233748
C	4.918272	0.549633	0.059663
C	-2.145749	-2.101565	-0.004964
C	0.005210	0.748818	0.023940
O	-4.681635	0.866863	-0.070855
C	-2.491307	1.577775	0.131456
C	2.544517	-1.643106	-0.117043

16

99 t67 scf done: -1006.845821

O	-8.360301	-1.051148	-0.061772
Mg	4.104222	-0.239478	0.106165
C	-7.213900	-0.838828	-0.038409
O	5.691635	-2.059487	0.013638
C	-5.962865	-0.607625	-0.012624
C	2.311436	-1.229919	0.029283
C	-4.702069	-0.373199	0.013867
C	6.281239	-3.020013	-0.043052
C	-3.460164	-0.142588	0.039090
Mg	3.500221	2.465070	0.259658
C	-2.190218	0.093114	0.065367
C	0.917375	1.873384	0.200132
C	-0.958413	0.321242	0.090655
C	1.509245	2.957287	0.269752
C	0.361068	0.565156	0.117567
C	1.350877	-0.455034	0.066583

16

100 t77 scf done: -1006.846741

C	-1.306630	-1.521513	0.534985
C	3.262244	-0.250292	-0.152226
C	-4.364066	1.103418	-0.508674
C	1.135441	-1.596459	0.286433
C	4.573549	-0.144706	-0.178051
C	2.323310	-1.161024	0.113803
C	-3.126807	-1.041513	-1.005880
O	5.681105	0.143938	-0.270885
C	-0.637879	1.928630	0.078328
O	-1.716630	-0.750017	1.456592
Mg	-2.415000	0.943987	0.528872
C	-0.031473	-2.059467	0.556532
C	-2.181120	-1.708186	-0.592119
Mg	1.536035	1.045619	-0.205462
C	-3.965525	0.022029	-0.993650
C	0.342468	2.625150	-0.258580

16

101 t89 scf done: -1006.848428

C	4.012128	-0.031446	0.409525
Mg	-4.074298	0.135381	0.621249
C	3.196961	0.885671	0.535445
C	-2.902336	-1.615780	0.219149
O	4.488177	-1.170381	0.182143
O	-2.782895	-2.791245	0.154726
C	-2.186338	0.728589	-0.069393
C	2.174926	1.763244	0.453504

C	-1.823505	-0.575449	-0.187953
C	1.075413	2.263728	0.280297
C	-0.540520	-1.077606	-0.494304
C	-0.193388	2.472463	-0.198079
C	-1.391616	1.843373	-0.350444
Mg	2.529520	-1.398361	-0.253412
C	-1.195858	3.106111	-0.954562
C	0.580965	-1.547543	-0.633219

16

102 t48 scf done:	-1006.845929		
O	-3.646988	-0.256524	-0.671906
C	3.902979	-0.427473	-0.087793
C	3.678951	0.895768	-0.105404
C	1.914536	2.716453	-0.074166
O	-1.825443	0.598113	0.416831
C	3.002553	1.915839	-0.101362
Mg	-1.101298	2.512970	0.098400
C	-3.150680	2.061795	0.158563
C	0.788195	3.213489	-0.033830
C	2.669397	-2.603339	-0.009280
C	-3.103705	0.771497	-0.191069
Mg	-2.175144	-1.381148	-0.009106
C	1.555943	-3.109963	0.029502
C	3.566318	-1.605775	-0.053893
C	-1.011573	-3.024586	0.077334
C	0.207937	-3.201165	0.059445

16

103 t45 scf done:	-1006.848326		
C	-4.166956	-0.704975	-0.005608
Mg	5.822295	-0.383160	-0.003382
C	-1.684031	-1.976186	0.001233
C	-2.805437	-1.179629	-0.001875
C	-2.246590	1.305420	-0.001635
C	-3.041948	0.168721	-0.003052
O	-5.340578	-0.915550	-0.008604
O	-0.064062	4.096623	0.002699
Mg	2.699510	-0.757243	0.008272
C	0.788438	-2.631836	0.006714
C	1.855396	1.108851	0.007460
C	-0.118958	2.889164	0.002705
C	2.025237	-2.689106	0.009630
C	1.010559	1.991421	0.005314
C	-0.549290	-2.416940	0.003796
C	-1.356841	2.124675	0.000140

16

104 t80 scf done:	-1006.847384		
C	0.887063	-2.575304	0.000114
Mg	-1.756103	2.530037	-0.000306
C	-0.395369	-2.099437	-0.000745
C	1.748571	2.606159	0.000110
C	2.061388	-2.130174	0.000846
C	0.310590	2.627408	0.000050
O	4.392080	0.361697	0.002101
O	-3.103790	1.352830	-0.000933
C	-1.693628	-2.610165	-0.001281

C	0.970706	1.446406	0.000060
C	3.359867	-0.097536	0.001604
Mg	-2.595725	-0.399196	-0.001109
C	2.143991	-0.735992	0.000982
C	0.886327	0.005393	-0.000020
C	-0.322291	-0.643131	-0.000878
C	-2.939886	-2.588083	-0.000923

16

105 c29 scf done: -1006.842496

C	-1.002775	2.656949	-0.009662
C	-1.646127	1.427368	-0.029541
C	-1.205679	0.167266	-0.036024
C	-0.975342	-1.088859	-0.045141
Mg	1.030079	-0.716665	-0.016081
O	2.324809	-2.602977	-0.005787
C	2.883918	-3.583646	0.008957
C	2.196897	0.955710	0.014609
C	1.336016	1.841114	0.012239
C	0.406746	2.914795	0.010746
O	0.901969	4.105794	0.028540
Mg	0.001179	5.759792	0.032941
C	-1.324404	7.412492	0.031609
C	-2.036861	6.387191	0.012649
C	-2.181778	5.011939	-0.002229
C	-1.762629	3.864231	-0.007826

16

106 c78 scf done: -1006.842243

C	-3.246723	-2.395971	0.288167
Mg	-3.175167	-0.373505	-0.467181
C	-2.277852	1.398968	-0.768741
C	-1.089645	1.611619	-0.518561
C	0.228086	1.724482	-0.230095
C	1.407776	1.639830	0.061173
C	2.688509	1.316592	0.368640
C	3.836216	0.946255	0.652323
Mg	3.875986	-1.042380	0.357793
C	3.276986	-2.995114	-0.333432
C	1.855530	-3.193231	-0.250249
C	0.652922	-3.054957	-0.070122
C	-0.678031	-2.941192	0.096611
C	-1.890114	-2.875246	0.263684
O	4.059690	-3.766439	-0.855640
O	-4.200569	-2.976872	0.760600

16

107 t72 scf done: -1006.841495

C	-4.694494	1.415400	-0.034893
C	2.311739	1.230484	0.025623
Mg	-3.008131	2.571630	0.014860
C	-2.351196	-1.373020	-0.095081
C	2.896948	-2.316156	-0.074450
C	3.408961	0.286421	0.008364
C	1.295337	1.893413	0.035497
O	4.575343	0.607684	0.029004
Mg	0.798006	-2.066581	-0.086579
O	2.412782	-3.444567	-0.113768

C	-1.037132	2.996752	0.045752
C	0.095023	2.527192	0.042692
C	2.917690	-1.068637	-0.036246
C	-4.114299	0.287686	-0.062804
C	-1.197549	-1.840880	-0.098331
C	-3.620134	-0.951523	-0.094458

16

108 t95 scf done: -1006.845141

O	2.139675	3.706117	-0.094503
Mg	-0.452347	-3.536971	-0.578780
C	1.897800	2.574157	-0.054119
C	2.780771	-2.023137	0.097500
C	1.744898	1.276154	0.005758
C	-0.798797	-1.605831	0.329492
C	-1.951623	1.376159	-0.279314
C	-2.008392	-1.046236	0.482469
C	-0.743159	1.238274	-0.216083
C	1.632308	-1.547256	0.122135
C	-3.311157	0.874415	0.009639
Mg	3.320607	-0.070500	0.010509
O	-4.352708	1.390489	-0.283547
C	0.387722	-0.840257	0.130452
C	0.482869	0.572316	-0.031959
C	-3.077524	-0.416036	0.691885

16

109 t92 scf done: -1006.839222

Mg	2.450853	1.516980	-1.101762
C	-1.816416	2.397289	0.421823
C	-2.953403	1.934675	0.391053
C	-3.786056	-1.403303	-0.081556
C	-0.488838	2.146042	0.151788
C	-1.473452	-2.452105	-0.310868
C	-3.994889	1.081880	0.354657
Mg	1.375445	-0.963692	-0.149830
C	-0.244153	-2.322183	-0.306396
O	4.211805	-1.548604	1.635026
C	3.162365	-1.491130	1.241664
C	-2.755832	-2.067234	-0.232333
C	-4.123425	-0.123192	0.114556
C	0.446315	1.125494	0.194834
O	2.881069	-0.222611	-1.000925
C	0.722187	2.391259	-0.434085

16

110 t69 scf done: -1006.839335

C	1.333185	-2.214377	-0.021386
C	2.661691	-2.339605	-0.024679
C	-1.090743	1.569133	-0.021654
O	-6.509619	-0.981069	0.000237
O	3.707201	1.260938	-0.033192
C	-0.884076	-0.951047	-0.017555
C	0.039120	2.308908	-0.026473
C	0.270593	-1.517928	-0.019756
C	-4.144404	-0.388724	-0.009455
C	-5.392165	-0.703686	-0.004288
C	3.915181	-2.480515	-0.027541

C	-1.240743	2.957839	-0.023311
C	-1.602185	0.220318	-0.017736
Mg	2.083988	2.022452	-0.030529
C	-2.929062	-0.087745	-0.013392
Mg	4.240517	-0.452339	-0.031587

16

111 c27 scf done: -1006.833772

C	-0.335322	2.497014	0.103415
C	-0.536938	1.175506	-0.039894
C	-1.006969	-0.003424	-0.124543
C	-1.337833	-1.268367	-0.124353
C	-0.223252	-2.086688	-0.180342
C	0.895022	-2.662188	-0.121471
Mg	1.397961	-0.579625	0.056758
O	2.412386	1.073783	0.314820
C	1.942662	2.202183	0.309918
C	1.038299	3.069095	-0.166456
O	1.231151	4.285439	-0.601684
Mg	0.051467	5.717779	-0.487378
C	-1.527569	7.065188	-0.085868
C	-1.941642	5.943499	0.278575
C	-1.825987	4.588669	0.488005
C	-1.287417	3.494632	0.380496

16

112 c40 scf done: -1006.844604

Mg	-0.000000	4.337491	-0.179255
Mg	-0.000000	-4.337491	-0.179255
C	-1.842768	3.526131	-0.179522
C	1.842768	3.526131	-0.179522
C	-1.381535	2.377899	-0.179940
C	1.381535	2.377899	-0.179940
C	-0.678839	1.151254	-0.180444
C	0.678839	1.151254	-0.180444
C	-1.842768	-3.526131	-0.179522
C	1.842768	-3.526131	-0.179522
C	-1.381535	-2.377899	-0.179940
C	1.381535	-2.377899	-0.179940
C	-0.678839	-1.151254	-0.180444
C	0.678839	-1.151254	-0.180444
O	1.427239	0.000000	-0.180913
O	-1.427239	-0.000000	-0.180913

16

113 t99 scf done: -1006.841411

C	4.658674	-1.469540	-0.063795
Mg	-2.980192	2.073809	-0.019752
C	4.376630	-0.256750	0.033040
C	0.357542	2.082535	0.110529
Mg	2.634293	-1.804486	-0.156612
C	-0.964401	1.728364	0.022797
C	0.655121	-1.392646	-0.188643
C	1.576887	2.200881	0.158141
C	-2.744683	0.018923	-0.073715
C	3.802271	0.974259	0.121744
C	2.829702	1.718404	0.156682
C	-3.230677	-1.288498	0.259678

C	-1.291995	0.383275	-0.075018
O	-3.561642	-2.134955	1.020284
O	-3.167962	-1.112530	-1.050816
C	-0.286509	-0.611049	-0.144845

16

114 t60 scf done: -1006.837907

C	0.139445	1.813679	0.000000
C	-1.856686	-1.424269	-0.000000
C	-0.722780	-0.796375	-0.000000
C	1.428299	2.418470	0.000000
C	0.734185	-0.758254	0.000000
C	2.590595	2.806745	0.000000
C	0.045970	0.389565	0.000000
Mg	2.763875	-1.103200	0.000000
C	-0.974664	2.555259	0.000000
O	-1.921587	3.197075	-0.000000
C	-4.081432	-2.659812	-0.000000
C	-2.975391	-2.043439	-0.000000
O	4.331806	-0.221266	0.000000
Mg	4.177816	1.574468	0.000000
C	-5.215130	-3.294484	-0.000000
C	-6.326781	-3.920855	-0.000000

16

115 t62 scf done: -1006.831120

C	-1.121241	1.694780	-0.319673
C	8.650156	-0.412823	-0.026966
C	-6.809211	-1.479799	0.203512
C	7.381720	-0.278296	-0.044478
O	-5.784981	-1.010467	0.124375
C	6.087645	-0.144858	-0.060948
C	-2.457658	1.902795	-0.346775
C	4.835873	-0.018396	-0.075561
C	0.006225	1.195571	-0.245789
C	3.548979	0.101540	-0.087975
C	-3.705205	1.895424	-0.340361
C	2.297326	0.243681	-0.105255
C	0.982989	0.240076	-0.098594
Mg	-0.710099	-1.060516	0.114398
Mg	-3.724776	-0.153456	-0.016326
O	-2.466398	-1.436178	0.181619

16

116 c14 scf done: -1006.835096

C	-0.373711	2.379601	0.007488
C	-1.268028	1.264185	0.027155
C	-1.085459	-0.015907	0.023688
C	-0.777462	-1.266987	0.017691
C	0.373715	-1.832710	-0.007154
C	1.652610	-2.041472	-0.034802
C	2.338731	-0.938787	-0.050221
C	2.668566	0.298701	-0.057740
C	1.905677	1.342121	-0.041594
C	1.044507	2.299520	-0.023244
Mg	0.342205	4.364809	-0.010063
C	-1.328367	5.620620	0.024101
C	-1.055532	6.896494	0.018215

O	-0.649000	8.001945	0.009189
O	-2.551074	4.983077	0.049449
Mg	-2.291361	3.157281	0.047840

16

117 c45 scf done: -1006.829229

C	1.995382	0.449118	0.220138
C	1.737717	1.704197	-0.021664
C	0.924119	2.678492	-0.400750
O	1.204439	3.719298	-1.137279
Mg	0.622895	5.464230	-0.828476
C	-0.117212	7.276201	-0.021933
C	-0.734739	6.363970	0.568839
C	-1.018970	5.044809	0.846813
C	-0.924944	3.844583	0.632723
C	-0.524210	2.579013	0.154185
C	-1.313686	1.533771	-0.079718
C	-1.225770	0.242606	-0.409229
C	-1.316552	-0.992661	-0.687258
Mg	0.591410	-1.458270	-0.250246
O	2.279863	-1.901649	0.742774
C	2.436269	-0.668389	0.659151

16

118 c51 scf done: -1006.826873

O	-4.554538	2.042272	0.001727
C	-3.751352	0.993093	-0.000180
C	-2.773762	0.285205	-0.001356
C	-1.543957	-0.276343	-0.002964
C	-0.339579	-0.458923	-0.003889
C	1.011737	-0.379696	-0.004315
C	2.209821	-0.110003	-0.005473
Mg	3.538753	1.395334	-0.003119
O	5.275851	2.506863	-0.000698
C	4.318032	3.307748	0.000808
C	3.148863	3.752568	0.001619
Mg	1.392740	4.701243	0.002870
C	-0.584545	5.084600	0.004324
C	-1.720250	4.623740	0.004132
C	-2.882576	3.913621	0.003571
C	-3.799218	3.131178	0.002942

16

119 c74 scf done: -1006.825602

C	-3.006853	-1.636726	-0.001065
C	-2.108417	-2.458558	-0.000697
Mg	-0.102265	-2.514525	-0.000189
C	1.846610	-1.993790	-0.000548
C	2.877492	-1.322530	0.000187
Mg	4.120468	0.239957	-0.003170
O	5.578282	1.613891	0.004375
C	4.554628	2.339132	0.003957
C	3.379429	2.711454	0.001687
C	2.070101	3.035447	0.001150
C	0.849328	3.078980	0.000297
C	-0.466629	2.807000	-0.000310
C	-1.579114	2.305748	-0.000899
C	-2.612766	1.435382	-0.001268

C	-3.362880	0.490178	-0.001634
O	-3.939037	-0.690437	-0.001711

16

120 c50 scf done: -1006.823105

C	2.344571	0.046349	-0.449168
C	1.605337	-0.903890	-0.207603
C	0.360311	-1.288861	0.121986
C	-0.828633	-1.308548	0.414601
C	-2.023069	-0.709902	0.669292
C	-3.065189	-0.057585	0.882989
Mg	-2.221052	1.737511	0.561702
C	-1.936974	3.826500	0.358887
C	-1.822616	5.088874	0.250371
C	-1.107594	6.177225	0.005806
C	0.099512	6.342347	-0.300386
Mg	0.783912	4.304641	-0.338097
O	-0.775765	3.074587	0.122415
O	2.544594	3.700225	-0.730870
C	2.747288	2.471346	-0.702144
C	2.894288	1.254232	-0.660712

16

121 t91 scf done: -1006.829159

Mg	-1.437619	2.661704	0.000000
O	4.689990	-1.573310	0.000000
O	-2.939804	1.566579	0.000000
C	-2.632760	0.316131	0.000000
C	3.664375	-1.021881	0.000000
C	0.300302	1.678411	0.000000
C	0.673150	-1.931946	0.000000
C	-3.603075	-0.786976	0.000000
C	-0.450937	-2.507189	0.000000
C	0.010021	0.317962	0.000000
C	2.584813	-0.307907	0.000000
C	-1.328646	-0.296224	0.000000
C	1.205596	-0.711036	0.000000
C	-3.007398	-1.867969	0.000000
C	-1.571811	-1.765661	0.000000
Mg	2.316208	1.714546	0.000000

16

122 c19 scf done: -1006.824480

C	-0.942056	2.269543	0.000931
C	-1.534886	1.033542	0.003919
C	-1.362245	-0.198428	0.004962
C	-0.971853	-1.469728	0.005556
C	0.226725	-1.866066	0.003008
C	1.547996	-1.873254	-0.000254
C	2.054860	-0.701008	-0.003133
C	2.195281	0.593971	-0.005128
C	1.365136	1.551203	-0.004364
C	0.440679	2.495550	-0.003077
Mg	0.961105	4.553080	-0.007550
Mg	0.720629	7.356101	-0.001342
O	-1.244386	7.042871	0.002520
C	-1.399580	5.805130	0.002240
C	-1.293832	4.569558	-0.000448

O	-1.817554	3.350428	0.002160
16			
123	c13 scf done: -1006.817738		
C	-0.926695	2.282763	0.026922
C	-1.445325	1.005673	0.039794
C	-1.269099	-0.224160	0.029450
C	-0.847939	-1.487685	0.010968
C	0.365451	-1.840267	-0.030148
C	1.682542	-1.794883	-0.073439
C	2.150438	-0.602280	-0.083766
C	2.258477	0.690447	-0.082093
C	1.425909	1.648835	-0.050038
C	0.479169	2.562384	-0.016865
Mg	0.370351	4.686849	-0.000725
O	0.152151	6.470491	0.783810
O	0.104742	6.476633	-0.756739
Mg	-1.625179	6.558745	0.067581
C	-2.199785	4.607109	0.077758
C	-1.729191	3.471838	0.057528

16			
124	c59 scf done: -1006.808350		
Mg	1.667629	-0.119524	-1.368910
C	-0.086912	-0.001863	0.013420
Mg	1.653343	0.059672	1.414823
C	-0.967383	1.100262	-0.060180
C	-1.884402	1.901337	-0.120501
C	-3.266982	2.226612	-0.150147
C	-4.308857	1.288432	-0.094529
C	-4.259113	0.005380	-0.009718
C	-4.325402	-1.279456	0.073528
C	-3.282627	-2.216337	0.139537
C	-1.899535	-1.893112	0.126225
C	-0.977378	-1.097129	0.079274
C	-3.748873	3.491821	-0.236640
C	-3.769902	-3.480257	0.218095
O	-4.178483	4.547971	-0.308999
O	-4.204209	-4.534872	0.283373

16			
125	c71 scf done: -1006.799876		
C	-0.000000	0.614026	0.416585
C	0.000000	-0.614026	0.416585
C	-0.000000	1.945671	0.350343
C	0.000000	-1.945671	0.350343
C	-0.000000	3.166123	0.228584
C	0.000000	-3.166123	0.228584
C	-0.000000	4.495796	0.041728
C	0.000000	-4.495796	0.041728
C	0.000000	5.716238	-0.134097
C	0.000000	-5.716238	-0.134097
Mg	0.000000	7.543045	-1.009129
Mg	0.000000	-7.543045	-1.009129
C	-0.000000	9.350588	0.338818
C	0.000000	-9.350588	0.338818
O	-0.000000	10.457477	0.582223
O	0.000000	-10.457477	0.582223

16
 126 c33 scf done: -1006.801338
 Mg -1.236280 2.673554 -0.000821
 O -1.025118 0.745188 -0.004596
 C 0.153951 0.220190 -0.003788
 C 0.429691 -1.104768 -0.006080
 C 0.766715 -2.304397 -0.008017
 C 1.111253 -3.565842 -0.010074
 C 1.452724 -4.791061 -0.011974
 C 1.218347 1.200486 -0.000030
 C 1.418454 2.418253 0.002903
 C 0.833389 3.691796 0.004660
 O 1.430799 4.804671 0.007946
 Mg 0.352923 6.379525 0.009546
 C -1.135925 7.733800 0.010038
 C -1.858352 6.715586 0.006733
 C -2.409177 5.458256 0.003187
 C -2.557373 4.237255 0.000366

16
 127 c86 scf done: -1006.799195
 Mg 0.093772 0.000000 1.000000
 C 1.706239 0.000000 1.000000
 C -1.575684 0.000000 1.000000
 C 3.000181 0.000000 1.000000
 C -2.915151 0.000000 1.000000
 C 4.493427 0.000000 1.000000
 C -4.370693 0.000000 1.000000
 C 5.881820 0.000000 1.000000
 C -5.796027 0.000000 1.000000
 C 7.256652 0.000000 1.000000
 Mg -7.171098 0.000000 1.000000
 C 8.611125 0.000000 1.000000
 C -9.249143 0.000000 1.000000
 C 10.056204 0.000000 1.000000
 O -10.688104 0.000000 1.000000
 O 11.483913 0.000000 1.000000

16
 128 c21 scf done: -1006.799877
 C -2.719300 5.190287 0.052883
 Mg -2.392898 3.000640 0.049510
 C -1.234965 1.183014 0.026203
 C -1.049960 -0.090868 0.023370
 C -0.745123 -1.347843 0.017320
 C 0.415422 -1.890477 -0.007617
 C 1.698454 -2.094094 -0.035314
 C 2.355439 -0.973247 -0.049956
 C 2.672919 0.268193 -0.057431
 C 1.898259 1.303485 -0.041789
 C 1.033670 2.257423 -0.024047
 Mg 0.362816 4.304428 -0.011401
 C -1.123206 5.945301 0.019297
 O -1.109135 7.125848 0.021181
 C -0.386946 2.324320 0.006790
 O -3.640683 5.928285 0.069357

16

129 c20 scf done: -1006.803856

C	-0.794432	2.426009	0.433751
C	-1.321701	1.190203	0.224581
C	-1.295332	-0.026154	-0.007747
C	-1.002265	-1.305872	-0.268166
C	0.173231	-1.728921	-0.407566
C	1.498678	-1.687976	-0.466505
C	2.048366	-0.570998	-0.274102
C	2.120108	0.722721	-0.029405
C	1.486405	1.758704	0.203481
C	0.578610	2.780703	0.457593
O	1.006962	3.986721	0.712544
Mg	0.492275	5.684546	0.123205
Mg	-0.931082	7.552887	-1.153751
C	-1.711407	5.690466	-0.425023
C	-1.683446	4.577059	0.119892
O	-1.718951	3.462396	0.757216

16

130 c64 scf done: -1006.802264

C	-0.943245	-0.000000	-4.084017
C	-0.213675	-0.000000	-2.972050
C	0.421594	0.000000	-0.251936
C	0.190532	1.254470	-2.364839
C	0.190532	-1.254470	-2.364839
Mg	0.947739	3.011800	-1.792536
Mg	0.947739	-3.011800	-1.792536
C	0.527966	1.242789	-1.000384
C	0.527966	-1.242789	-1.000384
C	0.216840	0.000000	1.064751
C	0.055333	0.000000	2.318615
C	-0.116162	0.000000	3.585945
C	-0.285854	0.000000	4.850601
C	-0.456615	0.000000	6.113890
O	-0.612008	-0.000000	7.270079
O	-1.561481	-0.000000	-5.056119

16

131 c58 scf done: -1006.802528

C	-0.112506	0.018507	2.213031
C	0.080504	-0.608124	-0.308721
C	0.017271	1.107579	1.371440
C	-0.086272	-1.372580	2.041005
Mg	0.197325	1.802712	3.354415
Mg	-0.344481	-1.007694	4.072468
C	-0.047626	0.789218	-0.047259
C	0.135473	-1.569771	0.653834
C	-0.116870	1.740935	-1.000121
C	0.163301	-1.972973	-0.712138
C	-0.127434	2.677610	-1.832006
C	0.208825	-2.907946	-1.650215
C	-0.169754	3.622341	-2.707252
C	0.201026	-3.228057	-2.884757
O	-0.202552	4.472784	-3.488403
O	0.206943	-3.653443	-3.974863

16

132 c56 scf done: -1006.796707

C	-0.420462	2.611909	-0.003879
Mg	-2.713244	0.748599	-0.068260
C	-1.731105	2.512639	-0.027706
Mg	2.500821	3.050458	0.063276
C	3.922668	1.579066	0.072748
C	3.134724	0.594097	0.044619
C	2.334834	-0.469864	0.015465
C	1.144100	-0.931554	-0.013975
C	0.000694	-1.500468	-0.043217
C	-1.324582	-1.374452	-0.067496
C	-2.583381	-1.293094	-0.090798
C	0.535595	3.513621	0.030010
C	-0.441623	4.705752	0.037439
O	-0.186748	5.859103	0.064913
C	-1.954573	4.037643	-0.001002
O	-2.979138	4.626001	-0.006090

16

133	c85	scf done:	-1006.789876		
C	-0.173706	0.000000	1.000000		
C	1.054086	0.000000	1.000000		
C	-1.522634	0.000000	1.000000		
Mg	3.067396	0.000000	1.000000		
C	-2.743731	0.000000	1.000000		
C	5.070197	0.000000	1.000000		
C	-4.091654	0.000000	1.000000		
C	6.320696	0.000000	1.000000		
C	-5.320114	0.000000	1.000000		
C	7.630392	0.000000	1.000000		
Mg	-7.301946	0.000000	1.000000		
C	8.896251	0.000000	1.000000		
C	-9.373821	0.000000	1.000000		
C	10.179852	0.000000	1.000000		
O	-10.521874	0.000000	1.000000		
O	11.348040	0.000000	1.000000		

16

134	c63	scf done:	-1006.795659		
C	-0.000000	0.000000	0.031382		
C	-0.000000	0.000000	1.358333		
C	-0.000000	-0.000000	4.238292		
C	-1.263750	0.000000	2.078524		
C	1.263750	0.000000	2.078524		
Mg	-3.090141	0.000000	2.828212		
Mg	3.090141	-0.000000	2.828212		
C	-1.245289	0.000000	3.484142		
C	1.245289	-0.000000	3.484142		
C	0.000000	-0.000000	5.568799		
C	0.000000	-0.000000	6.837059		
C	0.000000	-0.000000	8.113768		
C	0.000000	-0.000000	9.395416		
C	0.000000	-0.000000	10.667435		
O	0.000000	-0.000000	11.838922		
O	-0.000000	0.000000	-1.124954		

16

135	c62	scf done:	-1006.790896		
O	0.000005	0.168381	0.053433		

C	-0.000010	0.162136	1.244379
C	-0.000010	-0.140569	4.388542
C	-1.175412	0.118038	2.188505
C	1.175384	0.118342	2.188534
Mg	-3.181621	-0.143725	2.762856
Mg	3.181654	-0.142853	2.762969
C	-1.111772	-0.065339	3.486761
C	1.111767	-0.065053	3.486790
C	-0.000037	-0.114611	5.738597
C	-0.000036	-0.067843	6.984132
C	-0.000010	-0.033242	8.285588
C	0.000024	0.000333	9.543849
C	0.000148	0.035306	10.832306
C	0.000153	0.069600	12.101972
O	-0.000226	0.101100	13.270992

16

136 c68 scf done:	-1006.792235		
C	0.425680	-0.000000	1.408883
C	0.425680	0.000000	-1.408883
C	-0.098564	-0.000000	2.623543
C	-0.098564	0.000000	-2.623543
C	-0.579325	-0.000000	3.796637
C	-0.579325	0.000000	-3.796637
C	-1.079939	-0.000000	4.972444
C	-1.079939	0.000000	-4.972444
O	-1.532527	-0.000000	6.045696
O	-1.532527	0.000000	-6.045696
C	0.715415	1.242041	0.700581
C	0.715415	1.242041	-0.700581
C	0.715415	-1.242041	-0.700581
C	0.715415	-1.242041	0.700581
Mg	1.331675	-2.998770	-0.000000
Mg	1.331675	2.998770	0.000000

16

137 c70 scf done:	-1006.782855		
C	0.066798	0.000000	1.000000
C	1.297881	0.000000	1.000000
C	-1.262829	0.000000	1.000000
C	2.627508	0.000000	1.000000
C	-2.491976	0.000000	1.000000
C	3.856655	0.000000	1.000000
C	-3.831472	0.000000	1.000000
C	5.196151	0.000000	1.000000
C	-5.064484	0.000000	1.000000
C	6.429163	0.000000	1.000000
Mg	-7.043856	0.000000	1.000000
Mg	8.408535	0.000000	1.000000
C	-9.113023	0.000000	1.000000
C	10.477702	0.000000	1.000000
O	-10.261753	0.000000	1.000000
O	11.626432	0.000000	1.000000

16

138 c66 scf done:	-1006.786303		
C	0.000000	0.000000	1.453855
C	0.000000	-0.000000	-1.453855

C	0.000000	0.000000	2.776737
C	0.000000	-0.000000	-2.776737
C	0.000000	0.000000	4.048088
C	0.000000	-0.000000	-4.048088
C	0.000000	0.000000	5.324421
C	0.000000	-0.000000	-5.324421
O	0.000000	0.000000	6.493369
O	0.000000	-0.000000	-6.493369
C	0.000000	1.250247	0.702062
C	0.000000	1.250247	-0.702062
C	-0.000000	-1.250247	-0.702062
C	-0.000000	-1.250247	0.702062
Mg	0.000000	-3.087041	0.000000
Mg	0.000000	3.087041	-0.000000

16

139 c84 scf done: -1006.776749

C	0.000000	0.000000	0.628333
C	0.000000	0.000000	-0.596156
C	0.000000	0.000000	1.965175
C	0.000000	0.000000	-1.941480
C	0.000000	0.000000	3.190056
C	0.000000	0.000000	-3.170999
C	0.000000	0.000000	4.534024
Mg	0.000000	0.000000	-5.177905
C	0.000000	0.000000	5.764354
C	0.000000	0.000000	-7.189798
Mg	0.000000	0.000000	7.747578
C	0.000000	0.000000	-8.451504
C	0.000000	0.000000	9.816033
C	0.000000	0.000000	-9.750687
O	0.000000	0.000000	10.964832
O	0.000000	0.000000	-10.917354

16

140 c67 scf done: -1006.779149

C	0.000000	0.322282	-3.649647
C	0.000000	0.254216	-2.294407
C	-0.000000	0.096295	0.594564
C	0.000000	1.450698	-1.479522
C	0.000000	-1.029054	-1.611585
Mg	0.000000	3.260178	-0.691654
Mg	-0.000000	-2.913399	-1.012822
C	0.000000	1.383667	-0.071214
C	-0.000000	-1.109749	-0.206110
C	-0.000000	0.025597	1.942996
C	-0.000000	-0.036974	3.194426
C	-0.000000	-0.102191	4.489112
C	-0.000000	-0.165838	5.754884
O	-0.000000	-0.224585	6.926640
C	0.000000	-0.373511	-4.731583
O	0.000000	-0.836574	-5.807939

16

141 c65 scf done: -1006.778172

C	0.000000	0.000000	-3.617298
C	0.000000	0.000000	-2.269782
C	0.000000	-0.000000	0.621604

C	0.000000	1.244655	-1.521857
C	-0.000000	-1.244655	-1.521857
Mg	0.000000	3.091544	-0.823329
Mg	-0.000000	-3.091544	-0.823329
C	0.000000	1.248151	-0.112677
C	-0.000000	-1.248151	-0.112677
C	0.000000	-0.000000	1.971978
C	0.000000	-0.000000	3.224950
C	0.000000	-0.000000	4.521174
C	0.000000	-0.000000	5.788768
O	0.000000	-0.000000	6.962105
C	0.000000	0.000000	-4.881093
O	0.000000	0.000000	-6.060542

16

142 c54 scf done: -1006.766677

C	-0.000000	-0.000000	1.851273
C	-0.000000	0.000000	-0.874884
C	0.361211	1.209223	1.331453
C	-0.361211	-1.209223	1.331453
Mg	0.681546	1.290834	3.423209
Mg	-0.681546	-1.290834	3.423209
C	0.063801	1.199488	-0.100771
C	-0.063801	-1.199488	-0.100771
C	0.000217	2.312507	-0.861700
C	-0.000217	-2.312507	-0.861700
C	-0.048938	3.366590	-1.541234
C	0.048938	-3.366590	-1.541234
C	-0.107890	4.421996	-2.271157
C	0.107890	-4.421996	-2.271157
O	-0.160967	5.373621	-2.922863
O	0.160967	-5.373621	-2.922863

16

143 c6 scf done: -1006.765560

C	1.392105	-1.771411	0.119596
C	0.270218	-1.283954	0.078728
C	-1.010007	-0.697240	0.030529
Mg	-2.952345	-1.491749	0.056671
O	-4.200381	-0.278919	-0.800302
O	-4.217026	-0.187923	0.737444
Mg	-3.142908	1.190803	-0.104190
C	-1.107994	0.679023	-0.052002
C	0.076311	1.442040	-0.084804
C	1.118066	2.083768	-0.112133
C	2.458431	2.289481	-0.110578
C	3.652518	2.022703	-0.082133
C	4.555025	1.004664	-0.012273
C	4.640568	-0.214376	0.061278
C	3.892726	-1.351316	0.120977
C	2.747884	-1.783942	0.134744

16

144 c52 scf done: -1006.759914

C	-0.000000	0.000000	0.944807
C	-0.000000	0.000000	3.808541
C	-1.255680	-0.000000	1.541826
C	1.255680	0.000000	1.541826

Mg	-1.447807	-0.000000	-0.593611
Mg	1.447807	0.000000	-0.593611
C	-1.184491	-0.000000	2.983889
C	1.184491	0.000000	2.983889
C	-2.364348	-0.000000	3.651518
C	2.364348	0.000000	3.651518
C	-3.485622	-0.000000	4.208466
C	3.485622	0.000000	4.208466
C	-4.616945	-0.000000	4.821143
C	4.616945	0.000000	4.821143
O	-5.631727	-0.000000	5.367485
O	5.631727	0.000000	5.367485

16

145 c16 scf done: -1006.747521

C	-0.786262	2.512151	-0.409928
C	-1.458381	1.337472	-0.217338
C	-1.372317	0.117073	0.006989
C	-1.062719	-1.157236	0.226906
C	0.105520	-1.625213	0.316640
C	1.423912	-1.707473	0.333474
C	2.009273	-0.589368	0.150732
C	2.223248	0.677698	-0.066490
C	1.473789	1.680745	-0.236706
C	0.611452	2.679010	-0.378149
Mg	1.172510	4.698069	-0.192222
C	1.016210	6.628721	0.393846
C	-0.202770	6.389306	0.514365
Mg	-1.960797	5.405334	0.351715
O	-2.786342	3.782226	-0.080277
O	-1.460307	3.683979	-0.713556

16

146 c80 scf done: -1006.734059

C	1.148145	5.871990	0.052402
C	1.869566	4.818054	0.050640
C	2.573747	3.707917	0.048481
C	3.317824	2.693672	0.048520
C	3.720697	1.404348	0.034323
C	4.818108	0.697601	0.050287
O	5.691741	-0.055412	0.059311
Mg	1.589568	1.252118	-0.007518
C	-0.284791	0.588222	-0.037679
C	-1.451849	0.219182	-0.054484
C	-2.752777	-0.176023	-0.071801
C	-3.926847	-0.523917	-0.086970
Mg	-5.866061	-1.043645	-0.109663
C	-7.788745	-1.572013	-0.130538
C	-9.028635	-1.912400	-0.143166
O	-10.163139	-2.223641	-0.154929

16

147 c5 scf done: -1006.739512

C	1.471992	-1.793195	-0.004246
C	2.808277	-1.673418	-0.003502
C	3.976191	-1.269730	-0.002005
C	4.522358	-0.037189	0.000735
C	4.562583	1.198237	0.003414

C	3.465830	2.012792	0.004562
C	2.295200	2.367176	0.004776
C	0.990269	1.972915	0.003179
C	-0.074649	1.389558	0.001329
C	-1.152534	0.455462	-0.001133
O	-2.341402	1.110835	-0.000670
O	-3.448857	0.203169	-0.003110
Mg	-5.333461	-0.328481	-0.009154
Mg	-2.899632	-1.686494	-0.005494
C	-0.987009	-0.898602	-0.003378
C	0.318036	-1.371373	-0.003753

16

148 c75 scf done: -1006.733468

C	0.266143	-1.636172	0.021709
C	-1.064083	-1.380873	0.015727
C	-2.195855	-0.967704	0.005419
O	-3.358590	-0.364317	-0.006398
C	-3.211214	0.954407	-0.027949
C	-3.045323	2.159877	-0.047843
Mg	-1.579229	3.530759	-0.068707
C	0.271704	4.313053	-0.079819
C	1.503009	4.315601	-0.080440
Mg	3.349348	3.523108	-0.064550
C	4.808496	2.144940	-0.039473
C	4.969454	0.938877	-0.015635
O	5.111454	-0.380471	0.007273
C	1.481518	-1.638462	0.023686
C	2.812720	-1.388226	0.021195
C	3.946026	-0.979118	0.015781

16

149 c57 scf done: -1006.729833

C	-0.000000	0.000000	1.515259
C	0.000000	-0.000000	3.911074
C	-1.287270	0.000000	1.710249
C	1.287270	0.000000	1.710249
Mg	-1.466096	0.000000	-0.403131
Mg	1.466096	0.000000	-0.403131
C	-1.377038	0.000000	3.194065
C	1.377038	-0.000000	3.194065
O	-2.402447	0.000000	3.831200
O	2.402447	-0.000000	3.831200
C	0.000000	-0.000000	5.231293
C	0.000000	-0.000000	6.490367
C	0.000000	-0.000000	7.778123
C	0.000000	-0.000000	9.038903
C	0.000000	-0.000000	10.335282
C	0.000000	-0.000000	11.614283

16

150 c11 scf done: -1006.725950

C	-0.556174	2.399438	0.141711
C	-1.280757	1.231892	0.008513
C	-1.309758	-0.005343	-0.096863
C	-1.101887	-1.316989	-0.199285
C	0.032186	-1.874326	-0.198645
C	1.337319	-2.060835	-0.155150

C	1.999122	-0.969828	-0.036994
C	2.323422	0.279903	0.085836
C	1.656720	1.360553	0.144938
C	0.873444	2.413495	0.206198
Mg	1.139372	4.524043	0.236381
Mg	0.166006	7.048295	-0.359096
O	-1.702689	6.880743	-0.761436
O	-1.909938	6.062731	0.474416
C	-1.544860	4.848362	0.290388
C	-1.175513	3.690356	0.219087

16

151 c31 scf done: -1006.711524

C	-1.020867	3.061089	0.001025
C	-1.717928	1.875306	0.002924
Mg	-0.286130	0.331657	0.000697
O	-0.240843	-1.789785	0.001872
C	0.627098	-2.579518	0.001021
C	1.571162	-3.438164	-0.000106
C	2.492862	-4.328007	-0.001179
C	1.752459	0.980509	-0.003093
C	1.270088	2.123353	-0.002529
C	0.446213	3.277311	-0.001455
O	0.966960	4.440816	-0.002472
Mg	0.058770	6.115259	-0.001549
C	-1.187941	7.831681	-0.000163
C	-1.940399	6.834028	0.001298
C	-2.133414	5.463478	0.002001
C	-1.712072	4.313482	0.001707

16

152 c76 scf done: -1006.707712

C	-3.501321	-1.944166	-0.013309
Mg	-1.251611	-1.923773	-0.005926
C	0.765706	-2.123208	0.000856
C	1.994925	-2.052914	0.004307
Mg	3.951409	-1.569903	0.009036
C	6.057472	-1.001900	0.010568
O	7.205962	-1.327054	0.012621
C	5.415681	0.309777	0.007542
C	4.317054	0.903551	0.005211
C	3.094791	1.437343	0.002289
C	1.903281	1.732990	-0.000674
C	0.570167	1.694847	-0.003441
C	-0.625981	1.441767	-0.006067
C	-1.846075	0.872453	-0.008719
C	-2.855382	0.192914	-0.011422
O	-3.879122	-0.620501	-0.014243

16

153 c17 scf done: -1006.700389

C	-0.389142	2.389886	0.136804
C	-0.939508	1.181215	0.194860
C	-1.360387	-0.012522	0.238687
C	-0.814773	-1.190191	0.154818
C	0.013838	-2.157063	0.038597
C	1.267407	-1.771792	-0.121721
C	2.281942	-1.030165	-0.244943

C	2.223766	0.307275	-0.224286
C	1.849588	1.489166	-0.162910
C	1.030079	2.571975	-0.044957
Mg	1.403897	4.599418	-0.005532
O	-0.136266	5.549930	0.562728
O	-0.788701	6.720129	-0.044059
C	-1.985498	6.243348	-0.292423
C	-3.005875	5.545818	-0.414667
Mg	-1.704349	4.076066	0.229001

16

154	c9	scf done:	-1006.695426	
C	-0.432500	-0.101704	2.548529	
C	-0.551534	-1.340471	1.909916	
C	-0.125919	-1.568380	0.627564	
C	0.307001	-1.629986	-0.546439	
C	0.869225	-0.987401	-1.518248	
C	1.397388	0.020563	-2.121918	
C	1.387685	1.033589	-1.321607	
C	1.157376	1.681038	-0.226726	
C	0.650587	1.423944	0.895851	
C	0.096153	1.120839	2.108029	
O	-1.093510	-2.414719	2.499316	
O	-1.548865	-2.238229	3.820302	
Mg	-1.301564	-0.479133	4.522693	
Mg	-0.895374	2.120739	5.455115	
C	0.009792	3.125548	3.866888	
C	0.074058	2.232396	3.016045	

16

155	c53	scf done:	-1006.681623	
C	-2.108877	-1.486245	-0.216445	
C	6.509102	-0.194963	-0.113901	
C	-4.067774	0.126149	0.083955	
C	5.272351	0.087874	-0.049361	
C	-3.225183	-0.952787	-0.110700	
C	2.044832	1.332153	0.205741	
C	-6.632677	0.544999	0.189923	
O	3.372897	1.406065	0.200282	
C	-5.381561	0.281852	0.128240	
C	0.841634	1.488350	0.248612	
Mg	-2.123167	0.964198	0.199869	
C	3.942571	0.158016	-0.019628	
C	-0.822825	-1.875788	-0.300135	
O	-0.407440	1.600284	0.284631	
C	0.398633	-2.033512	-0.343564	
Mg	2.162983	-0.999379	-0.191947	

16

156	c55	scf done:	-1006.673615	
C	0.016366	0.777971	1.665060	
C	-0.009071	-0.379523	4.060080	
C	-1.137523	0.158955	2.116105	
C	1.141524	0.107794	2.115619	
Mg	-1.360793	0.207841	-0.031386	
Mg	1.365833	0.146638	-0.032001	
O	-1.151262	-0.436636	3.333851	
O	1.129095	-0.487779	3.333359	

C	-0.006599	-0.284107	5.381010
C	-0.004685	-0.212090	6.631857
C	-0.002584	-0.132306	7.921593
C	-0.000454	-0.054473	9.177064
C	0.001784	0.025205	10.464726
C	0.003906	0.105168	11.719490
C	0.006094	0.187810	13.016277
C	0.008371	0.269532	14.287759

16

157 c69 scf done: -1006.653705

C	-0.000000	0.027746	1.902974
Mg	-0.000000	0.017284	3.888527
O	-0.000000	0.002117	5.703215
C	0.000000	-0.014520	6.945099
C	-0.000000	0.029045	0.679764
C	-0.000000	0.029045	-0.679764
C	-0.000000	0.027746	-1.902974
Mg	-0.000000	0.017284	-3.888527
O	-0.000000	0.002117	-5.703215
C	0.000000	-0.014520	-6.945099
C	0.000000	-0.031364	8.177440
C	0.000000	-0.049813	9.503837
C	0.000000	-0.068004	10.782291
C	0.000000	-0.031364	-8.177440
C	0.000000	-0.049813	-9.503837
C	0.000000	-0.068004	-10.782291

16

158 c81 scf done: -1006.663171

C	-1.488307	2.601523	0.000000
C	-0.202606	2.158762	0.000000
C	-0.045301	0.737311	0.000000
C	-1.273640	-0.140448	0.000000
C	-2.559263	0.302972	-0.000000
C	-2.716554	1.724304	-0.000000
C	-1.888750	4.101191	-0.000000
C	-3.217380	3.933032	-0.000000
C	-3.697203	2.666967	-0.000000
C	0.935480	-0.205590	0.000000
C	0.455848	-1.471517	0.000000
C	-0.873657	-1.638709	0.000000
Mg	-2.890371	-1.715137	-0.000000
Mg	0.128987	4.177740	0.000000
O	1.873542	-1.271629	0.000000
O	-4.636202	3.731375	-0.000000

16

159 c88 scf done: -1006.629674

C	-1.517462	-1.940921	-0.000000
C	-2.409099	-0.855214	-0.000000
C	-3.850527	-1.040253	0.000000
C	-4.371235	-2.348021	-0.000000
C	-3.451979	-3.452600	-0.000000
C	-2.098069	-3.262595	-0.000000
C	-2.199725	0.519526	-0.000000
C	-2.863814	1.564980	0.000000
C	-4.251412	1.408799	0.000000

C	-4.704977	0.106872	0.000000
O	-5.147621	2.433471	0.000000
C	-6.468695	2.298553	0.000000
C	-6.983058	0.847957	0.000000
O	-6.057614	-0.095408	0.000000
Mg	-5.384726	-4.042661	0.000000
Mg	-0.087546	-3.312081	-0.000000

16

160 c48 scf done: -1006.612045

O	-4.178894	2.081699	0.001042
C	-3.332578	1.073840	-0.000932
C	-2.415846	0.291308	-0.002578
C	-1.268840	-0.426873	-0.004243
C	-0.132429	-0.863199	-0.005377
C	1.201424	-1.107205	-0.006085
C	2.431696	-1.190989	-0.006414
Mg	3.593566	0.450240	-0.003892
C	4.073070	2.383770	-0.000767
O	3.503079	3.469446	0.001177
C	3.001841	4.586234	0.003240
Mg	1.247573	5.517014	0.005375
C	-0.746281	5.780935	0.006465
C	-1.752474	5.079568	0.005582
C	-2.756938	4.157993	0.004405
C	-3.521950	3.228716	0.003002

16

161 c25 scf done: -1006.607174

C	3.071182	-0.163364	1.000000
C	1.833391	0.401205	1.000000
C	0.584933	-0.167762	1.000000
C	0.849906	1.274687	1.000000
C	2.963072	-1.554626	1.000000
O	0.975665	2.567397	1.000000
C	2.405920	2.873265	1.000000
C	2.701579	4.228779	1.000000
C	4.134925	4.366012	1.000000
Mg	6.187520	4.254861	1.000000
C	4.676446	3.033046	1.000000
C	3.642599	2.100576	1.000000
Mg	3.108176	6.129407	1.000000
O	4.071152	0.751806	1.000000
C	0.380079	-1.584939	1.000000
C	1.678934	-1.843673	1.000000

16

162 c87 scf done: -1006.565175

C	-4.624903	3.898474	0.000000
C	-3.257179	4.115979	0.000000
C	-2.368312	3.014495	0.000000
C	-2.752510	1.656999	0.000000
C	-4.340702	1.404329	0.000000
C	-5.127621	2.575689	0.000000
C	-4.730413	0.110585	-0.000000
C	-3.875192	-0.909616	-0.000000
C	-2.477345	-0.687340	-0.000000
C	-1.980494	0.547899	-0.000000

O	-4.291342	-2.284961	-0.000000
C	-3.589432	-3.340059	-0.000000
C	-1.994624	-3.086226	-0.000000
O	-1.655478	-1.864844	-0.000000
Mg	-1.344999	4.725585	0.000000
Mg	-6.632090	3.883235	0.000000

16

163 c24 scf done: -1006.542967

C	0.000000	-0.000000	-2.823190
C	0.000000	-0.000000	2.446865
C	0.008151	1.449044	-3.135217
C	-0.008151	-1.449044	-3.135217
C	0.006264	1.083877	-1.837991
C	-0.006264	-1.083877	-1.837991
C	0.004024	0.694368	-0.484618
C	-0.004024	-0.694368	-0.484618
Mg	-0.000000	-0.000000	-6.800452
C	0.008160	1.414575	3.067906
C	-0.008160	-1.414575	3.067906
C	0.007138	1.236498	1.758285
C	-0.007138	-1.236498	1.758285
Mg	0.000000	-0.000000	6.665610
O	0.009396	1.625595	0.498156
O	-0.009396	-1.625595	0.498156

16

164 c23 scf done: -1006.497508

C	3.265510	0.000000	1.000000
C	-1.861397	-0.000000	1.000000
C	3.733537	1.372862	1.000000
C	3.733537	-1.372862	1.000000
C	2.354648	1.165604	1.000000
C	2.354648	-1.165604	1.000000
C	1.071887	0.763490	1.000000
C	1.071887	-0.763490	1.000000
Mg	5.366314	0.000000	1.000000
C	-2.520705	1.367191	1.000000
C	-2.520705	-1.367191	1.000000
C	-1.201524	1.267576	1.000000
C	-1.201524	-1.267576	1.000000
Mg	-4.804723	-0.000000	1.000000
O	0.012498	1.683759	1.000000
O	0.012498	-1.683759	1.000000

Optimized geometries of C12O2Mg2 (triplets) obtained at the UPBE0-D3/def2-TZVP level

16
t21 scf done: -1006.883654
C -1.822680 1.176698 0.003082
O 6.475989 0.147372 -0.013938
C -4.047257 0.209338 -0.001864
C 5.327187 -0.020263 -0.008637
C -3.172143 1.275333 -0.000582
C 1.884664 -1.477371 0.004366
O -6.451650 -0.302264 -0.010350
C 3.025836 -1.012147 0.000573
C -5.343508 0.024179 -0.006491
C 0.601275 -1.922091 0.007118
Mg -2.218245 -0.960562 0.004844
C 4.036113 -0.070409 -0.002641
C -0.636298 1.788832 0.003734
C -0.603190 -2.179273 0.009629
C 0.565381 2.146901 0.004668
Mg 2.293999 1.093842 0.008659

16
c79 scf done: -1006.898275
C -3.051459 0.564981 -0.055571
Mg -1.405540 1.910086 -0.025376
C 0.087907 3.245484 0.002740
C 1.309298 3.412417 0.020337
Mg 3.104918 2.523699 0.040511
C 5.051219 1.668511 0.062736
C 4.286085 0.535422 0.045889
C 3.043260 0.171775 0.026614
C 1.833973 -0.272276 0.007407
C 0.568124 -0.444924 -0.011030
C -0.715910 -0.340047 -0.028230
C -2.010598 -0.321635 -0.046060
C -4.354772 0.580449 -0.073551
O -5.497480 0.767201 -0.088395
C 6.302714 2.032626 0.082101
O 7.353564 2.518733 0.099324

16
t3 scf done: -1006.889563
O -5.410735 -1.964823 -0.028408
O 5.390885 -2.140246 0.110376
C -4.293522 -1.663667 -0.019056
C 4.339465 -1.660850 0.089528
C -3.090607 -1.160147 -0.011907
Mg -2.155746 0.807195 -0.031272
C 1.750078 2.822902 -0.015048
C -1.786259 -1.570836 0.011135
C 3.236916 -0.967195 0.064597
C -2.073175 2.838045 -0.062254
Mg 2.550734 1.004246 0.024274
C -0.667738 -0.785238 0.012652
C 1.889367 -1.189692 0.051261
C -0.841687 2.970566 -0.049112

C	0.526813	2.964190	-0.032264
C	0.649814	-1.032676	0.033153
16			
t7	scf done: -1006.890796		
O	6.884004	0.434098	0.009803
O	-6.447721	-0.309365	0.007338
C	5.759496	0.106746	0.008283
C	-5.302739	-0.483914	0.006239
C	-4.001386	-0.497247	0.005892
C	4.568110	-0.349978	0.006029
Mg	-2.331114	0.798951	0.011543
C	2.145082	-1.144522	0.002175
C	-2.951738	-1.374733	0.001759
C	0.874430	-1.355853	0.001339
C	-0.670194	1.964074	0.015873
C	3.258633	-0.432881	0.005536
C	0.378407	2.636003	0.018456
C	-0.386733	-1.605993	0.000320
C	-1.673912	-1.471965	0.001074
Mg	1.556908	1.015206	0.011771
16			
t2	scf done: -1006.880576		
C	3.655132	-0.760710	-0.002485
C	1.281689	2.575761	0.000546
C	1.197490	-1.566091	-0.001043
O	-5.112740	-0.414643	-0.002148
C	-4.700744	0.763774	0.001352
C	-1.359299	-1.946074	0.001257
Mg	-3.162386	-1.039135	0.006279
C	2.410585	-1.360806	-0.002176
Mg	2.443850	0.925327	-0.000531
C	-1.292345	2.588539	0.006373
C	0.036343	2.638778	0.004022
C	4.898983	-1.113951	-0.004193
C	-3.355783	1.103938	0.009946
O	6.042714	-1.310121	-0.005390
C	-2.403205	1.996749	0.008372
C	-0.137757	-1.809452	0.000100
16			
c77	scf done: -1006.877117		
O	-3.740700	-1.647843	-0.134818
C	-3.911244	-0.405954	-0.109709
C	-3.544509	0.790240	-0.104714
C	-3.184648	2.069864	-0.098953
C	-2.274573	2.944175	-0.118237
C	-1.277753	3.763255	-0.143428
C	-0.038027	4.088226	-0.183657
C	1.238013	4.203696	-0.229622
C	2.538397	4.393566	-0.275535
C	3.617896	3.549500	-0.327094
C	4.921107	3.606391	-0.374296
O	6.071010	3.479923	-0.418216
Mg	2.059309	2.081798	-0.290882
C	1.007751	0.351584	-0.278748
C	0.084904	-0.462674	-0.255482

Mg -1.838835 -0.975652 -0.193203

16

c26 scf done: -1006.887976

C	0.602831	0.768471	-0.004108
C	-0.481544	1.600534	-0.003641
C	-1.778234	1.516188	-0.002411
C	-3.066294	1.524679	0.000308
C	-4.299244	1.085906	0.002955
C	-4.622328	-0.245211	0.004433
C	-4.527130	-1.503633	0.004622
Mg	-2.495813	-0.794148	0.000255
O	-0.652837	-1.270333	-0.003265
C	0.474269	-0.717722	-0.004122
O	1.531588	-1.442673	-0.004561
Mg	3.357461	-1.025306	0.000643
C	5.264229	-0.121759	0.007274
C	4.442785	0.820517	0.004494
C	3.157484	1.315094	0.000729
C	1.938209	1.213184	-0.001896

16

t63 scf done: -1006.877275

O	-5.892577	-1.099539	-0.291694
C	2.975806	3.207051	1.160358
C	-4.732754	-1.072064	-0.338257
C	2.250882	2.025879	0.675944
C	-3.451349	-0.926316	-0.338734
O	2.532374	4.198992	1.620436
C	-2.314878	-1.619157	-0.701976
C	2.884376	0.912133	0.152201
C	-1.112368	-1.878576	-0.877288
C	3.125254	-0.181655	-0.342830
Mg	0.782819	-2.459171	-1.229480
C	3.033045	-1.418616	-0.884196
Mg	-1.805643	0.322181	0.129155
C	0.858894	1.901355	0.691545
C	-0.336303	1.617168	0.626710
C	2.799007	-2.541816	-1.368129

16

c82 scf done: -1006.879589

C	-1.091551	-2.650525	-0.443176
O	5.348989	-1.129976	-0.262236
C	-3.654934	0.278243	0.104868
C	4.679248	-0.174350	-0.085703
Mg	-2.722162	-1.483141	-0.216537
C	1.593540	1.886255	0.316268
O	-6.115340	0.416232	0.162176
C	2.516317	1.093767	0.165195
C	-4.946066	0.350687	0.134946
C	0.406018	2.511881	0.441878
Mg	-2.518426	1.923371	0.378034
C	3.215617	-0.084702	-0.050555
C	0.109580	-2.368726	-0.409926
C	-0.760642	2.906039	0.526683
C	1.359066	-1.864962	-0.338130
C	2.356246	-1.162833	-0.228211

16
t4 scf done: -1006.888186

O	3.002041	1.334915	-0.019716
O	-4.490413	-1.512837	0.006325
C	0.664710	1.502395	-0.014135
C	-3.260971	-1.775372	0.003885
C	1.886760	0.775887	-0.015306
C	-0.693511	-1.548307	-0.003093
C	-0.481029	1.902742	-0.012372
C	-2.032107	-1.687681	0.000488
Mg	4.860902	0.375980	-0.021130
C	0.490840	-1.244271	-0.006525
C	1.756299	-0.684383	-0.010754
C	4.171377	-1.695274	-0.012879
C	-1.825322	2.098265	-0.009558
C	2.969688	-1.356647	-0.011364
C	-3.059436	2.180636	-0.006710
Mg	-3.795598	0.325798	-0.000195

16
c73 scf done: -1006.873802

C	-1.118622	2.094659	-0.004570
C	-2.280115	1.653550	-0.004681
C	-3.339817	0.843267	-0.004115
C	-4.328788	0.091672	-0.004021
Mg	-3.140488	-1.701254	0.002892
C	-1.351721	-2.565450	0.004250
C	-0.128635	-2.474053	0.004903
C	1.214458	-2.240029	0.005392
C	2.394738	-1.899992	0.005233
Mg	3.442940	-0.174256	0.003416
C	3.988495	2.121122	-0.000406
O	4.893222	1.261678	0.002942
C	2.632889	1.824520	-0.001529
C	1.406219	2.272426	-0.003039
C	0.152748	2.408916	-0.004197
O	-4.999276	-0.967934	-0.002469

16
c60 scf done: -1006.871304

C	2.547905	1.596735	-0.027163
Mg	3.614914	-0.074704	-0.026939
C	5.582895	-0.995418	-0.038883
O	4.600168	-1.777999	-0.026260
C	2.944216	2.762390	-0.036856
C	3.503681	3.994689	-0.048416
C	4.204143	4.991578	-0.059827
C	5.179505	5.933385	-0.073263
C	6.160802	6.687591	-0.085725
Mg	7.797411	5.488701	-0.093147
C	9.547337	3.890269	-0.099532
O	9.814459	5.101484	-0.108482
C	8.231212	3.390071	-0.085315
C	7.726014	2.158513	-0.074218
C	7.089460	1.089315	-0.062895
C	6.269734	0.038645	-0.050303

16

c28 scf done: -1006.877620

C	-0.759561	2.594044	-0.001512
C	-1.225023	1.308792	-0.008379
C	-1.211817	0.077818	-0.012879
C	-0.935879	-1.229015	-0.016407
C	-0.373915	-2.337775	-0.017841
Mg	1.757776	-2.572617	-0.008449
O	2.337444	-0.550829	0.000874
C	1.908998	0.572971	0.002631
C	1.577746	1.775306	0.005389
C	0.718432	2.834176	0.005686
O	1.132491	4.059470	0.011970
Mg	0.323481	5.731666	0.014716
C	-1.071615	7.315241	0.014702
C	-1.764243	6.273054	0.007900
C	-1.928059	4.911703	0.002142
C	-1.540237	3.748490	-0.000542

16

t6 scf done: -1006.864381

C	3.621962	0.636887	-0.005983
Mg	-4.482860	0.292108	0.013614
C	4.831230	0.188579	-0.012069
O	-3.790140	2.054156	0.023176
C	2.302683	0.302378	-0.004832
C	-4.721148	-1.675687	0.001467
Mg	0.907185	-1.268499	-0.011364
C	-2.536796	1.924668	0.019053
C	6.106284	0.041927	-0.016243
C	-3.501973	-1.923922	-0.003631
O	7.258708	-0.180341	-0.020626
C	-1.326719	1.727066	0.014453
C	1.168172	1.056160	0.003197
C	-2.152641	-2.149097	-0.008699
C	-0.928205	-2.143807	-0.011987
C	-0.035938	1.383148	0.008594

16

t5 scf done: -1006.872430

Mg	-1.999147	1.158057	0.007206
C	3.412827	1.731159	-0.008741
Mg	1.260691	-1.652535	0.015506
C	-4.426673	-1.009831	0.017669
C	3.572833	-2.157529	0.019812
C	-3.217497	-0.563954	0.014595
C	3.507463	0.454043	-0.002539
C	-0.018573	3.191100	-0.007710
O	2.734769	-3.077999	0.030147
C	3.274967	-0.814113	0.004810
O	-5.550823	-1.303546	0.019760
C	-0.679863	-1.081603	0.015602
C	2.404407	2.576115	-0.011162
C	-1.921677	-1.039519	0.016113
C	-1.254833	3.046431	-0.002650
C	1.321698	3.191020	-0.011065

16

c46 scf done: -1006.835602

C	2.559076	1.514062	-0.020855
C	2.954421	2.810412	-0.029884
C	3.416709	3.953402	-0.038960
O	3.505284	5.211162	-0.045395
Mg	1.546009	4.975078	-0.026473
C	-0.450882	5.021191	-0.007660
C	-1.517392	4.363050	0.005425
C	-2.650929	3.682635	0.019049
C	-3.146837	2.461005	0.029186
C	-2.808523	1.182919	0.031621
C	-2.502780	-0.032521	0.033889
Mg	-1.037725	-1.390421	0.025334
O	0.202719	-2.925515	0.019658
C	1.015734	-1.961861	0.008077
C	1.480678	-0.819924	-0.001360
C	2.100771	0.385182	-0.012072

16

t12 scf done:	-1006.877934		
C	4.134227	-1.143048	-0.035003
C	-2.121056	-2.401756	0.029175
C	2.878480	-0.815348	-0.023366
O	1.799084	3.911086	-0.022892
C	2.127402	0.328690	-0.018500
C	-2.346561	1.530313	0.022377
O	5.215008	-1.556357	-0.044725
C	1.140004	1.081282	-0.010416
C	-4.622510	-1.668277	0.051564
C	-0.896553	-2.424611	0.017282
C	-3.457147	-2.102623	0.041309
Mg	0.911681	-1.554898	-0.002462
C	0.212794	2.107239	-0.003498
C	0.694135	3.497527	-0.011213
C	-1.156295	1.833953	0.010383
Mg	-3.869946	0.211649	0.040098

16

c30 scf done:	-1006.865625		
C	-0.802604	2.662649	0.003906
C	-1.317332	1.370553	0.008221
C	-1.684844	0.191901	0.011581
Mg	-0.579253	-1.473262	0.006473
O	0.720400	-3.018963	0.000017
C	1.453969	-1.987658	-0.005378
C	1.774535	-0.791365	-0.008365
C	1.794785	0.551384	-0.009695
C	1.468435	1.747937	-0.008779
C	0.715626	2.878208	-0.005243
O	1.175983	4.111692	-0.008937
Mg	0.389966	5.771507	-0.005746
C	-0.990132	7.368798	0.000793
C	-1.704476	6.334500	0.005804
C	-1.913680	4.990330	0.008162
C	-1.555358	3.804282	0.007185

16

c43 scf done:	-1006.864317		
C	2.521758	0.709783	0.078799

C	1.501046	-0.107651	0.048174
C	0.438275	-0.755058	0.016930
C	-0.881466	-0.963712	-0.023480
C	-2.120736	-1.054314	-0.060637
Mg	-3.335205	0.542512	-0.101322
O	-4.816403	1.816091	-0.148608
C	-3.850569	2.631367	-0.119603
C	-2.729623	3.137776	-0.085311
C	-1.554582	3.829663	-0.049399
C	-0.465110	4.392038	-0.015582
Mg	1.525489	4.657466	0.042414
O	3.393044	5.494517	0.109835
C	3.872939	4.345095	0.123489
C	3.126944	3.181899	0.092841
C	2.973118	1.897580	0.090525

16

c37 scf done: -1006.865778

Mg	1.931256	-1.165624	-0.001771
O	1.068121	-2.995702	-0.004057
C	0.072737	-2.231177	-0.003996
C	-0.0636220	-1.220810	-0.003498
C	-1.055405	0.055374	-0.002585
C	-1.098348	1.283960	-0.001452
C	-0.704897	2.597279	0.000026
C	-1.512125	3.709726	0.000639
C	-1.921698	4.875545	0.001472
C	-1.778854	6.232001	0.002677
C	-1.107661	7.293194	0.003891
Mg	0.328320	5.747477	0.003235
O	1.208173	4.130177	0.002338
C	0.802618	2.878896	0.001109
C	1.659216	1.801976	0.000718
C	2.343691	0.762755	0.000318

16

t1 scf done: -1006.888911

C	3.814837	1.049033	0.000276
C	-4.277313	1.226581	-0.001201
C	2.979425	2.094779	0.000575
C	-3.026895	1.234421	-0.000888
C	1.807583	2.477304	0.000418
Mg	-4.308722	-0.948363	-0.001767
C	4.135416	-0.135670	0.000022
C	-1.672022	0.948546	-0.000669
C	3.286788	-2.590411	-0.000579
O	-0.106940	-0.849814	-0.000867
C	3.794469	-1.450976	-0.000538
Mg	1.389907	-1.908639	-0.000903
C	0.479703	2.381606	0.000210
C	-1.342126	-0.514493	-0.000970
C	-0.620926	1.830678	-0.000203
O	-2.263541	-1.346108	-0.001433

16

c39 scf done: -1006.871713

C	2.169833	-0.835627	-0.206051
C	2.150833	-2.094354	-0.242625

Mg	0.194445	-2.001071	0.160895
O	-1.530834	-1.232403	0.335710
C	-1.399974	0.016229	0.201812
C	-1.231568	1.219778	0.051999
C	-0.725407	2.499069	-0.092576
C	-1.452125	3.640869	-0.329971
C	-1.809665	4.822684	-0.432636
C	-1.652933	6.159311	-0.199687
C	-1.000536	7.184261	0.118595
Mg	0.315675	5.560942	0.423561
O	1.195680	3.929995	0.404706
C	0.768924	2.734019	0.085085
C	1.573291	1.647033	-0.071339
C	2.033280	0.504316	-0.208412

16

c8 scf done: -1006.885390			
C	-0.529179	2.496054	-0.000140
C	-0.943159	1.187985	-0.000382
C	-1.103994	-0.047679	-0.000311
C	-1.069309	-1.369964	-0.000731
C	0.018274	-2.207256	-0.000217
C	1.202607	-1.666526	-0.000965
C	2.059154	-0.729952	0.003238
C	2.089879	0.579158	0.001199
C	1.750133	1.776965	0.000731
C	0.869020	2.847054	0.000188
O	1.259428	4.082585	0.000110
Mg	0.099491	5.572318	-0.000375
O	-0.723483	7.218138	-0.001149
Mg	-2.415447	6.615338	-0.001053
C	-2.170116	4.577514	-0.000140
C	-1.447280	3.580761	-0.000003

16

t38 scf done: -1006.923454			
O	3.606106	0.516378	0.374576
C	-3.619203	1.948044	0.264140
C	2.110285	-1.236035	-0.037928
C	-2.281127	2.141669	0.372222
C	-0.428175	-1.831786	-0.287011
C	-4.814310	1.622539	0.138061
C	0.770550	-1.641717	-0.186468
C	-1.067954	1.999590	0.409533
C	-1.779742	-1.873375	-0.367508
C	0.214026	1.604899	0.402186
C	-3.006222	-1.796622	-0.418813
Mg	-4.358754	-0.320245	-0.208780
C	2.389202	0.168634	0.244043
C	1.294731	1.039387	0.351666
Mg	4.842170	-1.046776	0.142153
O	3.102172	-2.021782	-0.134836

16

t85 scf done: -1006.860490			
O	2.589459	3.768718	0.135660
Mg	1.900921	-2.944483	-0.193070
C	2.977426	2.572044	0.068058

C	2.947068	-1.242065	-0.126105
Mg	0.872128	2.773749	0.114770
C	0.220014	-4.062019	-0.220914
C	-1.001087	2.062142	0.111635
O	-5.071649	-0.500695	0.053018
C	2.955171	1.340970	0.005616
C	-4.219064	0.313425	0.078840
C	-1.877702	1.201699	0.083160
C	-0.673530	-3.200029	-0.161201
C	3.014143	-0.018879	-0.064698
C	-2.191279	-1.136456	-0.029901
C	-2.757516	0.121135	0.043701
C	-1.568808	-2.189428	-0.094222

16

c12 scf done: -1006.870568

C	-0.678044	2.418972	-0.001905
C	-1.333390	1.203306	-0.010887
C	-1.309308	-0.037374	-0.014399
C	-1.040902	-1.344536	-0.016502
C	0.119100	-1.843077	-0.009747
C	1.435139	-1.960327	0.000213
C	2.039247	-0.831922	0.008604
C	2.299295	0.441017	0.014467
C	1.582946	1.488291	0.012551
C	0.750364	2.509105	0.009208
Mg	0.836338	4.609522	0.012974
O	0.817142	6.439747	0.011800
Mg	-0.861699	7.037450	0.001900
O	-2.412095	5.937960	-0.008496
C	-1.922139	4.768842	-0.006155
C	-1.375976	3.675516	-0.003628

16

t10 scf done: -1006.868009

Mg	-3.839257	-1.327372	0.023361
C	2.104159	1.740044	0.010838
C	-2.171828	-2.400485	0.010545
C	3.422810	2.219753	0.008732
C	-0.942176	-2.418316	0.005178
O	4.416441	1.479194	0.002881
C	-3.992485	1.176302	0.033268
C	0.873808	2.209211	0.017025
C	-2.863386	1.901968	0.030958
Mg	3.128615	-0.117349	-0.000036
C	-1.667702	2.225230	0.026976
C	-0.365992	2.392589	0.022329
C	0.416822	-2.378323	-0.000779
O	2.870201	-1.976363	-0.010381
C	-4.963691	0.389091	0.035049
C	1.622885	-2.211291	-0.005737

16

t24 scf done: -1006.856045

C	-2.772286	1.513550	-0.019706
C	4.528151	-1.612225	0.040102
C	-4.103694	1.155457	-0.038300
C	4.167545	-0.416260	0.045523

O	-4.550962	-0.000346	-0.051622
C	3.710212	0.849273	0.050315
C	-1.791834	2.343320	-0.002031
C	-1.164211	-2.043980	-0.014830
C	-0.657236	2.934172	0.015802
Mg	2.762582	-2.566318	0.012018
Mg	-2.617279	-0.711151	-0.031082
C	2.880760	1.768695	0.048329
C	0.635025	2.846494	0.030477
C	-0.075176	-2.612456	-0.015431
C	1.871244	2.614426	0.042956
O	1.046889	-3.211877	-0.013956

16

t11 scf done: -1006.863183

C	0.596884	2.485117	-0.020466
C	2.552522	-1.834573	-0.018137
C	-1.652426	1.250457	-0.018235
C	1.691766	3.057743	-0.021964
C	3.019113	-0.702613	-0.019946
C	-4.122264	0.961263	-0.016735
Mg	2.896510	1.286218	-0.021771
C	1.215107	-4.066884	-0.013863
C	-2.522486	-0.958356	-0.015158
C	-0.621458	1.913188	-0.019202
C	-2.754367	0.418470	-0.016654
O	2.929791	3.267422	-0.023240
C	1.881102	-3.024508	-0.015937
Mg	-0.699988	-3.477076	-0.013044
O	-4.475324	2.087736	-0.017977
C	-2.203596	-2.145967	-0.013653

16

t8 scf done: -1006.898970

C	-4.294639	1.082655	0.001076
C	2.984450	0.758768	-0.014385
C	3.044185	-0.681307	-0.011876
C	-0.682908	-1.973598	-0.001690
C	1.822277	-1.412669	-0.008101
Mg	5.174764	0.600473	-0.018927
C	-3.142132	1.540812	-0.002098
Mg	-3.550346	-0.905273	0.002594
C	-0.642955	2.029146	-0.008351
O	4.179946	-1.233343	-0.013104
O	-5.206618	0.215117	0.004269
C	0.668030	1.888623	-0.011234
C	0.655706	-1.754691	-0.005033
C	1.808177	1.374267	-0.013031
C	-1.907942	-2.048994	0.000970
C	-1.879150	1.989018	-0.005562

16

c7 scf done: -1006.831678

C	-2.051376	-0.833565	-0.063883
Mg	-3.425111	0.636807	-0.098801
O	-4.998244	1.793818	-0.140072
C	-4.050064	2.645131	-0.112192
C	-2.914181	3.125857	-0.079841

C	-1.761555	3.861513	-0.045930
C	-0.707829	4.461603	-0.014101
C	-0.821971	-0.808263	-0.029361
C	0.499303	-0.536447	0.008289
C	1.607887	-0.025643	0.040557
C	2.624407	0.848981	0.071014
C	3.359633	1.823762	0.094038
C	3.816576	3.102209	0.110149
C	4.113340	4.311811	0.122852
Mg	2.196110	4.903598	0.070221
O	0.386036	5.099427	0.019682

16

c41 scf done: -1006.873299

C	1.871108	-0.706059	-0.000873
C	1.530627	-1.999409	-0.002539
C	0.834327	-3.044962	-0.004324
Mg	-1.045276	-1.877567	-0.005100
O	-1.194304	0.246365	-0.003142
C	-0.538719	1.282756	-0.001396
C	-0.797494	2.720535	-0.000288
C	-1.674876	3.775712	-0.000233
C	-1.944453	4.977701	0.000662
C	-1.665403	6.317403	0.002321
C	-0.910861	7.316568	0.004184
Mg	0.429575	5.721741	0.004113
O	1.289046	4.025660	0.003379
C	0.636806	2.934919	0.001549
C	0.921822	1.530193	0.000391
C	1.856994	0.533489	0.000366

16

t15 scf done: -1006.883378

C	-5.362433	0.948890	0.139158
O	7.796295	-0.846367	-0.265829
C	-4.146057	1.208966	0.207746
C	6.660528	-0.575722	-0.202098
Mg	-4.936461	-0.951315	-0.332380
C	5.417393	-0.280599	-0.132618
C	-1.418313	-1.107324	-0.360138
C	4.180395	0.015608	-0.062826
C	-2.523811	-1.872683	-0.554137
C	2.923106	0.308586	0.006097
C	-0.494323	-0.323759	-0.162124
C	1.712391	0.632056	0.082753
C	-3.611160	-2.447945	-0.700790
C	0.358132	0.778516	0.114883
O	-0.280423	1.896296	0.391098
Mg	-2.128547	1.445812	0.273080

16

c83 scf done: -1006.849211

C	-0.810051	0.000000	1.119039
C	0.660078	0.000000	1.149306
C	-1.558093	0.000000	2.293405
C	-1.522434	0.000000	-0.080252
C	-2.324171	0.000000	3.258574
C	-2.219848	0.000000	-1.096010

Mg	-4.287251	-0.000000	3.696197
Mg	-4.151056	0.000000	-1.656701
C	-6.209690	-0.000000	3.158578
C	-6.102699	-0.000000	-1.235601
C	-6.927472	-0.000000	2.169116
C	-6.867561	-0.000000	-0.281958
C	-7.618426	-0.000000	0.925987
C	-8.952024	-0.000000	0.893566
O	1.417236	0.000000	0.243425
O	-10.100234	-0.000000	0.865334

16

t65 scf done: -1006.861654

Mg	0.060162	0.706218	0.936449
C	1.681683	-0.376694	-0.240725
O	-9.061708	-0.022280	0.414621
C	2.939513	-0.286515	-0.178848
C	-7.900941	-0.088662	0.314888
C	5.487002	-0.053257	-0.000546
C	-6.636746	-0.162883	0.205101
C	4.238072	-0.164364	-0.084597
C	-5.354415	-0.233274	0.097596
C	6.768037	0.059287	0.084083
C	-4.104209	-0.303342	-0.008733
O	9.190484	0.278996	0.250218
C	-2.804229	-0.382301	-0.126550
C	8.030914	0.174408	0.171491
C	-1.545432	-0.430709	-0.211269
Mg	0.074160	-1.245140	-1.107585

16

c38 scf done: -1006.877779

C	2.727432	-0.501959	-0.008749
Mg	1.148435	-1.749013	-0.002108
O	-0.639231	-2.589615	0.004777
C	-0.937945	-1.349154	0.005230
C	-0.908237	-0.114708	0.004452
C	-0.397838	1.162068	0.001855
C	-0.692375	2.588897	0.002164
C	-1.611421	3.602136	0.005015
C	-1.940786	4.793333	0.005561
C	-1.714656	6.140711	0.003939
C	-1.014210	7.180570	0.000719
Mg	0.405795	5.640822	-0.003711
O	1.354375	4.022419	-0.006317
C	0.732779	2.887662	-0.003333
C	1.042170	1.501820	-0.003645
C	2.044630	0.539057	-0.006783

Optimized geometries of Cl2O2Mg2 (singlets) obtained at the PBE0/SDDALL level (through AUTOMATON)

16

0.000000 Kcal/mol 0.000000 eV -101.383681 H Child_4_40.log

6	4.059637	1.211947	0.004878
6	-4.285170	1.362850	-0.014551
6	3.082382	2.145231	0.015242
6	-3.030628	1.248122	-0.014324
6	1.869965	2.404103	0.011247
12	-4.347621	-0.655120	0.001589
6	4.403669	0.021937	-0.008320
6	-1.682247	0.785043	-0.005121
6	3.272687	-2.302470	-0.003620
8	-0.370653	-1.225084	0.003852
6	3.996800	-1.278855	-0.017500
12	1.276050	-1.966193	-0.000135
6	0.542452	2.175488	0.000369
6	-1.540885	-0.630211	0.007037
6	-0.553239	1.608097	-0.006504
8	-2.623558	-1.406409	0.017342

16

0.463557 Kcal/mol 0.020102 eV -101.382942 H MutD_10_74.log

6	3.193113	-0.691167	-0.029228
6	1.566662	3.040046	-0.127460
6	0.897974	-1.937903	-0.085382
8	-4.511973	-0.521119	0.059092
6	-3.950807	0.641881	0.098713
6	-1.585293	-2.704046	-0.071235
12	-3.478687	-2.085120	-0.010272
6	2.026561	-1.449235	-0.061862
12	2.656100	1.356188	-0.097635
6	-1.025427	2.933267	0.035202
6	0.320070	3.086511	-0.019733
6	4.467392	-0.983680	0.089059
6	-3.247979	1.646687	0.071405
8	5.652149	-1.107731	0.203789
6	-2.157074	2.446384	0.054877
6	-0.380254	-2.399082	-0.089050

16

1.517371 Kcal/mol 0.065800 eV -101.381263 H Child_9_11.log

8	-5.216659	-2.122420	-0.886757
8	5.443366	-1.967851	0.456925
6	-4.256604	-1.572857	-0.457533
6	4.376828	-1.469738	0.295127
6	-3.266215	-0.897298	0.057037
12	-2.997152	1.042606	0.797675
6	1.580691	2.551243	-1.010732
6	-1.893883	-1.168638	0.116262
6	3.267864	-0.821486	0.075240
6	-1.713259	2.592764	0.922389
12	2.906978	1.049048	-0.802052
6	-0.664959	-1.211966	0.218243
6	1.916471	-1.124174	0.239410
6	-0.656826	2.828512	0.313286
6	0.501783	2.760073	-0.434015

6	0.686180	-1.196047	0.247147		
16					
2.031357	Kcal/mol	0.088088	eV	-101.380443	H Child_1_29.log
8	3.046309	1.366615	-0.030654		
8	-4.419404	-1.311160	0.055101		
6	0.666162	1.440268	-0.055663		
6	-3.169513	-1.703658	0.034611		
6	1.867450	0.701552	-0.069754		
6	-0.606126	-1.722614	-0.041825		
6	-0.474190	1.892924	-0.020073		
6	-1.955582	-1.871623	-0.005636		
12	4.639583	0.404744	0.110619		
6	0.571095	-1.377853	-0.066223		
6	1.811268	-0.706585	-0.071531		
6	4.316337	-1.601952	0.020524		
6	-1.813791	2.122333	0.003839		
6	3.087917	-1.338871	-0.027478		
6	-3.057173	2.112800	0.016835		
12	-4.346114	0.584925	0.014270		
16					
6.730402	Kcal/mol	0.291858	eV	-101.372955	H MutD_9_72.log
12	-2.439497	1.457861	-0.147399		
6	3.390880	1.843417	0.051195		
12	0.925829	-2.822576	-0.077183		
6	-4.355727	-0.814444	0.103666		
6	3.467479	-1.804316	0.065924		
6	-3.090221	-0.543380	-0.063601		
6	3.843189	0.693164	0.053282		
6	-0.069184	3.339589	0.001311		
8	2.808599	-2.915024	0.059544		
6	3.911022	-0.657283	0.056345		
8	-5.529305	-0.932728	0.262142		
6	-0.888385	-2.001283	-0.169167		
6	2.412167	2.770905	0.041667		
6	-1.954570	-1.367164	-0.120061		
6	-1.297358	3.123156	-0.029463		
6	1.285653	3.277404	0.029150		
16					
8.018000	Kcal/mol	0.347694	eV	-101.370903	H Child_5_58.log
6	3.517739	0.218152	-0.045859		
12	-4.827752	0.478737	-0.074995		
6	4.789604	0.070684	-0.178338		
8	-3.798034	2.027650	-0.053245		
6	2.226297	0.213444	0.093103		
6	-4.513548	-1.493917	-0.049520		
12	0.954060	-1.474246	0.112305		
6	-2.505121	2.100346	0.006830		
6	6.065834	0.102572	-0.096200		
6	-3.392117	-2.036060	-0.047172		
8	7.259698	0.161702	-0.023056		
6	-1.278131	2.039177	0.067492		
6	1.110131	1.046367	0.129227		
6	-2.073109	-2.381720	-0.006896		
6	-0.832202	-2.436455	0.039554		
6	0.016456	1.629292	0.114892		

16
9.143178 Kcal/mol 0.396486 eV -101.369110 H Child_11_8.log
8 7.237847 -0.291129 0.304063
8 -6.414410 -0.995640 0.102658
6 6.056137 -0.410703 0.179441
6 -5.239484 -0.821721 0.084642
6 -3.980948 -0.494663 0.077059
6 4.796716 -0.533057 0.029468
12 -2.899505 1.311694 0.163319
6 2.234679 -0.533834 -0.202146
6 -2.758108 -1.149829 -0.001856
6 1.030621 -1.194064 -0.140017
6 -1.119839 2.299238 0.063815
6 3.518231 -0.603843 -0.067315
6 -0.029055 2.947198 0.102254
6 -0.196428 -1.404530 -0.111724
6 -1.542417 -1.385092 -0.057913
12 0.965495 1.188603 -0.412320

16
9.471244 Kcal/mol 0.410713 eV -101.368587 H MutD_11_78.log
6 -4.025768 1.057821 0.047073
6 2.915613 0.744393 -0.021407
6 2.946457 -0.654901 -0.034706
6 -0.727553 -2.145087 -0.007173
6 1.737215 -1.386473 -0.040216
12 5.005080 0.448785 0.077934
6 -3.078585 1.840944 -0.006826
12 -3.794510 -1.506164 0.000642
6 -0.584478 2.426055 -0.040553
8 4.143225 -1.296205 0.004888
8 -4.867467 0.061330 0.072827
6 0.724111 2.132229 -0.035199
6 0.593527 -1.831871 -0.017128
6 1.823077 1.556063 -0.031764
6 -1.962163 -2.298262 -0.038947
6 -1.816936 2.320347 -0.033925

16
10.899414 Kcal/mol 0.472644 eV -101.366311 H Child_8_52.log
6 -1.746536 3.055154 -0.223860
8 -5.100639 -1.638267 0.748731
12 -2.699773 1.273619 -0.158564
12 1.351276 -2.467795 -0.330054
6 -0.549175 3.386175 -0.121203
8 3.199196 -2.831380 0.090597
6 0.804040 3.406671 -0.032107
6 2.947920 2.047137 0.204600
6 -4.016815 -1.360699 0.318201
6 -2.884877 -0.850691 -0.132428
6 3.611634 -1.610701 0.303498
6 -1.645815 -1.412556 -0.455924
6 -0.491227 -1.816820 -0.707462
6 3.760605 -0.384147 0.325084
6 1.944064 2.942995 0.091605
6 3.498434 0.945362 0.288130

15.019167 Kcal/mol 0.651294 eV -101.359746 H Child_5_38.log

12	-3.590812	-1.727027	-0.192737
6	1.978372	3.079190	-0.105791
6	-2.074047	-3.035847	0.089505
6	2.666813	2.063923	-0.251546
6	-0.846766	-3.217261	0.140679
8	3.466738	1.071821	-0.377725
6	-3.618235	1.299679	-0.062174
6	0.715512	3.554692	0.092115
6	-2.756955	2.339208	0.115639
12	3.401966	-0.702293	0.080525
6	-1.768935	3.050114	0.329254
6	-0.501755	3.529641	0.316673
6	0.520586	-3.198089	0.152373
8	2.952125	-2.495504	0.083745
6	-4.211203	0.216988	-0.287299
6	1.715820	-2.925353	0.086970

16

16.929908 Kcal/mol 0.734151 eV -101.356701 H MutD_14_54.log

6	0.451963	2.338070	-0.118602
6	3.124213	-1.740517	-0.103708
6	-1.850630	1.191686	-0.237744
6	1.612388	2.703547	0.067778
6	3.890996	-0.763038	-0.109022
6	-4.160231	1.160972	0.004316
12	3.921041	1.221257	0.040865
6	1.095110	-3.363562	0.003938
6	-2.955713	-0.992944	-0.016273
6	-0.790364	1.798577	-0.204205
6	-3.047643	0.427704	-0.117492
8	2.900964	2.764599	0.232201
6	2.122242	-2.671629	-0.068517
12	-0.934144	-3.298636	0.121140
8	-5.054322	1.914621	0.139728
6	-2.594983	-2.173068	0.079615

16

18.063784 Kcal/mol 0.783321 eV -101.354894 H MutD_13_60.log

6	3.834398	-1.206647	-0.120516
6	-1.982334	-2.814857	0.242482
6	2.537669	-1.082854	-0.228233
8	1.264151	4.605106	0.396301
6	1.817325	0.132310	-0.235561
6	-2.295722	1.942090	-0.300759
8	5.005225	-1.313822	0.081485
6	1.184991	1.171027	-0.122227
6	-4.109699	-1.333036	0.133915
6	-0.797316	-3.187501	0.217923
6	-3.176046	-2.152243	0.216677
12	1.098717	-2.577757	-0.028959
6	0.329474	2.307799	-0.045551
6	0.849406	3.522986	0.197149
6	-1.086236	2.176384	-0.193594
12	-3.831255	0.645838	-0.170418

16

18.892522 Kcal/mol 0.819258 eV -101.353573 H MutD_12_72.log

6	1.220051	1.024594	0.187781
6	2.701481	-1.161373	0.169120
6	0.908621	3.317113	-0.315992
6	-1.045503	2.060038	0.275450
6	0.364107	2.160479	0.095659
12	-3.898686	0.628066	0.354712
6	-2.245776	1.798389	0.411796
6	-2.151336	-2.505766	-0.329342
12	1.006666	-2.309260	-0.191819
6	-3.405193	-1.975904	-0.217420
6	-0.943506	-2.753503	-0.401205
8	5.193051	-1.402694	0.219329
6	1.959429	0.040928	0.218833
6	4.004902	-1.276037	0.223285
6	-4.423904	-1.258677	-0.103687
8	1.437450	4.321774	-0.624377
16			
22.623145	Kcal/mol	0.981034	eV -101.347628 H Child_10_51.log
12	-3.489910	-1.210672	-0.030559
12	4.621847	1.081606	-0.662323
8	-5.009703	-0.085815	-0.585430
8	4.398652	-0.991446	-0.360506
6	3.139479	-0.706104	0.067183
6	-4.216640	0.952509	-0.456401
6	2.060012	-1.623259	0.144070
6	-1.694497	-2.107706	0.283290
6	2.777449	0.629635	0.290234
6	-3.234684	1.645526	-0.198827
6	1.602697	1.229799	0.613357
6	-1.980578	2.041086	0.152901
6	0.491325	1.757111	0.729311
6	-0.814329	2.037618	0.499022
6	-0.462487	-2.166747	0.284199
6	0.883114	-1.994986	0.238671
16			
23.775234	Kcal/mol	1.030993	eV -101.345792 H Child_14_22.log
6	-4.287693	0.671249	1.646460
8	7.087266	-0.783538	1.546912
6	-3.544470	1.595766	1.242278
6	6.103427	-0.512556	0.925307
12	-4.443344	-1.279637	1.147175
6	5.087468	-0.206462	0.208967
6	-1.488329	-1.284491	-1.419021
6	3.956956	0.073717	-0.324283
6	-2.541114	-1.992661	-0.923112
6	2.785151	0.334309	-0.787237
6	-0.578987	-0.459901	-1.552524
6	1.584511	0.544607	-1.156892
6	-3.482412	-2.415847	-0.226045
6	0.248368	0.654507	-1.236190
8	-0.411449	1.767228	-0.817843
12	-1.928637	2.122727	0.167925
16			
28.859863	Kcal/mol	1.251484	eV -101.337689 H MutD_10_66.log
6	2.572198	2.452454	-0.169858

6	-1.316478	-1.497237	-0.043293
6	-3.177583	0.139038	0.010955
6	4.384429	0.766742	-0.036772
6	3.751559	-1.720042	0.143631
6	1.346206	2.313053	-0.104346
6	3.784357	1.850196	-0.124444
6	4.264640	-0.581712	0.093991
12	1.745147	-1.987134	0.137350
12	-3.351095	-1.896197	-0.248474
6	-0.773971	0.882698	0.034933
6	0.143065	1.704878	-0.032406
6	-3.858049	1.233218	0.121149
8	-0.060701	-1.909566	0.004035
8	-4.578057	2.190836	0.220798
6	-1.723465	-0.151653	0.028933
16			
30.028553 Kcal/mol 1.302163 eV -101.335827 H MutD_7_64.log			
6	-1.184348	1.477429	-0.213403
6	3.831184	-1.567198	0.436217
6	-2.336656	0.719803	0.125022
6	1.311518	-2.055260	0.450359
8	-4.382174	-1.777802	-1.199055
6	-0.098343	2.013767	-0.472003
6	-1.174107	-1.498783	0.128624
6	-3.416083	-1.309558	-0.713226
6	4.903348	-0.927827	0.307293
6	-2.347960	-0.764436	-0.125937
8	-4.286678	1.773944	1.309146
6	2.541018	-1.979841	0.500121
12	1.940742	2.205735	-0.580421
6	-3.362014	1.274792	0.771031
6	-0.017003	-1.855586	0.329644
12	4.513215	1.033186	-0.254844
16			
36.958701 Kcal/mol 1.602683 eV -101.324783 H MutD_15_74.log			
6	1.568377	-1.247825	0.114184
8	-3.397637	-2.169509	0.397095
6	2.934471	-0.873433	0.124527
6	-1.026214	-1.365924	0.168252
12	-4.732883	-0.814551	0.055269
6	-2.168686	-1.816515	0.296307
12	-2.768316	1.177742	-0.524941
6	2.111905	2.735649	0.480022
8	4.711167	-2.509480	-0.661187
6	2.905510	1.650243	0.564846
6	1.004323	3.232434	0.257729
6	3.892643	-1.752219	-0.342542
6	0.334425	-1.264536	0.126195
6	-1.272491	2.576689	-0.680815
6	3.260505	0.477422	0.395156
6	-0.293744	3.160286	-0.212398
16			
37.515007 Kcal/mol 1.626807 eV -101.323897 H Child_15_9.log			
6	3.772851	1.046283	-0.046339
6	-3.816746	-0.965580	-0.057433

6	3.623427	-0.190090	0.136288
6	-3.586029	0.261339	0.066599
6	2.971974	-1.362836	0.254856
12	-1.979652	-1.849756	-0.206616
6	2.013850	-2.161287	0.285819
6	-3.034329	1.501228	0.163192
12	1.801267	1.899334	-0.222311
6	-2.169478	2.377668	0.238580
6	0.272138	3.198594	0.141749
6	-0.009004	-0.802155	-0.343261
6	0.645230	-2.168300	0.098278
6	-0.951024	2.984853	0.232456
8	-0.275040	-3.050528	0.212408
8	0.742973	0.186374	-0.447106
16			
38.031552 Kcal/mol 1.649206 eV -101.323073 H MutD_16_74.log			
6	-3.139176	1.125418	-0.093465
6	3.228406	-1.260030	-0.089197
6	-0.912987	2.156886	0.087057
6	0.099251	-3.264781	0.038698
6	-2.296895	2.035081	0.044067
6	3.621961	0.042734	-0.100889
6	2.458547	-2.225044	-0.053733
8	-0.094921	3.125715	-0.077794
8	-0.714308	-0.253730	0.273003
6	-3.596605	-1.385350	-0.233991
6	-3.628450	-0.125896	-0.202375
6	3.663007	1.297063	-0.110195
12	-1.574992	-2.091526	0.091734
6	-0.087909	0.822493	0.241047
12	1.757716	2.041222	0.020840
6	1.304371	-2.947282	-0.012450
16			
41.149582 Kcal/mol 1.784417 eV -101.318105 H Child_11_51.log			
6	-1.912683	-1.379703	0.586821
8	5.231888	0.838723	-1.687943
6	-4.059221	-0.336500	-0.399340
6	4.423642	0.224839	-1.076057
6	-3.004130	-1.011083	0.034079
6	2.300564	1.654651	0.954587
8	-5.742262	1.016121	-1.584884
6	3.064681	0.917061	0.350210
6	-4.915949	0.330787	-1.013102
6	0.997015	2.035829	1.059188
12	-1.859301	0.867928	0.954553
6	3.493433	-0.281812	-0.306544
6	-0.709695	-2.047857	0.630325
6	-0.249267	2.031619	1.092792
6	0.462862	-2.479864	0.660067
12	2.253924	-1.933475	-0.059180
16			
41.280038 Kcal/mol 1.790074 eV -101.317897 H Child_11_60.log			
6	3.410151	-0.819446	0.092367
8	-4.343565	2.052265	0.134915
6	3.476829	0.426754	0.114388

6	-3.234932	1.488190	0.039704
6	-0.293357	-4.071932	-0.019626
6	-1.984253	2.201178	0.068836
6	2.845272	-2.032769	0.120783
6	-3.095540	0.057588	-0.086783
6	0.886923	-3.674888	0.056009
6	-0.860540	2.712637	0.052127
12	-2.008828	-2.992091	-0.122460
6	-2.880819	-1.155887	-0.151200
6	2.888269	1.671343	0.096993
12	1.163412	2.834247	0.091363
6	2.043148	-2.974030	0.085601
8	3.210824	2.812946	-0.440167
16			
41.665464 Kcal/mol 1.806788 eV -101.317282 H Child_12_43.log			
6	-0.702366	-0.370034	0.002883
12	2.498489	2.761975	-0.004814
6	-1.990021	-0.205512	0.006990
8	2.811883	0.917371	0.005760
6	-3.283973	-0.163657	0.032980
6	0.516816	3.176814	-0.013924
12	0.251824	-2.216331	-0.034272
6	0.327434	1.932384	-0.001242
6	1.784541	0.041847	0.004082
6	-4.550880	-0.166139	0.017805
6	0.447834	0.513109	-0.001714
6	-5.856913	-0.201437	0.012262
8	4.335936	-2.501152	0.017949
6	2.116945	-1.370837	0.000243
6	3.303680	-1.910367	0.009092
6	-7.144146	-0.255752	-0.022897
16			
42.117184 Kcal/mol 1.826376 eV -101.316563 H Child_12_49.log			
6	-2.913120	1.852209	-0.140417
6	6.827704	-0.647566	0.078497
6	-3.968330	1.228532	-0.030522
6	5.669029	-0.092315	0.136346
8	-4.925838	0.376294	0.095842
6	4.437446	0.348255	0.171604
6	-1.604479	2.156646	-0.125096
6	-2.291065	-2.141650	0.096000
6	-0.370307	2.184714	-0.066690
12	1.784236	-1.004736	-0.259090
12	-4.078458	-1.349513	0.199042
6	3.172915	0.570044	0.103332
6	0.931387	1.875131	0.014106
6	-1.068461	-2.023040	-0.067029
6	2.067760	1.383628	0.104037
8	0.199314	-1.865860	-0.211396
16			
42.953979 Kcal/mol 1.862663 eV -101.315229 H MutD_17_64.log			
6	4.076319	-0.321999	0.067809
6	-1.252282	-2.005875	0.710813
12	2.355038	-1.195904	-0.685075
6	-4.122682	0.122413	-0.012372

6	-3.482956	-0.828213	0.521388
6	2.519466	1.705591	0.588226
6	0.003285	-1.842094	0.182548
6	1.464008	2.344053	0.559879
6	3.436698	0.717600	0.387705
12	-2.319093	1.286571	-0.540645
6	0.195853	-0.676795	-0.856755
6	-1.040207	2.755420	0.105914
8	1.097983	-2.476491	0.342931
8	-0.793589	0.054663	-1.092322
6	0.174603	2.725928	0.385598
6	-2.449855	-1.648260	0.809873
16			
44.781150 Kcal/mol 1.941897 eV -101.312317 H Child_6_60.log			
6	4.726260	-2.317180	0.013188
8	-6.352173	-1.012362	0.043609
6	4.201698	-0.953939	0.011855
6	-5.199293	-0.673462	0.022123
6	4.146974	0.423385	0.016525
6	-3.985618	-0.316980	0.004289
6	3.308077	-1.989614	0.000761
6	-2.699401	0.055643	-0.020290
6	3.827757	1.626593	0.019052
8	-2.273721	1.326753	-0.029009
6	1.942154	-2.135333	-0.011136
6	-1.617164	-0.887166	-0.028010
12	2.076539	2.709538	0.013844
12	-0.744100	2.376656	-0.014480
6	0.727023	-1.943577	-0.019938
6	-0.542153	-1.479945	-0.026614
16			
45.139009 Kcal/mol 1.957415 eV -101.311747 H Child_5_52.log			
6	-2.864342	2.462112	0.004220
6	4.818140	-0.739960	-0.000057
6	-1.506914	1.888650	0.000968
6	3.831849	-1.535540	0.000024
6	-2.590410	1.056096	0.000824
6	0.146826	-2.411420	0.001595
8	-5.508797	-0.807463	-0.003444
12	3.898586	1.121408	-0.001604
6	-4.370156	-0.571597	-0.001075
6	2.707794	-2.268590	0.000655
6	-3.029024	-0.310762	-0.000333
6	1.449730	-2.373514	0.001073
12	0.551178	2.150253	0.000066
6	-1.035056	-1.894149	0.001121
6	-2.238048	-1.459821	0.000426
8	2.343860	2.018842	-0.001330
16			
45.524210 Kcal/mol 1.974119 eV -101.311133 H Child_8_48.log			
6	2.662287	-2.233132	-0.329058
8	-0.892857	4.462774	-0.608677
6	1.457052	-2.328704	-0.555898
6	-0.331565	3.466956	-0.277183
6	-6.054903	-1.205142	0.622604

6	1.439966	1.846215	0.372479
8	3.886858	-1.928287	-0.039987
6	0.149286	2.301390	0.058869
6	0.119460	-2.126191	-0.598787
6	-4.790660	-1.202342	0.371367
12	-1.093334	0.618796	0.004029
12	3.919185	-0.114452	0.540226
6	2.533420	1.303238	0.605665
6	-3.511150	-1.255486	0.103465
6	-2.241769	-1.159248	-0.097034
6	-1.075127	-1.795554	-0.500113
16	45.598305 Kcal/mol 1.977332 eV -101.311015 H Child_4_53.log		
6	3.699259	0.253114	-0.002091
8	-5.112730	1.864010	-0.337405
6	4.987767	0.178849	-0.209882
6	-4.200130	1.098437	-0.196212
8	6.156691	0.010598	-0.387701
6	-3.264763	0.206196	-0.038202
12	2.048952	-1.087480	0.083346
12	-3.203504	-1.883610	-0.004841
6	0.054464	-1.711649	0.091638
6	-1.794722	0.325084	0.090090
6	2.741240	1.247310	0.185872
6	-0.890060	1.415715	0.170664
6	0.256161	1.852809	0.298331
6	-1.183610	-2.326198	0.029533
6	-1.099482	-0.848977	0.094106
6	1.611033	1.752014	0.295950
16	45.666460 Kcal/mol 1.980288 eV -101.310906 H Child_12_10.log		
6	3.803213	-1.095954	-0.036709
8	-5.584144	-0.540008	-1.126984
6	3.625286	0.199689	-0.654130
6	-4.554020	-0.742765	-0.569883
6	3.199147	1.316805	-0.970780
6	-3.448946	-0.670468	0.125835
12	1.788948	2.687372	-0.500633
6	-2.211263	-1.140968	0.418556
6	2.610099	-1.874348	-0.200309
12	-2.398317	0.992518	0.991259
6	1.399758	-2.117201	-0.002691
6	-1.118314	-1.841471	0.287097
6	0.085059	-2.203513	0.075359
6	-1.068387	2.479115	0.836646
6	-0.036326	2.957879	0.317265
8	4.784218	-1.429925	0.671353
16	45.902012 Kcal/mol 1.990502 eV -101.310531 H Child_12_62.log		
8	8.152171	0.736981	-0.034770
12	-4.503524	2.092618	-0.005886
6	6.968707	0.523301	-0.018977
6	-2.511394	2.244527	0.042542
6	5.721434	0.293837	-0.003537
8	-5.240549	0.275829	-0.043702

6	4.445899	0.068876	0.013092
6	-2.032380	1.086362	0.025068
6	3.201080	-0.161404	0.024800
6	-4.244477	-0.520504	-0.031760
6	1.918826	-0.392006	0.023339
6	-3.106008	-1.062217	-0.012008
12	-1.753950	-2.841136	0.004084
6	-1.808290	-0.324074	0.009344
6	0.676407	-0.610707	0.022195
6	-0.597017	-0.999370	0.014136
16	46.098627 Kcal/mol 1.999028 eV -101.310218 H MutD_15_54.log		
8	5.199695	-0.380390	-0.064583
6	4.242026	0.460605	-0.036776
6	0.616398	1.078273	-0.005094
12	1.838862	2.872017	0.064658
8	-8.113976	-0.739710	0.079607
6	-1.899694	0.465608	-0.052939
6	1.973435	-1.055534	0.046003
6	-3.175607	0.204453	-0.081811
6	3.127607	1.052407	0.010419
6	-4.408822	-0.080061	-0.074464
6	-0.662956	0.709618	-0.035804
6	-6.927092	-0.543922	0.018520
12	4.397569	-2.167796	-0.001154
6	1.804254	0.361723	0.013761
6	-5.678188	-0.335319	-0.047694
6	2.401481	-2.232825	0.098840
16	46.143229 Kcal/mol 2.000962 eV -101.310147 H Child_5_8.log		
6	-4.185621	0.733376	-0.095748
8	5.778521	1.350374	-0.193327
6	-4.157562	1.980512	-0.070719
6	4.703353	0.810416	-0.115302
6	-3.907277	-0.595891	-0.102788
6	3.574889	0.242219	-0.052419
6	-3.307620	-1.671037	-0.086820
6	1.478228	0.726994	0.193185
12	-2.383871	2.952337	0.024616
6	0.571469	1.679748	0.148489
6	-2.338443	-2.620404	-0.052368
6	2.324101	-0.312873	0.077723
6	-1.282341	-3.275462	-0.009647
6	-0.425897	2.453225	0.131692
12	0.678810	-2.857357	0.061515
8	1.993613	-1.605958	0.090172
16	46.428558 Kcal/mol 2.013335 eV -101.309692 H MutD_13_40.log		
6	1.809204	0.236451	-0.011605
12	4.776994	-1.868864	0.002379
6	3.030739	1.093344	-0.036798
6	-5.788620	-0.321826	0.005574
6	-4.499143	-0.198196	0.030306
8	5.311520	0.013573	0.008286
6	2.172311	-1.148069	-0.016320

6	-3.237570	-0.065611	0.050207
6	2.796159	-2.235307	-0.031026
6	0.543283	0.795201	0.017591
6	4.233227	0.695734	0.015754
12	1.516090	2.751392	-0.018228
6	-0.706252	0.338561	0.022550
8	-8.260619	-0.507536	-0.041161
6	-1.949795	0.123284	0.049508
6	-7.057581	-0.420003	-0.020207
16			
46.742519 Kcal/mol 2.026950 eV -101.309192 H MutD_16_36.log			
6	-1.851259	-1.020045	-0.136966
6	-1.789772	0.404469	-0.069438
6	6.809073	-0.644778	0.087137
6	-0.657087	1.209143	-0.075639
6	5.645415	-0.162026	-0.066743
6	4.398005	0.187200	-0.114304
6	-4.218545	0.305541	0.131150
6	1.889255	0.734516	-0.140411
6	-2.201544	-2.223344	-0.169051
8	7.892351	-1.132118	0.249997
8	-5.104221	-0.609786	0.171166
6	-3.160422	0.988890	0.051099
12	-2.011023	2.898405	0.081722
6	0.642966	0.924494	-0.126765
6	3.168818	0.487224	-0.134215
12	-4.185181	-2.332778	0.019576
16			
47.038663 Kcal/mol 2.039792 eV -101.308720 H MutD_2_68.log			
6	-3.452729	-0.251229	-0.053453
6	-3.101968	1.085849	0.028448
6	-4.505662	0.734497	-0.105631
6	6.004589	1.238089	-0.930684
6	-1.957786	-2.346181	-0.341802
6	-1.930747	1.822585	0.144895
6	-0.750874	2.178001	0.202214
8	5.033730	0.804857	-0.459811
6	0.610128	2.160968	0.207200
12	-0.023581	-2.925617	-0.139907
6	1.891501	-2.469034	0.295450
12	3.141686	0.294233	0.457438
6	2.829774	-1.701282	0.634597
8	-5.694548	1.022582	-0.213069
6	1.809601	1.849212	0.301830
6	-2.800945	-1.475292	-0.120952
16			
47.575410 Kcal/mol 2.063068 eV -101.307864 H Child_7_8.log			
6	2.338806	-1.878707	-0.611666
6	-2.253666	1.584276	-0.135906
6	1.177916	-2.302000	-0.548062
6	0.163875	2.476266	-0.096496
6	3.379946	-0.988602	-0.591733
6	-1.140771	2.094728	-0.093884
6	4.112399	0.018925	-0.523192
6	1.391060	2.658550	-0.136466

12	-0.797501	-2.772639	-0.484436
8	-4.595659	1.202276	-0.232816
6	-2.550356	-1.751673	-0.416772
6	-3.432053	0.757776	-0.227714
8	0.169399	-1.119488	2.304072
6	0.901647	-0.248031	2.466092
12	3.241358	1.824299	-0.274241
6	-3.074835	-0.635210	-0.328523
16			
47.587486 Kcal/mol 2.063591 eV -101.307845 H Child_9_42.log			
8	3.582387	-0.124296	0.715596
6	-3.354390	2.139983	0.115467
6	1.900180	-1.772304	0.178719
6	-2.017572	2.256752	0.296342
6	-0.718982	-2.015673	-0.184934
6	-4.523945	1.733490	-0.067471
6	0.497532	-1.951974	-0.017103
6	-0.818659	1.980284	0.418049
6	-2.066161	-1.929983	-0.326251
6	0.384685	1.387133	0.512628
6	-3.283289	-1.706424	-0.424058
12	-4.714424	-0.267728	-0.362206
6	2.376571	-0.346513	0.518153
6	1.359799	0.646729	0.559182
12	5.634793	1.932877	-0.962899
8	2.735231	-2.689551	0.088020
16			
48.506863 Kcal/mol 2.103459 eV -101.306380 H Child_11_55.log			
6	1.547265	-1.816092	0.358478
8	-5.579756	-0.477542	-0.431115
6	3.987706	-0.833303	0.028252
6	-4.394309	-0.400399	-0.362147
6	2.953917	-1.491595	0.243887
6	-3.133237	-0.170415	-0.144531
12	3.797503	1.115451	-0.550503
12	-2.031977	1.388014	0.780886
8	1.031067	-2.728751	1.023651
6	-0.309934	2.466059	0.911372
6	0.705089	-0.853915	-0.431301
6	-1.904115	-0.746199	-0.483161
6	0.789365	2.194449	0.384044
6	1.239797	0.349677	-0.710367
6	-0.693720	-0.982858	-0.564520
6	1.746045	1.552718	-0.480819
16			
48.531968 Kcal/mol 2.104548 eV -101.306340 H MutD_8_78.log			
6	2.864024	-2.119214	-0.155278
6	-1.105014	-2.330536	0.147791
6	0.101992	2.269770	-0.640960
12	-4.374922	-0.011704	0.258414
6	1.435025	-1.930675	-0.169440
8	3.228811	2.469078	0.513537
6	0.100672	-2.217985	-0.052642
6	-1.132705	2.351691	-0.531371
6	2.275605	-0.832497	-0.399303

6	-3.653897	1.820607	-0.166341
6	-2.442455	-2.196958	0.354647
8	3.842362	-2.855089	-0.018534
6	-3.634025	-1.888808	0.554896
6	3.345955	3.052501	1.513115
6	-2.479214	2.183564	-0.362781
12	1.822825	1.188315	-0.634582
16			
49.264516 Kcal/mol 2.136314 eV -101.305173 H MutD_14_46.log			
6	-4.484129	-0.293679	-0.040673
6	2.948923	1.095367	0.081733
6	3.018814	-2.128849	-0.482029
8	-8.212877	-0.393179	0.462028
6	-5.798221	-0.287825	-0.022122
6	-3.222035	-0.243080	-0.150839
12	4.877876	-1.752889	0.156409
6	0.513859	0.705750	-0.296073
6	-0.721747	0.224529	-0.364082
6	-1.950540	-0.061117	-0.313266
6	-7.034872	-0.360205	0.232151
6	1.796670	0.201161	-0.231243
6	2.259120	-1.137583	-0.395597
6	4.094837	0.742244	0.464553
12	1.429277	2.710500	-0.161867
8	5.186637	0.114227	0.684275
16			
49.500311 Kcal/mol 2.146539 eV -101.304797 H Child_9_47.log			
6	-2.285557	-2.516039	-0.131926
8	5.595311	1.571504	-0.458892
6	-1.131484	-3.226327	-0.075950
6	-0.209796	2.162347	0.272406
6	-3.074986	-1.568509	-0.169686
6	4.525609	1.074121	-0.210628
6	0.035910	-3.664434	-0.013666
6	0.815292	1.466760	0.259711
6	-3.696219	-0.368542	-0.178949
6	3.381523	0.556956	0.054243
6	-3.953867	0.831294	-0.140294
12	-2.147247	2.656807	0.090607
6	2.433815	-0.597000	0.287877
6	1.927206	0.645408	0.266712
8	-3.970126	2.131172	-0.097451
12	1.680068	-2.523275	0.170364
16			
50.790696 Kcal/mol 2.202496 eV -101.302740 H Child_18_23.log			
6	-3.089800	-1.533535	0.617548
6	2.177144	2.835535	0.157979
6	-2.130553	-2.059991	-0.104474
6	2.615504	1.724909	0.547290
6	-3.272925	-0.296728	0.871958
6	2.902167	0.409521	0.802080
6	-0.976697	-2.120353	-0.699469
12	0.487902	2.158060	-0.805911
12	1.023119	-2.556384	-0.274957
6	-3.064919	1.001171	0.907710

6	2.801061	-0.809567	0.742037
6	-0.431082	-0.923130	-1.261947
8	2.598421	-2.093941	0.617264
6	-2.248712	1.837453	0.437520
6	0.076314	0.191925	-1.518402
8	-1.383081	2.498520	-0.120833
16			
50.836363 Kcal/mol 2.204476 eV -101.302668 H Child_16_21.log			
12	1.551295	1.862740	-0.007436
8	-2.703153	-0.964955	-1.666235
6	3.820094	-0.262926	-0.146199
6	-1.538021	-1.302972	-1.524356
8	4.972203	-0.475376	-0.371628
6	-1.923660	-0.485419	2.022297
6	2.599514	0.045461	0.172158
6	-0.576636	-0.649930	2.046237
6	-0.305324	2.390198	-0.528597
6	-3.092781	-0.336227	1.591626
6	-1.488499	1.998016	-0.647339
6	0.701821	-1.446140	-0.496984
6	1.410276	-0.767259	0.417728
6	-0.342878	-1.632695	-1.246039
6	0.574966	-0.676424	1.586316
12	-2.983430	0.660640	-0.257412
16			
51.337998 Kcal/mol 2.226229 eV -101.301868 H MutD_16_72.log			
6	-4.236426	-0.704374	-0.011111
12	6.074423	-0.486775	-0.037537
6	-1.813618	-2.107117	-0.000625
6	-2.888940	-1.248603	-0.003371
6	-2.238707	1.240864	0.001062
6	-3.058094	0.125053	-0.001990
8	-5.447785	-0.857426	-0.021299
8	-0.106636	4.086797	-0.007449
12	2.950307	-0.619932	0.023315
6	0.699818	-2.609757	0.011060
6	1.994842	1.204532	0.024027
6	-0.114166	2.840775	0.004209
6	1.927582	-2.400848	0.018683
6	1.064526	2.019605	0.016444
6	-0.650806	-2.509802	0.005138
6	-1.329576	2.057256	0.003251
16			
51.345862 Kcal/mol 2.226570 eV -101.301856 H MutD_14_48.log			
8	5.442753	-0.873496	-0.051435
6	2.247406	1.247950	0.003489
6	3.060856	0.126765	-0.009604
6	-1.982461	1.197543	0.027389
12	-6.069983	-0.476512	-0.071015
6	-1.056676	2.017375	0.021538
12	-2.948557	-0.621312	0.026163
6	1.336233	2.062430	0.011454
6	2.880212	-1.244940	-0.009626
6	-1.936705	-2.408167	0.046619
6	4.232464	-0.711815	-0.033969

6	-0.708181	-2.613291	0.039893
6	0.642119	-2.508126	0.028736
8	0.107568	4.088273	0.006613
6	1.802304	-2.099024	0.009843
6	0.119080	2.842580	0.013706
16			
51.376066 Kcal/mol 2.227880 eV -101.301808 H Child_10_50.log			
8	-5.971637	-1.243969	-0.113106
8	3.536073	-2.813068	0.401911
6	-4.900518	-0.727099	-0.069913
6	1.670200	2.689966	0.073588
12	-1.700214	-1.017374	-0.070192
6	2.588394	1.859716	-0.004268
6	-3.682305	-0.292076	-0.032909
6	3.494227	0.835323	-0.154639
6	0.283058	-1.501620	-0.056281
6	3.646571	-0.507154	-0.129433
6	-2.974442	0.906049	0.053607
6	2.933756	-1.768275	0.104162
6	-2.040760	1.737753	0.120158
6	4.814028	0.247433	-0.492269
6	1.504211	-1.670617	0.003022
12	-0.344286	2.817366	0.170243
16			
51.533355 Kcal/mol 2.234701 eV -101.301557 H MutD_8_64.log			
8	-3.821186	-0.456136	-0.638562
6	4.060294	-0.373421	-0.351818
6	3.883026	0.970658	-0.148529
6	2.087538	2.717892	0.263552
8	-1.893241	0.545279	0.282191
6	3.227752	1.995303	0.044264
12	-1.000484	2.337781	0.279583
6	-2.938187	1.976443	-0.630461
6	0.901965	3.055147	0.474959
6	2.488252	-2.398941	-0.330532
6	-3.221942	0.680233	-0.553070
12	-2.366682	-1.443445	0.336941
6	1.443447	-2.973409	0.045704
6	3.343843	-1.401158	-0.541321
6	-1.071852	-2.980916	0.585983
6	0.149434	-3.175359	0.383381
16			
51.776036 Kcal/mol 2.245224 eV -101.301170 H MutD_15_48.log			
6	2.860697	-1.219785	0.049175
6	3.005919	0.154410	0.106644
6	4.177262	-0.656744	0.297881
6	-1.909972	-2.477584	-0.450133
6	2.182409	1.264404	0.031796
8	0.011707	4.083180	-0.114364
12	-5.823633	-0.442665	0.795078
6	-1.106112	1.990385	-0.246507
6	-2.010350	1.150351	-0.326153
6	-0.676572	-2.642283	-0.372110
6	1.813115	-2.094819	-0.103059
6	0.665001	-2.515266	-0.242384

6	0.047279	2.838720	-0.135833
6	1.271377	2.076433	-0.043258
12	-2.925966	-0.694142	-0.354093
8	5.372650	-0.779136	0.528342
16			
52.189789 Kcal/mol 2.263166 eV -101.300511 H Child_13_25.log			
8	-5.299236	1.283414	0.502813
6	1.923161	-1.526200	-0.052659
6	-4.139795	1.002399	0.235757
6	0.910477	-2.236426	-0.065504
6	-2.782735	1.423212	-0.068729
8	-0.512391	-4.141163	-0.097468
6	-1.634932	2.169571	-0.233719
12	3.024610	0.212585	-0.097664
6	-0.434658	2.429490	-0.307415
6	-3.065490	0.069689	0.021194
6	-0.359955	-2.908920	-0.064627
12	6.025721	0.811609	0.455205
6	2.118702	2.048332	-0.330512
6	-2.328153	-1.105932	-0.005522
6	-1.476787	-1.980753	-0.042794
6	0.918339	2.377483	-0.341013
16			
52.422381 Kcal/mol 2.273252 eV -101.300140 H Child_12_35.log			
8	6.078923	0.691097	-0.459097
6	-5.084611	-0.486441	-2.127803
6	5.060004	0.102396	-0.317999
8	-4.589204	-0.508450	-1.084457
6	3.822830	-0.321812	-0.183925
6	-1.953661	-1.715915	0.818172
6	3.174863	-1.542588	0.026225
12	-3.404799	-0.267307	0.724206
12	2.044852	0.832109	-0.190308
6	-3.341512	1.773668	0.859064
6	1.814338	-1.611479	0.158264
6	-0.719585	-1.842785	0.659140
6	0.357354	1.927350	-0.063620
6	-2.162682	2.058827	0.544331
6	0.601591	-1.826945	0.402109
6	-0.835328	2.112592	0.216317
16			
53.198924 Kcal/mol 2.306927 eV -101.298903 H Child_5_27.log			
6	-4.300582	-0.023726	-0.281221
8	5.035781	-1.780338	-0.399269
6	-3.631297	1.048925	-0.291591
6	3.977848	-1.262212	-0.255891
12	-3.773751	-1.940820	0.163204
6	2.755372	-0.826537	-0.093744
6	-0.291452	2.803375	-0.249719
6	2.247748	0.473505	-0.040511
6	-2.681863	1.955975	-0.465107
12	1.119527	-2.122446	0.165403
6	-1.515843	2.466655	-0.266347
6	1.714107	1.576234	0.032979
6	-2.024978	-2.924015	0.298710

6	-0.786490	-2.760432	0.322270
8	1.567250	3.854653	0.721054
6	1.041838	2.833033	0.203911
16			
53.484239	Kcal/mol	2.319299	eV -101.298448 H Child_6_8.log
8	4.497630	1.511732	0.263851
6	-4.021749	-1.456538	0.211702
6	0.342746	2.059443	-0.400845
6	-2.830344	-2.012219	-0.106232
6	1.365482	1.357266	-0.342870
6	-4.945308	-0.665389	0.520982
6	3.751679	0.582623	0.166945
6	-1.631165	-2.148913	-0.362855
12	-1.690267	2.392500	-0.226875
6	-0.303774	-1.970263	-0.465986
6	2.339344	0.365262	-0.188724
6	0.860198	-1.573989	-0.419086
6	3.311302	-1.795620	0.280146
12	-4.286572	1.309067	0.329276
6	2.093554	-0.993919	-0.188145
8	4.218656	-0.874889	0.553773
16			
53.685921	Kcal/mol	2.328045	eV -101.298127 H MutD_5_66.log
12	-4.386032	1.229129	0.037259
8	3.279174	2.081095	0.326637
6	2.574328	1.095008	0.082905
6	2.327440	-1.434920	-0.075318
6	-2.779366	-2.080502	-0.042282
6	-1.472723	1.866048	-0.254484
6	-2.669578	2.227457	-0.267444
6	-1.519201	-2.016793	-0.141841
6	-0.223377	-1.856252	-0.147069
6	1.025446	-1.553156	-0.117299
6	4.516883	-0.453206	0.039430
6	3.178566	-0.338218	-0.004399
6	-3.939986	-1.424869	0.262878
6	-4.982751	-0.720807	0.362925
12	0.394006	1.052670	-0.131270
8	5.682105	-0.486135	0.040877
16			
53.830097	Kcal/mol	2.334297	eV -101.297897 H MutD_5_64.log
6	4.030993	-0.406450	0.245414
6	-3.658677	1.772368	0.258115
6	1.852809	2.693547	0.150379
6	-2.881703	-1.615440	0.146439
12	-0.150930	2.380351	-0.182463
6	0.082821	-1.857675	-0.279496
6	2.798209	1.885114	0.217326
6	1.030760	-2.646985	-0.150700
6	-2.656495	0.769359	0.070975
6	3.555972	0.746046	0.247873
8	-0.026135	0.415126	-0.565369
8	-3.637912	-2.484047	0.324449
12	3.016712	-2.114768	0.047950
6	-2.090670	-0.542936	-0.046220

6	-2.234733	2.084513	0.059828
6	-0.675453	-0.654066	-0.329681
16			
54.091780	Kcal/mol	2.345645	eV -101.297480 H MutD_14_72.log
6	2.436697	0.048801	-0.306143
6	2.282509	1.428915	-0.288626
8	-0.306190	-2.251420	0.842634
6	1.861922	2.593321	-0.177641
6	-2.751524	-0.442022	-0.698433
8	3.999175	-2.003488	-0.067963
12	0.066491	3.481685	0.190842
12	-2.043649	-2.677254	0.234568
6	0.204483	-1.133496	0.238608
6	-1.916100	3.083193	0.432223
6	3.021481	-1.272478	-0.150476
6	-1.778818	0.498907	-0.193894
6	-3.357441	-1.533987	-0.849004
6	-1.999395	1.864704	0.157632
6	-0.576785	-0.046166	0.053083
6	1.603308	-1.025344	-0.101043
16			
54.387945	Kcal/mol	2.358487	eV -101.297008 H Child_4_45.log
12	-3.112941	2.019384	-0.107236
6	3.636083	-1.581822	-0.621480
6	-3.441772	-0.837107	-0.493554
8	3.363138	2.638437	-0.543136
6	-3.997791	0.279242	-0.522791
6	2.701920	1.726298	-0.243391
6	-2.615178	-1.919957	-0.379534
6	2.630168	-0.663105	-0.193036
6	-1.162563	2.488260	0.358972
6	2.307602	-2.007729	-0.157537
6	-1.658327	-2.687163	-0.174233
6	2.021281	0.606933	0.066672
6	-0.166810	1.778728	0.569556
6	0.675665	0.635833	0.608862
12	0.294303	-2.378483	0.386042
8	0.167109	-0.463595	1.011048
16			
54.778014	Kcal/mol	2.375403	eV -101.296386 H MutD_14_40.log
6	-0.215188	-1.026506	0.006034
6	1.084053	-0.923847	-0.070912
8	1.429266	2.173772	0.549251
6	2.364544	-0.845247	-0.069674
6	-3.615281	2.119145	-0.366912
6	-5.248350	-1.268052	0.081775
6	6.158112	-0.219383	-0.103391
6	0.449889	1.668870	0.198364
6	-1.503668	-0.952000	0.090301
8	7.332644	-0.014141	-0.125937
6	-4.451978	1.190655	-0.267138
6	3.629855	-0.644821	-0.074747
12	-1.785821	1.209127	-0.077124
6	-5.030081	-0.046037	-0.109264
6	4.903669	-0.457069	-0.074898

12	-3.318240	-1.946734	0.175146	
16				
54.987847	Kcal/mol	2.384502	eV	-101.296052 H Child_10_12.log
6	-2.911737	0.942586	0.181689	
6	2.682839	-0.518366	-1.821772	
6	-1.864951	1.600260	0.221749	
6	2.176984	-0.962629	-0.663375	
12	-2.074802	-1.277344	0.566570	
6	1.012738	-1.439423	-0.056251	
6	-0.624269	2.145951	0.193636	
6	-0.107939	-1.711203	0.394651	
6	0.583323	2.431662	0.199977	
6	3.391735	-0.195254	-0.131107	
6	-3.806040	-0.123605	0.192865	
8	-6.151036	-0.607740	-0.492873	
8	5.639119	-0.846733	0.716318	
6	-5.044069	-0.328739	-0.160921	
6	4.562964	-0.605704	0.287888	
12	2.390291	1.629224	-0.135048	
16				
55.295560	Kcal/mol	2.397845	eV	-101.295561 H Original2D_13_1.log
6	0.090929	1.892110	-0.000000	
6	-1.826407	-1.496278	0.000000	
6	-0.736610	-0.790617	0.000000	
6	1.417167	2.446230	-0.000000	
6	0.721624	-0.691820	-0.000000	
6	2.643495	2.629043	-0.000000	
6	-0.000000	0.458375	-0.000000	
12	2.717897	-1.107498	-0.000000	
6	-1.015777	2.657142	-0.000000	
8	-1.957063	3.354117	-0.000000	
6	-4.093195	-2.676823	0.000000	
6	-2.989289	-2.037452	0.000000	
8	4.318158	-0.267080	-0.000000	
12	4.357529	1.545179	-0.000000	
6	-5.190985	-3.374317	0.000000	
6	-6.319933	-4.007003	0.000000	
16				
55.501701	Kcal/mol	2.406785	eV	-101.295233 H Child_1_62.log
12	3.260922	-0.574309	-0.283277	
8	-4.677923	-0.391435	-0.069841	
6	2.309022	1.232234	0.211185	
6	-3.506513	-0.525693	-0.043647	
12	1.106100	2.853321	-0.330606	
6	-2.182790	-0.637235	-0.036906	
8	2.195759	-2.206475	-0.465947	
6	-1.443934	-1.804227	-0.414361	
6	1.360691	0.452323	0.807056	
6	-1.254472	0.471108	0.386845	
6	0.996333	-1.972483	0.060223	
6	-0.294479	-2.273118	-0.451961	
6	0.880547	-0.941616	1.006977	
6	-0.952437	2.972439	-0.450028	
6	-0.068744	0.123477	0.971977	
6	-1.267716	1.808648	-0.105209	

16
55.528004 Kcal/mol 2.407925 eV -101.295191 H Child_2_60.log
6 -1.115412 2.197551 -0.499080
6 7.706020 -1.646940 -1.171682
6 -5.157447 -2.935444 -0.207838
6 6.771110 -0.996349 -0.590618
8 -4.961965 -1.932839 -0.782711
6 5.730703 -0.404008 -0.086742
6 -2.440055 2.172554 -0.810420
6 4.642764 0.093607 0.321532
6 -0.016238 1.801006 -0.057238
6 3.423063 0.499071 0.527596
6 -3.642805 1.842569 -0.986760
6 2.199366 0.826673 0.606776
6 0.877164 0.951170 0.588096
12 -0.755956 -0.317392 1.210252
12 -3.777613 -0.040032 -0.103845
8 -2.471356 -0.832120 0.897885

16
55.549079 Kcal/mol 2.408839 eV -101.295157 H Child_9_12.log
8 -4.918220 -1.160183 -0.959556
6 1.776909 0.974880 0.843148
6 -3.849026 -0.951790 -0.474880
6 1.436591 1.847189 -0.113001
6 -2.722944 -0.574188 0.059826
8 2.083500 0.023628 1.507380
6 -1.532651 -1.250886 0.408788
6 2.183857 1.400575 -1.277525
6 -0.412771 -1.666277 0.750851
6 2.772599 0.339700 -1.570577
12 1.574418 -2.043562 0.806680
6 3.039715 -0.977860 -1.368034
12 -2.226098 1.434566 0.326946
6 0.250795 2.601499 0.053835
6 -0.892289 2.994991 0.356464
6 3.032203 -2.004434 -0.666578

16
55.570443 Kcal/mol 2.409766 eV -101.295123 H MutD_17_76.log
12 2.923131 -1.163860 0.648552
8 -4.999796 -0.298849 -0.687433
6 -1.671752 1.432668 0.057892
12 3.127683 -0.207061 -2.399670
6 0.702336 -2.872952 0.650660
6 1.589675 1.785696 0.679345
6 -1.652401 -1.956796 0.205725
6 -0.713413 2.173656 0.218228
6 0.578610 2.781654 0.454838
6 -3.819811 -0.286987 -0.368768
6 2.342808 0.808177 0.790912
6 -0.591769 -2.537770 0.428954
6 -2.588876 0.407084 -0.096889
8 0.779793 4.009798 0.437526
6 1.933572 -2.966117 0.845620
6 -2.583936 -0.974404 -0.031072

16

57.037849 Kcal/mol 2.473398 eV -101.292785 H Child_11_48.log

12	-1.121858	2.988484	-1.291350
6	1.876218	0.706895	1.362742
8	-8.192101	-2.449632	-0.015984
6	3.061287	0.390299	1.079441
6	-7.190405	-1.799787	-0.132362
6	5.389959	-0.448790	0.317990
6	-6.114876	-1.145941	-0.281789
6	4.284903	0.009408	0.737273
6	-5.055704	-0.408980	-0.262862
6	6.533781	-0.875117	-0.146398
6	-3.965347	0.236913	-0.247062
8	8.627299	-1.751889	-1.118636
6	-2.854630	0.895833	-0.074586
6	7.600539	-1.325797	-0.638554
6	-1.731165	1.505049	0.073768
12	-0.085554	0.942538	1.153962

16

57.085796 Kcal/mol 2.475478 eV -101.292709 H Child_4_15.log

6	-3.547273	2.376375	0.091661
8	1.830489	-2.898990	0.066303
6	-2.356669	1.969242	0.062260
6	2.428990	-1.735073	0.064075
12	-4.334955	0.512283	-0.038028
12	-0.032585	-2.878172	-0.017322
8	4.710156	2.390901	-0.096192
6	2.864936	-0.593126	0.035204
6	-2.890388	-0.996385	-0.065682
6	1.389049	1.316143	0.040280
6	3.783694	1.656284	-0.041490
6	-1.223184	1.082689	0.021130
6	-1.682936	-1.656540	-0.081924
6	-1.655102	-0.209450	-0.039215
6	2.735653	0.835126	0.019596
6	0.167448	1.363948	0.044656

16

57.181734 Kcal/mol 2.479638 eV -101.292556 H Child_1_42.log

8	-8.469227	-0.240364	-0.566692
12	4.317968	-0.133461	-0.561797
6	-7.304977	-0.342932	-0.302741
8	6.061065	-1.626546	-0.268335
6	-6.069456	-0.480295	-0.030907
6	2.562950	-1.147705	-0.079290
6	-4.796768	-0.482670	0.186299
6	6.535181	-2.455777	0.396994
6	-3.538541	-0.472082	0.356167
12	3.305365	2.497829	-0.275760
6	-2.248386	-0.331867	0.432836
6	0.754827	1.531829	0.420865
6	-0.998143	-0.170141	0.448832
6	1.336447	2.639590	0.421159
6	0.309592	0.175405	0.375022
6	1.421491	-0.702878	0.163248

16

57.337476 Kcal/mol 2.486391 eV -101.292307 H MutI_16_51.log

6	3.352525	0.295609	0.750623
8	2.273662	3.224699	-0.761795
6	-4.832283	0.009273	0.461128
6	0.893579	-1.367574	-0.385978
6	-3.981519	-0.799785	-0.031981
6	2.251210	2.112922	-0.372106
6	-0.273772	0.683564	0.002243
6	3.173156	-1.937202	0.324579
6	2.202918	0.871110	0.122786
12	-3.373866	1.452670	0.479173
12	-2.036348	-1.353983	-0.409625
6	2.082920	-2.166971	-0.202521
6	-1.388149	1.241571	0.123118
6	3.717722	-0.873227	1.024808
6	0.964995	0.020012	-0.111942
8	-0.280817	-1.939707	-0.621096
16	57.689566 Kcal/mol 2.501659 eV -101.291746 H MutD_8_66.log		
6	1.369100	-2.248236	-0.118935
6	2.695282	-2.339032	-0.081636
6	-1.116655	1.525958	-0.111860
8	-6.588594	-0.898331	0.254159
8	3.670620	1.223713	0.151725
6	-0.862217	-0.976178	-0.120063
6	0.032698	2.269488	-0.088692
6	0.280309	-1.566039	-0.120542
6	-4.196794	-0.372274	-0.045732
6	-5.441173	-0.654871	0.099562
6	3.967188	-2.445922	-0.005922
6	-1.272066	2.954327	-0.119303
6	-1.626251	0.180607	-0.112082
12	2.087922	2.076681	0.043156
6	-2.967146	-0.099640	-0.089974
12	4.426256	-0.407697	0.143844
16	57.924903 Kcal/mol 2.511865 eV -101.291371 H Child_15_20.log		
8	-5.530269	0.897647	0.241130
8	4.263112	-0.665340	0.425320
6	-4.355131	0.566487	0.194892
6	3.126201	-0.855185	-0.125228
6	-2.947608	0.886247	0.039835
6	1.939779	-1.539347	-0.398506
6	-1.786334	1.612403	-0.145998
6	0.869512	-2.396714	-0.249914
6	-3.324225	-0.440078	0.195360
6	-0.313364	-2.647165	-0.010590
6	-0.644479	2.066650	-0.328340
6	2.062305	-0.173960	-0.775225
6	-2.619882	-1.630578	0.217788
6	-1.626018	-2.352090	0.125214
12	4.229407	1.428108	0.664096
12	1.424986	1.868684	-0.478041
16	58.319843 Kcal/mol 2.528991 eV -101.290742 H MutD_15_40.log		
6	1.065504	-2.795900	0.356253

12	2.398418	1.514636	-0.013163
6	0.106017	2.457423	-0.050484
6	-1.409146	0.475029	0.545999
8	-6.087182	-0.702022	-0.808667
6	-4.983102	-0.372666	-0.540999
6	3.106212	-1.428569	-0.621701
6	-0.254795	1.224627	0.512947
12	-0.024336	-1.242207	1.079046
6	0.992713	3.263881	-0.447778
6	-3.795631	-0.015281	-0.232774
8	0.860426	0.565415	0.987397
6	-2.613478	0.280748	0.128259
6	2.046709	-2.197626	-0.171485
6	3.529343	-0.109901	-0.684448
6	4.430498	-1.144480	-1.163863
16			
58.586103 Kcal/mol 2.540537 eV -101.290318 H MutI_10_71.log			
6	-3.507699	1.268706	-0.273669
6	2.541837	1.551654	0.115486
12	-2.595206	3.024167	0.125059
6	-2.802082	-2.304414	-0.330836
6	2.403323	-1.772315	0.161110
6	3.483010	0.561178	-0.359702
6	1.617059	2.315786	0.373490
8	4.509898	0.887024	-0.991503
12	-0.148032	-3.148460	0.557741
8	1.653139	-2.780031	0.427550
6	-0.680576	3.513166	0.517805
6	0.454299	3.010509	0.519920
6	3.050737	-0.768164	-0.097185
6	-3.596780	0.038664	-0.527575
6	-2.097181	-3.349978	-0.088393
6	-3.596853	-1.292194	-0.624115
16			
58.754465 Kcal/mol 2.547838 eV -101.290049 H Child_11_23.log			
12	-2.080983	2.981101	-0.306559
6	6.383789	-0.508472	-0.021899
6	-3.911215	2.310758	0.284798
6	5.110259	-0.578862	-0.058929
6	-3.679962	1.113809	0.575103
8	7.583532	-0.470609	0.059442
6	0.564405	1.217765	-0.374793
6	3.839101	-0.345787	-0.121953
6	-3.157345	-0.132498	0.799031
6	-4.792123	-3.265890	-0.097294
6	1.264813	0.019592	-0.108792
6	2.585027	-0.151753	-0.119895
6	-0.248689	2.146170	-0.546886
12	-0.390469	-1.213848	0.440859
6	-2.368497	-1.093489	0.876474
8	-5.068526	-2.728778	-1.074618
16			
59.016662 Kcal/mol 2.559208 eV -101.289631 H MutI_13_39.log			
12	3.200422	1.312647	0.090019
6	-0.968897	1.407607	-0.113781

6	-0.006486	-0.856659	-0.063100
6	-1.316880	-1.384287	0.029315
6	3.686449	-1.506558	-0.079791
6	-3.495443	1.435396	-0.055389
8	1.389939	1.199036	-0.003271
6	4.584816	-0.489063	0.023686
6	1.116049	-1.572625	-0.120372
12	-4.337797	-1.019363	0.089262
6	5.217547	0.617658	0.161086
6	-2.496800	-1.748020	0.144509
6	0.150461	0.714028	-0.059303
8	-4.651597	0.880828	0.018127
6	-2.266583	1.632644	-0.105311
6	2.419395	-1.609842	-0.139917
16			
59.190855	Kcal/mol	2.566762	eV -101.289354 H MutD_13_44.log
6	2.360939	2.914889	-0.362033
8	-8.019873	0.080150	-0.106433
6	3.989526	-2.577165	-0.748294
6	4.533100	-0.320843	0.442309
6	-5.551060	0.019822	0.049681
6	-6.821333	0.038092	-0.036108
8	2.719191	3.726698	-1.080838
6	-2.992913	-0.179699	0.109694
6	-0.434781	-0.477625	0.160703
6	-1.716379	-0.333752	0.134456
12	1.976731	-2.252043	-0.506741
6	4.424320	-1.531620	-0.198615
6	-4.264631	-0.064097	0.076158
12	2.222539	0.893299	0.863431
6	4.274663	0.749499	1.046543
6	0.867583	-0.595809	0.195154
16			
59.266588	Kcal/mol	2.570046	eV -101.289233 H Child_7_55.log
6	2.300696	1.409526	-0.269389
6	-4.518024	-0.853402	0.457784
6	-2.769051	2.389560	-0.687805
6	-3.916112	0.186615	0.081041
6	3.084538	0.460077	-0.357697
6	-1.065203	-2.766943	-0.021111
12	-0.744108	2.462366	-0.367651
12	-2.987613	-2.216844	0.336158
6	-3.356499	1.337379	-0.324293
6	0.166552	-2.642855	-0.146030
6	3.653988	-0.856397	-0.160268
6	1.480215	-2.307044	-0.233666
6	1.329148	2.360336	0.127895
6	2.601089	-1.819365	-0.306303
8	1.563898	3.054619	1.157134
8	4.790181	-1.096019	0.269987
16			
59.705757	Kcal/mol	2.589090	eV -101.288533 H MutD_12_78.log
6	-1.356876	-1.454305	0.387253
6	3.392064	-0.286470	-0.128142
6	-4.512962	0.906649	-0.401894

6	1.182683	-1.549235	0.233741
6	4.714039	-0.271365	-0.091356
6	2.405148	-1.176049	0.131852
6	-3.325263	-1.255463	-1.001879
8	5.866730	-0.048611	-0.171731
6	-0.851065	2.237024	0.199028
8	-1.782438	-0.556714	1.247538
12	-2.579807	1.188966	0.654354
6	-0.044697	-1.858438	0.434418
6	-2.290086	-1.838537	-0.634027
12	2.109354	1.433217	-0.402973
6	-4.167750	-0.193288	-0.917801
6	0.349947	2.302212	-0.148365
16			
59.937069 Kcal/mol 2.599121 eV -101.288165 H MutD_7_66.log			
8	-0.187839	-2.302476	0.028544
8	6.599528	-0.069908	-0.102315
6	0.824968	1.838616	0.064066
12	-1.056029	2.636077	0.026146
6	2.817679	0.099677	0.044550
6	-3.863689	-1.197249	-0.030382
6	5.399184	0.032394	-0.052523
12	1.484865	-1.550450	0.067306
6	-3.778874	1.353804	-0.035091
6	-1.452718	-2.098798	0.007390
6	-2.653581	-1.850237	-0.012003
6	-4.331074	0.086724	-0.040594
6	4.139913	0.239050	-0.009232
6	1.842597	1.121725	0.055667
6	-3.041427	2.355381	-0.030910
6	-5.309568	-0.989163	-0.049480
16			
59.969286 Kcal/mol 2.600518 eV -101.288113 H MutD_6_74.log			
12	-1.507028	-1.568861	-0.095590
6	-2.811057	0.107442	-0.054196
8	-6.581946	-0.031348	0.153288
6	-5.385607	0.054645	0.080351
6	-0.787447	1.810697	-0.074722
6	3.834858	-1.201449	0.054783
6	-4.128400	0.286398	0.011513
8	0.166151	-2.328378	-0.069011
6	3.778248	1.355633	0.040609
6	4.308784	0.080303	0.066748
6	-1.816278	1.108374	-0.070873
6	1.425583	-2.103512	-0.025470
6	5.279839	-0.999853	0.117757
6	2.626869	-1.857946	0.009763
6	3.074926	2.381740	0.017351
12	1.084065	2.630775	-0.047401
16			
60.004694 Kcal/mol 2.602053 eV -101.288057 H Child_7_18.log			
6	0.905734	-2.662869	0.004894
12	-1.802042	2.708266	-0.001675
6	-0.383168	-2.153989	0.001897
6	1.754970	2.617149	-0.008512

6	2.051352	-2.134708	0.007960
6	0.276626	2.621473	-0.001313
8	4.414431	0.396026	-0.011721
8	-3.051206	1.413962	0.004550
6	-1.677469	-2.670781	-0.002175
6	0.950749	1.431055	0.004287
6	3.365420	-0.090350	-0.000795
12	-2.606156	-0.362506	0.004392
6	2.162137	-0.736468	0.006407
6	0.870324	-0.004928	0.008788
6	-0.336459	-0.678233	0.008503
6	-2.941453	-2.642188	-0.025816
16	60.291810 Kcal/mol 2.614504 eV -101.287599 H MutD_5_70.log		
6	-0.184800	-1.562197	-0.141318
6	4.515354	-0.946441	-0.038030
6	-3.258446	0.679370	0.396247
6	0.827213	-2.226559	0.117754
12	0.118591	2.445199	-0.228369
8	-0.569481	0.663420	-0.563561
6	3.112661	1.280553	-0.029730
6	-3.186971	-1.654797	-0.064207
6	-1.903925	2.937348	0.469367
6	3.939271	0.182653	-0.002311
12	2.845430	-1.950699	0.342771
6	2.158040	2.076416	-0.068376
6	-2.517730	-0.474547	-0.049736
6	-1.083051	-0.467835	-0.343676
6	-2.594707	1.863327	0.427605
8	-3.743732	-2.670638	-0.113233
16	60.292858 Kcal/mol 2.614549 eV -101.287598 H Child_11_37.log		
6	-4.500778	-0.971145	0.428904
8	5.850292	-0.043244	0.149682
6	-4.068122	0.069906	1.006014
6	4.700489	0.217075	0.103409
12	-2.606347	-1.070743	-0.758532
6	3.376720	0.262557	0.148654
6	-3.191566	1.097877	1.129524
6	2.406243	1.172320	-0.107403
8	-1.858681	0.715265	-1.305330
6	1.189731	1.555892	-0.234997
6	-0.874882	-2.109958	-0.295780
6	-0.035230	1.879995	-0.430495
6	-2.189876	1.736213	0.760834
12	2.064737	-1.437354	0.406653
6	0.295648	-2.276569	0.108714
6	-1.347303	1.486004	-0.372755
16	60.506888 Kcal/mol 2.623830 eV -101.287257 H MutD_13_52.log		
6	-3.003439	0.103227	-0.209072
8	2.846290	3.226807	0.054049
6	-0.430623	-0.000394	-0.155870
6	-5.562905	-0.096414	-0.018484
6	-1.713411	0.127011	-0.187624

8	-8.025179	0.084613	0.238231
6	4.002848	-2.305793	0.098284
6	3.293743	-3.348875	0.093452
6	3.382931	4.255922	0.095141
6	0.864072	-0.192514	-0.107402
6	-4.282538	0.049501	-0.137903
6	4.444507	-1.002072	0.095352
6	-6.833234	0.048865	0.106294
6	4.474784	0.249708	0.068345
12	1.556863	-2.204053	-0.017703
12	2.577363	1.052354	-0.047407
16			
60.527789 Kcal/mol 2.624737 eV -101.287223 H Child_8_54.log			
8	-6.080656	-1.018550	-0.374076
6	4.053385	-1.318015	0.801988
6	-2.447417	-1.026871	0.012331
6	4.576686	-0.251061	-0.211403
6	-4.925552	-0.780935	-0.223060
8	5.614686	0.035174	-0.770266
6	-1.258771	-1.388762	0.092196
6	2.343462	1.208440	0.004482
12	0.725599	-1.741830	0.184290
6	1.337379	1.917120	0.071239
6	-3.697524	-0.391020	-0.054338
6	3.144722	0.086729	-0.198856
6	0.079107	2.420112	0.136352
12	-2.826605	1.486995	0.154844
6	-1.147578	2.614174	0.188702
6	2.765407	-1.269073	0.227889
16			
60.935535 Kcal/mol 2.642418 eV -101.286574 H Child_8_27.log			
8	2.141775	3.002049	0.107528
12	2.562186	-2.921388	0.006943
6	2.917870	1.969444	0.035212
6	4.074666	-1.623605	-0.077910
12	0.327266	3.249395	0.062181
6	0.520692	-3.088709	0.055769
6	-1.551191	2.527998	0.069779
8	-5.157216	-0.565548	0.272052
6	3.555890	0.926861	-0.026801
6	-3.946756	-0.445631	-0.039780
6	-2.496014	1.719800	-0.189465
6	-0.651351	-2.681257	0.047068
6	3.924086	-0.385779	-0.063398
6	-2.928321	-1.463669	-0.014517
6	-3.306436	0.728745	-0.459639
6	-1.871451	-2.088880	0.019327
16			
61.290532 Kcal/mol 2.657812 eV -101.286008 H Child_10_18.log			
6	0.507343	-0.122136	0.516050
6	-3.951591	1.999546	-0.556169
6	0.221469	-1.388937	0.175655
6	-4.004610	0.769056	-0.751456
6	0.430794	1.083656	0.849964
12	-2.676404	3.292208	0.326087

6	0.635458	-2.686165	0.244280
6	-3.779632	-0.570137	-0.943233
8	7.514291	1.780690	-0.447368
6	-3.330132	-1.728516	-1.001129
6	7.913797	2.410636	-1.329621
6	-0.768008	3.371840	1.091062
6	-0.116006	2.310474	1.000407
12	-1.498764	-2.434923	-0.494469
6	1.575703	-3.542990	0.575253
8	2.247524	-4.496363	0.796644
16			
61.761266	Kcal/mol	2.678225	eV -101.285258 H MutD_18_64.log
12	2.823968	-0.005715	-1.169352
8	-5.239101	-1.765389	-0.874597
6	2.121667	1.907353	-1.047594
8	4.758970	-0.646499	1.857979
6	-1.352058	2.659889	0.092290
6	-0.670605	-1.333335	0.475748
6	-3.403698	1.325553	0.954581
6	-4.357761	-1.564908	-0.193563
6	1.075417	2.474788	-0.692721
6	0.491244	-1.642625	0.115044
6	1.662460	-1.967226	-0.515775
6	-0.177746	2.767481	-0.271617
6	2.818522	-2.090191	-1.008539
6	4.302263	-0.340524	0.871742
6	-2.506654	2.087213	0.521758
12	-2.505405	-0.528094	0.863087
16			
61.902559	Kcal/mol	2.684352	eV -101.285033 H MutD_9_76.log
6	-1.247969	-2.540262	-1.022737
6	4.031379	0.648725	-0.612505
6	0.929569	0.999120	0.731235
8	5.053263	1.030546	-1.138497
6	-0.297608	-3.276971	-0.650553
12	-1.567199	2.887516	0.244927
12	0.730677	-1.964767	0.599354
6	-1.437297	-0.313900	2.251534
6	3.004570	0.116026	-0.073687
8	-0.790270	-1.221549	1.912368
6	-2.967786	0.894130	-1.205489
6	-3.045011	2.096682	-0.872769
6	-2.668936	-0.426782	-1.341603
6	1.787131	-0.090649	0.446647
6	-2.115771	-1.527689	-1.288085
6	0.016782	1.830740	0.917621
16			
62.324255	Kcal/mol	2.702639	eV -101.284360 H Child_10_30.log
6	3.934395	0.025907	0.403647
12	-4.095017	0.146715	0.556323
6	3.247545	1.039038	0.553117
6	-2.905838	-1.606552	0.201339
8	4.375977	-1.175145	0.153024
8	-2.808723	-2.820064	0.152363
6	-2.154001	0.717444	-0.085562

6	2.203696	1.893598	0.480226
6	-1.792800	-0.604569	-0.169527
6	1.080265	2.360956	0.283449
6	-0.507118	-1.132860	-0.439419
6	-0.200592	2.532340	-0.170674
6	-1.390657	1.860132	-0.336187
12	2.605266	-1.805727	-0.372792
6	-1.248643	3.179539	-0.925060
6	0.623580	-1.620002	-0.569595
16			
62.444505 Kcal/mol 2.707853 eV -101.284169 H Child_4_22.log			
6	3.383698	-1.680911	0.092085
8	-3.610066	-2.223322	-0.471940
12	0.400424	3.335672	-0.023339
6	-2.590324	-1.660502	-0.203004
6	3.870718	-0.442232	-0.167912
8	-2.617375	0.231894	0.087028
6	3.477535	0.728257	-0.272746
12	-2.236434	2.202435	0.283275
6	1.058143	1.023713	-0.120665
6	2.357249	-2.383380	0.274070
6	2.266893	1.391078	-0.295974
6	1.029792	-2.605079	0.356951
6	-0.167833	-2.338690	0.208107
6	-0.287321	1.010716	0.049531
6	-1.240126	-1.457739	0.014136
6	-1.183150	-0.006209	0.058763
16			
62.474133 Kcal/mol 2.709138 eV -101.284122 H Child_1_55.log			
12	-1.419329	2.753918	0.000000
8	4.763666	-1.504795	-0.000000
8	-2.889384	1.610205	0.000000
6	-2.640054	0.318494	0.000000
6	3.682060	-0.996397	-0.000000
6	0.287631	1.663216	0.000000
6	0.692765	-1.999613	-0.000000
6	-3.609442	-0.777603	-0.000000
6	-0.470441	-2.513258	-0.000000
6	-0.000000	0.286003	0.000000
6	2.571610	-0.325096	-0.000000
6	-1.343113	-0.315125	-0.000000
6	1.193577	-0.745511	-0.000000
6	-3.056288	-1.899781	-0.000000
6	-1.613016	-1.795138	-0.000000
12	2.322164	1.725713	0.000000
16			
62.479123 Kcal/mol 2.709355 eV -101.284114 H MutD_17_36.log			
12	2.795394	1.559666	-0.735425
6	-1.736094	2.416836	0.366547
6	-2.903754	2.003078	0.391361
6	-3.830832	-1.394547	0.015991
6	-0.412420	2.091853	0.155005
6	-1.601329	-2.595022	-0.354787
6	-3.903103	1.098643	0.352438
12	1.248084	-1.132511	-0.375282

6	-0.355783	-2.511064	-0.455885
8	4.096071	-1.024759	1.507104
6	3.044452	-1.177049	1.022835
6	-2.869620	-2.160890	-0.190788
6	-4.169509	-0.104115	0.207205
6	0.353774	0.917486	-0.012257
8	2.932770	-0.255410	-0.837921
6	0.925475	2.267371	-0.168495
16			
62.514807 Kcal/mol 2.710902 eV -101.284057 H MutD_7_76.log			
6	-2.806119	-2.907583	0.166148
6	-0.566567	-1.581474	0.220984
6	4.386589	0.112729	-0.390602
6	0.040991	0.986099	0.439860
8	-3.820573	-3.559776	0.118189
6	3.987063	-1.185978	-0.416828
6	-1.751385	-2.197807	0.217279
6	2.970910	3.505895	0.147505
6	-0.345328	-0.196186	0.362011
12	1.110271	2.721818	0.417708
6	3.336745	-2.248408	-0.378218
8	-6.938038	2.869215	-0.299729
6	3.759444	2.559819	-0.082517
6	4.324114	1.338491	-0.283575
12	1.346928	-2.493892	-0.053551
6	-7.906041	2.279300	-0.488308
16			
62.850449 Kcal/mol 2.725457 eV -101.283522 H MutD_6_64.log			
6	-3.977104	1.835178	-0.538596
6	-0.046027	-0.354051	0.353709
6	-4.932642	-0.529223	-0.368755
12	-1.125794	2.320115	-0.128493
6	1.758245	1.327098	0.414429
6	9.919119	-0.885071	-0.480529
8	4.168243	1.712345	0.776631
6	0.481044	0.958244	0.271195
6	-4.681136	0.677089	-0.481545
6	-0.679216	-1.425190	0.403740
8	9.172947	-1.719951	-0.747607
6	-4.702521	-1.861432	-0.169863
12	-2.200095	-2.773492	0.340907
6	-3.079593	2.694706	-0.534884
6	3.007721	1.462868	0.607524
6	-4.204366	-2.983324	0.060048
16			
63.114749 Kcal/mol 2.736918 eV -101.283101 H Child_16_28.log			
8	2.138991	3.702367	-0.372267
12	-0.267197	-3.623954	-0.535263
6	1.881276	2.564198	-0.146179
6	2.802222	-2.035077	0.049369
6	1.727982	1.278398	0.083624
6	-0.808602	-1.668522	0.221011
6	-1.963933	1.475827	-0.129816
6	-2.047829	-1.121802	0.343561
6	-0.755689	1.254131	-0.119886

6	1.621382	-1.575062	0.066057
6	-3.317187	0.942399	0.039507
12	3.326604	-0.041650	0.349317
8	-4.390035	1.528864	-0.094502
6	0.371134	-0.877169	0.076508
6	0.465610	0.554358	0.000621
6	-3.093787	-0.435448	0.509872
16			
63.245954 Kcal/mol 2.742608 eV -101.282892 H Child_12_63.log			
6	6.114370	-1.052798	-1.171731
6	-0.065732	2.819159	-0.020932
6	2.726309	-1.678807	0.562326
6	1.225964	2.851542	0.120312
8	6.695146	-0.629162	-0.275264
6	-1.324921	2.620139	-0.075937
12	0.708442	-2.149077	0.353085
6	2.165219	1.932386	0.233811
6	2.900818	-0.428673	0.487007
6	-2.344868	1.784214	-0.116357
6	-3.923465	-0.274361	-0.103187
6	2.893276	0.915803	0.394010
6	-5.136359	-0.748074	-0.188627
6	-3.260779	0.920809	-0.115614
8	-6.169171	-1.321045	-0.282297
12	-2.044008	-1.381454	0.016081
16			
63.311591 Kcal/mol 2.745454 eV -101.282787 H MutI_4_73.log			
12	-1.312970	0.736309	0.247066
6	-2.224969	-1.163332	0.422404
8	-3.045856	1.538256	-0.845219
8	-4.675205	-1.517208	0.558821
6	-4.053670	1.956390	-1.225283
6	3.360223	1.710906	0.212428
6	0.175086	-2.045730	-0.186352
6	-0.187208	2.462475	0.415375
6	4.120445	-1.799191	-0.329255
6	-0.999270	-1.760697	0.129730
12	2.128755	-2.401871	-0.360553
6	2.416026	2.568345	0.393841
6	4.227902	-0.544249	-0.175264
6	4.240306	0.785422	0.031518
6	1.072768	2.573411	0.428125
6	-3.484460	-1.440688	0.491571
16			
63.342148 Kcal/mol 2.746779 eV -101.282738 H Child_12_57.log			
12	1.612047	2.112767	-0.206798
8	-7.718129	0.249310	0.848658
6	2.985929	-4.286169	0.637943
6	-6.603727	0.106080	0.420664
6	3.852491	2.420245	0.523713
6	-5.411903	-0.013245	-0.008902
8	2.692920	-3.232745	0.242553
6	-4.170908	-0.150175	-0.367868
12	2.580415	-1.125079	-0.246055
6	-2.936757	-0.279873	-0.664393

6	4.303193	1.123597	0.427774
6	4.289692	-0.095984	0.171501
6	-1.652954	-0.268781	-0.815201
6	3.129167	3.453381	0.448756
6	-0.366680	-0.122118	-0.775577
6	0.897813	0.115579	-0.547652
16			
63.513783	Kcal/mol	2.754222	eV -101.282465 H Child_3_41.log
6	4.550424	-1.415155	-0.040446
12	-2.971705	2.084893	0.054780
6	4.392551	-0.167650	-0.015604
6	0.378417	2.122961	0.066980
12	2.608050	-2.106565	-0.038975
6	-0.930503	1.712376	0.057728
6	0.687403	-1.454576	-0.005569
6	1.609433	2.259338	0.064259
6	-2.708660	0.029325	0.091773
6	3.855738	1.079673	0.013837
6	2.890064	1.852637	0.040206
6	-3.267685	-1.297464	0.122935
6	-1.264586	0.342224	0.052959
8	-3.621282	-2.222359	0.830720
8	-3.276933	-1.042610	-1.207235
6	-0.267665	-0.667052	0.021349
16			
63.526329	Kcal/mol	2.754766	eV -101.282445 H MutD_13_32.log
8	5.534907	0.565365	1.148608
6	-0.663887	-2.832158	-0.105591
6	-4.671166	0.194392	0.298390
6	0.731510	2.537413	-0.420933
6	5.251167	-0.438513	1.628759
6	-3.388632	-0.014632	0.388848
6	0.556614	-2.665954	-0.332000
6	1.803705	-2.254577	-0.637434
6	1.984599	2.137551	-0.720207
6	3.192527	-0.115856	-1.026517
6	-0.480832	2.690294	-0.131135
12	-2.386023	-1.791733	0.271868
6	2.674206	1.089291	-0.884598
8	-5.852670	0.371876	0.153901
6	2.558137	-1.261138	-0.839362
12	-2.176109	1.633847	0.250683
16			
63.629546	Kcal/mol	2.759242	eV -101.282280 H Child_5_15.log
8	5.501189	0.029801	-1.040235
6	-4.669378	1.380722	-0.511438
6	4.436036	-0.091268	-0.536862
6	-3.783868	0.245063	-0.333016
6	3.265436	0.067338	0.035804
6	-3.236222	1.495394	-0.256696
6	2.095425	-0.487650	0.494709
6	-3.438281	-1.092029	-0.257880
6	1.545634	-1.750440	0.478581
6	-2.043218	2.147261	-0.060682
12	1.743067	1.553228	0.594884

6	-2.971805	-2.239951	-0.174964
6	0.784384	-2.740399	0.408050
6	-0.880886	2.465866	0.169258
8	0.351475	2.783092	0.364444
12	-1.196471	-3.128444	0.128212
16			
63.747860 Kcal/mol 2.764372 eV -101.282092 H Child_10_57.log			
6	3.497109	-1.373995	0.150333
6	-0.744517	2.678978	-0.245821
6	2.582005	-2.196957	0.082252
6	-1.799441	2.029683	-0.332985
8	4.326372	-0.403867	0.207584
6	-3.173123	0.181797	-1.499663
6	1.336887	-2.688907	-0.019988
6	-2.809038	1.068529	-0.389357
6	0.115737	-2.866174	-0.131550
12	1.287614	2.793808	-0.105918
6	-1.175087	-2.524564	-0.244944
6	-3.049090	-0.803632	-0.400345
12	3.788999	1.432816	0.119898
6	-3.332080	0.186234	0.685920
6	-2.257900	-1.932692	-0.354083
8	-3.834887	0.245206	1.796618
16			
63.978715 Kcal/mol 2.774383 eV -101.281724 H Child_13_19.log			
6	-2.858555	-2.036006	-0.128299
8	5.311451	-0.429318	-0.819145
6	-3.350111	-0.803815	-0.373971
6	4.160764	-0.389122	-0.445458
8	-1.113249	-3.741161	0.497423
12	1.155502	2.453939	0.682516
6	-2.121065	-2.972631	0.199814
6	2.962424	-0.328765	-0.011635
12	0.232463	-2.362791	0.104900
6	-1.330592	3.481071	-0.047606
6	-3.448989	0.417094	-0.537748
6	1.563529	-0.826285	0.253327
6	1.788871	0.471399	0.500638
6	-0.212189	3.911645	0.317055
6	-3.107447	1.720377	-0.513278
6	-2.420170	2.733381	-0.358710
16			
64.126143 Kcal/mol 2.780776 eV -101.281489 H MutD_15_76.log			
6	-1.734719	1.475345	0.031170
6	2.542129	-0.499763	-0.021049
6	3.487162	-1.586629	0.072902
6	-2.977325	0.864726	0.024407
12	1.501700	1.335687	-0.007953
8	-5.564264	0.999844	0.098251
6	-4.408026	0.607971	0.046710
6	-0.522008	1.740805	0.027090
6	-1.692549	-2.299344	-0.090679
6	2.076376	-1.824464	-0.045150
6	0.841003	-2.435990	-0.092288
6	-3.424872	-0.444757	-0.013705

6	-2.737250	-1.647455	-0.063300
8	4.632767	-2.015604	0.189786
12	3.583179	3.671219	-0.071702
6	-0.377685	-2.609912	-0.100848
16			
64.376700 Kcal/mol 2.791641 eV -101.281090 H MutD_13_34.log			
12	-2.780745	0.801810	0.768922
6	0.082750	-1.901484	0.380700
6	2.513446	-1.133516	0.094368
8	5.866712	0.242404	-0.446437
6	-3.994737	0.072630	-1.242106
6	0.126212	2.072858	0.147841
6	3.439353	-0.170083	-0.115713
6	-3.035336	-0.897165	-1.175957
6	-2.058872	-1.550806	-0.776390
6	-1.230455	-1.484846	0.388820
6	4.750616	-0.072325	-0.249711
12	1.974837	1.418107	-0.110196
8	-1.767811	-0.862368	1.413008
6	1.289879	-1.515168	0.230802
6	-4.649621	1.030665	-0.720817
6	-1.086620	1.936026	0.431951
16			
64.382135 Kcal/mol 2.791877 eV -101.281081 H Child_1_61.log			
8	-4.708913	-1.911915	0.157031
6	3.666534	-1.822940	0.388151
6	-3.677069	-1.309388	0.057934
6	1.570575	2.169714	-0.056058
6	-2.658771	-0.541712	-0.020128
12	2.997736	0.146694	-0.126976
8	-1.547128	2.309538	0.099725
6	2.676402	-2.599420	0.332943
6	-1.372630	-0.183999	-0.154744
6	0.580187	1.233918	-0.291243
6	-0.896228	1.239446	-0.122799
12	0.044856	3.638103	0.292943
6	0.226102	-2.336459	-0.094786
6	0.950644	-0.144058	-0.521962
6	1.345102	-2.832669	0.129664
6	-0.154644	-0.972191	-0.321246
16			
64.772693 Kcal/mol 2.808813 eV -101.280459 H Child_10_61.log			
6	3.150625	-0.559857	1.417098
8	-5.447141	-0.766110	0.694616
6	2.932012	-1.816579	1.369997
6	-4.321745	-0.667026	0.316884
6	3.268962	0.783190	1.423397
6	-3.119483	-0.428165	-0.117439
6	2.486406	1.701003	0.917840
6	-1.912202	-1.146479	-0.141733
6	1.634511	2.537658	0.480258
6	-0.764984	-1.629578	-0.159742
8	3.011938	-0.654469	-2.543995
12	-2.235727	1.384450	-0.623235
6	0.422488	2.740161	-0.057962

12	1.173740	-2.043538	0.235014
6	2.349530	-1.071953	-1.710498
6	-0.755208	2.769909	-0.495821
16			
65.834701 Kcal/mol 2.854866 eV -101.278766 H Child_10_40.log			
6	-3.750666	1.124126	-0.506349
8	1.673370	0.082308	1.405586
6	-3.808804	-0.131373	-0.614805
6	0.604451	-0.539613	1.156891
6	-3.190639	-1.320925	-0.464894
12	2.632492	1.138929	-0.001223
12	-1.733161	1.669137	0.218810
6	0.442858	-1.756131	0.310658
6	-2.202973	-1.996223	-0.105994
6	1.435344	-2.144721	-0.557474
6	0.037752	2.550089	-0.365681
8	3.346805	-0.596501	-1.000213
6	2.474812	-1.447611	-0.783695
6	-0.823602	-0.243962	1.035234
6	1.287366	2.543335	-0.514389
6	-0.998129	-1.567533	0.434827
16			
66.071076 Kcal/mol 2.865117 eV -101.278390 H Child_18_15.log			
6	4.536354	-1.189027	-0.549943
6	-5.346933	-0.479164	-1.127909
6	4.429009	0.063264	-0.447283
8	-5.749389	0.595442	-1.111043
12	2.913124	-2.382009	-0.198347
6	-1.495959	1.753810	0.479970
6	4.149906	1.376382	-0.328213
6	-2.452623	0.968836	0.581781
6	3.185389	2.173937	-0.100873
6	-0.399003	2.497893	0.364071
6	0.935830	-2.707002	0.206490
12	-2.089229	-1.710938	0.591355
6	2.122432	2.912329	0.068766
8	-3.137309	-0.125958	0.690571
6	-0.290790	-2.570023	0.395268
6	0.827529	2.758681	0.232490
16			
66.319317 Kcal/mol 2.875881 eV -101.277994 H Child_5_41.log			
6	3.728619	-1.405677	0.139551
6	-7.416418	0.940328	0.238794
6	2.887619	-2.467657	0.063546
8	-6.510638	0.320968	0.580724
6	4.172348	-0.259351	0.212722
6	-1.670773	0.740372	-0.379639
6	1.928513	-3.258148	0.016322
6	-3.065611	0.276750	-0.494194
6	4.252913	1.095493	0.252672
6	-0.712188	1.738676	-0.337270
6	4.027401	2.320084	0.256727
6	0.228731	2.540176	-0.241269
12	-0.053722	-2.935200	-0.054114
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6	-4.569390	-0.105096	0.076846
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6	-3.265969	-0.007536	-0.124270
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6	4.533300	0.403566	0.354747
6	-3.974550	0.045884	0.185270
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6	1.731025	0.535906	-1.869457
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6	-1.904595	0.233166	-1.175656
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6	1.423026	-2.518813	-0.061074
6	-1.007400	-1.934345	-0.206632
6	0.986279	0.580206	-0.113900
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6	-1.425576	2.788285	-0.402101
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6	-2.572463	1.341737	0.355814
6	1.554572	-1.482481	-0.401867
6	-3.190237	-1.496347	0.380980
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6	3.503047	1.065896	1.026938
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6	1.318055	0.589060	0.024294
6	-2.828467	1.420616	-1.383789
6	0.318457	-0.351885	0.214213
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6	3.039432	-1.107528	-0.071379
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73.615148	Kcal/mol	3.192259	eV -101.266367 H Child_5_50.log
6	-2.934463	2.470635	-0.433227
8	3.932737	-1.293439	1.803401
6	-1.881708	3.038567	-0.046382
6	2.853762	-0.794032	1.552529
6	-3.904150	1.593310	-0.697686
6	9.607453	0.450246	-1.228519
6	-4.600356	0.559605	-0.784937
8	8.934294	-0.269447	-1.819282
12	-0.217526	2.229196	0.753663
6	1.682158	-0.391179	1.237980
6	-4.994666	-0.777742	-0.780928
6	-0.487751	-0.587479	0.367044
6	-5.032171	-2.033403	-0.614357
6	-1.471965	-1.186465	-0.016908
12	-3.052338	-2.466103	-0.461738
6	0.547545	0.215599	0.882715
16			
73.705860	Kcal/mol	3.196193	eV -101.266223 H MutI_13_43.log
6	-0.008670	2.677008	-0.169355
6	-1.287963	2.941715	-0.123654
6	-0.482109	-2.642166	-0.124419
12	-3.485900	-1.565718	-0.303483
12	2.163573	-1.605089	0.473479
6	2.071545	1.351371	0.287316
6	2.763615	0.336211	0.529174
8	0.807080	-2.765228	0.017105
6	-5.143750	-0.281639	-0.024490
6	-2.468245	2.402471	0.048081
6	-4.423705	0.763572	0.139709
6	-1.701235	-2.417937	-0.189986
6	-3.561857	1.783955	0.141186
6	1.202963	2.343238	-0.001613
8	5.835739	0.125858	-0.229147
6	6.826974	0.602976	-0.569217
16			
74.144800	Kcal/mol	3.215227	eV -101.265523 H MutI_10_67.log
6	3.459117	2.262776	0.030653
6	-2.198863	0.904142	-0.222753
12	-4.254833	0.815239	0.240797
6	-0.075321	2.411721	-0.136507

6	1.092920	2.875278	-0.144268
6	-1.157098	1.638180	-0.180174
6	4.188849	1.152355	0.157094
6	3.762237	-1.370431	0.228586
6	1.763568	-2.967702	0.072241
6	2.419069	2.959057	-0.085326
6	4.173653	-0.103118	0.222095
12	-1.808800	-1.225820	-0.432064
8	-0.713634	-2.757351	-0.157477
8	-5.858901	-0.011979	0.401757
6	0.537505	-2.960601	-0.048117
6	2.925008	-2.288057	0.163303
16			
75.167739 Kcal/mol 3.259586 eV -101.263893 H Child_14_28.log			
6	-3.632281	0.504623	0.588684
6	3.739436	1.770252	-0.146421
6	-3.555161	-0.673010	0.229623
6	3.177312	0.624383	0.511258
6	-2.910743	-1.790149	-0.188581
6	2.932414	-0.576411	1.104103
6	-3.092201	1.753074	0.681813
6	2.404347	1.328169	-0.457728
6	-1.983277	-2.527080	-0.607336
6	2.190593	-1.568821	0.959642
6	-2.278510	2.697416	0.595574
6	1.093785	1.044683	-0.848261
8	0.814597	-0.183598	-1.244939
12	-0.478286	2.435889	-0.285190
8	1.390387	-2.498969	0.710983
12	-0.034560	-1.941074	-0.570024
16			
75.170461 Kcal/mol 3.259704 eV -101.263889 H Child_18_24.log			
6	-2.058402	-2.507498	0.066232
8	4.443437	0.156448	-0.109420
12	-0.100944	-3.002342	0.190128
12	-0.250806	2.729757	0.537351
6	-2.841137	-1.547232	0.140255
6	1.612649	2.025545	0.832080
6	-3.282472	-0.240906	0.280908
6	3.242197	-0.006383	0.213479
6	2.370425	1.089608	0.567057
6	-3.871820	0.946449	0.885511
8	0.193666	0.499858	-2.080208
6	-2.726247	0.968288	-0.013061
6	2.555531	-1.270656	0.241493
6	-1.542923	1.509641	-0.582845
6	-0.707159	0.925833	-1.418311
6	1.770055	-2.222596	0.251747
16			
75.173807 Kcal/mol 3.259849 eV -101.263883 H Child_8_16.log			
6	1.347644	-2.583221	0.636734
6	-1.576663	2.485900	0.276048
6	0.218902	-2.896408	0.281737
6	0.988417	2.076101	0.588006
6	2.435962	-1.826273	0.941554

6	-0.216893	2.318291	0.425782
6	-1.071723	-2.874971	-0.123187
6	-2.769798	3.301925	0.305419
6	3.290039	-0.937878	1.182647
6	-2.792186	1.863943	0.072988
6	3.802738	0.599624	-2.381559
12	2.697440	0.943125	0.707766
6	-2.157628	-2.425902	-0.504124
12	-3.585001	-0.020738	-0.161140
8	3.476049	1.050323	-1.376877
8	-3.268817	-1.759750	-0.719596
16			
75.238541 Kcal/mol 3.262656 eV -101.263780 H Child_3_28.log			
12	3.868863	1.862650	0.073836
8	-6.728777	0.610459	0.170529
8	4.323304	0.074568	-0.088615
6	-5.569580	0.333941	0.094386
6	2.165793	2.895556	0.199803
6	-4.328727	0.052281	0.058377
6	3.533704	-0.949484	-0.058883
6	-1.810584	-0.414484	-0.278032
6	0.970207	2.539646	0.112626
6	-3.094346	-0.272992	-0.123557
6	2.745436	-1.874532	0.012262
6	1.525509	-2.596654	0.011349
6	-0.784226	-1.339254	-0.350084
12	-0.624588	1.320442	-0.106496
6	0.292800	-1.945174	-0.348125
6	1.072761	-3.708404	0.625981
16			
75.523092 Kcal/mol 3.274995 eV -101.263327 H MutI_14_65.log			
6	3.560369	3.972618	0.000000
6	2.077972	-0.782605	0.000000
12	-1.787373	-2.115207	0.000000
6	2.156076	1.795314	0.000000
6	1.239281	-1.845696	0.000000
6	4.145731	5.141238	0.000000
6	2.951647	2.860343	0.000000
6	2.396577	0.422918	0.000000
6	-1.974171	1.088679	0.000000
8	-5.218373	-4.785880	0.000000
6	0.214204	-2.555344	0.000000
6	-4.262399	-4.124035	0.000000
8	-3.281665	-3.456497	0.000000
6	4.651627	6.325491	0.000000
12	-0.000000	1.532261	0.000000
6	-2.248785	-0.143193	0.000000
16			
75.568675 Kcal/mol 3.276972 eV -101.263254 H Child_1_49.log			
6	3.231315	1.036153	0.069788
6	0.230517	-0.610041	1.941531
6	4.179941	1.087778	-0.805666
12	-1.175811	0.931392	2.041652
8	5.025802	1.310689	-1.616001
6	-0.171569	-3.451936	-0.717571

6	-2.563297	0.884629	-1.384277
6	1.320164	-0.057994	1.420787
6	-3.352897	2.123178	-1.508996
12	0.244433	-2.532795	1.078739
6	-1.520361	-1.458560	-1.728789
8	-2.241130	1.920652	0.898845
6	-2.638266	1.751462	-0.330796
6	-2.039816	-0.339568	-1.720592
6	-0.828324	-2.548713	-1.297792
6	2.302453	0.477965	0.777800
16			
76.133349	Kcal/mol	3.301459	eV -101.262354 H Child_1_21.log
6	-3.116671	-0.438652	-2.226069
6	0.864800	2.416973	0.237218
6	-2.075115	-0.823796	-1.544471
6	-0.368169	2.474235	0.255111
8	-3.976196	-1.680280	1.681383
6	2.137441	1.986424	0.122778
6	1.188222	-1.991532	-0.085604
8	-1.646661	2.330978	0.266646
6	0.031037	-1.599253	-0.354307
6	4.136146	0.378417	0.021834
6	-1.143238	-0.985980	-0.581952
6	3.223800	1.396683	0.060245
6	-3.500871	-0.726529	1.251489
6	4.852182	-0.665468	0.010859
12	-2.590972	0.774088	-0.147443
12	3.224761	-1.918647	0.265191
16			
76.598991	Kcal/mol	3.321651	eV -101.261612 H MutD_14_50.log
8	-1.077626	1.828136	-0.007607
6	2.215193	2.231772	-0.179850
6	-4.277622	-0.655153	0.046278
6	-5.480410	-0.254341	0.076271
6	-3.044744	-1.050688	-0.032210
6	4.669082	-0.152627	0.179939
12	0.772780	0.734311	-0.134280
6	0.772774	-1.440972	-0.141946
6	3.393098	1.770753	-0.016607
6	-1.713445	2.783689	0.133129
12	2.663538	-2.149234	0.005580
8	-6.614008	0.129410	0.117564
6	-1.823944	-1.371225	-0.117532
6	4.623595	1.204755	0.071589
6	-0.513740	-1.427345	-0.139852
6	4.563040	-1.418834	0.231581
16			
77.134149	Kcal/mol	3.344858	eV -101.260759 H MutD_17_32.log
6	3.721587	1.061815	0.162328
12	1.131818	-2.281583	-0.151973
6	-5.892535	-1.112834	0.381446
6	-3.314210	-1.121259	0.082658
6	3.764367	-1.459828	-0.062183
6	1.822921	2.818706	0.287228
8	0.232129	-0.377142	-0.048770

6	-1.897227	2.313733	-0.276620
6	-0.748085	-1.382117	-0.087845
12	0.250952	1.523172	0.100767
6	3.166574	-2.555340	-0.154110
8	-2.933021	2.741004	-0.481067
6	4.022278	-0.128649	0.044786
6	-4.615644	-1.100256	0.210537
6	2.858381	2.111731	0.243778
6	-2.052759	-1.080696	-0.023143
16			
77.269872	Kcal/mol	3.350743	eV -101.260543 H Child_8_15.log
12	2.011409	3.034310	0.061590
6	-5.621413	-1.075037	-0.044147
6	0.079596	3.588775	0.466872
6	-4.377087	-0.742171	-0.020266
6	2.969886	1.397243	-0.472254
6	-3.061887	-0.404332	-0.007952
6	-0.944616	2.881948	0.420500
6	-1.993929	-1.332695	-0.189961
6	2.753670	0.228714	-0.846021
6	-0.938600	-1.953399	-0.365857
6	3.122994	-2.505920	1.859218
6	-2.580698	0.913727	0.178114
6	-1.901537	1.928369	0.315828
8	2.283111	-2.629310	1.072040
12	1.070798	-2.084227	-0.633556
8	2.463795	-0.989732	-1.184646
16			
77.447822	Kcal/mol	3.358460	eV -101.260260 H Child_7_26.log
8	-5.145183	-1.255341	-0.387739
6	2.205122	2.759384	-0.226533
6	-4.041183	-0.922523	-0.183474
6	3.174366	1.983663	-0.189418
6	-2.775348	-0.544894	0.023258
6	4.030714	0.920540	-0.080350
6	-1.706719	-1.467405	-0.009991
6	4.594307	-0.187743	0.004596
6	-0.639578	-2.063333	-0.002750
12	3.692687	-1.987036	0.094360
8	-3.307482	1.891171	0.416179
6	-1.342908	1.574473	0.301563
6	-2.471088	0.862448	0.237359
6	1.837313	-2.795417	0.110027
6	0.627484	-2.548677	0.039555
12	0.196183	2.777891	-0.125240
16			
77.578694	Kcal/mol	3.364135	eV -101.260051 H Child_11_46.log
6	0.532696	-1.282682	-0.425228
8	-4.847484	0.983051	-0.707753
12	3.341897	-0.642124	-0.600150
6	-3.741099	0.903274	-0.336281
6	4.307321	1.123159	-0.278729
6	-2.475419	0.693605	0.032895
6	3.397705	1.885727	0.146842
8	-2.710939	-1.730021	0.395647

6	2.141199	2.356409	0.417989
6	-1.527280	1.710841	0.278125
6	-0.640517	-0.843520	-0.201023
6	-0.414647	2.168024	0.525272
6	-1.975337	-0.727129	0.083695
6	1.742775	-1.890114	-0.478601
6	0.918300	2.441085	0.542529
12	0.564203	-3.129235	0.654478
16			
77.686168 Kcal/mol 3.368795 eV -101.259880 H Child_12_42.log			
8	-6.594055	0.780604	1.193649
8	7.582896	0.613454	0.370022
6	-5.667708	0.452343	0.523946
6	6.424367	0.327671	0.251491
6	-4.632758	0.102437	-0.179910
12	1.078113	1.021722	-0.396753
6	5.197299	0.036492	0.105451
6	-3.156966	-0.079025	-0.335894
6	-0.919472	1.313130	-0.393683
6	0.435922	-1.686765	0.183257
6	2.657103	-0.356406	-0.091220
12	-1.589563	-1.473522	0.156295
6	3.942345	-0.228025	0.038350
6	-4.098679	-0.434579	-1.405430
6	-2.073377	0.840068	-0.377741
6	1.596369	-1.242487	0.077404
16			
77.820950 Kcal/mol 3.374640 eV -101.259665 H MutI_2_75.log			
6	-1.234726	1.897660	0.107373
6	0.286978	-1.868382	0.362470
6	-0.014035	1.747081	0.248871
8	4.664775	-1.959917	-0.672109
12	3.320605	2.093686	0.164237
6	3.351682	0.064538	-0.021591
6	1.083132	-0.934477	0.224595
6	-2.562415	1.764734	-0.098979
6	-3.537433	-1.699788	0.172845
6	3.994710	-1.025261	-0.360666
12	-1.665734	-2.327768	0.376485
8	-4.691558	0.508220	-0.493423
6	-4.177400	-0.712119	-0.193655
6	-3.712385	1.451445	-0.390304
6	1.907266	0.218850	0.165532
6	1.340596	1.499480	0.256105
16			
77.833793 Kcal/mol 3.375197 eV -101.259644 H MutI_10_75.log			
6	-0.730915	-2.842705	-0.013667
8	-4.730970	1.204748	-0.742185
12	1.252942	2.075645	-0.372080
8	-2.994949	-2.142760	-0.739563
6	0.681860	0.260561	1.327423
12	3.418110	-0.680509	0.006200
6	-0.139911	1.336857	1.085809
6	4.060869	0.857929	-1.248775
6	0.476810	-2.381378	0.204323

6	-2.641024	1.602112	0.554429
6	-1.912078	-2.523181	-0.423893
6	-1.433909	1.519502	0.964676
6	2.986962	1.538900	-1.149334
6	1.701872	-0.521155	1.215292
6	-3.719884	1.386802	-0.103964
6	1.628468	-1.773833	0.295104
16			
77.923500 Kcal/mol 3.379087 eV -101.259502 H Child_12_60.log			
6	-2.525836	-0.236319	1.073550
6	0.581668	3.436842	-0.354566
6	-2.039991	0.922496	0.690696
6	0.375580	-3.129496	-0.832141
6	-2.120617	-1.465950	1.112862
6	-0.468971	2.760389	-0.136061
6	-1.464632	1.961003	0.258898
6	4.036619	-0.165038	0.192984
8	-4.964654	0.839725	-0.395470
8	5.137308	-0.483848	0.576585
6	-1.716772	-2.578379	0.617565
6	2.836245	0.157155	-0.216536
6	-4.861783	-0.195962	-0.930722
6	-0.642266	-2.949673	-0.092004
12	2.133102	2.083972	-0.111813
12	1.757174	-1.579758	-0.701194
16			
78.091331 Kcal/mol 3.386365 eV -101.259234 H MutI_14_59.log			
6	2.491440	2.637839	0.383253
6	4.243219	0.745182	0.729729
8	-5.711682	-0.979219	1.296876
6	-0.585982	-1.749579	-0.778922
12	4.092725	-1.259748	0.463192
6	-1.611089	-1.077592	-0.873624
12	-1.920170	2.456737	-0.451244
6	-0.002881	3.120946	-0.143242
6	1.217597	2.871025	0.084026
6	3.364664	1.653210	0.545984
8	3.074808	-2.706373	-0.104907
6	-6.591016	-1.641831	0.986090
6	-2.532535	-0.074317	-0.852818
6	0.627085	-2.316927	-0.592534
6	-3.262401	0.931999	-0.716111
6	1.812621	-2.579809	-0.385019
16			
78.393821 Kcal/mol 3.399482 eV -101.258752 H Child_7_53.log			
6	-4.905441	0.232706	0.944455
12	-0.109777	-1.106709	-0.618335
12	-4.445985	2.119539	0.336269
6	6.842205	0.645309	0.346229
6	-3.869402	-0.372692	0.570233
6	2.019258	-0.803022	-0.480169
6	-2.735049	2.701981	-0.670907
6	3.243609	-0.594147	-0.260723
6	-2.598042	-0.720662	0.052386
6	5.666791	0.154780	0.168703

6	-2.244777	1.535604	-0.656390
6	-2.047882	-2.093575	0.056650
6	-1.756717	0.230683	-0.548178
6	4.485003	-0.242871	-0.041365
8	-2.667913	-3.124090	0.299875
8	7.926888	1.099276	0.512529
16			
78.479852 Kcal/mol 3.403213 eV -101.258615 H MutD_14_38.log			
6	-0.280666	2.847374	-0.016536
6	1.928836	-1.252055	-0.138489
12	-4.048950	-1.005165	1.909194
6	-2.635279	0.114961	-0.633813
6	2.999290	-0.346730	0.156573
6	4.247349	-0.810595	0.314737
6	-2.370020	1.483682	-0.368534
6	2.696391	1.037253	0.272311
6	0.943489	2.890314	0.245933
12	-1.106563	-1.750869	-0.855757
6	-1.523963	2.371574	-0.210132
8	-2.080169	-0.323944	-1.824512
6	0.870850	-1.839240	-0.405232
6	-2.926116	-0.977656	0.180218
6	2.029958	2.070888	0.283953
8	5.328349	-1.234332	0.483617
16			
78.829249 Kcal/mol 3.418364 eV -101.258058 H Child_14_16.log			
8	-5.482101	-0.811153	-0.080431
8	5.375779	-1.354782	-0.162748
6	-4.268083	-0.637145	-0.077196
6	4.232262	-1.122601	-0.109235
6	-3.106303	0.190074	-0.267691
6	2.913340	-0.797015	-0.056013
12	-1.460885	1.444968	-0.538426
6	1.886518	-1.721784	0.281278
12	0.667693	3.801650	0.819410
6	0.725321	-2.098636	0.430526
6	-2.938732	-1.147319	0.129793
6	2.653928	0.544388	-0.416493
6	0.514597	2.042523	-0.551086
6	-0.621502	-2.193167	0.470099
6	-1.817320	-1.911247	0.383576
6	1.554120	1.246607	-0.455289
16			
79.048568 Kcal/mol 3.427875 eV -101.257709 H MutD_4_70.log			
6	0.341827	-2.227013	0.197231
6	-1.282233	1.460554	1.395662
6	0.529395	-1.950242	-1.179917
6	-0.399746	2.434715	1.106940
8	1.399490	-2.311861	0.952467
6	2.112132	1.172670	-2.197097
6	0.684872	2.925661	0.710073
6	-5.767664	0.522303	-0.839503
6	0.964324	-1.071616	-1.940771
12	2.334996	1.970529	-0.227606
6	-0.921737	-1.975151	0.767144

12	2.670512	-0.738896	1.092319
6	1.543700	0.069622	-2.382347
8	-4.789774	-0.064678	-0.976292
6	-1.524551	-0.973478	1.192569
6	-1.770957	0.317429	1.472353
16			
79.155890	Kcal/mol	3.432529	eV -101.257538 H Child_8_38.log
6	-7.898178	-0.255887	0.425016
8	4.426956	1.873102	-0.535922
6	-6.621663	-0.174667	0.245822
6	3.448970	1.368493	-0.172615
6	-5.330060	-0.053519	0.074381
8	5.912817	-0.985852	0.686117
12	-1.047110	-1.173879	-0.640935
6	4.760941	-1.088188	0.368329
6	-4.075468	0.081796	-0.072772
12	1.259920	0.991449	0.261410
6	-1.793738	1.054966	0.061738
6	0.968169	-1.160831	-0.277836
6	2.234188	-1.224487	-0.119935
6	3.550323	-1.070175	-0.030858
6	-0.695714	1.620990	0.288467
6	-2.759756	0.083370	-0.230947
16			
79.268610	Kcal/mol	3.437417	eV -101.257358 H MutD_3_74.log
6	3.450386	-1.455219	0.442093
6	1.003934	-2.151487	-0.000403
6	-3.891481	1.209375	0.436725
6	0.007071	1.694713	-0.554143
6	2.324681	-1.832191	0.148562
6	-1.496431	-1.505005	-0.333886
6	-0.182208	-1.915140	-0.261400
6	-3.296471	0.153700	-0.032123
6	3.806126	1.736774	-0.033408
6	-0.921873	0.881422	-0.467965
6	4.250795	0.616997	0.235927
8	4.547775	-0.671826	0.543907
8	-4.544603	2.104282	0.895633
12	1.919437	2.304131	-0.438668
12	-3.505035	-1.897708	-0.158160
6	-1.887563	-0.156727	-0.305708
16			
79.402249	Kcal/mol	3.443212	eV -101.257145 H Child_16_8.log
6	-3.621830	-0.989250	0.298386
6	5.755742	1.067136	0.319719
6	-2.887689	-2.113226	0.063628
6	4.484344	1.122147	0.132673
6	-3.832246	0.221528	0.407547
6	3.185560	1.164101	-0.060543
6	-1.960778	-2.911134	-0.210820
6	1.936654	1.174953	-0.233971
6	-3.554503	1.550319	0.397811
8	2.863606	-2.683364	0.594962
6	-2.997736	2.661999	0.303843
6	0.593890	1.224216	-0.351974

12	-0.298468	-1.752668	-0.498506
6	1.843013	-2.439772	0.143009
8	-0.119807	0.104253	-0.580655
12	-1.002942	2.605567	-0.115687
16			
79.461681 Kcal/mol 3.445789 eV -101.257050 H Child_13_13.log			
6	0.684390	-2.830480	0.061928
12	-3.041922	2.530223	-0.042420
6	1.768748	-2.249769	0.087258
6	-4.597992	1.243126	-0.101715
6	5.921471	1.058151	-0.247802
6	-1.036438	2.777877	0.182935
6	-0.655148	-2.992050	0.025564
6	-4.397763	0.008281	-0.095974
8	4.779165	0.870824	-0.157901
6	0.203938	2.403821	0.130642
6	-1.878459	-2.820063	-0.012153
6	-3.893946	-1.252088	-0.079296
12	2.761533	0.384279	0.031376
6	1.362970	1.818126	0.194512
6	-3.045565	-2.149537	-0.050278
8	2.814266	-1.504123	0.102750
16			
79.593793 Kcal/mol 3.451518 eV -101.256840 H Child_1_48.log			
8	5.598555	-0.785403	0.081721
6	-2.885076	2.426796	0.492936
6	-4.040493	-1.674020	0.331629
6	-1.720155	2.073812	0.151510
6	4.528353	-0.351001	0.102011
6	-0.884886	1.042003	-0.296311
6	2.281632	-0.912346	0.110329
8	-1.584653	0.036034	-0.771889
6	3.243363	0.135592	0.119556
6	2.811762	1.495310	0.024604
6	-2.856959	-2.121834	0.283551
6	0.539561	0.800882	-0.131666
6	0.939733	-0.611665	0.006045
6	1.554031	1.741531	-0.043641
12	-3.561669	0.293825	-0.017075
12	-0.869698	-1.816776	-0.098089
16			
79.914445 Kcal/mol 3.465423 eV -101.256329 H Child_13_10.log			
8	3.567043	-3.302298	0.817128
6	-0.232995	3.478589	-0.030433
6	3.192884	-2.242174	0.649382
8	4.009509	2.305605	-0.281443
6	0.366659	-2.203048	-0.669852
6	0.431473	2.208200	-0.030857
6	-0.835846	-2.516258	-0.670956
6	2.863904	1.990779	-0.194496
6	-2.186486	-2.445876	-0.527196
6	-0.937433	2.184439	0.115829
6	-3.265842	-1.912362	-0.258102
6	1.649237	1.488255	-0.117137
12	1.564021	-0.613701	-0.214652

12	-2.899396	1.583321	0.371730
6	-4.044276	-0.874778	0.136253
6	-4.432597	0.233918	0.569162
16			
79.968907 Kcal/mol 3.467784 eV -101.256242 H Child_10_49.log			
6	0.873590	-2.435886	-0.497362
8	-0.278144	3.721694	0.380050
6	1.220342	-2.459266	0.693674
6	0.418477	2.764015	0.213338
6	-0.000255	-1.608727	-1.278278
6	1.009592	1.599886	0.153649
6	1.072836	-1.867583	1.889835
6	2.295653	1.204436	-0.299732
6	-1.140023	-1.147374	-0.880970
8	-4.525047	0.086146	-0.454701
6	3.294006	0.548282	-0.763304
6	0.514691	-1.030227	2.681035
6	-3.396645	-0.242494	-0.425118
6	-2.129068	-0.491765	-0.269592
12	-0.361489	0.287572	1.246380
12	1.547017	-0.242781	-1.805201
16			
80.945792 Kcal/mol 3.510146 eV -101.254685 H Child_8_14.log			
12	6.444191	-1.315655	-0.158595
6	-1.177806	3.405019	-0.390647
6	2.059389	0.861914	0.888987
6	-2.168439	2.828453	-0.890562
6	1.664533	-0.386561	0.551841
12	-2.197907	0.778116	-1.045159
6	1.875258	2.086276	0.904839
6	0.034310	3.589090	0.192222
8	-0.108350	-3.134555	-1.009341
8	-4.208048	-2.183519	1.485094
6	0.995335	-1.320054	0.105535
6	-3.290225	-1.815491	0.833731
6	1.106497	3.168047	0.649949
6	-2.457330	-1.179183	0.041508
6	-0.109143	-1.992834	-0.518230
6	-1.269751	-1.078832	-0.596002
16			
81.258784 Kcal/mol 3.523719 eV -101.254186 H Original3D_15_4.log			
6	-0.613805	-0.001485	1.098323
6	0.403210	2.179130	-0.262486
6	1.317436	1.214102	0.229895
6	-1.821433	0.029815	1.391146
6	0.707297	0.016824	0.688262
8	-1.590918	1.259776	-1.430729
6	-0.672187	1.874774	-0.831690
6	-3.171722	-0.014715	1.178673
12	-2.023054	-0.550117	-0.785180
6	0.406087	-1.922538	-0.457475
6	2.744703	1.211788	0.143825
6	-4.419290	0.021397	0.945136
6	3.969668	0.943028	0.044173
12	3.411161	-1.019255	0.301262

6	1.326402	-1.317666	0.217016
8	-0.623518	-2.081557	-1.131992
16			
82.231359	Kcal/mol	3.565894	eV -101.252636 H Child_2_63.log
6	3.182874	1.769059	-0.420397
6	-9.012889	0.263919	0.250568
6	1.932796	1.764330	-0.237987
6	-7.733742	0.085854	0.208902
6	0.623477	1.429173	-0.103197
6	-6.439893	-0.082584	0.163901
8	7.347238	0.048359	0.847083
6	-5.184192	-0.226126	0.112239
6	6.313347	-0.309718	0.448396
6	-3.888780	-0.315974	0.094022
8	5.267236	-0.707255	0.047487
6	-2.624327	-0.335729	0.054678
12	3.265636	-0.384056	-0.485940
6	-0.446210	0.793544	-0.016794
6	-1.303247	-0.296943	-0.032990
12	0.615107	-1.446083	-0.371110
16			
82.232563	Kcal/mol	3.565946	eV -101.252635 H Child_8_33.log
8	-0.583494	2.555290	-0.710899
6	-0.200918	-2.354088	-0.109063
6	1.490817	1.874086	0.307004
12	1.806488	-2.159340	-0.240386
6	0.086578	2.020379	0.340239
6	4.798543	-0.292808	-0.199836
6	-1.673756	0.632734	1.061944
6	3.564633	-1.060356	-0.189021
6	-0.645092	1.367392	1.307677
6	-1.389065	-2.044830	0.038016
6	-2.617251	0.025118	0.337160
6	3.515580	0.305492	0.058850
6	2.553256	1.261907	0.252599
6	-2.695961	-1.424190	0.139372
8	-3.758254	-2.038872	-0.052082
12	-2.305672	1.659643	-0.923430
16			
82.246741	Kcal/mol	3.566561	eV -101.252612 H MutI_15_77.log
6	2.998011	1.957858	-0.626597
6	3.352151	-1.414439	0.373022
6	1.856276	2.673056	-0.622122
8	1.220535	-1.324054	1.146048
8	-3.252315	1.472417	1.714409
6	-3.353812	-0.766438	-1.010053
6	3.677054	0.944947	-0.401815
12	-2.151009	-2.495141	-1.238216
6	-2.776413	1.331429	0.563083
6	-3.109826	0.234117	-0.295558
6	-0.646324	2.698889	-0.198948
6	2.133693	-2.116771	0.594946
6	-1.734713	2.200922	0.082211
6	0.650348	2.919480	-0.503882
12	0.068352	-2.759264	0.382891

6	3.827906	-0.352057	-0.057577
16			
82.321432	Kcal/mol	3.569800	eV -101.252493 H MutD_15_32.log
6	-4.659192	-1.228343	-0.080892
6	-3.063872	2.103884	0.131009
6	0.164195	-2.264497	-0.020263
6	0.688739	2.757265	0.016291
8	2.838295	1.490239	-0.337588
6	-1.876923	2.735834	0.179113
6	5.963133	-1.134110	0.521930
6	-0.653343	2.897380	0.130073
6	-4.485427	0.003303	-0.010227
8	4.952202	-0.854630	-0.002357
6	1.766917	2.172739	-0.147485
12	2.862582	-0.391137	-0.136191
12	-3.121556	-2.525430	0.007336
6	1.326228	-1.691617	-0.075816
6	-1.083764	-2.619063	0.008825
6	-3.956075	1.252882	0.058412
16			
82.365759	Kcal/mol	3.571722	eV -101.252422 H Child_4_54.log
6	3.439662	-0.914567	-0.175541
8	-6.948999	-0.949997	0.947900
12	1.316885	-0.885631	-0.012444
6	-6.006296	-0.681860	0.263603
6	4.151200	-1.985299	0.015990
6	-5.005638	-0.394662	-0.477517
8	4.756862	-3.007429	0.136963
12	1.984399	2.764722	0.251604
6	0.218003	0.426114	1.532056
6	-3.829054	-0.047306	-0.901320
6	-0.233799	0.593115	-0.327034
6	3.653366	0.466354	-0.276893
6	-1.423082	0.544798	-0.851105
6	0.423911	1.486869	0.763743
6	-2.648288	0.320295	-1.225159
6	3.580296	1.704537	-0.265629
16			
82.457459	Kcal/mol	3.575698	eV -101.252276 H MutD_6_68.log
6	-1.861562	-1.253313	1.232855
6	-1.397220	0.371582	-1.636968
6	0.669224	-1.834237	1.026113
6	-0.869201	1.951285	0.737064
6	-0.641623	-1.497164	1.162614
6	1.812864	-2.398617	1.001960
6	2.577425	1.311721	0.213017
12	2.473058	-1.006841	-0.492403
6	1.382764	1.843753	0.528780
6	-0.086169	0.464024	-1.096929
12	-3.309386	-1.018194	-0.131540
8	0.867595	-0.277431	-1.488757
6	3.676327	0.756849	-0.122338
6	-2.616630	0.123670	-1.689331
8	-1.715368	2.406971	1.386548
6	0.156820	1.371132	0.027329

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82.683311 Kcal/mol 3.585492 eV -101.251916 H Child_3_59.log
6 3.382287 -1.647634 0.591246
6 -2.143169 0.290849 0.622806
6 4.171961 -0.688089 0.433527
8 -3.178044 -0.777054 -2.422583
6 2.185741 -2.270146 0.534796
12 -1.301666 2.117727 0.520628
12 -0.559792 -0.882415 -0.223075
6 -3.194599 -0.095872 1.283929
6 0.953850 -2.280368 0.340134
6 3.955063 0.598838 0.066081
8 -4.167930 -0.478553 1.885360
6 0.691584 0.907219 -0.783963
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6 3.219177 1.488907 -0.392746
6 1.856520 1.660182 -0.519595
6 0.634145 2.234104 -0.193977
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82.695314 Kcal/mol 3.586013 eV -101.251897 H Child_8_53.log
6 -3.658350 -0.480252 -0.983098
8 4.229060 0.375955 -0.192195
6 -2.763424 -1.311177 -1.244982
8 2.459264 2.840688 -1.100286
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6 2.185086 1.877937 -0.498439
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6 3.167356 -0.099668 0.269822
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6 2.964543 -1.395622 0.830818
12 -2.557002 0.935356 1.129685
6 1.905506 0.753946 0.191282
6 -0.598425 0.186763 0.927776
6 0.584800 0.463543 0.617628
6 2.098795 -2.237062 0.269190
6 0.927080 -2.575392 -0.075705
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82.784548 Kcal/mol 3.589882 eV -101.251755 H Child_12_28.log
12 4.458528 -1.357701 0.819713
8 -4.573144 0.708256 0.372275
6 2.504394 -1.170124 0.253121
6 -3.477863 1.376428 0.510237
6 3.205997 0.039404 0.127478
12 -4.141275 -1.019850 -0.341907
6 1.203982 -1.519295 -0.037708
6 -2.279251 1.726448 0.476688
8 3.437672 1.901874 -1.341939
6 -0.995345 2.005983 0.505468
6 2.727745 1.300061 -0.478017
6 -2.519377 -2.137511 -0.551483
6 0.043127 -1.896136 -0.239087
6 0.253468 1.885125 0.217152
6 1.493390 1.750371 -0.020087
6 -1.280807 -2.085823 -0.426489
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83.021311 Kcal/mol 3.600149 eV -101.251378 H Child_8_21.log
 8 5.622215 0.606728 -0.121162
 8 -5.952099 -0.043505 -0.348720
 6 4.447176 0.538644 0.110790
 6 -4.795885 -0.025851 -0.129094
 6 3.219503 0.550011 0.559158
 6 -3.461581 0.053044 -0.027823
 6 1.983599 -0.245709 0.949415
 6 1.839780 1.010817 0.477862
 6 -2.737212 1.234199 -0.373574
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 6 -2.626993 -0.990600 0.493786
 6 0.813818 1.814518 0.034559
 6 -1.660998 1.832886 -0.488771
 6 -0.341012 2.065514 -0.329667
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83.249363 Kcal/mol 3.610039 eV -101.251014 H Child_7_17.log
 6 -1.945906 2.899021 0.078856
 8 11.005563 -0.393474 1.035605
 6 -2.986190 2.251853 0.276041
 6 0.242490 -2.182310 -0.896022
 6 -4.018867 1.386673 0.478996
 6 1.122459 -1.224183 -1.314919
 6 -4.820957 0.448227 0.547700
 6 11.095515 0.753771 1.071595
 12 -0.052959 2.778490 -0.582056
 6 -0.931493 -2.319689 -0.187229
 8 -5.395537 -0.718501 0.688297
 6 1.446404 -2.621151 -1.591568
 6 1.282716 1.382006 -1.208919
 6 1.294161 0.143833 -1.298598
 6 -1.938174 -2.277417 0.537322
 12 -3.608137 -1.357491 1.186160
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83.445092 Kcal/mol 3.618526 eV -101.250702 H Child_14_30.log
 6 -3.842945 -1.684696 0.085335
 6 0.211888 2.547605 -0.060475
 8 -2.944842 -2.681854 -0.011203
 6 -2.346991 2.579009 -0.052402
 6 -1.650594 -2.279031 -0.024059
 6 1.344040 2.053975 -0.078016
 6 -4.224284 -0.525145 0.122439
 6 -1.118281 2.739680 -0.068747
 12 4.205432 -1.710573 -0.028630
 6 -3.479672 1.855082 0.017486
 6 -0.513870 -1.805897 -0.075991
 6 2.486551 1.336379 -0.000878
 6 3.692351 0.979431 0.105053
 6 -4.170839 0.828449 0.077473
 8 4.767683 0.336601 0.187314
 12 1.385664 -1.038345 -0.112385
 16

83.784025 Kcal/mol 3.633224 eV -101.250162 H Child_9_15.log

8	4.598677	-1.576245	-0.010600
12	-3.612390	1.475057	-0.043715
6	3.402395	-1.561922	-0.052956
6	-1.562415	1.789917	-0.158939
6	0.892878	-1.945850	-0.052784
6	-0.383226	1.611697	-0.897764
6	2.130190	-1.339831	-0.098986
6	-4.851277	-0.141938	0.157762
6	-0.318414	-2.188693	-0.002993
6	-3.973823	-1.044302	0.144860
6	-1.663325	-2.141979	0.060617
6	-0.453867	1.404550	0.615586
8	3.042143	1.940075	0.135716
6	3.932833	2.639407	0.374781
6	-2.850852	-1.810397	0.113451
12	1.367961	0.647059	-0.141012
16			
83.866570	Kcal/mol	3.636803	eV -101.250031 H Child_7_39.log
8	-5.138400	-0.489049	0.354994
8	4.207780	1.810208	-0.203398
6	-3.978586	-0.454789	0.192839
6	5.180124	1.662698	-0.823007
6	-1.896301	-1.565106	-0.353364
6	-0.894335	-2.258761	-0.526111
6	3.495873	-1.204055	0.523869
6	-2.639835	-0.408712	-0.006320
6	-0.697566	1.011626	0.442899
6	0.368911	-2.737551	-0.515448
12	-2.742967	2.876833	-0.599655
6	1.591242	-2.707394	-0.342598
6	0.535984	1.156601	0.644916
6	-2.069817	0.889663	0.302220
6	2.741554	-2.088453	0.056773
12	2.494756	0.594511	0.700257
16			
83.870453	Kcal/mol	3.636972	eV -101.250024 H MutD_6_78.log
8	-6.679967	0.081007	-0.670126
6	-1.914940	-0.966062	-0.297787
6	1.390105	1.941854	0.804374
6	1.250407	-1.817711	1.078802
6	-5.491885	0.038248	-0.522534
6	2.144458	-1.621006	1.951332
6	-0.822274	-1.522808	-0.313000
6	-4.232030	-0.114677	-0.385780
6	-2.923926	0.061135	-0.176178
6	0.156973	2.092787	0.691475
6	-1.154909	1.824775	0.464547
6	-2.205380	1.236237	0.196671
6	0.577552	-1.458181	-0.113116
12	2.466926	0.190567	0.591844
8	1.302972	-0.746791	-0.922425
12	7.730663	0.405994	-1.219547
16			
84.019782	Kcal/mol	3.643447	eV -101.249786 H Child_12_31.log
6	3.742924	-1.163314	-0.093185

8	-4.278578	-0.468650	-0.203515
6	4.123313	0.074769	-0.380187
12	-4.110114	1.526010	-0.063403
6	3.799178	1.263361	-0.123699
6	-2.969540	-0.568690	-0.069828
8	3.032252	2.268324	-0.003810
6	-2.164122	-1.723771	-0.084251
6	-2.144935	0.588895	0.090684
12	1.127971	1.735920	0.147358
6	-0.983636	-2.093206	0.002842
6	2.772859	-2.010592	-0.075742
6	-0.784262	0.707408	0.186727
6	1.551872	-2.237911	0.269707
6	0.328783	-1.615520	0.146057
6	0.353621	-0.144855	0.239400
16			
84.256057 Kcal/mol 3.653693 eV -101.249410 H Child_1_8.log			
8	6.167829	-0.016447	-0.844757
6	-1.021340	2.967003	-0.485838
6	5.073189	-0.015212	-0.380388
6	-2.094534	2.322913	-0.468564
8	-0.925712	-3.331416	-1.368166
12	0.556103	2.013724	0.331068
6	-1.644795	-2.722850	-0.715796
6	-3.184227	1.478611	-0.469715
6	3.934305	-0.009658	0.193627
6	-0.573669	-1.490107	1.446304
12	-2.521799	-1.315948	0.867276
6	-4.484474	0.996253	-0.904099
6	2.687022	-0.012166	0.503530
6	0.428036	-0.824027	1.112433
6	-3.592085	0.229411	-0.041156
6	1.414474	0.148094	0.763540
16			
84.675441 Kcal/mol 3.671879 eV -101.248742 H MutD_10_78.log			
6	-2.667482	0.022002	0.073922
12	1.376219	-1.674033	0.276024
6	-6.425469	-0.699750	-0.139444
6	-1.419983	0.443047	0.103796
12	-0.445486	2.476947	-0.023090
8	-7.602631	-0.920710	-0.213973
6	0.959427	0.688447	0.127613
6	-5.176371	-0.479970	-0.057544
6	1.782493	2.005073	-0.004082
6	4.563750	-0.411568	-0.055031
6	5.800946	-0.710268	-0.184091
8	6.981015	-0.894396	-0.313985
6	2.349563	0.721450	0.070958
6	-0.133321	-0.142000	0.184265
6	3.246310	-0.400987	0.068414
6	-3.912509	-0.221160	0.009298
16			
85.129931 Kcal/mol 3.691588 eV -101.248017 H Child_8_45.log			
6	2.655322	0.032717	-0.222172
8	-5.266759	-0.409844	0.424679

6	1.673991	-0.957198	-0.303341
6	-4.107807	-0.470794	0.206841
6	2.481043	1.396129	-0.123741
6	-2.797794	-0.559474	-0.022848
8	2.046822	-2.262648	-0.119853
6	-1.866719	0.568525	-0.074981
6	0.250061	-0.740109	-0.396564
6	-2.011057	-1.762524	-0.242426
6	2.291938	2.635633	0.012646
6	-1.187377	1.752420	-0.000040
6	-0.482528	0.424958	-0.261796
6	-0.776494	-1.764506	-0.353255
12	0.362864	3.091043	0.085945
12	3.722472	-1.587270	0.601676
16			
85.151403 Kcal/mol 3.692519 eV -101.247983 H MutD_11_68.log			
6	-2.182772	-2.812130	-0.274353
6	-7.869567	7.317097	0.076643
6	3.439855	0.203475	-0.638920
6	0.059612	-1.593986	-0.448547
6	-3.333991	-3.446869	-0.173765
6	-1.078881	-2.214850	-0.368636
8	-7.007227	8.032782	0.330449
6	1.174426	-0.993769	-0.511553
8	7.950119	2.425806	-0.710732
6	2.310963	-0.388188	-0.572567
12	-6.438701	-4.006925	-0.438404
6	5.724737	1.358729	-0.699352
6	6.877277	1.908407	-0.703184
6	-4.366556	-4.165826	-0.007974
12	3.141891	-0.944596	3.190509
6	4.581326	0.786168	-0.674957
16			
85.316085 Kcal/mol 3.699660 eV -101.247721 H Child_5_21.log			
8	-0.669179	-2.617406	-0.310484
8	-6.544146	1.604505	-0.863515
6	1.231244	-1.640562	-1.451032
6	-5.902207	0.730507	-0.488616
6	0.049599	-1.594208	-0.687337
6	1.349388	1.600835	2.236027
6	2.341326	-1.089410	-1.465351
6	0.494888	0.684748	2.057965
12	-1.138903	-2.161659	1.516250
12	2.283624	2.007952	0.304728
6	-0.138740	-0.266633	-0.045575
6	-0.171982	-0.322897	1.373428
6	3.328138	-0.224457	-1.154957
6	0.658163	2.044325	-1.109788
6	3.835288	0.810112	-0.634823
6	0.253221	0.925587	-0.706568
16			
85.704555 Kcal/mol 3.716506 eV -101.247102 H Child_3_26.log			
6	-1.004811	-3.027369	0.629871
8	-2.502264	3.222755	-0.784695
12	0.825764	-2.480797	-0.340931

6	-2.355316	2.091187	-0.476721
6	-1.855081	-2.031624	0.331935
6	-2.211842	0.820719	-0.084704
6	2.558554	-1.617430	-0.937980
6	3.866751	1.683307	0.387750
6	-0.728777	-1.089488	0.421407
6	-3.246887	-0.140791	-0.143899
8	0.115640	1.190787	0.487320
6	3.666308	0.654086	-0.320138
6	3.120927	-0.517163	-0.808085
12	1.832439	1.686518	0.802129
6	-3.083166	-1.369504	0.128944
6	-0.860903	0.247905	0.345725
16			
85.911751 Kcal/mol 3.725491 eV -101.246771 H Child_10_62.log			
8	7.993769	2.008096	-0.723189
12	-7.148192	-2.293967	-0.574404
6	6.940668	1.448289	-0.713099
6	-1.407698	-1.791246	-0.454685
6	5.811579	0.849977	-0.702806
6	-2.634322	-2.040866	-0.332903
8	-5.816564	6.426240	0.829687
6	-0.153360	-1.449720	-0.530403
6	4.648498	0.314966	-0.746147
6	-3.931705	-2.262389	-0.184814
6	3.463376	-0.180350	-0.689456
6	1.055976	-1.071214	-0.606205
6	-6.371668	5.749046	0.086140
6	-5.141232	-2.465066	0.138601
12	3.419741	-1.557756	3.202555
6	2.273851	-0.643762	-0.662521
16			
86.295658 Kcal/mol 3.742139 eV -101.246160 H MutD_12_68.log			
6	-0.139500	2.806543	-0.109106
6	1.205825	2.641899	-0.137118
6	-1.345648	-2.602754	-0.041645
6	-3.785142	1.797396	0.068197
6	2.401856	2.309065	-0.133346
6	-3.862083	-1.996883	0.088427
8	4.351863	-0.848186	0.809071
6	-0.117844	-2.532665	-0.088021
6	1.195807	-2.249604	-0.179115
6	2.305479	-1.740156	-0.277313
6	-2.666011	2.337209	0.017148
6	-2.683680	-2.399558	0.041584
12	-4.525827	-0.081182	0.116615
6	-1.364641	2.712602	-0.047906
8	3.416004	-1.125139	-0.521315
12	3.775039	0.855186	0.090656
16			
86.589656 Kcal/mol 3.754888 eV -101.245691 H Child_8_30.log			
6	0.170939	3.724116	0.153721
8	0.804343	-3.512348	0.153676
6	1.349097	3.351107	-0.025687
12	-0.864017	-2.649750	0.147181

12	-1.445470	2.556358	0.409382
6	1.921565	-2.873805	0.051559
6	2.497280	2.647325	-0.187879
6	2.838780	-2.067976	-0.084931
6	3.218024	1.647691	-0.268528
6	-2.308144	-1.140083	0.189186
6	-2.457280	0.691323	0.469679
6	3.445831	-0.866837	-0.203707
8	-3.898718	-0.056645	-1.500032
6	3.602703	0.356493	-0.277426
6	-3.082995	-0.144596	-0.591759
6	-2.450994	-0.379316	1.457787
16	86.830389 Kcal/mol 3.765327 eV -101.245307 H Child_4_28.log		
8	-4.819522	-2.566218	0.145028
6	6.255846	-0.823182	0.474874
6	-4.081006	-1.624160	0.017342
6	5.003716	-0.638539	0.229930
6	-3.241516	-0.680673	-0.117464
8	1.490191	1.634268	-0.319700
6	-2.451794	0.398961	-0.119115
6	3.736299	-0.526906	-0.055672
6	-2.633131	1.716450	0.441747
6	1.368658	0.329601	-0.332369
6	-1.059376	0.457353	-0.599609
6	2.457276	-0.570058	-0.210153
6	-2.154213	2.824205	0.808575
6	0.013937	-0.273113	-0.312787
12	-0.280098	2.482744	-0.123933
12	0.892304	-2.156413	0.127732
16	86.845052 Kcal/mol 3.765963 eV -101.245284 H Child_8_60.log		
6	1.626769	2.122908	-0.503970
6	4.273406	0.183604	1.584919
6	-2.044759	1.047187	-0.361955
6	3.516473	-0.663892	1.002906
6	0.417491	1.852030	-0.489351
8	-1.086602	-2.149188	0.156751
8	-5.339537	1.047634	1.068802
6	2.670859	-1.212355	-0.048133
6	-4.347165	0.795341	0.466018
6	3.601044	-0.660466	-0.849035
6	-0.893469	1.475103	-0.456416
6	0.161705	-1.849740	0.053793
6	-3.284113	0.417476	-0.196132
6	1.365745	-1.663519	-0.063707
12	-2.745053	-1.558296	-0.661573
12	3.497152	1.370827	-0.224930
16	87.037128 Kcal/mol 3.774292 eV -101.244978 H Child_5_10.log		
6	6.198506	-0.407881	0.636291
12	-3.922665	2.155376	0.221386
6	4.968966	-0.233761	0.295199
8	-1.951160	1.774469	-0.041091
6	3.652042	-0.067274	0.036107

6	-0.680639	2.062878	0.043543	
8	-3.291522	-3.451123	0.821639	
12	-2.521436	-0.202366	-0.453204	
6	-3.242150	-2.322396	0.640879	
6	0.543007	2.143096	0.107322	
6	2.726452	-1.100475	-0.313285	
6	1.850959	1.791359	0.132656	
6	-0.929158	-1.438067	-0.929496	
6	0.268134	-1.676895	-0.769744	
6	2.904810	1.153615	0.113970	
6	1.617514	-1.574683	-0.570535	
16				
87.084331	Kcal/mol	3.776339	eV	-101.244903 H MutD_2_66.log
12	-0.606984	0.388059	-1.536474	
6	-2.485734	1.770179	1.013331	
6	-0.019645	1.958063	0.414916	
6	0.958169	1.310624	-0.315687	
6	6.911812	-1.103837	0.231657	
6	3.378711	0.471889	0.020385	
8	-4.888891	-2.904752	1.007726	
8	-4.384480	0.332660	0.272419	
12	-3.312342	-0.579138	-1.171854	
6	-4.364195	-2.405202	0.123305	
6	2.226411	0.978991	-0.108230	
6	5.695763	-0.602170	0.241904	
6	-3.527153	1.138004	0.790363	
6	8.065671	-1.679864	0.269918	
6	-1.182074	2.059860	0.867390	
6	4.545409	-0.084926	0.160546	
16				
87.225608	Kcal/mol	3.782465	eV	-101.244678 H MutD_16_32.log
6	3.621446	0.093581	2.539192	
6	-3.060230	2.255664	0.025822	
6	2.178144	-0.159193	-1.124892	
12	-4.383852	-0.402617	0.597008	
6	-0.591991	2.510506	-0.611182	
6	0.400453	-1.973094	-0.522636	
6	0.597771	1.917218	-0.861804	
8	-0.601697	-2.664895	-0.143432	
6	4.785929	-0.400936	-1.495230	
6	-4.096556	1.601976	0.293839	
6	-1.787755	2.600084	-0.320764	
8	4.482521	0.840510	2.678452	
12	-2.380937	-2.396578	0.399460	
6	3.516418	-0.253409	-1.364152	
6	1.474831	1.079996	-1.040210	
6	1.316686	-1.241489	-0.890946	
16				
87.418498	Kcal/mol	3.790830	eV	-101.244370 H Child_2_24.log
6	2.601019	0.424825	-0.276394	
8	-4.085118	-1.558799	-0.210890	
6	5.810682	-1.631548	0.755623	
6	-3.375462	1.772485	0.588074	
6	4.666696	-1.152181	0.429805	
12	-4.557068	0.194197	0.343440	

8	2.709091	2.808951	-0.362101
6	-2.845362	-1.850891	-0.286920
6	2.076320	-0.834109	-0.175218
6	-2.143386	1.859392	0.380044
6	3.491471	-0.638307	0.053118
6	-1.625450	-2.025565	-0.310250
6	2.018519	1.775959	-0.341399
6	-0.299001	-1.845610	-0.255358
6	0.883100	-1.499542	-0.186065
12	-0.155153	1.794916	-0.148976
16			
87.439313 Kcal/mol 3.791732 eV -101.244337 H Child_9_22.log			
8	-5.619643	-1.985013	0.397431
8	7.098092	-1.524571	0.327076
6	-4.515937	-1.589761	0.308217
6	2.512541	2.001560	-0.239357
6	-3.292026	-1.054788	0.186060
6	6.514737	-1.418975	1.312361
6	-2.105498	-1.800292	-0.094640
6	2.566883	0.685042	-0.522310
6	-0.969069	-2.199930	-0.365641
6	2.586040	-0.565711	-0.743854
6	-3.177457	0.369612	0.273850
6	1.457071	2.801037	-0.056834
12	0.992237	-1.861594	-0.741058
6	0.441852	3.548602	0.089194
6	-2.891919	1.572701	0.294474
12	-1.541479	3.026768	0.037294
16			
87.460419 Kcal/mol 3.792648 eV -101.244303 H Child_3_48.log			
12	-2.557196	0.560063	-1.459858
6	5.722148	1.425334	0.038748
6	-3.104045	-1.181123	-0.095654
6	4.484531	1.018217	0.027796
6	-3.580033	-0.195683	0.592839
6	3.272688	0.604448	0.016377
12	-1.281891	-2.024708	0.193352
6	2.004600	0.182035	0.025058
6	-1.532822	1.902646	-0.012358
8	2.701777	-2.110933	-0.001664
6	-3.724498	1.086803	1.029751
6	0.929814	1.090651	0.033082
6	-2.606109	1.735183	0.717258
6	1.759903	-1.313855	0.023044
8	0.480505	-1.660148	0.057628
6	-0.191045	1.602743	0.062456
16			
87.664038 Kcal/mol 3.801477 eV -101.243979 H Child_1_28.log			
8	5.628071	-1.688635	0.797077
6	-0.750438	1.267093	0.031017
6	4.739246	-1.248044	0.199813
6	-2.192619	1.242186	0.117395
8	3.774382	-0.842749	-0.385727
6	1.323781	2.509262	0.011175
12	2.031446	0.382530	-0.360751

6	-0.045021	2.539565	0.056409
6	-5.271260	-0.838710	0.460517
6	-3.368253	0.950753	0.229633
6	2.614150	2.454389	-0.076369
12	-3.358006	-1.616911	-0.044705
6	-1.526339	-2.105396	-0.660369
6	-4.509919	0.200455	0.305787
6	-0.805335	-1.168140	-0.253191
6	-0.091477	0.040528	-0.159372
16			
88.063536 Kcal/mol 3.818801 eV -101.243342 H MutD_6_66.log			
6	2.279077	1.345365	0.216096
12	-0.603533	-0.800063	0.035769
6	3.579189	-1.001300	-0.020637
6	1.488492	-1.052840	0.101620
12	0.183439	3.506829	-0.027326
8	4.778832	-0.976770	-0.209955
6	-4.686415	-1.305991	0.025917
8	-5.642314	-2.035596	0.103062
6	-3.752644	-0.434928	-0.055526
6	-2.189262	1.475818	-0.166731
6	-2.533762	0.110093	-0.088999
6	2.510133	-2.146370	-0.008296
6	2.448512	-0.041415	0.149028
6	1.924789	2.536725	0.225012
6	-1.605266	2.579432	-0.188358
6	2.528653	-3.461631	-0.063486
16			
88.096898 Kcal/mol 3.820248 eV -101.243289 H MutD_14_70.log			
12	-1.545854	-1.765037	-0.087304
6	2.762024	-1.303953	-0.006472
6	3.664224	-2.285321	0.147077
6	-2.906549	0.975864	0.248531
12	2.584273	2.147646	-0.185861
6	-1.182714	2.895130	0.195242
6	1.424708	-0.865351	-0.088397
6	-4.176815	-1.323875	-0.065766
6	-3.389420	-0.173298	0.244232
6	2.406902	0.106088	-0.083884
8	0.163316	-1.152563	-0.132990
6	-2.114236	2.075084	0.269526
6	0.055073	3.412509	0.063748
6	4.477693	-3.245283	0.363976
6	1.242004	3.700235	-0.205777
8	-3.418115	-2.397221	-0.268788
16			
88.312019 Kcal/mol 3.829576 eV -101.242946 H Child_5_46.log			
12	-7.811700	-0.187004	-1.072569
8	6.498562	0.437944	-0.988800
6	-2.395584	1.640254	1.711009
6	5.462093	0.154001	-0.443189
6	-1.477868	-2.036363	0.520340
6	2.017852	0.802878	0.101220
6	-0.241352	-2.267576	0.488979
6	0.981647	1.462832	0.086306

6	-1.345881	1.835187	1.026010
6	4.267985	-0.167939	-0.135991
6	1.091396	-2.057357	0.392209
6	-0.435898	1.500225	-0.010932
6	2.183516	-1.475892	0.272931
6	2.955969	-0.290876	0.085835
12	-2.404669	-0.208988	0.351243
8	-0.971916	0.831513	-1.000257
16			
88.346630 Kcal/mol 3.831077 eV -101.242891 H Original3D_8_3.log			
8	-2.227322	-1.067158	-1.006753
12	-1.327585	-2.681685	-0.817108
6	2.239401	-1.703628	0.491985
6	1.492967	-2.864107	0.546674
6	2.826240	-0.614261	0.391654
6	0.727268	2.789440	-0.058614
6	0.322178	-3.448029	0.138407
6	-1.215799	1.130147	-0.356281
6	2.003097	3.257647	-0.119729
6	1.221687	-4.233362	0.966060
8	-4.922403	2.257280	0.826028
6	-0.262950	2.062909	-0.142686
6	-1.773388	0.090347	-0.675656
6	3.246829	3.453288	-0.250821
6	-5.176290	1.143656	0.905383
12	3.268449	1.356246	0.019404
16			
88.461977 Kcal/mol 3.836079 eV -101.242707 H MutI_5_71.log			
6	2.029082	-2.909671	0.450109
6	4.825552	1.312445	-0.448767
6	-4.857031	-0.059288	-0.545375
12	0.009412	-2.638951	0.386481
6	-2.424575	-0.704485	-0.107580
6	3.669970	0.689937	-0.243127
8	-2.237282	2.972102	1.202937
6	2.605990	-1.821301	0.253821
6	-1.167207	-0.979714	0.042259
6	5.929061	1.922847	-0.658256
6	-3.665237	-0.358150	-0.260789
12	0.141360	0.673611	-0.133636
6	2.936476	-0.493383	0.036017
8	-5.984973	0.252913	-0.808336
6	2.231062	0.685584	-0.194055
6	-1.451680	2.345837	0.643916
16			
88.612892 Kcal/mol 3.842624 eV -101.242467 H Child_18_18.log			
8	4.188921	-2.014082	0.947494
6	-1.774384	1.944446	1.195804
6	3.368432	-1.305077	0.520509
6	-1.235833	3.047039	0.964792
6	2.605839	0.894677	-0.219156
6	-2.801039	-0.384551	0.747899
6	2.394234	-0.514001	-0.018714
6	-2.268365	0.682603	1.107268
6	2.181568	2.024882	-0.530235

6	-2.832536	-1.615634	0.035303
6	1.140243	-1.106289	-0.397593
6	0.297827	-0.201651	-1.005516
8	-3.811814	-2.085502	-0.563520
6	-0.380974	0.779083	-1.457386
12	-0.773264	-2.133687	-0.176921
12	0.174353	2.743978	-0.550550
16			
88.630566 Kcal/mol 3.843390 eV -101.242439 H Original2D_0_31.log			
6	2.979364	2.054551	-0.000000
6	0.394545	2.178040	-0.000000
6	-1.309639	-1.230763	0.000000
6	1.635426	2.363402	-0.000000
12	1.642185	-0.203825	-0.000000
6	0.000000	-1.653096	-0.000000
6	4.425646	1.917207	-0.000000
12	-1.645542	1.988584	0.000000
6	1.785265	-3.517989	-0.000000
6	3.527808	0.767888	-0.000000
8	-3.390237	1.358969	0.000000
6	-3.675249	0.038585	0.000000
6	0.791905	-2.668209	-0.000000
6	-2.426023	-0.716969	0.000000
8	-4.799309	-0.448882	0.000000
6	2.797060	-4.315613	-0.000000
16			
88.637831 Kcal/mol 3.843705 eV -101.242427 H MutD_7_74.log			
8	5.671332	0.174342	0.580152
6	-3.530784	2.806210	0.042643
6	-4.423438	3.645986	0.431579
6	-1.043392	-0.055657	-0.606345
6	3.132930	-2.331239	0.012787
6	-5.845028	-3.112548	0.099771
6	-0.342904	-1.087019	-0.658407
12	1.169467	-2.416619	-0.446325
12	0.453405	1.888369	-0.239940
8	-6.609380	-2.556147	0.749095
6	-1.556355	1.228761	-0.476998
6	3.443047	0.960380	0.272666
6	-2.592918	1.949704	-0.249701
6	4.466434	-0.054724	0.389494
6	3.872446	-1.359504	0.221690
6	2.424949	1.641891	0.121022
16			
88.797853 Kcal/mol 3.850644 eV -101.242172 H MutD_2_64.log			
6	3.708565	-1.260662	0.339202
8	-0.576680	-2.152436	0.171226
6	2.437715	-1.018435	0.147743
6	4.956977	-1.506750	0.526192
6	-1.576004	1.288025	1.148591
12	-2.453896	-1.882416	-0.343504
6	-0.584395	0.980632	-1.512483
6	-0.565346	2.110003	1.397525
6	1.248298	-0.612992	-0.084787
6	-1.123053	0.009026	-0.650134

6	-0.098580	-0.970360	-0.168606
6	0.172939	1.771151	-2.138602
12	1.510717	1.746299	-0.503394
6	-2.175699	0.350570	0.449211
8	-3.262238	-0.423102	0.591932
6	0.603498	2.566077	1.222396
16			
88.855483 Kcal/mol 3.853143 eV -101.242080 H Child_9_21.log			
12	-1.063411	-1.654906	0.161761
6	0.848853	2.834245	0.858240
8	1.320826	-3.850064	0.961589
6	-0.368240	2.857500	0.287533
6	0.794413	-2.996922	0.375794
6	2.014278	2.482726	1.111228
6	-2.904683	-0.342604	0.648913
6	-1.371001	2.611935	-0.422438
6	1.793542	-0.764936	-1.303014
6	2.965548	1.584357	0.799726
6	-0.744681	-0.550670	-1.739249
6	3.297671	0.525557	0.223709
12	-2.236247	0.892516	-1.147718
6	0.514835	-0.702972	-1.730837
6	2.758966	-0.376909	-0.611378
8	-3.570966	-0.377332	1.643675
16			
88.873788 Kcal/mol 3.853937 eV -101.242051 H Child_6_14.log			
8	6.772347	-0.706650	-1.081607
6	-4.151579	0.757208	-0.610590
6	5.685648	-0.397097	-0.660927
6	-3.336762	1.644418	-0.486356
6	4.539947	-0.066754	-0.169881
8	-4.786987	-0.420831	-0.687585
6	2.123847	0.356419	0.678574
6	-2.224823	2.403496	-0.249097
6	0.978059	-0.396136	0.972997
6	-1.076998	2.805430	0.028655
6	3.330767	0.125952	0.254018
6	-3.984740	-1.487386	-0.457022
6	-0.172865	-0.838601	1.224237
6	-3.154274	-2.410546	-0.252710
12	0.670168	1.938104	0.575405
12	-1.271856	-2.434651	0.468107
16			
89.062461 Kcal/mol 3.862119 eV -101.241750 H Child_6_17.log			
8	4.008302	3.060774	0.260574
12	0.179979	-5.118464	1.278345
6	3.040539	2.282704	0.193039
6	-5.531069	0.752770	-0.066393
6	1.698670	2.620985	0.593560
6	-2.336173	0.333236	-0.115303
6	3.118788	0.926743	-0.302435
8	-6.247657	1.612339	-0.333653
6	0.481150	2.527326	0.719537
6	-1.921307	-0.793691	-0.440378
6	3.053342	-0.240604	-0.707331

6	-0.954158	-1.704071	-0.671728
6	-0.817308	2.165121	0.667404
6	-1.799154	1.488715	0.350933
6	0.194931	-2.175542	-0.736441
12	2.198799	-2.088791	-0.971858
16			
89.075774 Kcal/mol 3.862696 eV -101.241729 H Child_12_40.log			
12	-4.003076	-0.214505	0.632886
6	-0.780228	1.951190	-0.811684
6	-0.522420	-2.555688	0.197223
12	0.676831	-0.676102	-1.488541
6	0.701439	-2.310565	0.209670
6	-0.307210	1.061834	-1.506583
6	-1.877139	-2.395063	0.263017
6	1.893118	-1.687235	-0.056731
6	-3.769537	1.785742	0.663662
8	5.671309	1.571291	0.714730
6	-2.686097	2.303339	0.355465
6	4.771606	0.783103	0.580326
6	-3.044904	-1.964659	0.240699
6	3.829210	-0.065350	0.424976
6	2.901871	-0.949445	0.278883
8	-1.514221	2.796719	-0.060440
16			
89.385240 Kcal/mol 3.876116 eV -101.241236 H Child_5_37.log			
8	-5.876518	1.780090	0.253922
8	4.977819	0.295185	0.071934
6	-2.081441	-2.288730	-0.066242
6	-4.766779	1.349396	0.119578
12	-0.411539	-3.391171	0.094308
6	3.344886	3.187384	0.119255
6	3.801678	0.567333	0.078228
6	-3.513964	1.073135	-0.034468
6	1.400885	-2.530247	0.031980
6	2.989462	1.920920	0.045501
6	2.012873	-1.451633	0.048072
6	1.765338	1.061519	-0.054463
6	2.486270	-0.133669	0.034842
6	-2.401871	0.339152	-0.177024
6	-2.334505	-1.067905	-0.125092
12	-0.340743	0.994327	-0.321628
16			
89.391993 Kcal/mol 3.876409 eV -101.241225 H MutD_9_66.log			
6	-4.315810	0.095460	0.271552
12	-0.599477	-1.819106	-0.207017
6	-3.198453	-2.142391	0.144739
6	-4.024280	-1.229580	0.216040
6	-4.097701	1.311041	0.275391
8	-2.152347	-2.900511	0.026054
12	-0.615108	1.856766	-0.047735
6	2.955546	0.148081	-0.816083
6	4.030231	0.352347	-1.719250
6	-2.211337	3.102415	0.175330
8	5.898755	-0.240264	1.598226
6	-3.222276	2.356767	0.225701

6	0.390824	0.003928	-0.287592
6	5.150137	-0.074299	0.685663
6	1.659068	0.069060	-0.542184
6	4.318012	0.119551	-0.285510
16			
89.439874 Kcal/mol 3.878485 eV -101.241149 H Child_18_13.log			
6	-4.364780	-0.583257	0.135309
6	5.820167	-1.874166	0.777832
6	-4.377289	-1.806485	-0.175991
6	4.809993	-1.148525	0.451761
6	-3.951292	0.679395	0.431466
6	3.831459	-0.354879	0.137632
6	-3.178462	1.641652	0.560369
6	2.731954	0.299183	-0.099871
6	-2.003169	2.301950	0.522369
8	2.648347	1.474159	-0.880801
12	-2.373695	-2.289798	-0.328588
6	1.585863	2.228568	-0.597447
6	-0.833256	2.500424	0.272175
6	0.457581	2.349955	-0.160673
8	-0.669773	-1.691860	-0.272584
12	0.790261	-0.681976	-0.029954
16			
89.453211 Kcal/mol 3.879063 eV -101.241128 H Child_11_15.log			
6	6.660448	0.431811	0.775632
6	-4.165955	1.725165	0.653653
6	5.472793	0.005449	0.438576
6	-4.737451	0.552864	1.034203
6	7.834560	0.936716	1.091275
6	-3.160939	2.212614	0.107417
6	4.327901	-0.383473	0.089751
12	-3.306400	-1.761220	0.521508
6	3.120020	-0.767790	-0.288362
6	-4.967293	-0.676997	1.228305
6	1.958832	-1.111184	-0.638170
6	-1.979901	2.325150	-0.493654
8	-0.160357	0.884168	-1.372325
8	-1.710181	-1.745943	-0.310613
12	-0.120359	-1.116417	-0.928700
6	-1.015447	1.653981	-0.940325
16			
89.853073 Kcal/mol 3.896403 eV -101.240491 H MutI_6_79.log			
12	-4.235837	-1.515087	0.241734
6	-1.645784	1.742429	0.324257
6	-3.834101	0.478472	0.587746
6	-2.483551	-2.404307	-0.346527
6	-2.880858	1.281503	0.621628
6	2.559661	0.707377	0.302438
6	1.185962	-1.392458	-0.301131
8	4.864132	-1.257982	0.121039
6	-1.323368	-2.070590	-0.538503
6	2.451759	-0.877405	0.009000
8	3.658821	1.169100	0.601547
6	-1.148220	2.783262	-0.404029
6	3.677447	-1.413336	0.009080

12	0.474731	1.219362	-0.044237
6	0.006529	-1.707504	-0.536666
6	-0.407199	3.582517	-1.085735
16			
89.926077 Kcal/mol 3.899569 eV -101.240374 H Child_12_36.log			
6	4.260976	-2.072933	1.702081
6	1.236906	2.509138	0.283742
8	3.605906	-1.505352	0.932120
6	0.054645	1.771634	0.522335
6	0.987153	-2.116612	-1.018221
6	-1.290249	1.518541	0.581141
6	-0.252665	-2.160485	-0.889839
6	-2.403973	1.009284	0.455626
6	-1.541179	-1.820959	-0.616294
12	3.196592	2.323213	-0.906216
12	2.322433	-0.587873	-0.566720
8	-5.768306	0.102707	0.247968
6	-2.586656	-1.252006	-0.305437
6	-4.600728	0.029322	0.187126
6	1.244240	1.058178	0.332839
6	-3.263320	-0.073588	0.137321
16			
90.595375 Kcal/mol 3.928592 eV -101.239308 H Child_16_13.log			
12	-2.741729	2.308445	0.094719
6	7.876540	-0.746930	0.103658
6	-0.651721	2.073137	0.008787
6	6.604083	-0.573119	0.148191
6	-3.384325	0.297312	-0.033968
6	5.302080	-0.389752	0.151035
6	0.560235	1.742025	-0.035331
6	4.052208	-0.272582	0.094061
12	-1.353863	-0.402979	-0.197814
8	0.376473	-1.308055	-0.220469
6	-4.425542	-0.491233	0.035944
6	-5.465788	-1.248187	0.126593
6	1.412627	-0.536374	-0.209955
6	1.604636	0.828459	-0.140636
6	2.741021	-0.079668	0.001439
8	-6.402624	-2.002460	0.187749
16			
90.787291 Kcal/mol 3.936915 eV -101.239002 H Child_4_42.log			
8	4.175112	-1.412392	-0.251508
6	1.160758	3.580809	0.351934
8	0.826729	-1.860531	-0.031961
6	1.853978	2.501738	0.253707
12	-0.693062	-2.915490	0.253874
6	-0.362090	0.234445	-0.204187
6	-4.942658	1.233570	-0.287187
6	0.812072	-0.504664	-0.122182
12	-0.482975	2.314220	-0.104858
6	3.229384	-0.743585	-0.155201
6	-4.057007	0.328509	-0.110633
6	2.150618	0.096846	-0.065170
6	2.629178	1.397910	0.138940
6	-2.282732	-1.667570	0.238646

6	-2.952279	-0.401936	0.108103
6	-1.556267	-0.489633	-0.066842
16			
91.169971	Kcal/mol	3.953509	eV -101.238392 H Child_6_44.log
6	-4.051013	-3.514111	-0.122828
6	3.740184	2.303346	0.337406
6	-3.227752	-2.589082	0.215782
6	4.266241	1.387674	-0.313579
8	-8.548201	1.911320	-1.347522
6	4.480270	0.180967	-1.085809
6	-2.315295	-1.703264	0.536695
12	1.905593	2.218952	1.215054
6	-8.078477	2.632909	-0.592760
6	3.480870	-0.799462	-0.719067
6	-1.288546	-1.014408	0.877918
6	2.518459	-1.477836	-0.361210
6	-0.586708	0.138824	1.166250
6	0.266001	1.027919	1.337866
8	5.332833	-0.002452	-1.965470
12	0.635869	-1.778269	0.355275
16			
91.373257	Kcal/mol	3.962324	eV -101.238068 H Child_3_37.log
6	-3.538198	1.257348	0.034351
8	3.527026	-0.787737	0.034790
6	-4.827640	1.290252	0.062630
12	1.488127	-1.428517	0.030347
6	-2.212463	1.108946	-0.000230
6	3.610149	0.439260	0.005368
6	-2.031772	-2.658818	-0.062047
6	3.467754	1.697475	-0.023187
6	-1.377039	-0.102488	-0.047809
6	-0.023601	0.250657	-0.023897
8	-1.348097	2.204931	0.020256
6	2.293490	2.332160	-0.026060
6	-1.857072	-1.419979	-0.087569
6	1.050206	2.516978	-0.016885
6	-0.038276	1.694351	-0.003213
12	-0.198515	-3.719350	0.027230
16			
91.495673	Kcal/mol	3.967633	eV -101.237873 H Child_1_59.log
6	3.576239	-1.230861	1.131624
6	-3.697931	1.430318	-0.247592
12	2.768385	0.722399	1.111971
12	-2.683484	-1.496153	-0.157548
8	3.756066	1.016073	-0.825833
6	-4.281548	0.374871	0.021676
6	2.699733	-1.833845	0.404338
6	-1.297367	2.205638	-0.067811
6	3.590501	1.094009	-1.981074
6	-0.772264	-2.093390	-0.581522
6	1.782713	-2.517214	-0.288967
6	1.181902	1.914770	0.651729
6	-2.506675	2.086447	-0.256699
6	0.014052	2.148194	0.263077
6	0.474951	-2.275354	-0.509901

8	-4.456647	-0.833129	0.490040	
16				
91.854606	Kcal/mol	3.983198	eV	-101.237301 H Child_3_11.log
6	4.813729	-1.383475	-0.418301	
8	-3.938232	2.352699	-0.693881	
6	3.363696	-1.472347	-0.260186	
6	-3.114227	1.544146	-0.217487	
6	3.947525	-0.212549	-0.386089	
6	-2.248522	-0.819463	0.078018	
12	1.323857	-1.637151	0.172455	
6	-2.217981	0.688549	0.141222	
6	3.585554	1.110935	-0.243464	
12	1.060537	1.824340	0.549803	
6	-0.076706	-0.093153	0.399403	
6	-3.307541	-1.630794	0.003408	
6	2.999117	2.220464	-0.057322	
8	-4.165921	-2.432374	-0.095175	
6	-0.862612	-1.319036	0.206235	
6	-0.845283	1.098579	0.362123	
16				
91.875911	Kcal/mol	3.984122	eV	-101.237267 H Child_12_30.log
6	-4.595665	-1.901221	0.225349	
8	3.379000	0.774100	0.263526	
6	-3.542449	0.644969	0.684902	
6	3.770081	-0.425374	0.489672	
6	-3.874077	-0.654607	0.398860	
6	0.856613	-1.061611	-0.711276	
6	-2.779606	1.618171	0.654353	
6	4.299218	-1.617154	1.133621	
6	-3.200454	-1.724747	-0.181246	
6	1.886550	-1.680297	-0.283552	
6	-0.555347	2.602566	-0.060490	
6	3.131595	-1.650702	0.277094	
6	-1.673499	2.347429	0.397707	
12	1.663173	1.073382	-0.608271	
8	0.635214	2.654633	-0.540421	
12	-1.200796	-1.607915	-0.719630	
16				
91.925296	Kcal/mol	3.986263	eV	-101.237188 H MutD_14_76.log
12	-1.186881	-2.195646	0.416849	
6	1.991126	2.734787	-0.118187	
6	-0.192415	-1.474174	-2.715498	
6	-1.751441	2.954280	0.172921	
6	1.988074	-2.341239	0.797596	
6	-3.218974	-0.347661	0.416417	
8	-0.688870	-1.455323	-1.666266	
6	3.233580	-1.949198	0.624378	
6	2.861939	1.849995	-0.322797	
6	0.765395	3.301705	-0.002464	
12	3.601316	0.054843	0.208665	
6	0.742999	-2.687413	0.738163	
8	-2.998239	-1.611635	0.470965	
6	-0.467078	3.356031	0.081930	
6	-3.230992	0.879973	0.382657	
6	-2.634937	2.093797	0.287590	

16
91.941694 Kcal/mol 3.986974 eV -101.237162 H MutD_5_74.log
8 -5.138039 2.696055 -1.684426
6 -1.439600 -2.777124 -0.016134
6 -4.920480 3.103648 -0.630953
6 1.882708 -1.820306 -0.802853
8 -2.072979 -3.756243 -0.070852
6 2.912384 2.572381 0.760412
12 4.526821 1.598219 -0.117562
6 -0.314992 0.584821 0.794537
6 -0.633807 -1.696756 0.039861
6 -3.738322 -0.550252 1.408201
6 0.600836 1.401178 0.882421
6 0.700822 -1.808472 -0.431255
12 3.738405 -0.964923 -0.984980
6 -1.205426 -0.492366 0.640631
6 -2.516022 -0.482735 1.027805
6 1.756138 2.112975 0.872780

16
92.143260 Kcal/mol 3.995715 eV -101.236841 H Child_2_8.log
8 -0.183966 -0.043879 0.061926
6 3.685833 0.728087 -0.924781
6 -0.709913 -2.632933 0.266357
6 3.112130 1.753901 -0.417351
6 -0.806800 -1.226283 0.067763
6 2.018655 2.440416 0.100205
8 3.281897 -2.904454 0.304167
6 0.837414 2.665428 0.424908
6 2.788878 -1.876799 0.414323
6 -3.180334 1.691849 0.162101
6 -3.995142 -0.639707 -0.333687
6 -3.271815 -1.641983 -0.455342
6 -3.906955 0.712595 -0.134717
6 -1.949576 -1.938355 -0.153965
12 -1.102721 1.854351 0.365578
12 1.726246 0.093096 -0.117547

16
92.175270 Kcal/mol 3.997103 eV -101.236790 H Child_15_8.log
6 0.521716 -3.394976 0.331898
12 -2.732817 0.975013 -0.133713
6 2.700867 -0.937727 -0.059627
8 -1.917966 2.844183 0.022417
6 0.630912 -2.073918 0.186400
6 -0.714162 2.409723 0.110799
6 1.354229 -0.836459 0.086571
6 -0.543652 0.921853 0.074251
6 3.812565 -0.311725 -0.214783
6 -3.946014 -0.674379 -0.338954
6 -0.787461 -2.602708 0.154952
6 0.741246 0.490649 0.138486
8 4.914967 0.126918 -0.385648
6 -3.145994 -1.627677 -0.173864
6 -1.994374 -2.302423 -0.009711
12 1.419877 2.514137 0.232658

92.184631 Kcal/mol 3.997509 eV -101.236775 H Original3D_0_34.log

6	-0.501206	-3.074305	-1.327279
6	-1.393159	-2.179518	-1.537977
12	-1.252041	2.922672	-0.782386
12	1.379055	-2.724577	-0.765950
6	1.568945	3.010725	0.288357
8	-3.299964	-0.722038	2.795372
8	-2.340424	1.445989	-1.016992
6	0.478080	3.515499	-0.001539
6	-4.173875	-1.461014	2.690898
6	3.125270	1.032011	0.606944
6	-2.281772	0.143376	-1.256585
6	2.570833	2.135439	0.580845
6	3.322378	-0.345691	0.685251
6	-2.130052	-1.036367	-1.497983
6	3.832148	-1.547811	1.290165
6	2.848900	-1.553803	0.204404

16

92.303366 Kcal/mol 4.002658 eV -101.236586 H Child_6_49.log

12	-1.060741	1.761723	0.166379
6	-4.245976	3.374529	-0.142289
6	0.190051	0.031634	0.089621
6	-3.815397	0.593975	-0.206494
6	1.473106	-0.204531	0.235927
6	-3.245736	-0.519341	-0.194720
6	2.787517	-0.254849	0.261462
6	-3.903920	1.978243	-0.156976
6	4.061258	-0.164872	0.170696
6	-4.045845	-4.003734	-0.119999
8	7.787289	0.207395	-0.344219
12	-1.341388	-1.304990	0.151936
6	6.605235	0.071014	-0.155410
6	-2.869320	2.874056	0.044583
6	5.356465	-0.078849	0.068436
8	-2.944674	-3.665449	-0.054381

16

92.532573 Kcal/mol 4.012597 eV -101.236220 H Child_7_10.log

6	4.345638	0.643966	-0.431934
6	-3.078766	-2.349089	0.145221
6	-0.558461	4.232044	0.604202
6	-3.902626	-1.450476	-0.094038
8	4.430073	-0.678035	-0.201870
6	-1.758505	-2.611417	0.304405
6	2.923997	0.985627	-0.167296
6	-3.925351	-0.109975	-0.350085
8	-0.892737	3.165933	0.295589
6	-0.609281	-2.134852	0.277502
6	1.742220	0.612852	-0.009416
6	0.537854	-1.363663	0.212381
6	0.454367	0.032326	-0.010143
6	-3.482572	1.053378	-0.526868
12	-1.398198	1.114932	-0.237270
12	2.695718	-1.543892	0.197826

16

92.889857 Kcal/mol 4.028091 eV -101.235651 H Child_4_19.log

12	2.330888	1.976238	-0.001165
8	-6.724332	0.556275	-0.015922
6	4.399563	1.895658	-0.025460
6	-5.660725	0.060551	-0.010675
6	4.427673	0.634048	-0.017237
6	-4.502558	-0.504115	-0.008982
6	0.600254	0.902024	0.021193
6	-3.322037	-0.936566	-0.006437
6	-0.643693	1.250867	0.020343
6	-2.112506	-1.436356	-0.003810
6	4.263066	-0.736240	-0.009934
12	1.183578	-1.156133	0.018782
6	4.591333	-2.143777	-0.008819
6	-0.884976	-1.733500	0.002134
6	3.218451	-1.650665	0.004539
8	-1.827751	1.512118	0.021855
16			
92.897931	Kcal/mol	4.028441	eV -101.235638 H Child_1_18.log
6	8.751446	-1.288172	0.429611
6	0.313346	1.598537	0.124784
6	7.568822	-0.804473	0.301095
6	-0.930319	1.780819	0.160417
6	6.359426	-0.337782	0.206822
8	-4.368987	0.397539	-0.445512
6	5.171842	0.085643	0.126674
8	-7.138997	-0.851074	1.445635
6	3.926863	0.429372	0.048358
6	-6.503678	-1.158823	0.536202
6	2.700333	0.708012	-0.036836
6	-2.238111	1.597508	0.014339
6	-3.435409	1.211674	-0.145325
6	1.369624	0.735109	-0.105984
12	-0.388981	-0.595679	-0.655667
12	-3.466122	-1.380675	-0.841160
16			
93.223510	Kcal/mol	4.042559	eV -101.235119 H Child_12_52.log
6	4.557179	0.668468	-0.469738
8	-5.721139	-0.600136	-0.750948
6	4.486314	-0.577946	-0.595404
6	-4.604500	-0.382391	-0.496930
8	3.891770	-1.701156	-0.598438
6	-3.292986	-0.162637	-0.257545
6	3.334883	1.250661	-0.160492
6	-2.613824	1.068359	-0.562195
6	2.103424	1.357577	0.099285
6	-2.557036	-1.115287	0.479390
12	2.020493	-1.013397	-0.060591
6	-1.315159	-1.106990	0.819244
12	0.107960	1.798284	0.544721
6	-1.702988	1.908413	-0.457482
6	-0.338433	-0.197582	1.604385
6	0.125379	-1.212029	0.828403
16			
93.272313	Kcal/mol	4.044675	eV -101.235042 H Child_3_53.log
8	5.604339	0.028632	-0.463657

6	-4.239386	-1.623374	0.196469	
6	4.468883	-0.230905	-0.211029	
6	-3.138371	0.846675	-0.559057	
8	-0.558327	2.144462	2.477327	
6	1.070916	-1.636465	0.603518	
6	-3.467948	-0.469491	-0.227014	
6	2.235518	-1.217814	0.421916	
6	-2.740638	2.053159	-0.624051	
6	3.180541	-0.335262	-0.023789	
6	-1.468827	-1.938054	0.416370	
6	-0.013593	1.709591	1.596209	
6	-2.774675	-1.583653	0.193561	
6	-0.237585	-1.870292	0.492833	
12	1.353732	0.795832	-0.622631	
12	-1.155158	0.903381	-1.857784	
16				
93.363695	Kcal/mol	4.048638	eV	-101.234896 H MutD_13_66.log
6	1.142373	1.138850	0.531885	
6	-0.097740	1.783035	0.548587	
12	2.946283	2.226839	-1.119239	
6	-2.584063	-1.337978	-0.258734	
12	2.270542	-0.576807	-0.213612	
6	1.044414	-2.148612	-0.814653	
8	-5.854468	-0.016466	0.199231	
6	-3.344856	-0.175909	0.112152	
6	1.045957	2.547993	0.198979	
6	5.132158	-1.626052	1.191647	
6	-4.688152	-0.117147	0.104099	
6	-1.436884	1.478286	0.606313	
8	4.057407	-1.315973	0.784832	
6	-0.204470	-2.174678	-0.744361	
6	-1.511770	-1.846810	-0.536601	
6	-2.534534	0.955543	0.414305	
16				
93.488741	Kcal/mol	4.054061	eV	-101.234697 H MutD_17_48.log
6	6.669524	-1.864038	1.592397	
6	2.668080	0.340597	-0.797989	
6	1.635221	1.322692	-0.512453	
6	-3.109310	0.183982	0.222305	
6	-0.521175	2.072129	0.710977	
8	0.332444	-0.198465	-1.957459	
6	-4.908418	-1.683908	0.246091	
6	3.792465	-0.230316	-0.379710	
6	-3.997012	-0.777472	0.207022	
6	1.389671	0.364092	-1.463383	
12	-1.306540	0.283638	-0.976904	
6	4.749707	-0.758508	0.242121	
6	0.640619	1.894265	0.282193	
8	-5.734423	-2.554937	0.271213	
12	-2.462181	1.778882	1.470957	
6	5.730712	-1.317354	0.910652	
16				
93.684343	Kcal/mol	4.062543	eV	-101.234385 H MutI_13_45.log
6	3.608614	0.597134	0.118338	
6	2.294354	2.815146	0.092240	

6	3.228938	-1.962164	0.031292
6	-0.145337	3.713188	0.089079
6	-5.614755	-1.386815	0.412614
8	-0.720938	-1.589031	-0.164079
6	-2.228963	0.481392	-0.266351
6	2.957800	1.718342	0.103776
6	1.053492	3.322792	0.064123
8	2.647301	-3.139094	-0.030407
6	3.388412	-0.719844	0.093418
6	-4.418074	-1.033578	0.179980
6	-1.762165	-0.810532	-0.188095
12	-1.765225	2.497916	-0.173680
6	-3.153786	-0.629831	-0.053063
12	0.876719	-2.398447	-0.035338
16			
93.758873 Kcal/mol 4.065775 eV -101.234266 H MutD_14_56.log			
12	-0.256864	2.156990	-0.284580
6	-1.298502	-2.582352	-0.450288
6	1.671760	1.616481	-0.670537
6	-2.197363	-1.687665	0.099930
8	2.893958	-1.440492	0.732807
6	-0.110190	-2.608993	-0.891022
6	3.965559	0.718296	0.202106
6	-2.341334	2.589500	0.030426
6	3.642694	-0.434967	0.585760
6	2.862933	1.379514	-0.326189
6	-2.976644	0.175861	0.431489
6	-3.001854	1.555093	0.308450
8	-0.505525	0.127671	0.283792
6	-3.635830	-1.148764	0.089107
12	1.208945	-0.868548	-0.320819
6	-1.669967	-0.398461	0.446101
16			
93.969040 Kcal/mol 4.074888 eV -101.233931 H MutI_15_79.log			
6	-3.776918	-1.304638	0.016687
6	-1.450028	1.635104	-0.067258
12	0.417587	-3.301879	0.313270
6	-1.157463	-1.698110	0.054699
6	3.532280	0.725244	0.006440
8	4.581923	0.182403	-0.001906
6	2.337026	1.232166	0.056385
8	-0.111931	3.725900	0.205579
6	-0.236057	0.776521	-0.000344
6	-0.947297	2.934894	-0.029588
6	-0.194468	-0.707655	-0.106655
6	1.085325	-1.263884	-0.328545
6	2.081057	-2.012630	-0.419650
6	-2.532372	-1.484153	0.029802
12	-3.301782	0.671605	-0.117756
6	1.067315	1.216619	0.125437
16			
94.083223 Kcal/mol 4.079840 eV -101.233749 H Child_3_23.log			
6	4.373637	1.261393	0.133529
8	-6.937417	1.480207	0.443049
6	2.500791	-0.629869	0.195659

6	-5.806087	1.230064	0.151266
6	3.254121	0.635662	0.138000
6	-4.610210	0.916048	-0.160127
6	5.530097	1.863191	0.078355
6	-3.409254	0.451928	-0.184936
6	1.775629	0.496886	-0.007167
6	-2.173712	0.056776	-0.282827
6	6.612785	2.568058	-0.054271
6	-1.513760	-1.183544	-0.181139
8	0.135921	-3.100217	-0.071534
6	-0.755052	-2.146029	-0.143002
12	1.902787	-2.585737	0.229906
12	-0.257949	0.905462	-0.319252
16			
94.137528 Kcal/mol 4.082195 eV -101.233663 H Child_14_17.log			
6	0.174303	2.563495	-0.334551
8	5.281212	-0.730435	0.176772
12	-1.538366	1.478988	-0.287621
6	4.072380	-0.451638	0.120063
12	-3.792836	-3.554139	-0.022919
6	2.966763	-1.363655	0.142295
8	-3.208915	2.722226	0.163566
6	1.762887	-1.672705	0.114349
6	1.385759	2.294752	-0.237688
6	3.500634	0.874808	0.007824
6	-4.005937	3.426530	0.635156
6	0.446429	-1.826748	0.063904
6	-1.945490	-0.565496	-0.145232
6	-0.805114	-1.632665	-0.011894
6	-2.258769	-1.860231	-0.072916
6	2.605495	1.708134	-0.114014
16			
94.724731 Kcal/mol 4.107658 eV -101.232727 H Child_5_33.log			
6	3.349509	1.874030	0.218279
6	-5.419737	-0.034311	-0.334555
6	2.576126	2.834147	0.095145
6	-4.072388	-0.027077	0.164064
6	3.954545	-0.604470	0.264442
6	-5.183481	-0.052854	1.080822
6	3.893543	0.630383	0.291901
6	-2.739064	-0.032081	-0.047224
6	3.482217	-1.872459	0.150099
6	-1.470595	0.618248	-0.227089
12	0.585105	2.899125	-0.206966
6	-1.502180	-0.741382	-0.184440
6	2.736038	-2.857554	-0.004952
12	0.744654	-2.661073	-0.187032
8	-0.895565	-1.896334	-0.206413
8	-0.802473	1.738294	-0.302459
16			
94.835905 Kcal/mol 4.112479 eV -101.232550 H Child_5_61.log			
12	-4.003403	0.154618	0.189006
8	5.302611	-0.299377	0.109816
8	-2.937865	-1.547055	0.077782
6	4.154619	-0.116422	0.075253

6	-1.714382	-1.134145	0.015274
6	2.808605	0.056122	0.023499
6	-0.487535	-1.921627	-0.029480
6	2.212696	1.365531	-0.100986
6	-2.298094	1.339971	-0.247073
6	0.889027	1.510978	-0.067524
6	-1.380583	0.294771	-0.092439
6	2.017590	-1.145838	0.116132
6	-0.458224	-3.238647	-0.220317
6	0.075415	0.354396	-0.105911
12	-0.818798	2.869252	0.022830
6	0.672271	-0.950922	-0.040229
16			
94.872154 Kcal/mol 4.114051 eV -101.232492 H MutD_16_62.log			
6	2.566043	2.620164	0.004053
6	0.309024	-2.731252	-0.001847
12	-2.546340	-1.204283	0.003589
6	3.680126	1.847247	0.004820
6	4.317227	0.787386	0.003214
6	-0.881553	-2.373649	-0.000529
6	1.388138	3.023308	0.001594
6	-3.499634	1.085814	-0.005404
6	4.425783	-0.556591	0.000205
6	-2.282012	1.366148	-0.004274
6	1.658676	-2.825982	-0.003238
6	2.857748	-2.525419	-0.003486
8	-4.498329	-0.949808	0.009288
8	-4.707937	0.593874	-0.003141
6	3.907005	-1.681096	-0.002192
12	-0.539434	2.423534	-0.004146
16			
95.337183 Kcal/mol 4.134217 eV -101.231751 H Child_3_58.log			
6	1.837809	-0.943852	0.286275
6	-3.295378	1.779959	0.782291
8	4.106098	-1.314932	0.931920
8	-3.780659	2.265952	1.703167
6	0.700999	-1.706855	0.238253
12	-2.141156	0.393302	-0.783522
6	3.254044	-0.542608	0.450317
6	1.612011	2.855297	-0.809420
6	-0.279856	-2.682703	0.244266
6	-3.440681	-1.304238	-0.837981
6	0.596464	-0.315559	-0.130926
6	0.802750	1.889320	-0.691270
6	-1.488020	-2.793520	-0.015065
6	-0.093625	0.781878	-0.561191
6	-2.647630	-2.191821	-0.419856
12	3.144754	1.560038	-0.241049
16			
95.481684 Kcal/mol 4.140483 eV -101.231521 H MutD_16_52.log			
8	4.642586	0.636364	0.268972
6	-3.673749	1.850424	0.125532
6	2.253792	1.367855	-0.196118
6	-0.282902	-2.762096	-0.174878
6	3.453086	1.089414	0.020134

12	2.551245	-1.206862	-0.076431
6	-4.372864	-0.571391	0.181801
12	0.513701	2.427034	-0.223027
6	-3.861453	-1.695784	0.098004
8	4.471603	-0.919619	0.278693
6	-2.825322	-2.547831	-0.016765
6	-1.631312	-2.852996	-0.113465
6	0.904666	-2.395691	-0.198427
6	-2.572375	2.635957	0.025563
6	-4.271474	0.772169	0.199540
6	-1.402238	3.047298	-0.082227
16			
95.523945	Kcal/mol	4.142316	eV -101.231453 H Child_10_20.log
6	4.309072	-0.897027	-0.176638
8	-3.900838	0.365731	0.345996
6	4.017961	0.325871	-0.430492
6	-2.936347	1.197776	0.727973
12	3.049452	-2.378683	0.408759
6	-1.998235	1.970057	0.944059
6	3.778929	1.596674	-0.736309
6	-3.519403	-0.735409	-0.505578
6	2.664642	2.311552	-0.519350
6	-2.351531	-1.418690	-0.101665
6	1.090287	-2.909496	0.483697
12	-0.275300	2.862099	0.427630
6	1.609922	2.976018	-0.302571
6	-1.320614	-2.033729	0.123306
6	-0.093280	-2.567883	0.350471
8	-4.198942	-0.952640	-1.493257
16			
95.658081	Kcal/mol	4.148132	eV -101.231240 H MutD_13_62.log
6	1.001736	-2.888750	-0.187516
6	2.175055	-2.504381	-0.248493
6	4.499582	-1.027779	0.095642
8	5.698209	-1.163332	0.326764
6	-0.340758	-2.745165	-0.123153
6	-1.402169	0.560545	0.135128
6	3.331704	-0.193074	-0.073381
6	-1.700964	-0.653415	0.075595
12	-0.262704	4.840234	-0.173615
6	-1.263185	-1.917848	-0.007748
8	-8.435833	-0.678673	0.299545
6	0.278540	2.555047	0.075283
6	-0.619103	1.645446	0.131716
12	2.073414	1.476602	0.009137
6	-9.137565	-1.417869	-0.230282
6	3.205873	-1.590425	-0.148914
16			
95.778472	Kcal/mol	4.153353	eV -101.231048 H Child_9_28.log
8	5.636667	0.718027	0.174975
6	-5.928677	1.279519	-0.393717
6	4.464831	0.654457	0.096658
6	-4.718019	1.462978	0.036462
6	2.405449	0.459604	-1.214760
6	-3.462819	1.330380	0.368538

12	-1.579147	-2.411145	-0.169647
6	1.133261	0.030491	1.477883
6	3.135069	0.562667	0.015475
6	-2.264667	0.982967	0.657639
6	1.442487	0.259504	-1.969234
6	-1.130019	0.393842	0.808172
12	-0.444727	-0.552128	-1.968850
6	-0.191256	-0.462708	1.320104
6	2.251615	0.397018	1.132454
8	-0.453798	-1.786157	1.281014
16			
95.886651 Kcal/mol 4.158044 eV -101.230875 H Child_5_28.log			
6	-4.612373	0.270536	0.189537
8	4.545710	-0.741175	-0.206445
12	-3.094665	-1.199736	0.153075
12	2.003076	2.626245	-0.017640
6	-3.635601	1.072810	0.151711
6	3.507312	-0.166872	-0.091500
6	-0.947247	-1.150897	-0.084108
6	2.475121	0.635424	-0.008031
8	-1.577763	-1.499868	-1.150136
6	1.036262	0.433720	-0.003302
6	-2.392404	1.629822	0.137065
6	0.208336	1.567842	0.080929
6	1.272033	-1.993681	0.157142
6	0.498923	-0.911429	-0.033682
6	-1.146622	1.598140	0.121190
6	1.962176	-2.850374	0.920954
16			
95.967472 Kcal/mol 4.161549 eV -101.230747 H Child_3_19.log			
8	-5.676752	-1.344512	-0.128283
6	4.861835	-0.822419	-1.392808
6	8.727591	0.677159	0.289324
6	3.646362	-0.650318	-1.056268
6	-4.704053	0.857165	0.206857
12	-0.179773	-1.840105	0.605389
6	-3.950969	1.847815	0.133207
6	2.394598	-0.608581	-0.626692
6	-4.718874	-0.588559	0.119848
6	1.190606	-0.566863	-0.176872
6	-2.747058	2.450683	0.045773
6	-2.096645	-1.135265	0.436481
6	-1.517092	2.516684	-0.119977
12	-0.272559	0.902025	-0.392985
8	8.041061	0.523634	1.190632
6	-3.334052	-1.006837	0.299852
16			
95.992135 Kcal/mol 4.162618 eV -101.230707 H MutD_4_72.log			
8	-0.581538	3.962843	-0.051524
12	-2.225738	3.090632	0.267457
12	7.984516	-0.702626	0.504358
6	-0.271454	-3.065779	-0.197750
6	1.557630	-1.312702	-0.408102
6	-3.525862	0.204614	0.280011
6	1.386147	2.439155	-0.386529

6	-1.380318	-3.569130	-0.078252
6	0.847740	-2.319304	-0.321749
8	-2.729228	-3.581835	0.084813
6	1.896602	1.189150	-0.464582
6	0.486706	3.265715	-0.246075
6	-3.491241	-1.157372	0.225834
6	1.998601	-0.042696	-0.470961
6	-3.246633	-2.346116	0.169111
6	-3.361120	1.430445	0.311029
16			
96.128461	Kcal/mol	4.168530	eV -101.230490 H MutD_8_74.log
8	-1.876472	2.022989	0.708293
6	4.470306	0.301056	0.169247
6	-4.216187	1.851051	-0.163288
12	-0.410903	-2.505184	-0.071269
6	-4.683715	0.658495	-0.600997
6	-3.069610	2.058332	0.294925
6	4.420619	0.015311	1.633054
6	-4.573691	-0.566852	-0.849136
12	-1.023070	0.237703	0.492415
6	5.102753	0.672960	-0.895574
6	3.272893	-0.194305	0.838299
6	1.997504	-0.549028	0.668954
8	5.666969	1.020162	-1.889811
6	-3.432240	-1.277883	-0.597550
6	0.781384	-0.897890	0.497964
6	-2.256068	-1.593820	-0.262832
16			
96.264717	Kcal/mol	4.174439	eV -101.230273 H Child_12_20.log
8	-3.611009	2.511640	-0.208993
6	8.357738	-0.403199	0.568838
12	-5.244192	-0.973198	1.021790
6	7.092923	-0.177925	0.413209
6	-3.035392	1.416664	0.007288
6	5.816638	0.031900	0.254910
6	-3.751658	0.196568	0.339088
6	4.570092	0.211326	0.108433
6	-1.585054	1.324486	-0.043593
6	3.291317	0.328107	-0.056616
6	-3.411341	-1.172384	0.156818
6	2.034740	0.376400	-0.229161
6	-0.403892	0.991135	-0.218908
6	0.743642	0.249370	-0.456897
8	-2.345885	-1.673076	-0.454287
12	-0.644423	-1.272068	-1.001307
16			
96.444784	Kcal/mol	4.182247	eV -101.229986 H Original2D_0_25.log
6	-1.104828	-0.091983	-0.000000
6	-3.403487	1.160684	-0.000000
6	0.000000	1.055346	-0.000000
6	-0.944839	-1.404955	0.000000
6	0.139128	-2.220032	0.000000
12	2.835100	-1.565424	0.000000
6	1.235059	-2.855366	0.000000
6	-2.076392	1.018276	-0.000000

6	1.375337	0.867806	-0.000000
6	-4.638533	0.832917	-0.000000
6	-0.966545	2.029339	-0.000000
6	2.555691	0.463353	0.000000
8	-5.826614	0.667902	-0.000000
6	4.935903	-2.603111	0.000000
12	-1.468819	4.078445	-0.000000
8	5.947321	-3.126640	0.000000
16			
96.638045 Kcal/mol 4.190628 eV -101.229678 H Child_9_8.log			
8	-6.788592	-1.236374	0.096279
8	7.534852	-1.088790	-0.049931
6	-5.586771	-1.015068	0.055257
6	6.362619	-0.822810	-0.001347
6	-4.349997	-0.692980	-0.003614
6	5.114787	-0.562603	0.042873
6	-3.034467	-0.542589	-0.058865
6	1.437951	0.660993	0.059091
6	-2.387378	0.778197	-0.102868
6	2.626183	0.092323	0.040805
6	-0.984550	1.073528	0.001176
6	3.863848	-0.228145	0.057494
12	-1.133023	-1.548767	-0.065371
12	0.456653	2.599988	0.054918
6	0.077258	0.183941	0.019457
6	-2.781757	2.072990	-0.150351
16			
96.847398 Kcal/mol 4.199706 eV -101.229344 H Child_4_20.log			
12	-1.211271	2.055442	0.607380
8	4.336189	-1.409791	-0.162175
6	-3.100380	1.755854	-0.038176
6	0.715985	-0.102835	-0.390468
6	-3.181686	0.512233	-0.225332
12	-0.987153	-0.737622	-1.546839
6	-1.555640	-2.265543	1.096040
8	2.446827	3.104542	0.082518
6	-2.882247	-0.827473	-0.490458
6	0.691543	1.304551	0.115204
6	-2.514940	-1.753207	0.388114
6	1.653307	2.194999	0.079390
6	-0.257286	-2.114353	1.069612
6	3.176738	-1.201166	-0.140616
6	1.888322	-0.992520	-0.056967
6	0.719110	-1.405847	0.578783
16			
97.396126 Kcal/mol 4.223501 eV -101.228470 H Child_6_9.log			
6	3.063612	1.934557	1.046251
6	-1.447074	-0.651232	-0.531160
6	3.584402	-1.778667	0.789401
6	-0.278859	-0.245894	-0.950630
6	3.511487	0.698649	1.377877
6	-2.624109	-0.717962	-0.079358
6	3.697199	-0.517503	1.305537
6	0.882735	0.170707	-1.361339
6	3.352020	-2.782830	0.055025

6	-3.891744	-0.685147	0.245490
6	2.499282	2.891679	0.483176
6	-5.088227	0.007759	0.231995
8	-4.718681	-0.408895	1.555625
12	1.361339	2.188613	-1.064750
12	2.090943	-1.558675	-1.088616
8	-5.905285	0.720899	-0.284774
16			
97.442199 Kcal/mol 4.225499 eV -101.228396 H Child_11_22.log			
6	-1.300856	1.300996	0.532835
8	-4.461461	-1.212023	-0.994474
6	-1.843119	2.350050	-0.005719
6	-3.452393	-1.043047	-0.404761
12	0.760480	0.832045	1.021890
6	1.454398	-2.370572	-0.096181
6	2.330106	2.105107	0.242412
12	-0.522765	-2.087601	0.488174
8	-2.144317	3.384916	-0.513633
6	2.554195	-1.550938	-0.350458
6	-1.301885	-0.088574	0.594190
6	3.560162	-0.848473	-1.018754
6	1.724133	-1.174893	0.728955
6	3.661282	0.398954	-0.995158
6	-2.293388	-1.027064	0.202192
6	3.239640	1.562375	-0.438873
16			
97.614890 Kcal/mol 4.232988 eV -101.228121 H Child_9_57.log			
12	1.902187	1.180658	-0.979436
12	-6.408466	-2.280076	0.306620
6	0.704583	2.720225	-0.396758
6	-1.365726	-1.611519	-0.261923
6	2.391350	-0.914278	-0.771906
6	-2.404453	-1.036206	0.101339
8	3.525712	-1.330788	-0.475818
6	-3.164421	0.032247	0.416481
6	6.994293	-1.222061	1.115303
6	-0.066899	-1.790070	-0.565610
6	-0.402791	3.220340	-0.114953
6	-3.262350	1.254300	0.620063
6	-1.687671	3.135002	0.312813
6	1.148550	-1.632348	-0.766301
6	-2.710321	2.483751	0.591949
8	6.103098	-0.499622	1.274669
16			
97.729990 Kcal/mol 4.237979 eV -101.227938 H Child_12_23.log			
8	-6.647655	-0.749754	0.504469
8	5.710118	-0.139068	0.160199
6	-1.191174	1.133813	-0.713623
6	4.484120	-0.199925	0.143107
6	-1.782071	-0.069857	-0.600900
6	2.407832	-2.030760	0.380845
6	-1.761698	-1.305421	-0.440320
6	3.269636	-0.964137	0.258645
6	-7.275854	-1.471484	-0.131653
6	1.361961	-2.689205	0.359977

6	-0.427069	2.140386	-0.587208
6	-1.064518	-2.414578	-0.139795
6	0.042320	-2.890446	0.173683
6	3.187666	0.410356	-0.035040
12	1.589797	1.688496	-0.453331
12	-1.590348	4.079681	0.676359
16			
97.981596 Kcal/mol 4.248890 eV -101.227537 H Child_10_47.log			
8	-3.413278	1.226827	0.247823
6	4.052792	0.656457	0.023018
6	-2.151274	1.544300	0.062674
6	3.591164	-0.500566	0.097985
8	-5.143925	-0.239349	0.277331
6	-3.965999	-0.114274	0.098730
6	3.039965	-1.761522	0.188669
6	-1.022180	2.016478	-0.053957
6	3.169085	-3.191722	0.379887
6	-2.972495	-1.085134	-0.205682
12	3.228505	2.491729	-0.034863
6	-2.010256	-1.832906	-0.409494
6	1.898484	-2.526399	0.130465
6	0.226064	2.558047	-0.130002
6	1.322110	3.112985	-0.167702
12	-0.112433	-2.587920	-0.322535
16			
98.577399 Kcal/mol 4.274726 eV -101.226587 H MutD_11_64.log			
6	11.381728	-2.113682	-0.451167
6	-3.097499	0.499671	-0.761828
6	-4.809100	-1.389171	-0.610803
6	-4.085230	-0.239626	-0.849979
8	0.958779	3.482329	-0.367560
6	1.271595	0.296167	1.371176
6	-1.774373	0.783862	-0.296013
6	-4.423457	-2.516671	0.125706
6	0.117208	0.004762	0.973157
6	-1.178914	-0.230749	0.484611
8	10.258469	-1.877376	-0.518443
6	-5.749730	-2.483401	-0.497677
6	-1.073863	1.987474	-0.569325
12	1.803188	2.116802	0.710445
6	-0.142852	2.789829	-0.533960
12	-2.499110	-1.881003	0.688274
16			
98.651888 Kcal/mol 4.277956 eV -101.226469 H Child_15_18.log			
6	-1.663250	0.090192	-0.462790
6	3.425970	-1.846171	0.025365
6	-0.732838	1.095310	-0.500736
6	2.311614	-1.043370	-0.446878
6	0.227702	1.877095	-0.571510
6	3.449727	-0.413327	0.046313
6	-2.927898	-0.095018	-0.244108
12	0.230172	-0.957191	-0.644561
12	2.215361	2.261610	-0.251226
6	-7.961022	-0.008631	0.762960
6	-4.175785	-0.309504	0.007453

6	-6.722039	-0.265881	0.466266
6	3.806973	0.976356	0.453111
6	-5.409236	-0.312820	0.234867
8	4.737228	1.199286	1.242451
8	3.872034	-2.964087	0.273496
16			
98.800247	Kcal/mol	4.284390	eV -101.226232 H Child_3_8.log
12	4.945743	-1.926466	0.051060
12	-2.724583	1.290031	0.065343
6	3.725867	-0.168003	0.021159
8	1.551909	3.920460	-0.132575
6	2.400117	-0.243337	0.031541
6	-4.464171	0.214698	0.121737
6	1.046890	-0.864332	0.037350
6	1.031477	2.866802	-0.049582
6	0.159578	-1.898225	-0.050591
6	-4.126402	-0.991537	0.026919
6	-0.892461	-2.548151	-0.094325
8	-0.976559	1.702281	0.021203
6	0.389037	1.684799	0.013921
6	-2.240616	-2.641219	-0.116859
6	-3.363656	-2.118615	-0.078064
6	1.124888	0.483001	0.052485
16			
99.502677	Kcal/mol	4.314850	eV -101.225113 H Child_10_26.log
6	3.442989	1.838026	-0.018877
6	-4.119786	-1.824514	0.524344
6	3.885124	0.445558	0.105927
6	-3.969039	-0.577287	0.391249
6	4.826339	-0.445930	0.226679
12	-1.950515	-2.021794	-0.195138
8	5.657789	-1.280406	0.332563
6	-3.123895	0.484587	0.067349
6	2.477511	0.791539	-0.091776
6	-3.021352	1.846705	0.325089
6	1.216197	0.341617	-0.257319
8	-2.002706	0.021022	-0.536015
6	0.754841	-0.979745	-0.174426
6	-2.291587	2.877154	0.418293
12	-0.565111	1.480657	-0.358689
6	0.080467	-2.036259	-0.137610
16			
99.764443	Kcal/mol	4.326201	eV -101.224696 H Child_2_50.log
6	3.896339	4.351266	-1.681846
12	-8.204523	1.586931	-0.310128
8	3.695115	3.844829	-0.666241
6	-1.037162	-2.906238	-0.351320
6	1.951923	1.177772	0.747031
8	-0.442736	-4.048079	-0.483431
6	2.821613	-1.195443	0.357321
6	-1.446792	-1.761318	-0.153904
6	2.561985	0.114291	0.606520
6	-1.487985	-0.426700	0.044363
6	0.883821	2.041817	0.817164
12	1.416993	-3.824527	-0.147777

6	2.809922	-2.413163	0.094065
6	-1.232845	0.761061	0.278250
6	-0.015275	3.158880	1.073508
6	-0.466988	1.843964	0.617553
16			
100.486028 Kcal/mol 4.357492 eV -101.223546 H Child_11_32.log			
6	0.457350	-2.116773	-0.185870
6	2.113447	1.936167	-0.455380
6	1.786823	-2.119958	0.046791
6	3.424837	1.703276	-0.213176
6	-2.123419	-1.944080	-0.497749
6	4.576881	1.363710	0.122330
8	-3.592146	1.440803	1.255955
6	0.886867	1.871326	-0.544071
6	-0.764826	-2.002954	-0.373264
6	-0.449245	1.758075	-0.488198
6	-3.358177	-1.912495	-0.521147
6	-1.648006	1.539158	-0.365094
6	3.003420	-2.028681	0.283973
12	4.455990	-0.628170	0.555859
8	-2.894376	1.278114	-0.274662
12	-4.084617	-0.207828	0.385373
16			
100.886830 Kcal/mol 4.374873 eV -101.222907 H MutD_11_72.log			
6	0.812060	2.789183	1.059830
6	-2.664103	-0.988416	1.029263
6	-0.398872	1.123616	2.629271
6	-1.645447	0.700304	-1.880964
12	0.575482	2.586258	-0.970691
6	6.058034	-2.873184	-0.438442
6	0.300122	2.082262	1.962221
12	-4.745193	-2.927254	-0.844638
6	-2.439237	-0.213062	-1.277862
6	2.634727	1.455074	-1.166360
6	-1.200216	0.189443	2.663141
8	3.497171	0.738595	-0.981015
6	-2.860584	-0.921282	-0.329636
6	-2.098537	-0.631645	2.071005
6	-0.793159	1.591656	-2.126546
8	5.978804	-3.455060	0.557820
16			
101.020676 Kcal/mol 4.380677 eV -101.222694 H Child_4_30.log			
6	4.521114	-1.827340	0.048727
6	-2.511142	0.916718	-0.019611
6	4.701498	-0.556806	0.022884
6	-4.025932	0.421605	0.025804
12	2.414949	-1.624762	-0.006566
8	-5.061860	1.020674	0.075566
6	4.837392	0.794770	0.042565
6	-1.568385	1.805934	-0.029782
6	3.674658	1.503466	0.007229
6	-2.130662	-0.502890	-0.041895
6	0.454159	-0.993954	-0.057989
6	-3.476116	-1.033155	0.000721
6	2.526269	2.024839	0.006439

8	-4.006297	-2.135440	0.018646
6	-0.794153	-0.905782	-0.056103
12	0.526139	1.544238	-0.030737
16			
101.055898 Kcal/mol 4.382204 eV -101.222638 H Child_9_26.log			
6	3.165996	-2.228567	0.057640
12	-2.257464	1.634829	-0.063303
6	1.927486	-2.369119	0.048360
6	-0.399032	2.364675	-0.043837
12	4.449309	-0.703219	0.067941
6	0.843049	2.354826	-0.004946
6	0.581196	-2.459541	-0.042396
6	2.193968	2.171125	-0.003736
6	-0.639163	-2.251803	-0.079726
6	-3.656899	0.117348	-0.083407
8	4.512004	1.172143	0.015572
8	-5.059314	-0.039925	0.105490
6	-1.871761	-1.737029	-0.154574
6	3.351834	1.762751	0.004598
6	-2.905610	-1.035952	-0.110556
6	-6.245007	-0.061558	0.241888
16			
101.164310 Kcal/mol 4.386905 eV -101.222465 H Child_8_59.log			
8	-4.351090	-1.196115	0.243235
6	2.170651	1.756052	-1.442296
6	-3.710994	1.204511	0.525153
12	3.406206	-1.400373	0.351306
6	-4.210640	0.070826	0.434878
6	2.424040	1.386257	-0.164142
12	-2.396497	-1.443005	-0.201855
8	1.730495	-1.651499	-0.534186
6	-2.510742	1.823857	0.369764
6	3.349778	0.883188	0.756547
6	-1.300674	1.776245	0.099798
6	4.124199	0.168626	1.462541
6	-0.560655	-0.552809	-0.430951
6	0.880807	-0.678497	-0.629069
6	-0.322265	0.863254	-0.283831
6	1.141200	0.782064	-0.609358
16			
101.535409 Kcal/mol 4.402998 eV -101.221874 H Child_12_53.log			
6	3.560642	-1.786769	1.067628
6	-0.994394	2.862842	0.089518
12	4.037603	0.018625	0.247505
6	-1.721300	1.871563	0.278806
6	2.358590	-1.838654	0.711708
6	-2.428264	0.681064	0.388674
6	1.220255	-1.220194	0.039781
12	0.924936	2.708903	-0.475217
6	-0.044557	-1.515413	-0.222873
6	-3.554461	-0.221029	0.597358
6	2.299106	1.165662	-0.531699
8	-4.711165	-0.407108	0.940509
6	-1.344602	-1.520444	-0.659137
6	-2.286475	-0.647853	0.086957

6	1.667223	0.071194	-0.374573
8	-1.781465	-2.110662	-1.703054
16			
101.622325 Kcal/mol 4.406767 eV -101.221735 H MutD_14_68.log			
6	2.040324	-0.555410	0.044584
8	2.635962	2.782281	0.426953
6	-3.013994	0.229450	-0.098790
6	3.123769	-1.180732	-0.257265
6	4.273428	-1.789887	-0.529894
12	0.201272	-1.467263	0.405432
6	-2.818059	-1.076164	0.454827
6	-0.683280	1.434049	-0.484488
6	-4.247434	0.614217	-0.446315
12	1.343072	1.315266	-0.416338
6	-3.174116	-2.355458	0.991601
6	-1.787947	-1.925090	0.765591
6	-1.827099	0.999399	-0.351100
6	5.393971	-2.349722	-0.818906
8	-5.335713	0.886192	-0.778311
6	3.231418	3.368046	1.220444
16			
101.781684 Kcal/mol 4.413677 eV -101.221481 H Child_11_28.log			
6	-0.231700	2.130145	-0.535199
6	0.215810	-1.981535	-0.027573
6	-1.436067	2.378272	-0.648537
12	-1.774476	-1.870851	0.464731
6	-2.740467	2.067266	-0.491283
6	1.302908	-2.488560	-0.561289
6	1.018777	1.642745	-0.212920
8	2.215721	-3.029426	-1.114235
6	-3.622668	1.281238	-0.116644
6	-3.718356	-1.225623	0.536304
12	3.045315	2.108850	0.158146
6	2.518908	-0.056944	0.630817
6	-3.870953	-0.025153	0.203458
6	1.188570	0.337970	0.218096
6	3.730681	0.226715	0.802005
8	0.111439	-0.542473	0.331994
16			
102.138546 Kcal/mol 4.429152 eV -101.220912 H MutD_12_70.log			
6	1.486451	3.441313	0.113448
6	-4.444250	-2.414280	0.179393
6	2.014577	1.603221	1.662502
8	-5.228696	-3.231200	0.522663
6	0.146730	-0.060466	1.077291
6	-3.741891	0.690969	-1.713596
6	-2.423819	0.615006	-1.044772
8	9.521166	-2.278048	-0.307285
6	0.535112	3.475819	-0.713848
12	-0.694728	1.766720	-0.804243
6	-3.368234	-0.386302	-0.828329
6	8.867222	-2.744278	-1.129722
6	-3.482856	-1.557214	-0.063368
6	1.148526	0.562735	1.499082
6	2.097950	2.685385	1.056148

12	-1.584677	-1.049843	0.613543
16			
102.532923 Kcal/mol 4.446254 eV -101.220284 H MutD_15_64.log			
6	-1.062896	-0.996532	-0.220619
12	-0.774156	1.080387	-0.386490
8	-2.766244	1.847966	-0.506140
6	-4.555990	-1.909972	1.208713
6	2.143744	0.815574	3.925880
8	2.582512	1.392580	3.032488
6	-2.227943	-1.302578	0.217135
6	1.711381	1.874844	-1.368554
6	2.672639	0.915644	-1.485477
12	0.541519	-2.292985	-0.338170
6	2.969092	-1.549623	-1.032838
6	-3.430273	-1.594118	0.684176
6	-3.782322	2.319514	-0.794686
6	2.548452	-2.651985	-0.601298
6	0.624932	2.422391	-1.070952
6	3.099434	-0.238692	-1.380624
16			
102.570953 Kcal/mol 4.447903 eV -101.220223 H Child_7_34.log			
8	-5.939003	0.174449	-1.018281
12	3.565184	1.535212	-0.530141
6	-4.846851	0.245466	-0.539168
8	2.056554	1.683919	0.564437
12	-2.082800	-1.299145	-0.001549
6	4.227904	-0.130658	-1.473317
6	1.176319	0.727768	0.739811
6	-3.637307	0.174651	-0.082278
6	3.439115	-0.913775	-0.894492
6	2.400764	-2.459164	0.905168
6	-0.175956	0.571379	0.955606
6	1.287910	-0.789821	0.334029
6	-1.442411	1.165361	0.839933
6	-0.068759	-0.925030	0.479331
6	2.465961	-1.555382	-0.088483
6	-2.614859	0.939246	0.492363
16			
102.928572 Kcal/mol 4.463411 eV -101.219653 H MutD_11_74.log			
6	-2.299451	-1.196537	-0.191445
12	-2.815251	1.338189	-0.091540
6	2.761728	-0.764855	-0.088923
6	4.162854	-1.242376	0.101054
6	1.478765	-1.274013	-0.217977
6	4.775042	-2.420555	0.248495
6	-1.284226	2.632992	-0.019484
6	-3.560090	-0.630524	-0.052021
6	3.208884	0.543842	-0.018493
6	0.262320	-1.443295	-0.289774
8	-5.926751	-1.261005	0.356752
6	-1.087802	-1.417618	-0.278221
6	-0.035883	2.770514	0.028909
6	-4.777295	-1.032998	0.155072
8	4.620574	0.136460	0.155248
12	1.883613	2.149220	0.061612

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16
103.246159 Kcal/mol 4.477183 eV -101.219147 H Child_6_32.log
8   -6.499971  0.136047  -0.095999
6    5.969686  -1.590402  0.037808
6   -5.326070  -0.096437  -0.067576
6    4.793345  -1.098632  -0.014724
6   -4.078450  -0.337852  -0.027461
6    3.556394  -0.582003  -0.100615
6   -2.813490  -0.591046  -0.019020
6    2.695052  0.543753  -0.310708
6   -1.572051  -0.940559  0.026526
6    2.152812  -0.732619  -0.018816
8    0.957496  4.717633  0.464315
12   0.805808  1.373773  -0.420868
6    0.809710  3.643644  0.114568
6    0.862762  -1.298917  0.105298
12   -0.512324  -2.837101  0.336875
6   -0.246702  -0.463847  -0.048384
16
103.587025 Kcal/mol 4.491964 eV -101.218604 H Original3D_10_6.log
6    3.825587  2.245646  0.055362
6    3.551151  -0.213690  -0.510427
6    4.247149  0.953874  -0.315303
6    2.605731  -1.017096  -0.594478
6    1.195225  -1.049929  -0.295477
6   -0.631353  -2.927881  -0.494137
6    0.347171  -2.204139  -0.456010
8   -1.810214  -3.480352  -0.324036
8   -6.139232  2.510720  -0.590920
12   1.816221  1.864508  0.482512
6    0.640191  0.122736  0.253261
12   -2.417557  -1.868924  0.612908
6   -6.769507  3.472160  -0.560063
6    5.253745  2.006000  -0.148501
6   -1.786194  -0.099155  1.329773
6   -0.676962  0.013151  0.765099
16
103.707782 Kcal/mol 4.497201 eV -101.218412 H MutD_16_70.log
6    4.032929  -0.204333  0.109421
6    3.563713  1.249541  0.344859
6   -0.353284  -1.109969  -0.689790
6    1.297936  2.300284  -0.203803
6    3.220781  -1.220983  -0.280624
6    2.132085  -1.757630  -0.562777
12   -2.301135  -2.151302  0.637223
6    0.061470  2.148998  -0.383729
6    2.567514  2.012814  0.077792
6    4.762136  0.599927  0.951854
8   -4.843048  1.604932  -0.022186
8   -2.827146  -0.421808  0.624349
6   -0.441841  -2.483097  -0.263579
12   -1.553903  0.762659  -0.223109
6   -3.698677  1.574706  -0.146355
6    0.792237  -1.910471  -0.584382
16

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103.792568 Kcal/mol 4.500877 eV -101.218276 H Child_2_36.log

6	1.731576	-2.821749	-0.306564
6	-4.893800	0.479568	0.586516
6	0.617707	-2.308377	-0.057213
6	-3.695633	0.268305	0.111255
12	3.203016	-1.437576	-0.047023
6	-2.382866	0.116097	-0.056004
6	-0.335035	-1.291296	0.247654
6	2.617050	1.958368	-0.126311
6	0.271525	-0.187314	0.811699
12	-0.919842	1.667505	-0.009291
6	1.507305	0.210945	0.971445
8	0.409897	3.011551	-0.627627
6	-1.735456	-1.235999	-0.198335
6	1.604731	2.626304	-0.418427
8	-2.296521	-2.190543	-0.763222
6	2.642048	0.630614	0.401378

16

104.246767 Kcal/mol 4.520573 eV -101.217553 H MutI_9_77.log

6	-4.159944	0.671888	0.171202
6	8.847894	-0.413988	-0.188065
6	-3.716169	1.789718	-0.120811
12	-0.098787	-3.064930	-0.170139
6	1.823178	-0.594139	0.673018
6	-3.040989	-2.864012	-0.179701
6	-2.046286	-3.578981	-0.426130
6	-1.663207	3.202391	-0.413737
6	-3.914465	-1.848275	0.033407
6	2.222454	0.637936	1.024158
8	-0.418460	3.469957	-0.254756
8	7.832057	0.011345	-0.487430
6	-2.819880	2.753411	-0.387418
6	-4.268031	-0.669955	0.178044
6	1.400076	-1.788445	0.406298
12	0.824074	2.095287	0.279797

16

104.335274 Kcal/mol 4.524411 eV -101.217412 H Child_5_53.log

6	3.973142	1.478614	0.024404
8	-2.434152	-2.482490	-0.074520
12	1.791329	1.698531	-0.157733
12	-2.643862	-0.441894	0.112405
6	4.018615	0.218464	0.119151
6	-1.193720	-2.595256	-0.115749
8	-1.532009	2.566174	-0.030704
6	0.063283	-2.580054	-0.112401
6	-3.813897	1.315500	0.142018
6	-0.408099	1.780682	-0.065860
6	1.053823	-1.627512	-0.026123
6	-2.745566	1.964186	0.052892
6	3.464040	-1.013701	0.172006
6	0.715408	-0.178197	-0.092536
6	-0.579328	0.343883	0.006517
6	2.445578	-1.731462	0.126638

16

104.658712 Kcal/mol 4.538437 eV -101.216896 H MutD_10_76.log

6	-0.724895	-2.719369	-0.003709
6	-1.910633	-2.396760	-0.075562
8	-3.113151	3.293861	0.154933
12	2.351753	1.851668	-0.134849
6	0.625447	0.645900	0.014284
6	-2.886939	-1.430282	-0.105381
6	-4.192122	-0.769228	-0.139938
6	-2.930455	-0.072208	-0.071637
6	-2.560709	2.262230	0.093203
6	3.785832	-0.876164	0.096763
8	0.537680	-2.884357	0.071052
6	-0.607652	0.839450	0.020207
6	-2.021309	1.035719	0.014171
6	4.152780	0.370203	-0.012470
12	1.730090	-1.397868	0.123454
6	4.540932	1.656905	-0.108454
16			
104.692617 Kcal/mol 4.539907 eV -101.216842 H MutI_18_35.log			
6	1.814014	1.436404	-0.810605
6	2.156262	-1.134203	1.083786
12	4.468151	0.765475	0.789710
6	3.262839	-0.716797	1.474795
6	4.235599	2.330886	-0.536118
6	0.982340	-1.520064	0.464600
6	-0.822481	-1.243891	-1.068888
6	-5.977570	0.947661	1.606105
6	3.003760	2.096635	-0.666984
6	-4.037779	0.311053	-1.238829
6	0.962382	0.546936	-0.825120
6	0.402796	-0.723543	-0.541316
8	-3.346945	1.092239	-1.714748
8	-5.721552	2.061595	1.790026
12	-0.550349	-2.976881	0.316581
6	-1.726436	-2.113377	-1.254380
16			
104.970539 Kcal/mol 4.551959 eV -101.216399 H MutI_15_57.log			
6	-6.023259	0.950453	-0.366854
6	5.355248	1.532512	-0.143767
6	0.934923	-2.093974	-0.007184
12	1.067210	0.290673	0.406301
6	-1.493060	-1.058751	0.141581
8	6.275837	2.267775	-0.365007
6	-7.271502	0.683851	-0.588312
6	-1.173993	0.397238	0.391901
6	-4.771278	1.099436	-0.067928
6	3.320577	-0.056431	0.064976
6	-3.536612	1.288294	0.232163
6	-0.269342	-1.798993	0.034744
6	4.323225	0.770738	0.047552
8	-2.625923	-1.516793	0.033687
12	2.949592	-2.189634	-0.276591
6	-2.295083	1.082238	0.443469
16			
105.095360 Kcal/mol 4.557372 eV -101.216200 H Child_5_9.log			
6	-3.667853	-0.580900	-0.428018

12	3.133711	1.437266	-1.491428
6	-2.677470	-1.408089	-0.187700
8	2.458801	-0.211189	-0.775950
6	-4.367109	0.483540	-0.427276
12	2.502195	3.296569	0.548551
6	-1.633754	-2.059259	0.069507
8	1.539239	-4.091536	0.258689
6	-4.951597	1.649565	-0.279067
6	1.379586	0.755348	1.027973
6	-5.174870	2.846080	0.163837
6	1.609218	-0.382434	0.212262
6	0.929227	-3.029057	0.224228
6	1.324927	1.889837	1.549288
6	-0.322982	-2.287408	0.300392
6	0.950146	-1.607928	0.350012
16			
105.322078	Kcal/mol	4.567203	eV -101.215839 H Child_6_59.log
6	-2.829764	-1.057520	-0.541077
12	3.180691	-1.167344	-0.495722
6	-2.812125	0.172221	-0.315550
8	3.645421	2.973895	0.682936
6	-2.390453	1.511915	-0.055118
6	2.691479	0.800885	-0.060228
12	-0.887155	-1.784663	-0.523262
6	3.134385	1.957739	0.324682
6	-3.196802	2.580125	0.162011
6	1.086627	-1.106448	-0.518565
8	-0.859966	-3.618882	0.648418
6	1.339278	0.247425	-0.241695
6	-0.657519	-4.574994	1.271763
6	-3.871053	3.650732	0.397765
6	0.171502	1.061316	-0.115483
6	-0.966568	1.520601	-0.045675
16			
105.507796	Kcal/mol	4.575257	eV -101.215543 H MutI_6_71.log
6	-3.267574	-0.375694	0.131857
6	1.062217	-2.761870	0.228950
6	2.976746	1.844507	-0.051896
6	-1.882422	-0.082041	0.307017
8	0.362156	4.493217	-0.062706
6	-0.959933	-1.177946	0.426536
12	-6.577132	-0.480797	-0.403063
6	-0.046847	-1.993147	0.388777
12	3.861503	-2.442409	-0.271100
6	2.212122	2.840850	0.071152
6	2.100599	-3.380738	-0.069685
6	3.693308	0.736606	-0.152616
6	4.191292	-0.418676	-0.191978
6	1.264383	3.714284	-0.040883
8	-1.434445	1.091651	0.320640
6	-4.482914	-0.546213	-0.042818
16			
105.712767	Kcal/mol	4.584145	eV -101.215216 H Child_12_17.log
8	5.640237	-0.181765	0.309839
6	-3.541647	0.368719	-0.155198

6	5.618216	-1.644100	0.156567
6	-2.283865	0.586572	-0.202857
6	4.560183	0.573344	0.229602
6	-4.808808	0.126329	-0.085175
6	4.290820	-1.994419	-0.068692
6	-1.003090	0.774180	-0.208202
6	3.468231	1.162479	0.133762
6	-6.056027	-0.155189	0.017633
6	3.070670	-2.259967	-0.265765
6	0.281176	0.934227	-0.189744
12	1.769445	2.393090	0.027949
6	-7.239364	-0.614933	0.157486
12	1.867681	-0.523877	-0.192707
8	-8.363299	-1.014987	0.297736
16			
105.957196 Kcal/mol 4.594745 eV -101.214827 H Child_16_24.log			
8	1.144304	-3.408212	-0.379025
12	-2.692796	-0.303854	0.445848
6	1.342176	-2.264022	-0.175384
8	-4.578630	0.615164	0.082001
6	2.845605	-0.497506	0.471756
6	-5.388595	1.238742	-0.464847
6	-1.370045	0.260839	1.948201
6	3.908878	0.111323	0.728014
6	-1.813246	-0.815565	-1.387310
6	1.569207	-0.983886	0.086732
6	-0.398008	0.236871	1.168014
12	3.466714	1.883820	-0.162095
6	-0.686686	-0.453658	-0.993138
6	0.400099	0.056269	-0.094602
6	1.619826	2.351252	-0.896029
6	1.002053	1.323474	-0.562883
16			
106.475609 Kcal/mol 4.617225 eV -101.214001 H MutI_2_79.log			
6	-3.499015	2.569930	0.226087
6	5.658830	-1.728704	0.492111
12	-4.504631	0.793711	0.031754
6	2.011506	-0.426864	0.441115
6	-0.071270	0.949770	0.382319
6	-2.269023	-2.683016	-0.946054
6	-1.041841	1.721317	0.331268
6	4.436900	-1.301129	0.425032
12	-0.916055	-1.643014	0.170304
6	0.706342	-0.205914	0.411730
8	5.406636	1.409424	-0.911199
6	5.202538	2.508976	-0.692896
6	3.202594	-0.886314	0.413853
8	-4.031407	-0.938363	-0.276420
6	-2.288480	2.293908	0.266074
6	-3.041347	-1.741435	-0.571263
16			
106.480760 Kcal/mol 4.617449 eV -101.213993 H Child_7_21.log			
6	2.120675	0.428374	-1.268477
6	-2.989421	1.784349	0.497023
6	1.067690	-0.234970	-1.365848

6	-1.971323	2.496348	0.579260
6	-0.185978	-0.782634	-1.352111
12	-2.950091	-0.066568	-0.321432
6	-1.390033	-1.052205	-1.204206
6	-4.036621	-2.016396	0.389265
12	1.986704	2.255111	-0.385202
8	-4.309823	-3.094772	0.647045
6	-0.718743	3.063266	0.543966
6	3.308566	-1.317940	1.407978
8	3.959834	-2.449813	-0.692536
6	0.475224	3.356082	0.384818
6	3.082722	-0.818946	2.575931
6	3.630670	-1.889636	0.286322
16			
106.612992 Kcal/mol 4.623183 eV -101.213782 H Child_2_9.log			
6	-4.787258	-1.885612	-0.812320
6	3.127801	0.437253	-0.052586
6	-3.994860	-0.927993	-0.470483
6	2.407069	1.634294	-0.012800
6	-3.069132	-0.035651	-0.207221
6	4.006105	-0.683506	-0.243028
12	-2.011582	3.020805	0.114563
6	2.616901	-0.868995	0.109657
6	-2.177736	0.844301	0.062515
6	1.283694	2.154203	-0.011509
6	-0.752289	0.947989	0.182597
12	0.539122	-0.764681	0.341948
8	5.110683	-1.117709	-0.575393
6	-0.103036	2.179774	0.110289
6	-1.537760	-3.360376	0.471036
8	-0.666617	-2.593236	0.546017
16			
106.884340 Kcal/mol 4.634950 eV -101.213349 H Child_5_35.log			
6	1.521094	-2.730039	0.961706
6	-2.175847	2.270590	1.284201
6	0.266118	-2.603366	0.820911
8	4.071422	0.836205	0.440798
6	-1.038191	-2.276960	0.560941
6	2.939083	1.178528	0.248023
6	-2.112827	-1.825154	0.177226
6	1.681322	1.416575	-0.029080
12	1.766023	-1.515645	-0.682977
6	-2.584051	1.309897	0.581720
8	-3.056050	-1.009895	-0.302277
6	-1.389258	0.464075	-1.235804
12	-0.257196	2.296352	0.358254
6	-2.447049	0.323342	-0.426269
6	1.104743	0.465019	-0.993873
6	-0.136618	0.677664	-1.484952
16			
107.055464 Kcal/mol 4.642370 eV -101.213077 H Child_15_12.log			
12	-3.104947	1.267961	0.347932
6	3.109316	-1.542292	-0.379461
6	-3.596876	-0.853893	0.532763
6	4.201348	-1.954607	0.141585

8	-1.428341	2.209386	0.137146
8	5.280338	-2.203914	0.602361
6	-2.304404	-0.809958	0.790720
6	2.089690	-0.804062	-0.535805
6	-0.349837	1.490729	-0.067586
6	1.180087	0.123783	-0.355534
6	-0.994154	-0.804819	0.772782
6	2.040425	2.533785	-0.504535
6	-0.198441	0.082726	0.130455
6	3.023749	3.289171	-0.134855
6	1.072627	1.608566	-0.434061
12	-4.099816	-2.451174	-0.819172
16			
107.075709 Kcal/mol 4.643248 eV -101.213044 H Child_1_53.log			
12	-2.837396	1.080292	0.382014
6	2.710019	3.380400	-0.772405
8	-2.498172	0.378557	-1.414938
12	1.730427	-1.737167	0.743203
6	-1.373021	-0.304679	-1.151033
6	2.331932	2.398775	-0.030388
6	-0.273691	-0.603035	-1.814770
6	1.753007	1.451646	0.644506
8	-1.118600	1.528297	1.216469
6	1.941182	-1.756632	-1.382219
6	-1.012572	-0.668389	0.286318
6	1.054825	0.450705	1.131734
6	0.910315	-1.193047	-1.878328
6	-0.361674	0.473514	0.980188
6	-0.566193	-1.918577	0.709313
6	-0.077828	-2.939404	1.291274
16			
107.440229 Kcal/mol 4.659055 eV -101.212464 H Child_14_23.log			
6	0.347935	1.645558	-1.107782
8	6.850416	-0.949328	-0.177311
6	1.176839	0.861424	-0.607620
6	5.666609	-0.795193	-0.093755
12	-1.587963	2.154253	-0.784586
6	4.411468	-0.625708	-0.007951
6	1.888970	-0.112627	0.120090
6	3.162878	-0.385924	0.067876
8	-4.811036	-2.820048	-0.185208
6	-2.002728	1.021089	1.213010
6	-2.834985	0.311642	-0.984119
6	-1.471672	2.010012	1.824690
6	-4.181852	-1.820053	-0.265847
6	-2.151452	-0.054020	0.247962
6	-3.401578	-0.779809	-0.312193
12	-0.076839	-0.279530	0.979084
16			
107.529685 Kcal/mol 4.662934 eV -101.212321 H Child_6_13.log			
12	-1.411233	-2.602358	0.270452
6	-7.015493	1.241349	-0.331717
6	-1.916700	-1.076024	-0.899463
6	2.263922	3.215578	0.735993
8	2.764071	0.065973	-1.256270

8	-6.603187	1.572615	0.686937
6	0.631556	-2.448023	0.636111
6	2.183335	2.035464	1.164290
6	1.575698	-0.532978	-1.139852
6	2.026101	0.795111	1.702541
6	0.393553	0.157127	-1.279031
6	1.783619	-0.395015	1.872267
6	1.503804	-1.526868	1.140653
6	-0.843092	-0.431016	-1.081814
12	1.926276	1.825555	-1.036455
6	1.502433	-1.665881	-0.228863

16

107.683095 Kcal/mol 4.669587 eV -101.212077 H Child_2_52.log

8	-4.776454	-0.351628	-0.929475
6	2.509884	0.148884	-0.483116
6	-3.765104	-0.240288	-0.417815
6	1.688620	0.265979	0.725941
8	-1.087550	-1.902200	0.242012
6	3.006863	-1.062493	-0.987287
6	-0.022353	2.289961	-0.727433
12	0.452339	1.560565	1.682169
12	-1.598371	-0.026984	0.405305
6	-1.043699	2.042964	-0.005339
6	1.229457	2.168676	-1.253220
6	0.220544	-1.791447	0.469244
6	0.631435	-0.562218	1.131637
6	2.198474	1.375351	-1.166714
6	2.256574	-2.032936	-0.467050
6	1.200040	-2.664491	-0.077178

16

107.706278 Kcal/mol 4.670592 eV -101.212040 H Child_4_49.log

8	-5.337250	0.886553	-1.047868
6	5.171556	2.937583	-0.040852
6	-4.470396	0.230316	-0.715048
6	4.477791	1.858836	-0.151441
12	-2.592801	-0.631213	0.264963
6	3.721403	0.801074	-0.118844
6	-2.019325	1.423534	0.771030
6	2.830600	-0.129835	-0.156975
6	-1.033928	-1.937409	0.007545
12	0.779463	0.598096	-0.351552
6	0.168947	-2.257424	-0.023663
6	2.623053	-1.508542	-0.024129
6	-1.020886	1.404632	0.005432
6	2.864696	-2.959931	0.143037
6	1.550409	-2.348077	0.014012
8	-3.090684	1.027055	1.395174

16

107.724493 Kcal/mol 4.671382 eV -101.212011 H Original2D_2_1.log

6	0.423922	1.020202	0.000000
6	1.727550	1.191163	0.000000
12	-1.303109	2.421545	0.000000
6	-2.430734	0.105514	-0.000000
6	-0.000000	-0.361381	-0.000000
6	-3.305192	1.005835	-0.000000

8	-0.038458	-2.600219	-0.000000
6	0.809237	-1.545962	-0.000000
6	3.142158	-0.707950	0.000000
12	-3.968108	3.024408	-0.000000
6	-1.357246	-0.808116	-0.000000
6	2.231631	-1.856893	0.000000
8	2.697678	-3.013062	0.000000
6	-1.458935	-2.235485	-0.000000
6	2.933349	0.708310	0.000000
6	4.281065	0.077230	0.000000
16			
107.792696 Kcal/mol 4.674340 eV -101.211902 H Child_9_39.log			
12	-2.274513	-1.725740	0.635364
8	-0.501920	2.827905	-0.403024
8	3.005629	-3.243482	-0.744657
6	0.723133	2.689615	-0.083611
6	-4.482285	-1.623784	0.502511
12	-1.691521	1.341194	-0.546419
6	2.551838	-2.194445	-0.506410
6	-0.601872	-0.632843	-0.034631
6	1.876526	2.385780	0.233958
6	0.630994	-0.823070	-0.121664
6	-4.106123	-0.384976	0.115481
6	2.039392	-0.997302	-0.161627
6	-3.722507	0.748836	-0.397458
6	2.902052	0.060477	0.297754
6	2.818896	1.417400	0.470891
6	3.963742	0.677508	1.037159
16			
107.856322 Kcal/mol 4.677099 eV -101.211800 H MutI_11_67.log			
6	3.631748	0.878283	0.013210
6	-2.091200	-1.373270	-0.423579
6	-0.337643	-2.463290	0.074931
6	-2.930478	1.774655	0.510487
6	3.772907	-0.348583	0.179103
12	-0.163297	2.265476	-0.078540
12	-3.592856	-0.019309	0.047445
6	-2.027000	2.627463	0.688054
6	1.898475	2.686287	-0.238997
6	2.156881	-2.279849	0.312923
6	0.892589	-2.672930	0.235837
8	-0.316147	0.376003	-0.693014
8	-1.660527	-2.721581	0.029733
6	3.142704	-1.521766	0.261983
6	-0.918593	-0.706992	-0.545443
6	2.957482	2.035096	-0.121945
16			
108.009914 Kcal/mol 4.683759 eV -101.211556 H Child_13_15.log			
6	-1.504649	2.072499	0.744790
6	1.303835	-1.570914	-0.257387
6	-0.593984	2.098305	-0.096833
6	2.418534	-1.321228	0.442235
8	-2.546425	1.648860	1.408299
12	1.892486	-0.279762	-1.827369
6	0.475170	1.979018	-0.935616

6	-0.017874	-1.791768	0.120914
12	-2.291301	0.003329	0.329618
6	3.556474	-0.846020	0.760913
6	1.408989	1.664319	-1.703164
6	-1.264462	-1.734796	0.252028
6	5.754007	0.460334	1.196093
8	-5.560402	-1.304679	-0.209380
6	4.722359	-0.298994	1.026543
6	-4.651668	-0.616798	-0.153571
16			
108.204716 Kcal/mol 4.692207 eV -101.211245 H Child_2_17.log			
6	-0.374804	2.274869	0.000202
8	5.177113	-0.454569	-0.007710
12	-1.321456	0.809920	1.408517
6	4.088633	0.014350	0.011065
6	0.733978	1.676016	-0.001964
6	-3.323330	0.325155	-0.701635
6	-0.369767	-0.780635	-0.014524
6	-3.328761	-0.909505	0.010010
6	-3.311256	0.324603	0.721486
6	-2.573744	-2.066181	0.001722
6	1.694487	0.616979	0.004600
6	3.028596	0.781626	0.015172
6	1.057832	-0.788912	-0.007342
12	-1.341809	0.829608	-1.412817
6	-1.332043	-1.764533	-0.006535
8	1.825417	-1.782597	-0.010032
16			
108.379813 Kcal/mol 4.699799 eV -101.210966 H Child_11_27.log			
8	-4.239090	1.187202	-0.014012
6	2.890636	-2.019355	-0.008085
12	-0.993309	1.985268	0.024062
6	3.889362	-1.302640	-0.015077
6	-2.781309	0.905316	0.023249
6	1.592265	-2.390359	0.006212
6	0.996170	2.440790	-0.002921
8	4.796587	-0.378340	-0.021600
6	-4.444855	-0.247925	-0.021871
6	0.359150	-2.434503	0.021326
6	-5.549958	-0.989751	-0.071402
6	-0.934991	-2.055684	0.033638
6	-2.969516	-0.462236	0.020680
6	-2.024210	-1.478775	0.032938
6	2.236831	2.303359	0.010269
12	3.991857	1.341373	-0.014798
16			
108.679216 Kcal/mol 4.712783 eV -101.210489 H Child_2_38.log			
8	-1.213286	-2.457298	1.484001
8	0.200294	3.921449	1.715388
6	-3.279369	-2.268904	-0.022071
6	-0.268869	3.394106	0.816472
6	-1.143692	-1.559714	0.603031
12	3.620732	-0.820193	-0.410440
6	-2.437236	-1.220307	-0.082127
6	2.859667	1.077259	-0.834197

6	0.166019	-1.011646	0.183619
6	1.679381	0.702910	-0.575433
6	-2.803347	1.010319	-1.484830
6	2.460723	-2.340374	0.244116
6	1.313607	-1.856193	0.296135
6	-2.716931	-0.053333	-0.833310
6	0.374955	0.294559	-0.269775
12	-1.047857	1.759751	-0.743302
16			
108.703346 Kcal/mol 4.713829 eV -101.210451 H MutI_17_37.log			
6	2.619299	1.089283	-0.062590
6	-4.003512	-1.008685	0.006996
12	-0.002554	-0.331259	0.017740
6	2.880031	-0.306052	0.021752
6	-4.851475	-1.997481	-0.022521
12	-2.587359	1.984870	0.019939
8	-1.794082	0.049206	0.017752
6	5.281298	-1.350194	-0.018652
6	-3.213668	0.017599	0.069274
6	-5.620388	-3.036731	-0.097289
6	4.099610	-0.849038	-0.006636
6	-0.686725	2.798842	0.000098
6	6.469508	-1.898701	-0.021231
8	1.722406	-1.036462	0.108488
6	1.764193	1.979134	-0.068277
6	0.537224	2.571143	-0.044599
16			
108.745095 Kcal/mol 4.715640 eV -101.210384 H MutD_16_58.log			
6	-1.532844	4.151118	-0.029347
8	-3.078994	0.952264	0.129103
6	1.918769	0.829668	-0.062345
6	-1.712767	2.880249	0.022866
12	-1.981041	-2.794528	-0.275013
6	-1.761030	1.536466	0.104382
6	-0.578543	-0.722611	0.199513
6	-3.268356	-0.321637	-0.152022
6	4.365057	0.259442	-0.242048
6	0.711677	1.082768	0.041891
12	1.877637	-1.550030	0.525519
8	5.542879	0.302072	-0.407950
6	-0.167866	-1.938123	0.292841
6	3.104345	0.091993	0.014575
6	-3.505878	-1.509759	-0.427583
6	-0.650936	0.677093	0.108059
16			
108.811105 Kcal/mol 4.718502 eV -101.210279 H MutD_15_70.log			
6	-2.484119	1.071054	0.850287
6	4.073382	0.895157	-0.637699
6	0.502509	-2.356280	0.365421
6	4.151436	-1.471032	-0.015189
6	2.150925	2.514678	-0.284095
6	1.850409	-2.440085	0.341882
6	3.062584	-2.254068	0.231810
6	4.554442	-0.357546	-0.395430
8	-4.406472	0.529848	-0.715328

6	-3.346740	0.895479	-0.033158
6	3.294592	1.853275	-0.591745
12	-2.589699	-1.389235	0.133189
6	1.024228	2.854560	0.122362
8	-4.187205	-0.979496	-0.955335
6	-0.720402	-2.131318	0.346735
12	-0.737806	2.152064	0.829996
16			
109.093404 Kcal/mol 4.730744 eV -101.209829 H Child_12_44.log			
8	5.994252	-1.756303	0.632997
6	-6.969524	-0.459696	0.624207
6	5.061137	-1.062032	0.367634
6	-5.685572	-0.485366	0.431483
6	4.036924	-0.337652	0.111208
6	-4.404415	-0.528149	0.198330
6	2.979584	0.343958	-0.096859
6	-3.139224	-0.612396	-0.065968
6	1.811291	0.999752	-0.222985
6	-1.998696	-1.459848	-0.496133
6	0.586836	0.219843	-0.276502
6	-1.780370	-0.135622	-0.220688
12	0.018008	-1.788264	-0.554167
6	-0.674638	0.777445	-0.101297
12	-0.088054	2.748133	0.135836
8	1.743317	2.371324	-0.194823
16			
109.472148 Kcal/mol 4.747168 eV -101.209225 H MutD_13_36.log			
6	2.510855	0.138330	-0.087395
6	-2.494868	0.772671	0.880977
8	-0.542386	-2.216335	-2.172922
6	-0.532643	-1.383698	-1.203800
12	5.175958	-1.222054	1.099327
6	0.384486	-0.368557	-1.031513
6	-2.335144	-0.582792	0.614289
12	-1.228067	3.370098	0.211853
6	1.274788	0.558169	-0.693645
6	0.957342	1.958674	-0.777917
8	-3.250914	-2.969439	1.055021
6	0.533529	3.127916	-0.740685
6	-2.515689	2.009736	0.991604
6	-2.612462	-2.015308	0.630918
6	3.576826	-0.177746	0.458805
6	-1.585068	-1.419117	-0.173464
16			
109.597896 Kcal/mol 4.752621 eV -101.209025 H Child_17_26.log			
6	-2.628939	-2.105587	-0.108479
12	3.178402	2.622526	-0.149887
6	-3.456740	-1.132036	-0.239752
12	0.123048	1.888964	0.313232
6	-1.566657	-2.730489	0.249379
6	2.907678	0.514500	-0.164110
6	-3.720866	0.137532	-0.443232
6	1.878195	-0.296597	0.004298
6	-0.253406	-2.800964	0.299589
6	-1.622401	3.028432	0.336346

6	-3.517919	1.364929	-0.209049
8	3.173606	-2.322573	-0.425421
6	2.109159	-1.798267	-0.003608
6	-2.640165	2.382035	-0.062976
8	0.546849	0.023749	0.097335
6	0.948554	-2.521369	0.452350
16			
109.743291	Kcal/mol	4.758926	eV -101.208793 H Child_5_12.log
8	-5.372684	-0.083947	-1.359469
6	5.152506	-0.934261	-1.499479
6	-4.344323	-0.274514	-0.789437
6	3.932050	-0.985748	-1.145607
6	-3.264262	-0.607436	-0.143116
12	4.915082	0.471625	0.251424
6	-1.179301	2.506597	0.162152
6	2.875156	-0.670522	-0.284550
8	-0.732872	3.613905	0.329404
6	1.625660	-0.439830	0.420225
6	-2.018361	0.075427	0.106034
6	0.347345	-0.655354	0.587896
12	-2.504196	-2.199308	0.998294
6	-1.778097	1.398742	-0.023927
6	2.904816	0.166313	0.814038
6	-0.934222	-0.830658	0.669755
16			
109.816099	Kcal/mol	4.762083	eV -101.208677 H Child_3_42.log
12	-8.084521	0.920857	-0.013069
6	3.160908	0.943964	-0.016840
6	-1.402304	-2.311999	0.041185
6	3.011793	-0.406426	0.070951
6	-1.682566	-1.009748	0.148799
6	3.032914	2.159520	0.075419
6	-0.643731	-3.288517	-0.092452
6	2.864055	-1.634261	0.102015
6	-1.607909	0.228938	0.128291
8	2.977633	3.487875	0.029547
8	0.304544	-4.142305	-0.161032
6	1.701149	4.063766	-0.168368
6	-1.072187	1.431492	0.093288
6	0.645942	3.287891	-0.139177
6	-0.351740	2.449057	-0.030080
12	2.068241	-3.441408	-0.005790
16			
109.855836	Kcal/mol	4.763806	eV -101.208614 H MutD_17_44.log
6	0.816350	-0.777669	-0.501489
6	4.604450	-0.497980	-0.917141
6	-3.904242	0.222993	0.079619
6	-4.094840	2.706542	-0.598359
8	-3.678356	-2.060506	0.500208
12	-5.536080	-1.285033	0.805837
8	5.947111	1.160416	1.506232
12	6.707305	-0.460180	-0.871010
6	-3.921402	1.454664	-0.281657
6	5.349184	1.600927	2.387030
6	-1.727097	-0.903294	-0.155072

6	2.031648	-0.680750	-0.670683
6	3.369547	-0.583912	-0.815782
6	-0.509834	-0.856724	-0.311344
6	-3.098423	-0.940167	0.140042
6	-4.282798	3.945918	-0.900072
16			
109.987092 Kcal/mol 4.769498 eV -101.208405 H Child_10_58.log			
6	-1.037029	-1.354646	0.377789
6	8.663949	1.684736	-0.640804
6	-2.091726	-1.644273	-0.351877
6	7.536092	1.096576	-0.427372
12	0.999705	-1.603520	0.403350
6	6.370968	0.530334	-0.193179
6	-3.193849	-1.705687	-1.045976
6	5.253304	-0.002668	0.019354
6	-4.215094	-0.850074	-1.136172
8	-5.375605	2.416542	-0.285497
6	2.897157	-0.989350	0.433101
6	4.044902	-0.518992	0.237525
8	-3.746976	1.184073	0.765885
6	-4.733439	1.382053	-0.138046
6	-4.936785	0.160829	-0.966897
12	-2.197209	0.308690	1.192669
16			
110.262529 Kcal/mol 4.781442 eV -101.207966 H Child_8_56.log			
6	5.064939	1.529405	-0.210239
8	-5.427047	2.054140	0.863778
6	4.262277	0.401769	0.223006
12	-0.770696	0.673162	-0.494623
8	3.974434	-0.782531	0.723299
6	-4.638212	1.225878	0.518735
12	2.247288	-1.508618	0.667998
6	1.012309	1.653317	-0.701687
6	-3.898078	0.227431	0.174904
6	-0.949210	-1.922330	-0.002384
6	2.252244	1.688727	-0.590473
6	0.258209	-1.831671	0.277169
6	-2.709137	-0.237674	-0.190471
6	-2.302923	-1.693283	-0.396478
6	3.590908	1.437255	-0.341899
6	-2.959694	-2.503392	-1.223034
16			
110.294851 Kcal/mol 4.782843 eV -101.207914 H Child_7_50.log			
8	5.653431	1.343394	0.289438
8	-6.795409	0.866269	0.705712
6	3.184340	0.989444	-0.325745
6	-5.694160	0.479210	0.406358
6	4.502943	0.978971	0.127280
6	3.865200	-1.564647	1.089646
6	1.830588	1.078692	-0.455251
6	-4.522071	0.106586	0.073499
12	-1.424679	0.965842	-0.271794
6	2.691203	-1.413752	0.448289
6	3.564271	-0.206356	0.227109
6	-3.240568	-0.118979	-0.160580

6	-2.432901	-1.296578	-0.351435
6	0.604563	0.882626	-0.572785
6	-1.350439	-1.939511	-0.495236
12	0.684513	-1.426804	-0.397214
16			
110.413956 Kcal/mol 4.788008 eV -101.207725 H MutD_16_50.log			
6	5.751658	-0.211897	-0.069140
6	-2.520272	0.032224	-0.309741
6	1.070322	-0.609845	-0.138204
6	-0.222934	1.373910	0.036757
6	-0.638388	2.698289	0.184101
6	1.112286	0.815206	0.004780
6	2.337741	1.420831	0.079776
12	-1.408270	-1.797259	-0.362480
6	-1.305679	-4.007194	0.162679
6	4.790923	0.640178	0.030396
12	-3.436614	2.005476	0.052128
8	-1.818972	3.184147	0.258005
6	-1.330208	0.509081	-0.147792
8	-0.855039	-5.001307	0.482504
6	0.639745	-1.778061	-0.272034
6	3.569922	1.123724	0.071781
16			
110.718761 Kcal/mol 4.801226 eV -101.207239 H MutI_4_65.log			
6	-3.176330	1.578653	0.067865
12	-0.201566	2.284597	0.052387
6	0.965588	-3.685884	0.082531
6	3.103810	0.595467	-0.000981
6	-3.138710	-1.055940	-0.153870
8	1.603387	2.479380	-0.005524
6	3.946503	2.817780	-0.253756
8	-1.960642	2.112022	0.095811
6	-0.272100	-3.542143	-0.040138
6	-2.461740	-2.212371	-0.183216
6	-4.499156	1.513249	0.164827
12	2.677048	-2.600006	0.133843
6	3.200005	-0.639268	0.097757
6	-1.504772	-3.002998	-0.129811
6	-3.512274	0.137864	-0.064155
6	2.874550	2.004538	-0.079895
16			
110.738381 Kcal/mol 4.802077 eV -101.207208 H Child_9_61.log			
8	4.828534	-2.068378	-0.022218
12	-1.763017	1.521982	-0.017682
6	4.013647	-1.185423	-0.010738
8	0.038020	1.748331	-0.017536
6	3.240394	-0.150691	0.009844
6	-3.703844	0.747311	-0.011519
6	-0.234051	-1.584582	0.010055
6	0.819401	-0.944088	-0.004342
6	-4.324427	-0.066791	-1.084867
6	-1.548939	-1.912716	0.018005
6	-4.326937	-0.049830	1.083868
6	-2.780110	-1.822466	0.018773
6	1.317390	1.407399	-0.005298

6	1.784716	0.078104	-0.004987
6	-3.886001	-0.959897	0.011290
12	3.333028	1.913218	0.029142
16			
110.882516 Kcal/mol 4.808327 eV -101.206978 H Child_17_8.log			
8	5.094653	2.213963	0.080721
6	-1.862683	-1.614130	0.103652
6	-8.619298	1.965006	-0.180740
6	-3.044734	-1.189848	0.144988
6	3.841088	2.605899	0.074387
6	-0.610383	-2.001417	0.048771
12	5.424327	0.260913	-0.040978
6	-4.235422	-0.672449	0.127962
6	-7.551029	1.234068	-0.104454
6	0.607899	-2.321142	-0.011790
6	2.771705	1.763338	0.083625
6	-5.360208	-0.114499	0.089554
6	-6.471730	0.544067	-0.006004
12	2.560396	-1.450768	-0.087711
6	1.918257	0.840121	-0.041547
8	4.390666	-1.208440	-0.133991
16			
110.989126 Kcal/mol 4.812950 eV -101.206808 H MutD_18_40.log			
6	-2.612457	-0.392350	-0.063582
6	-2.106376	0.923784	0.116028
6	2.257152	-1.205714	-0.204903
6	-0.276235	2.717714	0.315606
12	0.181457	-1.349980	-0.412643
6	0.837625	3.272112	0.173138
6	-5.177709	-0.800617	0.255352
6	4.773941	-1.335158	0.488125
6	6.009470	-1.337386	0.876932
6	3.514117	-1.268791	0.125657
6	-3.920236	-0.634445	0.074035
6	-1.332679	1.860139	0.337012
8	-1.679049	-1.347831	-0.342035
8	1.614335	0.023475	-0.655881
12	2.103376	1.811512	-0.402109
6	-6.449991	-0.956543	0.466659
16			
111.574873 Kcal/mol 4.838351 eV -101.205875 H MutI_1_65.log			
6	3.602250	2.918037	0.000000
8	4.578480	3.555841	0.000000
6	1.174577	-1.415784	0.000000
6	1.222806	2.939152	0.000000
8	-3.494243	0.751663	0.000000
6	-3.617301	-0.580125	0.000000
12	-1.958387	1.871283	0.000000
6	0.507838	4.186211	0.000000
6	2.455789	2.204270	0.000000
12	-1.702916	-9.042718	0.000000
6	-1.330329	-1.866444	0.000000
6	2.475057	0.792920	0.000000
6	0.000000	-1.837267	0.000000
6	1.968088	-0.332485	0.000000

6	-0.142948	2.870165	0.000000
6	-2.438870	-1.279118	0.000000
16			
111.675208 Kcal/mol 4.842701 eV -101.205715 H Child_10_34.log			
8	3.334431	2.946183	0.280744
6	-2.071888	2.417135	-0.348200
6	3.869138	-0.631000	0.386212
6	-2.209234	-0.932453	-0.376431
6	3.226415	1.792394	0.290008
6	-3.233944	0.020598	-0.075238
6	3.315840	-1.861134	0.250926
6	-2.755687	1.363767	-0.223027
6	2.862521	0.435045	0.231099
6	-4.425060	-0.296179	0.428332
6	2.782631	-3.012493	0.023520
6	-1.099231	-1.440149	-0.630573
6	1.513140	0.365120	-0.034960
8	-5.468328	-0.607033	0.863291
12	-0.364362	1.196887	-0.475947
12	0.899639	-1.866647	-0.247577
16			
111.874538 Kcal/mol 4.851345 eV -101.205397 H Child_7_22.log			
6	5.024759	-0.852652	0.249214
12	-6.506635	0.063825	0.598752
6	3.972737	-1.579385	0.166922
12	-3.640008	-0.679970	0.001327
6	6.001586	-0.004330	0.309702
6	-2.223875	-2.051284	-0.566577
6	2.793638	-2.075156	0.055920
6	-0.496487	2.433721	-0.136558
6	6.726749	1.081836	0.291853
6	-1.010966	-2.341557	-0.379161
8	1.401927	4.010543	-0.216357
6	-1.477818	1.665043	-0.181525
6	0.503559	3.250787	-0.172735
6	0.297063	-2.471198	-0.223898
6	1.545232	-2.396584	-0.075843
8	-2.424095	0.919242	-0.186748
16			
112.026141 Kcal/mol 4.857919 eV -101.205155 H Child_2_32.log			
12	1.693168	1.279611	1.056778
6	-2.550182	-1.657871	-0.161844
6	2.474626	-0.447041	0.139201
12	-2.116913	-0.024014	1.111917
8	0.916876	2.098423	-0.502571
6	-1.483193	-1.490905	-0.803174
6	1.538774	-1.569655	0.563780
6	1.774153	-0.590360	-1.078587
8	-2.113416	1.570250	-0.130223
6	0.656158	-1.071554	1.568506
6	-0.181652	-0.240316	2.020573
6	0.529619	-0.043412	-1.585856
6	-0.169022	-1.317681	-1.258399
6	-1.246216	1.686701	-1.035747
6	0.064659	1.236452	-1.108658

6	1.035153	-1.897114	-0.753460
16			
112.027307 Kcal/mol 4.857970 eV -101.205154 H Child_11_62.log			
6	3.104681	-2.969949	-0.564176
6	-2.547722	-0.987315	-0.622803
6	2.986342	-1.694627	-0.625147
6	-1.717982	-2.206861	-0.203523
6	2.730770	-0.399776	-0.706946
6	-1.947799	0.256514	-0.076770
6	2.371701	0.817214	-0.581291
6	-1.007869	-2.187849	0.851695
6	1.598086	1.899897	-0.945740
6	-1.060193	0.157285	0.963038
6	0.701677	2.764485	-1.085891
6	-0.296612	-1.079463	1.220863
8	-0.440874	1.314551	1.456998
12	-1.116533	2.270788	-0.252342
12	1.340889	0.381791	1.321589
8	-3.581969	-1.070587	-1.278350
16			
112.484681 Kcal/mol 4.877804 eV -101.204425 H Original3D_4_6.log			
12	0.591421	-0.541819	0.073304
6	2.563622	-0.431927	1.745936
6	-1.883569	-1.983781	0.153760
6	-0.875366	1.682806	-0.784628
6	2.688897	0.782832	1.339354
6	1.564574	-1.336601	-1.529323
6	-2.095345	1.338948	-0.636678
6	2.823284	-1.395461	-1.465500
6	-4.370342	0.536895	0.123131
6	0.374434	1.926695	-0.484046
8	-5.339161	0.096398	0.676403
8	-2.820828	-2.625870	0.300894
6	2.762275	1.834272	0.460886
12	3.939819	-0.815375	0.092218
6	1.593596	2.120128	-0.112244
6	-3.328557	1.012211	-0.444757
16			
112.682833 Kcal/mol 4.886396 eV -101.204109 H Child_12_46.log			
8	-2.607648	1.431439	2.465370
6	-2.683017	-1.722104	-2.008549
8	4.481062	2.419493	-1.198156
12	-0.980687	-1.356946	-0.695840
6	3.379631	2.128837	-0.834244
6	-2.501461	1.069100	1.283555
6	-3.384345	-0.761723	-1.588070
6	2.200756	1.859460	-0.411668
6	0.993546	-1.922292	-0.328840
6	1.057305	1.479290	0.018716
6	-3.731814	0.238029	-0.734230
6	-0.105552	1.110598	0.429947
6	2.197250	-2.030323	0.014027
6	-3.517587	0.937600	0.263980
6	-1.244040	0.535952	0.686269
12	3.401408	-2.671554	1.455584

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16
112.922282 Kcal/mol 4.896780 eV -101.203727 H Original2D_5_1.log
6 0.919500 2.309032 0.000000
6 1.287175 0.970921 0.000000
6 -0.369902 2.854097 0.000000
12 -0.000000 -0.740692 -0.000000
6 2.358116 2.852108 0.000000
6 -1.574287 3.183189 0.000000
6 -2.489892 -0.412680 -0.000000
6 -2.679421 -1.661453 -0.000000
6 2.753919 1.390773 0.000000
6 -2.307972 -2.977620 -0.000000
6 -0.982893 -3.372399 -0.000000
8 0.120501 -2.707785 -0.000000
6 -2.004407 -4.409110 -0.000000
6 3.919042 0.790657 0.000000
12 -2.811290 1.618453 -0.000000
8 4.974701 0.253006 0.000000
16
112.979184 Kcal/mol 4.899247 eV -101.203637 H Child_2_53.log
8 -2.698238 0.697102 -0.220864
8 2.862948 -1.475791 0.719351
6 -2.214275 -0.093015 0.707705
6 -0.480973 -2.679210 -0.488246
12 -0.516912 0.743819 1.822206
6 -1.621299 -2.323809 0.129532
6 0.488392 2.252989 0.018316
6 2.306888 -0.574887 0.066345
6 -2.397235 -1.481899 0.656542
6 0.462501 -1.960258 -0.892519
6 1.269163 1.420549 -0.822129
6 1.238894 -0.807503 -1.020419
6 0.657422 0.374344 -1.574127
6 2.222543 0.864594 0.276050
6 1.298724 1.502274 1.112296
12 -1.208267 1.528222 -1.239203
16
113.364488 Kcal/mol 4.915956 eV -101.203023 H Original2D_14_2.log
6 -2.774596 -1.086166 0.000000
6 -1.180500 0.447660 0.000000
6 -1.338338 -0.964556 0.000000
6 -0.131420 -1.678583 0.000000
6 1.062802 -0.916570 -0.000000
8 -3.427996 1.221786 0.000000
6 -3.645394 -0.165994 0.000000
6 0.000000 1.242294 -0.000000
6 2.567052 0.931017 -0.000000
6 1.198971 0.554154 -0.000000
12 1.164649 -3.402317 0.000000
6 -0.837843 2.507605 -0.000000
8 -0.720309 3.703185 -0.000000
6 -2.089924 1.473707 0.000000
6 3.808640 0.721172 -0.000000
12 3.281163 -1.413867 -0.000000
16

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113.492744 Kcal/mol 4.921517 eV -101.202818 H Child_2_30.log

8	5.312071	0.483097	0.188473
6	-3.843055	-3.016036	0.196757
6	4.086732	0.335781	0.160869
6	-2.815024	-2.270305	-0.046727
6	-4.445703	2.468136	1.128844
6	-2.082114	-0.999793	-0.483480
6	2.586120	-1.867391	0.251526
6	-0.507330	2.318678	-0.467861
6	3.389303	-0.928005	0.235986
12	-2.103338	1.056353	-0.600615
8	-3.805606	1.928616	0.330623
6	3.110640	1.393499	0.023257
6	-1.326070	-2.075617	-0.268845
6	2.025168	1.950306	-0.113224
6	0.722761	2.272435	-0.296165
12	0.648314	-2.455005	0.094082

16

113.499181 Kcal/mol 4.921797 eV -101.202808 H Child_9_16.log

12	-1.448533	-2.230194	-0.766793
6	6.901135	1.856975	0.270266
6	-1.507075	-0.222959	-1.343930
6	5.792719	1.159633	0.227006
6	-1.760490	0.926017	-0.900340
6	4.754789	0.376777	0.198980
6	-2.790951	-2.952642	0.678304
6	3.725243	-0.371108	0.150140
6	-2.239913	1.937751	-0.077432
6	2.646082	-1.080755	0.042655
6	-2.861602	-1.787911	1.169716
6	1.583030	-1.711362	-0.196410
6	-2.642066	3.172086	-0.174818
8	0.514221	-2.239173	-0.440289
8	-3.063746	4.276037	-0.172985
12	-2.652235	0.221033	1.153573

16

113.578284 Kcal/mol 4.925227 eV -101.202682 H Child_3_18.log

8	-4.052695	-2.189538	-0.391284
6	-0.853590	0.809064	-2.219148
8	-1.039533	-0.552022	0.932925
6	2.841976	0.010082	-1.658628
6	1.071831	-1.390707	1.728159
6	0.391352	0.808997	-2.099126
6	-3.451326	-1.225073	-0.464245
6	3.292035	-0.751172	-0.699358
6	0.170033	-0.396141	1.343559
6	2.215552	-1.564777	1.181344
6	1.603949	0.653461	-1.350539
12	-1.978462	0.588495	-0.451045
12	-0.932618	2.553952	1.477947
6	0.757391	1.020233	1.130827
6	3.238699	-1.525159	0.347379
6	1.333896	0.921711	-0.016214

16

113.866532 Kcal/mol 4.937726 eV -101.202223 H MutD_16_68.log

6	-3.983017	-0.157097	-0.168917
6	2.316491	2.826825	0.081238
6	4.500647	1.402641	0.180395
6	-5.246355	-0.219570	-0.056239
8	-0.227044	0.197704	-0.315044
6	-6.520796	-0.259898	0.070418
6	-2.690759	-0.067302	-0.260892
6	-1.446302	0.065676	-0.293292
12	1.612506	0.741063	-0.095033
6	-7.802125	-0.291539	0.209928
6	3.318053	-0.722503	-0.007746
6	4.546320	0.097464	0.133575
8	3.430697	-1.993310	-0.053592
6	-9.094856	-0.316252	0.358881
12	5.564796	-1.867570	0.151317
6	3.476557	2.288708	0.131598
16			
114.574866 Kcal/mol 4.968443 eV -101.201094 H MutD_17_66.log			
6	2.795269	1.096242	1.203443
6	1.539993	-0.748831	0.531865
12	1.619022	-4.053898	-0.230930
6	-0.447171	0.636608	2.181571
6	1.060123	-1.156339	-0.568542
6	2.929134	1.752849	0.153395
8	-6.028374	-0.083553	0.178132
6	-1.479384	0.818450	1.343783
6	0.746791	0.383001	2.474513
6	-1.623712	0.643869	0.109053
6	2.478836	2.004747	-1.100763
6	1.627727	1.794207	-2.000886
6	1.801171	0.155516	1.576210
8	-1.567676	0.586955	-1.137900
12	0.220516	0.214175	-1.972552
6	-4.979789	-0.372075	-0.216986
16			
114.685518 Kcal/mol 4.973241 eV -101.200917 H MutI_8_75.log			
6	1.357428	-2.281847	-0.844234
12	-3.410890	0.219241	-0.172473
6	-2.579734	2.001844	-0.790345
6	-1.368747	2.123505	-0.397858
8	3.415744	1.330860	-0.758207
6	-1.160213	-2.045487	-0.874621
6	2.392100	1.879031	-0.462150
6	2.389501	-1.685058	-0.193803
6	-0.086489	2.072560	-0.156080
6	-1.985159	-0.590131	1.178139
8	-0.795271	-0.421684	1.512197
6	-2.193125	-1.495561	-0.353673
6	0.125376	-2.377125	-1.042875
6	3.008141	-0.822175	0.506112
12	1.137749	-0.087524	1.332550
6	1.153239	1.744776	0.105913
16			
114.846078 Kcal/mol 4.980204 eV -101.200662 H Child_11_57.log			
6	0.964422	2.269967	1.935813

12	2.800483	-1.995205	-0.279376
6	0.178855	1.305872	1.720920
6	1.167064	-3.114484	0.444669
12	0.536972	2.373137	-0.255551
6	0.053820	-2.544939	0.676919
6	-0.924476	0.755751	1.063813
6	3.369604	-0.176055	-0.705304
6	-1.683919	1.392110	0.068442
8	-4.524038	-0.711911	-1.372235
6	2.571988	0.679044	-1.170671
6	-3.588104	-0.334803	-0.759327
6	-0.985393	-1.751513	0.873332
6	-1.602659	-0.589764	0.780545
6	-2.554765	0.098782	-0.079161
8	1.793029	1.652539	-1.462868
16			
115.210162 Kcal/mol 4.995992 eV -101.200081 H Child_11_43.log			
8	-3.368740	-2.393524	0.078777
12	4.592956	-0.586132	0.468655
6	-2.102250	-2.711198	-0.040247
8	2.447851	2.687673	-0.296847
12	-3.002685	-0.476301	0.064966
6	2.939959	0.385496	-0.033226
6	-0.869871	-2.679924	-0.154204
6	2.020887	1.507690	-0.251227
6	0.435077	-2.350530	-0.191241
6	0.562241	1.357390	-0.295906
6	-3.570524	3.584491	0.306043
6	1.490956	-1.705016	-0.170911
6	-0.660502	1.380371	-0.201398
6	2.653244	-1.001329	-0.010649
6	-2.804224	2.540510	0.221426
6	-2.047684	1.424717	0.045057
16			
115.428370 Kcal/mol 5.005454 eV -101.199734 H Child_8_61.log			
8	1.226714	2.539454	-0.936086
6	-5.621410	1.560645	0.228078
12	3.050230	2.366285	-0.229745
8	-5.571226	1.675898	1.387395
6	-0.439111	-2.578190	-0.102464
6	3.047266	0.421461	0.644764
6	0.658043	-1.912110	0.568846
6	0.838381	1.374804	-0.424125
6	-1.617301	-2.170898	-0.687338
6	1.733890	0.444379	0.332887
6	-1.088160	-3.433397	-1.118383
6	-0.232387	0.473777	-0.393024
6	-1.474154	0.187486	-0.987302
6	0.595002	-0.545606	0.360549
6	-2.100472	-0.891022	-0.824557
12	2.696318	-1.642184	1.129907
16			
115.437530 Kcal/mol 5.005851 eV -101.199719 H Child_13_8.log			
6	3.595173	0.416977	-0.030414
6	-1.855667	-3.510855	0.609638

6	4.826772	0.172937	-0.072097
8	-2.281610	-2.495534	0.219670
6	2.320892	0.772479	0.065855
6	-5.619936	-1.067392	-0.578476
6	1.112802	1.102997	0.184760
6	-5.669310	0.202161	-0.356432
6	6.104238	-0.089643	-0.115544
12	-3.470093	-0.806609	-0.244077
8	8.531417	-0.545105	-0.193191
6	-5.308655	1.488695	-0.084159
6	7.349529	-0.320326	-0.151891
6	-3.999344	1.641874	0.109664
12	-0.752785	1.754915	0.335577
6	-2.743815	1.347671	0.200793
16			
115.456693 Kcal/mol 5.006682 eV -101.199689 H MutD_18_52.log			
8	-3.875869	4.390582	0.126845
6	-5.640254	-1.263752	-0.163537
6	-2.018611	-1.879065	-0.001540
12	0.000062	-2.200144	0.084363
6	4.338805	-0.697817	0.165143
6	-6.808007	-1.785253	-0.218859
6	-4.287476	0.679221	-0.016428
8	6.555415	0.403123	-0.194221
6	-4.171202	1.935047	0.020930
12	8.047224	1.465022	-0.146522
6	1.936660	-1.662835	0.299021
6	-4.015658	3.219687	0.077832
6	-4.383453	-0.690932	-0.094831
6	5.429223	-0.161476	-0.001151
6	-3.145238	-1.380738	-0.074158
6	3.097911	-1.233448	0.221731
16			
115.499340 Kcal/mol 5.008532 eV -101.199621 H Child_11_29.log			
6	3.328631	-0.422395	-0.014680
8	-4.846708	-0.635933	-0.031444
6	1.947682	0.093925	-0.035006
6	-3.695065	-0.250065	-0.003274
6	3.234498	-1.823899	-0.003149
8	-3.458365	1.153604	0.007487
12	3.832514	1.674319	0.002689
6	-2.223297	1.669549	0.014647
6	0.748288	-0.414645	-0.028584
6	-2.497938	-1.026549	0.013497
6	2.178030	-2.552793	0.012090
6	-1.079823	2.132806	0.023706
6	0.033845	-1.621858	0.003225
6	-1.380499	-1.510510	0.011678
6	0.881332	-2.757804	0.029713
12	0.966360	2.222686	0.001351
16			
115.814552 Kcal/mol 5.022201 eV -101.199118 H MutD_13_56.log			
6	5.792350	-2.025970	-0.420900
6	-3.360297	1.104092	-0.050955
8	4.094217	0.793534	-0.185944

6	-2.879572	-0.040613	-0.086043
12	-2.446591	2.876520	0.197747
6	0.686306	2.664444	-0.031686
8	5.787773	-2.384963	0.672366
6	2.876035	0.893955	-0.146692
6	-2.532670	-2.543308	-0.117918
6	-0.688814	-1.001124	-0.166785
6	-0.433015	3.126901	0.224001
6	-2.101803	-1.245879	-0.135423
6	1.553801	0.286352	-0.127735
12	-4.655743	-2.977828	0.103398
6	1.657636	1.669195	-0.079875
6	0.458726	-0.563525	-0.110840
16			
116.264750 Kcal/mol 5.041723 eV -101.198401 H MutD_7_70.log			
6	1.003635	2.084148	0.007800
6	-2.875583	-2.852675	-0.052653
6	2.028810	1.401463	0.013885
8	-4.782487	0.641835	0.010986
6	1.166528	-1.821646	0.002243
8	6.599850	-0.348476	-0.010160
6	-0.272650	2.522953	-0.020276
6	-2.815166	2.202545	-0.016171
6	2.851485	0.243559	0.011633
12	-4.171402	-1.165560	0.030525
6	4.198449	0.241899	0.011993
6	-3.834134	1.512750	-0.005076
6	-1.507179	2.528256	-0.018883
12	-0.739039	-2.534951	-0.003445
6	5.419641	-0.116183	0.004629
6	2.033896	-0.937192	0.005616
16			
116.310611 Kcal/mol 5.043712 eV -101.198328 H Child_8_44.log			
6	-0.399138	2.314698	-0.241997
8	-5.236427	0.279675	-1.483693
6	-1.075547	1.250742	-0.191606
6	-4.980106	0.406249	-0.350337
6	-1.513459	-0.052470	-0.132206
6	2.431976	-0.192455	-0.033974
12	1.558239	1.709855	-0.115477
6	-4.710057	0.521371	0.911486
8	6.017143	0.814921	0.083906
6	2.253874	-1.560102	0.038919
6	4.849875	0.605034	0.074995
6	1.867442	-2.790900	0.083426
6	3.529191	0.639091	-0.009303
6	-1.688617	-1.289508	-0.102192
6	-4.345562	0.555493	2.142019
12	-0.188652	-2.643206	-0.045947
16			
116.444403 Kcal/mol 5.049514 eV -101.198114 H Child_2_48.log			
6	0.482951	-1.771873	-0.385709
6	-1.720863	5.329228	0.192491
8	1.201784	-2.866089	-0.476040
8	-1.919340	4.574040	-0.652371

6	-0.918840	-1.626896	-0.545643
6	2.213894	1.469766	0.471995
12	-8.267225	-1.966440	0.547368
12	2.986701	-1.910476	-0.050203
6	1.001567	0.789572	0.136288
6	-1.666885	-0.617406	-0.514707
6	3.415650	1.204589	0.613707
6	-1.391426	0.671001	-0.265829
6	1.239046	-0.581969	-0.067227
6	4.812237	-0.923571	0.338738
6	-0.329862	1.291082	-0.012559
6	4.380318	0.243040	0.548672
16			
116.474248 Kcal/mol 5.050808 eV -101.198067 H Child_4_39.log			
8	-6.465094	-0.689359	0.652993
8	4.057150	2.088969	1.481582
6	-5.285318	-0.544326	0.477211
6	3.717583	1.064165	0.974809
6	-4.021827	-0.478856	0.349801
6	-2.777944	-0.070207	0.040178
6	3.468371	-0.062177	0.376090
6	-2.424844	1.143329	-0.661624
12	0.152317	1.529571	-1.045966
6	-1.549421	-0.734199	0.326443
6	2.247446	-0.800514	0.108849
6	-1.821792	2.087936	-1.222292
6	0.941958	-0.263626	-0.129573
6	-0.306419	-0.727561	0.211156
6	2.145538	-2.129642	-0.253383
12	4.286313	-1.704805	-0.675916
16			
116.534474 Kcal/mol 5.053419 eV -101.197971 H Child_12_9.log			
8	-4.096029	-1.290407	0.976212
6	4.238041	-0.000374	0.101714
6	-3.050142	-1.036132	0.357041
6	3.671372	1.107251	0.332891
6	-1.890834	-1.858593	0.269103
6	3.007214	2.239691	0.598643
6	-3.452383	1.477276	-0.264524
6	1.728807	2.591607	0.440707
6	-0.757597	-2.323445	0.185665
12	3.509220	-1.843769	-0.302900
12	-1.261447	2.313965	-0.387345
6	-2.882217	0.274455	-0.292157
6	1.715995	-2.801477	-0.386864
6	0.534877	-2.670356	-0.058140
6	0.533627	2.985278	0.316344
8	-1.823200	0.596226	-1.141164
16			
116.558461 Kcal/mol 5.054460 eV -101.197933 H MutD_14_44.log			
6	0.333095	-2.570590	0.542731
6	-4.227313	-1.534886	-0.560094
6	1.300419	-0.193966	0.772400
6	-3.270609	-2.318154	-0.305447
6	0.346152	2.179271	0.578068

6	5.561098	-1.784746	-0.104275
12	-4.017721	0.505992	-0.471671
6	-0.921160	-2.887119	0.275713
6	0.892927	-1.397562	0.703567
6	0.922534	1.088672	0.708170
6	4.943442	-0.685047	-0.345868
12	-2.282308	2.749349	-0.011995
6	4.337569	0.425981	-0.615325
8	3.822835	1.442728	-0.885417
8	-0.431166	3.184003	0.400958
6	-2.140321	-3.001510	-0.036363
16			
116.781835 Kcal/mol 5.064146 eV -101.197577 H Child_6_52.log			
8	4.714796	1.172064	0.934161
8	-4.209326	1.548614	1.041857
6	3.744180	0.547690	0.630108
6	-3.311638	1.294550	0.375287
6	2.670412	-0.129674	0.353713
12	-1.832639	-1.800411	0.795239
6	0.419125	0.640208	-2.088625
12	-1.076820	1.311365	-0.311325
6	0.754604	-0.636109	-1.510753
6	-0.847633	-0.029008	1.438260
6	1.689210	-0.744264	-0.501001
6	-0.327903	-1.556906	-1.360530
6	0.342610	-0.522554	1.449989
6	-1.294261	-2.325666	-1.109295
6	-0.216670	1.726168	-2.189714
6	1.522924	-0.913914	0.910042
16			
116.895035 Kcal/mol 5.069055 eV -101.197396 H Child_3_40.log			
6	-3.796742	-1.043008	0.490541
6	4.005947	-1.017446	0.434780
6	-3.546824	-0.017937	-0.450246
12	2.704462	-1.625478	-1.023729
6	-4.795343	-0.712684	-0.532842
6	3.228886	-0.054930	0.689187
6	-2.514913	0.843414	-0.756553
6	2.161001	0.830387	0.604056
12	-1.801084	-0.785780	1.213429
6	0.769917	2.526376	-0.074256
6	-1.395754	1.377428	-0.753743
6	1.926639	2.141974	0.435755
6	0.756977	0.117610	0.016925
8	0.021126	-0.540689	0.990487
6	-0.058353	1.520860	-0.438905
8	1.067727	-0.726458	-1.023562
16			
116.930755 Kcal/mol 5.070604 eV -101.197339 H MutD_11_70.log			
6	1.963750	1.891827	-0.318803
6	-3.873796	-0.951661	-0.989650
6	-0.598437	-0.374824	-0.082229
8	3.260376	2.088513	-0.452043
6	-2.739675	1.934406	1.030049
6	-1.397807	-1.445842	-0.209593

6	0.795816	1.595749	-0.134729
6	-0.421417	0.954460	0.183365
6	3.552040	-0.191561	-0.055764
6	-2.696566	-1.317965	-0.746174
6	2.951285	-1.244207	0.192113
12	-4.111481	0.827150	-0.003720
6	-1.570295	1.578567	0.767012
12	0.346129	-2.418890	0.352208
6	4.248153	0.981148	-0.312374
8	2.227865	-2.258477	0.436896

16

117.551965 Kcal/mol 5.097542 eV -101.196349 H Child_8_58.log

6	-6.401428	0.274567	-0.125028
8	3.892368	2.744685	-0.686545
8	-1.084480	-3.084723	-0.216695
6	2.853907	2.272087	-0.344436
6	3.098958	-1.478404	0.666777
6	-5.109587	0.353316	-0.090022
6	1.665635	1.803286	-0.050938
6	-3.797590	0.386058	-0.114530
12	2.294196	-3.201465	-0.096877
6	-2.538694	0.422622	-0.099059
6	2.276865	-0.571237	0.405279
6	-0.009806	0.031952	0.015560
12	-0.250060	2.606617	0.550015
6	-1.223151	0.539640	0.033884
6	1.315801	0.416956	0.111724
6	0.036967	-2.807765	-0.111165

16

117.558863 Kcal/mol 5.097841 eV -101.196338 H Original3D_8_7.log

6	2.132442	-1.611831	-0.148915
6	1.128098	-2.336120	-0.254010
6	-0.690069	1.537919	0.465123
6	-0.093022	-2.918821	-0.369430
6	-1.283325	-3.283588	-0.467335
8	-1.616607	0.718250	1.220633
6	-0.981957	2.699826	-0.051778
12	-3.080677	-2.336957	-0.396704
12	1.229426	0.639143	0.410444
8	5.312643	0.285575	-0.040324
6	-1.194432	5.100077	-1.025178
6	-3.660592	-0.462638	0.166152
6	2.959917	-0.505794	0.058029
6	4.208470	-0.163116	-0.012691
6	-2.658454	0.122622	0.631544
6	-1.092619	3.878659	-0.592737

16

117.656576 Kcal/mol 5.102078 eV -101.196183 H Child_4_37.log

8	4.508542	1.219189	-1.588191
6	-4.818251	-0.683376	-1.319125
6	3.682340	0.812345	-0.842715
6	-3.647594	-0.347545	-0.753948
6	2.820044	0.203283	-0.078076
6	-3.271444	0.997777	-0.445810
6	2.902957	-1.749861	-0.324156

6	-2.756138	2.071060	-0.109251
6	1.717530	0.597118	0.637337
6	-2.713913	-1.381517	-0.412943
6	0.667338	1.442258	1.045400
12	-1.000933	2.614821	0.693751
6	0.589003	0.058877	1.326768
6	-1.789022	-2.097888	-0.008812
12	0.045905	-1.927279	0.863184
8	1.886860	-2.192399	0.216788
16			
118.021563 Kcal/mol 5.117906 eV -101.195601 H Child_10_8.log			
8	5.759067	0.566810	0.994989
6	-4.388797	2.472822	0.776199
6	4.682993	0.719087	0.494315
8	-4.227264	-0.018136	0.673969
6	3.467256	0.688908	0.037572
6	-3.766582	1.336483	0.423839
6	1.226856	1.644943	-0.834025
6	-3.010433	-0.495912	-0.007637
12	2.164038	-0.986675	-0.280239
6	-2.568903	0.785453	-0.255362
6	0.713220	-2.409837	-0.186214
12	-1.813519	-2.230896	-0.153792
6	2.423858	1.462774	-0.468367
6	-1.306792	1.250276	-0.696051
6	-0.103802	-3.300881	0.241790
6	-0.112317	1.549461	-0.883274
16			
118.053638 Kcal/mol 5.119297 eV -101.195550 H Child_14_12.log			
6	-3.934226	0.146731	-0.513269
6	1.786262	-0.230279	1.593082
6	-3.176380	-0.874201	-0.496040
6	1.190311	0.816009	1.861452
6	-1.953634	-1.554457	-0.435493
6	3.793822	0.618900	-1.487721
8	-0.962741	-0.654627	-0.184306
6	2.000345	-1.444401	1.018924
12	-0.043653	-2.483709	-0.151816
6	2.567368	1.022786	-1.446855
6	-0.850097	2.330668	1.457981
6	0.200556	1.745738	1.805457
6	1.946668	-2.539563	0.408417
6	1.316852	1.322257	-1.413728
8	0.165081	1.573550	-1.423970
12	-1.868497	1.190999	0.047897
16			
118.152138 Kcal/mol 5.123568 eV -101.195393 H Child_6_46.log			
6	-2.878782	-2.035899	-0.012258
8	6.682950	0.135392	0.026981
6	-3.951953	-1.432080	0.025058
6	5.491887	-0.028119	0.036005
6	-1.567308	-2.335317	-0.045611
6	1.320278	1.914020	0.017589
8	-4.969048	-0.643647	0.068560
6	2.154712	0.999229	0.028671

6	-0.332370	-2.347230	-0.065405
6	4.250527	-0.300290	0.036992
6	0.954110	-1.953093	-0.053220
6	2.906328	-0.223939	0.013797
12	-4.392169	1.184136	0.087019
12	-0.603870	2.565300	-0.024683
6	2.016467	-1.330479	-0.028084
6	-2.657020	2.251998	-0.205594
16			
118.323293 Kcal/mol 5.130990 eV -101.195120 H Child_14_29.log			
6	1.797510	2.451201	-0.187143
6	1.085200	-2.338072	-0.055782
12	-0.229912	2.523624	0.110779
6	-0.127655	-2.347624	-0.304448
6	2.814841	1.748477	-0.218452
12	3.077378	-1.804188	0.007586
6	-2.145392	2.056679	-0.724037
8	-1.417437	-1.944525	-0.393533
6	3.743297	0.744710	-0.196381
6	-1.888714	-0.925641	0.354877
6	-2.832507	1.022921	-0.642847
6	-1.189387	-0.322742	1.353456
6	4.424060	-0.310746	-0.182270
6	-0.605566	0.789587	1.514957
8	-4.269645	-0.854115	-0.171047
6	-3.187842	-0.276102	-0.195887
16			
118.595943 Kcal/mol 5.142813 eV -101.194686 H Child_13_21.log			
6	1.558439	-1.822050	2.461780
8	-4.672376	0.585985	1.102856
8	1.614711	-1.726874	1.304351
6	-1.748004	2.213093	-0.295687
6	-0.056666	-2.696226	-1.289923
6	-2.825815	1.722931	0.052449
12	1.503584	-1.457171	-0.809889
6	-3.627178	0.593365	0.432132
12	4.815530	1.416730	0.187537
6	-1.130572	-2.124751	-1.016176
6	-0.427800	2.168556	-0.659107
6	1.747616	0.617690	-0.551983
6	-2.170486	-1.364735	-0.589375
6	-2.950622	-0.585033	-0.047102
6	0.594609	1.428748	-0.659261
6	2.475135	1.450482	0.197347
16			
119.122366 Kcal/mol 5.165641 eV -101.193847 H Child_6_57.log			
6	-3.196486	-1.377461	1.508289
8	2.996635	1.337496	1.732074
8	8.002815	-1.180403	-0.748510
6	-0.958568	2.352187	-0.660484
6	-1.957291	-1.485308	1.708506
12	-3.014405	2.016606	-0.902486
6	7.813852	-0.107870	-1.072297
6	0.011860	1.783547	-0.123333
12	-4.095701	-0.578691	-0.355206

6	1.984645	1.099751	1.169088
6	-2.587709	-1.497544	-1.740410
6	0.845943	0.823772	0.523707
6	-0.761802	-1.288875	1.072751
6	-1.386376	-1.558386	-1.354178
6	0.253466	-0.512391	0.510741
6	-0.507256	-1.316712	-0.338414
16			
119.213803 Kcal/mol 5.169606 eV -101.193701 H MutD_13_42.log			
12	-2.619892	2.935011	0.264362
6	-4.037775	1.469115	0.619687
6	-3.831760	-1.130286	0.393304
6	-0.829916	-1.510609	-0.587146
6	0.107760	-0.729601	-0.707054
6	-4.270915	-2.556786	0.474977
6	1.049394	0.314697	-0.692826
6	2.357020	0.131609	-0.512629
8	-1.729914	-2.473704	-0.346387
8	7.185698	-0.434474	0.818330
6	4.825738	-0.158030	0.114896
6	3.590334	-0.007765	-0.220379
12	-0.008933	2.193236	-0.554480
6	-2.988488	-2.117974	0.054477
6	-4.025212	0.228139	0.538846
6	6.037089	-0.311431	0.474823
16			
119.379088 Kcal/mol 5.176774 eV -101.193438 H Child_8_51.log			
8	-4.012832	1.627065	-0.006175
6	3.763581	1.048510	0.397941
12	-1.330361	-1.677045	-0.628103
12	1.491931	2.652688	-0.032467
8	-3.750195	-0.946989	1.348657
6	3.476039	2.265429	0.182834
6	-2.975551	-0.579056	0.476876
6	4.006448	-0.273632	0.436481
6	0.169127	-3.121414	-0.493998
6	-0.341436	1.721190	-0.481673
6	-2.966261	0.978892	0.069456
6	1.347747	-2.841304	-0.132759
6	-0.666390	0.407972	-0.971499
6	-1.656761	1.278569	-0.459046
6	3.294334	-1.352793	0.368108
6	2.576686	-2.390420	0.138442
16			
119.493900 Kcal/mol 5.181752 eV -101.193255 H MutD_8_76.log			
6	0.580003	-0.339693	-1.543925
6	2.309438	0.614498	-0.218686
12	0.641305	2.046395	-0.442661
6	-1.958052	-3.005628	0.651009
6	-3.289896	3.134420	1.333332
6	1.710080	-0.563713	-0.786029
6	-1.530088	1.918749	-0.208649
6	3.383028	0.759677	0.520443
6	-2.359032	-0.535612	-0.179479
8	-0.639746	-3.229401	0.640087

8	4.316577	1.022173	1.207257
12	0.949665	-2.366431	0.085839
6	-0.590715	0.156004	-1.511659
6	-2.240197	-1.639947	0.372151
6	-1.661021	0.567314	-0.757059
6	-2.437929	2.516976	0.579070
16			
119.535227 Kcal/mol 5.183545 eV -101.193189 H Child_7_62.log			
8	3.982383	-2.426452	0.483306
12	-4.783950	0.194370	0.561944
6	2.976298	-1.728161	0.175504
6	-3.019661	1.544838	0.119060
6	2.954005	-0.277527	0.098104
6	-2.298426	0.370928	-0.390579
6	1.710543	-2.193091	-0.144343
12	-2.758734	-1.744780	-0.297804
6	2.742451	0.925632	0.048253
6	-1.644139	1.568908	-0.150753
6	0.451721	-2.466239	-0.221376
6	-0.823717	-2.492051	-0.345817
6	2.276738	2.278154	-0.041589
6	-0.370583	2.104095	-0.114030
6	0.830702	2.315555	-0.076302
8	2.992196	3.288787	-0.096614
16			
119.548130 Kcal/mol 5.184104 eV -101.193168 H Child_6_24.log			
12	-6.485941	-0.831946	-0.174825
6	4.623475	1.364961	0.089001
8	-0.947834	0.875175	-1.289372
6	3.503578	0.642805	-0.029215
6	-0.339873	1.537884	-0.357592
8	4.673111	-1.468961	0.048480
12	-2.533195	0.092447	-0.046697
6	-1.190184	1.938394	0.699214
6	3.573876	-0.902526	0.018881
6	-2.230580	1.852260	1.413192
6	2.306770	-1.534450	0.067650
6	1.075291	1.589157	-0.328392
6	-1.410908	-1.607661	0.302142
6	-0.219615	-1.981039	0.261917
6	1.133907	-1.888540	0.162554
6	2.245498	1.259466	-0.201786
16			
119.753951 Kcal/mol 5.193029 eV -101.192840 H Child_8_8.log			
6	5.467843	-0.732522	-2.057256
6	0.710587	2.956208	0.617739
6	4.612572	-0.886082	-1.064526
6	1.386571	1.985668	1.027364
6	0.075312	-1.870900	0.569976
6	-3.316025	0.022359	-0.596552
8	-3.068708	-3.507597	0.080002
6	-3.217045	1.364589	-0.790184
6	-1.089760	-2.203075	0.318318
6	-2.855244	2.549457	-0.852846
6	3.635904	-1.027423	-0.244933

6	-3.105373	-1.159535	-0.346899
12	1.817026	-0.874025	0.966101
8	2.051856	0.947695	1.388973
6	-2.484494	-2.409432	0.014237
12	-1.049549	3.285970	-0.242637
16			
119.760994 Kcal/mol 5.193335 eV -101.192829 H Child_8_26.log			
8	-4.035114	-3.795254	0.078625
6	6.716900	-0.909728	0.814557
6	-3.599514	-2.698868	-0.009781
6	7.253493	-0.476978	-0.268403
6	-3.307188	-0.214687	-0.114501
6	3.083260	0.352723	-0.341338
8	-3.507373	3.411337	0.033902
12	5.114167	-0.034362	-0.214788
6	-3.316746	1.019314	-0.107350
6	-2.838880	2.367322	0.047772
6	1.854301	0.492928	-0.129486
6	-2.959632	-1.560961	-0.082407
6	-0.355246	1.593679	0.215633
6	-1.395234	2.270109	0.205223
6	0.505578	0.527787	0.054030
12	-0.906388	-1.091013	-0.002204
16			
120.169648 Kcal/mol 5.211056 eV -101.192178 H MutD_18_44.log			
6	6.748517	-0.221594	-0.043513
6	4.193691	0.009253	0.026208
8	7.940709	-0.365826	-0.091364
6	-2.068478	-1.782472	0.031981
6	-4.161658	1.424249	-0.026875
6	-1.714766	2.106198	0.007538
6	2.931275	0.126409	0.046407
6	-0.417701	1.778826	0.028186
6	1.604882	0.152234	0.059375
12	-4.118475	-1.774155	-0.021143
12	-0.053870	-1.248866	0.067412
6	0.677814	1.179622	0.045742
8	-5.673973	-0.578826	-0.061224
6	5.495731	-0.005406	-0.005743
6	-5.017137	0.531987	-0.046921
6	-2.949795	2.006273	-0.011470
16			
120.653954 Kcal/mol 5.232057 eV -101.191406 H Child_7_40.log			
8	4.703148	-0.366661	-0.842192
6	-2.353725	-4.073774	-1.112485
6	3.629162	-0.166103	-0.365664
6	-2.645972	1.166903	-0.382511
6	2.430134	-0.080052	0.144956
6	-1.821168	-3.073483	-0.484405
12	1.045528	-1.788203	0.387960
6	-2.536931	0.040823	0.153194
6	1.558890	0.993924	0.569904
6	-2.645290	2.572101	-0.419327
12	0.388572	2.593356	-0.244023
6	-0.591645	-0.173353	1.344652

6	0.460020	0.527014	1.223377
6	-1.118088	-2.165065	0.204299
8	-1.448216	3.126489	-0.542112
6	-1.573496	-0.859011	0.681875
16			
120.655197 Kcal/mol 5.232111 eV -101.191404 H MutD_17_42.log			
6	1.572859	0.262083	0.034260
12	-0.072404	-1.137612	0.221548
12	-4.013081	-1.858952	-0.181766
6	-1.752152	2.193182	0.065486
8	7.890978	-0.461117	-0.114424
6	0.654560	1.299882	0.031589
6	-4.153076	1.374836	0.007412
6	4.156980	0.037217	-0.039638
6	-4.958093	0.440956	-0.090091
6	-0.442510	1.894910	0.042672
8	-5.574817	-0.684438	-0.245259
6	6.699233	-0.292832	-0.091903
6	5.443673	-0.096159	-0.071690
6	-2.052376	-1.814464	0.475288
6	2.891845	0.206862	-0.025129
6	-2.978190	2.014062	0.061758
16			
121.078612 Kcal/mol 5.250472 eV -101.190729 H Child_7_60.log			
6	-4.456672	-0.555079	0.029252
6	1.705163	2.382494	-0.359023
6	-3.968588	-1.668513	-0.169318
12	3.207614	0.983854	-0.077353
6	-2.771232	-2.303557	-0.289855
6	0.477465	2.595154	-0.190118
6	-4.149445	0.760085	0.217380
6	4.709170	-0.528301	-0.153690
6	-1.532654	-2.342072	-0.321973
6	3.811811	-1.392241	0.038235
6	-3.268289	1.627026	0.251629
6	-0.870545	2.544743	-0.010223
6	-2.051545	2.232073	0.134558
12	0.051661	-1.139056	0.042899
8	2.620135	-1.872854	0.308341
8	1.764971	-0.408202	0.360699
16			
121.203053 Kcal/mol 5.255868 eV -101.190531 H MutD_15_56.log			
6	0.503881	-1.355524	-0.027678
6	-5.010866	1.918891	0.094186
8	-5.573164	2.963110	0.146967
12	-1.603255	-0.623398	-0.553407
6	-3.704222	-0.309873	-0.049525
6	3.408749	0.489720	0.185444
6	-4.350935	0.791226	0.041090
6	2.151185	0.495654	0.182558
6	0.888371	0.049670	-0.058450
6	5.970755	0.390410	0.205254
6	-0.254330	-2.297944	-0.378306
8	-0.170670	0.782014	-0.452089
6	8.548866	0.097920	-0.004330

12	-4.639160	-2.382601	0.489212
6	7.274936	0.243115	0.136888
6	4.716886	0.505237	0.208088
16			
121.310717 Kcal/mol 5.260537 eV -101.190360 H MutI_13_63.log			
6	0.432347	3.432017	0.138361
6	-1.164625	0.810615	1.759548
8	-2.419831	-2.157298	-1.166130
6	-4.403707	0.998754	-0.994304
12	2.933234	-2.179074	-0.207033
6	1.561505	3.119052	-0.532392
6	-0.922074	-0.427714	1.748406
6	2.568173	2.648696	-1.139800
6	-3.907231	-0.190630	-1.111428
6	0.508114	-2.387329	0.907087
6	-3.144467	-1.237752	-1.114033
6	-0.446349	2.875016	0.863977
12	2.967923	0.610715	-1.002737
6	-0.197018	-1.481459	1.376631
8	1.355294	-3.192172	0.389701
6	-1.267603	2.110077	1.552726
16			
121.505830 Kcal/mol 5.268998 eV -101.190049 H Child_3_22.log			
6	2.698734	1.610345	1.166071
6	-2.467505	-1.821063	1.439266
6	3.429662	0.930678	0.383135
8	-2.263752	-0.531874	1.447682
6	1.560398	1.962893	1.773341
6	-1.295833	-2.524073	0.956254
6	3.143318	0.186692	-0.674337
6	-0.360045	-2.959137	0.259438
6	0.304314	1.888393	1.694260
8	-3.110020	2.152895	-2.133691
6	2.358744	-0.556599	-1.379618
12	-1.242800	0.830236	0.597028
6	1.010032	-0.091798	-1.509667
6	-2.641470	1.897634	-1.122709
6	-0.164448	0.232901	-1.219773
12	1.037365	-2.289350	-1.022519
16			
121.924392 Kcal/mol 5.287149 eV -101.189382 H MutD_17_34.log			
6	3.527356	1.669986	-0.076903
6	-0.244611	-0.608002	0.245948
12	4.675405	-2.596133	-0.252921
6	0.986369	-0.683321	0.189286
6	-2.729467	0.345587	0.627030
6	-2.916080	-0.931736	0.113140
6	4.056364	2.866235	-0.233725
6	4.553932	4.035700	-0.415204
12	-5.210192	1.008115	-0.256814
6	-4.095597	-1.274988	-0.525530
6	2.389425	-0.675243	0.189451
8	-3.482105	1.393269	0.698406
8	3.028165	-1.836218	0.310926
6	-1.585294	-0.445782	0.338446

6	3.036457	0.525597	0.060518
6	-5.304028	-1.057397	-0.838764
16			
121.994772 Kcal/mol 5.290201 eV -101.189269 H Child_4_27.log			
12	-3.377639	-1.504635	0.510829
8	2.600236	3.428995	0.748815
6	-1.654015	-2.530024	1.104766
6	2.994932	2.334454	0.458791
8	-5.039388	2.034433	-0.906790
6	-4.090816	1.411960	-0.584714
6	3.218999	1.111763	0.107395
6	-1.049744	-1.489155	0.704221
6	3.108006	-2.074953	-0.758905
6	-3.109241	0.644218	-0.228986
6	4.066944	0.085913	-0.262497
6	-0.743732	-0.184467	0.232964
6	1.872756	-2.388568	-0.868695
6	-1.760759	0.527934	-0.079642
6	4.099964	-1.136267	-0.559070
12	1.527093	-0.294054	-0.038327
16			
122.045668 Kcal/mol 5.292408 eV -101.189188 H Child_6_25.log			
12	-2.905602	-0.134184	0.497464
8	5.764083	3.866295	0.092283
6	-2.043001	-1.933157	0.516418
6	5.441839	2.715615	0.016728
6	-1.082525	-2.674627	0.273291
6	-2.217459	2.104989	0.201575
8	-7.127105	1.089308	-0.523762
6	5.111405	1.505580	-0.130969
6	-5.970135	1.296582	-0.331011
12	3.126037	-2.620495	-0.287687
6	4.665622	0.259803	-0.082655
6	-4.702801	1.332190	-0.076996
6	0.137399	-3.218809	0.003169
6	4.202817	-0.913749	-0.031588
6	1.323024	-3.495116	-0.238251
6	-3.489691	1.922584	0.036041
16			
122.112323 Kcal/mol 5.295298 eV -101.189082 H Original2D_0_13.log			
6	1.411291	-0.172274	-0.000000
6	-0.039167	-1.629617	0.000000
6	1.398605	-1.693945	-0.000000
6	2.742713	-2.049415	-0.000000
6	-2.616535	-0.411532	0.000000
6	-1.239379	-2.511178	0.000000
6	3.497384	-0.933653	-0.000000
6	-2.242718	0.937887	0.000000
6	-0.000000	-0.156989	0.000000
6	2.678699	0.396460	-0.000000
6	-0.850226	0.966520	0.000000
6	-2.393012	-1.631805	0.000000
12	1.762385	2.323451	-0.000000
8	-1.185702	-3.748406	0.000000
8	-0.198511	2.209036	-0.000000

12	-2.013403	3.147566	-0.000000
16			
122.264731 Kcal/mol 5.301907 eV -101.188839 H Child_9_31.log			
6	4.216873	-1.061546	-0.083355
12	-4.673031	-1.051879	-0.056770
6	4.019643	-2.333156	-0.001292
6	-4.586603	1.033983	-0.120397
6	4.378467	0.259391	-0.319835
8	-2.820843	-1.496285	-0.056632
12	1.945176	-1.946590	0.226703
6	-3.355569	0.763591	-0.067153
6	3.356191	1.123844	-0.179058
6	-2.281558	-0.191786	-0.024113
6	2.361285	1.878492	-0.136787
6	0.377883	-0.562059	0.122195
6	0.235849	0.796792	0.065776
6	0.950009	2.060472	0.074195
6	-0.955810	0.018360	0.046098
8	0.375129	3.154204	0.269526
16			
122.278502 Kcal/mol 5.302504 eV -101.188817 H Child_6_33.log			
8	7.250597	1.044046	0.458513
6	-3.276640	0.734987	0.039400
6	6.241319	0.418969	0.270987
6	-2.934532	1.996100	-0.028418
6	5.169687	-0.232977	0.079329
6	-4.173568	-0.422368	0.302780
6	4.067641	-0.886587	-0.114424
6	-2.519271	3.200626	-0.081329
6	2.989636	-1.518044	-0.299813
6	-1.978020	4.370454	-0.065731
6	1.765262	-2.007328	-0.442969
8	-1.476051	5.449485	-0.057738
6	0.573459	-2.395985	-0.522374
12	-3.951240	-3.475448	0.568779
12	-1.439699	-2.168189	-0.369195
6	-2.842490	-0.628615	-0.070974
16			
122.401550 Kcal/mol 5.307840 eV -101.188621 H MutD_10_72.log			
6	-1.504952	3.341001	0.054200
6	3.488206	-0.077286	0.017718
8	5.787438	0.866573	0.057498
6	-2.860624	-2.046779	0.055722
6	4.681622	0.402693	0.037261
6	-2.608647	-0.724237	0.017832
12	1.222210	-2.571075	-0.019312
12	-0.076593	1.767174	-0.075355
6	-2.608120	2.742102	0.031226
8	-1.307109	-0.194225	-0.049305
6	-3.227351	-3.274151	0.048586
6	-3.468920	0.382170	0.010778
6	2.303994	-0.639987	-0.018110
6	-3.362650	1.613485	0.021646
6	-0.079243	-0.940678	-0.041538
6	0.981681	-0.066996	-0.056911

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16
122.605614 Kcal/mol 5.316689 eV -101.188296 H MutI_1_69.log
12  1.569616  -1.013567  -0.418150
 6  -0.341001  1.372371   2.194223
 6  3.984602  -0.486781   0.495832
 6  -2.496282  1.926636   -0.796795
 8  -0.222734  -1.282385   -0.219714
 8  -1.433163  1.095556   1.947303
 6  -2.121770  -3.176610   -0.591937
 6  3.752113  -1.711291   0.833816
 6  -1.323410  -2.017844   -0.350403
 6  2.482822  1.245524   -0.653316
 6  3.417773  0.596544   -0.136883
 6  -1.278938  2.178110   -0.984795
 6  0.077371  2.143153   -0.998685
 6  1.278823  1.829144   -0.854712
12  -2.850969  0.125378   0.246724
 6  -2.661535  -1.873471   -0.116947
16
122.612616 Kcal/mol 5.316993 eV -101.188285 H Original3D_2_7.log
 6  -0.046336  -1.207725   0.096503
 8  1.179502  -0.518264   0.070921
 6  -1.309967  -0.519665   -0.111945
 6  -3.889413  0.777730   -0.275433
12  2.973399  -0.689328   -0.557607
 6  -0.102454  -2.520377   0.350268
 6  3.417337  1.350431   0.092444
 6  4.460804  0.806563   -0.387144
 6  -1.476828  0.861251   0.086376
 6  -2.770301  1.455321   -0.035194
 6  -0.576521  2.115644   0.308863
 6  -1.745406  2.641799   -0.069996
12  1.388746  1.510290   0.541702
 8  -0.133869  -3.700760   0.429879
 6  -2.521219  -1.267438   -0.348567
 6  -3.558161  -0.510095   -0.342098
16
122.847518 Kcal/mol 5.327179 eV -101.187910 H Original3D_18_4.log
 8  4.888797  -1.464777   0.404433
 6  -0.347883  -0.579138   -2.100402
 6  -0.591406  0.389780   -1.263938
 6  -0.706160  0.091241   0.269289
 6  1.974326  0.835301   0.796341
 6  0.563669  0.704325   0.771778
 6  3.174662  0.271578   0.766058
 6  -1.946743  0.839306   0.699711
 6  -1.765703  -2.333972   0.736834
 8  -0.152819  -1.436790   -2.899270
12  -0.309141  2.455145   -0.954688
12  -3.442578  -1.113643   0.920168
 6  1.061873  1.979913   0.604145
 6  4.019793  -0.663921   0.599367
 6  -3.171500  0.956979   0.937769
 6  -1.076128  -1.305640   0.578535
16

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123.149306 Kcal/mol 5.340266 eV -101.187430 H Child_10_25.log

12	0.581470	-2.864113	-0.122996
6	0.923068	3.675130	-0.952706
6	-2.430107	-1.709992	-0.075678
12	2.225099	2.284709	0.106295
8	2.425518	-2.952011	-0.042216
6	-0.176803	3.133589	-0.614035
8	-4.689070	-0.941003	-0.065838
6	0.120264	2.446604	1.074512
6	-3.470745	-0.718164	-0.014642
6	-0.978971	2.358089	0.311417
6	-1.396733	-2.384178	-0.106098
6	3.050843	0.428010	0.096231
6	3.522809	-2.200578	0.070143
6	-2.096272	1.528772	0.211102
6	-2.879047	0.599711	0.116436
6	3.216625	-0.807501	0.060793

16

123.204116 Kcal/mol 5.342643 eV -101.187342 H MutI_3_79.log

12	-0.460783	-0.477222	2.144397
6	0.301135	1.395332	1.101359
6	-1.519884	0.361490	-1.449567
6	-0.180656	2.010133	-0.099879
6	-0.313542	-1.778068	-1.937383
6	-1.255354	1.402320	-0.834953
6	2.537280	0.257533	1.215709
6	-3.456329	-0.276735	0.907159
12	2.229312	-1.856106	0.877260
8	1.770291	3.093306	-1.280566
8	-4.540187	-0.457614	0.574927
6	0.816369	2.650336	-0.791191
6	-1.169976	-0.878297	-1.890877
6	0.837631	-2.420056	-1.603298
6	1.912799	-2.730188	-1.033445
6	1.646664	1.158603	1.313903

16

123.286535 Kcal/mol 5.346217 eV -101.187211 H Child_2_51.log

6	-2.072720	-1.749593	-0.667060
6	2.886892	1.861087	-2.480508
6	-3.198983	-2.231187	-0.409046
6	3.063596	1.290397	-1.339535
6	-0.972609	-0.861931	-0.852625
6	-3.455276	1.468157	0.570061
6	2.691770	-0.693229	0.190122
6	3.236883	0.602731	-0.211866
6	1.545189	-1.134475	-0.409733
8	3.333024	-1.271554	1.229196
6	-1.402474	0.476466	-0.655768
6	-2.255112	1.242858	-0.145013
6	0.351887	-1.151995	-0.783703
12	4.428135	0.304976	1.567434
12	-4.234019	-0.647325	0.438853
8	-3.938481	2.445614	1.157378

16

123.353431 Kcal/mol 5.349118 eV -101.187104 H Child_5_18.log

6	-5.197559	-0.472075	1.008690
12	4.001682	1.089175	-0.391627
6	-3.209026	-1.371154	-0.374070
6	2.229152	2.056074	-0.667590
6	-2.264737	-1.872945	-1.091604
6	1.107326	1.612752	-0.371251
6	-1.295994	-2.392708	-1.777381
12	3.025921	-1.744267	0.751636
6	-4.194351	-0.925246	0.318709
6	-0.030183	0.856071	0.059877
8	-3.480831	2.443444	0.214473
6	0.383035	-0.439701	0.504528
6	1.008726	-1.449624	0.869049
6	-2.407960	1.909322	0.133387
6	-1.296545	1.309640	0.055305
8	4.315512	-0.576110	0.244776
16			
123.370146 Kcal/mol 5.349843 eV -101.187078 H Child_3_36.log			
8	-4.206432	-0.930653	2.102546
6	4.792743	-0.284490	-0.290592
6	-3.785683	-0.736832	0.967242
6	4.228683	0.844669	-0.207086
6	-3.800122	-0.122582	-0.333794
6	3.310074	1.807528	-0.112587
6	-2.777284	-1.005175	-0.024282
12	3.832071	-2.036552	0.020406
12	-4.525567	1.348355	-1.695501
6	2.335782	2.599971	0.024370
6	-1.575906	-1.577285	-0.318718
6	2.022524	-2.819393	-0.128145
6	-0.470662	-2.108835	-0.342461
6	1.328917	3.230624	0.361785
8	0.428804	4.002820	0.894444
6	0.814763	-2.548026	-0.241528
16			
123.659592 Kcal/mol 5.362394 eV -101.186616 H Original3D_18_7.log			
12	3.869384	1.502001	0.433700
6	1.043882	-1.335146	0.700421
12	-1.053361	-1.076322	0.361062
6	2.961917	-1.648016	-0.952365
6	1.666831	-0.262931	1.362893
6	-2.395496	0.832643	-0.358628
6	-3.031477	-0.411252	0.032668
6	2.346968	0.765889	1.603808
6	4.559481	0.349459	-1.150824
6	-4.231968	-0.908989	0.005859
6	-2.945176	2.091555	-0.437470
8	-5.261974	-1.494066	0.003581
8	-1.069012	0.669436	-0.520897
6	-3.102563	3.356123	-0.336583
6	1.999454	-1.826662	-0.161288
6	3.937416	-0.754525	-1.208259
16			
123.695690 Kcal/mol 5.363960 eV -101.186559 H Child_6_34.log			
6	-7.647924	-0.214151	-0.275183

8	4.289399	-0.646306	-0.393457
6	-6.356634	-0.144878	-0.232753
12	3.825855	1.097692	-0.478347
6	-5.062822	-0.067530	-0.154280
12	3.132460	-1.937464	0.136774
6	-3.795661	-0.008643	-0.037146
6	2.146687	2.289159	-0.086845
6	1.136895	-1.491611	0.526308
6	-2.517520	0.058642	0.036534
6	0.850123	1.933502	0.208856
6	1.195267	3.316075	0.372513
6	0.085438	-0.537812	0.485807
6	-1.233068	0.105004	0.201483
6	0.029343	0.801313	0.334810
8	1.150535	-2.623339	-0.129261

16

123.732887 Kcal/mol 5.365573 eV -101.186500 H Child_6_41.log

8	-5.399081	-2.030837	-0.411891
6	4.722729	-1.461637	0.028695
6	-4.420873	-1.364172	-0.235731
6	4.055734	-0.931919	-0.907049
6	-3.411366	-0.619372	-0.045061
12	3.107517	-1.024991	1.280609
6	-2.275167	0.030608	0.149711
6	3.045875	-0.266436	-1.568163
6	-2.104443	1.425255	0.330110
6	1.200620	-0.225112	1.122397
6	-1.846834	2.641341	0.444137
6	2.002264	0.351625	-1.305853
12	0.136805	2.699322	-0.074750
6	0.166129	-0.113495	0.322080
6	1.006932	0.855218	-0.443685
8	-1.073600	-0.722087	0.184411

16

123.774087 Kcal/mol 5.367359 eV -101.186434 H Original2D_0_26.log

6	-1.572794	1.234785	-0.000000
8	-1.831405	2.599875	-0.000000
6	-2.138844	-0.014972	0.000000
6	-1.338118	-1.129205	0.000000
6	0.513571	2.224079	-0.000000
12	-1.310440	-3.193531	0.000000
6	-0.000000	-0.478230	0.000000
6	-0.199241	0.934630	-0.000000
6	0.166345	-4.717243	0.000000
6	1.231803	-1.249258	0.000000
8	-0.507128	4.488414	-0.000000
6	1.025004	-3.781087	0.000000
6	1.845797	2.334387	-0.000000
6	1.465559	-2.501945	0.000000
6	-0.567644	3.280058	-0.000000
12	2.653742	0.400006	-0.000000

16

123.967935 Kcal/mol 5.375765 eV -101.186125 H Child_12_18.log

8	-5.258751	-0.234241	-0.434971
6	2.735471	-0.919611	-1.328719

6	-3.465313	1.256785	0.421807
6	3.706259	-0.174987	-1.041096
6	-2.256164	1.490841	0.591428
8	1.519041	-3.668106	1.360680
6	-4.100611	0.094404	-0.210102
6	1.109994	-2.853088	0.672113
6	-1.054957	0.722642	0.238117
12	3.722531	1.594037	-0.084520
6	-2.812654	-0.567605	-0.487948
12	0.775864	-0.961212	-0.698486
6	-1.532556	-0.520508	-0.425734
6	1.167114	1.890068	0.713954
6	2.190153	2.619809	0.859621
6	0.302754	0.898731	0.328292
16			
124.061112 Kcal/mol 5.379806 eV -101.185976 H Child_6_30.log			
12	0.914376	-3.142102	0.238927
8	-4.381131	2.809891	0.762602
6	-0.923561	-3.252877	-0.466354
6	-3.686064	1.883290	0.466640
6	1.874733	-1.346505	0.488545
6	1.049796	1.898847	-1.192054
6	2.826674	-0.557843	0.766924
6	-2.933943	0.901110	0.162306
6	3.785249	0.383419	0.872696
6	2.146038	2.432143	-0.858652
6	-1.801820	-2.375885	-0.399277
6	-2.066556	-0.049506	-0.127806
6	3.739034	1.591363	0.444262
6	3.406312	2.591556	-0.342086
12	0.081704	0.152523	-0.452118
8	-2.674906	-1.399856	-0.304173
16			
124.385833 Kcal/mol 5.393887 eV -101.185459 H Child_8_23.log			
6	4.215001	-1.951319	-0.031401
6	-2.783285	2.147462	0.059730
6	2.772992	-1.635154	0.079608
12	-0.847213	2.009001	0.486580
6	3.651203	-0.626141	-0.172159
6	-3.644487	1.284785	-0.190531
12	0.729170	-1.344482	0.362310
8	4.404286	1.601466	-0.746373
8	-1.089403	-1.533559	0.281720
6	-4.291718	0.082922	-0.372847
6	-2.336611	-1.545290	0.047519
6	2.200686	1.185154	0.139641
6	3.549286	0.828208	-0.304708
6	1.022371	1.087242	0.506885
6	-5.020961	-1.005336	-0.606858
6	-3.518238	-1.272113	-0.233123
16			
124.389466 Kcal/mol 5.394045 eV -101.185453 H Child_3_13.log			
6	-3.428773	1.043473	0.526618
6	1.671068	0.411418	1.741241
6	-2.542037	1.235433	1.406718

6	2.141996	-0.809550	1.145734
12	-2.439407	0.145460	-1.028877
6	1.605434	-2.046970	0.822703
6	-0.423688	0.830348	-1.645775
6	2.433052	0.393532	0.546748
8	2.961587	1.496017	-1.591581
12	-0.565397	0.835745	1.694553
6	0.769713	0.610015	-1.070079
6	0.563206	-2.285193	0.177279
6	2.181098	0.922380	-0.840122
6	-0.218683	-0.152539	-0.267453
6	-0.523692	-1.557267	-0.455110
8	-1.625900	-1.914133	-0.973309
16			
124.862321 Kcal/mol 5.414550 eV -101.184700 H Original2D_0_17.log			
6	-0.000000	-1.194665	0.000000
6	0.308911	1.402557	-0.000000
6	1.402871	-0.850475	-0.000000
8	0.553376	-4.026466	0.000000
6	-1.089280	1.057957	0.000000
6	1.488557	0.516747	-0.000000
6	-1.166291	-0.306586	0.000000
6	-0.776388	-3.729091	0.000000
6	-0.848614	-2.284332	0.000000
6	1.088954	2.573310	-0.000000
12	-0.310316	4.143192	-0.000000
6	-1.951026	2.190402	-0.000000
8	-2.086721	-1.345509	0.000000
6	-2.241689	3.407761	-0.000000
12	2.026399	-2.829297	0.000000
6	2.396288	1.751259	-0.000000
16			
125.152232 Kcal/mol 5.427121 eV -101.184238 H MutD_15_34.log			
6	1.776119	-1.771988	-0.644567
6	2.814723	-1.173442	-0.355935
6	-2.225691	-0.513228	1.566806
12	-0.396074	2.315408	0.640250
8	4.808420	0.074182	0.103530
6	0.420335	-1.951044	-0.832636
12	-1.936146	0.038351	-1.166654
6	-0.807177	-1.770659	-0.934373
6	-1.595413	0.586334	1.559177
6	2.617287	1.076403	0.275109
8	-2.003099	-2.652669	0.578093
6	-1.985796	2.295781	-0.768218
6	1.644838	1.809980	0.531533
6	-2.413480	-1.787315	1.287563
6	-2.896002	1.914856	-1.558009
6	3.574269	0.014785	0.017527
16			
125.801670 Kcal/mol 5.455284 eV -101.183203 H Child_10_38.log			
8	5.079114	1.009373	-1.341240
6	-3.016757	-1.308949	-1.097523
6	4.110124	0.590539	-0.754584
6	-3.486504	-0.259599	-1.661037

6	3.094308	0.322476	-0.013955
6	-2.589647	-2.405594	-0.476489
6	2.218701	-0.594880	0.796406
6	-1.522168	-2.811653	0.205455
6	1.664352	0.520262	0.284605
6	-0.507090	-3.211733	0.854552
12	1.297427	-2.358001	1.263038
12	-2.320019	1.432542	-1.440624
6	0.540512	1.182145	-0.139885
6	-2.094169	3.408674	2.459716
8	-2.003790	2.520400	1.732882
6	-0.466909	1.712863	-0.624281
16			
126.395965 Kcal/mol 5.481055 eV -101.182256 H MutD_15_78.log			
6	2.538766	2.817623	0.249340
6	4.343384	1.026321	-0.328127
6	-9.128423	-0.318055	-0.160166
12	6.055260	-1.470676	-0.833720
6	-2.705403	0.003114	-0.144699
6	3.497572	2.060571	-0.142801
12	1.586255	0.793572	0.440077
8	-0.255525	0.373502	0.003937
6	3.129532	-0.920393	0.564425
6	-6.544711	-0.293908	-0.090069
6	-5.258531	-0.247649	-0.121366
6	-1.464299	0.178255	-0.087939
6	-7.826219	-0.327607	-0.082771
8	3.104895	-2.039854	1.058993
6	4.329754	-0.252627	-0.138877
6	-3.993613	-0.149635	-0.146902
16			
126.517291 Kcal/mol 5.486316 eV -101.182062 H Child_10_35.log			
8	-4.788582	-2.218625	0.548311
6	3.236081	-0.310638	-0.685205
6	-4.716946	-1.039744	0.449584
6	3.471080	-1.547892	-0.573710
6	-4.473186	0.232794	0.364587
6	2.618692	0.882234	-0.682846
6	-4.763798	1.677778	0.391437
6	1.566299	1.535861	-0.579507
6	-3.420437	1.249720	0.123164
6	0.309957	1.963253	-0.388872
6	-2.106617	1.241933	-0.148192
6	6.149722	-0.293552	1.144461
6	-0.906914	1.844926	-0.239870
12	1.497291	-2.127591	-0.369591
12	-0.856685	-0.655159	-0.360329
8	6.104723	0.815245	1.165296
16			
126.592546 Kcal/mol 5.489579 eV -101.181942 H Child_12_14.log			
6	0.270635	-4.592645	-0.425850
6	-2.012653	2.404792	-0.539796
6	0.714877	-3.390036	-0.212277
6	-2.474119	1.140087	-0.297528
6	1.139941	-2.191383	-0.016977

6	-0.823710	2.803787	-0.373098
6	2.759843	-0.336995	-0.324502
12	-3.553552	-0.642312	-0.113538
6	3.639579	0.523989	-0.567445
6	0.289082	2.133724	0.085395
6	1.586621	-0.960906	0.157516
6	-1.423683	0.280997	0.214881
8	0.852103	-0.048235	1.001725
6	-0.121997	0.801295	0.403429
12	2.372513	2.043599	0.075708
8	-1.738856	-1.016225	0.477209
16			
126.714756 Kcal/mol 5.494879 eV -101.181748 H Original3D_0_67.log			
6	-1.498611	2.099168	-0.220058
6	0.890863	1.293346	-0.404838
12	3.459232	0.933005	0.528480
6	1.008944	3.163444	-0.500453
6	-2.649048	1.655068	0.124573
6	2.964825	-1.071301	0.495964
8	-2.418726	-2.639575	-0.611470
6	2.193989	-2.072031	0.559573
6	0.019757	-2.503702	-0.136966
6	-3.695757	1.037128	0.492702
12	0.914384	-0.712825	-0.930807
6	1.080126	-2.896848	0.670438
6	-1.266171	-2.708138	-0.306271
6	-0.222597	2.263092	-0.401369
8	-4.678829	0.456523	0.855425
6	1.889856	2.211150	0.106085
16			
126.755894 Kcal/mol 5.496663 eV -101.181682 H MutD_4_68.log			
6	-2.298338	-1.574593	0.000512
8	4.036430	-0.131376	-0.000956
6	3.011323	0.483345	-0.001374
6	-0.905705	-1.237822	0.000355
6	0.046905	-0.309735	-0.000694
6	-3.922859	0.551526	-0.001096
8	2.127547	-3.603447	0.001720
6	1.976372	1.264280	-0.001367
6	-2.774658	-2.836292	0.001909
6	0.512773	1.064154	-0.000972
6	1.333872	-2.703157	-0.000600
6	-0.380066	2.141521	0.000369
6	0.474030	-1.744301	-0.001230
12	-2.412594	1.935557	-0.000615
6	-3.235460	-0.490254	-0.000563
12	1.384182	3.249990	0.002480
16			
126.841530 Kcal/mol 5.500376 eV -101.181546 H Original3D_3_5.log			
6	-1.262490	0.303408	0.059367
6	2.510825	0.326280	-0.223339
6	-0.169530	-0.578124	-0.170983
6	-2.444815	-0.504487	0.166319
6	-3.648771	-0.016020	0.434082
6	1.532854	1.394827	-0.277483

12	-0.361370	2.244430	-0.022049
6	1.113125	0.070858	-0.275435
12	-1.719113	4.966427	0.069329
6	-1.947610	-1.947263	-0.048149
6	-2.673026	-3.069286	-0.034118
6	-0.547554	-1.965093	-0.249636
6	3.752616	-0.121408	-0.109954
6	4.734690	-0.881906	0.140638
8	-3.316137	-4.045529	-0.012293
8	5.724127	-1.529596	0.382892
16			
126.912421 Kcal/mol 5.503450 eV -101.181433 H Child_14_26.log			
6	2.416182	-1.054831	-0.030535
6	-1.773534	3.451828	0.043716
6	1.158209	-0.806062	-0.024568
8	2.939767	1.617587	-0.083418
6	3.704576	-1.042893	-0.003099
6	1.757473	1.717055	-0.036610
6	-0.117616	-1.201794	0.012895
6	-0.738262	2.383448	0.032040
8	-4.327521	-1.162416	0.008225
6	-2.184578	2.144709	-0.013200
6	4.983416	-1.159740	0.046305
6	0.488818	1.968548	0.016285
6	-1.359156	-1.463444	0.021209
12	-3.228382	0.341690	0.014381
12	-3.158554	-2.535161	-0.024608
6	6.288681	-1.156778	0.056271
16			
126.941697 Kcal/mol 5.504720 eV -101.181386 H Child_7_35.log			
6	1.003767	-3.171587	-0.201385
6	5.367731	1.441435	0.325698
6	0.295141	-1.908399	-0.125949
8	4.366846	2.092311	-0.051969
6	-0.240282	-0.568399	-0.129287
8	-7.732361	0.549861	0.340762
6	-1.539040	-0.231974	-0.171938
6	-6.552223	0.519879	0.164737
6	1.683117	-1.850032	-0.109768
6	-5.283417	0.495659	-0.009703
6	0.927930	0.347855	-0.097724
6	-4.030269	0.317914	-0.103610
6	-2.764063	0.091234	-0.195669
12	2.479558	1.634996	-0.291340
6	2.116605	-0.449294	-0.074578
12	4.271620	-0.913589	0.463400
16			
127.103701 Kcal/mol 5.511745 eV -101.181128 H MutD_3_72.log			
6	4.096201	0.562773	0.795236
6	2.922265	-0.366562	0.864844
12	-0.249189	-2.545730	-0.114375
8	1.940098	2.692122	-1.055559
6	-3.375257	-1.515696	-0.256329
6	-0.601964	0.542492	-1.238556
6	1.414219	-2.477597	1.138426

6	2.191333	-1.492825	1.139273
6	-2.844841	1.976710	1.061890
8	-3.015317	2.649001	1.990496
6	0.253589	-0.660653	-1.153625
6	-2.311268	-2.138493	-0.076242
6	1.905077	1.491653	-0.737844
6	0.771460	0.631047	-1.104138
6	2.851283	0.810084	0.125915
12	-2.670047	0.303515	-0.788341
16			
127.115342 Kcal/mol 5.512250 eV -101.181109 H Child_9_45.log			
6	3.480538	1.438100	1.146341
6	-3.649634	0.509016	-1.587131
8	3.554319	-0.618590	-1.749613
6	-3.133068	-0.229919	-0.515025
6	2.864109	0.573399	0.175617
6	-2.765429	1.115857	-0.538718
6	2.881030	-0.585663	-0.683925
6	-2.819934	-1.399684	0.161444
6	2.154827	1.670534	0.596051
8	-1.644507	2.944357	0.694011
6	2.037356	-1.653416	-0.222285
6	-1.770252	1.941647	-0.135229
6	1.216984	-2.464961	0.205592
6	-2.436022	-2.443200	0.710290
12	0.267640	2.419974	0.271592
12	-0.571100	-3.206340	0.775632
16			
127.166793 Kcal/mol 5.514481 eV -101.181027 H Child_3_25.log			
8	-1.246591	1.777159	-0.215398
8	6.299505	-0.874082	0.172381
12	-4.691755	-0.179119	0.170104
6	5.352900	-0.226569	0.073028
6	-3.955509	-2.059917	0.291749
12	3.035199	0.395170	-0.029917
6	-0.191851	-2.189682	-0.148489
6	2.064904	2.188661	0.245563
6	1.134452	-1.892412	-0.237940
6	0.849443	2.471462	0.138034
6	-2.746753	-2.311904	0.114673
6	-2.574029	1.757802	-0.222673
6	2.312865	-1.482017	-0.295415
6	-0.473439	2.913237	0.059756
6	-1.399781	-2.371700	-0.046236
6	-3.797308	1.566833	-0.195071
16			
127.241868 Kcal/mol 5.517737 eV -101.180908 H MutI_2_65.log			
6	-1.458439	6.277974	-0.000000
6	-0.986903	-3.513310	-0.000000
6	0.169556	-4.041825	0.000000
12	2.167016	-3.152645	0.000000
6	-2.369486	0.016517	-0.000000
8	4.657382	-1.484123	0.000000
6	-2.303164	-1.321596	-0.000000
6	4.932339	-0.363965	0.000000

6	-2.510720	1.275495	-0.000000
12	0.000000	-1.186370	0.000000
6	-2.527843	2.588517	-0.000000
6	-2.014745	5.113947	-0.000000
6	-1.939530	-2.533443	-0.000000
6	-2.291707	3.830841	-0.000000
6	0.738990	0.942711	0.000000
8	1.513335	1.788748	0.000000
16			
127.636480 Kcal/mol 5.534849 eV -101.180279 H Child_8_13.log			
6	4.207244	0.651587	-0.474618
12	-3.099269	1.627298	-0.009710
12	2.780524	-1.093001	0.184280
6	-1.446198	2.800538	0.080178
6	0.520978	-3.198330	-0.062878
6	-3.291501	-0.382222	0.663214
6	3.066894	1.175458	-0.320765
6	-1.964085	-2.556378	-0.076547
6	-0.832751	-3.047785	-0.075706
6	-0.216048	2.687031	0.007318
6	1.706815	-2.816162	-0.003924
6	-3.156261	-0.338650	-0.843787
6	1.744558	1.398635	0.107866
6	-2.787188	-1.454491	-0.096271
8	1.191325	0.424042	0.699549
8	1.122450	2.585090	-0.139463
16			
127.778505 Kcal/mol 5.541007 eV -101.180052 H Child_16_16.log			
8	-4.624941	3.185581	0.684665
6	6.897555	1.826952	-1.365321
6	-3.790134	2.403578	0.774357
6	5.860667	1.312870	-0.774382
6	-2.490745	-1.364853	-1.699254
6	4.834164	0.804743	-0.192630
6	-1.850245	-2.323690	-1.253907
6	3.809252	0.305092	0.384995
6	-1.015804	-2.980569	-0.397784
6	2.777511	-0.204290	0.915840
6	-2.985768	-0.090962	-1.744774
8	1.774927	-0.647685	1.400664
6	-3.252011	1.132099	-1.551450
12	-0.223511	-1.236611	1.369300
6	-0.254518	-3.213725	0.577748
12	-2.146442	0.741059	0.403763
16			
127.888986 Kcal/mol 5.545798 eV -101.179876 H MutD_3_66.log			
6	-0.421389	1.744716	-0.153625
8	-2.053708	3.521908	-0.767163
6	2.736905	2.757863	0.667355
6	0.924094	1.213913	0.100111
6	0.316289	-2.142651	-0.276804
8	-3.926869	0.253960	0.688330
6	-2.963442	-0.406172	0.435532
6	-1.251698	2.671833	-0.484251
6	2.303692	1.515057	0.362078

12	2.356245	-1.907044	-0.368597
6	-0.534808	-1.055815	-0.052819
6	3.889896	-0.620354	0.085283
6	-1.989385	-1.219113	0.165417
6	-0.031015	0.303718	-0.047200
6	3.225141	0.422263	0.260365
12	-1.471334	-3.202830	-0.109569
16			
128.086887 Kcal/mol 5.554380 eV -101.179561 H MutI_4_79.log			
6	-3.185765	-1.319171	0.125220
6	-2.436830	-2.443941	0.061220
6	-3.570209	-0.164023	0.164046
6	-1.446921	1.823834	0.001457
6	-2.832915	2.065524	-0.086790
8	-3.864149	1.117271	0.224545
12	4.680067	1.514214	0.110793
6	-0.092053	-3.369968	-0.098400
12	1.859943	1.590207	0.047580
6	2.149721	-2.179830	-0.116168
6	1.093769	-3.029500	-0.130328
6	-3.077928	3.332303	-0.464571
6	2.784194	-1.134768	-0.069228
8	3.237417	0.100733	-0.013495
6	-1.419422	-3.132356	-0.033431
6	-0.210016	1.719048	0.048828
16			
128.642166 Kcal/mol 5.578459 eV -101.178676 H Original2D_0_19.log			
12	-0.026199	-2.866641	0.000000
6	-3.002162	-0.690666	0.000000
6	-2.378136	0.431654	0.000000
6	1.297553	-0.118884	-0.000000
6	-2.191042	-3.046490	0.000000
6	-0.000000	-0.703651	0.000000
6	-2.930075	-2.021125	0.000000
6	1.934447	1.078576	-0.000000
6	2.749238	-0.081565	-0.000000
6	0.219382	2.832925	-0.000000
6	-0.797249	1.808176	-0.000000
6	-2.218168	1.972013	-0.000000
8	1.691797	2.376669	-0.000000
12	2.903599	-2.317375	0.000000
8	0.107775	4.031523	-0.000000
6	-0.838017	0.362813	0.000000
16			
128.734113 Kcal/mol 5.582447 eV -101.178530 H Child_7_43.log			
12	-3.278947	-0.057326	0.258437
8	1.939011	-1.833953	-0.380277
8	-3.529103	4.241741	0.043657
6	2.952411	-1.190203	-0.206720
6	-3.037391	3.156735	-0.040216
6	3.994834	-0.494467	-0.008734
6	-2.622438	1.932659	-0.087270
12	-0.100113	-1.724041	-0.437837
6	-1.458095	1.201872	-0.391415
6	4.919187	0.379416	0.152065

6	-2.974823	-2.100873	0.414928
6	-2.925163	-3.520171	0.629551
6	5.810999	1.304182	0.305374
6	6.680872	2.252616	0.441107
6	-0.680995	0.236432	-0.535190
6	-1.781153	-2.805845	0.134148
16			
128.844783 Kcal/mol 5.587246 eV -101.178353 H MutI_16_35.log			
6	-3.436738	-0.164667	-0.122529
6	1.806345	-1.395678	1.769576
6	-5.472260	0.979602	1.026608
8	1.067463	-0.368086	-1.570108
12	0.631434	-2.275890	-0.546166
6	1.768815	1.167067	2.170515
6	-4.501017	0.355341	0.426213
6	1.891406	-0.073953	2.122864
6	2.027333	0.598121	-1.583822
6	-0.205982	0.117980	-1.027116
12	1.484404	2.143909	0.389139
6	1.612163	-2.494095	1.201600
6	-1.118435	-1.008575	-0.899633
6	-2.371351	-0.691082	-0.576191
8	-0.184339	1.250501	-0.531011
6	2.590548	1.697346	-1.392537
16			
128.878615 Kcal/mol 5.588713 eV -101.178299 H MutI_10_79.log			
6	3.198801	1.103688	0.528704
6	-4.806347	1.569305	0.228474
8	-5.631383	2.418139	0.394988
12	5.777236	1.067184	-1.046869
12	-1.235693	-2.814734	-0.429049
6	4.414561	1.423130	0.528951
6	1.963705	0.555291	0.598112
6	-4.160827	0.468897	0.043942
8	1.985701	-0.709904	1.325545
6	0.491657	-2.614444	0.518864
6	-1.623477	0.110296	-0.760357
6	-3.041854	0.005710	-0.533163
6	0.765656	0.816243	-0.029788
6	1.233152	-1.708764	0.927212
6	-0.387436	0.606428	-0.436682
6	-2.269768	-1.118327	-0.956475
16			
129.012435 Kcal/mol 5.594516 eV -101.178086 H Child_7_20.log			
6	5.098019	-1.028228	-0.006227
8	-4.723768	-0.133385	0.002611
6	3.487909	1.278434	0.002866
6	-3.931016	-1.277824	0.007733
6	4.117227	0.049452	0.000439
6	-3.908485	0.903943	-0.002623
6	2.643455	2.192729	0.004211
6	-2.871820	-1.913843	-0.005229
6	3.652623	-1.235586	0.000611
6	-2.808156	1.448226	-0.002127
12	0.627355	2.129814	0.000498

6	-1.439893	1.676259	-0.003295
6	2.398050	-1.811450	0.002972
12	-0.821931	-1.527560	-0.001726
6	1.175776	-2.030838	0.003527
8	-0.694633	0.541548	-0.002912
16			
129.118367 Kcal/mol 5.599109 eV -101.177917 H Child_3_35.log			
6	-0.858352	2.210601	-0.816763
6	1.784143	-1.042537	0.994456
6	-1.266414	2.261594	0.569932
6	4.717807	1.600931	-0.338936
6	-2.363876	1.798896	1.242078
8	4.847994	0.674509	-1.015834
6	0.089908	2.138389	0.212246
6	1.118611	-2.037320	0.649186
12	-2.352707	0.929974	-1.660289
6	0.144245	-2.908461	0.062413
6	-2.877998	0.697242	0.760380
6	-1.160166	-2.318369	0.109130
6	-2.903386	-0.368265	-0.087784
6	-2.042981	-1.461192	0.057433
12	1.657978	0.985813	0.977675
8	0.407946	-3.976821	-0.520573
16			
129.165356 Kcal/mol 5.601147 eV -101.177842 H Child_18_28.log			
8	-7.399950	0.637701	0.116323
6	5.481534	0.656887	0.555555
6	-6.280547	0.230677	0.147578
12	4.494555	-1.218317	0.213597
6	-5.072019	-0.208213	0.187922
6	4.383080	1.241928	0.291724
8	-0.489690	2.672235	-0.217217
6	0.579616	2.142438	-0.194973
6	2.415070	-1.323933	-0.311749
6	-3.889606	-0.664435	0.160840
12	0.491125	-1.992663	-0.260869
6	1.682472	1.446383	-0.196384
6	2.356938	0.025442	-0.338178
6	3.063937	1.207801	-0.110962
6	-1.498315	-1.592541	-0.035791
6	-2.674000	-1.153722	0.073489
16			
129.284949 Kcal/mol 5.606333 eV -101.177652 H MutD_18_34.log			
8	9.189880	0.382251	-1.148893
6	0.756402	-1.617202	0.846185
6	-2.364886	-1.552605	-0.201214
6	1.423621	0.853584	1.090170
6	-5.926750	-0.701308	-1.346715
6	-0.108106	-2.724130	0.543820
6	-3.336862	-0.630048	-0.519084
6	1.199759	-0.484000	1.002958
12	-0.160070	3.373980	0.574047
6	1.376636	2.098751	1.079926
6	-3.655910	0.660738	-0.622132
12	-2.727505	2.522544	-0.289763

6	-1.390740	-2.219308	0.121609
6	10.019151	-0.378307	-0.911377
6	-4.726491	-0.371708	-0.959007
8	0.192113	-3.927879	0.628612
16			
129.479189 Kcal/mol 5.614756 eV -101.177342 H Child_3_16.log			
8	-5.719609	-1.080306	-0.156242
8	5.125336	-0.650865	-0.887851
6	-4.607953	-0.841391	-0.161186
6	3.982215	-0.654883	-0.611350
6	-2.125566	1.884749	-0.833933
6	2.691958	-0.626735	-0.226324
6	-0.917424	2.236798	-0.784004
6	1.763557	-1.591250	-0.590431
6	0.413216	2.138606	-0.497836
6	2.151930	0.551667	0.653384
12	-2.510440	-0.090480	-0.387065
6	0.465449	-1.512164	-0.210943
6	1.413600	1.548825	-0.065288
6	1.876392	0.328474	1.957664
12	-0.262932	0.115518	1.797516
6	-0.768267	-1.204546	-0.058531
16			
129.767041 Kcal/mol 5.627239 eV -101.176883 H MutD_3_78.log			
6	-1.150371	1.313833	0.140214
6	4.055715	0.809774	-0.563594
6	-3.390573	-0.996810	-0.311243
12	-0.859204	-1.732046	-0.294044
6	2.235443	2.434222	0.211708
12	3.186100	-1.113533	-0.645875
6	-0.238515	2.271167	0.430524
6	3.297151	1.754862	-0.161285
6	-2.916255	-2.138442	-0.540993
8	1.581175	-2.758492	1.451888
8	-0.623455	0.118306	-0.148790
6	-3.972272	1.756623	0.113588
6	0.991479	2.626900	0.402635
6	-2.586209	1.354809	0.125737
6	-3.493869	0.363463	-0.087306
6	1.237523	-2.338994	0.382387
16			
129.958522 Kcal/mol 5.635542 eV -101.176578 H Child_2_15.log			
8	3.682829	-2.259956	-0.150227
6	-5.503316	-2.136807	-0.269838
6	2.395215	-2.241528	0.046456
6	-4.422619	-1.414248	-0.155078
6	1.193282	-1.952570	0.171472
12	0.844023	2.919809	-0.202838
6	0.412167	-0.798290	0.302760
8	-2.439209	1.513409	-0.070377
12	3.639628	-0.263957	-0.216831
6	-3.360287	-0.700220	-0.043500
6	-0.877533	-0.211319	0.317212
6	-1.139610	2.136111	0.051738
6	1.061061	0.589444	0.280372

6	-2.274073	0.049088	0.071212
6	2.220607	1.250072	-0.002829
6	-0.330355	1.113958	0.363497
16			
130.105530 Kcal/mol 5.641917 eV -101.176344 H Child_4_61.log			
6	0.041400	2.529009	-1.216847
8	4.398519	-0.781037	1.187636
12	2.062246	2.191093	-1.161988
6	2.034989	-1.291484	0.402669
6	-0.215540	1.436568	-0.646517
12	0.472462	-2.527877	-0.320612
8	-3.913271	2.255515	1.617099
6	-4.714016	-1.883613	-0.725077
6	-3.070847	1.557921	1.263880
6	3.272144	-0.547501	0.764933
6	-0.084849	0.158587	-0.025428
6	-3.492012	-1.525891	-0.540397
6	2.518597	0.546100	0.114368
6	-2.233545	-1.207398	-0.377947
6	1.214321	-0.094525	0.366812
6	-0.987054	-0.970175	-0.154897
16			
130.504215 Kcal/mol 5.659205 eV -101.175709 H Child_9_40.log			
6	-1.024105	2.969114	0.777123
6	-4.344607	-1.190161	1.608588
8	-1.289118	2.199991	-0.055994
6	-1.553318	-0.978277	1.195877
6	4.121424	0.363645	0.502948
6	-2.928555	-1.061255	1.267461
8	3.786597	1.216300	1.304471
6	-0.475045	-0.759635	0.614023
12	-1.101276	0.480130	-1.460319
12	5.086636	-1.174079	-0.525108
6	-3.860172	-0.806418	0.288764
6	-3.038888	-0.028415	-2.040909
6	0.508912	-0.294528	-0.263128
6	3.120813	-0.546800	-0.351276
6	1.818029	-0.431883	-0.284669
6	-3.645179	-0.402541	-1.008581
16			
130.526548 Kcal/mol 5.660174 eV -101.175673 H Original2D_16_2.log			
6	-0.056967	1.981912	-0.000000
6	-1.231879	1.221167	0.000000
12	-3.318700	3.071744	0.000000
6	1.260577	1.585072	-0.000000
6	2.175154	0.759059	-0.000000
6	-1.731655	-0.077802	0.000000
8	2.970767	-0.257792	-0.000000
6	-1.260670	2.689853	-0.000000
6	-3.991780	0.803084	0.000000
6	2.168190	-1.679002	-0.000000
6	-3.132069	-0.256693	0.000000
12	-0.000000	-1.268356	0.000000
6	-4.932249	1.699213	0.000000
6	3.977944	-3.513059	-0.000000

8	4.830839	-4.337480	-0.000000
6	2.990664	-2.692548	-0.000000
16			
130.572866 Kcal/mol 5.662183 eV -101.175599 H MutD_18_66.log			
12	1.639065	-2.784753	0.195664
6	-2.890920	0.470924	0.492363
6	-7.829632	-0.681532	-0.372547
6	-4.131507	0.208439	0.337919
6	-1.630075	0.721421	0.620913
6	2.533023	-0.279724	-1.498398
8	3.279961	1.102312	1.388488
6	3.208876	-1.253601	-0.855293
6	0.856247	1.136161	1.010237
6	1.865904	0.697668	-1.998111
6	-0.400638	0.920831	0.718153
6	2.086262	1.120568	1.160899
6	-6.611725	-0.390974	-0.052152
6	-5.362345	-0.085057	0.164203
8	1.100203	1.532959	-2.374147
12	4.594091	-0.264657	0.597349
16			
130.672875 Kcal/mol 5.666519 eV -101.175440 H MutD_7_72.log			
8	-3.143025	3.016198	0.947652
12	1.550095	-1.635227	0.685752
8	-2.882505	-1.383221	-0.643748
6	6.451052	1.223319	-0.631326
6	4.586337	-0.459381	0.051423
6	7.295336	2.159440	-0.981864
6	-2.457093	0.657077	0.430251
6	-4.465514	0.362927	-0.985270
6	-0.161912	-0.505467	1.055775
6	-2.831578	1.910021	0.696363
6	5.526649	0.409442	-0.271475
6	-5.501821	0.931309	-1.468231
12	-1.241821	-2.250291	-0.261593
6	3.527060	-1.055632	0.428708
6	-1.219287	0.132897	0.870237
6	-3.331735	-0.172219	-0.448114
16			
130.728092 Kcal/mol 5.668914 eV -101.175352 H MutD_5_68.log			
8	2.912201	-0.025743	-0.155965
6	-5.488035	-1.258966	-0.112502
6	-0.656793	-0.578605	0.128512
12	2.739742	1.771502	-0.289515
6	-6.628169	-1.846441	-0.254338
8	1.535245	-1.846765	0.140990
6	4.881725	-2.972092	0.117685
6	3.870000	-2.202751	-0.003802
6	-3.080612	-0.348527	0.007388
6	0.467402	-1.077161	0.139549
6	-1.853114	0.151941	0.137373
12	-1.485485	2.249106	0.280299
6	1.353437	3.194499	-0.096671
6	-4.300624	-0.711248	-0.081435
6	0.136387	3.425474	0.077734

6	2.859953	-1.320661	-0.021094
16			
130.831381 Kcal/mol 5.673393 eV -101.175187 H MutD_14_64.log			
6	1.763381	0.087430	0.187389
6	-4.912222	-1.427548	-0.068087
6	1.751521	3.892311	-0.403108
6	2.837255	-0.650993	0.162630
8	-0.109773	1.475002	0.066450
6	-6.129773	-0.678757	-0.099237
6	3.786673	-1.505052	0.139825
12	-0.418352	3.454954	0.095093
6	-3.559005	-1.411475	0.075290
8	5.378833	-3.341590	-0.266148
6	1.295745	1.363465	0.000279
12	-0.497201	-0.442409	0.245228
6	1.836641	2.642869	-0.202544
6	4.613093	-2.464623	-0.061925
6	-2.320206	-1.323239	0.186848
6	-6.157411	-2.060693	-0.331739
16			
130.905860 Kcal/mol 5.676623 eV -101.175069 H Child_9_33.log			
8	4.793653	-1.951575	1.354905
8	-8.142912	-0.200881	0.540996
6	3.986474	-1.379036	0.696251
6	-7.921293	0.588053	-0.266384
6	1.533121	3.667202	0.158600
6	-1.798378	-2.697629	-0.577120
6	3.288747	-0.568792	-0.012630
6	-1.756628	-1.382708	-0.037364
6	0.520335	2.958305	0.412466
6	-1.627140	-0.206017	0.339385
12	2.657589	2.260131	-0.837295
6	-0.488042	-2.696407	-0.614142
6	-0.464115	2.051016	0.582027
6	-1.137830	1.035640	0.525985
6	2.489281	0.128211	-0.830130
12	1.262983	-1.574079	-0.615111
16			
131.016955 Kcal/mol 5.681440 eV -101.174892 H Child_11_63.log			
6	-1.326696	2.302129	-0.109903
12	-3.179605	-1.763694	0.112061
12	0.610230	1.687830	0.207248
8	-1.360222	-1.860702	0.053426
6	-2.541669	1.973000	-0.238122
6	-0.151162	-1.446883	0.101498
8	3.933698	1.165365	0.155819
6	2.537200	0.902392	0.316942
6	-5.010840	-0.725473	0.015545
6	0.984120	-0.977250	0.157679
6	4.476152	-0.056080	-0.157780
6	-4.382809	0.392923	-0.160763
6	5.061064	-1.342070	-0.471406
6	-3.832814	1.604784	-0.270301
6	3.580974	-1.085722	-0.230954
6	2.313926	-0.462905	0.129954

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16
131.025167 Kcal/mol 5.681796 eV -101.174879 H MutD_2_76.log
8   1.345774   -2.226345   -0.380301
6   4.321150   2.901485    1.259908
6   0.336716   -1.299075   -0.689737
6   2.960500   0.931226    0.264513
6   -1.066208  1.724897    -1.155451
8   3.483417   -2.135331    0.482010
6   -4.195046  -0.381391    1.198286
6   3.642935   1.912185    0.727197
12  -1.767132   -1.176756   -0.558834
6   -4.897951  -0.621405    2.279500
6   2.536059   -1.523724    0.024764
12  -3.033853   1.824849    -0.656638
6   -3.486961  -0.084655    0.117673
6   -0.045462  1.055088    -0.923145
6   0.841367   -0.019396   -0.652063
6   2.215953   -0.075852   -0.156112
16
131.031267 Kcal/mol 5.682061 eV -101.174869 H Child_4_60.log
6   -3.203288  -2.218808   -0.113430
6   -4.328297  1.871158    -0.121659
6   -1.838383  -1.995985    0.195716
6   -3.210888  2.351082    0.144680
6   0.377508   -2.293700   -0.182748
12  4.688792   2.720581    -0.408052
12  0.172190   0.067859    0.235054
6   -4.982413  0.720587    -0.366276
6   -4.270386  -1.623230   -0.333746
6   -1.872637  2.410911    0.373909
6   -0.697028  -2.830305    0.204381
6   -0.700036  1.983292    0.492617
6   9.424359   -1.440729   -0.528752
6   -5.041006  -0.515057   -0.463563
8   9.525202   -0.767391    0.403414
8   -1.559806  -0.729680    0.380236
16
131.570797 Kcal/mol 5.705457 eV -101.174009 H MutD_17_56.log
6   -0.080876  2.064353    -0.077640
6   1.734970   0.314791    -0.193032
6   2.606891   1.474826    -0.005720
6   2.327396   -2.025010   -0.095499
6   -1.303294  1.910164    -0.014999
8   -6.367611  -0.987490    0.301012
6   -2.726092  -0.053179   -0.087301
6   -3.977905  -0.411062    0.021766
12  4.485428   0.606348    0.232147
6   4.891484   -1.447154    0.317138
6   -5.228806  -0.671426    0.165653
8   -2.542575  1.537068    0.044771
6   1.327744   -1.028677   -0.287870
12  -0.759630  -1.019314   -0.331095
6   3.633836   -1.653893    0.091557
6   1.223303   1.619430    -0.097202
16

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131.739658 Kcal/mol 5.712779 eV -101.173740 H Child_4_17.log

12	0.355999	3.280708	0.046812
6	-2.570554	-2.952191	-0.001424
6	-1.672808	3.477963	0.009940
12	-0.581007	-3.280166	0.041102
6	2.149725	2.323680	0.051250
6	-3.287685	-1.916772	-0.026142
6	3.129452	1.554525	0.030132
8	1.147514	-2.780896	0.060121
6	-2.661776	2.696829	-0.009344
8	4.242514	-0.496570	-0.087012
6	4.352490	0.865365	-0.067769
6	3.082117	-1.201784	-0.025649
6	2.188901	-2.020193	0.016456
6	-3.647755	1.789862	-0.033550
6	-3.963467	-0.763356	-0.048882
6	-3.835327	0.514942	-0.034989

16

131.802472 Kcal/mol 5.715503 eV -101.173640 H Child_4_35.log

6	3.754313	-0.758826	2.314471
8	-3.380048	-2.128162	-0.497862
6	3.027574	-0.172387	1.451853
6	-1.005560	-1.936352	-0.310804
6	2.258308	0.558916	0.528210
6	-2.357385	-1.484174	-0.187638
8	-3.952361	2.012504	0.447446
6	0.210732	-2.112050	-0.482340
6	2.702591	0.574187	-0.819150
6	-2.439421	-0.090197	0.269757
12	1.672153	2.102224	-1.885600
6	-1.604478	0.914589	0.661677
6	0.943380	1.094176	0.798154
12	2.118185	-1.487618	-0.867350
6	-3.028516	1.202326	0.469561
6	-0.265669	1.134792	0.879370

16

132.440902 Kcal/mol 5.743188 eV -101.172622 H Child_9_58.log

8	-4.244991	-0.171076	-0.822658
6	4.562142	0.946584	-0.353785
6	-4.317563	-0.625005	0.505196
6	3.828596	0.822207	0.675435
6	-2.165337	1.184461	-1.517627
6	2.796340	0.722051	1.559056
6	-3.187126	0.552995	-1.246599
6	-2.163882	0.057889	1.826408
8	1.214254	-4.104573	-0.484911
6	1.645309	0.652654	2.028270
6	1.910353	-4.881329	-0.968697
6	0.334775	0.492554	2.254040
6	-3.217472	-0.205980	1.225569
6	-0.899490	0.350648	2.131414
12	-0.185805	1.625852	-1.792330
12	2.642973	1.189715	-1.395296

16

132.458101 Kcal/mol 5.743934 eV -101.172595 H Child_5_29.log

6	-3.211409	3.311059	-0.244702
6	0.488905	-3.471413	0.038601
6	-1.999867	2.518058	-0.333717
8	1.812536	-3.478472	-0.164755
6	-0.643863	2.338561	-0.513461
6	-0.692747	-3.218823	0.172438
6	4.101805	2.868204	1.317157
6	-1.947596	-2.703796	0.317827
6	0.563544	2.072006	-0.629225
6	2.345060	-2.244517	-0.344002
6	-3.172601	1.876352	0.016160
6	-2.988643	-2.033844	0.403835
8	3.580095	2.125892	0.603025
6	2.694931	-1.072058	-0.485122
12	2.222717	0.889742	-0.541975
12	-3.586564	-0.107917	0.391899
16			
132.510885 Kcal/mol 5.746223 eV -101.172511 H Child_5_54.log			
6	5.034773	-1.404136	-1.101180
6	-0.740848	-2.984882	0.973703
6	1.188008	0.894103	-2.943484
6	-0.076929	-2.104694	1.555894
6	0.506816	1.213077	-1.883307
6	0.527255	-0.977243	2.040284
8	5.274243	-0.549130	-0.373239
6	0.925423	0.173850	2.296818
6	-0.011097	1.649866	-0.751865
12	-2.158883	-2.781784	-0.421498
6	-1.315511	1.977593	-0.128382
12	0.508784	1.998000	1.497029
6	-2.298136	1.258725	-0.662362
6	-3.060932	-1.129429	-1.277894
8	-1.242547	2.742557	0.959939
6	-2.754218	0.076166	-1.051553
16			
132.678573 Kcal/mol 5.753495 eV -101.172244 H Child_3_24.log			
6	3.238424	0.130303	0.629462
6	-3.642428	-3.123580	-0.047150
12	3.332056	-1.874941	0.050710
6	-3.069752	-1.973955	0.002735
8	1.952694	2.057823	-0.393941
6	-0.896359	-0.896083	0.148781
6	2.365216	0.854412	-0.085256
6	-2.355491	-0.816981	0.092182
12	0.018395	2.258349	-0.035652
6	0.045565	-1.782044	-0.354901
6	1.377978	-0.302423	0.038638
6	-2.826405	0.510487	0.120361
8	-1.876463	2.827138	-0.034917
6	0.045844	0.145903	0.405312
6	1.379530	-1.719577	-0.460483
6	-2.464664	1.693441	0.052015
16			
132.751368 Kcal/mol 5.756651 eV -101.172128 H MutD_1_64.log			
8	0.391014	1.949431	0.004034

6	0.632759	-1.444053	-0.071229
6	-3.159200	1.872939	0.004232
8	-1.923894	2.481335	0.007078
6	-3.686858	-0.577090	0.002356
12	1.853950	0.701734	-0.008472
6	-1.344768	0.280810	-0.044626
6	6.147410	0.428170	0.073300
6	-0.837822	1.566535	-0.013053
12	2.546901	-2.242275	-0.027568
6	4.916383	-0.031558	0.047937
6	-2.790031	0.395294	-0.020327
6	-0.419619	-0.769747	-0.065193
6	-4.554214	-1.520537	0.037310
6	3.674849	-0.467907	0.016901
6	-5.336750	-2.559463	0.089656
16			
133.030911 Kcal/mol 5.768774 eV -101.171682 H Child_8_22.log			
8	-0.960213	-3.505303	0.059210
6	4.989430	0.242920	0.479136
6	-0.784934	-2.278137	0.217727
8	3.949843	0.779988	0.477908
6	1.830425	-1.744038	-0.650778
6	-1.989447	2.607002	-0.258206
6	0.506814	-1.625254	-0.030135
6	1.167341	-0.499252	0.153419
6	2.985571	-1.842762	-1.218445
12	1.921346	1.438096	0.185849
12	-2.582000	-1.162994	0.522715
6	-2.998098	1.882513	-0.285712
6	-4.412245	-0.299452	0.025431
6	-0.679183	2.935581	-0.242652
6	-3.836918	0.816057	-0.169885
6	0.556377	2.888369	-0.153189
16			
133.072127 Kcal/mol 5.770561 eV -101.171617 H Child_10_17.log			
6	1.952451	2.953589	0.057913
12	-3.421088	-1.208653	-0.067458
6	2.533836	1.760535	0.001521
6	-1.353451	-1.259500	0.121215
8	3.843479	1.145784	-0.162191
6	-4.233122	0.631461	-0.189444
6	1.868126	0.442050	0.115212
6	3.211680	-1.496038	-0.139409
6	3.132115	-0.138820	-0.038449
6	-3.975399	1.865293	-0.090767
6	0.693490	-0.294559	0.153689
6	0.848067	-1.715087	0.051569
6	-0.726000	-0.025514	0.190592
6	2.139551	-2.170341	-0.065546
12	-1.914904	1.709005	0.063082
8	-0.407998	-2.311112	0.042683
16			
133.259076 Kcal/mol 5.778668 eV -101.171319 H MutD_18_50.log			
6	-0.888959	2.322855	-0.009027
6	-5.341711	-0.135882	0.002784

8	7.349994	-0.856421	-0.011160
6	-3.320412	1.556464	0.008897
6	-1.213399	-1.560116	0.029164
6	0.394242	1.971330	-0.010378
12	0.742732	-0.900340	0.021075
6	6.203461	-0.533999	-0.006722
6	-2.122475	2.118681	0.001321
6	2.482355	0.441919	0.006444
6	4.975379	-0.194491	-0.005089
8	-5.241570	-1.452937	-0.019367
6	1.504740	1.391583	-0.004262
6	-4.170437	0.617308	0.009793
12	-3.276546	-1.654964	-0.015017
6	3.753611	0.194100	0.005661
16			
133.597990 Kcal/mol 5.793364 eV -101.170778 H Child_5_14.log			
6	5.358200	-2.213615	0.003173
8	-8.604025	-0.534952	-0.105465
6	3.883754	-2.346776	-0.016836
6	-7.415022	-0.329805	-0.085920
6	4.461105	-1.091241	0.010089
6	-6.164445	-0.126077	-0.050051
8	5.252294	2.367120	-0.201335
6	-4.886178	0.116599	0.005671
6	4.681907	1.360371	-0.076362
6	-3.652259	0.342987	0.056970
6	3.876944	0.241571	0.016811
6	-2.365720	0.636099	0.121164
12	1.901425	-1.682624	-0.007941
6	-1.131937	0.921132	0.184331
12	0.766258	1.485961	0.094449
6	2.487261	0.439190	0.067011
16			
134.039534 Kcal/mol 5.812512 eV -101.170075 H Original3D_15_7.log			
6	0.983127	-0.671902	1.097679
6	-1.073984	-0.060190	-0.289794
6	-1.214707	0.773592	0.750027
12	-3.177811	1.307903	0.904190
6	-1.960499	-1.034905	-0.987226
6	0.236087	0.413660	0.353311
6	-3.318816	-0.542975	-0.864065
8	0.586745	-1.189036	2.153356
6	2.201345	-1.129289	0.451819
6	3.317348	-0.671443	-0.209170
6	1.697788	2.471149	-0.642233
8	-1.598158	-2.112405	-1.462247
6	3.164588	-2.111985	-0.002004
6	1.068773	1.465299	-0.209436
6	-4.231497	0.245198	-0.528929
12	3.417310	1.319954	-0.824918
16			
134.143858 Kcal/mol 5.817036 eV -101.169909 H Original2D_6_2.log			
8	-0.560480	-1.693825	-0.000000
12	1.538569	-1.385899	0.000000
12	-2.319023	-2.609798	-0.000000

6	3.891809	-1.410034	0.000000
6	-3.987957	-1.448942	-0.000000
8	4.524750	-0.436095	0.000000
6	-3.263995	-0.411645	-0.000000
6	-2.066518	0.314761	-0.000000
6	-0.848297	-0.358488	-0.000000
6	1.361567	0.798818	0.000000
6	-1.327676	1.604953	-0.000000
6	3.564123	2.221782	0.000000
6	-1.831337	4.181465	-0.000000
6	-0.000000	0.807887	0.000000
6	-1.632196	2.904498	-0.000000
6	2.415690	1.626231	0.000000
16			
134.356802 Kcal/mol 5.826270 eV -101.169569 H Child_9_29.log			
6	5.330088	-2.356581	-0.008366
12	-6.107919	-0.867906	-0.242401
6	4.293827	-1.584532	-0.007616
6	-0.680647	-1.123044	-0.010010
6	3.405471	0.750852	-0.012147
6	-1.906800	-0.850924	0.036923
6	2.205080	1.436591	-0.001612
6	0.643232	-1.244525	-0.033553
6	3.222908	-0.758875	-0.017697
6	-3.083789	-0.136409	0.154549
6	1.060763	2.034017	-0.092179
6	1.882252	-1.156567	-0.027526
6	-0.192846	2.253272	-0.151813
12	-2.146635	1.766595	0.076430
8	-4.278358	-0.618774	0.344844
8	4.525537	1.323283	0.032399
16			
134.370338 Kcal/mol 5.826857 eV -101.169548 H MutD_18_76.log			
6	3.535204	-2.590525	2.330246
12	5.618178	1.572162	-0.703859
6	2.684347	-0.890520	0.526012
6	3.085283	-1.761129	1.465340
6	-2.324392	-0.721709	-0.546225
6	-3.569827	2.603132	0.869044
6	-3.277443	0.216851	-0.078178
8	-2.775810	-1.892764	-0.919752
6	1.636205	-0.288510	-0.250364
6	-3.827473	3.756472	1.391915
6	-3.361972	1.418715	0.373189
6	-0.935632	-0.463719	-0.565872
12	-4.717247	-1.530566	-0.431090
8	3.787102	0.976623	-0.889517
6	0.277144	-0.325732	-0.466211
6	2.928305	0.185004	-0.366639
16			
134.382721 Kcal/mol 5.827394 eV -101.169528 H Child_5_43.log			
12	-4.224367	-1.431242	0.271121
8	7.072705	0.005773	0.746448
8	-3.601930	0.391742	0.192040
6	7.538259	-0.058089	-0.302283

6	-2.061893	-1.413095	0.046636
6	0.536289	4.316553	-0.163382
6	-2.288102	0.019135	0.060616
6	1.029435	3.137447	-0.237520
6	-0.980943	-2.153783	-0.055020
12	-1.331905	3.151559	-0.001698
6	-0.019695	-2.981470	-0.139635
6	1.045114	1.773775	-0.257639
6	-1.282901	0.944445	-0.036171
6	0.964070	-3.829342	-0.230197
6	0.076831	0.963028	-0.172826
6	1.928378	-4.689258	-0.302742
16			
134.477088 Kcal/mol 5.831486 eV -101.169378 H Child_6_18.log			
12	-4.025768	1.318469	0.245591
6	6.462055	0.368789	1.061040
8	-2.173486	1.539071	0.080269
6	5.352618	-0.014325	0.512945
6	-5.340728	-0.249181	0.312126
6	4.177897	-0.369730	0.075076
6	-0.961157	1.241806	-0.114465
6	3.152001	-1.164951	-0.219122
6	-4.323858	-1.027450	0.300212
12	0.013749	-1.368270	-0.345337
6	0.259752	1.021528	-0.394971
6	2.031965	-1.697182	-0.398105
6	-3.128730	-1.662032	0.180146
6	-1.922584	-1.911423	-0.007743
6	1.526419	1.519762	-0.518351
8	2.727276	1.493921	-0.522240
16			
134.655773 Kcal/mol 5.839234 eV -101.169093 H MutD_14_62.log			
12	-0.257081	-0.806483	-0.390512
8	-1.685571	-0.091418	-1.531483
6	-2.527300	0.143285	-0.510678
6	-2.058258	-0.305920	0.763536
6	1.726550	-1.469717	-0.379885
6	-4.807705	1.412073	-0.857572
6	5.907488	3.371919	0.473171
6	4.326573	1.353865	0.038350
6	5.132860	2.365649	0.235972
6	-2.501818	-0.335926	1.978320
12	2.386016	-3.462786	-0.446613
6	2.637088	-0.565917	-0.265810
6	-3.710741	0.782228	-0.706305
6	3.532155	0.386002	-0.137439
6	-5.910916	2.092977	-1.078070
8	-2.817312	-0.427567	3.121978
16			
134.680511 Kcal/mol 5.840307 eV -101.169053 H Child_8_62.log			
6	-2.565544	-2.392190	0.003700
8	5.317751	-0.438217	0.859501
6	-1.796839	-3.364348	-0.241643
6	4.447152	0.099349	0.263039
12	-0.071053	-2.226314	-0.121832

6	3.399421	0.646091	-0.268456
6	1.113576	-0.457656	-0.144909
6	1.881728	0.731886	-0.242513
6	-3.200415	-1.199044	0.149761
6	2.755541	1.212651	-1.391276
8	-0.216956	-0.209151	-0.004163
12	-0.191364	1.769178	0.172805
6	-3.346268	0.018631	0.252889
6	-2.202601	2.344666	0.234942
6	-3.204117	1.377168	0.202112
6	-3.557859	2.760224	-0.060042
16	134.685849 Kcal/mol 5.840539 eV -101.169045 H Child_11_16.log		
8	5.627367	-1.563241	-0.047307
6	-1.977638	3.349004	0.536020
6	4.440418	-1.531776	-0.094597
8	1.436010	4.753255	-0.469840
6	3.170048	-1.499518	-0.156769
6	0.489584	4.098436	-0.163795
6	1.906763	-1.319426	-0.047028
6	-0.534168	3.375190	0.163766
6	0.615786	-1.233488	0.077466
6	-1.298407	2.154845	0.225245
6	-1.245904	0.802576	0.097968
6	-2.698565	-1.538458	0.596965
12	-4.054447	-2.061758	-0.831692
12	-0.964758	-2.970542	0.339595
6	-0.416074	-0.335762	0.127797
6	-1.831272	-0.510372	0.310689
16	134.714072 Kcal/mol 5.841762 eV -101.169000 H MutD_5_72.log		
6	1.567184	1.884481	0.022153
8	4.744421	0.206487	-0.074223
6	2.540534	1.115700	0.033267
6	-1.424804	-0.834676	0.072265
6	-2.575371	-1.665893	0.012940
8	3.522083	-2.349192	-0.034036
6	2.810691	-1.343811	0.012240
6	-3.616122	-2.542871	-0.112564
6	3.521009	0.056050	-0.004692
6	-4.050075	0.196592	0.004540
6	-1.717318	0.502040	0.034078
6	-1.947345	1.956961	-0.015087
12	0.642083	-1.152092	0.089112
6	-3.051919	1.101741	-0.007886
6	-3.950121	-1.103297	-0.030172
12	-0.206256	2.919053	-0.027481
16	134.800176 Kcal/mol 5.845496 eV -101.168863 H Child_8_31.log		
6	0.023354	-2.743763	-2.086261
6	-3.949596	-0.289103	0.784090
8	5.589371	-0.040090	0.290814
6	-3.247778	0.389599	-0.000286
8	-1.016274	-3.091928	-1.741251
6	4.388944	-0.088294	0.390033

6	-2.302493	1.146901	-0.701364
6	3.127798	-0.197191	0.560408
12	-2.346020	-0.896597	1.930334
6	1.809787	-0.032131	0.413183
6	-1.463242	2.263178	-0.282840
12	0.824284	1.332376	-0.911844
6	-0.335090	-0.733409	1.764991
6	0.764842	-0.531351	1.210802
6	-1.407350	1.083543	-1.698810
6	-0.463164	3.036486	-0.457010
16			
134.844249 Kcal/mol 5.847407 eV -101.168792 H Child_10_48.log			
6	-8.007958	0.277736	-0.870472
8	5.044786	-0.665504	-1.058973
6	-6.757281	0.109914	-0.541375
12	4.368866	1.048943	-0.453797
6	-5.500419	-0.018904	-0.210433
6	2.806379	2.203377	0.099487
6	-4.266643	-0.110187	0.097623
6	1.615781	1.948146	0.356370
6	-3.001280	-0.074730	0.365559
8	4.036745	-0.863198	0.214429
6	-1.718102	-0.092348	0.569111
6	0.364337	1.471167	0.551727
6	1.750835	-1.946343	0.074648
6	2.930769	-1.516902	0.017289
6	-0.709017	0.856695	0.617562
12	-0.176921	-1.583619	0.453278
16			
135.056962 Kcal/mol 5.856632 eV -101.168453 H MutI_9_79.log			
8	0.000000	0.000000	-0.847138
6	0.000000	0.000000	0.403179
8	0.000000	0.000000	10.748562
6	0.000000	0.000000	1.652186
6	0.000000	0.000000	2.954641
6	0.000000	0.000000	9.586988
12	0.000000	0.000000	-2.694741
6	0.000000	0.000000	-8.479622
6	0.000000	0.000000	-11.086236
6	0.000000	0.000000	-5.898070
6	0.000000	0.000000	5.523786
6	0.000000	0.000000	-7.229511
6	0.000000	0.000000	4.243343
6	0.000000	0.000000	-9.802159
6	0.000000	0.000000	-4.645199
12	0.000000	0.000000	7.482129
16			
135.610456 Kcal/mol 5.880633 eV -101.167571 H MutI_14_33.log			
6	1.479387	-1.302663	-0.406726
6	0.394351	-1.834719	-0.632723
6	0.166431	1.781880	0.456864
6	1.261225	2.091418	-0.099254
6	-0.908628	-2.209425	-0.716298
6	3.558391	-1.042099	0.773555
6	2.518731	1.683075	-0.655758

12	-3.277859	-0.809680	-0.018269
12	-5.830553	0.837081	0.271920
6	-2.153169	0.703202	0.792551
6	-2.146313	-2.371184	-0.693327
6	2.687252	-0.658488	-0.157168
6	-1.065175	1.314479	0.663043
8	3.125622	0.493768	-0.904661
8	4.356588	-1.415444	1.553369
6	2.448059	3.018623	-0.697004
16			
135.655403 Kcal/mol 5.882582 eV -101.167500 H Child_16_22.log			
8	2.419926	-2.052856	-0.602437
8	-3.558125	1.573032	-0.253463
12	4.226299	-2.198860	0.217717
6	-2.298140	1.419127	-0.273011
6	2.176851	-0.784695	-0.313653
12	-5.266487	0.753607	-0.112531
6	3.296045	-0.005289	0.058939
6	-1.743654	0.007813	0.006370
6	3.841529	1.147956	0.137518
6	-3.937705	-1.162373	0.343134
6	4.490354	2.279423	0.222831
6	-5.223927	-1.296688	0.484574
6	-0.354665	-0.163724	-0.105310
6	5.132269	3.386839	0.230592
6	0.844763	-0.355623	-0.263537
6	-2.625746	-0.942496	0.402380
16			
135.773236 Kcal/mol 5.887692 eV -101.167312 H Child_2_11.log			
8	6.311856	0.926606	0.125079
12	-3.651071	2.141274	0.180774
6	5.141480	0.692351	0.086154
6	-2.501698	0.288313	0.156410
6	3.893024	0.448529	0.047016
8	-1.978010	3.137711	-0.326564
6	2.634428	0.209713	0.012586
12	-2.767590	-1.803947	0.255662
6	-1.258937	0.831490	-0.025625
6	1.383955	-0.132500	0.010152
6	-0.993918	2.344453	-0.408406
6	-0.096545	-2.510897	-0.042184
6	-0.152764	-3.891147	-0.576162
6	0.377805	-1.216426	0.078167
6	-0.064471	0.046730	0.044171
6	-1.303500	-3.204353	0.013497
16			
136.166989 Kcal/mol 5.904767 eV -101.166685 H Child_6_29.log			
8	5.094560	0.595489	-0.337594
8	-3.541824	3.061827	-0.305212
6	3.942485	0.392419	-0.100090
6	-2.895142	2.051939	-0.300115
6	2.679858	0.120805	0.088801
6	-1.720548	-3.083876	-0.128818
12	1.404281	-1.528184	-0.388979
6	-1.683968	-1.547543	-0.196921

6	1.596157	0.942800	0.622433
6	-2.015348	1.094573	-0.275906
6	0.536517	0.416849	1.266959
6	-0.582693	-2.193289	-0.638501
6	-1.698670	-0.174508	0.361744
12	-0.000534	2.154916	-0.261192
6	-2.350121	-4.159835	0.184970
6	-0.686336	0.009780	1.272861
16	136.183697 Kcal/mol 5.905491 eV -101.166658 H Child_15_13.log		
6	2.401769	2.288618	-0.596392
8	-3.549264	-1.892166	-1.399084
6	1.180796	2.061278	-0.673366
6	-2.654694	-2.092182	-0.709458
6	3.674811	1.905060	-0.375644
12	-0.496946	-1.930895	0.077510
6	-1.352811	1.388565	-0.021976
12	-3.360561	1.686659	0.599989
6	-0.005178	1.441470	-0.401292
6	1.378284	-2.484698	0.664635
6	4.367714	0.930456	-0.033655
6	2.574311	-2.129847	0.665039
6	-0.609712	0.180801	-0.208483
6	3.703843	-1.393828	0.520445
6	4.379999	-0.374701	0.316836
8	-4.943823	0.967777	1.022819
16	136.268304 Kcal/mol 5.909160 eV -101.166523 H Child_6_36.log		
8	4.786789	1.171820	1.233337
8	-4.525828	1.690468	0.770910
6	3.768597	0.834805	0.721160
6	-3.478946	1.145402	0.618645
6	2.646626	0.494991	0.146890
12	-0.677332	1.315606	-0.859161
6	1.513952	1.041379	-0.660449
6	-2.323339	0.610872	0.356981
6	1.853307	-0.713585	-0.168161
6	-1.893086	-0.733198	0.526541
6	0.242121	-0.503889	-2.273364
6	1.315422	-0.172566	-1.434614
6	-0.625326	-1.245600	-1.579899
12	0.444209	-1.889863	0.990607
6	-1.181316	-1.547973	-0.437923
6	-1.719714	-1.878509	1.248972
16	136.572293 Kcal/mol 5.922343 eV -101.166039 H Original3D_0_74.log		
6	-1.754080	-0.538833	0.045947
8	3.185491	1.178142	1.064079
6	2.898561	-2.132547	-0.292463
6	2.344909	1.701209	0.028346
12	-0.192340	-1.976292	0.002516
6	0.955625	1.649871	0.012993
6	-1.530030	0.819373	-0.045907
6	-0.239015	1.388134	-0.056774
6	1.724534	-2.576539	-0.247622

6	-3.854071	0.629606	-0.026108
6	-2.845080	1.519171	-0.115346
12	3.791184	-0.339648	-0.051066
6	-4.235017	2.031584	-0.247557
6	-3.242103	-0.759719	0.110308
6	3.372818	1.798196	-0.824906
8	-3.781544	-1.851362	0.253065
16			
136.678471 Kcal/mol 5.926947 eV -101.165869 H Child_7_38.log			
8	14.433920	-0.274708	-0.309828
6	-6.206293	3.968177	-0.011329
6	15.160055	0.614030	-0.354608
6	-5.607166	2.832329	-0.099839
8	3.599265	1.757336	0.599732
6	-4.991191	1.685508	-0.187771
12	-1.250583	-3.008002	0.485453
12	-5.413228	-1.774355	-0.438314
6	-0.665576	-0.845870	0.007337
6	-4.404999	0.557392	-0.230400
6	2.589989	1.157783	0.416754
6	-3.355488	-0.296627	-0.126656
6	0.396785	-0.107946	0.092620
6	1.508794	0.511270	0.215262
6	-2.025751	-0.779800	-0.132076
6	-3.115785	-1.708371	-0.070110
16			
136.838664 Kcal/mol 5.933894 eV -101.165614 H MutD_18_62.log			
6	-0.726602	-3.378491	-0.144710
6	1.381601	1.369567	-0.431048
6	5.261544	0.877166	-0.029909
6	-1.564541	-2.385302	-0.066167
6	0.313839	-4.127870	-0.312483
6	-1.074394	0.622698	-0.268124
6	-2.410749	-1.416753	0.020208
12	3.428549	1.431037	-0.325691
6	-3.533434	0.796797	0.103560
6	0.157478	1.032547	-0.365723
6	6.270310	0.145643	0.298514
8	7.214713	-0.554742	0.603582
12	-4.429088	-1.022203	0.341200
6	-3.824626	2.064839	0.151966
6	-2.263827	0.064952	-0.072012
8	-4.203852	3.192148	0.210100
16			
136.964999 Kcal/mol 5.939372 eV -101.165413 H MutD_16_60.log			
6	3.627227	-1.685389	-0.341114
6	4.170669	-0.551045	-0.307772
6	3.824280	0.793624	-0.197803
12	-0.818600	0.728923	0.517908
6	2.572040	-2.473767	-0.111344
12	2.414674	2.348495	0.201285
6	-4.388732	-0.035684	-0.036900
6	-5.452481	0.561964	-0.410063
6	1.356924	-2.721059	0.052149
8	4.144772	1.866808	-0.854593

8	-6.448863	1.135776	-0.742900
6	-2.064074	-1.083819	0.275211
6	-1.070409	-2.003997	0.274112
6	0.043572	-2.559256	0.221791
6	0.535942	2.259200	1.135674
6	-3.274983	-0.659054	0.137664
16			
136.980591 Kcal/mol 5.940048 eV -101.165388 H Child_6_23.log			
8	3.618866	-1.641727	-0.826533
6	-1.855555	3.066989	-0.647351
8	4.431001	0.891614	-0.024110
6	2.767326	-0.903043	-0.303386
6	-1.769676	1.875486	-0.074792
6	3.239827	0.582536	-0.027607
6	-2.794885	0.808612	-0.025807
12	0.790605	-1.554968	0.288952
12	-3.977594	-0.714397	-0.704753
6	2.099143	1.422575	0.236616
6	-2.128632	-0.256657	0.577953
6	0.893160	1.655325	0.312051
6	-0.466209	1.285564	0.431119
6	-1.230196	-2.303804	0.318763
6	-0.719099	0.004540	0.857025
6	-2.394382	-1.699241	0.311207
16			
137.227104 Kcal/mol 5.950738 eV -101.164995 H MutD_10_70.log			
6	-4.491688	1.100083	-0.334946
12	3.557736	1.365878	0.152288
6	2.794300	-3.143121	0.334731
6	3.187475	-1.879472	0.257068
6	3.471431	-0.668182	0.242866
8	-5.767030	2.848593	0.917280
6	-3.292731	-1.155741	-0.524182
6	3.230501	3.312904	-0.023528
6	-3.905833	-0.050279	-0.467821
12	-2.014832	-2.812674	-0.388994
6	2.793687	4.507480	-0.237891
6	2.240238	-4.263230	0.328018
6	-5.169932	1.963428	0.381720
6	0.847021	-4.293718	0.073605
6	-0.275664	-3.839094	-0.195370
8	2.381070	5.628307	-0.437924
16			
137.239857 Kcal/mol 5.951291 eV -101.164975 H Child_4_47.log			
6	7.045585	-0.203450	-0.566689
8	-5.154618	1.344877	-0.671790
6	5.770673	-0.096348	-0.385821
6	-4.113659	0.902596	-0.402580
6	4.483606	0.014103	-0.203038
6	-3.356184	-2.479968	-0.236330
6	3.215613	0.126004	-0.025767
6	-2.949757	0.304584	-0.071190
6	1.980488	0.901252	0.136797
6	-2.883822	-1.134735	-0.094353
12	0.251342	1.979295	0.343830

6	-1.948394	-2.141571	0.023825
6	1.856658	-0.457473	0.175217
6	-1.775161	1.078570	0.243503
8	-0.759577	0.318877	0.640145
12	0.028632	-1.495245	0.380480
16			
137.412218 Kcal/mol 5.958765 eV -101.164700 H Child_11_39.log			
6	4.530307	1.245358	-1.770788
8	-4.981192	0.230673	-0.392792
8	3.664921	1.429294	-1.013856
6	-2.953138	1.295013	0.326288
6	0.661556	-1.585617	-1.679042
6	-3.757471	0.242040	-0.211735
6	-1.801495	-1.496245	-0.639330
6	-1.907993	1.856398	0.652493
6	0.522545	-2.047918	0.325554
6	0.631219	2.171832	0.951196
6	-0.458184	-1.846413	-0.651013
6	-0.612593	2.180913	0.888657
6	1.170486	-0.940186	-0.514760
6	-2.839384	-0.835435	-0.539390
12	2.195739	-1.979833	1.826812
12	2.088848	0.753319	0.541887
16			
137.469849 Kcal/mol 5.961264 eV -101.164608 H Child_1_25.log			
12	2.416662	1.696493	0.000000
6	-2.179175	-2.979274	-0.000000
6	2.793915	-0.322801	0.000000
6	-2.431944	-1.756991	-0.000000
6	0.395487	2.244566	0.000000
6	-2.435724	4.971209	0.000000
6	-0.919918	2.842748	0.000000
12	-0.097734	-3.031998	-0.000000
6	2.328368	-1.678276	-0.000000
8	-2.320775	-0.413804	-0.000000
6	1.381962	-0.665572	-0.000000
6	0.000000	-0.895575	-0.000000
8	2.202084	-2.950758	-0.000000
6	-0.987417	0.034708	-0.000000
6	-0.728435	1.435949	0.000000
6	-1.696719	3.926399	0.000000
16			
137.515105 Kcal/mol 5.963227 eV -101.164536 H MutI_18_73.log			
6	-4.007548	-1.793814	-0.140650
12	1.336246	1.413254	0.088433
6	-0.720302	1.885057	0.115662
6	-1.373726	-2.026918	-0.137740
6	1.194046	-1.777998	-0.014076
6	-2.707143	-1.912425	-0.159924
6	4.984382	0.948368	-0.034406
6	2.411730	-1.661000	0.080847
6	-3.343532	1.870954	0.410261
12	-4.436814	0.175438	0.198864
6	-0.150128	-1.928261	-0.083123
8	3.683602	-1.453505	0.288460

8	-0.288013	1.574694	-1.075547
6	3.452786	1.109374	0.062757
6	-2.104929	2.050560	0.290312
6	4.038050	-0.102866	0.084937
16			
137.571382 Kcal/mol 5.965667 eV -101.164446 H Original3D_16_6.log			
8	-4.473601	0.052804	-0.335092
6	2.047411	0.895236	0.710360
6	4.572098	1.167075	0.538814
6	3.313342	1.333417	0.131946
6	3.537914	-2.672799	-0.837824
8	3.099450	-1.699864	-1.258553
6	-0.212526	1.541589	-0.306422
6	-1.612492	-2.082319	0.558212
12	-3.506727	1.501083	0.012932
6	1.193768	1.613323	-0.185725
6	-1.416545	1.274271	-0.303592
6	2.343851	1.753059	-1.043841
6	0.592545	-1.001062	1.287787
12	-3.278434	-1.312777	-0.408942
6	-0.565800	-1.693985	1.047362
6	1.608957	-0.308336	1.319801
16			
137.582509 Kcal/mol 5.966150 eV -101.164429 H Child_11_59.log			
8	-10.278460	-0.932325	-0.325519
8	2.746806	-4.863639	-0.263829
6	-9.166039	-1.201270	-0.405631
6	2.438763	-3.667779	-0.166139
12	-1.190107	1.437613	0.897605
6	2.784107	-2.295296	-0.041525
6	0.417529	3.489071	0.283211
6	3.563020	0.127147	-0.066250
6	3.463657	-1.103198	0.007243
6	1.585228	3.355446	-0.575494
6	3.273665	1.452114	-0.173920
12	-0.159606	-1.267242	0.475457
6	2.648390	2.480952	-0.322843
6	0.893948	3.910339	-1.586964
6	1.429655	-2.651069	0.042785
6	-0.590290	3.490751	1.045202
16			
137.720977 Kcal/mol 5.972154 eV -101.164208 H Child_16_27.log			
6	2.188405	-2.742101	-0.026039
6	-4.317037	-0.531412	0.026325
12	3.523041	0.853477	-0.165537
6	-3.648231	-1.584287	0.044026
8	3.962308	-0.967312	-0.086042
6	-2.702899	-2.556478	0.052541
6	3.112677	-1.934096	-0.058328
12	-3.649564	1.365303	-0.046768
6	2.326593	2.401247	0.614954
6	-1.605602	-3.121182	0.051023
8	1.293618	2.958350	0.157741
6	-0.288857	-3.399849	0.038554
6	0.305422	3.752157	-0.193438

6	-2.104437	2.690167	-0.122613
6	-0.956128	3.175460	-0.114909
6	0.935238	-3.241904	0.016916
16			
137.851748 Kcal/mol 5.977825 eV -101.164000 H Child_6_58.log			
6	-5.254013	-0.199000	-0.258221
6	1.497453	-2.852018	0.786284
6	-4.013455	0.084170	-0.175530
6	2.138911	-1.961476	-0.047345
6	-2.695115	0.338240	-0.059385
6	0.406007	-3.321242	1.224598
8	-2.332223	1.687603	0.193103
6	2.701486	-0.806245	-0.559329
8	-1.708087	-0.479811	-0.150496
6	3.410697	0.365284	-0.355397
6	-1.071139	2.081941	0.268881
6	1.507206	-1.276059	-1.143259
12	-0.523584	-1.877693	-0.278900
6	3.640246	1.550967	-0.060838
6	0.070806	2.540126	0.342012
12	2.047580	2.800153	0.269259
16			
137.896577 Kcal/mol 5.979769 eV -101.163928 H Child_2_45.log			
6	3.082121	-1.180694	-0.212702
12	-5.112875	1.885388	0.117276
6	3.537902	0.120770	-0.225045
6	-4.117971	0.055524	0.536531
6	2.999073	1.334421	-0.374462
6	-2.877382	-0.268674	0.097974
6	2.090887	-1.909888	-0.149251
6	-1.854017	0.644999	-0.255250
6	4.304405	1.242134	0.357590
6	-0.788683	1.245902	-0.426258
6	1.713708	1.792612	-0.485937
8	1.010010	-2.578510	-0.050494
6	0.485484	1.679690	-0.532972
12	-0.816994	-2.377765	0.073553
6	5.201496	1.784702	1.153882
8	-2.447972	-1.589049	0.151176
16			
138.028217 Kcal/mol 5.985478 eV -101.163718 H Child_16_9.log			
12	4.527810	0.132228	-1.052271
6	-4.940437	-0.903193	-0.265573
6	6.219305	-0.051788	0.304135
6	-4.846280	0.350033	-0.201115
8	7.264283	-0.207239	0.780079
6	-4.222722	1.553477	-0.057689
6	2.699610	0.225025	-0.275069
6	-3.154917	2.158760	0.121221
6	1.474303	0.385260	-0.074961
12	-3.056695	-1.729218	-0.064013
6	-0.635842	-0.783083	0.416147
6	-1.814830	2.108608	0.285132
6	-1.254465	-1.488941	1.375927
6	-0.701937	1.571192	0.222497

6	0.134206	0.444474	0.210369
8	-1.187950	-1.574644	-0.651418
16			
138.149011 Kcal/mol 5.990716 eV -101.163526 H MutD_5_76.log			
12	0.087457	-3.180133	-0.673782
6	2.716337	-1.330336	-0.068503
6	-2.820716	1.186174	-0.331525
6	-3.754304	0.350679	-0.437592
6	1.020477	1.562596	0.368337
8	3.877048	-1.032246	-0.084696
6	-0.946994	-1.883143	0.545493
6	0.224059	-1.163802	0.413230
6	0.237365	0.291702	0.499022
6	-1.655971	2.016703	-0.200993
12	-2.862918	-1.216860	0.529843
6	2.076403	2.258632	0.091318
6	-0.438213	1.411799	0.251376
6	1.498002	-1.773986	-0.070068
6	-1.828518	3.302867	-0.580083
8	3.040198	2.955322	-0.059404
16			
138.245957 Kcal/mol 5.994920 eV -101.163371 H MutI_14_49.log			
6	0.256343	-2.717870	0.291448
6	5.583145	-2.244018	-0.179349
6	-4.973173	0.299459	-0.144937
6	-6.007407	-2.035902	0.083611
12	3.247994	1.212944	0.094829
6	-3.191525	2.118649	-0.334019
6	-4.137371	1.305648	-0.249570
6	-5.557978	-0.805480	-0.015023
6	-1.997008	2.652986	-0.210483
6	-0.783101	2.870027	-0.028263
8	5.135216	-3.225432	-0.570134
6	-6.349861	-3.235868	0.358255
6	1.774266	2.575292	0.195643
6	0.539106	2.784053	0.109796
12	6.028620	0.356769	0.273743
8	-0.416716	-1.804368	0.109445
16			
138.368319 Kcal/mol 6.000226 eV -101.163176 H Child_11_58.log			
6	1.522682	-1.022500	-1.746486
8	-12.110700	-0.537392	-0.673815
6	1.875249	-1.844882	-0.735889
6	-11.013761	-0.344090	-0.392612
12	4.000690	-0.079748	-0.712810
12	0.047491	2.418090	1.153430
6	3.194046	-1.979341	-0.083242
8	-0.305901	0.794316	2.035577
6	1.933289	0.195543	-1.894063
6	1.272539	3.240794	-0.193576
6	1.525591	-2.228371	0.613831
6	1.901692	2.390888	-0.872931
6	0.690388	-1.419543	1.393671
6	2.560896	1.308154	-1.471503
6	2.827728	-2.954496	0.943722

6	0.168765	-0.361404	1.742157
16			
138.408177	Kcal/mol	6.001954	eV -101.163113 H Child_4_51.log
12	3.879989	1.019636	-0.294002
12	-1.646763	2.656586	-0.101128
6	0.151993	0.408385	0.382148
6	3.641428	-2.201046	-1.045567
6	0.463323	-0.910341	0.710553
8	-5.435956	-1.508608	-0.857695
6	1.651046	-1.596153	0.742514
6	-4.538562	-0.805691	-0.468257
8	-0.892457	-1.275756	1.004260
6	-3.629096	-0.007896	-0.045483
6	2.776994	-1.621432	0.165321
6	2.118343	2.035494	-0.169871
6	1.031586	1.442074	0.021367
6	-2.452691	0.539684	0.199242
6	-1.244632	0.108637	0.612532
6	4.001700	-1.031673	-0.509660
16			
138.506853	Kcal/mol	6.006233	eV -101.162956 H Child_4_29.log
8	4.130748	-1.652625	0.015103
6	-3.898475	1.166177	1.348891
6	2.889683	-2.145182	0.205826
6	-4.818863	-1.384975	-1.590286
6	4.139975	-0.315693	-0.179772
8	-3.876778	-1.060784	-1.003093
6	3.993969	0.896738	-0.341992
6	-2.821078	1.612236	0.780592
6	1.687862	-2.274098	0.343687
12	-2.330134	-0.552495	0.368632
6	0.329786	-2.234489	0.458809
6	-1.619984	1.563218	0.166763
12	2.609833	2.343902	-0.409552
6	-0.881179	-1.971680	0.518040
6	-0.527592	2.329490	-0.078700
6	0.627870	2.793325	-0.232697
16			
138.627101	Kcal/mol	6.011448	eV -101.162764 H Child_5_63.log
6	4.773192	0.910909	-0.299667
8	-2.548220	2.795867	-1.995420
8	3.711105	1.240228	0.004195
6	-1.707232	0.743728	-0.886967
6	-0.225203	1.297717	2.311031
6	-1.930706	-0.364757	-0.219682
6	0.426340	2.154765	1.656090
6	-1.823929	-1.366307	0.633950
6	-1.018425	0.188463	2.476112
6	-2.250402	1.782992	-1.457897
6	-1.536693	-0.792360	1.923221
12	-0.752924	-3.100210	0.000389
12	0.766768	1.112256	-0.147385
6	1.408615	-0.687047	-0.983910
6	1.245892	-1.973078	-1.038461
6	1.060349	-3.300577	-1.164862

16
139.055206 Kcal/mol 6.030012 eV -101.162082 H MutD_17_58.log
12 -2.985189 -1.639460 -0.087534
8 -4.850511 -1.617060 0.469293
8 7.030559 -1.203489 0.394745
6 -4.432649 0.556597 -0.061069
12 0.953156 -0.804166 -0.423154
6 0.237689 2.025931 0.070611
6 3.745123 0.504196 -0.043630
6 -2.301103 2.004257 -0.027458
6 2.464931 0.733224 -0.105622
6 6.007834 -0.556523 0.206280
6 -3.489735 1.381680 -0.061649
6 -1.077818 2.217265 0.055171
6 1.404096 1.571992 0.026965
6 -5.377404 -0.363972 0.426186
6 -0.979529 -1.504742 -0.607521
6 4.955899 0.078081 -0.008938
16
139.233982 Kcal/mol 6.037765 eV -101.161797 H Child_17_27.log
6 5.637167 0.538760 -0.051971
8 -7.205863 -0.424145 -0.603484
6 4.374051 0.393689 -0.283720
6 -7.871953 0.496123 -0.793789
6 3.179608 -0.492302 -0.463843
6 -1.214629 -2.218534 0.956239
6 2.007077 1.824781 -0.493832
6 -1.188929 -0.990922 1.075168
6 0.990128 2.464536 -0.336900
6 -1.027644 0.352395 1.041104
6 2.983917 0.833373 -0.461421
12 -0.138517 -3.696577 0.035517
12 2.130837 -2.329941 -0.430202
6 -0.766775 1.538381 0.846813
6 -0.279049 2.755623 0.273532
8 -0.899843 3.841996 0.214976
16
139.394492 Kcal/mol 6.044725 eV -101.161541 H MutI_18_55.log
6 0.883612 1.159044 0.035149
6 4.769339 1.305827 -0.329020
8 -2.377388 2.839640 0.875047
12 1.026923 -4.761876 0.727199
8 -3.252388 -1.555531 -0.834716
6 3.463421 1.256829 -0.180160
6 -1.112401 2.662152 1.088376
6 -0.394171 -1.965413 -0.251132
6 -2.494007 -0.607472 -0.596604
6 6.051310 1.330413 -0.455273
12 -3.152750 1.476757 -0.316493
6 2.214556 1.192460 -0.061569
6 0.081495 -3.049666 0.110751
6 -0.335451 1.840509 0.271215
6 -0.335933 0.448497 -0.143327
6 -1.033748 -0.715086 -0.363593
16

139.565099 Kcal/mol 6.052123 eV -101.161269 H MutD_18_72.log

6	0.669006	-0.585815	-0.253655
6	3.544401	4.349138	0.090133
6	-1.222983	-0.787491	1.406108
6	-2.748834	0.128985	-1.420842
6	-0.630068	-0.509619	-0.106826
6	3.329376	3.078733	0.151574
8	-2.471957	-0.498692	1.472680
6	2.974598	1.806103	0.119299
6	-5.245393	0.574424	-0.839841
6	2.001688	-0.627535	-0.015780
6	-1.607840	-0.156115	-1.055722
8	2.632983	-1.813977	0.076766
12	4.236016	-2.639391	-0.349669
6	2.666881	0.592331	0.092141
6	-4.094159	0.387027	-1.331316
12	-4.161703	0.056088	0.899068

16

139.861677 Kcal/mol 6.064984 eV -101.160797 H Child_4_10.log

6	-4.643978	2.611389	0.315939
6	-1.442156	-4.657009	0.273357
6	-3.394526	2.418297	0.130446
8	-1.004512	-3.603452	0.056805
6	-2.114207	2.184153	-0.045677
6	4.326627	-0.450149	0.187179
8	-3.256627	-0.599052	-0.058588
12	-0.071036	-1.654233	-0.284885
6	-0.871136	2.012266	-0.121097
6	3.121178	-0.816561	0.100355
6	-2.110805	-0.725930	-0.164583
6	1.699261	-0.803440	0.022952
6	0.437143	1.658011	-0.141077
12	3.851485	1.535656	0.091643
6	1.296639	0.525784	-0.070251
6	1.816581	1.883682	-0.098679

16

141.286243 Kcal/mol 6.126759 eV -101.158526 H Child_2_33.log

8	5.748400	-0.198198	0.273827
12	-2.098601	2.575372	0.373545
6	4.585847	-0.246073	0.175978
8	-0.250085	2.338773	-0.331157
6	2.305642	-1.342587	0.107686
6	-2.572877	0.505103	0.095262
6	3.263299	-0.284976	0.060715
6	-0.178139	1.026161	-0.396039
6	0.989041	-1.224973	-0.091854
6	-4.617706	-1.465214	0.152927
12	-1.078944	-1.889740	-0.180517
6	-3.501708	-0.558923	0.183385
6	2.334208	0.820330	-0.129972
6	-1.363575	0.212147	-0.467704
6	-3.240858	-1.931332	0.235807
6	1.020828	0.264973	-0.235805

16

141.430813 Kcal/mol 6.133028 eV -101.158296 H Child_4_46.log

8	4.993870	1.516305	-1.274378
8	4.053509	-2.117426	1.740645
6	3.983070	1.700973	-0.760870
6	1.040415	-0.020445	0.799252
6	-3.647660	0.329872	1.071846
6	4.688319	-1.703745	0.877964
12	-3.122548	-1.577534	-0.886880
12	-0.248587	1.810554	0.391986
6	-1.863999	2.119485	1.647225
6	0.572794	-1.112575	0.338720
6	-2.819288	1.328717	1.506219
6	-0.086148	-1.648781	-0.684405
6	-0.845159	1.262962	-1.620137
6	-1.061501	0.044552	-1.849072
6	-4.195512	-0.644775	0.509064
6	-1.086233	-1.320783	-1.467709
16			
141.652278	Kcal/mol	6.142632	eV -101.157943 H MutD_17_40.log
6	-3.519252	-0.886191	-0.489867
6	-3.314964	-2.117739	-0.381227
6	-2.740381	-3.366443	-0.073963
6	-1.582492	-2.937273	0.291451
6	6.170306	0.452176	-0.148592
6	-1.906205	3.411952	0.470391
8	1.282367	-0.892908	0.151371
6	4.939931	0.067020	-0.215230
6	2.468721	-0.586951	-0.016162
12	-3.799082	2.502667	-0.355799
6	-1.706162	2.151123	0.412615
12	-0.635547	-0.989754	0.523305
8	7.328676	0.767929	-0.144765
6	-3.189674	0.427998	-0.302710
6	3.675290	-0.244223	-0.133953
6	-1.907253	0.769361	0.243426
16			
141.695707	Kcal/mol	6.144515	eV -101.157874 H MutD_17_62.log
6	1.388781	2.918070	0.807378
6	-0.804686	-1.176197	1.434254
12	2.781196	1.805809	-0.210574
6	-0.455752	1.311229	1.634891
6	-0.276444	-2.192458	0.964012
6	-2.509542	3.588979	-1.121562
12	2.956611	-1.590395	-0.901713
8	-2.605771	2.488358	-1.436724
6	-0.868819	0.147987	1.689208
6	0.408845	2.298863	1.280236
6	1.727108	-3.135652	-0.351749
6	-3.879301	-1.624223	-0.425457
6	-2.780730	-2.151602	-0.896891
6	-5.022858	-1.098303	-0.094280
8	3.287503	0.179918	-0.804551
6	0.688808	-2.875219	0.292899
16			
141.766431	Kcal/mol	6.147582	eV -101.157761 H Original3D_5_7.log
6	-1.372354	-1.263704	0.105316

6	-1.568136	2.335868	-1.066294
6	-1.579734	2.539715	0.228391
8	-1.459825	2.165387	2.643990
6	-0.100584	-1.154842	0.366644
12	1.041868	0.563559	-0.638952
6	-1.533413	2.362778	1.496873
6	0.903527	-1.941107	0.929745
6	3.029316	-1.281974	-0.156050
6	-2.575430	-1.221781	-0.338570
6	3.287836	-0.318873	-0.927576
6	2.264821	-2.052368	0.709035
6	1.692468	-2.795292	1.825347
8	-4.705830	-1.207544	-1.563897
12	3.679559	1.809023	-1.176545
6	-3.670298	-1.230707	-0.981991
16			
141.862308 Kcal/mol 6.151740 eV -101.157608 H MutD_2_70.log			
6	4.524855	-0.287389	-1.158559
6	1.567806	-0.210476	0.585285
12	0.175009	-2.626363	0.485786
6	-2.492718	0.888430	0.463232
6	-2.394510	1.093275	-0.988862
6	-2.611268	-0.206306	1.263127
6	0.478727	3.636052	0.241802
12	-2.199106	-0.889120	-1.652862
6	1.347897	0.999874	0.527090
6	0.710251	2.202763	0.367205
8	5.275032	-0.068717	-0.315726
8	1.696985	-1.484239	0.632716
6	-0.562425	2.646201	0.099575
6	-1.765318	-2.276223	-0.108723
6	-1.772988	1.966722	-0.099967
6	-2.278138	-1.351350	0.720293
16			
142.076587 Kcal/mol 6.161032 eV -101.157267 H Child_6_56.log			
6	-4.161540	4.604814	-0.628798
8	4.409416	3.613958	1.604184
6	-1.989077	-2.807419	-0.056276
6	4.663195	2.680549	0.927673
6	-2.359167	-1.589522	-0.233839
6	4.891717	1.685992	0.149234
6	-2.730232	-0.355804	-0.403668
12	-1.128701	-3.590940	1.773477
6	-3.782063	3.354583	-0.569195
6	5.003217	0.498916	-0.301554
6	-3.093961	0.861857	-0.480159
6	5.104257	-0.705417	-0.701007
6	-3.422159	2.106028	-0.551000
6	5.127795	-1.930666	-1.055593
8	5.148597	-3.068717	-1.381029
12	-6.869299	-0.974508	0.029846
16			
142.162752 Kcal/mol 6.164768 eV -101.157130 H Child_7_9.log			
6	-2.825080	0.246908	0.512739
6	3.929382	0.970455	0.453071

6	-1.789309	2.170494	-1.173414
6	2.612664	1.060469	0.217202
6	-2.389077	1.382065	-0.218444
6	3.035440	-0.341830	0.009127
12	-2.929964	-1.790504	0.202733
6	2.316919	-1.518298	-0.277852
6	-1.726520	1.017191	0.966478
6	3.662535	-1.783622	-0.060848
8	-1.407607	-2.657654	-0.320382
12	0.759202	1.938191	0.009102
6	-0.671809	2.605561	-1.562907
6	0.999129	-1.924094	-0.418926
8	-0.581981	1.259772	1.461872
6	-0.159966	-2.316830	-0.391882
16			
142.216928 Kcal/mol 6.167117 eV -101.157043 H Child_13_30.log			
6	16.643967	-1.389565	-0.361728
6	-1.446360	2.254181	0.549792
8	17.178441	-0.391466	-0.136831
12	0.557150	2.223745	0.237202
8	-6.311598	-2.869546	-0.143602
6	-2.474617	1.559063	0.623201
6	-5.516134	-2.018463	-0.014886
6	-4.678851	-1.021815	0.149606
6	-4.316429	0.235597	-0.553538
12	-1.144284	-0.723169	0.623193
6	0.750739	-0.253558	0.294945
6	-3.980516	0.518643	-1.838926
6	-3.533091	0.664018	0.645315
6	1.676070	0.555047	0.565308
6	-3.525363	-0.677329	1.034542
6	-2.914272	0.921045	-2.440511
16			
142.458344 Kcal/mol 6.177586 eV -101.156659 H Child_12_12.log			
6	-2.976169	1.471380	-0.001676
6	4.553108	-1.436301	0.057277
6	-4.054411	0.896756	0.064395
6	3.085784	-1.300673	-0.024707
6	-1.726939	1.988347	-0.036087
8	5.167878	-0.270636	0.108852
8	-5.125558	0.104643	0.097593
6	1.900352	-1.701354	-0.057542
6	-0.529765	2.263273	-0.055390
6	0.564057	-1.894583	-0.055448
6	0.822484	2.344724	-0.056081
12	3.645346	0.959902	0.018614
6	-4.984480	-1.309231	0.060604
6	-0.676242	-1.991602	-0.051385
6	2.056034	2.215129	-0.043349
12	-2.690466	-1.622172	-0.056550
16			
142.512301 Kcal/mol 6.179926 eV -101.156573 H Child_9_25.log			
6	3.223938	2.363740	-0.020102
6	-3.070331	-2.008703	0.034357
6	2.000205	2.789382	0.005896

6	-1.735810	-2.379031	-0.040012
6	3.887237	1.198889	-0.037103
6	-0.582428	-2.826043	-0.001603
6	0.795670	3.212072	0.026244
8	-3.208621	-0.714002	-0.095324
6	4.437089	0.063493	-0.051218
6	0.761869	-2.992683	0.019293
6	-0.518672	2.982289	0.036059
6	2.004578	-2.954061	0.074895
6	-1.731648	2.671370	0.029451
12	-3.182106	1.269732	0.001532
12	3.698185	-1.825794	0.010103
8	-4.669271	-0.042442	0.020751
16			
143.028915 Kcal/mol 6.202329 eV -101.155749 H MutD_18_74.log			
6	3.704585	0.158728	-0.058585
6	4.066590	-0.990504	0.243656
12	2.747201	-2.620442	0.287142
6	1.056097	-1.635724	-0.456362
6	-5.039910	-0.427239	-0.142438
6	-2.656100	-1.023461	0.230788
12	-2.397164	1.509976	0.476795
6	-1.472130	-1.367365	0.111013
8	2.020794	1.555950	0.674576
6	-0.172282	-1.567925	-0.141386
6	-0.471273	2.105741	0.498123
6	-6.015087	-0.597543	-0.987588
8	2.802408	1.899356	-1.485263
6	-3.758843	-0.186643	0.169100
6	0.737836	1.874274	0.528842
6	2.889510	1.271518	-0.442119
16			
143.356043 Kcal/mol 6.216514 eV -101.155228 H Child_5_51.log			
12	3.013689	-1.271505	-1.050947
6	-1.567096	-4.053217	-0.644492
6	1.619013	-1.671147	0.688974
8	-0.521013	-4.327211	-0.254495
6	1.775580	0.872183	0.131662
6	-2.782024	2.317326	-0.716322
6	1.130740	-0.375832	0.604347
6	-3.687520	1.425429	-0.208543
6	2.900442	1.466188	0.434063
6	-3.471969	0.350581	0.427734
6	-0.272565	-0.292982	0.768703
6	-1.735088	2.943686	-1.043980
8	3.873247	2.131628	0.621927
6	-2.813170	-0.652408	1.004336
6	-1.490079	-0.626973	0.973584
12	-0.051644	1.883810	-0.404039
16			
143.453613 Kcal/mol 6.220745 eV -101.155073 H Child_18_30.log			
8	4.800925	0.563313	1.069865
6	-4.737071	1.361338	0.471611
6	3.876180	0.351273	0.257912
6	-3.642765	0.444560	0.350527

6	3.207765	1.321546	-0.533887
6	-3.301637	1.778094	0.384423
6	3.138669	-0.878697	0.054977
6	-2.750952	-0.627955	0.107213
6	2.231467	-1.707288	-0.098449
12	-1.226910	1.844712	-0.227516
6	2.015367	1.894099	-0.467503
6	-1.450837	-0.504415	-0.485422
6	0.781371	2.195353	-0.513459
6	-1.957156	-1.744788	0.061305
12	0.316968	-2.212959	-0.455636
8	-1.493813	-2.923281	0.262926
16	143.561900 Kcal/mol 6.225441 eV -101.154900 H Original3D_0_40.log		
6	1.887559	-0.605018	0.448745
6	0.760063	-1.160209	-0.433480
6	1.243753	0.017168	1.558905
12	-0.668136	2.360632	1.026272
12	-0.773347	-1.643882	1.004733
8	4.198265	-0.522259	-0.516637
6	0.224638	0.620532	1.972955
6	-2.902978	-1.823050	0.664167
6	0.407278	1.159358	-1.319109
6	-1.980133	0.024914	-0.967458
6	0.251883	-0.274705	-1.327566
6	-2.728814	-0.908140	-0.181204
6	3.134905	-0.577921	0.027018
6	-1.838666	1.253992	-0.429403
6	0.239442	2.323779	-0.890780
8	-1.060238	-0.590890	-1.871962
16	143.565569 Kcal/mol 6.225600 eV -101.154894 H Child_7_28.log		
12	2.624997	-3.218788	1.536989
8	-3.413931	3.530597	1.474385
6	-0.772597	-2.901984	-0.612637
8	4.529726	2.688762	-1.831216
6	0.268265	-2.378119	-0.167529
6	-3.623632	2.537118	0.813879
6	3.790381	2.271250	-1.006476
12	-2.640741	-2.338476	-1.139186
6	-3.867437	1.522357	0.098868
6	1.833392	-0.552364	0.378963
6	2.986930	1.795018	-0.097127
6	-3.876159	-0.771477	-1.098335
6	2.225410	0.700118	0.465376
6	1.394916	-1.765735	0.363490
6	-3.903480	0.354792	-0.512055
6	2.087773	2.011074	1.053751
16	143.583862 Kcal/mol 6.226393 eV -101.154865 H MutI_18_69.log		
6	-3.134019	0.156425	-0.217087
6	-0.098875	2.584529	-0.068687
6	-1.324427	2.023924	-0.210384
6	-6.527855	-1.447704	0.740879
6	-4.302064	-0.281604	0.109949

6	4.560577	-1.238602	0.400356
6	3.680084	-0.247637	0.447602
6	1.111003	2.815733	0.116665
12	2.750485	1.616774	0.225521
6	-2.312503	1.272601	-0.241945
8	2.340632	-0.380834	-0.164079
12	-1.294645	-0.865314	-0.446732
8	0.439590	-1.429884	-0.551148
6	1.680787	-1.715881	-0.409161
6	-5.421634	-0.861480	0.429194
6	5.470281	-2.148932	0.298676
16	143.632624 Kcal/mol 6.228508 eV -101.154787 H Original3D_0_59.log		
6	-0.045182	-1.649906	-0.386427
6	-0.245948	-0.189269	-0.495645
6	3.400325	0.391659	0.096364
6	2.193415	1.060478	-0.256756
6	0.879147	0.706233	-0.486447
8	3.299923	-0.936035	0.449444
6	1.200262	2.093350	-0.363180
12	1.789888	-1.998241	0.476809
6	-1.488777	0.479162	-0.363343
6	-1.305039	-2.180110	-0.375199
6	4.619831	0.966082	0.180516
8	-4.796691	0.422362	0.864074
12	-0.872252	2.490276	0.155102
6	-2.493955	-1.762328	-0.505791
6	-2.674148	-0.346304	-0.235384
6	-3.879509	0.131782	0.176114
16	143.661755 Kcal/mol 6.229771 eV -101.154741 H Original1D_2_0.log		
6	0.000000	0.000000	3.029627
6	0.000000	0.000000	4.318047
6	0.000000	0.000000	1.721340
6	0.000000	0.000000	5.600562
6	0.000000	0.000000	0.455669
12	0.000000	0.000000	7.546666
6	0.000000	0.000000	9.661961
12	0.000000	0.000000	-1.527918
8	0.000000	0.000000	10.822331
8	0.000000	0.000000	-3.335550
6	0.000000	0.000000	-4.604473
6	0.000000	0.000000	-5.839401
6	0.000000	0.000000	-7.168593
6	0.000000	0.000000	-8.420949
6	0.000000	0.000000	-9.741779
6	0.000000	0.000000	-11.031884
16	143.951196 Kcal/mol 6.242323 eV -101.154280 H Child_13_11.log		
12	-3.396642	-1.802250	-0.264940
8	3.205929	-2.112056	-1.700175
6	-4.065049	0.092512	-0.639824
6	2.846708	0.980160	-1.429771
6	-1.723664	-2.441940	0.641088
6	3.052812	-1.644664	-0.660835

6	-3.325448	1.118919	-0.608950
6	2.096947	1.527668	-0.553380
6	-0.495409	-2.186429	0.959793
6	1.147346	1.978403	0.394488
6	-2.433402	2.096916	-0.490376
6	0.001693	2.667015	0.054581
6	0.652314	-1.685637	1.315748
12	2.111009	-0.262226	0.950345
6	-1.227405	2.443943	-0.240549
8	1.326940	1.498618	1.615558
16			
144.695848 Kcal/mol 6.274614 eV -101.153093 H Child_12_16.log			
12	-0.703310	-2.560277	0.381686
8	-9.542285	-0.051899	0.789397
6	-0.615467	-0.557063	-0.650799
6	-8.434698	-0.132489	0.505684
6	-1.360968	1.270062	-1.760246
6	4.057944	0.288105	1.810526
6	0.489304	0.168223	-0.155699
6	3.531977	1.386254	1.451108
6	-0.459892	2.111996	-1.393465
12	2.300595	-0.555355	0.820198
6	2.630912	2.196199	0.802858
6	-1.543138	0.009911	-1.426327
6	1.622700	2.265907	0.099818
6	4.351041	-1.974204	-1.406214
6	0.531410	1.614888	-0.534167
8	3.545514	-1.760495	-0.599531
16			
144.719785 Kcal/mol 6.275652 eV -101.153055 H MutI_14_55.log			
6	1.515484	-1.694629	-0.542839
8	0.224605	-1.377538	-0.489811
6	-0.848811	-2.325489	-0.008459
6	-5.392137	-0.091685	0.951764
6	-2.588001	1.771821	-0.664259
6	-4.354446	-0.794198	0.655483
8	-3.463789	2.481393	-0.823490
6	4.656850	1.301419	0.678862
12	4.283459	-0.621183	0.011853
6	3.458241	1.673331	0.570599
12	-0.692989	0.453836	-0.193720
6	-1.921180	-1.448892	0.136891
6	2.742171	-1.798744	-0.509854
6	-3.156284	-1.245959	0.402899
6	0.916558	1.674514	0.068523
6	2.109528	1.841399	0.375191
16			
145.062717 Kcal/mol 6.290523 eV -101.152508 H Child_1_20.log			
6	1.306707	-1.119491	-0.797386
6	-4.670436	2.132645	-0.029841
8	3.685541	-0.638796	-1.091668
6	-3.503718	1.576711	-0.108996
6	0.113668	-1.318989	-0.483425
6	-2.317912	0.947935	-0.188872
6	-1.520015	-2.034354	1.131029

6	-1.081945	1.490608	0.172440
6	-1.916544	-2.525035	2.257467
6	0.077742	1.771947	0.520242
6	2.493719	-0.441826	-0.676886
6	-2.273413	-0.504560	-0.638412
6	-1.170571	-1.360753	0.004936
8	-3.091610	-0.999633	-1.409472
12	2.051482	1.255083	0.780772
12	4.783923	0.529784	0.305506
16			
145.075886 Kcal/mol 6.291094 eV -101.152487 H Child_9_14.log			
8	-1.551287	-3.128094	-0.089382
8	5.228236	1.609371	0.139603
6	-0.243688	-2.851662	-0.232614
6	4.160850	1.065773	0.094457
6	-2.391413	-2.099702	0.145924
6	-3.604619	4.086170	-0.504170
6	-3.725019	-1.680541	0.460611
6	3.008081	0.466059	0.047022
6	0.950274	-2.573312	-0.331424
6	-2.929894	3.023674	-0.270283
6	-2.580338	-0.777292	0.234621
12	1.172844	1.304771	0.259682
12	2.655650	-1.500062	-0.284559
6	-2.218593	1.924865	-0.023684
6	-2.063967	0.533284	0.166138
6	-0.921263	1.298232	0.196193
16			
145.321649 Kcal/mol 6.301751 eV -101.152096 H Child_7_56.log			
6	2.338076	-1.777503	0.247758
12	-2.424519	1.870589	-0.116792
6	1.325876	-2.516586	0.191458
8	0.334858	3.141697	0.266546
12	6.522011	0.233418	-0.493726
8	-3.896944	0.682022	-0.330847
6	0.056374	-1.860819	0.144490
6	-0.273406	2.047341	0.182697
6	0.414532	0.772336	0.232757
6	-1.254543	-1.490417	0.055707
6	1.855924	0.524106	0.280438
6	-2.644816	-1.497030	-0.132277
6	-0.212966	-0.456515	0.193226
6	-4.036097	-2.004278	-0.151404
6	2.640832	-0.446535	0.318279
6	-3.655325	-0.600406	-0.256360
16			
145.321980 Kcal/mol 6.301765 eV -101.152095 H Child_16_25.log			
8	5.522933	-1.549926	-0.061990
6	-6.663264	-0.123901	1.140604
6	4.451335	-0.925540	0.000061
8	-5.353726	-0.350472	-1.160409
6	3.136436	-1.527750	0.015956
6	-5.665801	-0.171622	0.275194
6	4.322440	0.513318	0.055079
6	-4.311426	-0.141890	-0.138018

6	1.932758	-1.804306	0.052766
6	-3.031778	-0.066509	-0.036465
6	3.936981	1.689810	0.079367
6	-0.840267	1.065834	-0.034188
12	2.076540	2.468389	-0.005494
6	-1.722888	-0.035995	0.034256
12	-0.043186	-1.338851	0.132975
6	0.163159	1.803340	-0.069708
16			
145.817460 Kcal/mol 6.323252 eV -101.151306 H Child_7_33.log			
6	-5.843577	-0.342389	-0.231895
6	0.974448	6.507259	-0.220437
12	-3.845265	-1.364115	-0.453183
6	6.564839	-0.165995	0.662481
6	-6.894651	0.127504	0.457409
6	5.482494	-0.770999	0.601267
6	-1.915129	-1.931775	-0.167740
6	4.320595	-1.441956	0.604468
6	-7.943802	0.500398	1.164090
8	-0.002425	6.748733	0.337481
6	-0.707064	-2.078114	0.082025
6	3.141897	-1.856095	0.727906
8	-5.359573	-0.448062	-1.425395
6	0.609610	-2.148813	0.300037
6	1.819193	-2.094084	0.524845
12	7.615504	0.011198	-1.073770
16			
145.944672 Kcal/mol 6.328768 eV -101.151103 H MutD_18_42.log			
6	2.717380	-0.164326	-0.474382
6	-0.430969	2.252530	-0.684054
8	1.521415	-0.395180	-0.679808
12	-5.273591	1.993290	0.614993
12	-0.344754	-0.687783	-0.460329
6	6.382137	0.389765	0.459179
6	5.192134	0.225097	0.029213
6	-2.223459	-2.581946	0.258502
6	-3.502153	-2.090007	0.338448
8	7.511560	0.522121	0.840189
6	-0.971481	-2.585561	0.127097
6	-2.610826	0.856370	-0.194508
6	3.934185	0.033535	-0.252016
6	-3.772525	0.369212	0.067960
6	-4.056301	-0.988893	0.240143
6	-1.465399	1.503957	-0.438750
16			
145.946616 Kcal/mol 6.328852 eV -101.151100 H Child_9_41.log			
8	3.610047	-3.057095	-0.419305
6	-6.992119	0.904537	-0.018079
6	2.818479	-2.184938	-0.219455
6	-5.752266	0.517709	-0.000033
6	1.845926	-1.333027	-0.003931
6	-4.510365	0.154070	-0.013415
12	-0.206303	-1.865096	-0.306962
8	2.943996	3.334618	-1.376916
6	1.857328	0.070074	0.410563

6	-3.259279	-0.195394	-0.009192
6	0.571540	0.575963	0.499798
6	3.118566	2.564476	-0.528447
6	-0.665598	0.760034	0.413362
6	-1.860034	0.121012	0.174215
6	-2.171813	-1.165348	-0.221101
12	3.336758	1.285497	1.262300
16	146.527752 Kcal/mol 6.354053 eV -101.150174 H Child_17_14.log		
12	-2.854442	1.937186	0.165367
6	3.832982	-0.570698	-0.350533
6	-3.769062	-1.130682	-0.271341
12	3.157595	-2.415573	-0.099366
8	-4.636730	-1.924724	-0.469235
6	3.383304	0.573544	-0.228636
6	-2.928579	-0.158538	-0.076138
6	1.252681	-2.806131	0.488587
6	-1.483847	-0.096711	0.124747
8	2.973622	1.825132	-0.105503
6	-0.909126	1.245126	0.204535
6	0.215645	-2.077900	0.387404
6	1.632983	2.176662	-0.054998
6	-0.733983	-1.181625	0.362164
6	0.816750	3.274156	-0.044920
6	0.301423	1.842362	0.093445
16	146.949586 Kcal/mol 6.372345 eV -101.149501 H Child_4_34.log		
12	-5.563838	-1.556416	-0.160168
8	6.518529	-1.507122	-1.141397
8	-2.719804	-1.537818	0.230259
6	5.490974	-1.221953	-0.657037
6	-1.547113	-1.118336	0.715856
6	1.906449	2.257447	0.959134
6	-3.608426	-0.701877	-0.572846
6	0.968441	2.651212	0.202979
6	4.345851	-0.927879	-0.114734
6	-0.447572	-0.709264	1.114825
6	-0.201703	2.723865	-0.458645
6	-3.131183	0.553333	-0.774770
6	3.237352	-0.623851	0.408022
12	1.385142	0.210407	1.232010
6	-2.395459	1.551300	-0.953119
6	-1.325186	2.317940	-0.798499
16	147.014753 Kcal/mol 6.375171 eV -101.149397 H Original3D_14_3.log		
6	1.465437	0.748986	-1.053424
12	-0.571452	1.096015	-1.710087
8	2.550254	1.676050	-0.567794
6	2.062939	1.294312	0.738728
6	1.772669	2.108530	1.755602
6	0.896788	2.795085	2.404527
6	1.322744	0.143014	0.189942
12	-4.336389	-0.734736	0.151677
6	-2.601018	1.033125	-1.559937
6	-1.925851	-1.841692	1.115676

6	0.342617	-0.715481	0.668828
6	-3.153825	-2.059938	1.132947
6	4.470609	-2.672538	0.041305
6	-0.666530	-1.362740	0.949109
6	-3.720740	0.707254	-1.109903
8	4.612130	-2.351406	-1.049642
16			
147.187159 Kcal/mol 6.382647 eV -101.149123 H MutI_17_61.log			
6	2.073244	-2.020509	-0.016865
12	2.429179	0.499392	-0.042902
6	0.622420	1.468206	0.103510
6	3.350616	-1.635431	0.206614
6	4.666293	1.225277	-0.186094
6	0.845487	-2.120145	-0.158282
6	-0.482176	-1.987239	-0.209831
6	-0.563785	1.817619	0.214564
8	5.704835	1.712998	-0.366522
6	4.490496	-1.066272	0.346134
6	-5.843903	0.422145	-0.206925
6	-4.688913	0.961603	-0.012682
6	-6.896956	-0.357904	-0.392407
12	-2.500960	1.226191	0.284188
8	-2.601172	-0.755028	0.226590
6	-1.567480	-1.435809	0.016267
16			
147.330334 Kcal/mol 6.388856 eV -101.148895 H Original3D_0_73.log			
6	-0.262671	1.014622	-0.364885
6	0.092564	-0.287037	-0.750818
12	-0.671052	-2.776792	-0.526700
6	-2.557867	-0.934684	0.257704
8	2.661385	-0.954335	1.439668
6	-3.969044	0.875241	0.013247
6	0.930199	1.755700	-0.422445
6	2.167329	-0.907245	2.481640
6	0.734261	-1.359743	-1.029733
12	2.652941	-0.472870	-0.794245
6	2.289946	1.526482	-0.658276
6	-1.517234	1.464000	0.187705
6	-2.697082	0.486934	0.173132
6	1.911830	2.856541	-0.360577
8	-1.671310	2.588781	0.693945
6	-2.406108	-2.170747	0.270377
16			
147.400942 Kcal/mol 6.391918 eV -101.148782 H Child_4_59.log			
8	2.372100	2.240448	-1.095539
8	2.591513	-3.781205	0.327364
12	3.089154	0.499143	-1.140634
6	2.210387	-2.616753	0.196306
6	1.377653	2.757721	-0.505960
6	-4.442897	-0.923338	-1.317547
12	-3.360213	-0.395329	0.223890
6	0.317683	3.079175	0.043734
6	-5.001342	-1.706226	-2.149067
6	0.371322	-0.833938	1.239195
6	-1.850032	0.531551	1.421920

6	-1.550077	1.865904	1.275585
6	1.424049	-1.481917	0.628146
6	2.513936	-1.275881	-0.240543
6	-0.684297	-0.243267	1.516045
6	-0.762419	2.693682	0.749908
16			
147.606913 Kcal/mol 6.400850 eV -101.148454 H Original3D_12_7.log			
8	0.808087	-1.061967	-1.290190
12	0.970197	-2.020430	0.426952
6	-0.933261	-2.508841	1.119254
6	-1.506040	0.652634	-1.098149
6	-2.022142	0.721969	0.260200
6	-2.343471	-0.649628	0.007915
6	0.865601	0.273018	-1.277219
6	2.094139	0.689636	-0.527575
6	-1.839001	-1.752641	0.714079
6	-0.195872	1.154006	-1.256280
6	1.821555	0.998522	0.895165
12	0.056110	2.231542	0.645361
6	3.363304	0.088224	-0.253969
8	-1.793826	1.577643	1.186605
6	2.383417	-0.314188	0.900701
6	-2.426524	-0.462503	-1.490637
16			
147.645571 Kcal/mol 6.402526 eV -101.148392 H Original2D_8_2.log			
8	0.000000	-0.808132	0.000000
12	-1.491138	0.989973	-0.000000
6	1.986438	0.273875	0.000000
6	1.385946	-0.953323	0.000000
6	2.591291	1.361077	0.000000
6	2.746650	2.699254	-0.000000
8	-0.798333	2.659569	-0.000000
6	-2.859223	-0.611927	-0.000000
6	2.585240	3.950212	-0.000000
6	-0.757358	-2.059687	0.000000
6	-2.125919	-1.802484	0.000000
12	0.477554	3.910741	-0.000000
6	0.878915	-5.605387	0.000000
6	-0.121285	-3.221088	0.000000
6	0.338233	-4.420230	0.000000
6	-3.557315	-1.880300	-0.000000
16			
147.724088 Kcal/mol 6.405931 eV -101.148267 H Child_3_33.log			
6	-4.942736	-4.427979	-0.869635
8	4.452380	-0.695228	0.778454
8	-4.463626	-3.382472	-0.841828
6	2.145514	-0.173654	0.230061
6	2.009404	0.905634	-0.483145
12	-2.935408	2.450879	0.495227
6	1.526556	1.970796	-1.066196
12	-1.818249	0.165984	1.832586
6	3.484801	-1.122653	0.145366
6	-1.795289	3.563839	-0.887864
6	0.593429	2.777755	-1.302634
6	0.042558	-0.689219	1.737414

6	3.172348	-2.207665	-0.618084
6	-0.605525	3.370541	-1.247407
6	1.090873	-0.540203	1.090447
6	2.800375	-3.223987	-1.299450
16			
147.881079 Kcal/mol 6.412739 eV -101.148017 H Child_5_25.log			
8	0.855025	3.695955	-0.030177
6	3.331523	-2.666263	-0.180804
6	-0.882729	2.084777	0.040405
6	2.176623	-2.153837	0.081155
6	0.472245	2.509460	0.062526
6	-5.323332	-1.838415	-0.172736
6	-1.979853	1.484851	-0.070034
6	1.021990	-1.352417	0.300055
8	-3.084748	0.836925	-0.188362
6	-4.190343	-1.233861	-0.145459
6	1.381451	1.356411	0.154663
6	-3.004743	-0.621729	-0.042046
6	2.589172	0.796825	0.018516
6	1.364823	-0.042880	0.253898
12	4.037348	-0.732364	-0.298652
12	-1.029279	-1.451017	0.294276
16			
147.927936 Kcal/mol 6.414771 eV -101.147942 H Child_2_44.log			
6	-2.490108	-2.052296	0.820977
8	4.788126	-0.684482	1.262241
12	-4.046327	-0.612209	0.825561
6	3.759533	-0.352752	0.855391
6	-1.435614	-1.583145	0.273946
6	2.243048	2.732508	0.045476
6	-4.231499	1.305314	0.271912
6	2.095475	1.313383	0.094229
6	-0.507055	-0.893472	-0.398599
6	2.540038	-0.048823	0.259391
6	0.780792	-1.269658	-0.962141
6	0.972595	2.020326	-0.242135
6	-3.039979	1.466372	-0.121582
6	1.959943	-1.225410	-0.154417
8	0.817459	-1.518016	-2.203043
12	-1.014314	1.374368	-0.569585
16			
147.985445 Kcal/mol 6.417264 eV -101.147851 H Child_5_48.log			
6	1.142755	3.304706	0.414765
6	1.738246	-2.630605	0.764042
6	-5.308092	1.408358	0.402414
6	0.591035	-2.959969	0.303438
6	0.130814	2.459358	0.223070
6	-0.577588	-3.237162	-0.161853
8	-4.246576	1.030474	0.153657
6	2.417313	-1.521749	1.110188
6	-0.736566	1.504506	0.013387
6	-1.668841	-2.521781	-0.497392
8	3.001122	0.820055	-1.350776
6	2.950306	-0.398300	1.334290
6	3.672134	0.519580	-2.228011

6	-2.650305	-1.766978	-0.767364
12	-2.301321	0.234344	-0.376616
12	2.281018	1.451987	0.719208
16			
147.996309 Kcal/mol 6.417735 eV -101.147833 H MutD_3_70.log			
12	4.141820	-0.594892	-0.655326
6	-1.076746	2.008930	0.099802
8	-4.926131	-0.826175	-1.003109
12	0.950280	1.426022	0.318374
6	2.625034	-2.067381	-0.792947
8	-0.509763	-1.377506	2.091465
6	-2.646710	-0.094354	-0.152719
6	-2.220806	1.281112	-0.088358
6	4.260280	1.321784	-0.081678
6	0.528632	-0.862613	0.147010
6	-1.974983	-1.234866	0.225377
6	-2.370970	2.700708	-0.119743
6	3.030367	1.497287	0.157547
6	1.507916	-1.591777	-0.400942
6	-3.897203	-0.473281	-0.614619
6	-0.701151	-1.209567	0.844030
16			
147.998345 Kcal/mol 6.417824 eV -101.147830 H Child_8_19.log			
6	-1.782346	2.695911	0.003162
8	5.874961	0.608498	-0.036196
6	-3.033569	2.418746	-0.033678
6	4.676353	0.478798	-0.015239
8	-3.912294	1.376400	-0.037057
6	3.400329	0.338375	-0.001275
12	0.217105	1.912440	0.034656
6	0.801399	-2.694119	0.001398
6	-2.887494	0.356980	0.001906
6	1.529273	-1.689335	0.008000
6	-1.665454	0.984340	0.024731
12	-1.131984	-3.252648	-0.004724
6	2.167443	-0.461530	0.016490
6	1.991572	0.871135	0.027602
6	-2.893437	-2.245618	0.003772
6	-3.091198	-1.019801	0.000940
16			
148.065269 Kcal/mol 6.420726 eV -101.147723 H Child_2_12.log			
6	-1.140902	-2.919487	0.196467
12	-2.016272	1.628444	0.049985
6	0.071149	-3.318510	0.140900
6	3.140817	0.930648	-0.277535
6	-2.525604	-0.903921	0.306021
6	2.331409	1.843384	-0.158735
8	-2.163850	-0.038586	1.237474
8	0.896817	3.796360	0.642619
6	-3.074542	-0.314013	-0.859598
6	3.639489	-0.343562	-0.300077
6	-2.242482	-2.254882	0.412537
6	1.176492	2.595678	0.026809
6	3.764636	-1.575930	-0.256363
6	-0.125980	2.435359	-0.160863

6	-3.324893	0.620168	-1.666263
12	2.016167	-2.531094	-0.005028
16			
148.362087 Kcal/mol 6.433597 eV -101.147250 H Original3D_3_4.log			
6	3.695525	0.542400	-0.641162
6	-1.706371	-1.853702	0.929802
12	2.299631	1.920128	0.025936
6	-2.687487	-1.071589	1.089158
6	-2.360879	1.725629	-0.516473
6	0.952829	0.499016	0.809034
6	1.566271	-0.666303	0.349159
8	-2.639232	2.491721	0.347944
6	-0.406105	-2.230510	0.646719
8	-1.767134	-1.487028	-2.134390
6	0.759228	-1.847667	0.447781
12	-1.015212	0.265273	1.537274
6	-1.952303	0.864202	-1.375392
6	-1.835920	-0.360881	-1.825611
6	4.351699	-0.753003	-0.453158
6	2.929832	-0.557984	-0.204350
16			
148.898364 Kcal/mol 6.456852 eV -101.146396 H Child_11_44.log			
8	-5.536056	1.434428	-0.053054
6	3.121994	-1.967817	-0.037822
6	-4.443089	1.008138	0.047320
8	5.708935	0.491183	0.288090
6	-3.219409	0.453309	0.056208
6	3.289515	-0.487427	-0.076433
6	-3.092547	-0.973451	0.083276
6	4.455223	0.616458	0.057290
6	-3.417245	-2.377882	0.013397
6	2.022089	-1.110308	-0.132620
6	-1.958414	1.125714	0.094357
6	3.251031	1.171248	-0.294860
12	1.294255	1.729702	-0.042077
12	-0.018006	-1.518173	-0.085228
6	-0.739293	1.401771	0.008242
6	-2.052855	-1.850292	0.122873
16			
148.926533 Kcal/mol 6.458074 eV -101.146351 H Child_17_28.log			
12	-7.307125	-0.971091	0.653461
6	6.745188	-0.498883	1.771800
8	-5.914953	0.273910	0.426421
6	5.690710	-0.268636	1.067619
6	-4.682584	0.539831	0.259798
6	3.962760	1.114047	-0.105358
6	-3.483708	0.766949	0.077934
6	4.562719	-0.093857	0.341810
6	-2.181957	1.027650	-0.130767
8	0.315925	-2.005814	-1.359058
6	-0.983331	1.292949	-0.351412
6	1.224197	-1.434847	-0.801309
6	2.524407	-1.537923	-0.396294
6	3.016424	1.835899	-0.479387
12	1.017955	1.324291	-0.648026

6	3.648886	-1.140374	-0.021788
16			
149.111411	Kcal/mol	6.466091	eV -101.146056 H Child_5_24.log
12	-8.320089	-0.678887	-0.012433
8	4.966982	-2.327956	-0.802530
6	-1.094666	-3.253457	-0.479524
6	4.158684	-1.743108	-0.194182
8	-0.759056	-2.330490	0.117805
6	3.259026	-1.104308	0.490872
6	0.068664	1.613079	-2.112392
6	2.388498	-0.406631	1.091201
6	-1.589121	0.766022	0.768848
6	2.399959	2.276533	0.548162
6	1.178585	2.003909	-1.716235
12	1.043408	1.184934	1.780084
6	-1.692341	0.864128	-0.590290
6	2.009524	2.204157	-0.648758
6	-1.129479	1.142165	-1.661007
6	-1.014538	0.836678	1.880970
16			
149.455164	Kcal/mol	6.480997	eV -101.145508 H Child_5_19.log
8	0.944379	5.078249	-1.100523
8	4.542360	-1.549589	-0.857883
6	3.423832	-1.383848	-0.544846
6	0.809277	3.987159	-1.061262
6	0.326439	1.416140	2.205629
6	-3.819066	0.245153	-0.784960
6	2.249105	-1.229039	-0.020667
6	-3.405186	-0.920669	-0.764647
12	1.620743	0.067442	1.479634
6	-2.551958	-2.002425	-0.349027
6	1.087665	-1.910758	-0.272832
6	-0.614426	1.528396	1.376464
6	-0.058929	-2.381190	-0.450263
12	-2.305215	1.295307	0.230576
6	-1.305619	-2.368905	-0.991207
6	-2.087842	-2.410392	0.848406
16			
150.032849	Kcal/mol	6.506048	eV -101.144588 H Child_4_11.log
6	-2.093138	-2.035257	-0.046392
8	3.667788	2.330232	-0.138953
6	-3.141005	-1.117580	0.026635
6	2.785753	1.556152	0.026858
6	-4.171681	-0.225137	0.168793
8	5.051389	-0.290648	0.167336
12	-0.173358	-2.610838	-0.083327
12	0.588245	0.803802	-0.063272
6	-1.831916	-0.536006	-0.100817
6	-3.700515	2.492820	0.040934
6	-4.056925	1.063767	0.127081
6	3.835975	-0.383430	0.087498
6	1.396707	-1.253722	-0.023209
6	2.683863	-1.112478	0.068796
6	-1.515805	0.800070	-0.098491
6	-2.646657	1.645427	-0.022334

16
150.134267 Kcal/mol 6.510446 eV -101.144426 H MutD_12_64.log
6 1.173078 -2.887280 -0.097932
12 -0.764824 -3.287283 -0.334201
6 1.701375 -1.771347 0.021588
6 4.566456 0.364134 0.357476
6 3.348934 -0.025966 0.290606
6 -2.706836 0.427125 0.237121
6 -2.378943 -0.754637 -0.302373
6 -0.289670 3.123094 -0.518726
8 -0.061028 4.270921 -0.634151
6 -2.340535 -1.997243 -0.476512
6 2.069740 -0.398466 0.139883
6 -5.224961 0.908351 0.888632
6 5.795374 0.766038 0.321567
12 -0.753407 0.909091 -0.004710
6 -4.017203 0.621266 0.522534
8 1.065768 0.515065 0.104618

16
150.280823 Kcal/mol 6.516801 eV -101.144193 H Child_1_44.log
12 3.665952 -0.767664 -0.427952
6 -4.125265 -1.533665 -0.072091
6 3.833580 1.013390 0.619968
6 -3.144835 -0.757593 -0.380971
6 2.632715 1.377977 0.654206
6 -2.195669 0.175801 -0.462314
6 1.301392 0.982330 0.265937
12 -2.552434 2.292990 -0.084622
6 -1.172271 -3.294608 1.040533
6 -0.783526 0.124792 -0.494034
6 1.372679 -0.254608 -0.358130
6 0.202410 -0.856732 -0.836714
8 -0.730747 2.392253 0.482159
6 1.653595 -1.429523 -0.959374
6 -0.067971 1.303936 0.154678
8 -0.569656 -2.318865 0.907930

16
150.449953 Kcal/mol 6.524136 eV -101.143923 H MutD_3_76.log
8 -7.963678 -2.337030 1.000227
6 0.881321 1.334843 0.347987
6 3.365495 -3.543517 -0.745603
6 1.987151 1.070468 1.189969
12 3.628748 -1.281197 1.268401
6 2.983203 0.584303 1.742655
6 -1.113968 2.252985 -0.695427
12 1.467508 -1.361937 -1.186556
8 -2.074496 2.937079 -1.024036
6 2.964471 -2.431303 -0.286562
6 -0.673348 -0.067570 -2.129744
6 -0.115466 2.454442 0.423362
6 0.571114 0.475441 -0.683569
6 -6.886052 -2.063998 0.716692
6 -0.116990 3.437892 1.323162
6 -0.655210 0.982217 -1.334868

16

150.455893 Kcal/mol 6.524393 eV -101.143914 H MutI_16_79.log

8	-3.347617	2.301824	0.606431
6	-3.313759	-0.746306	0.139022
6	2.734957	-1.203404	1.092964
6	4.045899	-1.189002	0.846426
6	1.327548	2.170473	-0.919885
6	2.557493	2.005063	-0.956612
8	-0.417227	-3.126947	-1.744891
6	-0.009422	2.175930	-0.684364
6	-4.154282	-1.648351	-0.281562
6	-1.175767	2.044257	-0.321632
6	-2.403105	1.578206	0.260596
6	-0.560120	-2.425237	-0.853449
12	-0.518273	-0.910594	0.941941
6	-2.342448	0.110257	0.484120
6	1.453963	-1.316784	1.249284
12	3.947691	0.683125	-0.210422

16

150.545539 Kcal/mol 6.528281 eV -101.143771 H MutI_4_67.log

6	1.664355	-1.485971	-0.028994
6	0.922353	-0.298555	-0.068029
12	-3.333332	1.898313	-0.080605
6	1.520533	3.106342	0.070392
12	-0.419611	2.391148	0.124647
6	3.466501	-0.103750	-0.040262
6	-1.276262	-0.966665	0.019527
6	-0.336907	0.080444	-0.042330
6	-0.639857	-2.410294	0.056880
8	3.096350	-1.395101	-0.049353
8	-1.410048	-3.373132	0.133772
6	-3.790138	-0.243380	-0.116642
6	2.453884	2.278651	0.008792
6	-2.636562	-0.744100	0.029357
6	0.824213	-2.505206	-0.045305
6	3.085370	1.071206	-0.044027

16

150.694330 Kcal/mol 6.534733 eV -101.143534 H Child_2_46.log

8	-4.621234	0.838222	-2.387512
12	3.442088	1.756516	-0.726321
6	-4.524463	0.005700	-3.166687
6	3.970398	-0.189655	-0.635929
6	-1.880254	-0.619937	1.654472
6	1.913446	3.017103	-0.373944
6	-1.236681	-1.693978	1.076016
6	3.287570	-1.229157	-0.557362
6	-2.926353	-0.081618	2.477179
6	0.795230	3.084182	0.185892
6	-1.876313	0.743325	1.877868
6	2.362349	-2.225228	-0.451445
6	-0.639414	-2.615846	0.544250
12	-0.806538	2.386271	1.213170
8	0.189758	-3.476016	-0.035915
6	1.392020	-2.963408	-0.372773

16

150.735522 Kcal/mol 6.536519 eV -101.143468 H Child_10_55.log

6	-3.802605	-1.157758	-0.666435
8	0.587346	1.282932	1.389446
6	-4.182704	1.271510	-1.534478
6	1.670650	-1.986732	0.730135
6	-4.220115	0.161801	-0.628062
6	0.641038	-2.597194	0.338296
6	-2.961079	-2.055980	-0.614444
8	10.347095	0.560187	-0.965732
6	-1.783357	-2.686375	-0.423116
6	9.181646	0.783250	-0.825574
6	-4.478146	1.121236	0.425540
12	1.776433	-0.042435	1.403873
6	-3.600331	2.157701	-0.302649
6	-2.493217	2.812668	-0.081048
6	-0.604815	-2.869046	-0.105866
12	-0.749542	1.336148	0.157502
16			
150.737708 Kcal/mol 6.536614 eV -101.143465 H Child_8_41.log			
8	3.508303	-1.846354	0.173738
6	-5.259652	1.254921	0.384092
6	-0.281100	-1.986762	-0.295445
6	-4.037954	0.883919	0.259829
6	2.274238	-2.116351	-0.027715
8	-1.641087	1.065135	0.226504
6	1.058822	-2.175847	-0.206639
6	-2.756786	0.409975	0.111237
6	-1.475390	-1.673389	-0.319628
6	2.201672	1.320324	0.102480
12	3.852474	0.030606	0.352016
6	-2.716172	-1.024327	-0.210329
6	2.199397	3.845822	-0.672454
6	-3.993875	-1.500939	-0.326596
6	2.222952	2.594144	-0.265753
12	0.184639	0.574462	0.114617
16			
151.107244 Kcal/mol 6.552639 eV -101.142876 H MutI_17_47.log			
6	-1.635158	0.099724	-0.558773
6	0.401560	1.027619	-0.247382
8	-0.292433	-3.661649	-0.052661
6	0.174941	-2.596361	-0.252370
6	-2.416178	1.198598	-0.343334
6	-0.250840	-0.165858	-0.511614
6	-3.077097	-0.139940	-0.585347
6	1.959632	-1.064645	-0.941699
12	2.663935	1.553803	-0.922033
8	1.318615	-0.887065	2.845040
6	-4.190150	-0.826509	-0.661276
6	0.454322	-0.125135	2.828625
6	0.833413	2.199532	0.018823
6	2.978184	-0.432429	-1.309703
12	-1.269378	2.578219	0.633949
6	0.610014	-1.373688	-0.582955
16			
151.238351 Kcal/mol 6.558324 eV -101.142667 H Child_12_33.log			
8	6.328280	-3.863328	-0.030894

6	-6.883000	-3.252785	1.006304
6	4.164561	0.671703	0.122656
6	-5.955152	-2.491711	0.495602
6	3.416719	1.765717	0.065248
6	-5.045386	-1.778281	-0.063318
6	5.848532	-2.764229	0.027856
6	-4.106060	-1.033437	-0.597612
6	4.742986	-0.444039	0.125662
8	-3.069097	1.215687	0.073778
6	5.333537	-1.604079	0.093144
6	-3.323574	0.158256	-0.601249
6	2.643558	2.755281	0.008734
6	-3.096543	-0.718325	-1.665842
12	-1.826746	2.579812	0.426663
12	0.783869	3.553246	0.036155
16			
151.395412 Kcal/mol 6.565135 eV -101.142416 H Original3D_0_47.log			
6	-0.131105	0.666224	-1.496684
6	-0.078255	-0.583118	-1.212597
6	-0.307283	1.743784	-0.682615
6	0.611905	1.731292	0.528270
8	-0.343233	-1.687009	-0.755268
6	-0.619336	-0.097397	1.983885
6	-0.046286	0.888200	1.471990
12	-2.446572	1.639130	-0.712938
6	-3.595639	-1.170351	0.120930
8	2.913694	-3.148759	-0.349023
6	1.922745	1.889039	0.477794
12	-1.801393	-1.537497	1.028774
6	3.224388	-2.044304	-0.257359
6	3.204009	1.802919	0.311423
6	4.405897	1.439253	-0.047310
6	-3.522390	-0.021117	-0.357012
16			
151.423290 Kcal/mol 6.566344 eV -101.142372 H Child_7_52.log			
6	0.588247	-2.422765	0.253161
6	-4.134986	0.004580	-2.547744
6	1.734733	-2.249455	-0.260705
6	-3.287925	0.532518	-1.666540
12	-1.189189	-1.679348	1.063367
8	-2.436554	1.218545	-1.084679
6	2.839981	-1.757432	-0.725730
6	1.598496	1.919971	0.725337
6	-0.316275	0.606693	1.968708
6	2.666655	2.047625	0.113509
6	3.704678	-0.943164	-1.074752
12	-2.082176	0.939912	0.795497
6	3.740959	1.512042	-0.501496
6	0.478377	1.318352	1.283874
6	4.049186	0.397193	-0.929333
8	-2.902993	-0.834011	0.817666
16			
151.448254 Kcal/mol 6.567426 eV -101.142332 H Child_18_31.log			
8	2.803983	-2.736619	0.376828
8	-2.568371	2.013858	-0.187951

6	1.759181	-2.060510	0.283437
6	-2.851276	0.740003	-0.305351
6	0.428632	-2.655493	0.269720
6	-2.870997	-0.515814	-0.329397
6	4.350232	2.099039	-0.764606
6	-0.260370	4.611444	0.672375
6	-0.767025	-2.958287	0.158614
6	-0.718243	3.443232	0.347958
6	3.473787	1.190974	-0.449419
6	2.608304	0.266667	-0.130626
6	-1.098394	2.189242	0.151205
6	1.682247	-0.608488	0.101354
12	-2.685986	-2.507229	-0.255685
12	-0.339128	0.118065	0.127134
16			
151.761490 Kcal/mol 6.581009 eV -101.141833 H Child_1_32.log			
8	4.754682	-1.305558	1.477320
6	-0.271883	3.160892	-0.516700
6	5.854874	-1.078760	1.251188
12	-1.768976	2.605744	0.723910
6	0.299942	-1.599270	-1.224331
6	0.682361	2.493395	-0.938829
6	-0.479532	-2.553368	-1.402436
8	1.723354	1.784989	-1.415335
6	0.152107	0.126976	0.303469
6	-2.108857	0.611509	1.354214
6	-3.512098	-1.532743	0.699905
6	-0.819230	0.292514	1.098921
6	0.806975	-0.326328	-0.795852
6	1.876325	0.395868	-1.489399
6	-2.979378	-0.489709	1.149563
12	-2.300518	-2.675853	-0.510090
16			
151.879718 Kcal/mol 6.586136 eV -101.141645 H Child_1_36.log			
6	-3.515400	-0.514209	1.285306
6	4.344571	0.042946	0.211340
6	-3.077873	0.597875	0.835805
6	3.280566	-0.560771	-0.276981
6	-2.468197	1.714473	0.324090
6	2.039253	-0.972139	-0.558556
6	-1.604168	2.438806	-0.224660
12	2.588126	0.896154	1.395061
12	-2.022848	-1.471788	0.281965
6	1.046106	-1.357107	-1.418919
6	-0.566879	3.024076	-0.808616
6	1.049318	-0.811232	0.966296
6	0.399558	3.525434	-1.475119
6	-0.186627	-1.564014	-1.594541
8	-0.000001	-1.436899	1.076589
8	-1.403087	-1.872753	-1.541211
16			
151.975308 Kcal/mol 6.590281 eV -101.141492 H Child_6_40.log			
6	-11.904397	-3.104127	0.525925
12	0.670839	2.749399	0.185580
6	4.267423	-1.877809	-0.115522

6	1.063606	0.426651	-0.202921
8	4.013179	-4.259741	0.733951
6	2.139250	-0.355361	-0.181148
6	6.916169	-1.484722	-0.282662
6	-1.621232	3.431398	-0.641663
6	4.080827	-3.183780	0.318662
6	-0.266133	0.368877	-0.311350
6	5.638851	-1.621751	-0.243482
6	-1.752633	2.173600	-0.636404
6	-1.418756	0.878631	-0.483968
6	3.148724	-1.089192	-0.186815
8	-11.118441	-3.219442	-0.302595
12	-1.079847	4.955515	0.747523
16			
152.089414 Kcal/mol 6.595230 eV -101.141311 H MutI_9_75.log			
6	-2.765792	-1.552928	-0.132112
12	2.739501	-2.549509	-0.205471
6	3.075169	0.252582	-0.041364
6	-1.637399	-2.121911	-0.077125
8	-4.919410	-0.339578	-0.252758
6	1.264394	0.891984	1.933382
6	-0.431296	-2.646201	-0.036550
8	-2.625308	1.939683	0.264660
6	3.728893	-0.825229	-0.186743
6	-3.880692	-0.906166	-0.195278
6	2.232483	1.318130	0.010737
6	0.940030	1.415926	0.735649
6	-0.148274	2.143492	0.111254
12	1.431116	2.990035	-1.005619
6	-1.430688	2.033512	0.241633
6	0.771562	-3.017715	0.042830
16			
152.284096 Kcal/mol 6.603672 eV -101.141000 H Child_8_18.log			
8	-6.098889	1.823767	1.023207
6	4.231365	2.462385	-0.300064
8	-5.907281	-0.447753	-1.435677
12	5.518134	0.873704	-0.420283
6	-5.135018	0.013346	-0.496052
6	5.057385	-1.113748	-0.129612
6	-3.829193	-0.442787	-0.171760
6	3.902057	-1.514696	0.131733
6	-5.584222	1.086178	0.265198
6	-2.695322	-0.848393	0.113226
6	2.545863	-1.434913	0.353293
12	-0.835527	-1.531239	0.371835
6	1.215393	-1.567573	0.340618
6	3.117616	1.905859	-0.046703
6	2.080187	1.081828	0.225227
6	1.736901	-0.147101	0.361752
16			
152.438243 Kcal/mol 6.610356 eV -101.140755 H MutI_17_55.log			
6	-1.287682	-0.062679	0.510218
12	-1.112885	-2.136847	-0.062870
6	-0.611876	1.103192	0.806608
6	-3.166579	-1.107558	-0.538498

6	3.462004	-0.843362	-0.203757
6	-3.106082	-2.327850	-0.846235
6	-3.063705	1.455793	-0.126323
6	0.953087	-2.854977	0.388281
8	1.302485	2.248942	-0.360918
6	-2.641802	0.114089	-0.027382
6	0.260838	2.111002	0.338890
12	2.975133	1.310161	-0.584070
6	-1.077805	2.480444	0.559792
8	2.070082	-2.914392	0.618158
6	4.441633	-0.020368	-0.047374
6	-2.383283	2.492913	0.136674
16	152.681511 Kcal/mol 6.620905 eV -101.140367 H MutD_18_54.log		
6	7.247256	-0.545874	-0.617714
12	-1.794573	-1.763506	0.258022
6	-3.050681	1.907475	-0.243531
6	-4.000522	-1.540858	-0.327849
6	6.002346	-0.423873	-0.337175
6	-2.138203	2.721185	-0.085623
6	-3.357270	-0.338262	-0.191967
8	0.000585	-1.414223	0.500056
8	-3.902320	0.873981	-0.435435
6	2.177116	0.023129	0.283599
6	0.852128	-0.440135	0.432264
6	4.715888	-0.290390	-0.101864
6	1.038078	0.928082	0.371631
12	-0.139911	2.607187	0.198932
6	-3.901781	-2.823878	-0.281123
6	3.486927	-0.143642	0.099281
16	153.007071 Kcal/mol 6.635023 eV -101.139848 H Child_15_17.log		
8	7.255625	1.785336	-0.556640
6	-5.636442	1.232647	-0.701742
6	6.213096	1.211967	-0.334598
6	-5.056586	0.120230	-0.851970
6	5.379130	0.208615	-0.186934
6	-4.101716	-0.843652	-0.878780
8	4.140384	-0.041405	0.056844
12	2.548548	-0.857464	0.391891
6	-2.979219	-1.242991	-0.527363
6	0.034535	-3.032028	0.197690
6	-2.316486	1.497010	0.967245
6	0.754314	-1.781141	0.349656
6	-1.756226	-0.940381	0.107649
6	-0.618440	-1.741734	0.187507
6	-1.861936	0.377411	0.640383
12	-4.172899	2.161866	0.456934
16	153.099198 Kcal/mol 6.639018 eV -101.139701 H Child_17_15.log		
6	1.998712	2.745046	-0.139887
6	-7.319894	-0.343863	-0.386620
6	2.967198	1.988476	-0.242697
6	-6.046833	-0.395314	-0.248368
12	0.026638	2.526793	0.234513

6	-4.743613	-0.347659	-0.061856
8	3.892307	1.006377	-0.269906
6	-3.501453	-0.301000	0.107535
6	-1.062054	0.785631	0.362872
8	0.039777	-1.523303	0.188268
6	3.377276	-0.243439	-0.177945
6	-2.184696	-0.135662	0.242422
6	4.206671	-2.658778	0.072059
6	-0.842277	-0.576066	0.272266
6	4.135143	-1.377851	-0.057618
12	1.859883	-1.751936	-0.051168
16			
153.192194 Kcal/mol 6.643051 eV -101.139553 H MutD_2_72.log			
6	-2.314479	-1.002869	-0.662837
6	-0.250282	-0.595794	-0.181107
12	4.875678	1.676729	-1.521837
6	-2.152745	2.401665	0.500320
6	1.019928	-0.127654	-0.547059
6	-3.697949	-0.558208	-0.670404
6	-1.081488	-1.818423	-0.804675
6	-3.822913	0.605801	-0.206309
6	3.056441	-0.971720	2.063684
8	-0.741519	-2.932448	-1.159040
6	2.869858	-0.428035	0.922122
6	-2.512147	1.181848	0.100172
6	-1.577997	0.073111	-0.178082
8	-1.784304	3.458724	0.830699
12	0.924180	-1.399156	1.688504
6	2.231822	-0.016570	-0.231371
16			
153.484678 Kcal/mol 6.655734 eV -101.139087 H Child_7_30.log			
6	-2.117839	2.002195	0.556424
12	-0.850248	0.069306	-0.240538
12	-0.222592	2.868377	0.512524
8	-2.265324	-1.198390	-0.518091
6	-3.156209	1.274393	0.404864
6	4.317696	0.165395	-1.584683
6	-3.976107	0.347508	-0.128064
6	2.083498	0.780883	-0.333596
6	-3.551365	-1.016099	-0.225889
6	4.445660	-0.528060	-0.247386
6	-4.468665	-1.990955	0.049543
6	3.284617	0.239858	-0.581421
6	-5.428746	-2.818447	0.285141
6	5.128882	-1.317982	0.508597
6	0.907492	1.281008	-0.159233
8	5.772900	-2.022905	1.201891
16			
153.530022 Kcal/mol 6.657700 eV -101.139015 H MutD_10_68.log			
6	-3.022781	1.043113	-1.018178
12	-7.068504	-1.397140	-0.268842
6	-0.292353	2.023535	0.564136
6	-0.441525	-1.231749	1.095156
12	-2.091311	1.165551	1.050832
6	3.319712	0.721297	-0.170542

6	0.852004	-1.396150	0.740184
6	-1.599173	-0.814413	1.325967
6	3.258478	-0.799989	-0.102823
6	2.015267	-1.282716	0.351887
8	-3.233518	0.714571	-2.095552
6	0.955595	1.851281	0.341422
6	4.304579	-1.550381	-0.486357
6	5.347009	-2.191128	-0.903348
8	4.355874	1.358519	-0.508296
6	2.126344	1.326357	0.170313
16			
153.835638 Kcal/mol 6.670953 eV -101.138528 H Child_7_25.log			
6	-4.816080	-0.476535	-0.299757
6	0.488241	3.199036	0.081028
6	-3.941191	-1.364234	-0.144312
6	1.666213	2.833189	0.011791
8	-2.779121	-2.078649	-0.001733
6	3.441479	1.016491	-0.149835
6	-1.703310	-1.260405	0.121680
6	2.752284	2.039920	-0.086032
12	-3.046765	0.846742	-0.013688
6	3.783224	-0.315528	-0.142298
12	0.235227	-2.202863	0.192193
6	-2.002742	2.596580	0.133430
6	-0.864902	3.090881	0.128132
6	3.187695	-1.531712	-0.025326
6	4.622970	-1.517652	-0.127276
8	2.036016	-2.119694	0.108056
16			
153.876742 Kcal/mol 6.672735 eV -101.138462 H Child_4_25.log			
8	-3.861886	2.024152	0.300559
6	2.782236	0.749561	-0.119464
6	-4.844600	-1.150052	-1.262545
12	3.996233	-1.002461	-0.537620
6	-4.343794	-0.142959	-0.634749
8	2.439769	-2.034879	-0.118820
6	-3.583510	0.864457	-0.001224
6	1.423649	-1.337111	0.289008
6	-2.238572	0.252114	0.251479
6	0.241305	-1.903267	0.702931
6	-0.971447	0.857848	0.130473
6	-1.006549	-1.718791	0.688024
6	-2.172350	-1.096925	0.564268
6	1.577315	0.223432	0.192770
6	0.274288	0.820855	0.225142
12	3.382860	2.800032	-0.096596
16			
154.055807 Kcal/mol 6.680500 eV -101.138177 H Child_11_12.log			
6	1.461233	0.946367	1.424481
6	4.985456	-2.533921	0.563260
6	0.129443	0.855377	1.506625
6	4.646313	0.242571	-2.267438
6	-1.093935	0.707308	1.374960
6	5.679656	0.912497	-1.929932
6	2.651414	0.956036	1.044503

8	-4.692996	-1.712356	-0.722918
6	-2.321506	0.360515	0.864921
6	-3.747974	-1.579942	0.156924
6	-3.237354	1.258608	0.199327
8	4.644951	-1.443329	0.488097
6	-2.839811	-0.942237	0.720449
6	-4.226298	1.647491	-0.469146
12	4.267209	0.620040	-0.223941
12	-5.278498	0.068415	-1.213978
16			
155.244507 Kcal/mol 6.732047 eV -101.136283 H Child_15_11.log			
6	0.961135	-1.677182	-0.390490
6	-0.767391	1.548458	-0.147944
6	-1.550549	-2.065231	-0.788495
8	1.612475	1.733476	0.505039
6	2.235710	-1.368666	-0.197454
6	-1.975952	1.611857	-0.571238
12	5.497353	-0.571766	0.049735
6	-3.187746	1.744108	-0.962315
6	3.422552	-0.955217	-0.003065
6	0.444487	1.602441	0.191700
6	-0.255154	-1.901457	-0.593176
6	-4.391755	1.902349	-1.458418
6	-2.823817	-2.146070	-0.929948
12	3.531068	1.182185	0.638335
8	-5.701131	-1.036040	1.663591
6	-4.716820	-0.446140	1.583198
16			
155.401627 Kcal/mol 6.738861 eV -101.136032 H Child_4_41.log			
6	-2.522326	-3.648106	-1.413157
6	2.186286	-0.645497	0.719356
8	-2.114607	-3.236448	-0.417385
8	2.650544	1.608615	-1.678080
6	-3.119290	1.342088	0.767327
6	3.314467	2.559226	-1.588908
12	-1.603587	1.241393	2.159564
12	1.355413	-0.108302	-1.185536
6	-4.182047	1.207023	-0.217298
6	1.262702	-0.023371	1.577291
6	-2.781515	1.019915	-0.535886
6	3.247554	-1.390807	1.074239
6	0.301286	0.554125	2.124907
6	-1.662841	0.685066	-1.276462
6	4.296066	-2.100878	1.350979
6	-0.558579	0.345478	-1.736489
16			
155.504855 Kcal/mol 6.743337 eV -101.135868 H Original3D_0_51.log			
6	1.051690	-2.296015	-0.668181
12	2.909543	0.005995	-0.060739
6	0.520725	1.414390	-0.008127
6	0.148217	0.037619	-0.167763
6	2.464147	2.995789	0.070617
6	1.213397	-4.687240	-1.645236
6	1.089535	-3.525913	-1.116954
8	-1.188201	-2.189218	2.633043

6	1.817661	1.849204	0.028553
6	-2.459201	0.050644	-0.349601
6	1.104516	-1.074477	-0.274123
6	-1.194626	-0.090632	-0.229587
8	3.179323	3.940879	0.099718
6	-0.893582	-1.126179	2.967687
6	-3.743545	0.129919	-0.543201
12	-4.796425	1.987676	-0.793143
16			
155.737904 Kcal/mol 6.753443 eV -101.135496 H Child_10_19.log			
8	3.796270	-1.691475	0.209323
6	-0.611092	3.396426	-0.006152
6	1.017176	-3.904831	-0.164488
6	-1.699929	2.807400	0.015119
6	1.409339	-2.532206	-0.043459
6	0.728076	3.579993	-0.027029
6	2.438407	-1.553204	0.030156
6	-2.727987	1.952555	0.028574
6	0.066575	-2.767638	-0.055161
6	1.976570	3.522006	-0.048964
6	2.601494	-0.244578	-0.027371
6	-3.386023	0.894280	0.041555
12	-1.904878	-2.173639	0.008037
6	-4.218312	-0.218459	0.014918
12	2.971486	1.763087	-0.043340
8	-3.591902	-1.391507	0.025359
16			
155.880275 Kcal/mol 6.759617 eV -101.135269 H MutI_9_71.log			
6	1.522797	-2.669449	-0.037043
12	-2.833160	-2.526791	0.185877
6	-0.991460	-3.274222	-0.262478
8	4.494581	-0.238125	-0.081812
6	-0.341474	2.790480	-0.000806
12	3.164834	-1.538293	0.119616
6	-3.964137	-0.845935	0.137063
6	0.887219	2.668562	0.066083
6	0.265438	-2.931217	-0.216741
6	-2.856958	2.318050	-0.101574
6	3.257534	1.695223	0.096783
8	-4.048230	1.725492	-0.125912
6	-4.048058	0.377488	0.025053
6	-1.672655	2.607830	-0.052320
6	4.507408	1.097507	-0.074067
6	2.175864	2.312693	0.086026
16			
156.057605 Kcal/mol 6.767307 eV -101.134987 H Child_14_19.log			
6	-5.963244	-1.737974	0.261797
6	5.126346	0.312732	0.043501
6	-6.702964	-0.646951	-0.158431
12	4.681418	-1.620937	0.252550
6	-5.323399	-0.464753	0.146707
6	2.727048	-2.247390	0.062653
6	-4.211716	0.300679	0.204143
6	4.068587	0.989383	0.019866
6	-3.178220	0.994176	0.233808

6	1.544581	-1.807594	-0.095427
12	-1.211071	1.376445	-0.039002
6	2.880918	1.641670	-0.005826
8	0.451177	2.244879	0.045818
8	-0.504277	-0.445734	-0.518207
6	0.481125	-1.169617	-0.495792
6	1.681045	1.925764	-0.014244
16			
156.107099 Kcal/mol 6.769453 eV -101.134908 H Original3D_1_4.log			
6	-0.858859	-1.339916	-0.803713
8	1.476640	-1.620798	-1.787888
6	0.387270	1.817424	-0.082397
6	3.928035	2.124440	0.699656
6	-1.858215	-1.420912	0.069524
6	2.494045	-1.213839	-0.936262
6	-3.005945	-0.611429	0.071414
12	-2.755159	1.940482	-0.316550
6	1.430768	-0.417987	-0.050119
6	0.387187	-0.996985	-1.043372
6	2.782725	1.630409	0.361126
6	-3.866692	0.297972	0.147710
6	1.589514	1.090606	0.055827
6	-0.750918	2.290383	-0.217600
8	1.241247	-0.968027	1.230701
12	-0.386223	-1.839681	1.552111
16			
156.149837 Kcal/mol 6.771306 eV -101.134840 H Child_8_29.log			
8	4.385876	0.493380	0.502028
8	-8.592026	-0.262218	-0.379518
6	3.866686	1.698863	0.784586
6	-8.865021	0.700836	0.186520
6	2.500159	1.874699	0.480840
6	1.883134	-2.328742	0.548569
6	3.582706	-0.594872	-0.018574
12	2.939380	-0.149074	-2.142331
6	1.306762	2.224112	0.353621
6	0.678532	-2.646294	0.444991
6	2.972757	-1.556038	0.572892
6	-0.630512	-2.357997	0.359418
6	-1.615372	-1.617517	0.232622
12	-0.725838	2.069519	0.092788
6	-2.169226	-0.390142	0.056579
6	-2.329488	0.843987	-0.066324
16			
156.702247 Kcal/mol 6.795261 eV -101.133959 H MutI_13_35.log			
12	-0.278676	1.970346	0.171238
6	1.682946	1.584941	0.771735
6	-3.882795	-1.140313	0.790217
6	-1.232854	0.438728	-1.052502
8	-0.036132	-0.118398	-3.164024
6	2.649944	-4.444525	-0.372757
8	-2.183661	2.002362	0.429685
12	3.621023	2.363856	0.430667
6	-0.680835	0.077997	-2.158582
6	2.332772	-3.336487	0.184679

6	1.779292	-0.995950	1.062430
6	1.654455	0.304800	0.959475
6	-3.110975	-0.222407	0.358500
6	-2.249593	0.735996	-0.113793
6	2.050866	-2.163066	0.666501
6	-4.718192	-2.020070	1.346073
16			
156.741861 Kcal/mol 6.796979 eV -101.133896 H Child_5_42.log			
6	6.250520	-1.283031	0.404598
8	-13.029054	-0.118521	-0.092137
6	5.496283	-0.043681	0.339284
6	-13.475918	-0.055108	0.964246
6	5.038384	1.257823	0.305260
6	-2.549778	-0.646835	-0.536933
6	4.795163	-1.217076	0.247668
6	-1.325902	-0.901468	-0.412745
6	4.281703	2.256193	0.233285
6	0.042569	-0.475622	-0.260110
6	3.466972	-1.513981	0.098641
12	-1.654240	1.303960	-0.408547
6	2.243188	-1.472629	-0.036520
8	0.970032	-1.656101	-0.179589
12	2.351591	1.517232	0.015787
6	0.420809	0.819196	-0.198855
16			
156.773584 Kcal/mol 6.798355 eV -101.133846 H Child_13_18.log			
6	6.381119	-1.949532	-0.008319
8	-6.950488	-1.239724	-0.000456
6	5.169653	-1.499399	-0.004473
8	-1.757929	1.592479	-0.000799
6	3.952391	-0.935307	-0.000378
6	-5.817982	-0.886499	-0.001090
6	-4.591795	-0.504631	-0.000487
6	2.662240	-1.384521	0.001576
6	-3.382742	-0.131254	0.003264
12	3.413877	1.177642	0.005775
6	-2.093883	0.267108	0.002424
6	1.409547	-1.411145	0.003096
12	-0.012892	2.255522	-0.015883
6	0.115494	-1.101975	0.004558
6	-1.050128	-0.666407	0.004644
6	2.055339	2.866892	0.017074
16			
156.846018 Kcal/mol 6.801496 eV -101.133730 H Child_9_17.log			
6	2.362757	2.752352	-0.143012
6	-3.137337	0.195016	0.204294
6	1.139489	2.945524	-0.176709
6	-3.773419	-2.407507	-0.454542
12	3.361097	1.011026	0.053345
6	-3.148653	-1.165753	-0.007829
6	-0.223795	3.059498	-0.154932
6	-2.367664	-2.280917	-0.090065
6	3.783050	-1.136421	0.269047
8	2.569954	-0.743524	-0.288440
12	2.114243	-2.604553	0.039894

6	-3.004496	1.399282	0.209477
6	-1.416095	3.020259	0.004666
6	-1.079400	-2.763017	0.052749
6	0.114705	-3.045501	0.228487
8	-2.719819	2.704203	0.192358
16			
156.863122 Kcal/mol 6.802237 eV -101.133703 H MutD_6_76.log			
6	4.081267	-1.002173	-0.878553
6	0.158116	2.093373	0.638321
6	1.533720	1.850162	0.576007
12	2.181197	-1.596612	-0.351064
12	-1.949076	0.613984	0.594249
6	0.085339	-1.681025	-0.080748
8	-5.243001	1.149096	-1.318737
6	3.852249	1.454724	-0.118917
6	-3.024215	-1.115733	1.085194
8	-1.047717	-2.517152	0.113150
6	-0.177424	-0.350194	0.091365
6	0.653662	0.763671	0.342523
6	4.217924	0.240325	-0.615754
6	2.897896	2.069569	0.376234
6	-2.166762	-1.901685	0.593895
6	-4.188389	1.368315	-0.888486
16			
156.940404 Kcal/mol 6.805589 eV -101.133580 H Original3D_11_3.log			
8	3.522897	2.191654	-0.113114
12	1.901812	1.008080	0.596806
8	-1.252660	-2.675978	-0.567157
6	3.856493	-0.142830	-0.844052
6	-1.355390	0.572613	0.227568
6	3.915699	1.092113	-0.643417
6	-2.785829	0.364822	0.166575
6	-2.245753	-1.876886	-0.551546
6	2.296176	-1.493171	0.759970
6	-3.018381	-0.929654	-0.358732
6	-3.734101	1.053779	1.161157
6	-3.734005	1.680068	-0.104153
6	3.151856	-1.051438	-0.077090
12	0.298610	-1.865141	0.360672
6	-0.113478	0.514904	0.294417
6	-3.661111	2.575566	-1.038626
16			
157.054433 Kcal/mol 6.810533 eV -101.133398 H Original3D_3_3.log			
6	-2.931317	1.771412	-0.386506
8	-0.268954	3.715460	-0.167430
6	-1.029141	-0.117342	-0.719677
12	1.907498	-0.608984	-1.749233
6	3.285194	-0.418596	0.546989
6	-1.934158	0.898669	-0.556478
8	-2.562921	-1.723906	0.391547
6	-1.847081	-0.616187	0.519496
6	3.670531	-0.575263	-0.649289
6	1.348417	-0.168680	2.181096
6	0.331657	4.635841	-0.494734
6	-0.060091	-0.805025	-1.392582

6	-0.000249	-0.171380	2.225304
12	-1.116402	-2.659664	-0.697956
6	-1.114187	-0.276123	1.697203
6	2.474067	-0.275435	1.624733
16			
157.095163 Kcal/mol 6.812300 eV -101.133333 H Child_7_48.log			
8	5.024258	-0.108308	0.463226
6	-6.298099	-0.858883	0.030464
6	3.834993	0.010096	0.164849
6	-5.051008	-0.610900	0.008739
6	3.014278	1.185072	0.145865
6	-3.716468	-0.297608	0.077979
8	3.422039	-2.148642	-0.850133
6	-2.588595	-1.115745	0.291692
6	2.938402	-1.236758	-0.185375
6	-3.031198	0.917457	-0.130320
6	1.994339	1.887052	0.053273
6	-1.276764	-1.168503	0.178758
12	0.017623	2.317086	-0.205907
6	-1.826347	1.415775	-0.356043
6	-0.945679	0.257832	-0.043601
12	0.827586	-1.004895	0.345705
16			
157.130503 Kcal/mol 6.813832 eV -101.133277 H Child_7_51.log			
6	-6.427973	0.924502	1.394816
6	5.582419	0.298742	1.787094
6	-5.316582	0.581969	0.844876
6	4.493334	-0.087836	1.189944
6	-2.209531	-1.268287	-0.365667
8	2.341571	2.948353	-0.734954
6	-4.186699	0.157728	0.340130
6	3.410156	-0.539599	0.629496
6	-1.260488	-2.057808	-0.560584
6	1.708645	1.930997	-0.727845
6	-3.033195	-0.168254	-0.141251
6	2.366388	-1.112021	0.097061
12	-1.194698	0.873804	-0.528943
6	0.880289	0.924309	-0.649688
8	1.338770	-0.446870	-0.731421
12	0.737757	-2.333682	-0.412665
16			
157.348807 Kcal/mol 6.823299 eV -101.132929 H MutD_9_68.log			
6	1.422922	2.745854	0.815467
6	-1.326353	-1.517544	1.110519
6	1.199454	-1.742266	0.494339
6	-3.188952	1.774469	-1.618306
6	-2.451493	-1.720013	2.024759
6	-2.954999	0.645929	-0.891477
6	0.000282	-1.634739	0.798311
6	0.281322	2.430041	0.353058
6	-0.839156	2.034407	-0.150803
12	3.105589	-1.688581	-0.216244
6	-2.570557	-1.183366	0.684475
8	-4.129201	-1.404818	-1.074078
8	2.509966	3.042510	1.246361

6	-3.308069	-0.689595	-0.469808
6	-1.939330	1.612725	-0.678214
12	5.811365	-0.781166	-1.134772
16			
157.367367 Kcal/mol 6.824104 eV -101.132900 H Child_3_52.log			
6	-0.160294	-1.700848	-1.968835
6	-2.141785	1.206742	1.231044
6	-1.261216	-1.135847	-1.850345
6	-3.417650	1.665930	0.926719
6	-2.368945	-0.429730	-1.476830
6	-0.995896	0.921036	1.590636
12	1.590920	-2.070350	-0.951148
12	3.727743	3.806121	-0.825835
6	-3.242598	0.245754	-0.963448
6	0.243229	0.338137	1.557640
8	-3.951772	1.114739	-0.211017
8	1.973350	-0.038900	-0.358440
6	1.640649	-3.107024	0.987703
6	1.277434	-2.170885	1.732911
6	1.049624	-0.801578	1.799067
6	1.378019	0.062318	0.746978
16			
157.416527 Kcal/mol 6.826235 eV -101.132821 H MutD_4_76.log			
6	0.291283	1.454792	-0.194379
6	2.863115	-2.056853	-0.671379
6	-1.725262	2.489928	0.022552
6	-0.689890	0.393069	-0.373287
6	1.583411	0.998668	-0.152729
6	2.874496	1.288736	0.192679
12	4.462091	-0.888594	0.177630
6	-3.158707	0.392872	-0.092249
12	0.893650	-1.072219	-0.523683
6	-2.000392	1.060787	-0.161050
6	4.081318	1.142500	0.566994
6	-5.255925	-1.020939	0.205865
6	-0.494114	2.723880	0.046872
8	-6.200978	-1.709227	0.365716
8	2.554122	-1.783922	0.602051
6	-4.218344	-0.288282	0.011859
16			
157.565388 Kcal/mol 6.832691 eV -101.132584 H Original3D_2_4.log			
6	-0.360331	0.348188	0.087538
8	0.919167	2.680382	-0.187027
6	1.878765	1.947856	-0.548702
6	0.957144	-0.065264	-0.079323
12	-1.077915	2.334063	0.238971
6	2.260882	0.607703	-0.158098
6	-3.431926	1.003112	-0.006941
6	4.398519	-0.853942	0.077798
8	5.341906	-1.599064	0.161099
6	-3.217642	2.165545	0.551441
6	-0.718597	-2.219367	0.275149
6	-1.406028	-3.198880	0.211067
6	-3.327375	-0.259712	-0.420800
6	3.501398	0.017625	-0.051832

12	-3.334019	-2.306601	-0.267850
6	-0.059036	-0.989546	0.155032
16			
158.238810 Kcal/mol 6.861893 eV -101.131511 H Child_16_10.log			
6	-2.897044	-1.791001	-0.459619
6	-0.109300	2.592622	0.808437
12	1.416269	-2.380641	0.400707
6	1.086462	2.449813	0.509133
6	-1.759467	-1.648969	0.369404
6	2.315980	2.012728	0.110930
6	-3.595302	-0.857939	-0.894527
6	3.238540	1.397057	-0.387310
6	-0.652773	-2.309390	0.735366
12	-1.823654	1.528089	0.498904
6	-3.867682	0.458156	-1.066190
6	3.791385	-0.716230	-0.582992
6	3.172269	-1.747250	-0.311902
8	-1.453056	-0.416742	0.887939
6	-3.583026	1.655194	-0.799624
8	4.209101	0.574476	-0.760685
16			
158.785976 Kcal/mol 6.885620 eV -101.130639 H Original2D_0_27.log			
6	1.034176	-0.094139	0.000000
8	-0.820345	1.333141	0.000000
8	1.553351	-2.887681	-0.000000
6	-0.000000	-1.013282	-0.000000
6	-0.430614	2.577435	0.000000
6	-1.461082	-0.807078	-0.000000
6	2.200778	0.447972	0.000000
12	2.889570	-1.576145	-0.000000
6	-2.016355	0.467004	-0.000000
6	-4.403135	1.549744	-0.000000
6	0.289771	-2.425804	-0.000000
6	0.253741	3.635919	0.000000
6	-3.246977	1.009899	-0.000000
6	-1.913403	-2.159579	-0.000000
12	1.969508	2.536043	0.000000
6	-1.002399	-3.035165	-0.000000
16			
159.216728 Kcal/mol 6.904299 eV -101.129952 H MutI_6_77.log			
6	-4.188878	-0.218021	-0.159250
6	0.678867	-0.142329	0.147865
6	-2.537987	1.781277	0.010890
8	-2.295805	-1.728704	-0.069966
6	3.985228	-1.786240	-0.724975
12	-0.462822	-2.113572	-0.018837
6	-0.509619	0.296558	0.176698
6	4.160032	-0.522096	-0.452146
6	-1.907101	0.584874	-0.001411
6	4.182494	0.761092	-0.205984
6	-2.869506	-0.541316	-0.088682
6	-5.395395	0.208209	-0.183669
6	4.173835	2.040234	-0.028521
12	2.301497	-1.425911	0.744022
8	-3.271002	2.697293	0.042227

6	3.973091	3.325274	0.095800
16			
159.272297 Kcal/mol 6.906709 eV -101.129864 H Child_2_27.log			
6	6.943291	1.339215	-0.818393
12	-4.562400	2.329559	-1.750288
6	5.804113	0.801460	-0.467120
6	-4.290222	0.765421	-0.357354
6	4.675094	0.251879	-0.182865
8	-4.867803	0.374955	2.131989
6	3.391294	0.058487	0.252728
6	-4.434258	0.283631	0.991350
6	2.902722	1.210464	0.869727
6	-2.613312	-1.288759	-0.307347
6	1.931328	-2.140481	-0.054223
6	-1.734929	-2.156613	-0.403498
6	2.616852	-1.127501	0.105073
6	-3.595668	-0.373029	0.011331
12	0.112955	-2.918107	-0.378120
8	2.844742	2.289736	1.331068
16			
159.627925 Kcal/mol 6.922131 eV -101.129297 H Original3D_0_57.log			
6	0.002103	-0.898021	-0.820596
6	2.493090	0.188259	-0.081676
6	3.782630	-0.082597	0.148462
6	-2.028983	0.422902	-1.795775
6	-2.877379	0.522933	0.632550
8	-2.962974	-0.627839	1.252547
8	-0.153079	-2.194961	-0.274222
6	-2.228331	1.746972	0.509244
12	-1.811953	-2.010633	0.590190
6	-2.597882	0.956442	-0.665002
6	5.161269	-0.052415	-0.284741
6	4.860693	-0.464745	1.030928
6	1.151910	-0.112131	-0.467672
6	-0.970333	-0.295706	-1.540094
12	-0.196703	2.342086	0.446806
6	1.423263	1.168932	-0.044053
16			
159.977210 Kcal/mol 6.937277 eV -101.128740 H Child_10_56.log			
6	9.415290	-0.592082	-0.957878
12	-4.201713	0.799551	0.030580
8	9.142376	-0.154366	0.064737
6	-4.262363	-1.220922	0.000945
8	2.156869	0.713415	1.387441
6	-3.433780	-2.139203	-0.098214
6	1.187869	0.430581	0.636760
6	-2.853994	2.295381	-0.157659
6	0.695584	-0.894519	0.408933
6	0.008289	-1.885768	0.166149
6	-2.309645	-2.935807	-0.197566
12	0.119936	2.166023	-0.069954
6	-1.961311	3.209225	-0.393619
6	-0.952997	-2.827445	-0.102838
6	-1.514192	-4.119308	-0.490574
6	-0.920855	4.003322	-0.671929

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16
160.030035 Kcal/mol 6.939568 eV -101.128656 H Child_10_22.log
6   4.049455   -1.690480   -1.167187
6   -5.711268   1.493755   -1.144704
6   4.127548   -0.452757   -0.904595
6   -4.846877   0.670520   -0.595400
6   3.654642   0.782740   -0.553468
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6   0.784815   0.102980   0.146764
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6   -1.125159   1.620428   -0.612133
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6   3.179873   -4.015422   -0.659761
6   -2.318515   0.970304   -0.131353
6   -2.007491   -0.438191   0.102736
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6	1.019013	0.519916	1.829376
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6	3.583354	1.396141	-0.085919
6	-1.943470	-1.665458	0.527766
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6	3.952238	-3.550485	-0.062469
6	3.707413	0.157070	0.064543
6	4.100818	1.342361	0.201553
6	1.651939	-0.904129	-0.209332
6	3.556679	-2.330618	-0.084668
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6	6.021422	-0.329159	-0.243716
6	-3.291411	-2.782710	-0.056533
6	3.609103	-0.371751	0.617930
6	-1.935609	-0.622816	0.479492
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6	-2.421475	1.462802	-0.260187
6	3.200549	-1.722000	-0.603313
6	-1.726367	2.233516	-1.125679
6	3.501301	-0.758492	-1.662774
6	-0.689605	2.815710	-1.537854
6	2.588137	-0.405657	-0.598267
6	-2.068665	0.859762	0.775690
6	1.776552	0.421167	0.072768
6	0.471818	2.685183	-0.778846
12	0.450598	0.836466	1.783369
8	-1.477944	0.349889	1.775832
6	1.389904	1.747559	-0.267295
6	0.837363	2.731198	0.600688
16			
164.268983 Kcal/mol 7.123386 eV -101.121901 H Child_7_32.log			
6	-3.483512	-1.110957	0.032076
6	4.463981	2.738878	0.199207
8	-4.670014	-1.278391	-0.007356
6	3.149460	2.190134	0.482599
6	-2.240122	-0.851622	0.024607
6	4.042711	1.413249	-0.237669
6	-0.931375	-0.944106	0.221747
6	4.046591	0.163182	-0.817810
6	-0.011650	-1.920126	0.845675
12	1.295105	1.364363	0.809585
6	1.034525	-2.580799	1.157917
6	3.827912	-0.983097	-1.272680
6	-5.675906	1.979043	-0.191302
6	0.332816	-0.361152	0.053532
12	2.038968	-1.763587	-0.657105
8	-6.747668	2.077756	-0.594787
16			
164.352005 Kcal/mol 7.126986 eV -101.121769 H Child_13_22.log			
6	-13.550766	1.289318	-1.395676
6	5.378453	0.561489	-1.921115
8	-13.831779	1.068105	-0.303794
12	3.434831	-0.004253	-1.246753
6	-1.145499	-1.785226	1.228934
6	5.330598	1.386511	-0.972489

6	-0.812226	-2.571862	0.302738
6	1.698686	-1.120712	-0.979472
6	-0.983507	-0.684345	1.971783
8	5.088847	2.191245	0.127066
6	-0.049330	-3.067074	-0.684045
6	3.886113	1.809044	0.612014
6	-0.679798	0.310245	2.735269
12	1.022451	0.179044	0.998602
6	0.895944	-2.109917	-0.972551
6	2.774011	1.287148	0.806549
16			
164.961251 Kcal/mol 7.153406 eV -101.120798 H Child_3_9.log			
8	1.495856	0.407404	1.162344
6	-3.842494	-1.144210	-1.246748
6	0.291878	0.317108	0.881138
12	2.966704	-4.323902	-0.158419
6	-0.461904	2.305203	2.158001
12	-4.237078	0.873346	-0.895990
6	0.678582	-2.043434	0.295200
6	-2.920256	2.163205	-0.050890
6	-0.636050	1.463253	1.135872
6	-2.662096	-1.223147	-0.745011
6	-0.256969	-0.961387	0.320109
6	-1.851580	1.768580	0.451428
6	4.758925	3.298153	-0.666403
6	1.554132	-2.919886	0.255427
8	5.529122	3.317608	-1.523514
6	-1.478058	-1.089010	-0.197744
16			
165.040001 Kcal/mol 7.156821 eV -101.120672 H Child_13_28.log			
6	4.841486	-0.250935	1.004612
6	-2.967211	-3.670756	-0.963208
8	3.142954	3.313498	-1.117429
8	-2.230675	-2.794893	-0.782786
6	2.882134	2.228746	-0.776422
6	-3.287272	0.173602	0.167083
6	3.615822	0.209586	0.363863
6	-4.103542	1.108133	0.388893
6	3.617462	-1.040622	0.940775
12	-1.620894	-0.773666	-0.281464
6	2.633260	0.983984	-0.340139
6	-4.942509	2.130801	0.623626
6	1.386803	0.298265	-0.453811
6	-5.626960	3.195308	0.842410
12	1.748980	-1.974762	0.830391
6	0.477982	-0.560730	-0.361918
16			
165.972315 Kcal/mol 7.197250 eV -101.119187 H Child_1_37.log			
6	-3.615933	2.639900	0.661346
6	3.791129	-0.938761	0.994285
6	-3.280841	1.351975	0.561405
6	2.723950	-1.560062	0.847362
8	-3.701592	0.055897	0.944341
6	1.490241	-2.036485	0.532124
6	-2.052793	0.930856	-0.127117

12	4.151998	0.929885	0.288925
12	-0.263689	1.798862	-0.853663
6	0.357506	-2.290856	0.132131
6	-2.434598	-0.400566	0.236307
6	2.904756	2.238865	-0.593453
6	1.685236	2.300236	-0.860050
6	-0.927924	-2.312787	-0.508342
6	-1.967083	-1.636027	0.163691
8	-1.136106	-2.863734	-1.627002
16	166.063531 Kcal/mol 7.201205 eV -101.119041 H Child_5_30.log		
6	-5.796786	-0.689640	-0.016685
6	2.872888	2.726737	-0.029532
6	-0.988210	-2.756195	-0.019964
6	1.821825	3.318210	0.001193
6	0.322724	-3.159551	0.042507
6	0.437361	3.715654	-0.035014
8	-4.823394	-0.026397	-0.028857
6	3.533048	1.524896	-0.003845
6	-1.602310	-1.540048	-0.092804
6	-0.764248	3.429743	-0.006200
6	1.630554	-2.932806	-0.027693
6	3.976054	0.385993	0.013840
6	2.816861	-3.420179	-0.035864
12	3.272550	-1.317481	0.031124
12	-2.490691	1.447731	0.035314
8	-2.544216	-0.621088	0.086747
16	166.299308 Kcal/mol 7.211430 eV -101.118666 H Child_3_27.log		
6	-2.156056	2.118682	-0.124006
8	3.766846	-2.613731	0.015970
12	-4.031041	1.491759	-0.024455
6	-0.029642	-1.616598	-0.166389
6	-0.959200	1.748577	-0.119580
12	1.908782	-2.371345	-0.026204
6	0.252619	1.133913	-0.001802
6	-1.421389	-1.682208	-0.107974
6	-4.749790	-0.357581	0.164802
6	-2.660691	-1.692487	0.035338
8	4.502949	2.740083	-0.026502
6	3.033702	0.711836	0.097180
6	-3.891552	-1.188646	0.162322
6	0.490164	-0.241323	-0.073783
6	3.713230	1.967891	0.138728
6	1.596732	0.688648	0.110524
16	166.761583 Kcal/mol 7.231476 eV -101.117929 H Child_15_10.log		
12	4.190746	0.159266	1.325352
8	-6.820995	2.331142	0.542854
6	2.433676	0.648533	-0.710957
6	-5.012892	-2.336140	-1.355082
6	3.657884	0.526759	-0.964623
6	-3.818617	-2.285244	-0.807034
6	5.012821	0.347522	-1.010743
6	-5.717137	2.420067	0.857790

6	1.119444	0.703007	-0.297768
6	-2.684014	-2.121592	-0.218868
6	0.029127	1.149103	-0.806469
6	-1.558795	-1.898838	0.417504
12	1.393091	-0.667321	1.494922
6	-0.519501	-1.584058	1.045130
6	6.306221	0.259912	-0.891980
8	-0.990924	1.559165	-1.215940
16	166.819489 Kcal/mol 7.233987 eV -101.117837 H Original2D_0_10.log		
6	-1.529296	-0.695062	-0.000000
6	-2.931465	-1.044612	-0.000000
8	-0.530883	-1.601569	-0.000000
6	2.689511	1.752854	0.000000
12	-3.161928	0.892952	-0.000000
6	-3.103210	-2.421247	-0.000000
8	3.951967	-1.559049	-0.000000
12	-0.788324	-3.468876	-0.000000
6	-2.858109	-3.663027	-0.000000
6	-1.130545	0.565883	0.000000
6	1.199353	1.796654	0.000000
6	4.953366	-1.072686	0.000000
6	1.978549	4.307563	0.000000
6	2.116800	3.007722	0.000000
6	1.954104	5.632474	0.000000
6	0.000000	1.199492	0.000000
16	166.903311 Kcal/mol 7.237622 eV -101.117703 H Child_9_62.log		
6	3.506533	-3.507158	-0.570876
6	-3.854256	-1.196452	1.536520
6	2.479325	-2.763613	-0.411886
6	-2.744453	3.513214	-0.389638
6	1.390978	-1.996252	-0.269058
6	-3.653355	-0.090800	0.954824
6	-0.002804	-1.876030	0.013145
6	-2.743292	2.131689	-0.009796
8	7.438258	1.813618	1.004016
6	-2.952995	0.746498	0.090488
6	0.730569	-0.734359	-0.373999
6	-1.512521	2.766171	-0.261978
6	6.756962	2.126419	0.134002
8	-2.087032	0.048495	-0.676404
12	-0.212904	1.053279	-0.731494
12	-2.054926	-1.854351	0.292212
16	167.010170 Kcal/mol 7.242256 eV -101.117533 H Child_10_14.log		
8	6.407147	-0.606888	-0.852672
8	-2.271985	-2.603582	1.344683
6	5.379746	-0.104306	-0.578666
6	-2.626899	-2.417078	-2.444790
6	4.246687	0.470760	-0.265068
6	-2.096383	-1.777577	-1.461032
6	3.152606	0.969643	0.110735
6	-1.588574	-1.627701	1.004964
6	-1.732289	-1.030027	-0.390231

12	1.159747	1.242987	0.841877
12	-4.106525	2.468546	-0.338088
6	0.334515	-0.170336	2.095429
6	-1.469465	0.358381	-0.527632
6	-1.994240	1.652686	-0.668449
6	-0.631885	1.474863	-0.303883
6	-0.593811	-0.941746	1.765031
16			
167.062957 Kcal/mol 7.244545 eV -101.117449 H Original3D_18_3.log			
8	0.092985	1.612444	-0.059703
6	-0.664407	0.638870	0.214200
6	3.381410	0.173786	0.883968
6	1.932607	-1.025112	-1.396191
6	2.958282	-0.980885	0.371714
6	2.157679	-1.848155	-0.217857
6	-1.940811	0.130139	0.351997
6	-0.845909	-0.697259	0.639223
12	1.882842	1.779124	-0.627187
8	-3.563556	1.668200	0.784007
6	-3.365501	0.522256	0.272686
6	-4.714871	-1.302871	-1.108988
12	0.364032	-2.357149	0.804809
6	1.921978	0.105373	-1.961005
6	-4.155492	-0.371015	-0.423583
6	3.468715	1.436731	1.052851
16			
167.140551 Kcal/mol 7.247909 eV -101.117325 H Child_9_48.log			
8	-7.538880	-3.978117	0.170371
8	4.720718	-1.588363	-0.550620
6	-7.878878	-4.882932	-0.451293
6	3.705551	-0.893820	-1.160297
6	-2.633143	3.043901	-0.095464
6	-1.625931	2.275117	-0.052951
6	2.556976	-0.496035	1.073921
6	-3.643304	3.873536	-0.127011
6	3.674701	-0.683002	-2.493519
6	-0.547634	1.529192	0.110227
6	2.613418	-0.349812	-0.309018
6	-4.598659	4.742370	-0.130860
6	1.521208	0.397868	-0.908140
12	4.304440	-1.613034	1.277452
6	0.441772	0.994607	-0.702795
12	0.781296	0.548525	1.599648
16			
167.194014 Kcal/mol 7.250228 eV -101.117240 H Child_6_12.log			
6	3.003390	1.807477	-1.323940
6	-3.050018	-1.799093	-0.055643
6	1.879587	1.614094	-0.627602
6	-3.586652	-0.554233	-0.088675
6	1.423496	2.108740	0.628780
6	-2.183806	-2.679609	-0.016081
8	4.592071	-1.135490	0.297245
6	-3.447786	0.670533	-0.111763
6	0.505191	2.329503	1.491216
6	-0.874751	-3.055490	0.025203

6	3.457689	-0.986073	0.227311
8	-3.068832	1.902438	-0.095411
6	0.587356	0.871470	-0.543647
6	0.382618	-3.107102	0.059047
12	-1.167053	2.079869	0.033434
12	1.103403	-1.201276	-0.000093
16			
167.413639 Kcal/mol 7.259752 eV -101.116890 H Original2D_10_1.log			
12	-0.000000	-0.393874	-0.000000
6	-2.121365	-0.487975	-0.000000
6	-3.413508	0.263124	-0.000000
6	0.290002	1.792008	0.000000
6	-3.263892	-2.393099	-0.000000
6	-4.509859	-1.947497	-0.000000
6	-2.004157	-1.951610	-0.000000
12	-1.884775	1.744847	0.000000
8	3.539161	3.795852	0.000000
6	2.900641	-1.678422	0.000000
6	2.430666	3.275157	0.000000
6	5.327926	-2.619459	0.000000
6	4.071031	-2.225096	0.000000
6	1.399747	2.489632	0.000000
8	1.767305	-1.227527	-0.000000
6	-4.412969	-0.643141	-0.000000
16			
167.579674 Kcal/mol 7.266952 eV -101.116625 H MutI_17_69.log			
6	-3.365550	-1.211013	-0.084724
6	7.387939	0.591844	-0.607800
6	-1.043157	1.890518	0.256152
8	-3.805535	-0.005679	0.560059
12	1.194204	-1.974972	0.214166
6	3.633069	-0.066498	0.139994
6	6.130426	0.345530	-0.350923
6	-3.588022	1.263459	-0.103949
6	2.349263	-0.244961	0.344372
6	-2.016857	-1.608890	-0.067047
8	-4.501543	1.778976	-0.714000
6	-4.398634	-1.885209	-0.621438
12	0.895874	1.289042	0.454843
6	-2.256430	1.717801	0.097077
6	4.881457	0.121344	-0.104688
6	-0.817555	-1.906462	-0.029792
16			
167.678135 Kcal/mol 7.271221 eV -101.116468 H Child_11_33.log			
6	3.620000	-2.628432	-1.893763
6	-5.488134	-2.376754	-0.058439
6	3.231660	-1.983283	-0.847798
6	-4.496773	-1.567473	0.141493
6	2.566716	-1.230765	0.024695
6	-3.606103	-0.629354	0.202974
6	2.704953	-0.203429	1.069077
6	-2.713385	0.275963	0.266537
6	2.456768	1.108585	0.448219
6	-1.710520	1.216781	0.024690
6	1.928747	1.964588	-0.261514

12	0.386341	-1.378998	-0.186207
12	0.226617	2.987154	-0.738842
6	-1.073773	0.045330	0.125755
8	-1.546574	2.519802	-0.326348
8	2.562019	-0.425853	2.282478
16			
168.562468 Kcal/mol 7.309570 eV -101.115059 H MutI_13_75.log			
8	-5.498504	-1.719219	0.672068
6	-4.564514	1.754551	1.009147
6	0.047768	1.302265	-1.587616
6	8.613597	-0.921223	0.826006
6	-3.277467	-1.049568	-0.068095
6	3.763500	0.488012	-0.117460
6	-4.750098	0.552365	0.682348
6	-0.704909	1.259243	-0.566205
12	1.765181	1.119473	-0.563285
8	-1.247177	-1.933711	-1.191982
6	-2.287532	-1.571511	-0.671394
6	4.902357	0.043611	0.164254
6	6.137556	-0.323156	0.404825
6	-4.622967	-0.861880	0.416351
6	7.349837	-0.647852	0.612313
12	-2.571626	1.303384	0.357658
16			
168.598240 Kcal/mol 7.311121 eV -101.115002 H Original3D_4_7.log			
6	-2.622900	1.423431	1.337923
6	-4.463979	-0.388963	-0.093456
6	-0.487570	0.863821	0.014915
6	0.172884	-2.143668	0.449598
12	-1.382687	-1.084827	-0.743846
12	0.247722	0.397984	-2.552158
8	3.828403	-1.693134	1.010934
6	-1.483125	1.246164	0.707633
8	-3.525223	-1.063803	-0.302755
6	0.781888	1.091545	-0.505015
6	-3.690281	1.557180	2.028411
6	2.695070	-1.863988	0.838234
6	1.973458	1.403582	-0.181684
6	3.229340	1.694173	0.036346
6	4.342418	2.230619	0.382340
6	1.418486	-2.064295	0.632524
16			
169.075727 Kcal/mol 7.331827 eV -101.114241 H Child_14_10.log			
8	-5.731975	-0.144379	-0.350863
6	1.538074	-2.872810	-0.256079
6	-4.539618	-0.128551	-0.298131
6	2.530665	-2.151332	-0.423128
6	-3.234294	-0.089903	-0.241163
8	3.396511	-1.115921	-0.583264
6	-1.988907	0.673188	-0.128973
6	3.053980	1.313672	-0.451231
6	-1.936562	-0.712196	-0.056341
6	2.836708	0.062710	-0.014751
12	-0.339417	1.880393	0.407092
6	1.280505	3.156442	-0.264546

6	1.696380	-0.071688	0.805501
12	-0.159281	-1.851770	0.419092
6	0.595588	0.055613	1.410020
6	2.278830	2.388008	-0.488045
16			
169.961910 Kcal/mol 7.370255 eV -101.112829 H Child_9_60.log			
6	-3.764318	-1.203061	-0.398516
6	5.014078	2.374890	-0.514723
6	-2.999347	-2.184351	-0.398077
6	5.028600	1.165640	-0.132216
12	-4.267803	0.765475	-0.226350
6	4.626774	-0.045410	0.198540
6	-1.990553	-3.181050	-0.323830
6	4.150768	-1.184895	0.504195
6	-1.811651	-4.492397	-0.606102
12	2.528596	-2.389242	0.699055
6	-4.099440	2.760346	0.088249
8	-2.903151	4.883493	0.660825
6	-0.625643	-2.941662	0.088601
6	-3.456442	3.831303	0.373531
6	0.569162	-2.870401	0.414929
8	5.030470	3.530443	-0.840818
16			
170.348416 Kcal/mol 7.387016 eV -101.112213 H Child_11_36.log			
6	4.038973	1.330059	0.028105
8	-3.853346	0.493933	-0.250407
6	2.301275	-3.239345	-0.235680
6	-3.073628	1.486449	-0.126651
6	2.546218	-2.002211	-0.179473
6	-2.200849	2.353853	0.002291
6	2.964791	0.506592	-0.083406
6	-0.958940	2.828233	0.095718
6	2.155511	-0.645499	-0.079906
12	-3.341159	-1.341762	-0.125642
6	2.601490	1.923250	0.027311
6	0.275613	3.004398	0.137311
12	0.169858	-2.455127	0.032542
6	1.533861	2.603916	0.103104
8	0.856940	-0.505984	0.039887
6	-1.846504	-2.539850	0.778170
16			
171.454310 Kcal/mol 7.434972 eV -101.110451 H Child_6_26.log			
6	-5.060413	-1.182013	-0.716871
6	3.309433	-2.445092	0.000041
6	-5.060553	-1.180748	0.715476
12	4.258929	-0.649710	-0.001657
6	-3.884647	-0.768249	-0.001062
6	2.158963	-1.939275	0.000604
6	-2.619813	-0.299882	-0.000495
6	2.911041	0.950085	-0.000642
6	-1.679454	0.782071	0.000433
6	1.130909	-0.956361	0.001239
8	-1.460552	2.069942	-0.000443
6	1.570542	0.308740	0.000237
6	-1.206983	-0.488933	0.000912

6	1.833744	1.770066	0.001069
8	-0.233611	-1.398276	0.002066
12	0.169128	2.926728	0.000105
16			
171.736122 Kcal/mol 7.447192 eV -101.110001 H Original3D_4_4.log			
6	1.085643	-0.164791	-0.133849
6	2.373451	1.925103	0.409136
6	-0.320199	-0.100959	0.304791
6	2.024960	-1.051310	-0.610296
12	0.831252	-2.706923	-0.390426
6	-1.252458	-1.112054	0.622767
6	-4.636271	1.082833	-2.100689
8	-0.832673	-2.378500	0.389318
6	3.627899	2.035316	0.243646
12	3.738674	0.092074	-0.769702
8	-3.720780	1.296340	-1.446627
6	1.169606	1.274217	0.334568
6	-0.244818	1.360892	0.649897
6	-3.477280	-0.216208	1.728733
6	-0.937601	2.404125	1.142799
6	-2.481512	-0.764586	1.138496
16			
171.750759 Kcal/mol 7.447827 eV -101.109978 H Child_3_43.log			
6	-2.979999	0.512234	-0.201154
12	4.431124	-1.165454	-0.448299
6	-4.127533	-0.035659	-0.241332
6	4.389380	0.888938	-0.268812
6	-1.762296	1.032006	-0.108462
6	3.190699	1.185185	0.018775
6	-1.352765	2.441248	-0.068405
6	2.490147	-1.788472	0.221051
6	-5.236762	-0.672009	-0.098735
6	1.896785	0.798590	0.357474
6	-0.509076	0.221868	0.048850
12	0.304287	-1.738583	0.101586
6	0.549951	1.199361	0.174510
6	-0.107548	2.500198	0.072006
8	-6.263779	-1.285747	0.009115
8	1.829923	-0.570813	0.581629
16			
172.000346 Kcal/mol 7.458650 eV -101.109580 H Child_2_18.log			
12	-4.486205	1.678050	0.272863
12	2.235457	0.189386	-1.632555
6	-1.236100	-4.266047	0.734643
8	1.898156	3.193656	1.089559
6	-1.534178	-3.040425	0.418994
6	2.520601	-1.453226	-0.096012
6	-2.894994	0.540584	-0.692568
6	0.949266	1.609851	-0.511552
6	-1.846230	-1.819909	0.110142
6	1.775740	2.051612	0.637979
6	-1.491697	0.730920	-0.513917
6	2.679884	-0.376890	0.835424
6	-2.094884	-0.590609	-0.214437
6	-0.309071	1.305424	-0.549283

6	2.459118	0.831665	1.044087
8	2.244873	-2.637023	0.047356
16			
172.386788 Kcal/mol 7.475408 eV -101.108965 H MutD_17_60.log			
6	1.965420	-1.805670	1.446488
6	-3.109800	-0.326246	0.009587
6	1.262109	-2.283459	0.518978
6	1.788405	0.467862	-1.043056
6	-1.809849	0.887091	1.678852
6	0.818429	2.929410	-1.660829
6	-0.943536	0.495781	-0.662846
12	2.352559	0.136853	1.070341
12	0.365466	-1.086341	-1.595446
8	-4.079712	-0.890993	-0.271126
6	0.530067	1.567977	1.184773
6	-1.980565	0.368679	0.332135
6	1.207589	1.704216	-1.285840
8	0.540264	-2.655194	-0.512738
6	-0.657432	1.430408	1.791411
6	0.212375	1.191176	-0.214292
16			
172.467246 Kcal/mol 7.478897 eV -101.108836 H MutD_18_56.log			
6	1.955976	-1.874540	1.395152
6	-1.973051	0.381845	0.358411
6	0.555107	1.517742	1.229864
6	1.217792	1.719948	-1.240325
6	-1.787044	0.838366	1.725196
12	2.366937	0.070904	1.059123
6	0.224590	1.200339	-0.180627
6	-0.623371	1.357865	1.844119
6	1.785127	0.464601	-1.036229
6	1.218194	-2.304226	0.470061
6	-3.116139	-0.273895	0.002719
6	-0.942753	0.532236	-0.640023
6	0.939987	2.964086	-1.652113
8	0.464375	-2.629767	-0.553956
12	0.327208	-1.045935	-1.619963
8	-4.096406	-0.800963	-0.311938
16			
172.953158 Kcal/mol 7.499968 eV -101.108062 H Child_12_21.log			
6	2.833754	0.811153	0.216749
6	-6.424133	-0.961337	0.262213
6	3.346158	-0.287890	0.606469
8	-5.341581	-0.572401	0.222997
6	1.987938	1.790106	-0.020815
6	-1.940925	-1.537331	-0.182820
8	5.795167	0.190218	0.438194
6	-0.782498	-2.078616	-0.312018
6	0.902458	2.473457	-0.234742
12	-3.289973	-0.018340	0.024041
6	-0.355835	2.667608	-0.274510
6	0.424492	-2.446688	-0.126366
6	5.608942	-0.454655	-0.423552
6	-2.781911	1.972687	0.080858
6	-1.678111	2.481681	-0.212933

12	2.417418	-1.941959	-0.154102
16			
173.046102 Kcal/mol 7.503999 eV -101.107914 H MutI_8_71.log			
6	-2.963308	-1.114446	0.013567
12	2.743834	-0.220169	0.491117
6	-0.579947	-1.350718	-0.005535
6	-4.216457	-0.649238	0.330096
6	0.810513	-1.346826	-0.183044
6	0.746602	0.578800	1.431587
6	1.756637	1.137057	1.955064
6	-3.089866	0.327735	-0.016619
6	-1.525890	2.289253	-0.561944
6	-2.414526	1.394563	-0.270641
6	-1.881735	-2.007651	-0.204486
8	-1.920885	-3.213977	-0.556340
6	0.133105	-0.373489	0.653505
12	5.121451	-1.133703	-0.874970
8	0.446651	3.763652	-0.759475
6	-0.540055	3.089801	-0.619422
16			
173.085454 Kcal/mol 7.505705 eV -101.107851 H Child_6_11.log			
12	3.422207	1.630415	0.622736
8	-5.751250	0.968405	-0.475084
6	3.190451	-0.760837	-0.423088
6	-5.594807	-0.093239	-0.051819
6	1.754436	2.768200	0.292078
6	-2.364144	-0.441047	2.346115
6	3.969620	-0.328193	0.481659
6	-1.711961	-0.025328	1.321816
12	1.342118	-1.343858	-1.078217
6	-1.012429	0.393669	0.260082
6	0.604679	2.375884	-0.009908
8	0.666047	-3.212067	-0.022106
6	-0.666780	1.012250	-1.794070
6	-0.072721	-3.894505	0.532812
6	-0.388685	-0.151303	-0.964333
6	-0.456035	1.562883	-0.417461
16			
173.205065 Kcal/mol 7.510892 eV -101.107661 H MutD_17_74.log			
6	-1.341361	0.136298	3.025534
6	-1.626544	0.044672	1.627181
8	-1.354803	-1.502948	-1.513393
6	-0.272724	0.165316	2.057600
6	-3.476023	1.099839	-0.855689
6	2.383615	-1.412454	0.642357
6	2.113741	0.898333	-0.444391
12	3.607453	2.220146	-1.070922
8	-4.564033	1.437382	-0.775573
6	0.713650	1.025813	-0.079190
12	-1.359873	0.230272	-0.501152
6	1.701028	-2.266203	0.027827
6	-0.377465	-2.211624	-1.156667
6	2.086860	-0.041875	0.744376
6	0.656529	-2.728781	-0.682982
6	0.835317	0.477252	1.290146

16
173.272512 Kcal/mol 7.513817 eV -101.107553 H MutI_15_55.log
6 -3.584989 1.289322 0.697905
6 -1.764774 -0.123151 -0.039740
8 0.749671 0.006480 -0.575991
12 1.295423 1.886902 -0.530600
6 -0.898253 -1.919766 -0.751672
8 4.370572 -1.654702 1.281619
6 -0.361831 2.948320 -0.012494
6 -4.795040 1.256835 1.120096
12 -1.800949 -3.711208 -0.188891
6 3.459771 1.346220 -0.568761
6 4.150729 0.420590 -0.053636
6 -0.415745 -0.580578 -0.473635
6 -2.242607 -1.493049 -0.277968
6 -1.382688 2.253776 0.014258
6 -2.314633 1.152603 0.201943
6 4.334121 -0.704877 0.641846
16
173.705853 Kcal/mol 7.532608 eV -101.106862 H Child_6_54.log
12 -4.534459 -1.537800 -0.195735
8 8.324606 -0.082820 -0.011879
6 -5.194522 0.336854 -0.123962
6 7.198563 0.283377 -0.039777
6 -2.969291 -2.816998 -0.059252
6 5.983779 0.644204 -0.048135
6 -5.281401 1.587029 -0.042874
6 4.741404 0.949396 -0.104155
6 -1.894374 -3.449768 0.119305
6 3.487393 1.194498 -0.104618
6 -5.317182 2.910122 0.052522
6 2.218862 1.022184 0.015752
6 -5.206237 4.188285 0.138089
6 0.923962 0.757581 0.137722
12 -0.510605 -2.004137 0.203562
8 0.224772 -0.309348 0.044676
16
173.880940 Kcal/mol 7.540201 eV -101.106583 H Child_15_24.log
6 -7.521588 1.202271 0.288573
12 2.601213 -1.751916 0.756611
6 -6.293508 0.800798 0.247950
8 0.902718 -1.275014 0.132709
6 -5.051461 0.419146 0.191459
6 3.653177 -0.067360 0.510162
6 -3.825473 0.100268 0.080587
6 -0.385964 -1.579901 -0.368512
6 5.762573 1.701472 -0.101182
6 3.202493 1.026091 -0.120048
8 2.169992 1.685527 -0.570524
6 4.644459 1.047948 0.095549
6 -1.320292 -0.483862 -0.113426
6 -2.595080 -0.286946 -0.009509
6 -0.755655 -2.370821 -1.387985
12 0.593473 0.723689 -0.121545
16

174.097429 Kcal/mol 7.549589 eV -101.106238 H Child_5_40.log
8 -1.167181 2.980293 0.533353
12 -1.286400 -5.022834 -1.421090
6 2.325772 1.174079 1.780161
6 3.034716 -1.094534 -0.832844
6 1.363377 1.400616 1.017782
6 1.896794 -0.461134 -1.209749
6 -0.692853 2.097299 -0.260705
6 -4.693345 -0.831191 2.480081
6 0.492078 1.323845 -0.095780
6 -2.977641 1.662684 -3.487396
12 3.846148 -0.162483 1.520610
6 4.026271 -1.409293 -0.123481
6 -1.419148 1.855215 -1.435712
6 -2.212232 1.787360 -2.427990
6 0.990752 0.360708 -1.000954
8 -4.273348 -1.101557 3.514806

16

174.128539 Kcal/mol 7.550938 eV -101.106189 H Child_1_51.log
12 4.841213 -0.031203 -1.259314
8 -1.489801 -3.364136 -0.057482
8 -0.806324 3.486696 -0.683033
6 2.296245 -0.574739 -0.193000
6 -1.397353 -2.163276 -0.215047
6 2.226914 0.837027 2.073081
6 -2.346629 -1.016907 -0.383947
6 2.516944 0.086855 1.013184
6 -3.563835 -0.270446 -0.195461
6 -1.329291 2.468138 -0.477795
6 -0.204381 -1.125200 -0.149399
6 -1.297864 -0.089747 -0.367954
6 -1.924828 1.285348 -0.231270
6 1.141300 -1.096567 -0.469385
6 -3.345056 0.981394 -0.199763
12 0.303455 0.288557 1.651369

16

174.273520 Kcal/mol 7.557225 eV -101.105958 H Child_3_38.log
8 1.906311 2.191634 0.073515
8 -4.801668 -3.115767 0.079808
6 2.927610 1.429089 0.082876
6 -4.632105 -1.931086 0.057357
12 0.183680 2.760039 -0.039038
12 -5.528864 0.058570 0.220408
6 3.859422 0.634123 0.069425
6 -3.252938 -1.054984 -0.164957
6 7.872321 -2.678983 0.016594
6 4.926007 -0.194516 0.047905
6 -3.477985 0.349572 -0.087526
6 -1.736138 2.300300 -0.116673
6 -2.195658 -1.834799 -0.338536
6 5.890168 -0.970562 0.009786
6 6.924870 -1.804381 -0.004934
6 -2.554729 1.351186 -0.138488

16

174.779958 Kcal/mol 7.579186 eV -101.105151 H Child_5_62.log

6	-3.628175	0.511965	-0.356071
6	3.935889	-2.257431	0.064866
6	-2.683657	1.154030	0.159810
8	2.952275	-1.656602	-0.031377
6	0.208691	0.551269	2.338469
6	2.617514	2.508246	-2.297455
12	-3.505824	-1.643324	-0.628018
6	1.701593	2.027951	-1.506077
6	-1.047402	-2.030580	-1.338252
12	1.230168	-0.543978	0.319470
6	-1.506568	1.636187	0.634623
6	0.893248	1.513885	-0.580444
6	1.029266	-0.394377	2.520838
6	-0.147729	1.912565	0.258430
6	-0.478533	1.469647	1.561576
8	-0.209394	-1.514963	-0.601036
16	174.972933 Kcal/mol 7.587554 eV -101.104843 H MutD_18_48.log		
6	-1.603508	1.112984	-0.056545
6	-0.184247	-2.351054	0.631447
12	1.913758	-0.675084	1.483620
6	-2.858247	0.616183	-0.276582
6	0.988629	1.450347	1.154153
6	2.474971	2.104871	-1.654511
8	-0.723880	-2.559188	-0.550039
6	-0.460732	0.795900	-0.875143
6	-1.463805	1.717912	1.256682
12	0.199440	-1.216095	-1.578855
6	0.789451	1.089433	-0.265681
8	-3.927000	0.168820	-0.304780
6	2.080649	0.955875	-1.099937
6	2.018946	-0.383339	-0.697351
6	-0.220938	1.865311	1.533678
6	0.413608	-2.004906	1.680018
16	175.063689 Kcal/mol 7.591490 eV -101.104699 H Child_1_35.log		
8	-2.855788	2.217515	1.096561
6	5.888242	-1.698352	0.057130
6	-4.807032	-0.759960	-0.905724
6	4.744302	-1.098983	-0.023558
6	-2.137724	1.605946	0.273701
8	-1.374392	-2.803589	0.341162
6	-3.670654	-0.221838	-0.569180
6	3.582120	-0.500660	-0.077672
6	-2.448628	0.221782	-0.278127
6	-2.112381	-3.468347	1.031128
6	-0.824567	1.925199	-0.183732
6	2.501895	0.198392	-0.092770
6	0.346461	1.394937	-0.217611
12	2.385052	2.432120	0.077451
12	-0.655035	-0.953581	-0.421141
6	1.118172	0.226239	-0.243165
16	175.356505 Kcal/mol 7.604187 eV -101.104232 H MutI_17_79.log		
12	-4.747986	0.088252	0.617022

6	-3.270390	2.474944	0.219474
6	5.573905	0.618792	-0.238943
6	-0.022753	-1.561688	0.107521
12	-3.208038	-1.613886	-0.959270
8	2.266475	-2.158911	0.728145
6	1.155955	-1.992834	0.413364
6	6.632162	-0.045923	-0.370100
6	-1.798467	-0.386525	-0.103631
6	0.508736	0.907352	0.023616
6	1.758412	1.197268	0.046702
6	3.055071	1.337143	0.097248
6	4.327340	1.044367	-0.021908
6	-1.407263	-1.800352	-0.179335
6	-0.395380	-0.079520	0.058783
8	-2.420434	3.162593	-0.254366

16

175.514942 Kcal/mol 7.611058 eV -101.103980 H Child_6_43.log

6	-3.753531	3.585105	1.676401
6	11.013821	-0.164728	1.900715
6	-3.188043	2.541679	1.186818
8	10.813366	-0.106464	0.770352
6	-2.613039	1.424452	0.695083
12	1.069612	-0.457642	-2.275747
6	-3.079775	0.139243	1.006297
6	1.315658	1.668650	-2.262341
6	-3.416838	-1.015920	1.256774
6	0.347134	1.457196	-1.491704
6	-3.412983	-2.379215	1.193330
6	-0.656443	-0.707027	-0.972913
6	-3.097640	-3.559196	0.853343
6	-0.658371	0.653430	-0.821580
12	-1.674820	-2.343160	-0.284518
8	-1.505515	1.574916	-0.095122

16

176.115208 Kcal/mol 7.637088 eV -101.103023 H Original3D_9_6.log

6	0.043359	2.080480	0.641072
8	-1.175378	2.515348	0.560807
12	-2.669966	1.676203	-0.135191
6	2.271270	0.770689	0.524495
8	-2.681370	-2.168854	1.375922
6	-1.410813	-2.120140	0.562096
6	4.633284	-0.262676	0.170974
6	-1.688709	-0.109838	-1.444685
6	3.459702	0.319353	0.426510
6	1.124554	1.495456	0.667242
6	-0.155890	-2.051174	0.231137
12	1.219493	-0.624293	-0.792850
6	-0.515076	-0.046159	-1.866772
6	5.699875	-0.869710	-0.191489
6	-2.815281	-0.356070	-0.607566
6	-2.602999	-1.416024	0.160764

16

176.199737 Kcal/mol 7.640753 eV -101.102888 H Child_3_39.log

6	-7.345591	-2.104123	0.627606
6	2.069065	-1.644735	-2.653375

6	-6.431473	-1.193661	0.440222
6	4.201320	0.606260	0.626496
6	-5.493143	-0.322498	0.276233
6	1.942940	-2.270269	-1.539857
6	-4.507970	0.498221	0.112185
8	2.491655	2.325842	-0.093064
6	-3.513551	1.265149	-0.032696
6	3.387111	1.469671	0.262238
6	-2.374613	1.926916	-0.155946
6	1.778130	-2.887768	-0.411684
6	-1.261484	2.499619	-0.253562
8	1.585270	-3.430064	0.611401
12	0.730882	2.705984	-0.289403
12	5.325799	-0.891227	1.294915
16			
176.331758 Kcal/mol 7.646478 eV -101.102678 H Child_11_45.log			
6	3.673722	2.676344	-0.050261
8	-6.276851	2.127198	0.461567
6	3.390451	1.407197	0.090122
6	-5.207585	1.636980	0.208585
6	3.069573	0.200363	0.221393
6	-4.077767	1.112683	-0.040013
6	3.734428	3.983100	-0.079438
6	-2.898917	0.600048	-0.314963
6	3.392611	5.244187	-0.072978
6	-2.036368	-0.527086	-0.372816
12	2.492479	-2.806919	0.054238
12	-1.494683	-2.453225	-0.022385
6	1.191290	-4.291913	-0.120153
6	0.029317	-3.803217	0.052635
6	-1.494230	0.707147	-0.763473
8	2.705264	-0.946357	0.421672
16			
176.736165 Kcal/mol 7.664015 eV -101.102033 H Original2D_9_2.log			
6	0.000000	-0.836897	0.000000
6	-2.425843	-0.546482	0.000000
6	1.384913	-1.157870	0.000000
6	-3.375204	1.785708	-0.000000
6	-0.883606	1.577527	-0.000000
6	-1.036660	0.107857	-0.000000
6	3.035267	2.277162	-0.000000
12	3.267461	-0.398138	0.000000
6	-2.094389	2.107117	-0.000000
12	1.060839	2.470296	-0.000000
6	-0.344413	-2.207967	0.000000
6	-3.334974	0.504787	-0.000000
6	-2.757553	-1.937118	0.000000
6	4.025369	1.495892	-0.000000
8	0.886646	-2.741706	0.000000
8	-1.523779	-2.743820	0.000000
16			
176.739201 Kcal/mol 7.664147 eV -101.102029 H Original3D_0_42.log			
6	3.824788	-0.316416	0.667040
8	4.746636	-0.783540	1.166217
12	1.860272	0.381322	-0.347267

12	-0.555022	-3.513758	-0.677456
6	-5.208628	0.940234	1.114202
6	-3.128157	-0.283419	0.225906
6	-4.243181	0.105220	0.786324
8	0.736482	0.652382	1.382499
6	0.531485	-1.216104	-0.957802
6	2.037816	2.424592	-1.144117
6	-0.691020	-1.016008	-0.691011
6	-1.897404	-0.177353	-0.344315
6	-0.489254	1.824575	-1.158832
6	0.779554	2.343174	-1.303367
6	-1.451567	1.109484	-0.842579
6	0.014245	0.701772	2.299710
16			
177.161531 Kcal/mol 7.682461 eV -101.101356 H Child_13_27.log			
8	8.290573	0.174187	-0.483523
12	-5.022320	1.524439	0.461689
6	7.091851	-0.000413	-0.202707
6	-3.300897	-0.101254	0.142343
6	5.877365	-0.245740	0.090485
6	-4.369922	-0.472778	-0.412898
6	4.597562	-0.052784	0.194881
6	-6.713603	0.514998	-0.605552
6	3.337134	0.127620	0.245638
6	0.017216	1.965188	-0.071054
6	2.035775	0.340318	0.221567
6	-5.700691	-0.246942	-0.748699
12	-0.312839	-0.207874	0.160693
6	1.156291	1.400489	0.085734
6	-1.583898	-2.049910	0.059729
8	-2.120972	-3.033130	0.300348
16			
178.141578 Kcal/mol 7.724960 eV -101.099794 H Original2D_0_20.log			
6	0.000000	0.580957	0.000000
6	-1.365683	1.021986	-0.000000
6	-2.288766	-1.360709	-0.000000
6	0.579588	-0.683582	0.000000
12	1.135974	2.417510	0.000000
6	-1.415950	2.423762	-0.000000
6	3.054321	0.031222	0.000000
6	3.961928	1.289518	0.000000
6	-2.424525	0.086691	-0.000000
8	0.087848	-1.985462	-0.000000
6	-0.866296	3.565321	0.000000
6	-1.357732	-2.264813	-0.000000
8	3.065421	2.261011	0.000000
6	1.998676	-0.609497	0.000000
12	-1.371126	-4.351002	-0.000000
6	-3.609615	-0.581271	-0.000000
16			
178.343798 Kcal/mol 7.733729 eV -101.099471 H Child_8_20.log			
6	-1.893982	3.132983	0.099410
6	3.635552	-0.760592	-0.092105
6	-1.733107	1.808076	0.048041
8	2.969913	-1.855072	0.025721

8	-3.253458	-1.646506	-0.180793
6	4.278768	0.317573	-0.206484
6	-2.868097	0.917709	-0.055410
6	-3.398516	-0.315957	-0.139455
12	3.091127	1.874284	-0.112960
6	-0.350437	1.391322	0.111785
12	1.070869	-1.832218	0.192005
6	1.001027	1.696846	0.092612
6	-0.838433	-2.524536	0.058738
6	-4.321692	0.754219	0.002757
6	-2.005435	-2.157282	-0.076366
6	0.548418	0.324278	0.205149

16

178.457553 Kcal/mol 7.738662 eV -101.099290 H Child_3_62.log

8	5.033077	1.071086	-0.506619
8	-4.370866	0.032970	-1.119778
6	3.333088	-0.516068	0.237686
12	-4.334890	1.388922	0.689886
6	3.894744	0.784034	-0.277897
6	-3.242826	-0.361753	-0.684246
6	2.551210	-1.574997	-0.302663
6	-2.170583	0.230044	0.061016
6	1.967564	-0.290861	0.811939
6	-2.345462	-1.264374	-0.085362
6	2.618002	1.526948	-0.442233
6	-1.030350	1.006894	0.134677
6	1.418664	-1.580066	0.682451
12	-0.464637	-2.262693	0.080362
6	0.172956	1.267874	0.237609
6	1.549097	1.047793	0.255055

16

178.472908 Kcal/mol 7.739328 eV -101.099266 H Child_4_8.log

6	5.286007	-0.015148	0.809276
6	-6.669036	0.045438	0.193302
6	5.272568	1.295697	0.427451
6	-4.021376	0.181322	0.243126
6	4.752456	-1.131063	0.855949
6	-1.704268	-0.657145	-0.448307
12	2.939145	1.764665	-0.647494
6	-5.395192	0.299850	0.367843
6	4.887238	2.397536	-0.055106
6	-7.918993	-0.230789	0.016564
6	3.754754	-1.994590	0.525616
6	-2.848874	-0.298427	-0.095101
6	2.669572	-2.386225	0.028335
8	-0.573870	-0.960817	-0.777143
12	1.424461	-0.873189	-0.693988
8	-4.520181	1.493758	0.637655

16

178.608585 Kcal/mol 7.745211 eV -101.099049 H Original3D_0_75.log

6	1.319080	-1.489431	0.139634
6	2.534964	-1.198724	-0.216545
8	-3.107219	2.540525	-0.631026
12	-0.048082	-3.215699	-0.446164
8	3.671517	-1.033393	-0.508988

6	-1.926407	2.113010	-0.443495
6	0.372721	0.916908	0.198129
6	-0.964045	-1.045276	0.744124
6	0.343917	-0.541828	0.453189
6	3.630239	3.076789	0.272675
6	-0.874775	1.499328	-0.137202
12	-2.831779	-0.046479	-0.175045
6	1.525490	1.599996	0.153274
6	-1.694315	-1.896359	-0.239634
6	2.628017	2.259990	0.124299
6	-1.887561	-0.779557	1.713989
16			
179.454079 Kcal/mol 7.781875 eV -101.097702 H Child_16_17.log			
12	2.899641	4.280841	-0.235027
6	-0.799887	-2.987242	-0.251247
6	4.739282	-3.006766	0.698413
6	-5.199601	0.255721	-0.583907
6	2.272031	1.036160	-0.069032
6	-3.940710	-0.228735	-0.436347
6	3.807957	-2.125329	0.448863
12	-2.039864	-1.080192	-0.517959
6	1.940894	-0.345144	-0.015733
6	0.094205	-2.098173	-0.177819
6	2.505577	2.247159	-0.116345
6	-4.464522	0.796906	0.534595
8	-4.232353	1.461090	1.516770
6	0.571845	-0.762624	-0.204867
6	2.886482	-1.273707	0.217236
8	-0.367478	0.106766	-0.420148
16			
179.576694 Kcal/mol 7.787192 eV -101.097507 H Child_10_37.log			
6	3.241122	-1.259099	1.229634
8	-6.097252	1.663369	0.158560
6	3.243280	0.049945	0.942517
6	-2.621267	-1.846441	0.979255
6	2.502274	-2.240973	0.830510
6	-5.093576	0.994154	0.178817
6	2.482430	0.256683	-0.274994
6	-3.153849	-0.653593	0.299113
6	1.638111	-2.010545	-0.212161
6	-3.989250	0.309398	0.167682
6	2.378464	1.664843	-0.736253
6	-1.945502	-1.452251	-0.160734
6	1.640499	-0.737527	-0.839001
12	-0.236400	-1.435072	-1.347019
8	2.419206	2.093216	-1.870933
12	2.527064	2.393386	1.286409
16			
180.254205 Kcal/mol 7.816572 eV -101.096427 H Child_2_13.log			
6	-2.350282	3.910338	0.717812
12	3.708994	-2.742959	0.632654
6	-1.491332	2.989943	0.471822
6	2.852496	-0.890730	0.355466
6	0.664159	2.308934	-0.447845
6	1.544249	-0.661929	0.578155

6	1.767492	2.415647	-1.020790
6	0.384087	-0.167293	0.717219
6	-0.556411	2.048229	0.218827
6	-3.463720	-2.412059	-0.271963
6	-4.234124	-3.090061	0.512594
8	-1.936090	0.202373	0.984306
6	-0.781807	0.596774	0.680265
6	-2.636930	-1.760610	-1.028944
8	-1.885235	-1.243257	-1.763994
12	2.989617	0.793291	-0.854170
16			
180.305138 Kcal/mol 7.818781 eV -101.096346 H Original3D_0_79.log			
6	-1.014544	0.907040	0.961795
6	-0.612521	0.227602	-1.540662
8	1.091734	2.048010	1.057559
6	0.515329	0.398441	-0.745910
6	1.568398	-0.526025	-0.545611
6	-2.524032	-1.550211	0.280322
8	2.817971	-0.264854	-0.426003
6	-1.727698	-0.455742	1.034837
6	0.947278	-1.726365	-0.067856
12	4.650589	0.169348	0.010929
6	0.268027	1.296050	0.433454
6	0.008227	-2.294488	0.487358
12	-3.308727	0.693513	-0.656891
6	-1.735458	0.534893	-1.990514
6	-1.278916	-1.812961	0.795644
6	-2.310753	0.898502	1.346990
16			
180.307565 Kcal/mol 7.818886 eV -101.096342 H MutI_14_75.log			
6	-0.515444	-1.006475	-1.079861
6	2.118873	-2.551574	0.821511
6	-1.327617	2.489518	0.339923
6	1.362744	0.527981	-0.712327
6	1.121601	1.883327	-0.244991
6	-2.991390	0.959865	0.460793
8	-2.779336	-1.434328	-0.356851
12	0.090663	-2.885908	0.592293
6	-0.190397	2.287914	-0.094876
8	-2.573593	2.243453	0.733565
6	-1.349559	-1.840577	-0.452769
6	-2.942718	-0.176954	0.015520
6	2.389645	-1.403093	0.345707
6	2.459531	-0.049613	0.024337
6	0.449729	-0.242664	-1.437000
12	3.185457	1.907664	0.163581
16			
180.549371 Kcal/mol 7.829372 eV -101.095957 H Child_6_50.log			
12	2.565228	1.228191	-0.861897
8	-5.486538	-0.151683	-0.317678
6	3.070497	-0.427660	-1.954397
6	-4.329795	-0.108552	-0.117948
6	1.127425	2.560137	-0.213236
6	-3.005443	-0.062196	0.154191
8	2.398447	0.266666	1.034732

6	-2.155552	-1.202707	0.031853
6	-0.059599	2.345117	0.129972
6	-1.107722	-1.874286	0.030437
6	-1.305773	1.850498	0.201973
6	1.914473	-0.992615	1.569356
6	2.376046	-1.350279	-1.436711
12	0.944264	-2.130765	-0.151532
6	-2.329159	1.171236	0.327636
6	2.903074	-0.256856	2.347661
16			
180.718220 Kcal/mol 7.836694 eV -101.095688 H MutD_7_78.log			
6	4.195074	0.265460	0.003558
6	-0.708692	1.085893	0.784813
12	-2.785871	1.986773	-1.006416
6	-1.119607	2.388149	0.619835
12	-2.807829	-2.074744	-0.596778
6	5.324333	0.209752	-0.639892
6	-0.390474	-0.891164	0.585618
6	-1.769076	3.409208	0.236010
6	6.401300	-0.132071	-1.278657
6	-1.541238	-0.026729	0.251410
8	-1.248424	-3.035917	0.076674
6	0.476993	0.228770	0.912997
6	1.811341	0.312733	0.924078
8	-0.117363	-2.160194	0.519277
6	3.024079	0.303668	0.530474
6	-2.695583	-0.049581	-0.518460
16			
180.856128 Kcal/mol 7.842674 eV -101.095468 H Child_14_21.log			
8	5.080079	-2.203728	-0.012945
8	-4.036632	-1.166146	-1.028580
6	4.077574	-1.562855	-0.058383
12	-3.388458	-1.653695	0.790003
6	2.963548	-0.905806	-0.187711
6	-2.237774	-0.391188	1.926045
6	2.427008	0.421789	-0.213963
6	-3.401966	-0.063074	-1.202321
6	2.540553	1.657322	0.449103
6	-1.923016	0.524176	1.114942
6	1.141352	0.114052	-0.838347
6	-2.634182	0.884902	-0.948367
6	2.144592	2.832648	0.693464
6	-1.692162	1.350291	-0.015589
6	1.382851	-1.182685	-0.314605
12	0.298637	2.060492	-0.297788
16			
180.971892 Kcal/mol 7.847694 eV -101.095283 H Original2D_0_14.log			
6	-2.803162	-1.124208	-0.000000
6	-1.913932	-1.971420	-0.000000
8	0.000000	-0.199943	0.000000
6	-0.585471	-2.497376	-0.000000
12	-1.753901	2.072676	-0.000000
6	0.451056	-1.493477	0.000000
6	0.818025	0.903920	0.000000
6	1.721533	2.755805	0.000000

6	0.339172	2.185566	0.000000
6	2.253288	1.249414	0.000000
6	-3.419107	0.089351	-0.000000
6	2.300491	3.940489	0.000000
8	3.321213	0.677105	0.000000
12	1.890403	-3.131400	0.000000
6	-3.639506	1.326387	-0.000000
6	-0.223674	-3.883217	-0.000000

16

181.178553 Kcal/mol 7.856656 eV -101.094954 H MutD_11_76.log

6	6.508814	0.369998	1.480019
6	-4.891168	2.253185	-0.014428
6	-3.753681	2.847541	-0.138726
6	6.818341	0.883701	0.176426
8	-2.677312	3.401932	-0.237258
6	5.585914	0.060284	0.508686
6	-3.069668	-2.295093	0.094448
6	4.406068	-0.454251	0.054578
6	-5.468213	-1.377175	0.379728
8	7.387443	1.466755	-0.718289
6	-4.278078	-1.826211	0.248574
12	-5.950468	0.630351	0.225549
6	-0.543177	-2.093450	-0.376365
6	-1.782630	-2.161366	-0.139775
12	1.389540	-1.527081	-0.567338
6	3.309161	-0.905286	-0.315525

16

181.327492 Kcal/mol 7.863114 eV -101.094717 H Original2D_0_11.log

6	-1.599497	-1.315654	-0.000000
6	-1.965273	0.013124	-0.000000
12	0.191695	-2.336670	-0.000000
6	-2.030859	2.463404	0.000000
6	3.716924	1.818582	0.000000
6	-1.328649	1.300083	0.000000
6	-2.735719	3.531680	0.000000
6	-3.085657	-1.569627	-0.000000
6	3.204897	-1.685419	0.000000
8	0.000000	1.251722	0.000000
12	1.658939	2.053433	0.000000
6	3.946135	0.561676	0.000000
6	4.188449	-0.761244	0.000000
8	-3.408129	-0.175059	-0.000000
6	2.221111	-2.475367	-0.000000
6	-3.688959	-2.750313	-0.000000

16

181.427520 Kcal/mol 7.867452 eV -101.094557 H MutI_17_53.log

6	3.004936	1.538526	0.230651
6	-0.449137	-0.931058	-0.661356
6	-6.515344	-0.560860	0.896387
6	-5.337242	-0.866037	0.460840
6	2.289689	2.571158	0.229411
12	3.269196	-0.463672	-0.099994
6	1.439341	3.610102	0.252951
8	-0.961058	4.211922	0.040719
6	0.763324	-1.595217	-0.946754

8	-0.470327	0.286253	-0.274530
12	3.450004	-3.431415	1.061594
6	1.994685	-1.768039	-1.080664
6	-2.977856	-1.469791	-0.423144
6	-4.182621	-1.191067	-0.009474
6	-1.748213	-1.449288	-0.678154
6	0.188550	3.904179	0.117854
16			
181.826209 Kcal/mol 7.884741 eV -101.093922 H Original3D_7_4.log			
6	2.502646	-1.355230	-0.897268
6	0.815570	-0.255403	1.065788
6	-1.538521	-0.172464	0.160194
12	2.221219	1.637337	0.557696
6	-1.935331	-1.608532	0.428002
6	-0.286585	0.476137	0.600958
6	1.579354	-1.590949	0.074847
8	3.264573	-1.176088	-1.768357
6	0.428499	-2.364834	0.033813
6	0.064933	1.838313	0.341929
6	1.973283	-0.690758	1.590202
6	-0.530869	2.861240	-0.214826
6	-2.303558	0.376317	-0.849666
8	-0.852252	3.931674	-0.643000
6	-0.799017	-2.386435	0.283450
12	-3.814635	-1.038095	-0.258837
16			
182.095058 Kcal/mol 7.896399 eV -101.093493 H Child_10_21.log			
6	5.857868	-0.373240	-0.719157
12	-4.112128	-2.410835	0.254546
6	4.955697	0.004591	0.048687
8	-2.334281	-2.191150	1.314841
6	6.796213	-0.774998	-1.544138
6	-3.109166	-0.451973	-0.065529
6	3.934695	0.437306	0.801522
6	-2.266729	-1.093817	0.767320
6	7.734799	-1.176620	-2.338906
8	-6.670838	1.342922	-2.008188
6	2.947584	0.857920	1.458397
6	-1.917517	0.160732	0.329009
6	-5.573399	1.390060	-2.240063
12	1.150449	1.712592	1.590620
6	-1.033472	1.230109	0.404672
6	-0.396392	2.317388	0.332316
16			
182.163779 Kcal/mol 7.899379 eV -101.093384 H Child_2_59.log			
6	-0.271305	-2.577223	0.346790
6	0.466361	2.531990	0.081426
12	-8.726707	-1.009338	-0.321276
6	1.760249	2.113673	-0.082632
8	0.729350	-3.372851	0.216661
6	-0.767813	2.047571	0.237726
6	-1.102726	-1.671424	0.434795
6	2.765205	1.416712	-0.203966
6	-1.459994	-0.369692	0.423218
6	-0.645416	3.513510	0.041579

12	2.418143	-2.648914	-0.259283
6	-1.441318	0.864323	0.376916
6	-1.184863	4.705598	-0.096983
6	3.480160	-0.966327	-0.634376
6	3.609735	0.321714	-0.325676
8	4.827291	-0.087588	0.205065
16			
182.430257 Kcal/mol 7.910935 eV -101.092959 H Original3D_4_3.log			
8	-1.353746	-1.028719	0.007453
12	-0.437967	-2.372799	0.840365
8	-1.741877	1.104867	-0.687077
6	1.313928	2.499722	0.866913
6	-4.799591	-0.688928	-0.370050
6	-3.569563	-0.352631	-0.379489
6	2.092797	0.798311	-1.103554
6	1.437676	-3.071407	1.042966
12	2.997708	-1.044154	-0.889196
6	2.258349	-2.484956	0.286636
6	-0.453782	1.482727	-0.311274
6	-2.235417	-0.137214	-0.336201
6	0.465644	3.294653	1.735236
6	1.851696	1.890070	-0.266896
6	0.744518	1.274675	-1.002012
6	-0.098242	2.227354	0.841554
16			
182.489422 Kcal/mol 7.913500 eV -101.092865 H MutI_14_51.log			
6	2.880934	-0.871332	-0.105674
6	-2.565588	3.771588	-0.077249
6	-1.155472	3.302524	0.024084
6	0.138764	3.257118	0.039992
12	-3.161409	-2.793375	-0.897083
8	5.220586	-1.560225	-0.463338
6	1.408038	2.998265	0.073795
12	-1.939429	0.287337	-0.173290
6	0.394430	-0.311787	0.245055
8	-1.740791	-3.396948	0.822149
6	2.574753	2.449884	0.252459
6	1.675989	-0.525797	0.098222
6	4.101492	-1.223286	-0.280253
6	-0.982539	-2.428717	0.882960
6	-2.324545	2.420515	-0.124630
6	-0.584307	-1.217334	0.633572
16			
182.521547 Kcal/mol 7.914893 eV -101.092814 H Child_16_26.log			
12	3.167589	2.059037	-0.578633
6	-8.491394	1.159710	-0.514683
6	3.801640	0.063536	-0.543640
6	-7.315161	0.589050	-0.525659
6	4.759088	-0.556866	-1.188993
6	-6.115349	0.106518	-0.480032
8	5.640584	-1.036910	-1.832934
6	-4.898154	-0.321242	-0.351404
8	3.141811	-0.723418	0.496341
6	-3.704105	-0.753328	-0.178344
6	2.169271	2.485364	1.219319

6	-2.443748	-1.114768	0.058036
6	2.138053	1.207937	1.373825
6	-1.272927	-1.513420	0.239447
6	2.241683	-0.171587	1.381954
12	0.543033	-1.475938	1.224782
16			
182.755975 Kcal/mol 7.925059 eV -101.092440 H Child_1_45.log			
12	3.380508	-1.711286	0.000000
6	-4.467885	2.424079	-0.000000
6	2.397729	0.203188	0.000000
6	-3.473165	1.579725	-0.000000
6	2.952415	1.500235	0.000000
8	-3.544211	-1.311708	-0.000000
6	0.916190	-3.949082	0.000000
6	-2.368948	0.829920	-0.000000
8	1.696197	-3.077995	0.000000
6	-2.475514	-0.693505	-0.000000
6	2.085440	2.534200	0.000000
6	-1.158099	-1.359304	-0.000000
6	1.081238	-0.074877	0.000000
12	-0.454972	1.868280	-0.000000
6	0.000000	-0.841087	0.000000
6	1.123545	3.385458	0.000000
16			
182.966926 Kcal/mol 7.934207 eV -101.092104 H Original3D_0_72.log			
6	1.083965	-1.767161	-0.782413
6	-0.154724	1.668013	0.328684
6	2.801398	-0.068929	0.493223
6	-0.742121	0.683862	0.980626
12	-0.947663	-1.891149	-0.160104
6	2.317499	1.231132	0.038120
6	2.294307	2.292306	-0.868824
12	-3.436599	-0.166287	1.144091
6	-1.395800	-0.387989	1.359454
8	-1.987034	1.674601	-1.310176
6	2.225999	-1.125116	-0.335400
6	2.372216	-2.190285	-1.308906
6	1.107111	1.899905	-0.082084
6	-2.452663	0.560692	-1.137850
6	-2.859573	-0.649810	-0.823514
8	3.615216	-0.198413	1.438360
16			
182.986617 Kcal/mol 7.935061 eV -101.092073 H Child_2_49.log			
6	0.289516	1.184146	-1.265903
6	-1.256096	-1.540119	-0.459435
6	1.023569	1.135360	-0.085805
8	-4.284605	-0.925037	1.561083
6	-0.802917	1.081061	-1.916466
6	-0.145784	-2.023888	-0.229673
12	-0.992298	1.597054	0.761892
12	-2.552550	0.069878	-1.293331
6	5.985939	0.147205	0.621567
6	1.207277	-2.277596	-0.276747
6	4.686575	0.349345	0.563618
6	-3.646637	-0.015495	1.090705

6	3.375451	0.436273	0.557679
6	-2.939279	0.922456	0.515830
6	2.163028	0.398114	0.195976
8	2.146395	-1.423007	-0.247433
16			
183.735199 Kcal/mol 7.967522 eV -101.090880 H MutI_9_69.log			
6	0.349634	2.572979	0.039636
8	-4.065600	-1.293561	-0.112967
6	2.448931	-2.298813	0.199852
6	-3.849934	0.022695	-0.005043
6	-2.861817	-1.957366	-0.055993
6	-1.687315	-2.333388	-0.001893
8	2.426353	1.207731	-0.350612
6	0.858382	3.806478	0.193206
6	0.535096	0.105282	-0.273890
6	-3.248778	1.071387	0.129503
6	-2.188313	1.918270	0.162703
6	1.087172	1.330085	-0.198424
12	3.688200	-0.119333	-0.015779
12	0.365292	-2.090299	0.007996
6	-1.062044	2.399193	0.151750
6	3.697665	-2.103100	0.292264
16			
183.831316 Kcal/mol 7.971690 eV -101.090727 H Child_1_27.log			
6	3.091829	-0.668549	2.863149
6	-5.070321	1.723433	0.905448
6	1.973340	-0.619690	2.172237
6	-3.945041	1.248558	0.463035
6	0.970473	-0.605188	1.318250
6	-2.816020	0.812892	0.010363
12	-0.928441	-1.544270	1.294321
6	-1.695696	0.333707	-0.581823
6	2.896021	1.863231	-0.586287
6	0.518757	-2.016901	-1.903056
8	3.763547	2.582838	-0.428880
6	1.721291	-1.561119	-1.914507
6	-1.603169	-1.114821	-0.838179
8	-0.610408	1.060297	-0.881609
6	-0.721802	-1.768455	-1.442888
12	1.166518	0.301965	-0.653533
16			
183.835526 Kcal/mol 7.971873 eV -101.090720 H Original3D_0_55.log			
6	-0.258366	1.197463	0.597463
6	-0.645181	2.408398	0.193599
6	0.973386	0.576287	1.013903
6	-1.397504	0.445826	-0.035905
6	1.192205	-2.023154	1.352433
6	-1.204933	-0.278689	-1.230981
6	1.264667	-3.296130	1.636889
6	2.181663	1.343536	1.130073
6	3.076767	1.023803	0.171028
6	1.099504	-0.801439	0.932344
6	-2.734750	0.356490	0.584423
8	-0.056495	-0.282918	-1.866971
8	-3.156785	0.935452	1.577649

6	3.651695	0.678810	-0.926999
12	-3.215709	-0.983130	-1.044581
12	1.758320	-0.267492	-1.471673
16			
183.967525 Kcal/mol 7.977597 eV -101.090509 H Child_8_34.log			
6	0.210302	2.489405	0.795629
12	3.077763	-2.831468	-0.519629
12	2.131921	2.116522	0.510619
6	1.268371	-1.545701	-0.555508
6	-1.011156	2.408053	0.468405
6	-2.310458	2.275329	0.123317
8	4.654047	-1.574443	-0.031248
6	3.056725	0.260303	-0.113811
6	4.238130	1.101389	0.329115
6	-3.469893	2.061612	-0.322537
6	-6.400831	-2.968404	0.630349
6	4.302131	-0.335604	0.083487
6	-4.689622	1.845605	-0.796980
6	1.958970	-0.479470	-0.406163
6	-5.926724	1.737361	-1.154162
8	-5.888030	-3.990547	0.733907
16			
184.021994 Kcal/mol 7.979959 eV -101.090423 H MutI_15_75.log			
6	0.184644	-1.974505	-1.688886
12	-1.671922	-1.151245	-0.861696
6	-2.511599	0.609449	1.031237
6	-3.404229	0.063747	0.079091
8	2.773006	1.068494	-0.424344
12	1.336698	-1.846018	1.098476
6	0.404588	3.772410	-0.268666
6	0.951685	2.609681	-0.281876
6	1.382109	1.345412	-0.306085
6	-0.225972	-0.195614	0.983840
6	0.646531	-1.005069	-1.012507
6	-1.306598	0.498814	1.438982
8	-4.596271	0.124333	-0.170665
6	3.231606	-1.292251	0.490414
6	0.607247	0.133714	-0.120879
6	3.141454	-0.161698	-0.024880
16			
184.087701 Kcal/mol 7.982808 eV -101.090318 H Original3D_9_4.log			
6	-1.807989	0.031024	-0.480968
6	-0.465574	-0.078336	-0.763974
6	2.149294	-3.663601	0.386184
8	1.416063	-2.926033	0.875568
6	0.752032	-0.036915	-1.001347
12	1.170346	2.238047	0.106669
6	-2.758031	0.958858	-0.036415
6	3.181970	0.134730	-1.546552
8	1.527722	-0.115369	2.736447
6	-4.011314	-1.419101	-0.389286
6	1.427457	0.694986	1.938465
6	4.366423	-0.207383	-1.932504
12	-1.664070	2.776212	0.328051
6	-3.144083	-0.407719	-0.334093

6	-4.651545	-2.523313	-0.491154
6	2.023765	0.543455	-1.033816
16			
184.157555 Kcal/mol 7.985837 eV -101.090207 H Child_3_49.log			
8	2.388261	-3.849530	0.271049
6	-6.092194	-0.501966	-0.136719
6	2.303204	-2.476855	0.059767
6	-4.822593	-0.366773	-0.249202
6	3.126275	-1.356359	0.115481
6	-3.520424	-0.385405	-0.147988
6	1.023331	-2.703436	-0.197005
6	0.740045	3.247930	0.013008
6	3.362211	-0.157510	0.036372
6	-2.234013	-0.441513	-0.008191
6	3.208409	1.182023	-0.099960
6	-0.414231	3.059496	0.427143
12	-0.876072	-1.971841	-0.163541
8	2.031038	3.411378	-0.381433
6	2.752294	2.292338	-0.317355
12	-1.786285	1.567958	0.489455
16			
184.251401 Kcal/mol 7.989907 eV -101.090057 H MutD_16_40.log			
6	-2.665707	-1.844091	-0.005582
8	-3.895956	-1.337807	0.060959
6	-1.035284	2.278794	0.001165
6	-0.203781	-2.602083	0.005694
12	2.971729	-2.302561	0.032566
6	-4.893772	1.138208	-0.060649
6	1.510096	2.556896	0.044134
6	4.719066	-1.007431	-0.147654
6	1.017346	-2.814694	0.020301
6	-2.196335	1.873432	-0.039987
6	-3.390801	1.209084	-0.046048
12	3.973170	1.009680	-0.003579
6	-4.028384	0.026766	-0.008982
8	2.785477	2.451126	0.041086
6	0.282392	2.550790	0.047266
6	-1.523992	-2.264336	-0.003693
16			
184.823051 Kcal/mol 8.014696 eV -101.089146 H Child_6_15.log			
12	0.388299	2.706351	-0.079426
6	-5.927632	-0.197384	0.519033
6	2.163574	1.573043	0.200802
6	-4.684659	-0.217535	0.228581
12	3.859884	0.414072	0.133918
6	-3.366223	-0.259730	-0.107427
6	1.366543	0.470704	0.097648
6	-2.443028	-1.377030	-0.250807
6	-1.191790	1.183810	-0.156757
6	-1.257805	-1.757207	-0.284843
8	2.323238	-1.951971	0.318831
8	3.698686	-1.469558	-0.154111
6	-0.119463	0.335790	-0.005307
6	-2.431341	0.738255	-0.368362
6	1.378182	-1.056692	-0.027537

6	-0.011956	-1.114833	-0.173638
16			
185.015320 Kcal/mol 8.023034 eV -101.088840 H Child_7_54.log			
8	4.680389	6.282793	-0.158497
6	-2.112756	0.549498	1.958757
6	5.136843	5.268462	0.131344
6	-2.950845	1.114101	2.775918
6	-3.310027	0.394796	-1.582103
8	2.789301	-3.233398	2.101559
6	-2.073347	0.282772	-1.719607
6	2.440046	-2.520737	1.222961
6	-4.574857	0.402887	-1.131087
6	2.054527	-1.813153	0.201879
6	-0.819167	-0.062068	-1.588653
6	1.195850	-1.101861	-0.431926
6	-5.812223	0.163807	-0.875854
6	0.268158	-0.476903	-1.092496
12	4.242089	-3.576696	-1.218264
12	-3.942984	0.442966	0.988323
16			
185.269717 Kcal/mol 8.034065 eV -101.088434 H MutD_17_54.log			
8	-1.328028	-0.094837	-1.275903
6	-2.692745	1.042184	0.132098
6	-3.714911	0.526769	0.634952
6	2.099823	1.371976	0.338598
6	1.897789	2.343512	1.150283
6	-0.142301	-0.370378	-1.813068
12	2.482732	-0.444273	-0.952222
6	1.410945	3.367575	1.813942
6	1.784789	-2.020853	1.018660
6	2.944275	-1.669004	0.668975
6	-0.800241	-2.239890	1.126877
12	-2.517038	-1.294920	0.624648
6	-1.502727	1.225722	-0.611454
6	0.976570	-0.497451	-2.355847
6	0.443502	-2.245427	1.168105
8	-0.649087	2.077575	-0.686825
16			
185.413448 Kcal/mol 8.040298 eV -101.088205 H Original1D_0_4.log			
12	0.000000	0.000000	6.660115
12	0.000000	0.000000	3.855425
6	0.000000	0.000000	8.678098
8	0.000000	0.000000	9.976276
6	0.000000	0.000000	1.804546
6	0.000000	0.000000	11.219461
6	0.000000	0.000000	0.556084
6	0.000000	0.000000	-0.780509
6	0.000000	0.000000	-2.026061
6	0.000000	0.000000	-3.342936
6	0.000000	0.000000	-4.599068
6	0.000000	0.000000	-5.903415
6	0.000000	0.000000	-7.169281
6	0.000000	0.000000	-8.461866
6	0.000000	0.000000	-9.733425
8	0.000000	0.000000	-10.930808

16
185.419856 Kcal/mol 8.040576 eV -101.088195 H MutI_12_77.log
12 4.807782 0.276735 -0.028836
6 -0.997157 0.993969 0.113071
6 1.410236 1.840841 0.011977
6 0.151366 1.452687 0.024461
8 -1.906837 -1.354130 0.283900
6 -7.427621 0.120529 -0.411933
8 3.886333 1.942089 0.033433
6 3.057304 -1.849134 -0.226629
6 -2.132944 0.318818 0.206496
12 -4.274142 0.564226 -0.012642
6 1.744659 -1.991378 -0.052432
6 2.651812 2.005222 0.006756
6 -0.802123 -1.962392 0.295365
6 0.502248 -1.862504 0.139310
6 4.329119 -1.702403 -0.346107
6 -6.193504 0.169878 -0.100494
16
185.509610 Kcal/mol 8.044468 eV -101.088052 H Child_12_22.log
8 8.112900 -1.809812 0.110245
6 -6.261794 -2.196064 -0.027444
6 6.968818 -1.738777 0.135015
6 -5.111815 -1.602739 -0.076156
12 2.495013 -0.171693 -0.161729
6 -3.986820 -0.906354 0.015293
6 0.700981 3.287250 -0.017048
8 -2.716678 -1.765378 -0.014101
6 2.877716 1.852316 -0.192775
6 -1.655527 -0.961282 0.047188
6 1.793492 2.526485 -0.076728
12 -2.786844 0.950243 0.136423
6 -0.359923 -1.433850 -0.003185
6 -0.608456 3.045042 0.054221
6 0.888890 -1.471898 -0.067046
6 -1.856864 2.809692 0.131084
16
185.590275 Kcal/mol 8.047966 eV -101.087923 H Child_1_22.log
6 3.668207 -1.615193 1.217693
6 0.266125 1.970444 -1.542006
6 2.866721 -0.798701 0.509100
8 -1.780549 1.586530 3.047259
8 3.094898 0.443152 0.012117
6 1.605111 -1.471899 0.336417
6 -1.694390 1.587897 1.905756
6 0.642094 -2.563683 0.502149
12 -2.331833 1.454982 -0.561252
12 2.186912 1.687553 -0.929866
6 -3.651662 -2.690788 -0.512993
6 0.341165 -1.350931 -0.192071
6 -2.780154 -1.738364 -0.544798
6 -2.007014 -0.671799 -0.767685
6 -0.603237 -0.463740 -0.798799
6 -0.115591 0.815445 -1.209695
16

185.784108 Kcal/mol 8.056372 eV -101.087615 H Original2D_0_30.log

6	3.158421	0.231099	0.000000
6	0.000000	-0.881037	0.000000
6	2.668329	-0.920431	0.000000
6	0.702988	-2.154716	0.000000
12	1.301260	1.157509	-0.000000
8	-1.299788	-0.856827	-0.000000
6	-0.936660	-4.147529	0.000000
12	-2.717932	0.347225	-0.000000
6	-1.979162	-4.928987	0.000000
8	2.115087	-2.143427	0.000000
6	-0.014367	2.897450	-0.000000
6	-1.393776	2.696283	-0.000000
6	0.012035	-3.283036	0.000000
6	0.673922	4.049666	-0.000000
6	1.457523	5.085097	-0.000000
6	-2.602976	2.347011	-0.000000

16

186.291910 Kcal/mol 8.078392 eV -101.086805 H MutI_13_47.log

6	2.909587	1.551213	0.000000
6	2.506520	4.167454	-0.000000
6	0.492428	0.682632	-0.000000
6	1.976020	0.618702	0.000000
6	-0.359105	1.789705	-0.000000
12	0.488130	3.688369	-0.000000
6	-0.000000	-0.765386	0.000000
6	-2.586064	-3.799116	0.000000
6	-2.885499	-2.523711	-0.000000
12	-1.895278	0.438142	-0.000000
6	2.697071	2.896381	-0.000000
6	0.066339	-2.304298	0.000000
8	2.350101	-0.877257	0.000000
6	-3.062889	-1.281353	-0.000000
6	1.199208	-1.505533	0.000000
8	-2.454590	-4.957526	0.000000

16

186.978764 Kcal/mol 8.108177 eV -101.085711 H MutI_13_67.log

6	-1.395288	1.411170	-0.027303
6	-2.401175	-1.679675	-0.316554
6	2.978016	1.246699	0.472378
8	4.152101	0.583628	0.752529
6	4.163157	-1.861055	-0.188332
12	2.087649	-1.705277	-0.433573
6	-3.788055	-2.140687	-0.105969
6	-0.982374	2.648746	-0.326611
6	-1.385578	-0.980592	-0.403124
6	0.795120	0.126028	-0.336812
6	4.102213	-0.708097	0.308270
8	-4.369904	-1.075466	0.478457
6	-0.668745	3.836813	-0.752637
6	1.852522	0.911641	0.005477
6	-0.579844	0.198144	-0.306932
12	-3.287431	0.528601	0.601989

16

187.408362 Kcal/mol 8.126806 eV -101.085026 H Child_9_53.log

6	2.871826	-1.062405	0.613520
8	-4.677496	0.510927	0.583792
12	2.799531	0.727156	-0.370991
6	-3.544131	0.815968	0.491075
6	2.002916	-1.927252	0.834120
6	-2.226317	0.868686	0.428976
6	1.093421	0.762862	-1.678165
6	2.507145	2.898998	0.819114
8	1.032853	-2.877110	0.975331
6	1.312313	2.469162	0.578138
6	-0.139311	0.545412	-1.995959
6	-1.151097	1.622914	0.362411
6	-0.042526	-2.716569	0.186668
6	0.090795	2.006689	0.357541
6	-1.045832	-2.864957	-0.564106
12	-1.234370	-0.859455	-0.885091
16			
188.292852 Kcal/mol 8.165161 eV -101.083617 H Child_8_50.log			
6	-2.991253	-0.790958	-0.110869
6	9.103234	-1.118227	1.136038
6	-1.713397	-0.476552	-0.173724
6	5.552326	0.069903	0.557798
6	-4.232478	-1.086963	-0.037060
8	-3.631088	3.501728	0.687448
6	-0.496499	-0.177780	-0.248842
8	9.072759	-1.574609	0.083345
6	-3.940835	3.511845	-0.407943
6	0.770879	0.152061	-0.325393
6	4.619931	0.672145	-0.137810
6	1.973365	0.486472	-0.423244
6	4.183087	1.740893	-1.142919
12	-5.761976	-2.390995	-0.943103
12	-5.896215	-0.834338	1.370570
6	3.232460	0.898333	-0.568690
16			
188.417753 Kcal/mol 8.170577 eV -101.083418 H Child_15_15.log			
8	-7.426446	-0.416056	-0.007230
6	3.271010	-2.821678	-0.567573
6	-6.228132	-0.369725	0.000792
6	4.091172	-2.342032	0.562790
6	-4.957125	-0.327405	0.007694
6	2.434950	-1.648314	-0.140076
6	-3.666611	-0.237841	0.012497
6	3.653368	-1.003682	0.183176
6	-2.400439	-0.151518	0.013242
12	3.321526	1.867511	-0.138016
6	-1.096354	0.122322	0.052476
6	1.116673	-1.267204	-0.010188
12	-0.086940	2.020539	0.032356
6	1.708119	3.307791	0.015587
6	-0.002120	-0.737063	0.032485
8	4.131184	0.191243	0.043545
16			
188.444081 Kcal/mol 8.171719 eV -101.083376 H Child_9_23.log			
8	-4.958829	-0.025506	-0.484996

6	2.882085	-1.575042	0.593744
12	-0.670133	2.089272	0.212414
6	4.031355	-1.107027	0.877436
6	1.255944	2.595831	-0.095359
6	2.548174	-1.077828	-1.160398
6	-2.718497	1.177995	-0.108252
6	1.749774	-1.727440	-0.299691
6	-3.807429	0.132797	-0.166796
6	0.382048	-1.958967	-0.141716
6	2.468590	2.320018	-0.231519
12	3.726886	0.745059	-0.231489
6	-1.943332	0.537269	0.939510
6	-0.824281	-1.950281	-0.031083
6	-2.666100	-0.605550	0.490890
8	-2.145050	-1.797322	0.013534
16	189.366761 Kcal/mol 8.211730 eV -101.081905 H MutI_4_75.log		
8	-0.301698	1.846514	-0.340720
6	-4.973293	0.085874	-0.214848
6	1.652311	-1.471375	-0.510959
6	-3.977707	0.857557	-0.413899
12	1.418494	1.801008	0.194799
6	3.792097	0.795980	0.544177
6	-1.573564	1.732036	-0.429787
8	-0.849066	-1.617248	-0.140576
6	4.432049	-1.709162	-0.590539
6	3.368261	1.924118	0.911620
6	-1.462843	-1.725072	1.159897
12	-3.598167	-1.270446	0.553645
6	-2.776720	1.507581	-0.498339
6	0.448264	-1.550616	-0.326113
6	3.023642	-1.347550	-0.487912
6	3.941201	-0.466182	0.001540
16	189.835463 Kcal/mol 8.232055 eV -101.081158 H Child_5_49.log		
6	-3.879430	3.619149	-0.135469
6	1.887702	-1.318821	-0.555933
8	-3.430276	2.593056	-0.390166
12	2.951392	2.104711	-0.093426
6	-0.552734	-0.176183	1.711276
12	0.247066	-2.592121	-0.141286
6	0.155454	0.948167	1.561515
6	2.774113	-0.250139	-0.820909
6	-2.788339	-1.431411	-0.993784
6	1.672013	0.014376	-0.023474
6	-0.462007	-1.588796	2.080954
6	-1.746162	-1.688583	-0.208460
6	1.205198	1.115812	0.719660
8	3.766207	0.500270	-1.204273
6	-1.312953	-1.186197	1.036901
6	-3.797680	-1.206987	-1.776934
16	189.873684 Kcal/mol 8.233713 eV -101.081097 H Child_10_29.log		
6	4.525522	0.989813	-0.101806
8	-2.842315	1.737846	0.807818

6	3.141942	-1.447046	0.293965
6	-0.406101	1.598845	0.100000
6	3.605782	-0.155669	0.103919
6	-1.697062	1.595916	-0.136132
6	2.438095	-2.481093	0.446796
6	-3.441164	0.616490	0.133545
6	3.097699	1.076014	-0.086114
6	-2.456420	0.554535	-0.867469
12	0.712757	-1.292332	0.034457
12	-3.300397	-1.451978	0.489456
8	1.946111	1.753576	-0.183850
6	-1.860866	-0.707982	-1.128803
6	0.762268	0.990536	0.115876
6	-1.339475	-1.796968	-0.753560
16			
189.939354 Kcal/mol 8.236560 eV -101.080993 H Child_16_23.log			
8	-2.478680	3.283104	1.713548
8	3.744960	1.344838	-0.364668
12	-4.698501	-1.855928	-0.445039
6	3.611646	0.059660	-0.006498
6	3.158001	-1.029469	0.279704
6	-2.561147	-0.967377	-0.507488
6	2.544781	1.929571	-0.648500
6	-1.828966	2.973685	0.907922
6	2.405857	-2.153844	0.536110
6	-1.707743	0.064775	-0.580459
6	2.074208	-3.478081	0.915777
6	-1.151321	-1.299202	-0.188655
6	1.393510	2.289060	-0.863322
12	-0.566689	1.828055	-0.693931
6	1.051908	-2.494804	0.471766
6	-0.148725	-2.008816	0.163075
16			
189.947340 Kcal/mol 8.236907 eV -101.080980 H Child_6_27.log			
12	4.047393	1.693837	1.261845
6	-6.473898	1.421619	-0.048309
6	2.395038	-1.536231	-1.593699
8	-5.379545	1.758364	-0.029827
12	3.627246	-0.136423	-0.772682
6	-1.903994	-3.733155	1.893709
8	2.232204	1.486544	0.655678
6	-2.133455	1.751864	-0.916173
6	0.922233	1.498544	0.511799
6	-1.450181	-2.780938	1.163820
6	1.200867	-1.688060	-1.311823
6	-1.003084	-1.861875	0.284121
6	-0.179991	1.062680	0.146406
6	-1.358420	0.701763	-0.606468
6	-0.085116	-1.601974	-0.789220
6	-1.082821	-0.675609	-0.546958
16			
190.017902 Kcal/mol 8.239966 eV -101.080868 H Child_2_28.log			
6	7.864338	-0.974222	0.395514
8	-1.672585	-3.556559	-0.622557
6	6.613084	-0.622337	0.370988

6	-2.093929	-2.473429	-0.292977
6	5.365927	-0.244771	0.288785
12	-4.865775	-0.258329	0.228258
6	4.177751	0.150596	0.181175
6	-1.932958	-1.088217	0.107792
6	2.951595	0.605046	0.025222
6	-4.707372	1.734171	0.579183
6	1.777909	0.999516	-0.112754
6	-3.209888	-1.566712	-0.011710
6	0.524465	1.617625	-0.479276
6	-3.446262	1.628915	0.612126
12	-1.441727	1.130031	0.309226
8	0.720342	2.424370	-1.431722
16			
190.500118 Kcal/mol 8.260877 eV -101.080099 H Child_10_63.log			
8	4.987738	0.989335	0.023379
6	-5.836926	-0.429033	-0.056857
6	2.537409	1.539071	-0.047894
8	-3.522086	-1.580511	-0.050587
6	3.754274	1.547422	-0.005618
6	-5.117460	0.674802	0.069731
6	1.185567	1.363237	-0.045255
6	-2.567903	-0.857290	-0.027382
6	4.847697	-0.391053	-0.018563
12	-0.333688	-1.306764	0.000334
6	-0.032837	1.065192	-0.024419
6	-4.175289	1.540139	0.085021
6	3.976459	-1.257190	0.007817
12	-2.109125	1.301581	0.001853
6	2.794445	-1.910942	0.024213
6	1.565988	-2.085757	0.071108
16			
190.776656 Kcal/mol 8.272869 eV -101.079658 H Child_8_43.log			
8	4.803863	2.402246	-0.973710
8	-4.471425	0.412555	-0.117413
6	3.881360	1.767044	-0.553498
6	-3.641302	1.484647	0.390888
6	3.974943	-2.241665	1.497692
6	-3.892222	2.610434	1.048293
6	2.999221	-1.718071	0.840574
12	-2.351502	-2.084715	-0.819853
6	2.809701	1.214093	-0.115940
6	-3.198443	-0.306851	-0.317327
6	1.980017	-1.106524	0.194019
12	-0.294798	0.767277	0.342615
6	0.800092	-1.751937	-0.274394
6	1.834208	0.365811	0.178206
6	-0.327333	-2.144080	-0.614756
6	-2.370894	0.708906	0.135550
16			
191.217209 Kcal/mol 8.291973 eV -101.078956 H MutD_14_78.log			
6	3.590414	0.047777	0.237873
8	0.145107	2.724475	-0.859458
8	1.529418	-1.213737	-1.352742
6	1.864531	1.866828	0.541580

6	-0.046911	-0.020879	1.603699
6	-2.728465	0.911766	-0.350373
6	2.976429	1.143392	0.534654
6	-0.292952	0.866732	0.583840
12	0.252730	-1.990534	0.104730
6	0.549047	1.946973	0.064937
6	2.234532	-1.714491	-0.500303
12	-3.679289	-1.060453	0.210244
6	-3.957241	0.906803	-0.803927
6	-1.555784	0.316933	0.125427
6	-1.563622	-1.062603	0.518560
6	3.550441	-1.121575	-0.236314
16			
191.318186 Kcal/mol 8.296352 eV -101.078795 H MutI_16_41.log			
6	-2.238374	-0.528260	0.250576
12	-6.230450	-1.585606	-0.001342
6	4.615363	2.286111	0.131237
8	2.464916	-1.392516	1.012006
6	-0.031659	-1.339549	0.880389
6	-0.449844	1.099644	0.134721
6	-0.880695	-0.348021	0.471809
6	0.827376	1.551578	0.111879
6	1.282345	-1.285943	1.012753
6	-1.646412	1.814411	-0.180026
8	5.703933	-1.598345	-1.084681
6	-2.851705	2.056664	-0.455010
6	5.310284	-2.677944	-0.979783
6	3.332437	2.099993	0.237379
6	2.029624	1.903373	0.158112
12	-3.864819	0.263485	-0.837226
16			
191.619286 Kcal/mol 8.309409 eV -101.078316 H Child_6_61.log			
6	-1.322479	-3.371321	-0.286543
12	4.140618	0.974299	0.113970
6	-1.678469	-1.945426	-0.029151
6	0.930145	1.106535	0.673282
8	-5.176949	0.830605	0.096540
6	-0.381965	1.402712	0.744637
6	-2.723786	0.394277	0.288692
6	6.130741	0.725612	-0.288133
6	-2.383049	-0.895622	0.168486
6	2.060796	0.559469	0.547870
6	-0.296962	-2.498300	-0.080841
6	-1.587381	1.149952	0.633656
6	-4.041696	1.038974	-0.325119
6	5.533401	0.038335	-1.203614
12	1.529278	-1.470588	0.287651
8	-3.507367	1.634932	-1.331387
16			
191.857867 Kcal/mol 8.319755 eV -101.077935 H Child_10_27.log			
6	-2.053099	-2.265730	0.162789
8	1.183591	2.208110	0.376901
6	-0.802899	-2.117644	0.116942
6	2.302148	1.677452	0.222851
6	0.505268	-1.492081	0.073488

12	-0.675375	1.699671	0.199296
12	-3.941918	-1.381465	0.181336
6	3.388505	1.087283	0.055018
6	1.853966	-1.720203	-0.118086
6	-2.578415	2.284897	-0.479290
6	-0.245885	-0.396924	0.264905
6	4.590184	0.463714	-0.169474
6	3.062596	-1.542871	-0.215989
6	-3.534966	1.392219	-0.364597
6	-4.537346	0.527880	-0.393674
8	4.279804	-1.108914	-0.314010
16			
192.003894 Kcal/mol 8.326087 eV -101.077703 H MutD_14_66.log			
12	-3.969401	-0.563997	0.297628
6	1.466485	-1.226998	-0.803448
6	-7.508875	1.687697	-0.269959
6	7.424913	0.930457	0.074867
6	6.363400	0.363332	-0.464954
6	9.311046	2.182111	1.351897
8	-8.484310	2.381763	-0.493803
12	3.392342	-0.777310	-1.202725
6	5.314986	-0.159428	-0.921683
6	-0.806992	-1.673833	0.424248
6	-2.145339	-1.435572	0.601539
6	8.353994	1.549783	0.691847
6	0.362000	-1.442488	-0.264792
6	-6.784207	0.713786	0.195970
8	-5.579218	0.246329	0.225026
6	-1.445923	-2.310358	1.553032
16			
192.386490 Kcal/mol 8.342678 eV -101.077093 H Child_5_16.log			
12	-2.186770	-0.542018	0.112854
6	4.977163	1.447993	-0.577847
6	-4.178313	-0.492918	-0.716525
6	3.496811	1.478574	-0.326019
6	-5.319906	-0.406299	-1.485968
6	2.258361	1.785504	-0.133927
6	-5.314293	0.262645	-0.119323
6	4.354807	0.266907	-0.291182
6	-0.535348	-1.791641	0.238802
6	0.986072	1.826825	0.148702
6	-5.685827	0.985223	0.944828
8	4.141621	-0.973696	-0.065206
6	0.642570	-2.195951	0.355367
6	-0.207595	1.561188	0.433821
12	2.608898	-2.011869	0.255907
8	-1.380690	1.258490	0.659019
16			
192.930711 Kcal/mol 8.366278 eV -101.076226 H MutI_11_71.log			
8	0.984453	-1.875608	0.158642
6	-4.257730	0.794601	1.900342
6	-1.432978	-2.283607	-0.548024
6	-2.915347	-0.252280	-0.083112
6	0.465403	2.717132	-0.765167
6	-2.296676	-1.443360	-0.376274

6	-3.697441	0.175283	0.931558
6	2.958733	2.162642	-0.349248
6	2.194360	-1.494835	0.613628
6	3.318613	-1.149365	0.975974
6	-0.766928	2.863179	-0.679567
8	-0.464359	-3.131884	-0.888896
12	3.975584	0.749247	0.663469
12	-2.451778	1.815606	-0.337619
6	1.804432	2.482544	-0.668172
6	0.884489	-3.024983	-0.629966
16			
192.967658 Kcal/mol 8.367880 eV -101.076167 H Original3D_16_4.log			
8	1.927751	0.180908	0.689089
6	-0.893391	-0.158345	-0.809719
6	-1.144434	-1.123822	0.301139
6	-1.503937	0.779200	1.912793
6	1.532117	0.844129	1.673180
12	-3.720939	1.129126	-1.721923
6	0.839253	-2.556161	-0.265686
12	1.259190	-0.671656	-1.002958
6	-1.850304	0.055337	0.803152
6	0.148954	-3.644461	0.237793
6	2.731948	0.893741	-1.620443
6	0.895475	1.540583	2.486508
8	3.370140	1.818231	-1.799584
6	-0.426366	-2.290912	0.420083
6	-1.996443	0.730701	-0.566016
6	-0.473228	1.349551	2.357641
16			
193.184306 Kcal/mol 8.377275 eV -101.075822 H Child_2_26.log			
8	-4.416973	-2.944912	-0.708551
12	2.134598	2.805329	-0.057609
6	-3.887915	-1.975016	-0.327664
6	0.307540	2.177495	0.491052
6	1.715671	-4.259681	0.616270
6	4.152309	2.333612	-0.438790
8	-3.319738	-1.006220	0.064579
6	4.476072	1.118699	-0.488652
6	2.688168	-3.425868	0.364786
12	-2.784506	1.096923	0.415968
6	3.494767	-2.458846	0.112012
6	4.564876	-0.193073	-0.349139
6	4.143362	-1.374756	-0.162766
6	-0.806371	1.694515	0.744680
6	-4.809550	1.889013	0.410021
6	-4.423499	1.937576	-0.829896
16			
193.327966 Kcal/mol 8.383505 eV -101.075593 H Child_1_52.log			
6	-2.379557	-1.594697	0.059586
6	1.976955	1.119797	-1.689850
6	-1.549553	-2.504356	0.514574
6	2.623903	1.959236	-0.852648
6	-2.496121	-0.142875	-0.058872
6	2.345721	1.945688	0.475065
6	-0.744847	-1.151057	0.933318

6	3.568656	-2.061591	0.458055
6	-3.538883	0.618054	-0.340207
8	2.579790	-2.253845	-0.104971
6	-1.215313	0.193413	0.628935
6	1.987755	1.944734	1.699206
8	-4.424600	1.361160	-0.541064
6	1.346541	0.344005	-2.488609
12	0.265992	0.801917	1.921467
12	0.001252	-0.541969	-1.160053
16			
193.626809 Kcal/mol 8.396464 eV -101.075116 H Original3D_0_70.log			
6	0.170058	-0.899722	0.347661
6	0.614473	-2.310073	-0.061499
6	0.891103	0.081190	0.827835
6	-1.399773	-1.020009	0.149762
6	-2.354677	0.051484	0.063595
6	-1.924870	1.430027	0.013208
8	3.011955	-3.047241	-0.170859
6	-3.689812	-0.287331	0.066672
12	-4.393721	1.703267	-0.861553
6	-1.567633	2.640724	-0.051879
6	-1.601501	-2.361372	-0.078523
6	6.183045	1.840893	-0.037313
8	6.080895	2.652592	-0.842287
12	-0.008476	1.877064	1.129025
6	1.906231	-2.681484	-0.151818
6	-0.546051	-3.118791	-0.271785
16			
193.674235 Kcal/mol 8.398520 eV -101.075041 H Child_7_46.log			
6	-3.757271	1.683646	-0.203806
8	6.473906	0.371100	-0.128990
6	-2.479323	2.119942	0.015236
6	5.282522	0.308935	-0.101853
6	-4.837204	1.080926	-0.400993
6	0.675670	-1.775592	-0.207264
6	-1.251992	2.208728	0.188373
6	3.990432	0.193840	-0.094553
12	0.451783	1.072662	0.374796
6	1.925719	-1.671674	-0.357132
12	-4.524419	-0.914578	-0.335362
6	2.611605	0.679177	0.145950
6	2.803991	-0.637400	-0.205706
8	-1.673806	-1.531816	0.264320
6	-2.810595	-1.884673	0.736812
6	-0.408417	-1.074401	0.225630
16			
194.034157 Kcal/mol 8.414128 eV -101.074467 H MutD_17_52.log			
6	-7.784084	-1.292401	0.167730
6	2.862740	0.744769	0.613218
6	1.265797	-3.486101	0.346671
6	-1.260874	0.582556	-0.805871
8	-0.431870	-1.816909	-0.486747
6	0.138424	3.790542	0.058484
6	2.735795	-3.042467	0.055516
6	2.101736	-1.692598	0.003729

6	2.541706	-0.434849	0.414926
8	-6.824178	-1.001260	0.734786
12	-1.342084	2.568092	-0.570768
6	3.910755	-3.606969	-0.126836
6	1.214943	4.449455	0.216799
12	2.282463	2.699879	0.370356
6	-0.772981	-0.540860	-0.633969
6	0.840013	-2.249459	-0.240292
16			
194.881829 Kcal/mol 8.450887 eV -101.073116 H Child_13_14.log			
6	4.951445	2.480558	-0.000077
12	-3.176049	-2.795898	0.169336
8	6.580125	-0.613997	0.221199
6	-1.724840	-1.267442	0.127055
6	3.732081	2.086195	0.040634
6	-6.257038	2.516821	0.023983
6	5.475816	-0.929883	0.013909
8	-5.654915	1.533087	-0.086350
6	4.268740	-1.339345	-0.231983
12	-4.511640	-0.330647	-0.100530
6	2.508432	1.627010	0.040757
6	-2.430441	-0.081846	-0.005725
6	3.071311	-1.768103	-0.462579
6	-0.966296	-0.023457	0.052442
6	1.334105	1.146478	0.042448
6	0.178449	0.580651	0.041724
16			
195.109064 Kcal/mol 8.460740 eV -101.072754 H Child_1_31.log			
12	1.107662	-2.874546	0.141172
8	4.214628	2.898334	-0.713356
6	-2.772996	-2.946752	-1.078530
6	3.610307	1.928858	-0.408745
6	-2.052672	-2.130537	-0.379555
6	-5.821846	1.767787	0.174970
6	2.623783	-1.640811	-0.333852
8	-6.451067	2.047295	-0.711868
6	-0.155194	-1.317689	0.755713
6	2.860665	0.836020	-0.144229
6	0.561111	1.954493	0.502559
6	3.262256	-0.431224	-0.438736
6	-1.371094	-1.170905	0.229141
6	1.442077	0.923199	0.410058
6	0.856861	-0.436048	0.614811
12	-1.138331	0.909264	0.857174
16			
195.109701 Kcal/mol 8.460768 eV -101.072753 H Child_5_11.log			
6	1.132727	3.968522	0.462104
6	-4.194059	-0.341396	-0.084886
6	1.817992	2.725137	0.240698
12	-2.097457	-1.176407	0.118528
6	0.427133	2.617262	0.331120
6	-3.432622	0.671808	-0.196697
6	2.332897	1.481128	-0.210299
8	-0.908865	-2.555550	0.262454
6	0.038564	1.315583	-0.086913

6	0.319171	-2.929339	0.221134
6	2.580362	0.147242	-0.332116
6	-2.410949	1.627733	-0.302180
6	1.173759	0.599701	-0.432989
6	1.516614	-3.293934	0.169615
12	2.896520	-1.926936	-0.117527
8	-1.265923	0.768479	-0.097900
16			
195.366552 Kcal/mol 8.471906 eV -101.072344 H Child_10_33.log			
6	4.106143	0.364376	1.079327
8	-1.687950	0.015616	2.583062
6	3.326654	1.105431	0.411369
6	-1.202426	-0.524840	1.706010
12	2.983307	-1.350196	0.269433
8	-2.560716	2.111872	0.527939
6	2.271738	1.318030	-0.455789
6	-3.229254	2.904098	0.025531
6	1.268013	1.918838	-1.135486
12	0.071536	-1.679901	0.105315
6	1.688085	-0.031311	-1.092030
6	-3.742413	-2.172591	-0.356605
6	0.479314	0.501952	-1.400959
6	-2.823305	-1.457527	-0.876407
6	-1.816339	-0.681847	-1.288863
6	-0.771008	-0.021067	-1.513595
16			
195.835349 Kcal/mol 8.492235 eV -101.071597 H MutI_11_65.log			
6	2.725125	-0.384741	0.198216
8	4.110797	0.090768	0.236888
12	-0.039925	1.403730	0.569143
6	2.436717	-1.870899	-0.001304
6	1.804913	0.573221	-0.232072
6	-2.568797	-0.408179	0.246723
6	1.885334	1.972853	-0.549730
6	-6.457125	-0.041968	-0.059261
6	4.127425	1.339683	-0.037967
8	3.195806	-2.798094	0.292426
6	-3.922181	-0.351026	0.187483
6	-7.545624	0.593963	-0.242757
6	-1.248570	-0.373884	0.180335
6	3.412925	2.385421	-0.227288
12	0.405270	-1.216089	-0.720041
6	-5.122970	-0.199956	0.133667
16			
196.413098 Kcal/mol 8.517289 eV -101.070676 H Child_2_25.log			
6	-1.340286	-2.174879	-0.000000
8	-1.186362	3.089130	-0.000000
6	-2.670741	-2.200821	-0.000000
6	6.485653	1.213007	0.000000
6	-3.935708	-2.062190	-0.000000
6	-3.399007	1.772237	-0.000000
6	-0.212728	-1.531927	-0.000000
6	5.356716	0.577698	0.000000
12	1.902793	-2.362256	0.000000
6	-2.357847	2.436108	-0.000000

6	0.000000	-0.167333	-0.000000
6	4.197127	0.027992	0.000000
12	-4.299198	-0.023885	-0.000000
6	0.068183	2.458230	0.000000
6	-0.039652	1.075269	0.000000
8	3.167187	-0.577462	0.000000
16			
196.685063 Kcal/mol 8.529082 eV -101.070243 H Original3D_6_7.log			
6	0.939213	-1.407305	-0.349251
6	0.402975	-0.222800	0.174062
12	-1.332486	2.244827	0.407701
6	-2.344061	-2.262547	-0.113548
6	-3.360552	2.555227	0.066396
6	0.085325	0.793506	0.878495
6	-3.566871	0.001851	-0.406320
6	0.143503	-2.384578	-1.032729
8	-1.156956	-2.237125	-0.728950
6	4.101060	1.988317	-2.212366
12	1.899510	0.065608	2.047455
8	4.030748	1.505301	-1.173652
6	3.074680	-1.347184	1.152463
6	-3.105540	-1.142249	-0.526373
6	2.265276	-1.563869	0.206167
6	-3.600777	1.346525	-0.210506
16			
196.792736 Kcal/mol 8.533751 eV -101.070071 H Child_1_63.log			
6	2.884567	-3.597813	0.140931
8	1.022322	3.334287	-0.062733
6	2.177654	-2.507348	0.068878
6	1.455469	2.185339	-0.071178
8	2.939014	0.473776	0.081066
6	-3.799085	-0.272916	0.054527
6	1.289610	-1.498501	0.016076
6	-2.772083	-0.269255	-0.984536
12	-0.841911	-1.855151	0.266314
6	-0.720037	0.755915	-0.389970
6	1.546150	-0.124597	-0.146333
6	2.968303	1.789628	0.131335
6	-2.932625	-1.378655	-0.033205
6	-1.625297	0.347047	-1.289792
6	0.680016	0.928824	-0.260108
12	-2.375300	1.137608	1.103151
16			
197.510601 Kcal/mol 8.564881 eV -101.068927 H Original3D_16_3.log			
6	-0.392588	-1.202188	1.296378
6	0.048213	-1.046752	-0.092129
6	0.669744	-0.729173	1.970100
6	0.297168	-2.753822	-0.709105
6	-0.657908	-1.946927	-1.215957
6	2.064580	0.120654	0.433695
12	-0.588134	1.081264	-1.429145
6	-1.891124	1.816981	0.423857
6	-1.452354	-0.858194	-1.243681
8	-0.631140	2.161888	0.244888
6	1.139323	-0.268384	-0.593082

6	1.785023	-0.114372	1.820753
6	-3.087680	1.445407	0.291844
6	3.249459	0.564715	-0.075187
8	4.242672	0.817822	-0.603673
12	-2.705482	-0.581710	0.514592
16			
198.087454 Kcal/mol 8.589896 eV -101.068008 H MutD_13_64.log			
6	-2.107510	2.183394	-0.107300
6	-1.181096	-3.131064	-0.466836
6	-0.026099	-2.407040	-0.144644
6	-1.149909	-1.667605	-0.064985
6	1.289918	3.155418	-0.053850
6	0.044892	3.668832	-0.117031
6	-1.074392	2.922896	-0.118454
8	-5.590256	-0.664554	0.299482
6	2.123651	-1.398035	0.013720
6	-4.474318	-0.462997	0.200606
6	2.429569	2.608351	0.013370
6	4.732878	-1.268938	0.232079
8	1.340275	-2.506400	-0.031408
12	-2.197084	0.135152	-0.025456
6	3.475861	-1.543959	0.181768
12	2.988681	0.649191	0.062519
16			
198.983713 Kcal/mol 8.628761 eV -101.066580 H Child_5_34.log			
12	-0.080872	2.716148	0.019136
6	0.192220	-1.627915	0.118436
6	1.762075	1.458179	-0.017382
6	1.493185	-1.974210	0.119803
8	-1.591441	1.637478	0.065759
6	2.731505	-2.180295	0.071042
12	3.747498	0.808601	-0.090481
6	-5.079548	-0.862440	-0.102870
6	0.806099	0.614219	0.001069
6	3.951527	-1.575794	-0.027338
6	-1.588319	0.267366	0.053985
8	-3.885516	-0.544914	0.413776
6	-6.291907	-1.048853	-0.447095
6	-0.251314	-0.326194	0.054598
6	4.991680	-0.861050	-0.182378
6	-2.747846	-0.389262	-0.138561
16			
199.125634 Kcal/mol 8.634916 eV -101.066353 H MutD_18_46.log			
8	2.635399	2.878582	-0.380602
6	10.412502	-2.349293	-0.040817
12	-5.101316	-0.269101	0.440599
6	8.085728	-1.214602	-0.050538
6	9.252198	-1.779126	-0.054492
6	6.939741	-0.672292	-0.043982
6	-1.917676	0.828338	0.357015
6	5.771108	-0.146705	-0.037238
6	1.572760	2.396093	-0.204737
6	-3.041122	0.302879	0.576968
8	4.691946	0.328554	-0.028651
6	-0.731535	1.364685	0.161974

12	-7.857841	-0.892092	0.062184
6	0.406111	1.874907	-0.021355
6	-9.775118	-1.334351	-0.192586
6	-10.826175	-1.224329	-0.910108
16			
199.316690 Kcal/mol 8.643201 eV -101.066049 H Child_13_29.log			
6	-1.619388	-0.781072	1.530100
6	4.784355	-0.791055	-1.302746
12	-3.073543	0.188767	0.450240
6	5.235554	0.262586	-0.774985
6	-4.856412	0.755211	-0.548801
12	3.147802	-2.028539	-1.190556
6	-0.988106	-1.340749	2.727337
6	5.539804	1.404737	-0.195338
6	-6.152349	0.955148	-0.723123
6	5.615558	2.497786	0.475173
6	1.375743	-2.279679	-0.298999
8	-3.735993	0.978473	-1.253057
6	0.478451	-1.973920	0.498327
6	5.657481	3.673865	1.109221
6	-0.469539	-1.516931	1.382799
8	-7.326258	1.131741	-0.545693
16			
199.401125 Kcal/mol 8.646862 eV -101.065914 H Child_17_13.log			
6	-1.366429	-2.806327	0.284435
8	4.162532	0.655578	-1.195868
6	-2.314240	-2.040741	0.110479
6	1.510680	2.979581	1.688578
8	-3.299020	-1.153516	-0.074958
6	2.023632	2.113623	0.858738
6	-4.253344	2.469682	-0.520762
6	3.182376	0.283313	-0.528308
6	-3.502989	1.419572	-0.347810
6	2.120208	1.192115	-0.109057
6	-2.908583	0.152534	-0.186698
6	2.836525	-1.063155	-0.173647
12	0.583945	-3.220285	0.373241
6	2.281086	-2.125606	0.129944
6	-1.897384	0.989147	-0.188871
12	-0.015389	1.770374	-0.034534
16			
199.628621 Kcal/mol 8.656727 eV -101.065552 H Original3D_5_4.log			
6	-2.135655	1.586112	0.130918
6	-0.693166	1.029663	0.405724
12	1.266121	1.819216	0.008011
6	5.683136	-1.192213	-0.077173
6	-3.086851	0.436467	0.059885
6	-2.353569	-2.071522	0.367204
6	-2.079262	2.897144	-0.030160
6	-1.026592	-1.660613	0.163180
6	-0.957251	-0.273000	0.739419
6	5.044910	-0.093247	-0.188260
8	-4.286402	0.209403	-0.427568
6	3.261142	1.790561	-0.309455
12	-4.346649	-1.846074	-0.541205

6	4.161368	0.885190	-0.306690
6	-2.370272	-0.621209	0.619320
8	6.321240	-2.204115	0.046923
16			
199.725064 Kcal/mol 8.660909 eV -101.065398 H Child_4_9.log			
6	-2.713160	0.092402	0.145051
12	3.661796	2.555894	-0.082718
6	-7.254539	2.308070	-0.701760
8	5.776586	-1.067422	-1.072131
8	-1.827263	-5.354331	0.447334
6	4.844942	-0.444040	-0.663829
6	-3.907908	0.391802	-0.145734
6	3.920794	0.363197	-0.237097
6	-6.192080	1.538499	-0.611933
6	2.604990	0.244708	0.222129
12	-0.725046	0.043028	0.656571
6	1.846405	1.476993	0.809257
6	1.407103	-0.350999	0.260679
6	-5.074606	0.935654	-0.427961
6	0.684619	1.512003	1.375248
6	-1.305825	-4.703792	-0.338694
16			
199.821963 Kcal/mol 8.665111 eV -101.065244 H MutI_6_75.log			
6	1.732127	-0.839674	0.246515
6	3.526181	1.958638	0.083724
8	-2.127037	-0.544222	0.607589
6	0.776647	0.251741	0.146349
12	-3.259345	0.848173	0.047669
6	0.385462	-1.092416	0.191079
6	-2.767613	2.905952	-0.341144
8	-1.899645	-1.865021	0.032907
6	-0.181923	2.529955	-0.224028
6	0.190747	-4.624160	-0.472667
12	3.682832	-0.084836	-0.000837
6	-1.500318	2.553579	-0.262059
6	0.864703	1.644525	-0.040133
6	2.277809	1.980109	-0.036238
6	-0.202368	-3.424281	-0.252801
6	-0.579518	-2.158317	0.013746
16			
199.885747 Kcal/mol 8.667877 eV -101.065142 H MutD_17_38.log			
12	5.927881	-0.059476	0.242226
6	1.332152	-0.925571	-0.010607
6	-7.035918	0.358525	0.588714
12	8.686108	0.607221	-0.091015
6	-9.476795	0.655674	-0.092357
6	-1.160826	-1.389803	-0.315439
8	-2.315118	-1.618137	-0.438363
6	-10.716948	0.826245	-0.423875
6	10.611869	1.091712	-0.147077
6	-11.954662	0.956642	-0.770686
6	0.100180	-1.145423	-0.179952
6	-8.260554	0.514473	0.238192
6	3.839950	-0.509864	0.412879
6	11.845098	1.027238	-0.410179

8	-5.909618	0.227140	0.906773
6	2.614789	-0.700674	0.183417
16			
200.803854 Kcal/mol 8.707690 eV -101.063679 H MutI_17_35.log			
6	4.574452	0.242524	-0.372841
6	1.009851	1.588404	-0.223369
12	-3.193259	-0.563530	-1.630741
6	3.418066	0.790072	-0.444964
6	-0.193918	1.903013	0.048787
6	2.229176	1.249552	-0.445989
8	-2.472748	2.511120	0.766889
6	-1.384319	2.194244	0.434337
6	6.813596	-0.990136	-0.111522
6	-5.389598	-1.321973	-1.653319
8	-0.805825	-1.431592	1.926287
12	-4.758789	-0.918210	0.543300
6	-2.685223	-0.908049	0.350004
6	7.900297	-1.677446	0.049873
6	-1.709620	-1.195162	1.164350
6	5.692768	-0.350936	-0.211367
16			
201.158122 Kcal/mol 8.723053 eV -101.063114 H Child_2_31.log			
6	-0.071853	-2.439425	0.119368
8	-2.861007	3.452685	0.567919
6	0.507332	-2.750270	1.542095
6	-2.865584	2.330419	0.236693
6	1.056050	-1.621871	-0.051177
6	-2.715607	1.003020	-0.097351
6	2.074472	0.418772	-1.234346
6	-3.644572	0.019363	-0.572160
6	0.817162	-1.348298	1.384359
6	-1.384704	0.716038	0.140829
6	1.745595	-0.745690	-0.872106
12	0.642417	0.758204	0.595748
6	6.667968	1.128461	-0.819972
6	-4.007066	-1.115129	-0.959032
8	6.165062	1.094142	0.212913
12	-1.934717	-1.587117	-0.524903
16			
201.359034 Kcal/mol 8.731765 eV -101.062794 H Child_2_56.log			
6	7.651983	-0.707096	0.226455
6	-3.430791	-2.194664	0.294039
8	1.921224	2.221585	-0.984425
12	-4.090883	-0.282289	0.776221
8	6.738789	-0.751053	0.854718
6	-2.351431	-1.968991	-0.299806
6	1.024692	1.618794	-0.394265
6	-1.250015	-1.224740	-0.802895
6	-2.398368	0.891483	-0.574823
6	0.165156	-1.288082	-0.349675
6	-1.559991	0.055034	-1.167923
6	-2.910998	1.488702	0.481246
6	1.145025	0.101277	-0.270080
6	0.581833	-0.612195	0.872806
6	1.457524	-1.071457	-1.055873

12	-0.744769	1.757902	0.830647
16			
202.520350 Kcal/mol 8.782125 eV -101.060944 H Child_6_22.log			
6	4.263805	-0.504380	-0.294250
6	-4.369598	-1.650946	0.129331
6	4.069026	0.710277	-0.052867
8	-3.906958	0.861474	-0.240063
6	3.368577	1.830889	0.140780
6	-3.972756	-0.412043	-0.029302
6	3.531163	-1.595735	-0.393486
12	-2.432267	1.915140	-0.302004
6	2.160776	1.774433	0.252794
6	-2.833220	-1.479463	0.199195
6	2.535785	-2.406455	-0.410869
6	-1.582433	-1.590351	0.270291
6	0.880454	1.413169	0.248819
6	-0.373577	1.997605	-0.227948
12	0.412115	-1.536949	-0.007089
8	1.178684	0.005991	0.829337
16			
203.344829 Kcal/mol 8.817877 eV -101.059630 H Original3D_2_5.log			
6	-1.809398	-1.110795	-0.281237
8	-5.465642	0.736451	-0.379148
6	-4.864771	1.061246	0.552542
6	-1.399182	0.235188	0.091641
8	-3.176235	-1.840447	-0.040431
6	-1.035356	1.533215	-0.150730
12	1.972312	2.149540	0.042716
6	2.017616	-1.105310	0.820382
6	-2.551401	-1.976301	-1.245915
12	4.246896	0.462246	-0.831018
6	-0.174037	2.408426	-0.251238
6	1.584592	0.231618	1.151539
6	0.657668	-0.813197	0.952077
6	-0.704912	-0.814999	0.609279
6	4.193585	-1.742475	-0.426010
6	3.169682	-1.658193	0.313712
16			
203.387923 Kcal/mol 8.819746 eV -101.059561 H MutD_6_72.log			
12	-3.755164	0.618973	0.272403
6	2.743304	0.049337	0.056232
6	-3.568875	-2.000608	-0.141679
6	5.990783	-1.448731	0.477940
8	1.382168	1.961442	-0.141210
6	-2.329560	-2.590442	-0.079130
8	3.732805	-0.513684	-0.481106
6	4.859899	-1.009721	0.067921
6	-4.494057	-1.149080	-0.325506
6	1.535716	0.610031	-0.069153
6	-1.871295	1.494396	0.306719
6	0.267128	-0.128916	0.065234
6	-0.005742	-1.468833	0.006392
6	-1.157147	-2.127022	0.019298
6	-0.854151	0.729522	0.211850
12	-0.212819	2.935889	-0.155584

16

204.183703 Kcal/mol 8.854255 eV -101.058293 H Child_3_57.log

6	4.140878	-1.627359	0.067316
12	-8.054423	-2.954199	-0.921940
6	4.683624	-2.774585	0.159408
6	0.422712	3.430612	-0.608599
6	3.168973	-0.728592	-0.002065
6	-2.413880	1.310263	0.633014
6	1.766309	-0.369205	0.089870
6	-3.538642	0.960632	1.134385
6	0.529749	-0.059673	0.685102
6	-4.635478	0.502448	1.685533
6	2.718639	0.559699	-0.399475
6	-1.221278	1.538731	0.117273
8	5.262842	-3.828653	0.202527
6	-0.508312	2.690850	-0.244199
8	-0.364333	0.370777	-0.230213
12	2.232104	2.542539	-0.718384

16

204.202345 Kcal/mol 8.855063 eV -101.058263 H Original3D_0_53.log

6	-1.930028	0.585617	-0.207782
6	-0.314957	-0.795293	-1.019211
8	0.786896	-1.143495	-1.625225
6	-2.311562	-0.729688	0.260422
6	-1.304962	-2.979226	-0.103477
6	3.689048	1.925338	0.507100
8	3.822346	-2.245608	1.353958
12	-4.056052	-0.031814	1.187411
12	1.227728	0.903990	-1.558164
6	-0.747116	0.575619	-0.994658
6	-1.295768	-1.654491	-0.256460
6	-2.849141	1.605774	0.205608
6	2.817109	1.654478	-0.400790
6	-3.897542	2.064299	0.722408
6	4.570933	2.022229	1.493477
6	3.084978	-1.500204	0.896558

16

204.237734 Kcal/mol 8.856598 eV -101.058207 H MutD_11_66.log

6	-3.404607	-1.380098	0.105447
6	-2.957602	-0.224935	0.100422
6	5.829157	0.472504	0.808919
6	-2.169394	0.965057	0.071038
8	-0.817225	0.792560	0.170648
6	-2.719179	2.169467	-0.089152
6	7.469582	-0.011520	-1.158230
6	-0.686113	-3.838473	-0.257906
6	-0.069854	-2.748117	-0.103915
6	1.806215	0.922264	0.414707
12	-2.606024	-3.234306	-0.087003
6	6.652613	0.249929	-0.174119
12	0.227045	-0.755212	0.216436
6	-3.268297	3.316627	-0.290307
6	-3.804247	4.483551	-0.519034
8	2.376987	1.909525	0.454301

16

204.357522 Kcal/mol 8.861792 eV -101.058016 H Child_9_49.log

6	-5.450064	-0.813088	0.557170
6	7.889877	-0.964171	0.404272
6	-4.333701	0.027800	0.279360
6	6.668074	-0.592784	0.239149
8	-3.652027	1.230955	0.205371
6	5.406843	-0.232263	0.086348
6	-4.070898	-1.278624	0.161754
6	4.206786	0.096133	-0.044617
6	-2.330141	1.136478	-0.050512
6	2.908068	0.375167	-0.148982
6	-1.858518	-2.577179	-0.379530
6	1.709442	0.643669	-0.243363
6	-2.983637	-2.092513	-0.108539
8	0.400098	0.807552	-0.249327
12	-1.009846	-0.621689	-0.309317
12	-0.703267	2.398372	-0.037634

16

204.475422 Kcal/mol 8.866905 eV -101.057828 H MutD_18_36.log

6	-5.103198	-0.198066	0.801610
8	-1.934247	-1.754572	-0.184170
12	1.769727	1.959026	0.184997
6	-5.197344	-0.035480	-0.461688
6	0.509854	-2.141627	-0.325286
6	3.005181	-1.560858	-0.087575
8	3.350673	0.920223	0.402432
6	-1.306137	1.137639	0.286642
6	-0.744466	-1.975073	-0.262013
6	4.464553	-1.435346	0.081931
6	3.684426	-0.290453	0.221316
12	-3.062940	-0.089632	0.181898
6	-0.184058	1.268664	0.955331
6	0.334010	2.633611	-1.273208
6	-0.559262	1.967822	-0.693409
6	1.794299	-1.997155	-0.268457

16

204.830424 Kcal/mol 8.882299 eV -101.057262 H Child_1_60.log

6	1.642187	2.405936	0.039720
6	-4.710647	0.249106	-0.356633
6	2.813315	1.929735	0.177063
6	-5.620516	0.009545	-1.227465
6	3.967886	1.253447	0.211947
6	-3.505725	0.366529	0.220211
12	-0.242633	1.526922	-0.272766
6	-0.482331	-1.414840	0.403361
6	4.138540	-0.046071	-0.035738
6	-2.210222	1.079304	0.271474
6	4.206866	-1.270643	-0.443032
6	0.065544	-2.439877	-0.237912
6	-2.367695	-0.134629	0.855783
8	-1.528508	-1.180154	1.266454
12	2.092656	-1.501875	-0.448472
8	0.300572	-0.348074	-0.093682

16

204.928454 Kcal/mol 8.886550 eV -101.057106 H MutI_14_69.log

6	-3.352757	-0.270196	0.267663
12	-1.627793	2.404072	0.635508
6	0.614949	-2.370480	-0.306890
6	3.097327	1.008979	-0.223281
12	-0.900716	-0.919899	-0.432807
6	-2.723108	0.785023	0.462422
6	0.555465	1.248010	-0.275473
6	-0.004075	3.170665	-0.315083
6	1.257308	2.950827	-0.451343
6	2.914709	-2.211393	0.541288
8	-2.452723	-2.167191	-0.459290
6	3.784339	-1.330528	0.516102
6	1.666444	-2.677200	0.288271
6	1.862205	1.616372	-0.385625
6	3.670623	-0.044603	0.078693
8	-3.762087	-1.465675	0.007680
16			
204.959935 Kcal/mol 8.887915 eV -101.057056 H MutI_16_55.log			
6	-5.542031	3.827036	0.243608
6	4.573134	0.812894	-0.126936
8	-2.544221	1.589496	0.223972
6	-3.406061	2.394804	0.221078
6	-3.889424	-4.711606	-0.221011
6	0.644356	-0.077532	-0.149581
6	-0.182118	-1.076428	-0.247541
6	-1.987813	-2.928127	-0.142055
6	-2.940215	-3.838273	-0.191944
6	5.399998	0.319739	0.986577
6	-1.114898	-2.006015	-0.094509
12	3.148014	1.026282	-1.564283
12	2.032880	-0.554937	1.326489
6	3.974298	0.031756	0.888818
6	-4.405533	3.225490	0.223838
8	1.430110	0.723185	-0.910037
16			
204.974227 Kcal/mol 8.888535 eV -101.057033 H Child_2_42.log			
6	0.601903	-2.167363	0.267148
12	-4.946897	1.810165	0.430951
6	-0.580646	-2.211889	-0.072127
6	5.138399	0.548693	-0.140483
8	-3.632389	0.462838	0.632493
6	4.421710	1.790720	0.643983
6	-2.903171	-1.496128	-0.418389
6	-1.531400	0.577102	-0.460116
12	2.500478	-1.574804	0.551855
6	-0.442990	1.077777	-0.718488
8	-1.839456	-2.372176	-0.505136
6	0.847408	1.449967	-0.779191
6	-2.648671	-0.156608	-0.020788
6	3.302837	1.246268	-0.037237
6	2.066301	1.512550	-0.570822
6	3.916952	-0.096027	0.171090
16			
204.995359 Kcal/mol 8.889451 eV -101.056999 H Child_10_42.log			
6	3.849984	1.410585	0.198658

6	-2.855111	-1.248173	0.709138
6	2.578578	1.951563	0.291466
6	-4.135896	-1.218499	1.042089
8	4.773648	-0.953006	0.050349
6	-1.884060	-0.845209	-0.093066
8	3.644824	0.093172	0.341632
6	-4.820644	-0.298227	0.447433
6	1.361747	2.179902	0.151816
6	-2.171763	0.704111	-0.355504
6	0.045937	1.991648	0.024835
12	0.094472	-1.571675	-0.534929
6	-1.106544	1.556450	-0.149566
6	-4.697253	0.530927	-0.598517
12	2.946458	-1.707742	-0.228278
6	-3.471464	0.990200	-0.665010
16			
205.126131 Kcal/mol 8.895122 eV -101.056791 H Child_2_41.log			
6	1.938902	-0.566643	-1.819051
6	-3.232943	-0.301094	2.417456
6	2.643193	-1.482819	-0.883196
8	-4.315390	1.024759	-0.801561
12	-0.106181	0.173945	-1.008546
6	-3.236153	0.862345	-1.086306
6	2.764287	-0.095063	-0.729866
8	-2.089163	0.679552	-1.454595
12	1.427841	-2.501682	0.480245
6	-2.271240	-0.810825	1.767047
6	2.444209	0.917522	0.168601
6	2.727510	3.244633	1.600382
6	1.206549	1.384039	0.356072
6	-1.255685	-1.291071	1.075762
6	-0.297724	-1.649102	0.313479
6	2.465176	2.171139	0.884429
16			
205.262575 Kcal/mol 8.901039 eV -101.056574 H Child_3_15.log			
6	1.691196	3.611195	-0.076779
6	0.891792	-3.141854	-0.038189
6	0.548856	2.705153	-0.109641
6	-0.296570	-2.758450	-0.170943
8	-0.792364	2.619561	-0.282747
12	2.722925	-2.307118	0.138346
6	1.740952	2.128959	0.125193
12	-1.796225	-1.383570	-0.178263
6	2.489055	-0.184165	1.096552
8	-6.193350	-0.743632	-0.214452
6	-2.313807	0.610406	0.138497
6	-6.004401	0.153648	0.485205
6	3.496650	0.239642	-0.420648
6	-1.417917	1.411976	-0.043725
6	4.144772	-0.842947	-0.598487
6	2.490309	0.946573	0.355733
16			
205.681974 Kcal/mol 8.919226 eV -101.055905 H Child_1_56.log			
6	1.920913	-1.042638	-1.779241
6	-1.375711	3.322746	-0.059832

12	0.977780	-2.444910	-0.447428
6	-1.244384	1.877350	-0.032186
8	-5.410734	-1.052392	0.018872
6	-0.096819	2.676046	-0.077941
8	-0.908994	-1.865850	-0.374972
6	-1.486092	0.542744	-0.036012
12	2.490025	-0.270340	1.668219
6	1.229469	2.264308	-0.124965
6	2.391610	-2.369276	1.201412
6	2.245188	1.592379	0.608854
6	-4.968381	-0.353770	0.826514
6	2.093744	0.182643	-1.553752
6	-1.231506	-0.663003	-0.199524
6	2.012663	1.291961	-0.740109
16			
206.317974 Kcal/mol 8.946805 eV -101.054892 H MutD_18_70.log			
6	-1.925224	2.343422	-0.035219
6	-0.581386	2.483759	0.012038
6	-3.106613	1.979878	-0.081496
8	-4.226874	0.097995	-0.213978
6	4.176445	-1.766534	-0.604165
6	4.431634	0.726203	0.205282
6	-4.136643	-1.123561	-0.493313
12	-2.714545	-2.352972	0.513282
6	2.892079	-1.592331	-0.438539
12	2.096361	0.955607	0.032924
6	0.448749	-1.823837	0.001566
8	5.569362	0.777860	0.328082
6	-0.690483	-2.271017	0.243159
6	0.662717	2.418364	0.059404
6	1.653903	-1.165005	-0.138345
6	-4.378795	1.417582	0.025076
16			
206.355333 Kcal/mol 8.948425 eV -101.054832 H Child_9_59.log			
8	1.222648	1.742600	-1.954224
6	0.796459	-1.820581	-0.212616
6	0.328985	1.242177	-1.443541
6	-0.428563	-2.051193	-0.150818
6	-7.896816	2.496185	0.435516
6	2.065889	-1.382068	-0.224122
6	-6.983008	1.531344	0.493070
6	-1.777010	-2.065348	-0.041852
6	-6.065449	0.639987	0.450374
6	3.148207	-0.817120	-0.162177
6	3.971586	1.381378	0.324328
6	-3.002611	-1.894230	0.077550
12	6.015807	1.295353	1.208508
6	4.224357	0.055020	0.069201
8	5.578281	-0.304969	0.080714
12	-4.740774	-0.911550	0.233042
16			
206.521823 Kcal/mol 8.955645 eV -101.054567 H Child_10_31.log			
6	1.061488	-1.733076	0.457556
6	0.199098	2.027104	0.091273
6	2.253771	-1.768846	0.149610

6	1.379335	2.353930	-0.131350
12	-0.473092	-0.591574	1.093584
12	3.287969	1.684884	-0.497750
6	-4.285675	-2.661753	-0.897217
6	-4.642559	1.008148	-0.373169
6	-0.977804	1.355484	0.466033
6	4.538456	-2.116882	-0.617025
6	-2.248320	1.491193	0.106878
6	-3.473207	0.648044	0.405002
6	-3.469636	1.820890	-0.582820
6	3.575503	-1.316163	-0.123810
8	3.724132	0.024876	0.096282
8	-3.379286	-2.495896	-0.203252

16

206.705540 Kcal/mol 8.963612 eV -101.054274 H Child_3_55.log

8	-3.153982	-2.290264	0.008633
8	1.462573	4.013981	0.047087
6	-1.932645	-2.678869	0.011957
6	1.411588	2.659091	0.015853
6	-0.729029	-2.924509	0.018649
6	2.395497	1.661953	0.005482
12	-3.818343	-0.532060	0.000270
6	3.034683	0.617439	-0.002226
6	0.616596	-2.864005	0.014820
6	0.080622	2.668072	-0.001843
6	1.819581	-2.592665	0.009669
6	3.517285	-0.672575	-0.012314
6	-3.924064	1.611168	-0.004188
6	4.479849	-1.752784	-0.040194
6	3.025716	-1.950792	-0.008397
12	-1.951890	2.492154	-0.041051

16

206.992995 Kcal/mol 8.976077 eV -101.053816 H Original3D_17_4.log

8	-0.369378	-0.758792	-1.149581
6	0.765567	-0.966390	-1.760075
6	0.793887	-0.245493	1.853304
6	2.412301	-2.245783	1.395611
6	1.783237	-1.256221	1.667513
6	-4.304080	3.165990	0.233568
6	-4.559816	1.942962	-0.331978
12	-1.240118	-0.886858	0.551031
12	2.773579	-1.774244	-0.525432
6	-4.485483	0.780648	-0.438547
6	4.759919	2.736994	-0.172659
8	4.603723	3.885126	-0.153097
6	1.880678	-1.091363	-2.343264
6	-3.350034	-1.486774	0.004902
6	-4.079402	-0.529376	-0.394730
6	-0.329489	0.348564	1.972060

16

207.209279 Kcal/mol 8.985456 eV -101.053471 H Original3D_7_6.log

6	-2.014539	0.308811	-0.052825
6	-2.786512	-0.136694	1.147627
6	3.346996	-0.843759	1.078361
6	0.976586	-0.013975	0.425757

6	1.208496	-2.008254	-0.252564
6	0.126274	-0.992914	-0.160495
12	0.779233	2.156434	0.054295
6	-2.405962	-0.802214	-1.251799
6	2.147255	-0.980135	0.487751
12	3.611874	1.393528	-0.358394
6	-3.492230	-0.177833	-1.694352
6	-1.229345	2.826871	-0.231971
6	-1.203008	-0.798122	-0.521398
8	1.413671	-3.079810	-0.768625
8	-2.753831	-0.774928	2.147268
6	-1.669344	1.657944	-0.204086
16			
207.593612 Kcal/mol 9.002122 eV -101.052859 H MutI_18_53.log			
6	2.628520	0.070484	-0.133593
8	-3.708732	-1.036647	2.545722
6	-0.876981	-1.373183	0.601202
12	0.556786	-2.469077	-1.621676
6	2.420473	-1.659337	-2.044643
12	-3.904896	0.965539	-0.171370
6	-0.314692	-0.325148	1.288448
6	1.933487	0.545245	0.778782
6	2.744511	-0.824345	-1.161973
6	-4.006552	3.486031	-2.188011
6	-3.729840	-0.555122	1.502924
6	0.706879	0.377868	1.351131
6	-0.948403	-2.294188	-0.243215
6	-4.052649	2.539095	-1.324575
8	6.342356	1.697398	1.187655
6	6.679968	2.138675	0.181781
16			
207.673996 Kcal/mol 9.005608 eV -101.052731 H Child_14_18.log			
6	5.079487	0.645606	0.206620
6	-5.952869	0.190024	0.629602
6	3.901271	-0.207170	0.227996
8	-4.833527	0.115328	0.345719
6	3.725488	1.154363	0.120579
8	-2.296243	1.595603	-0.265503
6	3.008996	-1.261879	0.181888
12	-2.784113	-0.244878	-0.183056
6	2.620379	1.959600	0.000189
6	-1.101630	2.045692	-0.233105
6	0.087496	2.357474	-0.184225
6	1.954686	-1.913637	0.826603
6	-2.004645	-2.214467	-0.453870
6	2.115795	-1.937724	-0.653484
6	1.429002	2.274729	-0.100178
12	0.105565	-2.442050	-0.154727
16			
207.743323 Kcal/mol 9.008614 eV -101.052620 H Child_4_18.log			
6	0.293005	1.287585	-0.077368
6	-2.080686	1.403880	0.312753
12	-0.505794	3.016563	0.841686
6	-1.045296	0.597308	-0.302538
6	-10.287099	-2.000507	0.248044

6	4.698317	-1.248818	-0.331064
8	-9.902678	-1.469101	-0.694700
8	-1.136775	-0.489973	-0.888480
6	1.435364	0.685238	-0.277318
12	4.230493	-0.044850	-1.930965
6	-2.531182	2.487837	0.768698
6	3.297736	-1.735100	1.252717
6	2.561703	-2.299570	2.167733
6	4.978599	-1.729205	0.983753
6	2.571731	0.103164	-0.541288
6	3.377679	-0.883138	0.085342
16			
208.034187 Kcal/mol 9.021228 eV -101.052157 H Child_14_27.log			
12	-3.833274	-2.386720	0.596889
6	7.476930	-0.444028	2.325029
6	-5.176566	-0.885575	0.927712
6	6.641197	0.082852	1.497028
6	-1.992730	-2.834503	-0.073604
6	5.776063	0.611072	0.638902
6	-0.966920	-2.516291	-0.713836
6	4.952151	1.089435	-0.154912
6	-5.226864	0.372244	0.804246
8	4.030960	1.502878	-0.993641
6	-5.123349	1.677483	0.643230
6	3.013940	0.683755	-1.319547
6	-4.653468	2.782912	0.213631
6	2.061740	-0.048689	-1.576857
12	0.601699	-1.465165	-1.416072
8	-4.270188	3.846950	-0.185851
16			
208.051257 Kcal/mol 9.021968 eV -101.052130 H Child_18_11.log			
6	6.704666	-1.332108	0.065654
12	-4.068940	-0.757764	-0.384576
6	5.448015	-1.062562	-0.070765
6	-2.938481	0.913735	-0.465569
6	4.226756	-0.620866	-0.291667
6	-3.897071	-2.916578	0.005607
6	2.974716	-0.384768	-0.425485
6	-1.902395	1.503217	-0.142315
8	1.791738	-0.031841	-0.543859
6	-0.165537	4.499397	-0.304921
12	0.120717	-0.627129	0.372330
6	-2.607531	-2.579978	0.173167
6	-0.285002	3.308811	0.104561
6	-1.430318	-2.065932	0.326212
6	-0.636596	2.017985	0.335308
8	0.012180	1.148917	1.079889
16			
209.114528 Kcal/mol 9.068076 eV -101.050435 H Child_11_50.log			
8	-5.053571	0.948040	0.490559
6	5.170559	-3.643064	-0.070679
6	-3.763930	0.854877	0.120841
6	4.084339	-2.746898	0.170612
6	-2.849757	1.772675	-0.210475
6	5.259275	-2.787220	0.995778

12	-5.270057	-0.963834	0.726182
6	2.870217	-2.233362	-0.129140
6	-1.636967	1.926406	-0.680064
6	5.747126	4.774042	-0.071940
6	-3.173063	-0.528169	0.062283
6	1.762741	-1.752656	-0.417294
6	-0.584142	1.289624	-1.018418
8	4.908556	4.765830	0.716342
6	-2.067983	-1.088331	-0.241885
12	-0.042474	-0.764374	-0.785592
16			
209.456528 Kcal/mol 9.082906 eV -101.049890 H Original3D_5_5.log			
6	2.371509	-0.076360	1.073230
6	0.285343	-1.695871	-1.101340
8	3.678361	-1.331841	-0.583660
6	2.611182	-0.897400	-0.129500
12	-3.370264	-0.027217	-0.232745
6	1.354365	-1.227380	-0.747750
8	-0.943940	-1.996714	-1.465837
12	-0.395692	-0.679850	1.876708
6	-2.450765	1.787976	-0.009021
6	-1.338277	2.380156	-0.176620
6	1.516959	0.145100	1.958915
6	2.389606	2.694057	-0.867682
6	-1.944611	-1.401969	0.793753
6	1.155333	2.941049	-0.514965
6	-0.097820	2.738934	-0.323722
6	-1.966806	-1.536083	-0.510562
16			
209.759796 Kcal/mol 9.096057 eV -101.049407 H MutD_16_38.log			
6	0.560665	2.446343	-0.353134
6	-4.500749	-0.186170	0.138139
6	4.472342	1.513915	0.927520
6	2.976739	-0.223328	-0.262046
6	-5.599040	0.177715	-0.414256
8	3.349006	-2.390614	-1.086918
12	-2.496995	-0.527940	0.719776
6	-1.568268	1.275846	0.364543
8	-1.110983	-1.819063	0.686120
6	0.117873	-1.866416	0.385613
6	1.309464	-1.893945	0.070994
6	3.901778	0.450077	0.433476
6	-0.624647	2.104303	0.018108
6	2.597055	-1.624082	-0.443503
12	2.557216	1.978964	-0.400109
6	-6.747683	0.536599	-0.970393
16			
209.829885 Kcal/mol 9.099096 eV -101.049295 H MutD_17_46.log			
6	-2.943748	-0.289492	-0.038888
8	-3.553117	-2.523266	0.472099
6	-3.563107	0.319623	-1.071921
6	-2.656100	-1.710027	0.170423
6	-1.265138	-1.925308	0.043040
8	1.205743	-1.608188	0.145854
6	1.422801	1.414192	1.018151

6	6.954624	0.187770	-1.053258
6	0.332112	2.124265	0.949733
6	5.706540	0.026499	-0.624549
6	4.513580	-0.134522	-0.196141
6	-0.916361	2.451598	0.858782
6	-0.044107	-1.774021	0.086534
6	-3.940424	1.307245	-1.834484
12	2.496702	-0.259703	0.432314
12	-2.732122	2.015095	0.002006
16			
210.581548 Kcal/mol 9.131692 eV -101.048097 H Child_7_45.log			
6	-3.014320	3.181308	-0.636460
6	-1.000878	-2.611142	-0.060632
6	0.224654	2.498435	0.500866
12	-3.006142	-2.423036	0.266799
6	-2.424408	2.111962	-0.089927
6	8.131967	-1.114575	-0.042892
6	-1.007661	2.104397	0.201084
6	-0.303495	-1.571373	0.010924
6	-3.138042	0.864041	0.172679
8	9.020772	-0.389234	-0.117297
6	-0.028169	0.975678	0.221776
6	-3.115704	-0.237626	1.053759
6	-3.765496	-0.279033	-0.240474
6	0.045698	-0.271222	0.070655
12	4.497081	0.695551	-0.131801
8	-4.210290	-1.257676	-0.956217
16			
210.681558 Kcal/mol 9.136029 eV -101.047938 H MutD_18_32.log			
6	-1.195780	-2.141239	0.130186
6	1.580670	1.481729	0.290071
6	-3.718899	-1.761360	-0.508213
6	-2.381748	-1.411591	-0.052011
6	1.669060	0.092077	0.317267
12	8.168857	-0.851977	-0.320142
6	-4.121553	-0.221160	-0.251218
8	1.092584	2.192914	-0.875809
8	-2.007055	1.064321	0.016812
6	-0.396828	-3.344066	0.314146
6	0.154442	-2.000522	0.288402
12	-0.645521	2.309217	0.003845
6	1.088520	-0.994743	0.323422
6	-5.188975	0.536029	-0.161950
6	1.363219	2.532661	1.107442
6	-2.679503	-0.025273	-0.019621
16			
210.742692 Kcal/mol 9.138680 eV -101.047840 H Original3D_0_56.log			
6	-1.700101	-0.327184	0.828350
6	-1.040132	0.165426	-0.343099
12	-0.185625	1.534779	1.109456
6	-2.359657	-1.455323	0.136213
8	-1.563583	0.218117	1.995308
6	2.717157	1.111045	1.281839
8	-2.244112	3.035901	-2.236752
6	3.585943	0.207338	0.740187

6	-1.759109	3.160074	-1.211389
6	-1.655304	-0.943334	-1.141767
6	-3.192639	-2.450814	0.426020
6	-3.876827	-3.485355	0.773969
12	5.124208	-1.696825	-1.343887
6	-1.566247	-1.230566	-2.440164
6	4.259573	-0.628753	0.119084
6	1.787102	1.862847	1.621545
16			
210.762123 Kcal/mol 9.139522 eV -101.047810 H MutI_15_45.log			
6	-7.237945	-0.341224	1.516807
12	6.784522	-0.366850	1.627457
8	5.576154	-0.297769	0.294257
6	1.978455	0.161159	-0.935810
6	0.598942	2.300296	-0.369888
6	-2.629439	-1.310609	-0.346464
6	-4.932484	-0.344534	0.198863
6	-3.844063	-0.981333	-0.033081
6	-0.134949	-1.336178	-0.840713
6	1.368942	1.316878	-0.716784
8	-5.500485	1.007370	-0.022869
6	-1.420248	-1.545024	-0.624719
12	4.074617	-0.107939	-0.694906
6	-0.388715	2.994651	0.114501
6	-6.196590	-0.040146	0.770977
6	1.018923	-0.870492	-0.960643
16			
211.037097 Kcal/mol 9.151446 eV -101.047371 H Original3D_5_6.log			
8	0.323775	-0.873454	0.024272
8	4.983108	-1.352887	0.517297
6	1.193256	1.264698	-0.413393
6	-1.930750	-1.634149	0.138102
6	-1.011236	-0.521953	0.456931
6	0.254617	1.799740	-1.366388
6	-0.761919	2.318360	-1.935153
6	-1.497786	0.605694	1.054452
6	3.857505	-0.968254	0.392819
6	-1.880696	-2.359085	-0.955650
12	-3.225801	-0.600328	1.438857
12	-1.108751	2.458412	0.345009
6	1.451922	-0.101957	0.005682
6	1.227292	2.496905	0.113197
6	-1.953093	-3.044134	-2.071519
6	2.644146	-0.603579	0.291094
16			
211.310571 Kcal/mol 9.163305 eV -101.046936 H Child_18_14.log			
6	-3.418102	3.029701	0.020109
8	8.749938	0.952039	-1.317992
6	-2.175704	2.658092	0.354722
6	9.022488	1.707604	-0.497946
12	0.310427	0.818861	1.372849
6	1.570229	-1.643529	0.793206
6	-1.040746	2.327043	0.877093
6	0.653137	-2.569322	0.177159
6	-0.943809	-1.040303	1.211148

6	0.986139	-3.717099	-0.422576
8	-3.746693	-0.462030	-1.321268
6	1.908152	-0.574406	1.346363
6	-2.837749	-1.230381	-0.894328
6	-0.703679	-2.002146	0.316435
6	-1.882409	-1.891717	-0.466152
12	-4.214898	1.327698	-1.020960
16			
211.420547 Kcal/mol 9.168074 eV -101.046760 H MutD_16_44.log			
12	4.861255	-1.555780	0.220601
8	-5.432463	0.373598	-0.028378
8	-1.687978	0.553937	0.304311
6	1.867539	-2.295801	-0.195576
6	5.526043	0.390740	0.406386
6	3.768476	2.259747	0.078524
6	4.714980	1.358411	0.243625
6	-0.506628	-1.310411	-0.418418
6	1.507855	3.419016	-0.440260
6	0.591676	-1.872820	-0.334389
6	-1.725397	-0.632971	-0.344640
6	3.090129	-2.482642	-0.060915
6	-7.847982	-0.372688	0.482680
6	-6.643789	0.092224	0.263311
6	2.650974	2.848734	-0.156056
12	-3.611233	0.236654	-0.166693
16			
211.427186 Kcal/mol 9.168362 eV -101.046750 H Original3D_9_5.log			
6	1.515559	-0.157456	0.247813
12	-1.113082	0.979403	0.498391
8	1.158840	-2.525384	-0.418679
6	3.045187	-0.077695	1.149447
6	0.786838	1.670175	-1.098616
6	-3.267852	0.652138	0.307712
6	1.965726	-1.617984	-0.541936
6	-4.368652	0.189619	0.002098
6	-5.484095	-0.476802	-0.179027
6	-0.411084	2.031476	-1.174609
8	-6.433349	-1.148222	-0.272268
6	1.921831	1.032456	-0.525598
12	3.960098	-0.775127	-0.692628
6	1.841592	-0.019612	1.803132
6	3.270048	1.195752	-0.178634
6	0.523546	0.067523	1.497955
16			
211.812571 Kcal/mol 9.185074 eV -101.046136 H Original3D_17_3.log			
12	-0.439414	0.058805	1.597385
12	0.510849	0.239855	-1.976694
8	1.995872	-1.128660	1.737162
6	1.282790	-0.130331	0.394882
6	3.253542	-1.084451	-0.615028
6	-3.743357	-1.098807	0.280379
6	2.110324	-0.351489	-0.723686
6	-3.243367	-0.425679	1.348525
8	0.188067	4.148584	-0.156194
6	0.519050	3.097173	-0.426679

6	-3.380213	-1.288303	-0.902329
6	-2.368646	0.140714	2.034077
6	-2.421385	-1.056825	-1.848314
6	2.200029	0.086687	1.739885
6	-1.372867	-0.485119	-2.149266
6	4.109313	-2.027455	-0.481787
16			
211.992619 Kcal/mol 9.192882 eV -101.045849 H MutI_12_71.log			
6	2.634945	-2.523361	0.772563
6	1.034390	0.830848	-0.946999
6	-0.195010	0.515250	-0.715845
8	3.379712	1.475931	-1.329893
6	-4.010661	-1.816561	-0.110255
6	-3.657214	-0.611757	-0.140338
6	1.336536	-2.633730	0.530538
6	-2.906357	1.836560	0.049476
6	7.145048	0.539731	1.274000
6	-1.375973	0.039725	-0.472302
6	-2.752867	0.511132	-0.195999
12	-1.901054	-2.192913	-0.224245
6	2.242933	1.186021	-1.159139
6	0.079139	-2.674557	0.286262
8	6.526075	1.212276	0.572073
12	-4.490259	2.801124	1.143476
16			
212.088474 Kcal/mol 9.197038 eV -101.045696 H Child_15_21.log			
8	-8.565373	-2.442785	-0.055877
12	1.199655	3.542665	-0.053227
6	-7.502471	-1.897123	-0.062501
6	-0.833537	3.144505	-0.000522
6	-6.350322	-1.325164	-0.051000
6	-1.396547	2.042640	0.064987
6	-5.214651	-0.759844	-0.026978
12	3.197963	1.414162	-0.092619
6	-4.023473	-0.220354	0.018038
6	4.729533	0.020276	-0.044547
6	8.360954	-3.621023	-0.040335
6	5.690614	-0.810321	-0.006979
6	-2.818209	0.083747	0.141458
6	6.675383	-1.686991	0.038725
6	7.549682	-2.590596	0.065414
8	-1.681271	0.722730	0.202826
16			
212.750218 Kcal/mol 9.225734 eV -101.044641 H MutD_15_58.log			
6	-8.167389	1.108749	-0.640420
6	0.042643	-0.197867	0.697440
6	-1.167125	-0.463589	0.873250
12	1.576127	-1.340977	0.042219
6	-5.171531	-0.855509	0.559510
6	-7.461296	0.095378	-0.175160
12	-3.183554	-0.620696	0.903709
6	6.983005	2.342967	0.230370
6	3.471034	-1.893550	-0.529899
8	5.937636	-1.216997	-0.780614
6	-6.308538	-0.408579	0.231587

6	4.667474	-1.605317	-0.616913
6	6.273381	0.016235	-0.502625
8	-8.753348	2.016053	-1.119167
6	7.192875	3.562901	0.706374
6	6.614605	1.156121	-0.192331
16			
212.759952 Kcal/mol 9.226156 eV -101.044626 H Child_12_51.log			
8	-2.669740	3.531539	0.038549
6	5.203279	0.116699	-0.071507
6	-2.467171	2.367488	0.034435
12	3.711125	-1.229841	-0.102591
6	-4.752578	-0.487236	-0.195029
8	1.868702	-1.809161	0.053459
6	-2.319725	1.004363	0.019793
6	4.316303	1.044770	-0.040444
6	-3.439948	0.108805	-0.100505
6	0.736429	-1.340593	0.070834
6	-3.490379	-1.252314	-0.187720
6	3.338229	1.994333	0.016766
6	-1.032350	0.628709	0.120191
6	-0.382196	-0.727524	0.068026
6	2.159350	2.503506	0.068196
12	-2.111722	-2.898913	0.139735
16			
213.100313 Kcal/mol 9.240916 eV -101.044083 H Child_11_14.log			
6	7.876822	0.441383	-0.244015
6	-4.376951	0.624474	0.210337
6	6.606868	0.274962	-0.125334
6	-8.033073	-0.473891	-0.194911
6	5.289388	0.185036	-0.069285
6	-6.797095	-0.169144	-0.000030
8	4.716147	-1.153595	-0.081371
6	-3.127819	1.037669	0.170408
6	3.357786	-1.116933	-0.099883
6	-9.292884	-0.678401	-0.437149
6	2.173530	-1.385225	0.210334
6	-5.575386	0.214546	0.170727
8	0.892355	-1.339223	0.282867
6	-1.934015	1.459432	-0.024506
12	-0.151888	0.231852	0.093131
12	3.329300	1.223073	-0.010809
16			
213.102686 Kcal/mol 9.241019 eV -101.044080 H Child_10_15.log			
8	4.308453	-1.460032	0.102723
6	-3.320940	2.428828	-0.054746
6	3.152613	-1.019434	0.032474
6	4.079121	2.556102	0.780477
6	1.959609	-1.816151	-0.044022
6	-1.948886	2.356803	-0.334518
6	0.813536	-2.256715	-0.090664
8	-3.674207	1.237638	0.429343
6	-0.504034	-2.585639	-0.118610
6	-0.784070	2.062539	-0.661317
6	2.812812	0.424768	-0.029789
6	-3.964480	0.124186	0.925868

6	-1.740017	-2.703392	-0.111657
12	1.107058	1.375675	-0.771329
6	3.455689	1.428695	0.593795
12	-3.535364	-1.727706	-0.027027
16			
213.258436 Kcal/mol 9.247773 eV -101.043831 H MutI_4_69.log			
12	3.734040	1.880767	-0.137905
6	-1.572052	0.800638	0.765642
8	0.606599	1.790564	-0.277540
6	-0.522278	1.312264	0.265235
6	-3.973537	-1.512944	-1.215153
8	-5.513514	1.592433	0.033435
6	-4.200210	-0.351724	-0.721850
6	3.430680	-1.603694	-0.262718
12	-1.830624	-1.212377	0.900863
6	1.009983	-2.359829	0.143867
6	4.432307	-0.678215	-0.359609
6	2.318515	-2.098141	-0.086553
6	-4.817490	0.734564	-0.334443
6	-0.214413	-2.331652	0.388865
6	5.140540	0.350589	-0.310013
6	1.703675	1.890703	0.526286
16			
213.278468 Kcal/mol 9.248641 eV -101.043799 H Original3D_17_7.log			
6	-1.796061	-0.405721	-1.386743
8	1.405759	1.279009	-1.287240
6	2.114879	2.006431	-0.380952
6	-0.268137	0.975901	0.398403
6	0.210677	0.837670	-0.942897
8	-0.174127	-2.291304	-0.009043
6	1.819684	-1.355487	-0.609200
6	-2.977733	-0.175872	-1.095418
6	-0.279310	0.321100	1.664700
6	-0.385101	-0.396389	-1.428671
6	0.405940	-1.467562	-0.853096
6	-1.426096	0.991883	1.210491
12	1.103312	-1.259407	1.543962
6	2.813623	-1.317455	0.166613
6	2.778709	2.541457	0.563212
12	-3.429937	0.656293	0.667006
16			
213.532748 Kcal/mol 9.259668 eV -101.043394 H MutI_13_71.log			
6	-4.229453	1.835241	0.072983
8	7.123529	0.482714	0.313059
12	-5.554150	-0.298929	0.338799
6	-5.478739	1.711920	0.253818
6	-4.080145	-1.761715	0.275057
6	-1.556036	-1.907634	-0.073855
6	4.788636	-0.347303	-0.051396
12	0.176093	-0.757383	-0.324380
8	-0.552255	0.989912	-0.514502
6	-1.726269	1.469928	-0.335145
6	-2.879604	1.810878	-0.087338
6	8.246423	0.983954	0.487097
6	-2.829878	-2.075502	0.134038

6	3.499549	-0.672713	-0.205432
6	2.272053	-0.870087	-0.298333
6	5.967879	-0.027845	0.068261
16			
213.821219 Kcal/mol 9.272177 eV -101.042935 H Original3D_1_6.log			
6	2.744196	1.150418	-0.795778
6	3.336874	2.311030	0.025674
6	0.435443	-0.084961	-0.537622
6	1.893068	0.132989	-0.638504
6	-0.697107	0.598761	-0.646852
6	2.203280	-1.239741	-0.185205
6	3.759545	1.971884	-1.296439
12	-2.422108	-1.758583	-0.263771
8	0.485881	0.692583	2.088741
6	0.638305	-1.593791	-0.193661
6	-3.271259	0.239921	-0.690140
12	-4.708727	1.582950	0.037923
6	-1.975751	0.513123	-0.512917
8	3.210017	-1.784572	0.199415
6	-0.378376	-2.403631	-0.237386
6	0.645589	0.211250	3.109655
16			
214.311716 Kcal/mol 9.293447 eV -101.042153 H Child_2_14.log			
6	-4.489933	4.219388	-0.057385
12	5.217411	0.486794	-0.162710
6	-4.497247	2.888275	-0.016720
6	3.277746	-0.410006	0.329346
6	-4.585331	1.613088	-0.049679
6	2.851578	0.906897	0.168499
12	-4.263882	-0.392016	0.021970
6	3.655340	2.073849	-0.100364
6	-2.979975	-1.955024	-0.114581
6	1.870855	-0.166585	0.283197
6	-0.299899	-4.869180	-0.548097
8	3.366385	3.265483	-0.201907
6	-1.822806	-1.460707	0.061752
6	0.613229	-0.615634	0.222110
6	-0.550988	-1.049334	0.183692
8	0.421396	-4.288921	0.141691
16			
214.659891 Kcal/mol 9.308546 eV -101.041598 H Child_9_43.log			
8	3.860947	1.476607	0.240484
6	-3.884220	-0.649137	0.177707
6	1.962851	3.120439	-0.251460
6	-2.494066	-0.552447	-0.088635
6	2.492961	1.913856	-0.045946
6	-5.023681	-0.141639	0.389014
6	3.317226	0.094393	0.222715
12	-3.710094	1.619644	0.165842
6	2.035646	0.512535	-0.039674
8	-0.313459	-2.272091	-0.112024
12	3.003426	-1.944817	0.236381
6	-1.863011	0.688659	-0.177659
6	-0.510750	-0.036463	-0.489350
6	0.974203	-1.700838	-0.034296

6	-1.166043	-1.246255	-0.442858
6	0.842235	-0.292113	-0.195283
16			
214.735728 Kcal/mol 9.311834 eV -101.041477 H MutI_12_75.log			
8	0.409199	-1.180397	-1.113313
6	1.808134	2.613058	-0.383504
8	1.697028	-1.880081	0.695918
12	-0.230536	2.723082	-0.169243
6	-0.663896	-1.146000	1.123685
6	-1.846817	-0.585918	1.263840
12	-2.605210	1.500412	0.612460
6	-2.038157	-1.074946	-1.625054
6	-3.126626	-0.935512	0.644767
6	2.667125	-0.963103	0.409833
6	4.036569	-0.694793	0.123071
6	0.421441	-1.418450	0.423199
6	-2.945496	-0.915847	-0.621048
6	2.427538	1.557384	-0.183420
6	-0.807292	-1.105343	-1.573711
6	2.930666	0.303121	0.068436
16			
215.152509 Kcal/mol 9.329908 eV -101.040813 H Child_10_53.log			
6	-3.923069	1.456370	-0.106930
6	4.164864	1.788415	0.809776
6	-3.982511	0.228892	0.016776
6	3.379599	0.857096	0.026330
8	-3.980668	-1.110803	0.143569
6	2.817153	-1.610724	-0.172557
12	-2.236110	2.529354	-0.121988
6	2.494645	-2.827215	-0.218685
6	-2.757863	-1.676246	0.104251
6	2.608767	-0.243928	-0.044514
6	-0.285660	2.009249	-0.005821
6	4.014535	2.002701	-0.559865
6	-1.598262	-2.079651	0.040337
8	1.153309	-0.111930	0.078569
6	0.479193	1.046473	0.041902
12	0.415322	-2.189916	0.008396
16			
215.197545 Kcal/mol 9.331861 eV -101.040741 H MutI_15_71.log			
6	-3.076771	-2.318281	-0.068794
8	1.753266	2.669655	-0.667633
12	-0.350211	-1.868972	-0.762563
6	-3.740760	-3.260549	0.482236
6	-2.805118	0.076980	-0.300554
6	-0.360029	3.495352	0.458333
12	3.924206	-1.322213	0.304611
8	1.177147	-2.580668	0.108370
6	3.249808	0.608854	-0.106686
6	0.744197	3.090918	-0.003569
6	2.450756	1.556729	-0.349507
6	2.131371	-2.828854	0.886238
6	-2.594638	2.501526	0.422991
6	-1.701564	3.288467	0.614738
6	-2.345353	-1.206053	-0.428615

6	-3.007107	1.258631	0.054777
16			
215.400380 Kcal/mol 9.340656 eV -101.040418 H MutD_16_48.log			
6	-1.674867	2.451910	-1.334118
6	-1.492210	1.127580	-0.850647
6	1.984248	-1.844587	-0.055856
8	-0.498611	-2.097909	-0.190437
6	2.889025	0.236640	0.144375
6	-0.389748	2.035421	-0.896792
12	1.598621	1.922366	-0.307562
6	2.643686	2.049279	1.996582
6	3.230443	-1.164794	-0.092884
12	-1.908203	-0.852478	-0.322957
6	0.762162	-2.005476	-0.127270
6	-6.328179	0.015248	1.028750
8	4.367156	-1.594601	-0.351798
6	-5.128538	-0.385543	0.638237
6	-3.954166	-0.765349	0.299989
6	2.919246	1.033243	1.233655
16			
215.924527 Kcal/mol 9.363386 eV -101.039583 H Child_12_38.log			
6	-5.139110	-1.091118	0.302699
8	4.585234	0.807534	0.217119
6	-4.256013	-0.107971	0.152681
6	3.969478	-0.381233	0.169976
8	-4.298681	1.355346	0.152369
6	3.412894	-1.481633	0.113454
6	-2.751484	0.004940	-0.035093
6	3.947944	2.053896	0.085093
6	-2.890292	1.421781	-0.013178
6	2.557205	1.924236	-0.070715
6	-1.507169	-0.538342	-0.142372
12	1.784304	-2.611796	-0.033387
6	-0.968638	-1.790255	-0.189948
6	1.318944	2.021892	-0.176545
12	-0.696033	1.563342	-0.221041
6	-0.252371	-2.823124	-0.179846
16			
216.654028 Kcal/mol 9.395020 eV -101.038420 H Child_12_55.log			
6	-3.074583	2.897640	-0.260942
8	3.420310	-1.210897	-0.929981
6	-1.759418	2.206733	-0.131204
6	4.574731	-0.643168	-0.763275
6	-2.839100	1.546286	-0.704432
6	-1.366223	-2.299547	0.820174
12	0.044974	2.025088	0.876645
8	-3.157560	-1.983042	-0.906916
6	1.239205	0.028196	2.087210
6	-0.327439	-1.892423	1.583983
6	1.547812	1.247849	1.960608
6	-2.224901	-2.229074	-0.057231
6	0.559773	-1.180353	2.057243
6	5.397536	0.156891	-0.970151
12	-3.584404	-0.255933	-1.480063
6	5.001135	0.881246	-1.965948

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16
216.904612 Kcal/mol 9.405886 eV -101.038021 H Original3D_13_3.log
8   0.118411   0.997232   -3.011785
6   0.454958   -0.180979   0.337975
6   -0.442597   1.811464   0.877603
6   0.084039   0.463288   -1.945969
6   2.702775   -0.525309   0.239353
6   -4.329309   0.878510   0.213251
8   -1.683838   -1.634340   0.186155
6   1.424677   -0.939889   1.214016
6   -0.783599   0.480694   0.532215
6   -1.974021   -0.331759   0.336949
6   0.469434   2.689378   1.003995
6   2.071909   -1.616847   -0.355100
6   1.262485   -0.237179   -0.862076
12  2.158788   1.503859   0.734756
6   -3.227528   0.206572   0.282251
12  0.028218   -2.428093   0.211766
16
217.335415 Kcal/mol 9.424567 eV -101.037334 H Child_15_27.log
6   1.629584   2.732714   0.038579
8   -4.095614   -2.027917   0.781968
6   1.547545   1.315095   -0.026920
6   -3.112970   -1.418614   0.331070
6   0.389126   2.084235   0.288419
6   -1.876420   -1.935793   -0.146681
6   4.148423   -0.559229   0.035808
6   -3.527314   1.011086   -0.468471
12  2.029699   -0.685064   -0.343255
6   -2.973602   0.038929   0.290925
6   5.385823   -0.312237   0.230888
6   -3.686669   2.195884   -0.987862
6   6.697270   -0.255567   0.335948
6   -0.664863   -1.911379   -0.393871
8   0.585337   -1.866075   -0.617259
12  -1.667480   1.788497   0.469533
16
217.410162 Kcal/mol 9.427809 eV -101.037215 H Child_13_20.log
6   -0.378685   3.225523   -1.816367
12  -4.651257   -1.275048   -1.549377
8   -1.125452   3.027611   -0.965303
6   2.065821   -1.357917   -0.751997
6   -5.827468   0.372599   2.088424
6   0.881118   -1.319752   -0.395478
8   7.671724   0.768192   1.225962
6   -0.378069   -1.068232   -0.004630
6   -4.740021   0.297807   1.393896
6   -1.493663   -0.743573   0.375095
6   6.728648   0.238485   0.689193
6   -2.719866   -0.295717   0.743722
6   -3.345650   0.951487   1.224083
6   -4.040213   -0.594299   0.418562
6   5.720155   -0.336615   0.140795
12  4.051022   -0.940385   -0.677045
16

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217.741072 Kcal/mol 9.442158 eV -101.036688 H Child_13_9.log

6	-5.898385	-2.810494	-0.025970
8	0.007573	1.868443	-0.114612
6	-6.219325	-1.605424	0.612874
6	1.923541	0.540903	0.353063
6	-4.934443	-1.766794	0.005807
6	2.322645	-0.669395	0.582767
6	5.396447	-3.429526	-0.586604
6	1.492131	1.762864	0.141754
6	-2.541285	-0.871834	-0.477835
6	2.692245	-1.890666	0.826509
6	-3.701500	-1.274844	-0.266508
6	2.006208	3.085786	0.071913
8	5.678024	-4.426008	-0.089042
6	1.926011	4.345331	0.012278
12	-0.198371	3.822701	-0.093139
12	-0.824172	0.174388	-0.396116

16

217.893612 Kcal/mol 9.448773 eV -101.036445 H MutI_18_67.log

12	-0.550006	-2.769694	0.053975
6	-2.556595	1.764285	-0.039514
6	-1.342664	2.266174	-0.043630
12	4.483751	-1.084088	-0.153195
6	-5.293946	0.570753	-0.101496
6	2.214282	-1.252075	-0.013617
6	3.674386	1.515679	0.103530
6	-2.134206	-1.324388	0.047279
6	-4.169915	-0.156956	0.012921
8	-3.428878	-1.387972	0.079162
6	2.416654	1.985150	0.065644
6	-3.668546	1.136828	-0.039836
6	-0.097036	2.409628	-0.023845
6	1.220316	2.328270	0.020523
8	1.223624	-1.986163	-0.013762
6	4.810118	0.963062	0.123280

16

218.191353 Kcal/mol 9.461684 eV -101.035970 H MutI_10_65.log

6	-6.191419	0.106544	1.015233
6	-4.997606	-0.281616	0.638628
6	1.362033	2.753984	0.530019
8	2.239442	-2.247569	0.046064
12	4.060632	-0.863308	0.122766
6	-0.568639	2.562732	-0.756645
6	0.301429	3.233630	-0.129074
6	2.148506	1.832648	0.827845
6	-2.718935	-1.221695	-0.173134
12	0.587448	-1.588365	-0.683520
6	-0.692851	1.398884	-1.444587
6	-3.864321	-0.744386	0.239778
6	2.364254	0.440209	0.814575
8	1.758229	-0.538321	1.219008
6	-0.214947	0.263982	-1.778400
6	-1.553891	-1.727051	-0.349494

16

218.488057 Kcal/mol 9.474551 eV -101.035497 H MutI_1_79.log

6	2.669995	-2.239973	-0.176206
6	0.093494	0.307032	-1.786778
6	-3.567330	3.203758	0.085964
6	5.089738	-1.286745	-0.084864
8	3.617462	1.813479	1.514289
6	1.461079	-2.637846	-0.149997
6	2.780858	2.381782	0.901840
6	-0.927689	0.914508	-1.387527
6	-2.609117	-0.131769	-0.247774
12	-4.153155	-2.081446	1.546416
8	1.952161	2.959366	0.279277
6	-2.902500	2.247136	-0.519383
6	-2.729054	-1.287293	0.229355
6	3.921871	-1.773193	-0.184345
12	-0.112243	-1.511814	-0.702898
6	-2.176711	1.125328	-0.758743
16			
219.539713 Kcal/mol 9.520155 eV -101.033822 H Child_18_27.log			
12	-2.831994	3.481246	-0.191819
6	3.844955	0.234691	0.595021
6	-1.365137	-0.771674	0.646509
6	5.063114	0.559538	0.809417
6	-2.783363	-0.838956	0.544443
6	6.335515	0.874915	1.050573
6	-3.423952	-2.041688	0.544959
12	1.832207	-0.196031	0.253075
6	-3.387047	0.437066	0.399236
6	1.558537	-2.395982	-1.001080
6	-0.137255	-0.613769	0.657694
6	-3.689692	1.636165	0.294587
8	1.021691	-3.294702	-1.459582
6	-3.833614	-3.254545	0.430083
6	0.698485	2.113948	-1.748382
8	1.317580	1.412098	-1.049598
16			
220.352312 Kcal/mol 9.555393 eV -101.032527 H Child_17_19.log			
12	-4.271719	-1.141045	-0.238640
6	9.018313	0.641200	0.321159
12	-1.752704	-2.568939	0.115320
6	7.915633	0.857955	-0.353332
6	0.736241	-0.888463	0.495406
6	-1.669064	2.331438	0.248327
8	1.444130	-0.877971	1.530573
6	6.839476	1.256559	-0.978914
6	-4.850239	0.825297	-0.509616
6	-2.081537	3.707156	0.059521
6	-4.087365	1.796453	-0.317192
6	-0.790254	1.271790	0.324618
6	0.450578	-2.188132	-0.204259
6	-0.130339	0.232526	0.238780
6	-2.964267	2.571342	-0.059949
8	1.302123	-2.868393	-0.794005
16			
220.637429 Kcal/mol 9.567757 eV -101.032072 H Child_3_45.log			
6	5.492224	0.512274	1.088228

12	-0.185226	-3.151253	0.269772
6	4.350771	0.755854	0.592897
6	-2.026199	-2.442491	0.011012
6	-0.356541	1.890837	-0.315436
6	1.727669	-2.338172	0.203002
6	3.225205	1.128183	-0.005813
6	-2.785586	-1.456687	-0.156241
6	-1.521066	1.897521	0.075796
6	2.346485	-1.403956	-0.392343
12	1.558637	1.741655	-1.026945
6	-3.599673	-0.566926	-0.809262
6	-2.812129	1.560979	0.517502
6	2.472528	-0.128011	-0.709066
8	-3.519011	0.817569	-0.517691
8	-3.426370	1.739775	1.578244
16			
220.813205 Kcal/mol 9.575379 eV -101.031792 H Original2D_0_22.log			
6	-0.000000	-0.887616	-0.000000
12	-2.110127	-0.489453	-0.000000
6	-2.258540	2.644202	-0.000000
6	0.233589	1.796071	0.000000
6	1.302022	-0.382133	0.000000
6	-4.436909	1.427410	-0.000000
6	-5.741164	1.337372	-0.000000
12	1.656860	-2.643937	-0.000000
8	-2.734036	3.786024	0.000000
6	6.205689	-4.045978	0.000000
6	2.782601	1.248828	0.000000
6	1.432394	1.034569	0.000000
6	-3.102481	1.380068	-0.000000
6	-0.594641	-2.104059	-0.000000
8	7.182833	-3.442277	0.000000
6	-0.847753	2.359715	0.000000
16			
221.286506 Kcal/mol 9.595903 eV -101.031038 H Original3D_1_7.log			
6	-0.024302	-0.917029	0.450822
8	3.290169	-4.598949	1.244957
12	-2.960461	0.327327	1.075957
6	-0.413793	2.322202	1.035085
6	-3.974095	-0.688760	-0.435308
6	-1.753667	1.976622	1.469529
6	-1.260011	3.305796	1.635562
6	-1.718828	-1.473709	-1.575805
6	-0.831785	-1.245287	-0.457580
12	0.967193	0.899222	0.326964
8	-1.306063	-1.795491	-2.699635
6	3.495288	-3.539164	1.634630
6	-3.060407	-1.128686	-1.156011
6	4.717262	3.115398	-1.534300
6	2.592904	1.830143	-0.740252
6	3.572496	2.515299	-1.192643
16			
221.963996 Kcal/mol 9.625282 eV -101.029958 H Child_1_40.log			
12	-5.966399	0.342451	-1.296298
12	0.736808	-1.354701	1.155437

6	-4.280650	-0.362730	-0.369568
6	2.753795	-1.470069	0.455541
6	-3.256625	-0.940539	-0.016135
6	1.718166	0.835141	0.887356
6	-2.020528	-1.403784	0.437862
6	4.453602	-0.637650	-1.483902
6	1.380419	2.065119	0.724503
6	-1.422987	-2.172108	1.357032
6	0.659701	3.135630	0.543966
6	3.602816	-0.718155	-0.449822
6	5.094302	-0.469842	-2.582242
6	2.695597	-0.071320	0.440488
8	0.055286	4.126193	0.299472
8	-0.744104	-0.950087	-0.046990
16			
222.199726 Kcal/mol 9.635504 eV -101.029583 H Child_15_23.log			
6	-1.646644	-0.285080	-2.158750
8	5.770954	2.420323	0.212279
6	-2.362288	-0.141371	-1.053247
6	4.986269	1.526699	0.176570
6	-4.221003	1.199174	0.086346
8	-3.290138	-1.570040	1.778080
6	-3.473943	0.099816	-0.119815
6	4.171547	0.529913	0.156975
12	0.162901	-1.293425	-0.910184
6	-2.970854	-1.070158	0.705439
6	2.996259	0.036824	-0.362540
12	3.919706	-1.560299	0.827640
6	-5.230723	2.172859	0.157371
6	-1.791579	-1.247371	-0.178481
6	-4.030644	2.595823	0.682123
6	2.100636	-0.843391	-0.580715
16			
223.155249 Kcal/mol 9.676940 eV -101.028060 H Child_18_8.log			
6	4.652562	0.214097	0.215147
12	-3.318200	-1.114158	1.322314
6	3.375068	0.198889	0.175014
6	-4.032275	-0.858853	-0.655034
6	5.957294	0.266273	0.288933
8	-3.643108	0.378803	-0.764405
6	2.058918	0.320335	0.096041
6	-3.159494	1.526799	-0.987305
6	1.449558	1.589249	-0.033281
12	-1.142371	1.773320	-0.143971
6	0.761823	2.628583	-0.076474
6	-0.212515	-0.631828	0.635478
6	1.299260	-1.943393	-0.597527
8	1.419019	-2.946719	-1.165227
6	1.102809	-0.826581	0.106520
6	-1.366414	-0.378008	1.048646
16			
223.579745 Kcal/mol 9.695348 eV -101.027383 H Child_5_57.log			
12	3.131314	-0.865348	-0.814257
6	-8.040180	3.326977	-0.596687
6	3.384377	0.933072	0.280471

6	-0.966420	-1.238403	1.671199
6	1.695052	-2.324284	-1.100220
6	0.147592	-0.722833	1.738241
6	3.882801	2.104810	0.004937
8	-7.069388	3.448778	0.028898
6	0.568747	-2.852772	-0.806449
6	1.334905	-0.131749	1.507388
6	4.360134	3.276074	-0.363194
6	2.345040	0.442196	1.049704
6	4.610179	4.486619	-0.720062
12	-2.311565	-2.013941	0.294782
6	-0.625053	-3.248555	-0.343949
8	-3.683115	-2.168208	-0.990720
16			
223.795152 Kcal/mol 9.704689 eV -101.027040 H MutI_13_73.log			
6	-4.990399	2.566786	0.813562
6	-4.933469	1.302790	0.608621
6	1.111390	1.675056	-0.332434
6	-5.402767	-0.689306	-0.863671
6	7.089411	-0.785314	0.101031
6	-0.178882	1.877295	-0.398243
6	2.316690	1.316990	-0.280205
12	-4.599602	-2.619800	0.155492
8	-4.475403	-0.991490	1.188425
6	9.633230	-1.335939	0.290720
6	-4.963029	-0.019194	0.354798
12	4.209587	0.610628	-0.098794
6	5.901647	-0.358362	0.031462
6	8.364706	-1.150325	0.177642
8	-1.337879	2.012759	-0.488136
6	-5.417455	-1.743826	-1.550396
16			
224.716995 Kcal/mol 9.744663 eV -101.025571 H Child_11_11.log			
6	5.553464	1.142345	1.747998
12	-3.086703	0.202573	-0.892490
6	5.114082	0.332219	0.846968
6	-2.036672	-1.028508	0.543220
8	-2.145532	3.221266	0.838111
12	1.830549	-1.361835	-1.413526
6	4.440226	-0.372288	-0.066540
6	-2.505967	-2.121551	1.061160
6	-0.563566	1.102418	0.583733
6	-1.590689	1.747799	-1.153014
6	-1.609346	2.328301	0.223899
8	-2.991985	-3.133623	1.449108
6	-0.760223	-0.368054	0.414840
6	-0.423115	0.890393	-0.897118
6	0.047754	-0.482294	-0.849323
6	3.696381	-0.969114	-0.893415
16			
224.921673 Kcal/mol 9.753539 eV -101.025245 H MutI_2_71.log			
12	3.396524	0.662298	0.642946
8	-1.978634	4.101974	-2.047959
6	0.146914	0.051616	0.886350
6	-2.028236	-3.530148	-1.036492

8	-1.251229	1.906057	1.784289
6	-1.625163	-1.239849	0.124309
6	5.982675	0.312855	-1.107638
12	0.009671	-3.121644	-0.683871
6	-3.549957	0.307055	0.600467
6	-1.163076	0.837494	1.209352
6	4.919118	0.090928	-0.436585
6	-2.263964	-0.019786	0.651325
6	1.369877	0.483104	1.096292
6	-1.886337	3.226822	-1.308213
6	-0.241723	-1.204633	0.246465
6	-2.166035	-2.407474	-0.492222

16

226.291824 Kcal/mol 9.812955 eV -101.023061 H Child_1_24.log

6	-1.470059	0.856793	0.977900
6	3.831660	0.430210	-2.027445
6	-0.273640	1.243786	1.464046
6	-1.312179	-0.726204	-1.600320
12	-2.136892	-1.115663	1.445749
6	3.299203	0.723103	-0.901021
6	0.946674	1.378352	1.779838
6	-1.572173	-1.860564	-0.836797
6	-1.815814	-2.677941	0.092578
12	2.740238	0.763124	0.987494
6	-1.470731	0.610016	-1.398519
6	-0.770614	0.197709	-2.602267
8	2.347073	-1.526225	0.877732
8	-2.862356	2.297407	-0.375817
6	2.089565	-1.914887	-0.194946
6	-2.001538	1.416461	-0.288755

16

226.706647 Kcal/mol 9.830943 eV -101.022400 H MutI_18_63.log

6	2.084393	1.955761	0.503072
12	4.172464	0.138535	-1.215396
6	-2.616186	1.579114	-0.365007
6	-0.747811	-1.803679	0.298115
6	-1.640658	2.198511	0.052817
8	-3.310146	-1.841220	-0.019723
6	-5.017764	0.159842	-0.415921
6	-3.864480	-0.658195	-0.281757
6	-3.624985	0.658604	-0.464712
12	2.258993	-1.055094	0.470077
6	0.829259	2.500454	0.643165
6	4.715936	-1.926843	0.074683
8	0.526962	-1.719217	0.478486
6	3.080536	1.288794	0.213769
6	-1.952058	-1.894952	0.164693
6	-0.398184	2.522956	0.456037

16

226.723289 Kcal/mol 9.831665 eV -101.022374 H Original3D_13_4.log

6	-1.039836	2.311178	-1.024993
8	0.106896	2.341043	-0.987246
6	0.921153	-0.455517	0.907147
12	-3.803437	0.757435	-0.421530
8	-0.537175	-1.781351	-0.140953

6	-0.333847	-0.920777	1.082348
6	1.603990	0.581475	1.648063
6	2.745439	0.928604	1.225392
12	-2.105183	0.098245	1.702911
6	0.901601	-1.783765	-1.211984
6	-2.799706	-0.953947	-1.008264
6	-1.736577	-1.519551	-0.706404
6	3.479388	0.575934	0.133192
6	2.887872	-0.414276	-0.655169
6	4.150050	0.153898	-1.079274
6	1.611418	-0.960874	-0.368551
16			
227.514447 Kcal/mol 9.865973 eV -101.021113 H Original3D_13_6.log			
6	-0.553405	1.199939	-1.227229
6	0.282894	2.048026	-0.582975
12	-3.570741	0.095133	-1.047560
8	0.930137	-0.304039	0.826869
6	-1.376846	0.169367	-1.298310
12	2.218825	0.968912	-0.138325
6	4.356728	1.064772	0.074465
6	-1.429350	0.288064	1.554336
6	-1.361986	-0.608813	-0.063031
6	-1.125968	1.667542	1.557634
6	-0.287995	-0.519841	0.933184
8	0.440013	-3.620488	-0.098507
6	-2.510892	-0.315714	0.796889
6	4.135214	0.379046	-0.981280
6	-0.476154	2.182716	0.602118
6	1.224724	-4.450491	0.034818
16			
227.740187 Kcal/mol 9.875762 eV -101.020753 H Original2D_0_9.log			
6	-1.496679	-1.334948	0.000000
6	-2.006379	-2.675696	0.000000
6	-1.113982	-3.832559	0.000000
6	0.800558	-2.245534	0.000000
6	0.000000	-1.061034	0.000000
12	1.047551	0.851335	0.000000
6	-1.896728	4.563323	-0.000000
6	0.096525	-3.389806	0.000000
12	2.794998	-1.314332	0.000000
8	3.101301	3.176979	-0.000000
6	4.047572	3.831865	-0.000000
6	-2.327647	-0.287238	-0.000000
6	-0.251825	2.546693	-0.000000
6	-1.028277	3.567285	-0.000000
6	-2.639393	-3.896060	0.000000
8	-3.002934	0.677800	-0.000000
16			
228.489896 Kcal/mol 9.908272 eV -101.019558 H MutI_4_77.log			
8	4.805765	1.139188	1.005605
6	-3.085015	-2.391804	0.111206
6	1.361653	-1.780573	-0.449719
6	-1.314773	2.429151	-0.495921
6	0.517588	-0.769089	0.060031
6	3.685414	-0.628925	-0.284667

12	-2.955587	-0.225026	0.586134
8	-3.583728	1.668069	0.213012
12	-0.957704	-2.546179	-0.294744
6	-0.777295	-0.428672	0.677343
6	2.604526	-1.295139	-0.538399
6	1.267763	1.885765	-0.995970
6	-0.012750	1.855755	-0.546427
6	-2.458733	2.107062	-0.166287
6	0.081983	0.531736	0.059135
6	4.326839	0.284133	0.362072
16			
228.609500 Kcal/mol 9.913459 eV -101.019368 H MutI_15_43.log			
8	-0.158784	-2.645933	0.367029
6	4.383645	0.769896	-0.393613
6	-2.670148	0.429842	-0.283747
6	-1.500665	0.737099	0.127428
6	0.242870	-1.245406	0.454563
6	0.524510	2.419289	0.338168
6	3.605614	-1.602450	-0.105049
12	-1.852913	2.725676	0.309940
8	4.287314	1.976616	-0.601856
12	-5.518045	-1.158275	-0.567426
6	4.311681	-0.519793	-0.266149
6	-0.226848	0.027506	0.377960
6	1.286113	-2.105542	0.292128
6	2.560118	-2.439132	0.041230
6	0.606664	1.190270	0.302559
6	-3.886344	0.096042	-0.057404
16			
228.835573 Kcal/mol 9.923262 eV -101.019008 H Child_5_60.log			
6	5.991164	1.140092	-0.172108
8	-7.010077	0.477495	0.031986
6	4.877156	1.819223	-0.184206
6	-5.807004	0.599835	-0.013767
12	3.226580	0.650928	-0.127800
6	0.045316	-3.572408	-0.318315
6	1.666900	-0.339323	-1.369674
6	0.587787	-2.347724	-0.132929
6	1.163919	-1.424605	-1.104465
6	0.636445	-1.731382	1.195271
6	-2.001590	0.883417	-0.216396
6	-4.555670	0.709873	-0.076436
6	-3.219931	0.814239	-0.142447
6	1.141245	-0.659686	1.466767
8	1.704001	0.535746	1.312591
12	0.047936	0.727802	-0.234232
16			
229.079145 Kcal/mol 9.933824 eV -101.018619 H Child_17_18.log			
6	-4.331263	3.438207	-0.119894
6	5.063881	1.863030	-0.127704
6	-3.510277	2.451495	-0.060358
6	4.016601	1.647365	0.719192
6	-2.633691	1.442193	-0.009584
6	-0.190006	-2.336466	0.097509
8	-3.205771	0.116450	0.054050

6	0.933534	-1.729945	0.168076
6	-2.372231	-0.913164	0.087916
8	1.990190	-1.110530	0.206009
6	-1.233696	1.487038	-0.007353
6	-1.435237	-1.685037	0.094813
6	0.004015	1.408945	0.002359
6	3.995091	1.444957	-0.864318
12	2.051128	0.919515	0.042349
12	-0.394100	-4.516104	-0.206048
16			
229.530858 Kcal/mol 9.953413 eV -101.017900 H MutI_17_39.log			
6	3.511594	1.389147	-0.070495
6	-4.617566	1.844049	-0.293401
6	2.368942	1.990342	-0.036550
6	-1.587558	-1.144231	0.013668
8	3.302835	-1.130189	0.131390
6	1.092749	2.224559	0.013569
6	4.910108	0.905276	-0.234974
12	1.613816	-1.990246	0.209990
12	-2.916387	0.554778	0.009736
6	-2.148675	-3.846472	-0.320576
6	3.917212	-0.019030	-0.004996
6	-0.415005	-1.782033	0.057268
6	-0.159443	2.071931	0.045970
6	-1.659341	-2.652633	-0.146355
8	-1.356793	1.860103	-0.010939
6	-5.202598	0.916813	0.376818
16			
229.576009 Kcal/mol 9.955371 eV -101.017828 H Child_13_24.log			
6	3.479447	4.195216	-1.256282
8	-5.107320	1.794753	1.381502
12	5.603713	-1.461400	-0.320508
6	-4.339807	1.041889	0.880976
6	2.409824	3.542938	-0.940815
6	-3.341837	0.368541	0.328604
6	4.430966	-1.861741	1.190639
6	-2.998328	-1.983142	-0.747818
6	1.298432	2.872474	-0.641037
6	-2.784855	-3.140714	-1.338652
6	3.142739	-1.739154	1.359726
6	-3.201394	-0.869579	-0.201813
6	0.252062	2.228024	-0.366756
6	-2.596951	-4.268569	-1.958231
12	-1.395327	1.214553	0.103994
8	1.982018	-1.714119	1.711861
16			
229.727662 Kcal/mol 9.961947 eV -101.017586 H Original2D_15_1.log			
6	-1.244726	-0.303806	0.000000
6	-0.740235	-2.260009	-0.000000
6	-1.448351	1.050872	0.000000
6	-2.001653	-1.692488	0.000000
6	-0.000000	-0.983770	-0.000000
6	2.459604	-0.121573	-0.000000
12	3.682302	1.441159	-0.000000
8	-0.738310	-3.627661	-0.000000

8	-0.650337	3.425975	0.000000
6	-2.143207	-3.864882	-0.000000
12	1.229186	3.729039	0.000000
6	-2.937373	-2.736849	0.000000
6	3.328685	3.524556	0.000000
6	-3.438903	-4.355302	-0.000000
6	1.306880	-0.567570	-0.000000
6	-1.112166	2.239340	0.000000
16			
230.643059 Kcal/mol 10.001642 eV -101.016127 H			
Original3D_15_5.log			
6	-0.805983	0.280628	-0.857273
6	0.657429	-1.402360	0.313581
6	2.837760	-0.438333	-0.521810
12	-1.095283	-2.200670	1.138723
6	-2.743944	-1.172674	0.396137
6	1.743634	0.194114	-1.047134
12	-4.194745	0.294670	-0.003460
6	1.237937	2.213430	1.610372
6	4.168276	-0.584306	-0.626471
6	-1.327937	1.520173	-1.349455
6	-2.016092	-0.292867	-0.279237
8	1.950407	3.070727	1.339558
6	1.955155	-1.121714	0.617214
8	-2.718320	1.154273	-0.798477
6	0.454698	-0.308707	-0.688135
6	5.443009	-0.708719	-0.559757
16			
231.426900 Kcal/mol 10.035633 eV -101.014878 H			
Original3D_8_6.log			
6	-0.095172	-1.520503	-0.106915
12	-1.546078	-0.136772	0.803263
6	0.190932	1.917422	0.035583
6	1.316362	-1.935843	-0.254697
6	1.115383	0.782938	0.103013
8	3.360848	-3.273030	-0.666986
6	0.902993	-0.545188	-0.121056
6	2.351830	-2.694976	-0.424415
6	-5.033745	-2.504994	0.445229
6	2.264933	1.645359	0.122551
8	-5.400354	-1.465010	0.067645
6	1.376887	2.814188	-0.333882
12	-2.728242	2.377438	-0.906898
6	-1.148757	2.085671	0.324003
6	3.532144	1.253860	0.365533
6	4.494193	0.538122	0.851442
16			
231.601180 Kcal/mol 10.043190 eV -101.014600 H			
Original3D_0_62.log			
12	1.070064	1.068409	2.043720
6	-1.243224	-0.430860	-1.412823
6	1.416242	2.256892	-1.414412
8	-2.478258	1.465589	-0.273878
6	-1.985866	0.426731	-0.970518
12	2.352393	-2.184043	-0.432251

6	0.458050	3.108689	-1.145256	
6	0.733882	-2.088814	-1.664746	
6	2.896640	-1.531488	1.398069	
6	-3.068015	-2.622938	0.823972	
6	-0.254380	-1.349000	-1.660336	
6	2.317007	1.366901	-1.688812	
6	-0.632988	2.002332	1.441613	
6	-1.607591	1.837129	0.687937	
6	2.374556	-0.468806	1.807854	
8	-3.708661	-1.672214	0.704767	
16				
231.763446	Kcal/mol	10.050227	eV	-101.014342 H Child_11_30.log
6	0.913636	2.717574	-0.483699	
6	-3.346343	-1.695052	-0.261636	
8	0.963769	3.780509	-0.984185	
6	-2.032577	-2.176508	-0.564095	
6	0.653649	1.510243	0.016083	
8	-2.981252	-0.330752	-0.132181	
6	2.868260	0.198947	0.369456	
6	-0.783928	-2.271943	-0.569899	
6	1.378702	0.347917	0.230916	
6	-3.469397	0.763004	0.561007	
12	-1.100650	0.307668	-0.022631	
6	3.321507	-2.397559	0.162460	
12	1.218591	-2.099037	-0.031808	
6	3.492781	1.319096	0.754662	
6	3.295896	-1.151199	0.200033	
6	-3.838090	1.818541	1.182079	
16				
232.655005	Kcal/mol	10.088889	eV	-101.012921 H Child_17_20.log
6	-1.442604	1.612841	-1.038061	
12	3.490472	-1.482183	-0.299347	
6	-0.706399	1.804838	-2.087445	
6	1.704909	-2.428857	-0.306599	
12	-2.265829	0.975785	0.834656	
6	0.470892	-2.328485	-0.238173	
6	-0.438241	1.775232	1.422166	
6	4.134981	0.346651	0.398667	
6	0.830137	1.849002	1.266532	
6	-0.863402	-2.122572	-0.122982	
6	-0.070004	1.976706	-3.239580	
6	3.176004	1.125746	0.725755	
6	2.122200	1.773597	1.181272	
6	-2.043883	-1.806050	-0.059266	
8	-3.320811	-1.557020	-0.077125	
8	-3.672097	-0.367370	0.847446	
16				
233.913385	Kcal/mol	10.143457	eV	-101.010916 H Child_2_40.log
6	5.253735	1.099061	1.113308	
8	-0.576645	-3.126287	-1.470905	
6	4.190900	1.627645	0.496752	
6	-0.141887	-2.070540	-1.420385	
6	5.290349	-0.273405	1.136273	
12	0.309746	0.231134	-1.061104	
6	3.110939	1.346081	-0.124902	

6	-4.013203	-1.755374	2.673473	
6	4.369225	-0.963588	0.482044	
6	-4.299878	0.180990	0.926795	
6	2.376204	0.192787	-0.527259	
6	-4.228710	-0.805736	1.828450	
6	3.253044	-0.874447	-0.141175	
6	-4.567647	1.030399	0.028889	
12	-2.378492	1.234794	-0.591825	
8	-4.265040	1.876990	-0.903897	
16				
234.058592	Kcal/mol	10.149754	eV	-101.010684 H MutD_9_78.log
6	-2.013273	-2.370352	0.085521	
6	-3.688368	-0.584974	0.133924	
6	-3.157712	-1.793356	0.171162	
6	-1.749631	1.750645	-0.180787	
6	-2.848831	2.614630	-0.072163	
6	-0.646458	1.189486	-0.279805	
6	-0.787284	-2.807252	-0.028361	
8	3.851331	1.793231	0.135280	
6	3.255663	0.568655	0.005076	
6	1.687289	-2.053823	-0.117782	
12	3.631913	-1.390997	0.138401	
12	1.220568	0.212925	-0.321025	
6	-4.211393	0.555251	0.164770	
6	0.504044	-2.513375	-0.087753	
8	-4.119914	1.889708	0.106742	
6	4.309103	2.890024	0.248750	
16				
234.412268	Kcal/mol	10.165091	eV	-101.010121 H Child_11_47.log
8	-5.429060	0.114252	0.431704	
12	1.316851	3.316941	0.034627	
6	-3.773870	-1.705482	-0.297368	
6	4.877240	-0.844506	0.199149	
6	-4.960110	-1.132510	0.021763	
6	6.067802	-1.329999	0.317100	
6	-4.339542	0.921029	0.542981	
8	7.167137	-1.743822	0.441608	
12	-2.127503	-0.381834	-0.048314	
6	3.768751	-0.277066	-0.027576	
6	-5.090626	-2.453595	-0.436066	
6	2.663740	0.366072	-0.374094	
6	1.219626	0.158420	-0.427212	
6	-3.171558	1.365082	0.529964	
6	0.023703	-0.242937	-0.266022	
6	2.018711	1.478037	-0.919662	
16				
234.820620	Kcal/mol	10.182799	eV	-101.009470 H MutD_1_76.log
6	-0.125509	-0.164771	2.025597	
6	1.142189	-0.063784	1.388631	
8	1.270837	1.446347	1.120957	
12	-3.255268	-0.232566	0.660085	
6	1.343404	-1.634004	-0.665375	
6	-0.873254	-0.384413	-0.074184	
6	-1.311101	0.747616	-1.102961	
8	-1.979925	-1.205519	-0.646572	

6	-0.400767	1.743112	-1.360377	
6	0.779994	2.001561	-1.012219	
6	-2.520919	0.132497	-1.410758	
6	0.557208	-0.755145	0.042669	
6	2.403985	-2.223409	-1.069321	
12	2.998819	-0.295556	0.037277	
6	-1.303595	-0.128388	1.428529	
6	1.766714	1.464269	-0.217469	
16				
235.025628 Kcal/mol 10.191689 eV -101.009143 H				MutD_13_48.log
12	5.017184	1.015655	-0.058143	
6	-5.897762	-2.774606	-0.043095	
6	-4.601597	3.389092	-0.070481	
8	-4.431486	-0.589672	0.076860	
8	-3.711998	2.673900	-0.200084	
6	0.577229	0.177196	0.074557	
6	4.188267	-0.966705	-0.084744	
6	3.469807	2.471186	0.129170	
6	-3.164849	-0.472016	0.079494	
6	1.929024	0.316203	0.066323	
6	2.599104	1.557115	0.119388	
6	2.790184	-0.885909	-0.012909	
6	-1.955712	-0.224464	0.093312	
12	3.353058	-2.823632	-0.080207	
6	-5.161406	-1.738168	0.008620	
6	-0.654794	-0.011941	0.081363	
16				
236.103256 Kcal/mol 10.238419 eV -101.007426 H				Child_8_12.log
6	2.911524	-2.342845	-0.490582	
6	-0.553027	2.370038	-0.062181	
8	4.218131	-1.804626	-0.141130	
6	0.742513	2.566284	0.178083	
6	1.871382	-1.415189	-0.415693	
6	-1.735609	2.013206	-0.269806	
6	0.730549	-0.927883	-0.386527	
6	-4.323228	-2.821587	0.803679	
6	4.500902	-0.535605	0.242175	
6	1.938234	2.224615	0.397642	
12	-1.260615	-0.260639	-0.217738	
8	-3.926794	-1.772993	0.373976	
6	3.115701	1.646528	0.511569	
6	3.691811	0.491687	0.358146	
12	-3.725541	1.315337	-0.360897	
6	-3.306889	-0.608489	-0.019697	
16				
236.144590 Kcal/mol 10.240212 eV -101.007360 H				
Original3D_0_50.log				
8	0.923282	-1.870530	1.549945	
6	-1.559066	-0.764092	-0.515934	
6	1.087742	-2.944768	1.142162	
6	0.757853	0.729261	-0.746403	
6	-0.432326	0.090413	-0.311784	
6	-2.713173	-0.119446	0.035515	
6	-1.386837	-3.172349	-1.600680	
8	1.002437	1.260679	-2.093132	

6	2.312983	0.455448	-0.653518	
6	3.072155	0.302788	0.409104	
6	-0.098100	1.261766	0.421774	
6	2.368480	0.942065	-2.090938	
12	1.463420	0.482416	1.883475	
6	-3.462447	0.728367	0.578835	
6	-1.489753	-1.989230	-1.107269	
12	-1.975988	2.164039	0.698218	
16				
236.228075 Kcal/mol 10.243832 eV -101.007227 H				Child_12_25.log
12	-3.630092	-2.804301	-0.159120	
6	6.415581	-2.294499	0.343545	
6	-4.234103	-0.874920	0.068197	
6	5.413889	-1.529613	0.139346	
12	-4.907709	1.151260	0.287033	
6	4.128368	3.468966	-0.110980	
6	-2.841648	-0.938841	-0.088080	
8	3.374535	2.602101	-0.084406	
6	-1.885073	0.192623	-0.091310	
6	-3.252615	2.465895	0.034503	
6	3.209115	-0.619940	-0.062673	
6	-2.455767	1.477603	-0.066686	
6	1.983030	-0.467876	-0.076493	
6	-0.545526	-0.026874	-0.089969	
6	0.681488	-0.263028	-0.078635	
8	4.469612	-0.564661	-0.048037	
16				
236.813979 Kcal/mol 10.269239 eV -101.006293 H				MutI_15_33.log
12	2.572123	1.800300	-0.022783	
12	5.911850	-0.724838	0.142912	
6	2.685390	-0.765387	0.006845	
6	3.690536	0.022347	0.031146	
8	-0.053241	1.574482	-0.036049	
6	-6.105893	0.707270	0.223713	
6	-1.328255	1.255701	-0.040739	
6	-2.436039	0.752365	0.010581	
6	1.582924	-1.526437	-0.037141	
6	0.430002	-1.977965	-0.070783	
6	-0.911511	-2.054164	-0.081262	
8	-3.362646	-1.456161	-0.101997	
6	0.572104	2.861676	-0.194806	
6	-4.869615	0.352231	0.161628	
6	-3.596770	-0.026806	0.036353	
6	-2.126303	-1.909517	-0.101732	
16				
237.189355 Kcal/mol 10.285517 eV -101.005695 H				MutI_16_43.log
6	-3.361714	-0.134629	0.859929	
8	-3.144936	0.992352	-0.013275	
6	1.797861	1.259170	-0.613683	
6	3.907638	-0.157164	-0.033209	
12	1.082747	2.922706	0.737647	
6	-4.231329	-0.784962	0.026324	
6	2.902961	0.543313	-0.385245	
6	4.872331	-0.930001	0.341861	
6	5.747079	-1.826818	0.711679	

6	-2.455140	-0.339464	1.871039
6	-1.433231	-0.450264	2.623551
6	0.723616	0.944870	-1.413050
6	-1.140717	-1.934617	-0.523672
12	-2.272804	-0.126671	-1.304554
8	-0.302807	-2.691597	-0.322444
6	-0.352251	0.484157	-1.884086

16

239.302119 Kcal/mol 10.377135 eV -101.002328 H

Original3D_0_44.log

6	-1.212301	-0.334724	-0.604822
6	1.629932	0.683341	0.735851
6	-2.448817	-0.856450	-0.767332
6	1.950874	-1.732371	1.195656
6	1.128372	0.293569	-0.690805
6	-1.325759	1.014103	0.174718
6	0.361087	-2.378511	-0.584450
6	-3.600736	-0.631278	-0.228368
6	0.131891	-0.728565	-0.767574
12	0.382534	2.304770	-0.750040
6	1.099797	-2.438808	0.479796
6	2.432061	-0.533404	1.237805
8	-2.153618	1.317734	1.005258
12	3.462543	-0.001328	-0.804514
6	1.295807	1.915041	1.219830
8	-4.695654	-0.476856	0.276345

16

241.093203 Kcal/mol 10.454804 eV -100.999474 H

Original3D_0_52.log

12	0.414406	-0.911826	-0.107918
6	-0.856627	0.538563	1.064238
12	-2.790035	-0.558809	0.953601
8	-1.300653	-3.369969	-0.098991
6	-1.880258	1.292130	0.426609
6	2.515802	-0.829777	0.030009
6	2.631470	0.228932	0.861179
6	1.656861	1.014559	1.496736
6	-2.139534	2.537016	0.050223
6	-2.436778	-3.369696	-0.346167
6	3.864840	-0.142111	0.158173
6	0.070335	0.100480	-2.173933
6	5.103954	0.148462	-0.165089
6	0.407751	1.031339	1.461039
8	-0.063013	0.858109	-3.022408
6	-2.368340	3.740519	-0.392520

16

242.014036 Kcal/mol 10.494735 eV -100.998006 H

Child_1_54.log

6	-4.983170	-0.092092	-0.047660
6	5.518583	1.161460	-1.079559
6	2.156258	1.908410	1.444388
6	4.541302	0.321962	-0.832302
6	-3.800444	-0.593143	-0.052772
6	3.608838	-0.524319	-0.572527
6	0.816875	1.457791	1.227355
8	-2.850617	2.622025	-1.517503

6	1.921128	0.611306	0.884369	
6	-2.519426	2.081758	-0.566828	
6	-2.542461	-1.011283	0.003991	
6	-0.183555	-2.203096	-0.065468	
12	-1.144245	0.888803	0.869544	
12	1.785881	-1.365264	0.090124	
6	-1.281017	-1.165190	0.153610	
8	-0.551520	-3.372507	-0.294447	
16				
242.421959	Kcal/mol	10.512424	eV	-100.997356 H Child_13_16.log
6	5.561353	-0.194741	1.241322	
8	-3.144331	1.195700	1.793535	
6	4.560430	0.021025	2.019976	
8	-3.188547	1.391646	0.103883	
12	3.770963	0.145105	0.086924	
12	-3.069468	-0.550544	0.976080	
6	1.974822	0.247767	-1.112527	
6	-2.138700	1.953598	-0.371173	
6	1.193242	-0.876892	-1.147559	
6	-1.043620	2.318222	-0.809004	
6	-2.115672	-2.187200	0.087127	
6	0.270034	-1.680094	-0.883444	
6	0.220817	2.083847	-1.201897	
6	1.245342	1.399451	-1.366688	
6	-1.821459	-3.416105	-0.562780	
6	-0.865744	-2.307794	-0.549251	
16				
242.610555	Kcal/mol	10.520603	eV	-100.997056 H
	Original3D_14_4.log			
6	1.877658	-1.988105	-0.736454	
6	3.063403	-1.197869	-0.399439	
6	2.718704	-2.807226	-1.582784	
12	3.295590	0.894584	-0.248130	
6	-1.734442	-1.911890	1.086357	
6	3.651767	-2.511957	-0.370321	
6	-2.775696	-1.322822	0.380456	
6	2.766234	2.778260	0.110815	
6	2.194125	3.819092	0.555805	
6	-3.647894	-0.487849	-0.079521	
6	-4.543147	0.241229	-0.620079	
8	-1.911418	-2.335294	2.286439	
12	-4.934139	2.198420	-1.231790	
6	-0.508819	-2.044554	0.397018	
6	0.586349	-2.058963	-0.160663	
8	1.633059	4.815280	0.997547	
16				
243.301551	Kcal/mol	10.550567	eV	-100.995955 H MutI_13_55.log
6	-2.554303	-2.348648	0.010432	
6	-1.117620	2.105616	0.201469	
6	-1.234953	-2.296891	0.124681	
6	4.980910	0.250835	-0.071491	
6	6.144538	-0.210441	-0.159432	
8	-2.286245	2.750292	0.098650	
6	7.419492	-0.533512	-0.263515	
6	-4.429151	1.316633	-0.043439	

6	0.014041	-2.124084	0.285363
12	-4.667603	-0.691502	-0.255389
8	3.786863	0.344549	0.142369
6	-3.817618	-2.459887	-0.185370
12	2.007010	1.059957	-0.054578
6	1.335601	-2.276082	0.361375
6	-3.425068	2.056391	0.079716
6	0.004494	1.656706	-0.041211

16

243.490572 Kcal/mol 10.558764 eV -100.995653 H

OriginalID_7_0.log

6	0.000000	0.000000	-0.832418
6	0.000000	0.000000	0.403145
6	0.000000	0.000000	1.737197
6	0.000000	0.000000	-2.176129
6	0.000000	0.000000	-3.418846
6	0.000000	0.000000	2.967370
12	0.000000	0.000000	-5.463840
8	0.000000	0.000000	4.226035
6	0.000000	0.000000	-7.449564
6	0.000000	0.000000	5.507262
6	0.000000	0.000000	-8.707663
12	0.000000	0.000000	7.435161
6	0.000000	0.000000	9.521635
6	0.000000	0.000000	-10.042450
6	0.000000	0.000000	-11.330096
8	0.000000	0.000000	10.682403

16

243.751101 Kcal/mol 10.570061 eV -100.995238 H

Child_10_36.log

6	-2.767993	-3.089241	0.743279
6	5.612371	1.584894	-0.834583
8	-3.739699	-0.929637	-0.299032
6	4.421762	1.195335	-0.618402
6	-2.641875	-1.873971	0.214764
6	-3.576053	2.262811	0.802206
6	-2.638000	0.012271	-0.700479
6	3.445287	0.302844	-0.229015
6	-1.658684	-0.851399	-0.232794
8	-3.122022	2.203288	1.859603
12	5.757551	-0.370022	0.482341
6	2.258622	-0.357928	-0.021623
6	-0.299611	-0.685193	-0.150280
6	0.914636	-0.478754	-0.096702
6	3.481464	-0.960460	0.464138
12	-4.459034	0.990317	-1.192975

16

244.454843 Kcal/mol 10.600579 eV -100.994117 H

Child_12_19.log

12	5.325347	-2.629204	-0.677287
6	-0.607406	0.370003	0.463552
6	4.629214	-1.190914	0.802227
8	-3.320194	-4.025900	-0.426528
6	3.853359	-0.152921	0.542112
6	-1.649928	1.814657	0.950596
6	2.942215	0.748358	0.477666
6	-1.954059	0.471313	0.486710

12	1.101303	1.712564	0.471735
6	-0.753368	2.653270	1.289429
6	0.245161	2.890313	-1.301241
6	-3.431899	-2.844653	-0.264294
8	-0.423047	3.462646	-2.034619
6	-3.105283	-0.259734	0.232367
6	-4.480645	-0.347857	0.123966
6	-3.549676	-1.567549	-0.110458

16

245.211992 Kcal/mol 10.633412 eV -100.992910 H

Original1D_0_5.log

8	0.000000	0.000000	11.037518
6	0.000000	0.000000	9.879174
12	0.000000	0.000000	7.759942
6	0.000000	0.000000	5.811709
6	0.000000	0.000000	4.507711
6	0.000000	0.000000	3.222524
12	0.000000	0.000000	1.196525
6	0.000000	0.000000	-0.804282
6	0.000000	0.000000	-2.049199
6	0.000000	0.000000	-3.391813
6	0.000000	0.000000	-4.629149
6	0.000000	0.000000	-5.961611
6	0.000000	0.000000	-7.194090
8	0.000000	0.000000	-8.435603
6	0.000000	0.000000	-9.746329
6	0.000000	0.000000	-11.026800

16

245.499067 Kcal/mol 10.645861 eV -100.992453 H

MutI_14_71.log

8	-3.248538	-3.082720	-0.275167
6	-4.409656	1.207173	-1.810460
6	2.872243	-0.439817	0.467016
6	-4.745558	0.961894	-0.568848
12	-0.274155	-1.830467	0.502784
6	4.157229	0.016227	0.384198
6	5.389580	0.282073	0.185991
6	-5.281573	1.641410	0.442041
8	8.955019	1.338917	-0.562098
6	-2.218148	-2.466528	0.232610
6	6.627931	0.631161	-0.057526
6	-5.776043	2.690848	0.960479
12	-3.874413	-1.217039	-0.470137
6	-5.506329	3.912302	0.443121
6	7.826481	0.974446	-0.313576
6	1.752336	-0.991104	0.686016

16

246.454135 Kcal/mol 10.687276 eV -100.990931 H

Original3D_0_38.log

6	-1.299592	1.889900	-0.265981
6	-1.683537	0.574974	-0.507027
8	0.956981	0.379111	-0.097821
6	-1.303864	-1.660871	-0.198154
6	1.093814	-0.864549	-0.314947
8	-4.179804	-0.841995	1.509411
6	-0.382609	-0.825382	-2.430417

6	-3.004413	-0.361716	1.645383	
6	-1.889139	-0.546986	0.330446	
6	-0.735816	3.004584	-0.194258	
12	3.515002	0.212107	1.246061	
6	-0.175653	-1.492874	-1.018924	
6	-1.204836	-0.135790	-1.696545	
12	1.283644	2.337016	-0.032652	
6	2.249940	-1.549828	0.021689	
6	3.035510	-2.512530	0.319797	
16				
247.510865	Kcal/mol	10.733101	eV	-100.989247 H Child_10_39.log
12	-2.277434	-1.458200	0.599535	
6	0.083677	3.635999	0.881453	
6	-3.901455	-0.915983	-0.519122	
6	-0.472563	2.570245	1.249061	
6	-0.658099	-2.782241	0.132991	
12	0.562062	4.466567	-0.895751	
6	-4.910132	-0.195232	-0.905854	
6	-1.043531	1.374922	1.528227	
6	0.527479	-3.158951	-0.044567	
6	6.922329	1.273147	-0.813882	
8	-5.825838	0.500706	-1.278024	
8	6.092191	1.030564	-0.059010	
6	1.825274	-3.409484	-0.184130	
6	3.051841	-4.005918	-0.322583	
6	-1.536136	0.226385	1.563420	
6	3.186924	-2.671317	-0.189871	
16				
248.352103	Kcal/mol	10.769580	eV	-100.987906 H MutI_17_43.log
6	-1.286692	-1.600848	0.250721	
6	0.873963	-1.334659	-0.643188	
6	1.490334	-2.313937	-1.201292	
6	4.836781	0.642268	-0.052588	
6	-1.954384	-2.580550	0.720065	
6	3.084962	0.346088	1.547165	
6	-0.344537	-0.678997	-0.289574	
8	-4.796248	0.539107	0.118759	
6	-4.783182	1.665044	-0.233402	
12	2.901141	-0.197568	-0.412038	
6	6.068137	0.971057	-0.250783	
6	-0.724791	0.637560	-0.317050	
6	4.147773	0.583818	1.012105	
12	-3.445299	-1.069442	0.343757	
6	-1.359691	1.738807	-0.220750	
8	-1.924020	2.804671	-0.257409	
16				
249.118591	Kcal/mol	10.802818	eV	-100.986685 H MutI_16_71.log
6	-0.906306	3.164320	0.197010	
6	-3.383801	0.402216	-0.201372	
6	4.806191	0.275450	-0.112767	
8	3.703074	0.969424	-0.028072	
6	5.933043	-0.339493	-0.169693	
6	-1.991977	4.138577	0.153860	
6	-2.222837	2.708768	-0.044325	
12	0.342044	-1.512171	0.147568	

12	0.290655	1.416193	0.041102	
6	-0.751462	-3.567081	0.031844	
6	-2.885633	-2.131716	-0.072997	
6	-1.870013	-2.970455	0.048508	
6	-2.911341	1.541175	-0.189822	
6	-3.385444	-0.956713	-0.141230	
8	0.538663	-3.691386	0.101567	
6	2.648532	1.556189	0.025650	
16				
249.356391 Kcal/mol 10.813130 eV -100.986306 H				
Original3D_10_5.log				
6	1.045348	-2.211719	-1.615382	
6	2.748354	0.948227	0.436085	
12	1.140602	2.010068	-0.197207	
6	3.384036	-0.266080	0.816386	
6	-1.969098	1.204934	-0.328099	
12	1.833013	-1.515401	0.330843	
6	-1.312477	-1.047936	1.257133	
8	-3.054284	1.023406	0.431006	
6	-0.903426	1.937529	-0.645272	
8	-2.654177	-1.126452	1.261585	
6	-3.642721	-0.314231	0.909927	
6	-1.204911	0.592113	-1.373521	
6	0.231330	-1.309474	-2.081069	
6	4.033625	1.008189	1.101937	
6	-0.081077	-1.055181	1.087758	
6	-0.664930	-0.338309	-2.089943	
16				
249.696531 Kcal/mol 10.827880 eV -100.985764 H				
Child_16_31.log				
6	5.935343	2.010670	0.940151	
12	-3.769286	1.155914	-2.468846	
6	5.350583	0.917635	0.350140	
6	-3.406370	0.360240	-0.582703	
8	5.371501	-0.383917	-0.060206	
12	-1.618303	-0.669258	-0.383126	
6	4.563045	2.047107	0.486714	
6	-4.021340	0.861589	0.432069	
6	4.160736	-0.839628	-0.422695	
6	-4.599276	1.394412	1.498305	
6	2.959908	-0.882793	-0.625214	
6	-1.743060	-3.288589	1.569089	
6	1.604757	-0.912720	-0.725503	
6	-4.946643	2.033040	2.558618	
6	0.366005	-0.876191	-0.726535	
8	-1.957883	-2.464646	0.773837	
16				
249.764723 Kcal/mol 10.830837 eV -100.985655 H				
Child_18_10.log				
12	-7.974572	-0.156359	-0.018055	
6	3.724778	-0.549173	-0.027737	
6	-2.625741	-0.042897	-0.228023	
6	3.747209	0.689427	-0.194237	
6	-1.448066	0.801690	-0.204564	
8	3.468441	1.914049	-0.314004	
6	-1.206056	-0.504651	-0.175554	
6	2.517057	-1.276867	0.072233	

6	-0.397421	2.934141	0.870204
6	2.173701	-2.592304	0.269420
8	-0.574010	1.839686	-0.156214
6	1.241652	-0.561994	0.001567
6	-0.002386	-1.263518	-0.060992
6	1.215573	-3.492750	0.125245
12	1.458638	1.895374	0.058339
6	0.232328	-2.624112	0.098829

16

250.630104 Kcal/mol 10.868364 eV -100.984276 H

Original3D_8_4.log

6	-0.589617	-0.652418	0.751534
12	2.385706	0.958823	1.044489
6	-1.045672	1.905370	1.796338
6	-3.986031	1.503808	0.263927
6	-0.762464	-0.694846	-1.733213
6	0.517355	-1.534590	1.223329
8	-3.517734	0.516224	-0.089486
6	1.617121	-1.062735	1.760731
6	-0.664143	0.665975	1.218507
6	0.046877	-2.494523	0.009941
6	-0.710993	-1.316339	-0.479485
8	0.258862	-3.651308	-0.249753
6	0.355484	1.535068	1.611388
6	-0.446953	0.110756	-2.633500
6	2.889787	1.612684	-0.959280
12	1.176500	1.342128	-2.233437

16

251.345184 Kcal/mol 10.899372 eV -100.983136 H

MutI_18_75.log

6	-1.354004	-1.248858	-1.037443
6	-2.663135	-0.915385	-1.012081
8	1.286919	1.396654	0.422556
6	4.454315	0.739032	-0.455375
6	-0.779972	-2.717738	1.312307
6	1.642757	-2.045890	1.190606
12	2.647772	-0.070162	-0.359163
12	-4.070077	1.176842	0.108554
6	-1.088895	2.041357	0.745904
6	0.163568	1.726335	0.623988
6	0.479163	-2.511882	1.332236
6	-3.838931	-0.490763	-0.923611
6	-0.118606	-1.153223	-1.060553
6	5.091939	1.823165	-0.338940
8	1.116059	-1.124396	-0.833302
6	-2.347559	2.177482	0.671843

16

251.992771 Kcal/mol 10.927455 eV -100.982104 H

Original3D_0_41.log

6	-0.580100	-1.175041	1.068423
6	-2.762805	-1.576043	0.210380
6	-3.074104	-0.544279	-0.624522
8	-0.142685	-0.108656	1.908019
6	-1.937781	0.410656	-0.853251
6	0.373066	0.535893	0.653724
6	0.276929	-0.812250	-0.150832

12	3.777285	1.007905	-0.177815	
6	-0.680069	0.291721	-0.420056	
12	1.949775	-1.592585	-1.152884	
6	-1.794121	-1.749753	1.012881	
6	-3.285235	0.866198	-0.616188	
6	3.933211	-1.230190	-0.301953	
6	2.233367	2.336179	0.221189	
6	1.392318	1.502874	0.646313	
8	-4.018913	1.843703	-0.546550	
16				
252.775527	Kcal/mol	10.961398	eV	-100.980857 H Child_4_63.log
8	3.675850	2.251491	-0.153732	
6	4.673433	-1.567096	-1.214070	
6	-1.898085	2.473160	-0.005397	
12	2.854684	-0.916580	-0.124357	
6	2.556026	1.799135	-0.091528	
6	0.842277	-1.446341	0.589853	
12	-3.263808	0.985593	0.408822	
8	1.253673	-2.442419	1.201919	
6	-0.891618	1.754440	0.123487	
6	-0.256665	-0.577655	0.421584	
6	-4.163659	-0.612902	-0.560523	
6	1.473988	1.084662	-0.082926	
6	-1.641480	-0.916958	0.329509	
6	-3.846317	-1.546738	-1.442457	
6	0.154958	0.776326	0.147424	
6	-2.757306	-1.103490	-0.181469	
16				
253.514639	Kcal/mol	10.993449	eV	-100.979679 H MutI_16_37.log
8	-4.761211	-0.633164	0.220786	
6	-0.703560	2.006493	-0.238914	
6	-6.732032	-2.263647	0.602755	
6	0.533711	4.268946	-0.032530	
6	-5.761468	-1.380013	0.439573	
6	5.184953	-0.207782	0.358223	
6	-0.108426	3.135070	-0.132364	
6	0.226892	-1.438191	-0.597638	
6	1.298858	5.328319	0.065557	
6	4.013393	-2.909711	-0.131074	
6	-0.438362	-0.394334	-0.460443	
6	-1.204204	0.765039	-0.339795	
12	2.033575	-2.350494	-0.488440	
12	-3.256177	0.330043	-0.050773	
6	4.112592	-1.660519	0.120704	
8	6.278353	-0.273412	0.847494	
16				
254.085850	Kcal/mol	11.018219	eV	-100.978769 H MutI_17_57.log
6	-2.825942	1.490324	0.472281	
12	4.563086	-0.880331	0.100446	
8	1.959267	1.935188	-0.624711	
6	-0.768256	-1.586804	0.074894	
6	-5.370844	1.049726	0.741320	
6	-4.109611	1.289830	0.632326	
6	0.946069	1.142927	-0.031507	
6	4.298613	0.886888	-0.841971	

6	3.170175	1.396465	-0.715332
8	-4.285710	-1.767678	-1.132875
12	1.279624	-0.962155	0.580684
6	3.107327	-1.899557	1.332614
6	-0.296295	1.516676	0.089846
6	-1.579047	1.586268	0.276602
6	-3.197465	-1.716717	-0.735423
6	-1.958217	-1.694401	-0.314463

16

254.853882 Kcal/mol 11.051524 eV -100.977545 H

Original3D_11_6.log

12	2.038242	1.121653	1.223958
6	-2.255680	-1.503876	0.613171
6	1.593665	-1.459097	-0.019071
6	-3.045311	-0.501313	0.678597
6	2.373902	-2.299043	-0.724117
6	-1.349666	-2.433055	0.746972
6	-3.764815	0.578835	0.752030
6	4.279651	0.731788	0.257302
8	1.845840	1.479521	-2.120379
6	1.627178	1.751679	-1.031520
6	4.027877	1.674571	1.081187
6	0.887273	-0.686203	0.783864
6	-6.212485	0.045123	-1.581031
12	4.132298	-1.076799	-0.685015
8	-6.508262	0.221697	-0.491476
6	-4.286107	1.742593	0.847204

16

254.983203 Kcal/mol 11.057132 eV -100.977339 H

MutI_15_61.log

6	0.648399	-2.236076	0.138934
12	-1.122759	0.654311	0.152349
6	3.466617	0.162247	-0.109620
6	-5.237608	-1.479833	-0.445398
6	1.788240	2.167023	-0.081719
6	3.202140	2.830797	-0.274469
6	-3.988826	-1.272036	-0.178518
6	3.174910	1.508594	-0.170202
6	-0.507667	-1.517005	0.130909
6	1.834767	-2.588851	0.106086
6	0.580695	1.821950	0.062240
8	-1.734125	-2.032480	0.085708
12	-2.664554	3.540655	0.170079
8	3.141347	-2.360034	0.054654
6	3.469915	-1.047358	-0.026467
6	-2.733250	-0.882697	0.016220

16

255.008450 Kcal/mol 11.058227 eV -100.977298 H

MutI_7_69.log

12	3.563420	-2.167066	-0.007112
8	0.241991	3.031631	-0.250692
6	4.228966	0.346510	-0.644089
6	2.962622	0.839948	-0.193354
6	2.512179	-0.485221	-0.225787
6	-2.607687	0.729436	0.121924
6	-0.811927	-1.405474	0.765105
6	-4.656378	-0.617853	-0.185353

6	-1.360412	0.943818	0.443297	
6	2.252313	1.965602	0.201391	
6	0.290338	-0.619860	0.551699	
12	-2.540192	-1.300526	-0.464024	
6	1.553484	-1.433129	0.112186	
6	0.820904	1.954274	0.116127	
6	0.035281	0.787276	0.462431	
8	-5.691595	-0.084237	-0.186786	
16				
255.127572 Kcal/mol 11.063393 eV -100.977109 H				Child_8_10.log
6	-2.952113	-1.915095	1.646260	
8	3.937238	-0.599564	2.717674	
6	-3.421420	1.616720	-0.539903	
6	3.926100	0.045251	1.778333	
6	-3.434061	0.584623	0.167222	
12	3.450246	-1.422661	-1.610232	
6	-2.468550	-1.929034	0.153227	
6	2.084648	3.470051	0.260861	
6	-3.124083	-0.623578	0.777118	
8	0.973536	3.169253	0.119812	
12	-1.372611	1.502585	-0.865991	
6	1.474210	-1.358781	-2.352051	
6	-1.214008	-1.179475	0.115816	
6	0.610722	-0.896100	-1.529603	
6	-0.409181	-0.459989	-0.769116	
6	-1.775233	-0.940694	1.460970	
16				
256.271694 Kcal/mol 11.113006 eV -100.975285 H				
Original3D_15_3.log				
6	-1.132425	-0.635641	0.928164	
6	0.222810	-0.241197	1.199421	
6	1.141587	-0.162809	0.026392	
6	2.075287	0.754293	2.091017	
12	-0.642111	0.293107	-1.885443	
6	0.889062	-2.293628	-0.673738	
6	2.627050	0.705244	0.821125	
8	0.757348	1.767176	-1.482783	
6	-2.396735	-0.676879	0.514252	
6	1.537663	1.221644	-0.655881	
8	0.786118	-3.396569	-0.187319	
12	-3.996565	0.758195	0.710157	
6	2.911365	1.602433	-0.236544	
6	0.916090	-0.974801	-1.068770	
6	-2.437937	0.480499	-0.696543	
6	0.865578	0.290762	2.328481	
16				
256.476383 Kcal/mol 11.121883 eV -100.974959 H				Child_6_55.log
6	0.320685	2.709755	0.107960	
6	-5.230234	-0.799473	-0.017475	
12	3.448784	0.386244	-0.094317	
6	-3.932357	-0.791662	-0.035544	
6	2.837251	2.359052	-0.225384	
6	-2.638537	-0.889838	-0.056041	
6	1.663415	2.760653	-0.087150	
6	-6.480389	-0.441039	-0.106701	

6	-0.842598	2.310443	0.247125	
6	4.807390	-1.386501	0.075158	
6	1.541044	-1.152329	0.005944	
6	3.670965	-1.935546	0.041485	
6	-2.122702	1.729001	0.102992	
8	2.327254	-2.259383	0.110304	
12	-0.624679	-1.353946	-0.056129	
8	-1.758861	0.356547	0.076088	
16				
257.162932 Kcal/mol 11.151654 eV -100.973865 H				Child_12_41.log
6	-4.374458	-3.457411	1.314482	
8	-7.445075	2.340020	0.562475	
8	4.217501	-0.844396	-0.541810	
6	-6.341953	1.965468	0.434881	
6	-3.465711	-2.645432	0.862881	
6	5.178767	-0.290206	0.116331	
6	-5.118378	1.560556	0.279061	
12	2.575262	0.122883	-1.056972	
6	7.887972	1.726183	1.947349	
6	-2.458730	-1.954328	0.440640	
6	7.032583	0.995293	1.310401	
6	-1.429419	-1.322435	-0.026093	
6	-3.908074	1.173298	0.085246	
6	-0.393744	-0.746114	-0.527953	
6	6.102905	0.309556	0.664639	
12	0.220573	0.222821	-2.407738	
16				
257.766454 Kcal/mol 11.177825 eV -100.972903 H				MutD_15_72.log
6	-0.484775	-0.225829	0.044942	
6	2.509793	-4.641887	-0.595778	
12	-2.749276	-0.001408	2.108332	
6	2.713114	-3.340650	-0.481367	
6	-0.695966	0.429261	2.580859	
8	-5.220664	1.208780	-1.398297	
6	2.718297	-2.053072	-0.328924	
6	-2.984768	-0.971556	0.210968	
6	3.837292	2.978111	-0.199959	
6	-5.818171	0.839083	-2.307380	
6	-1.805119	-0.717578	-0.125141	
6	-0.310826	0.155908	1.397924	
12	2.306042	-0.014096	-0.431559	
8	0.396334	-0.037217	-0.862301	
6	4.368813	4.190026	-0.226277	
6	3.271223	1.827105	-0.309284	
16				
259.282431 Kcal/mol 11.243565 eV -100.970487 H				Child_4_12.log
8	6.192067	-0.880978	-0.485136	
8	1.205908	3.323994	0.839801	
6	5.031539	-0.806389	-0.234599	
6	-3.956210	0.132953	-0.228428	
6	3.792246	-0.748111	0.037617	
12	0.011671	2.486348	-0.177283	
6	-4.545006	-0.880634	0.184532	
6	-1.039075	-2.023225	-0.035373	
6	-0.844239	0.178501	1.011528	

6	2.533987	-0.754289	0.237713	
6	-1.985046	1.950600	-1.039517	
6	0.070622	-1.415677	0.131833	
6	-2.807439	0.901724	-0.567689	
6	1.278901	-0.853339	0.358403	
12	-3.014863	-2.278374	0.074538	
6	-1.387864	0.644584	-0.123416	
16				
259.520649	Kcal/mol	11.253895	eV	-100.970108 H MutI_5_69.log
6	-2.445040	5.039723	0.273883	
6	0.415797	0.074706	0.509259	
6	-4.554648	-0.369197	0.323953	
12	-2.557223	2.011457	0.010721	
12	-5.276421	-3.327703	-1.188633	
6	1.447668	-0.745454	0.498207	
6	-1.845735	3.955210	-0.022660	
8	-3.607694	0.481876	0.594074	
6	-0.591288	0.802831	0.276668	
6	-5.406841	-1.318016	0.025938	
6	5.836756	-3.418942	0.366114	
8	7.680070	1.838249	-0.718076	
6	6.840288	2.472865	-1.186201	
6	2.457115	-1.587514	0.439059	
6	4.579143	-3.022077	0.493969	
6	3.504238	-2.345145	0.522971	
16				
259.723448	Kcal/mol	11.262689	eV	-100.969785 H Child_7_27.log
6	7.230148	-0.242587	-0.728204	
6	-3.623269	-3.725552	0.447799	
8	6.577872	0.287609	0.039435	
8	-3.154106	-3.266619	-0.527355	
6	-1.931900	1.001565	1.937755	
6	3.012635	-2.278515	0.006788	
12	-2.946158	2.073299	0.442660	
6	2.188087	-1.338740	0.249743	
6	-0.894754	0.270415	1.837291	
6	1.203660	-0.424654	0.455957	
6	-0.990640	2.370122	-0.593747	
12	-2.822327	0.270459	-1.760719	
6	0.261910	-0.170064	1.398568	
6	0.817853	0.737937	-0.420448	
6	0.390707	1.980159	-0.229816	
6	-0.692489	1.104410	-1.075010	
16				
260.099398	Kcal/mol	11.278992	eV	-100.969186 H Child_9_24.log
12	5.576075	0.127361	0.687915	
8	-4.064532	-1.288008	-0.350098	
6	5.209539	1.206442	-1.076917	
6	-3.041860	-2.192989	-0.593219	
6	3.975203	1.109288	-1.351761	
6	-3.467290	-0.017999	0.024099	
6	4.006419	-0.829076	1.593601	
6	-1.792276	-1.515952	-0.387633	
6	2.777639	0.615674	-1.016003	
6	-4.245115	1.017394	0.301098	

6	2.999789	-0.579480	0.885034	
6	-4.706613	2.340143	0.648122	
6	2.140754	-0.100053	-0.140277	
6	-2.025257	-0.158244	0.003840	
12	-0.009908	-0.598267	-0.127879	
8	-5.657917	1.323005	0.342557	
16				
260.152404	Kcal/mol	11.281290	eV	-100.969101 H MutD_10_64.log
6	-3.807837	1.378534	1.136391	
8	5.608601	1.367815	-0.362620	
6	2.011380	-0.195213	-0.023060	
12	-5.593342	0.123381	-0.553327	
6	1.811960	-1.546090	0.406460	
8	4.075616	-1.255626	0.402166	
6	-2.672609	0.735370	0.840975	
6	-2.142051	-0.182771	0.092947	
6	-4.165350	-1.118261	-1.336380	
6	-3.098027	-0.810977	-0.749346	
6	4.640013	2.347647	-0.724159	
6	3.447133	-0.012179	-0.022892	
12	0.010244	-0.679510	0.087207	
6	3.078174	-2.179578	0.654564	
6	4.202152	1.032550	-0.323625	
6	-5.051031	1.513638	0.927636	
16				
260.656142	Kcal/mol	11.303134	eV	-100.968298 H Child_12_27.log
6	-0.319279	-2.108413	-1.350965	
6	0.390864	3.299132	-0.036794	
6	-1.609240	-1.899890	-1.175775	
12	2.225073	2.789454	-0.618993	
6	-3.029108	-1.963717	-1.003776	
6	-0.408669	2.393277	0.310824	
6	0.904400	-1.947971	-1.062058	
6	3.050372	0.919813	-0.877693	
6	-2.370019	-0.906630	-0.398472	
12	-1.102391	0.501758	0.736766	
6	1.771718	-1.265699	-0.289699	
6	2.613136	-0.228901	-0.681505	
6	-7.788469	1.842202	0.497686	
6	1.389708	-1.320688	1.239970	
8	2.111617	-1.857446	2.068574	
8	0.257800	-0.688758	1.375959	
16				
261.359156	Kcal/mol	11.333620	eV	-100.967178 H Child_5_22.log
8	-5.305722	-1.823966	0.299073	
6	6.310507	-0.570718	-0.449352	
6	-4.251342	-1.293168	0.135800	
6	5.012619	-0.568760	-0.241758	
6	-3.138615	-0.620413	-0.024894	
6	3.757979	-0.466838	0.046903	
12	-3.108783	1.624354	-0.159573	
6	2.443224	-0.236320	0.289703	
6	-1.786119	-0.751430	-0.125558	
8	1.200816	-2.255351	-0.227337	
6	-1.190844	2.522021	-0.507681	

6	1.211433	-1.117662	-0.001908	
6	-0.766262	1.301019	-0.404117	
12	1.121872	1.511653	0.208008	
6	-0.643446	-0.113455	-0.266533	
6	2.487898	1.082802	1.356877	
16				
261.665389	Kcal/mol	11.346900	eV	-100.966690 H MutI_15_67.log
6	-0.836865	3.048057	-0.169282	
6	-2.475438	-2.558674	0.223544	
12	-3.945953	0.074073	0.511719	
6	0.882444	1.205043	-0.369797	
6	-3.152926	1.913699	0.206146	
6	0.933119	-0.025123	-0.353635	
6	5.351601	-0.014477	0.545155	
6	-2.118644	2.585129	0.064913	
6	6.493624	0.567241	0.305304	
6	0.402230	2.478886	-0.359947	
6	0.266236	3.932658	-0.457020	
8	0.555695	-1.231553	-0.202860	
8	1.371636	-2.575891	-0.717489	
6	-3.527149	-1.892323	0.357913	
12	-0.569252	-2.841827	-0.321377	
6	4.242403	-0.628012	0.853154	
16				
262.045135	Kcal/mol	11.363367	eV	-100.966085 H MutD_1_74.log
6	3.254486	-2.036749	0.152097	
12	-2.276237	1.077637	0.753428	
6	0.109080	-0.685956	1.394762	
6	-0.295713	-2.697181	0.224406	
6	4.586453	1.747643	0.620523	
6	0.695759	-1.838722	0.789005	
6	2.026361	-1.955313	0.568644	
6	-0.604462	0.297876	1.651656	
6	-3.443045	0.265619	-0.918510	
8	1.974913	0.621816	-1.843406	
6	3.744435	1.386475	-0.291502	
6	-1.316568	-3.139211	-0.339527	
6	-1.600100	4.030782	-0.367159	
6	2.873172	0.978699	-1.132216	
8	-1.919856	3.194884	0.362239	
12	-2.775396	-1.799085	-0.942072	
16				
262.355146	Kcal/mol	11.376810	eV	-100.965591 H Child_5_56.log
12	2.452347	0.532597	-0.884789	
12	0.799242	-2.346913	0.451347	
6	0.344069	0.259354	-1.143343	
8	-4.380293	0.863241	-0.446248	
6	3.607230	-1.043398	-0.331464	
6	-3.378002	-0.159161	-0.122511	
8	1.770823	2.641761	-0.115632	
6	-1.066998	-1.463167	-0.158306	
6	1.050532	3.513183	0.130397	
6	-2.207594	-0.624322	-0.520408	
6	0.316989	0.004094	0.198247	
6	0.684286	0.638169	2.725246	

6	-0.924553	-0.518456	-1.205194	
6	0.431074	0.400559	1.478664	
6	2.736314	-1.919114	-0.009046	
6	-4.617233	-0.132444	0.573775	
16				
262.514339	Kcal/mol	11.383714	eV	-100.965337 H MutD_16_42.log
6	2.125260	2.552707	0.136788	
12	0.149417	2.749628	0.417465	
12	3.784197	0.126572	-0.876611	
6	-4.427397	-0.481711	-1.060340	
8	-1.533039	2.180335	-0.314859	
6	3.105736	1.943931	-0.344907	
6	-4.329201	-0.883621	-2.293091	
8	-1.525056	1.432927	1.125752	
6	-0.172358	-2.187298	0.818355	
6	-0.858521	-0.995195	0.921107	
6	0.994396	-2.715998	0.348764	
6	2.160849	-2.344870	-0.288514	
6	0.107364	-3.580836	1.121196	
6	-1.233627	0.165576	1.006294	
6	-4.444093	-0.235373	0.219616	
6	3.181822	-1.807394	-0.748167	
16				
262.600564	Kcal/mol	11.387453	eV	-100.965200 H MutD_14_34.log
6	3.844295	2.073637	-0.546304	
6	-0.406892	-0.974597	-0.168607	
6	4.370201	0.935889	-0.388066	
6	3.283861	3.271127	-0.441506	
6	4.903918	-0.196215	-0.195322	
6	-5.059516	1.705475	0.503733	
6	-1.843271	-1.156914	-0.242453	
8	1.724849	0.231452	0.128088	
6	-4.212281	-2.122102	-0.552887	
8	5.762943	-2.313830	0.728164	
6	-1.652299	0.104376	0.188462	
12	-5.315297	-0.443226	-0.047444	
12	-2.821801	1.841636	0.545066	
6	-3.004590	-1.929621	-0.469126	
6	5.343144	-1.325688	0.295523	
6	0.723904	-0.405684	-0.120360	
16				
262.724130	Kcal/mol	11.392811	eV	-100.965003 H Child_9_55.log
8	0.329892	0.941081	-1.362142	
6	0.099749	-3.261929	0.014644	
6	-0.478834	1.560842	-0.635889	
6	1.426332	-3.145686	0.040192	
6	-1.888162	1.422293	-0.204794	
6	2.583748	-2.656429	0.054550	
6	-0.303687	2.777094	0.200750	
6	-1.107563	-2.912908	0.014035	
6	-1.685783	2.875799	0.357666	
6	-2.171033	-2.156441	0.035301	
12	1.771510	2.624819	0.365908	
12	3.310140	-0.712603	0.145307	
6	-2.799493	-1.029741	-0.017870	

6	3.502244	1.381855	0.260962	
6	-2.681353	0.372802	-0.157035	
8	-3.824490	-0.230067	0.623435	
16				
263.099458 Kcal/mol 11.409087 eV -100.964405 H				Child_14_20.log
8	-2.559426	-2.733336	-0.259019	
6	1.081219	4.645514	-0.361410	
6	-3.047701	-1.568382	0.172850	
8	0.879973	3.478623	-0.293903	
12	-0.754732	-2.158822	-0.483355	
6	2.302629	-0.120587	0.216480	
6	-3.722147	-0.557554	0.402740	
6	3.460749	-0.701540	0.410458	
6	-4.121240	0.654943	0.813745	
6	4.668055	-1.164711	0.599944	
6	1.145091	-0.836398	-0.277246	
6	5.880777	-1.719687	0.707182	
6	0.015832	-0.212411	-0.882294	
12	0.829732	1.358579	-0.159741	
6	-4.281102	2.026718	1.169440	
6	-1.292893	0.160864	-0.948468	
16				
263.661016 Kcal/mol 11.433438 eV -100.963510 H				
Original2D_4_1.log				
6	3.022116	0.005803	0.000000	
8	1.532510	-4.430092	-0.000000	
6	-1.398058	-1.900526	-0.000000	
6	-2.891815	-4.029819	-0.000000	
6	2.117806	-0.926430	-0.000000	
12	-0.000000	-0.327905	-0.000000	
8	-4.166093	0.169555	-0.000000	
6	-2.164598	-2.929365	-0.000000	
6	0.393143	1.749208	0.000000	
6	1.564168	4.891453	0.000000	
6	1.747859	2.274036	0.000000	
12	-0.262944	3.778083	0.000000	
6	2.670008	1.263913	0.000000	
6	1.965776	3.699858	0.000000	
6	-5.296891	-0.040328	-0.000000	
6	2.307816	-5.277444	-0.000000	
16				
265.725273 Kcal/mol 11.522953 eV -100.960220 H				Child_18_20.log
6	-4.324680	-1.786113	-0.511587	
6	-1.417885	4.667540	1.101524	
6	-3.099353	-2.072345	-0.220758	
12	1.733717	3.184800	-1.001390	
6	-5.480979	-1.215249	-0.732694	
8	-1.085282	3.717557	0.460360	
6	4.423656	-1.405454	0.183127	
6	-2.186837	0.297523	0.976417	
6	3.200743	-1.936614	0.185131	
6	1.109531	1.237485	-0.793227	
6	2.011074	-2.303746	0.156320	
6	-1.011616	0.319001	0.401222	
8	0.775228	-2.584017	0.165164	

6	0.096045	0.821912	-0.211024	
6	5.559664	-0.761124	0.146279	
12	-0.966696	-1.871901	0.244010	
16				
266.513007 Kcal/mol 11.557112 eV -100.958965 H				MutI_17_67.log
6	-3.438575	2.197160	0.255116	
6	1.617579	3.235634	0.023681	
6	0.374728	3.218861	0.077013	
6	3.826077	0.221394	-0.162949	
6	-0.962116	3.030088	0.125000	
6	-0.375690	-3.232071	0.121314	
12	3.295357	2.159267	-0.024622	
6	-3.930173	-0.177613	-0.588624	
6	-2.129539	2.619795	0.129661	
8	3.605631	-0.986472	-0.084990	
6	-1.620612	-3.220864	0.145505	
8	-3.619409	0.954488	-0.160409	
12	-3.249362	-2.059896	0.077147	
6	2.137665	-2.682915	0.029193	
6	3.461474	-2.292954	-0.012545	
6	0.965563	-3.072612	0.079782	
16				
266.852654 Kcal/mol 11.571841 eV -100.958424 H				
Original1D_15_0.log				
6	0.000000	0.000000	-2.044904	
6	0.000000	0.000000	-3.331199	
12	0.000000	0.000000	-0.030595	
6	0.000000	0.000000	-4.608458	
12	0.000000	0.000000	2.758142	
8	0.000000	0.000000	4.648420	
8	0.000000	0.000000	-5.843117	
6	0.000000	0.000000	-7.111887	
6	0.000000	0.000000	-8.351577	
6	0.000000	0.000000	-9.673812	
6	0.000000	0.000000	-10.957301	
6	0.000000	0.000000	5.889510	
6	0.000000	0.000000	7.139145	
6	0.000000	0.000000	8.439101	
6	0.000000	0.000000	9.720981	
6	0.000000	0.000000	11.028238	
16				
266.963323 Kcal/mol 11.576640 eV -100.958247 H				Child_17_16.log
6	3.926314	-0.208935	-0.741471	
6	-4.975474	-0.648951	0.140788	
6	3.868194	-1.560228	-0.593089	
6	-4.209463	0.389156	-0.217990	
6	3.451683	0.929786	-0.431438	
12	-3.031342	-1.639195	0.260687	
6	2.607830	-1.788075	-0.321549	
6	-3.513036	1.434477	-0.589627	
6	2.339051	0.977534	0.373066	
6	-1.057907	-1.048833	-0.069414	
6	0.223312	2.488845	0.401762	
6	0.178961	-1.226307	0.077886	
12	-1.392973	1.174254	-0.499071	

6	1.549648	-1.230259	0.310540	
8	1.968325	-0.085487	1.218968	
8	1.376313	1.901742	0.384009	
16				
267.276824 Kcal/mol 11.590235 eV -100.957748 H				MutI_5_75.log
6	-1.649989	-1.897641	-1.476691	
6	-0.219213	-2.314381	-0.610358	
6	-0.833009	-1.875886	1.735380	
6	1.717210	-0.977804	-1.267605	
6	1.079604	-2.003989	-1.010867	
12	-1.956426	-0.016425	2.380807	
12	-2.385265	1.698996	-0.242127	
8	-2.377854	-1.048461	-1.555410	
6	4.660817	0.047163	1.257650	
6	-2.802838	1.604952	1.816594	
6	0.376566	2.353774	-1.212808	
6	1.908805	0.334489	-1.439021	
6	-0.772097	2.761032	-0.947353	
6	1.360530	1.445249	-1.400875	
6	-0.452099	-2.372040	0.695513	
8	5.609677	0.695914	1.242720	
16				
268.130709 Kcal/mol 11.627263 eV -100.956387 H				Child_12_50.log
6	9.289098	-2.188327	-1.478996	
6	-6.440740	-1.716940	2.913484	
6	8.186856	-1.722953	-0.963331	
6	-6.666934	-1.538965	1.656163	
6	7.106374	-1.243503	-0.446307	
6	-6.899942	-1.323675	0.388925	
6	6.036593	-0.754523	0.073920	
6	-7.094774	-1.355638	-0.887168	
6	4.970154	-0.258396	0.555789	
8	-7.394598	-0.388003	-1.782429	
6	3.837846	0.269084	0.980578	
6	-7.634775	0.297510	-2.735406	
6	2.748183	0.749264	1.368385	
12	0.389335	2.328829	-1.363728	
12	0.929271	1.675069	1.585205	
8	-0.161764	2.472452	0.380685	
16				
268.731388 Kcal/mol 11.653311 eV -100.955430 H				MutI_14_41.log
8	-7.684063	-1.644472	1.136535	
6	-1.086783	0.573479	-1.475577	
6	3.580353	0.371160	1.419177	
6	4.027170	-0.900148	1.274578	
6	4.174358	-2.100964	0.954754	
6	1.965243	2.292377	0.988451	
6	-1.167807	1.924656	-1.134323	
6	-1.582501	2.593705	0.111132	
6	-0.832663	-0.626098	-1.651323	
12	2.867394	-3.077756	-0.313426	
8	-6.512511	-1.235887	1.235098	
6	-0.435993	3.102492	-1.643060	
6	0.977811	2.869148	0.530723	
6	2.929543	1.415437	1.335689	

6	-0.198916	3.015251	-0.190898	
12	0.422081	-2.267252	-1.527325	
16				
269.178119	Kcal/mol	11.672683	eV	-100.954718 H Child_4_13.log
6	-1.739667	1.652903	0.165840	
8	2.876400	-1.167358	1.156309	
12	0.409945	1.856567	0.032192	
6	1.536807	-1.993177	1.124894	
12	-4.244970	-0.785058	-0.720850	
6	3.031849	-0.477865	0.008328	
6	-2.876938	0.968221	0.638740	
6	1.056751	-1.759827	-0.215340	
8	-4.053475	0.703274	1.008846	
6	3.613092	0.817199	-0.231691	
6	-1.921185	0.224184	-0.182925	
6	-0.396798	-1.914143	-0.378667	
6	2.098781	0.513780	-1.072295	
6	4.052042	2.046457	-0.155468	
6	-1.116671	-0.834073	-0.327878	
6	1.901420	-0.767899	-0.883097	
16				
269.207225	Kcal/mol	11.673945	eV	-100.954671 H Child_3_46.log
6	3.319675	0.222344	-1.320761	
6	-8.140030	-0.480682	-1.054705	
6	2.469258	4.113130	-1.276111	
6	-6.909836	-0.359773	-0.685431	
12	3.641194	-1.778383	-1.259550	
6	-5.650273	-0.235977	-0.307342	
8	2.861419	4.171757	-0.191852	
6	-4.456124	-0.118611	0.051112	
6	3.109120	0.569738	-0.116791	
6	-3.188646	0.005963	0.431578	
6	3.445690	-3.547585	-0.279464	
6	-2.011089	0.121698	0.785051	
6	3.314113	-4.484332	0.580871	
8	-0.801112	0.240621	1.148257	
6	2.823384	1.047605	1.104513	
12	0.922647	0.410039	1.665686	
16				
269.431079	Kcal/mol	11.683652	eV	-100.954315 H Child_9_37.log
6	4.288230	1.680600	-0.586605	
6	-5.098286	-1.805142	-0.815783	
6	3.648606	0.401249	-0.456598	
6	-5.986253	-0.880966	-0.711603	
6	2.818465	1.481411	-0.342199	
12	-4.210602	0.053859	-0.323408	
8	4.560378	-1.827630	-0.383255	
8	-2.826585	1.568539	0.037966	
6	3.593384	-1.071125	-0.484622	
12	0.737433	1.384758	-0.148902	
6	-0.003370	-0.541372	0.451486	
6	2.187285	-1.431371	-0.538924	
6	-0.263214	-0.626190	1.789963	
6	1.020717	-1.284640	-0.142616	
6	-1.777274	2.057799	0.218783	

6	0.206325	-0.512033	3.023724	
16				
269.453280	Kcal/mol	11.684615	eV	-100.954279 H MutD_3_64.log
12	-2.329663	0.402246	0.355315	
8	-2.568659	2.031909	-0.758126	
6	-1.622394	2.585162	-1.408369	
6	1.077573	-0.534058	2.992058	
6	-3.044945	-1.465821	-0.371031	
6	-3.670495	-2.585498	-0.743984	
6	0.152847	0.072466	2.106841	
6	3.787378	-0.495394	-0.666686	
6	0.923891	1.940015	-1.160736	
12	2.321574	0.906470	0.028287	
6	4.635634	-1.419527	-0.963388	
6	-0.278101	2.193460	-1.328289	
8	-1.011859	0.339516	1.655673	
6	5.447974	-2.396610	-1.358027	
6	-4.146465	-3.847377	-0.904170	
6	1.527305	0.173849	1.841845	
16				
269.505061	Kcal/mol	11.686860	eV	-100.954197 H MutD_14_52.log
6	-5.703988	0.680161	2.055576	
12	-3.975629	-1.187969	-1.607764	
6	-1.341741	-0.883355	0.325182	
8	7.165623	1.077868	1.131993	
12	3.459712	-1.170151	0.215628	
8	-1.164407	3.080941	-0.902080	
6	-0.222043	-1.141889	-0.155232	
6	-4.594221	0.129843	1.372149	
6	2.086415	-1.283332	-1.374432	
6	-3.970147	-0.739415	0.411716	
6	0.989144	-1.248166	-0.736793	
6	-0.446197	3.359722	-1.754280	
6	-2.600832	-0.443453	0.754598	
6	5.505905	-0.372277	-0.078239	
6	6.515639	0.318910	0.418869	
6	-3.187722	0.794413	1.238607	
16				
270.342232	Kcal/mol	11.723164	eV	-100.952863 H MutI_14_39.log
6	0.475546	2.213536	2.096434	
12	1.673905	-0.110692	-0.293517	
6	-4.951133	-1.016312	0.237119	
6	-2.470307	-1.100991	-0.010919	
6	3.376266	-1.007575	0.491525	
6	3.292065	1.482796	-0.506893	
6	-5.950724	-0.256712	-0.010120	
6	3.903186	0.342155	-0.292964	
8	-0.084114	-0.664822	-0.286305	
6	-7.482180	1.566252	-0.904287	
6	-3.723345	-1.225136	0.163788	
12	5.772697	0.428064	-1.281289	
8	4.015792	-1.787861	1.154063	
6	1.374240	1.766380	1.270945	
6	-1.269634	-0.800610	-0.134695	
6	-6.709422	0.671718	-0.407332	

16

271.187607 Kcal/mol 11.759822 eV -100.951515 H

Original1D_3_0.log

6	0.000000	0.000000	-9.509686
6	0.000000	0.000000	-8.189936
6	0.000000	0.000000	-6.949713
6	0.000000	0.000000	-10.793027
8	0.000000	0.000000	-5.677757
6	0.000000	0.000000	-4.453635
6	0.000000	0.000000	-3.177564
6	0.000000	0.000000	-1.916641
8	0.000000	0.000000	-0.672687
12	0.000000	0.000000	1.217135
12	0.000000	0.000000	4.003655
6	0.000000	0.000000	6.029350
6	0.000000	0.000000	7.295748
6	0.000000	0.000000	8.604260
6	0.000000	0.000000	9.888651
6	0.000000	0.000000	11.197872

16

271.856531 Kcal/mol 11.788830 eV -100.950449 H

Child_6_21.log

6	2.626405	3.178843	-1.462784
6	-2.502023	-1.437032	-0.342856
6	2.090409	2.232594	-2.135519
6	-1.508948	-2.201021	-0.529305
12	0.850014	2.409972	-0.355854
6	-0.296205	-2.679216	-0.500291
8	4.566634	0.827845	1.371426
6	0.904551	-3.047352	-0.409361
6	-0.775321	1.830119	0.699962
12	-3.602702	0.266360	0.517822
6	-5.524372	1.058061	-0.050781
6	2.173960	-3.265763	-0.228227
6	5.665519	1.140323	1.465225
6	-5.954042	-0.040610	0.448050
6	-1.894733	1.317560	0.955900
8	3.308500	-3.407222	-0.046888

16

272.038588 Kcal/mol 11.796725 eV -100.950159 H

MutI_16_75.log

6	-1.062661	2.289678	0.611012
6	-7.826586	-1.064406	0.816310
6	-1.217795	-0.338560	-0.099660
6	-2.017001	2.673074	1.368885
8	0.138186	2.174442	-0.015054
6	2.159411	-1.753233	0.500961
6	4.728534	-1.805748	0.706511
8	-2.347975	-0.283788	-0.402732
6	1.052539	-1.295591	0.273784
6	0.745560	1.036666	-0.305970
12	5.289872	-0.135108	-0.378358
12	2.832393	1.086914	-0.821279
6	3.492676	-1.990687	0.686054
6	-6.395899	-0.984673	-1.334526
6	-7.089986	-0.940555	-0.234867
6	0.133062	-0.250448	-0.032172

16
272.971576 Kcal/mol 11.837183 eV -100.948672 H

Original3D_3_6.log
6 4.584224 0.448727 -0.039958
6 5.925843 -0.064380 0.537738
12 2.640339 -0.117381 -0.548624
6 0.222197 -1.377851 0.924093
6 -0.461275 -2.306218 1.443710
6 -0.247224 0.935988 0.430119
6 -1.642455 1.149615 0.584863
6 5.680077 1.212551 0.022585
6 0.920953 -0.504694 -1.616151
6 0.491097 -0.249031 0.077947
6 -0.340414 -0.756158 -1.471602
12 -1.903833 -1.120493 0.070729
6 -4.326358 0.507431 -0.191672
8 -4.775099 1.575945 -0.103027
6 -0.685306 2.199381 0.791621
8 -3.920679 -0.615655 -0.300101

16
273.055133 Kcal/mol 11.840806 eV -100.948539 H

Original3D_0_33.log
6 -1.434884 0.876723 0.100845
8 1.206236 -0.886786 0.470829
6 -1.906877 -1.584305 -0.099716
6 -1.118472 -0.493759 -0.128498
6 2.630673 0.669798 -0.764620
6 2.526856 -0.450438 0.232262
6 0.278080 -0.249785 -0.323548
6 -1.369103 2.135328 0.265847
6 3.509997 -0.874251 1.031203
12 -3.284989 3.164789 0.661292
6 -2.008227 -3.007229 -0.315994
6 -3.256444 -2.085243 -0.108361
6 -3.364213 -3.535961 -0.326757
12 0.782857 1.880668 -0.488817
8 3.326419 0.617739 -1.785762
6 4.473337 -1.133063 1.845630

16
274.808724 Kcal/mol 11.916849 eV -100.945745 H MutD_13_50.log

6 -3.774553 -1.369475 2.402219
8 9.228905 -0.436610 0.348664
6 1.690559 -0.473490 -1.469825
12 -2.312565 0.396722 -0.273725
6 -0.213462 0.852874 0.188558
12 0.942710 2.416605 0.941453
6 -0.455863 -1.585235 -0.522821
6 -3.627537 -1.600058 1.023748
6 -0.508266 -0.399146 0.224263
6 8.350246 0.190665 0.852733
6 -2.747180 -2.223228 0.175123
6 -4.649241 2.412620 -0.883549
6 -1.636211 -2.417967 -0.445409
6 2.409580 0.682739 -1.604064
6 0.710695 -1.529610 -1.416467

8	-3.835697	1.811103	-0.243638	
16				
275.001940	Kcal/mol	11.925228	eV	-100.945437 H Child_17_17.log
6	-3.837854	-0.411637	-0.019113	
6	5.438801	2.721408	-0.537976	
8	-3.378666	-1.544056	-0.291715	
6	4.532001	1.787875	-0.224373	
6	-3.959270	0.807496	0.302821	
6	3.667239	0.889270	0.065433	
6	-2.840374	1.619429	0.035460	
12	2.402709	-0.711286	0.551728	
12	-1.353592	-0.798069	-0.355253	
6	0.255132	-2.119045	-0.023680	
6	-2.025523	2.764661	0.160242	
8	0.487566	-0.894064	0.534955	
6	-1.233218	3.812926	0.245880	
6	1.960890	-4.053657	-0.201865	
6	1.401587	-2.914577	-0.049838	
6	-1.602847	1.365389	-0.470260	
16				
277.827617	Kcal/mol	12.047761	eV	-100.940934 H MutD_15_42.log
12	2.230395	0.200440	0.375186	
6	-0.405671	0.256047	0.718924	
6	3.416758	-1.534772	-0.004348	
6	3.550471	1.419650	-0.783970	
12	-5.070942	0.613640	0.367536	
6	4.261892	-2.460405	-0.276291	
6	4.485835	1.885487	-1.615169	
8	-7.020416	-1.073028	-1.649646	
6	5.122187	-3.433612	-0.516716	
6	-3.038543	0.460369	0.577299	
6	-6.349465	-0.906934	-0.719026	
8	0.287379	0.111256	-0.368686	
6	0.367334	0.329955	1.896255	
6	-1.814072	0.341723	0.671180	
6	3.666021	2.952608	-1.379691	
6	1.395731	0.344088	2.637218	
16				
279.178677	Kcal/mol	12.106349	eV	-100.938781 H MutD_14_60.log
6	1.847547	3.254019	0.690492	
6	-4.871828	1.135951	-0.609102	
6	4.859550	-1.201650	-1.116892	
6	3.058033	3.069633	0.075684	
6	3.717355	-0.951141	-0.590048	
6	-3.254285	-1.204918	0.217929	
6	1.061098	-0.916902	2.459128	
8	-4.506372	2.171507	-0.945347	
6	6.059666	-1.487292	-1.592460	
12	1.925768	-0.191827	0.331415	
6	-0.637998	-0.900437	0.451104	
6	2.591307	1.830616	0.207921	
6	0.082039	-0.996334	1.658845	
8	0.090264	-0.561520	-0.574674	
12	-5.224238	-1.143322	-0.411448	
6	-2.027400	-1.107895	0.334160	

16
 281.251092 Kcal/mol 12.196217 eV -100.935478 H MutI_18_65.log
 6 -0.932585 -2.561658 0.206635
 6 -2.144104 -2.081312 -0.051184
 6 0.343487 -2.443401 0.221898
 6 1.596337 -2.163399 0.516851
 6 -3.221206 -1.465972 -0.044143
 6 2.917018 2.396987 -0.160977
 12 1.802739 0.730554 0.170215
 6 -1.094332 1.720710 0.468519
 6 -3.147686 1.687446 -0.110573
 8 2.425339 -1.154870 0.147765
 6 -0.229927 0.768497 0.378525
 6 -3.952570 0.789558 -0.382999
 8 -4.111495 -0.544060 -0.470645
 12 4.206922 -0.937107 -0.561655
 6 2.306264 3.444170 -0.071085
 6 -2.211809 2.586721 0.241919

16
 281.360609 Kcal/mol 12.200966 eV -100.935304 H Child_7_44.log
 6 1.441054 -3.035287 0.050096
 6 1.388902 3.008673 -0.742657
 6 0.243558 -2.706215 -0.002210
 6 0.473407 2.289655 -0.074144
 6 -0.959238 -2.078714 -0.066779
 12 3.008831 1.457120 0.001042
 12 3.235000 -2.046722 -0.011423
 6 -0.818511 1.768533 -0.138153
 6 -1.905838 -1.304572 -0.126488
 6 -4.841239 0.015105 1.360273
 6 4.375169 -0.216009 0.018008
 6 -4.079363 -0.020324 0.288521
 6 -2.664045 -0.098030 -0.195062
 6 -1.803389 1.051171 -0.171317
 8 -3.866830 -0.052509 -1.110477
 8 1.363233 1.931421 0.975982

16
 282.382517 Kcal/mol 12.245280 eV -100.933675 H MutI_3_65.log
 6 -1.939890 2.532644 0.000000
 6 3.042493 1.512600 -0.000000
 6 -1.284194 -1.798734 0.000000
 12 -2.992092 -3.243978 0.000000
 6 -0.575942 2.570728 0.000000
 6 0.652090 2.446750 -0.000000
 6 2.504599 -1.381459 -0.000000
 8 0.000000 -1.524146 0.000000
 6 1.236509 -1.482819 -0.000000
 6 1.925878 2.006307 -0.000000
 12 -3.216171 -0.425528 0.000000
 6 4.037262 -1.993796 -0.000000
 6 -3.027080 1.667397 0.000000
 6 -3.281785 3.090413 0.000000
 6 3.707163 -0.679981 -0.000000
 8 4.064566 0.660870 -0.000000

283.161357 Kcal/mol 12.279054 eV -100.932434 H MutI_2_73.log

6	2.535262	-0.494784	0.681954
6	-0.475350	-0.344668	-0.616050
8	1.517742	3.966065	-0.718982
8	-3.963280	0.783044	1.787990
6	3.449040	0.648062	1.017592
6	-0.891720	-1.599367	-0.731383
6	1.320829	2.857384	-0.414436
6	1.118243	1.540534	-0.149803
6	2.175579	0.801952	0.506751
6	2.681980	-3.140468	0.481488
6	-0.010414	0.872022	-0.573481
12	1.153036	-1.968073	-0.748518
12	-2.975156	-1.128829	-0.664448
6	-4.577480	0.387797	-0.608184
6	2.755071	-1.848842	0.633905
6	-3.176083	0.182038	1.172235

16

284.158760 Kcal/mol 12.322306 eV -100.930844 H Child_6_35.log

6	14.390954	1.159729	0.711470
12	-0.666924	-2.291381	-0.350366
8	13.307159	1.278390	0.347784
8	-1.628440	-0.605329	-0.376600
6	-4.274903	5.033711	0.057728
6	0.883944	-3.428840	-1.171036
6	-1.584918	0.670375	-0.885831
6	-3.822976	3.827832	0.088308
6	-3.581762	1.203009	0.630310
6	-2.900082	-2.756435	1.900472
6	-2.575599	1.528604	-0.290234
6	-3.439394	2.545469	0.137522
12	-3.124101	-0.838546	1.013645
6	1.692406	-2.657388	-1.779300
6	-1.924461	-3.045752	1.143869
6	-0.852785	1.282127	-1.831412

16

284.537731 Kcal/mol 12.338739 eV -100.930241 H MutD_13_72.log

12	0.838856	2.080773	-0.422351
6	-4.129779	-0.368633	-1.315969
6	3.173547	-1.369575	0.403383
8	2.908623	2.280075	-0.384799
6	1.352810	-3.201489	-0.080129
6	-1.089422	1.459192	-0.000661
6	2.614069	1.062295	-0.066417
6	-1.819636	-0.140149	1.191734
6	-3.505066	-0.242190	-0.137464
6	-0.981173	0.062710	-0.732791
12	-0.028255	-1.779445	-0.643140
6	-3.146699	-0.300208	1.286252
6	3.243070	-0.106283	0.318251
8	-0.980550	1.020348	1.483246
6	-2.217273	0.546000	-0.466917
6	2.313586	-2.404890	0.267114

16

288.829416 Kcal/mol 12.524845 eV -100.923401 H

Original3D_16_7.log

6	1.778637	0.299260	-2.168008
6	1.793200	1.098652	0.019280
6	2.434929	-0.058468	0.473710
6	1.273951	1.280595	-1.289663
6	2.450579	-0.187683	1.887673
6	2.922279	-1.158180	-0.529198
6	0.223623	2.276170	-1.165346
6	-6.381135	-0.365267	0.347615
8	-0.944221	-1.723927	-1.058531
8	-5.295827	-0.857557	0.216213
6	-7.637716	0.132171	0.499709
6	-1.386375	-2.553184	-0.397375
6	-0.344634	2.955358	-0.257868
6	2.481947	-0.659200	-1.698518
12	3.596610	-2.004645	1.268347
12	0.758778	2.195522	1.432193

16

289.099056 Kcal/mol 12.536537 eV -100.922972 H

Child_11_53.log

6	-0.802367	-3.995941	-0.309645
6	-2.693369	4.870247	-0.168692
12	-2.519233	-3.025982	0.097227
6	4.949537	2.298169	0.063381
6	0.384823	-3.605220	-0.379897
6	4.442769	0.938296	-0.110219
6	-0.591136	0.084062	0.424479
8	-3.033505	3.762014	-0.291237
6	-1.865994	-0.381667	0.500130
6	3.522179	2.153614	0.230518
6	0.631186	0.205718	0.287911
6	3.009262	0.792641	0.062644
12	1.771348	-2.139997	-0.290956
6	1.986643	-0.057193	0.057688
6	-2.910628	-1.069554	0.515159
8	-3.391847	2.312075	-0.298261

16

289.390180 Kcal/mol 12.549162 eV -100.922508 H

MutI_17_77.log

8	-3.319256	1.294598	-0.587968
6	3.288081	0.971920	0.181092
6	1.232232	2.478896	0.031617
6	-4.391809	1.344583	-0.170580
6	0.195918	3.253149	-0.051762
6	7.532344	-1.904136	0.038755
8	-0.067276	-1.613090	0.079978
6	-0.830963	4.042054	-0.079589
6	2.252307	1.723769	0.120556
6	-1.403269	-1.761578	-0.545191
6	6.444155	-1.224894	0.157134
6	5.379229	-0.488361	0.203395
6	-0.372828	-2.589768	-1.031428
12	-6.237606	-0.963616	0.608424
12	-3.334475	-1.866384	0.188600
6	4.334141	0.239023	0.229272

16

289.906409	Kcal/mol	12.571548	eV	-100.921685	H	Child_17_31.log
6	-6.757291	-1.001521	0.317632			
8	4.320822	-2.579352	-0.693044			
6	-5.542107	-0.554043	0.126684			
6	3.758570	-1.643549	-0.274475			
8	-4.345910	-0.170892	-0.067569			
12	3.189516	1.635903	-0.358868			
12	-2.564083	0.142155	-0.210754			
6	3.182202	-0.559233	0.158429			
6	-0.512207	0.992995	-1.033090			
6	0.034699	-0.060096	-0.391475			
6	1.785770	2.179132	1.469234			
6	0.787399	-0.892545	0.573482			
6	1.683580	0.900982	1.301911			
6	-0.827321	2.186177	-1.433623			
6	1.871817	-0.424846	0.834038			
6	-0.682528	-1.012576	0.504647			
16						
290.982286	Kcal/mol	12.618202	eV	-100.919970	H	MutD_5_78.log
6	-1.995233	-2.321054	1.131719			
6	9.058694	2.201276	-1.459384			
6	-0.518190	-3.477884	-0.629888			
6	-2.742010	2.255417	-0.288356			
8	3.055247	-1.361229	1.218022			
6	8.900126	2.167807	-0.159386			
12	-5.262176	1.350524	0.149136			
6	8.795020	2.150463	1.130587			
12	-2.901839	-0.401609	1.159658			
6	-1.323917	-2.958226	0.262064			
6	1.085453	-4.485389	-2.397137			
8	-4.037543	4.043907	-1.294508			
6	0.282808	-4.017064	-1.472089			
6	2.044673	-1.329742	1.753739			
6	-2.088708	1.333595	0.275748			
6	-3.860961	3.006067	-0.663223			
16						
291.336504	Kcal/mol	12.633562	eV	-100.919406	H	Child_4_57.log
6	-0.107915	-1.729824	0.102586			
6	-1.084687	3.297700	-0.362688			
12	-2.206605	-1.331795	-0.064427			
6	-1.858703	2.033751	-0.426482			
6	1.266042	-1.556066	0.184312			
6	-0.491484	1.881074	-0.193190			
6	-4.019934	-0.403272	-0.040911			
12	1.302326	0.941405	0.156528			
6	2.493532	-1.283380	0.093814			
6	3.598461	1.001062	0.280324			
6	-5.158801	0.145909	0.115593			
6	-6.352827	0.742178	0.367700			
6	3.710078	-0.644302	-0.057040			
6	4.751473	-1.227666	-0.563661			
8	4.547259	1.741054	0.347758			
8	-0.749767	-2.848343	-0.111176			
16						
291.402235	Kcal/mol	12.636413	eV	-100.919301	H	Child_14_8.log

12	-3.849985	1.296249	0.530441		
6	1.287787	3.661780	-0.046580		
6	-1.547528	-2.086468	-0.496862		
6	2.094487	2.676697	-0.097897		
6	-0.316302	-1.480730	-0.481162		
6	3.673824	0.733698	-0.491226		
6	-2.769656	-1.956248	-0.344827		
8	2.908509	1.668207	-0.289177		
6	1.046552	-1.070376	-0.480368		
12	3.147179	-1.516411	-0.056954		
6	-3.942416	-1.302619	-0.132679		
6	-0.015217	-0.146440	-0.257051		
6	-4.846174	-0.483965	0.168347		
6	-0.808484	0.942239	0.044429		
6	-1.827205	1.585406	0.316964		
8	4.123447	-2.142694	1.303130		
16					
292.654909	Kcal/mol	12.690734	eV	-100.917305 H	Child_12_37.log
8	-4.778816	2.845036	-0.788764		
12	5.294135	2.541587	-0.461720		
6	-3.750100	2.395770	-0.333427		
6	5.183284	0.424346	-0.004674		
6	-1.359842	2.128177	0.885970		
6	4.039415	-0.243085	0.110634		
6	-2.666427	1.908792	0.184910		
6	2.978024	-0.973807	0.248363		
6	-1.839757	0.846813	0.612334		
12	1.120192	-1.685498	0.741533		
6	-1.659979	-0.510532	0.751079		
6	0.187849	-2.606773	-1.216986		
8	-0.907954	-2.677185	-1.568637		
6	-0.772658	-1.502244	0.891430		
6	-3.412773	-1.755425	0.108837		
6	-2.173331	-2.048013	0.345107		
16					
293.178836	Kcal/mol	12.713454	eV	-100.916470 H	Child_18_17.log
6	3.319489	-3.402039	-0.045353		
6	-4.358364	0.792069	-1.334709		
6	2.721917	-2.246456	-0.156351		
8	-4.782453	3.606597	0.216096		
6	2.795099	-0.726278	-0.398182		
6	-3.684904	3.935875	0.203291		
12	4.149080	0.759739	-0.100465		
6	-4.014597	-0.132165	-0.534904		
6	1.602878	-1.316483	-0.177794		
6	-3.511104	-1.182320	0.234001		
12	6.171298	2.887784	0.291152		
6	0.247546	-1.250233	-0.040262		
6	-2.043889	-1.321375	0.169424		
6	-0.838812	-0.452287	-0.076160		
6	-0.991357	-2.145558	0.202418		
8	-4.131040	-1.992444	0.963809		
16					
293.790811	Kcal/mol	12.739991	eV	-100.915495 H	Child_14_13.log
8	7.768777	-0.302701	-0.042612		

6	-5.153764	-2.111209	-0.001809
6	6.549440	-0.263305	-0.023218
6	-3.976195	0.276345	-0.002939
6	5.298760	-0.227387	-0.006185
6	-4.378258	-0.957203	0.002049
6	3.999442	-0.180983	0.050906
6	-3.388038	1.317916	-0.006095
6	2.753481	-0.204219	0.062178
6	-2.353551	3.761222	-0.007180
6	1.413532	-0.296273	0.036429
6	-2.598322	2.413859	-0.009120
6	0.155842	-0.353911	0.028037
12	-2.468005	-2.818276	-0.016370
12	-1.574231	-0.360189	-0.011760
8	-0.447201	2.689260	-0.007482

16

293.935299 Kcal/mol 12.746257 eV -100.915265 H

Original2D_3_2.log

6	1.612544	4.011911	-0.000000
8	-0.000000	-1.346774	0.000000
6	0.701555	3.031589	-0.000000
6	-0.700953	1.511889	-0.000000
6	-1.520705	0.429321	0.000000
12	1.691788	-0.272906	-0.000000
6	-1.303572	-0.886959	0.000000
6	2.529501	4.913914	-0.000000
6	-1.823203	3.877372	-0.000000
6	0.752774	1.580459	-0.000000
12	0.513110	-3.427323	0.000000
6	-1.847605	-3.126123	0.000000
6	-0.832707	2.998712	-0.000000
6	2.460680	-2.381364	0.000000
8	-2.289834	-1.855572	0.000000
6	-1.384996	-4.290468	0.000000

16

293.995668 Kcal/mol 12.748875 eV -100.915168 H

MutD_15_52.log

6	1.647861	-0.961808	0.146950
8	4.018274	-1.547506	0.596168
6	-4.851702	-0.216726	-0.623707
6	8.227522	0.820570	0.168153
8	10.650195	0.577674	-0.310478
6	-11.038428	0.786599	0.916533
6	0.427939	-0.719524	-0.029385
6	-3.561295	-0.284221	-0.522008
6	5.611673	0.868027	0.203297
6	-6.146038	-0.194652	-0.708181
6	2.908529	-1.246696	0.386748
12	-1.583472	-0.300642	-0.281443
6	6.921840	0.823123	0.178690
6	9.477517	0.689810	-0.126839
6	-9.786821	0.816548	0.690646
12	-8.114806	0.356671	-0.249464

16

294.443721 Kcal/mol 12.768304 eV -100.914454 H

Child_6_28.log

6	2.782360	-2.231518	-0.027521
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12	-3.025736	1.976905	0.140806		
6	1.719709	-2.947101	0.006827		
6	-1.284275	3.015838	-0.183549		
6	3.757111	-1.342818	-0.076463		
6	-0.020328	2.981538	-0.195814		
6	4.681417	-0.394952	-0.128951		
6	-4.134706	0.329695	0.300321		
12	-0.289737	-2.464360	0.184348		
6	1.253969	2.721949	-0.163748		
6	-2.337956	-2.241571	-0.288278		
6	-3.762622	-0.843282	0.037495		
6	2.450086	2.301201	-0.045225		
8	0.214221	-0.634937	0.446317		
8	3.584965	1.936169	0.091779		
6	-3.539399	-2.109043	-0.602865		
16					
294.514396	Kcal/mol	12.771369	eV	-100.914342	H Child_3_10.log
8	2.849514	-0.709126	2.958587		
8	-8.074845	0.008432	0.361780		
6	2.862402	-0.466754	1.804260		
6	-6.913627	0.012500	0.223599		
12	3.476844	2.160585	-0.171344		
12	-4.853279	0.023347	-0.025137		
6	3.244106	-2.504275	-0.730092		
6	-2.909878	0.053139	-0.277948		
6	3.061829	-0.195110	0.530167		
6	-1.690472	0.082616	-0.476148		
6	-0.362890	0.091862	-0.689194		
6	3.001064	-1.201115	-0.608164		
6	0.844528	0.051770	-0.870842		
6	3.175372	-3.598471	-1.418525		
6	2.245584	-0.042709	-0.807388		
6	3.161960	4.282941	-0.713920		
16					
294.819665	Kcal/mol	12.784607	eV	-100.913855	H Child_11_49.log
8	-3.763108	0.639835	-0.298220		
6	7.867475	-1.252116	1.330133		
6	-1.943726	1.614038	-0.165486		
6	6.678206	-0.887074	0.778609		
12	-2.902184	-1.543060	-0.638692		
6	-5.180802	-0.681108	1.692952		
6	-1.245554	2.636494	-0.213509		
8	-6.299332	-0.716737	1.502727		
6	5.485942	-0.581569	0.281792		
6	0.106397	2.758416	-0.237550		
6	4.375827	-0.182063	-0.133099		
6	-1.246147	-2.501861	-1.377390		
6	-2.452798	0.366087	0.021561		
6	1.317014	2.457008	-0.287113		
6	0.005195	-2.446920	-1.183185		
12	2.726963	0.944662	-0.418170		
16					
295.082541	Kcal/mol	12.796006	eV	-100.913436	H MutI_17_45.log
6	2.358625	0.202353	1.121529		
6	1.145115	-3.066319	-0.555581		

6	-2.255961	1.345874	-0.188844
6	-0.047189	2.876498	-0.899956
6	-0.972441	1.863784	-0.412699
8	0.848780	-1.702801	-0.105663
6	1.547288	-0.573804	0.234081
6	0.364135	1.672153	-0.229118
6	-3.490765	1.984545	0.235246
8	-2.245986	-1.133969	0.022050
12	8.101953	0.596772	0.082965
6	-5.329848	-0.015338	0.534539
12	-1.031632	-2.485175	-0.224760
6	1.294442	0.750064	0.214373
6	-2.759082	0.037792	0.017257
6	-4.132021	0.481563	0.324250
16			
295.191128 Kcal/mol 12.800715 eV -100.913263 H MutI_14_45.log			
8	1.671341	-2.658250	-0.598101
6	-8.007878	0.396826	-0.034266
6	-0.391173	-0.623622	0.197627
6	0.885710	-0.565185	0.336051
6	-6.782160	0.251490	0.022582
6	3.924949	-2.051565	-0.102573
6	2.944920	-2.677622	-0.730543
6	-4.234277	-0.099419	0.111525
6	-1.619871	-0.536815	0.171863
6	4.033747	-0.894481	0.405622
6	-5.440100	0.069580	0.078487
6	3.501301	0.301147	0.805357
12	3.276942	2.404445	0.930905
6	2.101100	0.060620	0.444060
8	-2.908746	-0.313541	0.146741
12	2.089860	2.761272	-1.482894
16			
296.962766 Kcal/mol 12.877541 eV -100.910440 H			
Original3D_0_63.log			
6	0.426353	-1.829759	0.194632
6	2.215629	-1.443803	-0.315564
6	0.391744	-1.326653	-1.335243
12	-1.261591	-0.128450	-1.573245
6	0.900107	-0.942766	1.329782
8	-3.355223	-1.073239	0.666981
6	-4.407260	-0.801674	1.070604
6	1.730751	-0.847241	-1.540416
6	-0.148110	2.636639	0.214608
6	-1.542596	2.482314	-0.044578
6	2.219729	-0.537239	0.746755
8	-1.793694	1.515832	-0.937084
6	1.066017	2.846665	0.456357
6	0.376678	-0.541984	2.473770
6	1.056840	-2.966323	-0.223599
12	2.551261	1.469301	0.239760
16			
299.284919 Kcal/mol 12.978239 eV -100.906739 H			
Original1D_18_0.log			
6	0.000000	0.000000	1.750737

6	0.000000	0.000000	2.996238	
12	0.000000	0.000000	4.987441	
8	0.000000	0.000000	6.809044	
8	0.000000	0.000000	8.177263	
6	0.000000	0.000000	9.447611	
6	0.000000	0.000000	10.760043	
12	0.000000	0.000000	-0.275429	
6	0.000000	0.000000	-2.304236	
6	0.000000	0.000000	-3.551983	
6	0.000000	0.000000	-4.886895	
6	0.000000	0.000000	-6.134114	
6	0.000000	0.000000	-7.448170	
6	0.000000	0.000000	-8.706679	
6	0.000000	0.000000	-10.016670	
6	0.000000	0.000000	-11.311650	
16				
300.460724	Kcal/mol	13.029227	eV	-100.904866 H MutI_12_73.log
6	-2.188161	-2.610791	-0.437559	
12	-4.438328	1.408368	-0.437902	
6	-2.951860	-1.400030	-0.287164	
12	1.593659	-0.978693	0.586077	
6	0.781850	4.414834	0.019189	
6	3.318793	-0.102428	-0.153935	
6	-2.556833	1.119809	0.653815	
6	2.513154	0.995116	0.059193	
6	-4.067686	-0.729548	-0.612367	
6	-0.020090	-2.283438	0.877759	
8	-1.068300	-2.418241	0.256739	
6	-2.641711	-0.100451	0.337751	
6	4.478761	-0.583908	-0.496453	
6	1.913913	2.094702	0.146201	
8	5.443938	-1.271730	-0.694978	
6	1.275025	3.246742	0.181540	
16				
300.478954	Kcal/mol	13.030017	eV	-100.904837 H Child_8_55.log
12	2.177708	-0.605386	0.177233	
6	-6.136904	3.143879	1.412828	
12	5.080557	-1.456410	0.767418	
6	-5.611379	2.248306	0.637199	
6	0.239903	-1.375480	-0.080844	
6	-5.031804	1.423897	-0.160753	
6	-1.017531	-1.921386	0.108943	
6	-4.445425	0.596828	-0.955055	
6	4.014365	0.303330	0.246922	
6	-3.862287	-0.251697	-1.743348	
6	4.430543	1.485210	-0.019025	
6	5.158831	3.879048	-0.724597	
6	-2.285943	-2.040974	0.366093	
6	4.851493	2.694238	-0.330516	
8	-3.412087	-2.287773	0.664101	
8	-0.203208	-2.258432	-1.149463	
16				
300.546918	Kcal/mol	13.032964	eV	-100.904728 H MutI_14_53.log
12	3.071680	2.270656	-1.405323	
6	-4.037841	1.466347	0.601275	

6	1.405336	-0.628660	-0.405981	
8	4.444295	1.358791	-0.190881	
6	-3.995480	2.697401	0.994462	
6	0.241010	-0.991757	-0.844029	
6	-3.935511	-2.156412	-0.652143	
6	-4.050972	0.251736	0.214765	
6	-3.857975	3.907692	1.426231	
6	3.581455	0.419947	0.100170	
6	2.302416	0.415008	-0.549223	
12	2.926783	-1.345064	1.130235	
8	-0.823402	-1.437850	-1.208569	
6	3.220823	-2.802274	2.790375	
6	-3.996880	-0.955704	-0.198001	
6	-3.701164	-3.369097	-1.061794	
16				
300.679454	Kcal/mol	13.038712	eV	-100.904517 H Child_1_46.log
12	-3.834241	0.936322	-0.595612	
6	9.718583	0.534425	0.775407	
6	-3.462106	-1.333135	-1.085561	
8	-1.711912	-2.427631	3.430032	
6	0.631373	-2.073196	-2.367480	
6	-3.436745	3.205303	0.709008	
12	-1.309525	-1.157948	-1.677324	
6	1.173951	-1.344069	-1.472922	
8	8.994768	0.683511	-0.107113	
6	0.438868	0.394302	0.007707	
6	-1.302185	-2.652881	2.375939	
6	1.325480	-0.271036	-0.657086	
6	-2.353259	2.550343	0.572965	
6	-1.155609	1.831248	0.428071	
6	-0.010033	1.286447	1.168241	
6	-0.991262	0.640996	-0.338978	
16				
300.746657	Kcal/mol	13.041626	eV	-100.904410 H MutI_11_75.log
6	-1.244086	-2.041248	0.582279	
6	-5.539297	0.267289	0.292866	
6	-2.221267	0.931342	-0.614523	
6	6.263257	2.031147	0.610462	
6	5.541565	-0.076013	-0.697305	
6	-3.353176	1.464849	-0.539487	
12	-3.194330	-1.392070	0.739170	
6	-0.031569	-2.105361	0.215356	
8	5.531890	-1.416603	-0.464241	
8	-5.667603	1.507282	-0.230466	
6	-5.150197	-0.814372	0.757223	
12	-0.528114	-0.303367	-0.642663	
6	-4.549648	2.195529	-0.670670	
6	5.367058	-2.601017	-0.453637	
6	6.604048	3.116269	1.205272	
6	5.939152	0.901555	0.045426	
16				
302.631255	Kcal/mol	13.123350	eV	-100.901407 H MutI_14_47.log
6	1.587238	-2.796296	-0.160616	
6	3.102010	-1.281214	-0.703713	
6	-1.067413	-1.126565	0.716320	

6	0.540038	-2.718304	0.420353	
6	1.599187	1.939014	0.251366	
12	-0.442520	1.707444	0.640664	
6	3.659519	3.695933	-0.163005	
6	-5.430762	0.274311	-1.250138	
6	2.940976	2.611620	-0.041393	
8	-0.676901	-2.376970	0.925845	
12	-3.705580	0.179805	-0.171808	
8	2.804021	-2.597068	-0.722059	
6	-5.534975	1.189606	-0.342937	
6	3.035586	-0.100263	-0.416071	
6	2.632441	1.188287	-0.125874	
6	-1.603807	-0.018578	0.606282	
16				
303.475475	Kcal/mol	13.159959	eV	-100.900061 H MutI_13_41.log
8	1.050789	3.022158	0.143120	
6	-2.676508	-2.333813	0.500708	
6	-2.455475	0.936037	-0.607068	
6	3.224959	-2.239021	-0.349485	
6	-3.434302	-1.206424	0.421385	
6	-2.419245	-0.317240	-0.246561	
8	3.248657	-3.304621	-0.796380	
6	4.333268	1.403714	0.988147	
12	-5.420713	-0.828823	0.882349	
6	-0.267887	-1.803232	-0.577462	
6	-2.797595	3.448254	-1.157754	
6	3.212700	1.901877	0.609358	
6	-2.611844	2.189729	-0.887956	
6	2.084211	2.496121	0.360931	
6	-1.477857	-1.443313	-0.249722	
12	5.197203	-0.499213	0.150897	
16				
304.145713	Kcal/mol	13.189023	eV	-100.898993 H MutI_16_67.log
6	-2.190764	-2.344511	0.867568	
8	-0.742913	0.166471	-0.015697	
6	-3.630832	-1.376863	-1.172594	
6	-3.087514	0.118346	-1.066527	
6	-1.830220	-0.450054	-0.688613	
6	5.699585	-0.334317	-0.627896	
6	1.720940	-0.561320	0.074715	
6	0.525053	-0.233209	-0.091224	
8	-1.391293	6.747401	0.764507	
6	-0.674710	7.139774	-0.058993	
12	3.787133	-0.237138	-0.202265	
6	-4.584888	-2.021904	-1.817262	
6	-2.488671	-1.625893	-0.283963	
6	6.807087	-0.721562	-1.124689	
12	0.276909	-1.783986	1.767650	
6	-1.547544	-2.764734	1.860295	
16				
305.175939	Kcal/mol	13.233698	eV	-100.897351 H Child_14_11.log
6	6.934132	-1.402006	-0.162297	
8	-6.602079	-1.133372	0.234193	
6	5.849461	-0.757897	0.087748	
6	-5.409764	-1.083977	0.225413	

6	4.677851	-0.175806	0.250333	
6	-4.145528	-0.678393	0.098984	
6	3.510808	0.319416	0.378799	
8	-2.935880	-1.246161	0.204148	
12	1.970065	-1.302887	0.005042	
12	-2.528943	0.678890	-0.203003	
6	2.280910	0.929089	0.400454	
6	-1.153992	2.216531	-0.289133	
6	0.427158	-2.630783	-0.973859	
6	-0.666579	3.533196	-0.474596	
6	1.318847	1.743827	0.316605	
6	0.211732	2.407508	-0.046984	
16				
305.256191 Kcal/mol 13.237178 eV -100.897224 H				Child_11_31.log
6	10.726381	-1.078553	-1.066512	
6	0.780180	0.998463	0.028322	
6	-3.379573	-2.317176	-0.008047	
6	1.816201	1.721160	0.240349	
6	-3.490345	-1.173090	-0.578289	
6	-2.528408	2.240321	0.559019	
6	9.844847	-0.694413	-0.183702	
6	-3.661744	2.542790	0.060710	
6	-3.211631	-3.510014	0.536531	
6	2.916260	2.365505	0.546636	
6	8.933708	-0.307050	0.659902	
12	-1.179122	0.055662	0.057834	
6	-2.558271	-4.529082	0.996658	
8	-2.569987	-0.258669	-1.203989	
12	-4.261330	0.809297	-0.832638	
8	-1.410039	1.767085	1.022510	
16				
306.833390 Kcal/mol 13.305572 eV -100.894710 H				Child_2_57.log
6	7.423518	-0.493312	0.456386	
8	-5.382715	1.274971	-0.167381	
12	5.441233	-0.175372	-0.274249	
6	-0.526320	1.949130	0.207455	
6	3.220356	-0.362805	-0.834007	
6	-1.345105	0.999393	0.138164	
8	2.142541	-0.652991	-1.120754	
6	-4.423314	0.585906	-0.231952	
6	0.988457	-1.780189	1.411936	
6	0.343416	2.953000	0.250996	
6	-0.188219	-1.630962	0.898804	
6	1.224037	3.905497	0.315479	
6	-2.046584	-0.160442	0.065255	
6	-1.381044	-1.457897	0.331583	
6	-3.447973	-0.281941	-0.251917	
12	-3.201731	-2.351971	-0.246086	
16				
307.259242 Kcal/mol 13.324039 eV -100.894031 H				
Original2D_0_8.log				
6	-0.000000	-0.600357	0.000000	
6	3.925781	-0.120189	0.000000	
6	-0.118769	0.805145	-0.000000	
6	0.014394	-1.864613	0.000000	

8	-3.010251	-0.361825	-0.000000	
12	2.335247	-1.255399	0.000000	
6	3.935430	1.138759	0.000000	
6	-1.501415	1.360510	-0.000000	
6	3.835276	2.474754	0.000000	
6	-3.610369	-1.521712	-0.000000	
8	0.796382	1.686073	-0.000000	
6	-1.555264	2.725251	-0.000000	
12	-1.704571	-2.802806	-0.000000	
6	3.539162	3.727468	0.000000	
6	-2.943103	1.012904	-0.000000	
6	-3.830650	-2.787174	-0.000000	
16				
311.820384	Kcal/mol	13.521829	eV	-100.886763 H MutI_8_69.log
12	2.489441	-1.966182	0.522376	
6	1.377905	2.115841	-0.143818	
6	0.088158	1.727766	0.188693	
6	-2.548722	-0.514110	-1.048413	
6	3.972469	-0.451468	-0.319783	
6	-1.620947	-0.023208	-0.160041	
6	0.401771	-3.267866	0.320202	
6	0.622750	-0.725093	0.457095	
6	-0.246957	0.250684	0.137817	
8	-0.211322	-2.185593	0.376488	
12	-4.546849	-0.867149	-0.545564	
6	-2.917900	0.223667	0.227706	
6	2.488667	2.660494	-0.561604	
6	-0.933036	2.549503	0.548987	
8	4.155150	0.536122	-0.868453	
6	-1.827778	3.319746	1.055490	
16				
314.888967	Kcal/mol	13.654895	eV	-100.881873 H Child_4_33.log
6	1.494957	-3.229516	-0.491824	
12	-7.576122	-1.014152	-0.824428	
6	1.489939	-2.683839	0.649890	
6	-2.604172	0.207556	2.325952	
12	2.229505	-1.549191	-1.509346	
6	-1.715186	0.963526	1.665848	
6	1.726873	-1.579466	1.471744	
6	1.551566	4.164731	-0.951832	
8	2.892941	-0.261073	-0.218407	
6	-0.836598	1.636968	0.927320	
6	2.393385	-0.482246	0.970482	
6	0.721504	3.264183	-0.421848	
6	0.684665	0.223626	-2.079549	
6	-0.015620	2.287460	0.107615	
6	1.545039	-0.261292	2.123979	
8	0.299720	0.722320	-1.004265	
16				
315.818386	Kcal/mol	13.695199	eV	-100.880392 H Child_12_11.log
6	5.313310	-0.492859	-0.869234	
6	-2.623992	-2.289815	-0.604708	
8	3.791997	1.373038	-0.193834	
6	-4.037990	-0.301040	-0.238713	
6	4.214025	-0.021736	-0.280602	

6	-4.730219	0.740270	-0.102300
6	2.517223	0.903548	0.331533
8	-3.164120	-1.240885	0.157120
6	2.911519	-0.432898	0.295642
6	-1.416411	-2.577812	-0.015388
12	0.632075	1.913758	0.389180
12	-3.030149	1.923594	-0.146668
6	2.108250	-1.548687	0.388882
6	-0.197398	-2.583376	0.231966
6	1.070345	-2.223111	0.462740
6	-1.169685	2.976609	-0.035891

16

317.613424 Kcal/mol 13.773039 eV -100.877531 H

Original2D_1_1.log

12	-1.105732	2.198597	0.000000
6	0.709250	0.468197	-0.000000
6	0.000000	-0.719619	-0.000000
6	-1.423704	-0.498769	0.000000
6	0.362060	-2.127163	-0.000000
6	-0.863118	-2.816908	-0.000000
8	4.403822	-0.237376	-0.000000
6	3.772440	-1.264958	-0.000000
6	-1.958402	-2.461614	-0.000000
6	1.641590	-2.511814	-0.000000
6	-2.286278	0.362946	0.000000
6	0.381882	5.148162	0.000000
8	-0.534434	4.446362	0.000000
6	2.882327	-2.235325	-0.000000
6	0.942529	1.671016	0.000000
12	-3.554148	-1.511664	0.000000

16

317.720142 Kcal/mol 13.777667 eV -100.877361 H

MutI_13_61.log

6	4.610661	-1.303800	0.593303
12	-1.494679	-1.457204	-1.118140
6	-2.449611	-3.359289	-0.715801
6	-2.941088	-2.015058	1.459473
6	-2.873533	-2.875021	0.400257
6	3.585632	-0.570351	0.910105
6	-0.109976	-0.167819	-1.765416
6	1.681343	1.619795	-1.845672
12	-0.925397	4.583909	0.387071
6	-1.463405	1.433374	0.551070
6	-1.999776	0.195231	0.624397
8	0.798178	0.748228	-1.742607
6	-0.819360	2.518477	0.444367
6	-2.576518	-0.771950	1.295705
8	2.632794	0.055445	1.185302
6	5.621153	-2.028562	0.253423

16

318.911191 Kcal/mol 13.829316 eV -100.875463 H

Child_12_24.log

6	7.734623	-0.136773	0.075327
12	-7.807603	-1.917286	-1.050046
6	6.902057	-0.222390	-0.901414
8	-4.418298	0.493489	1.614819
12	5.086270	-0.827677	-0.361445

6	-3.802169	1.209425	0.883466	
8	2.391348	1.890634	0.302856	
6	-3.130209	1.941938	0.067903	
6	1.714883	2.548323	0.964247	
6	-2.451670	2.692720	-0.736726	
6	1.869821	-1.680595	0.109314	
6	0.582184	-1.848855	0.273249	
6	-1.735112	3.428747	-1.561461	
6	-0.676227	-2.012300	0.453463	
6	3.108334	-1.465867	0.014028	
6	-1.971248	-2.143278	0.624684	
16				
321.222707	Kcal/mol	13.929553	eV	-100.871779 H MutI_3_73.log
6	3.068364	0.134686	-0.333468	
6	-3.953716	0.842563	0.825605	
6	3.536245	-1.113950	-0.272218	
6	3.642985	-2.388621	-0.217053	
6	3.237141	1.625254	-0.010272	
12	-1.616499	-1.690645	-0.779967	
6	0.104764	-2.201987	1.002381	
8	0.858528	-1.781328	1.751834	
6	4.045912	2.554239	0.436059	
6	-0.416677	0.060014	-0.816889	
6	2.017346	0.975586	-0.514846	
12	-2.304480	2.136029	0.476819	
6	0.671940	0.948096	-0.642665	
8	-3.734101	-0.150661	0.019373	
6	-0.652605	1.408005	-0.434621	
6	-3.625644	-1.158665	-0.777328	
16				
321.589367	Kcal/mol	13.945452	eV	-100.871195 H Child_1_23.log
6	9.080129	-1.690588	1.512574	
6	0.692376	3.316501	0.438189	
8	8.991913	-2.034668	0.439201	
6	-0.175273	2.479377	0.846800	
12	-3.075810	-2.641364	-0.886955	
6	-1.073780	1.456386	0.687562	
6	-3.836160	-1.311806	0.654523	
12	1.326281	1.801205	-0.936335	
6	-3.164480	-0.134148	0.924162	
8	-0.185699	0.502791	-0.533662	
6	-1.323667	-1.680324	-1.235801	
6	2.925808	2.029807	-2.480662	
6	-0.733461	-0.623586	-0.936781	
6	-2.249237	0.915902	1.032590	
6	-3.448855	0.955305	1.794928	
6	-4.935963	-1.990003	0.534442	
16				
327.749516	Kcal/mol	14.212582	eV	-100.861378 H MutI_6_69.log
6	-0.898164	-0.787955	0.248478	
6	2.676952	0.387436	-0.060452	
6	3.546658	-0.779393	-0.062811	
6	-2.310599	-0.759956	0.172275	
6	-0.881974	2.771210	0.090467	
6	2.126937	1.557825	-0.113517	

6	2.976688	-2.110596	-0.028262	
6	2.869290	-3.360616	-0.045330	
6	1.516552	2.729891	-0.149915	
6	-1.479999	1.741768	0.194205	
6	-1.639148	0.413296	0.288519	
12	-4.208037	-0.837388	-0.070108	
8	0.275589	3.399720	-0.110523	
8	-5.790520	-1.394411	-0.266004	
6	4.898029	-0.622090	-0.054601	
12	1.184048	-1.089894	0.081598	
16				
327.874268 Kcal/mol 14.217992 eV -100.861179 H				Child_11_41.log
6	-5.368544	1.338829	-0.616734	
12	2.009471	0.079337	0.527185	
6	-4.387705	0.492847	-0.723265	
6	3.759754	-1.380939	0.684699	
6	-3.238547	-0.128972	-0.895451	
12	-1.553032	0.633954	1.416050	
8	-1.635132	-2.602027	0.475789	
6	-2.185440	-2.668499	1.461493	
6	-2.073270	-0.648748	-1.174740	
8	2.926401	2.429440	0.419914	
6	-0.872679	-0.201204	-1.032100	
6	2.964023	3.451421	-0.167101	
6	4.111575	-1.804229	-0.470743	
6	4.734135	-1.951689	-1.669337	
6	-0.213819	1.760425	0.068323	
6	0.135947	0.544293	-0.545784	
16				
328.464215 Kcal/mol 14.243574 eV -100.860239 H				MutD_15_50.log
6	4.907933	-2.577849	-0.402229	
6	0.988753	4.094140	0.036186	
6	3.124060	-0.806285	0.031269	
6	-0.795281	0.126386	2.338391	
8	-2.841010	0.825615	-1.142154	
6	-1.749762	-2.878157	-0.466192	
6	-0.172899	3.387631	-0.038712	
12	1.724618	0.783949	0.264896	
6	-0.261092	-0.725138	-0.001667	
6	1.494908	2.893463	-0.184108	
8	0.569137	-0.394097	-0.934355	
6	-1.216031	-1.751156	-0.210837	
6	-0.153527	-0.036662	1.220304	
12	-3.457417	-1.865548	0.411946	
6	3.999173	-1.637819	-0.251672	
6	-3.671473	1.499289	-0.655739	
16				
328.624179 Kcal/mol 14.250511 eV -100.859984 H				
Original3D_2_6.log				
6	0.564541	1.555743	-1.664446	
6	-0.706436	1.258605	0.590029	
12	3.247679	-1.206909	0.296328	
6	1.577956	1.805579	-0.627438	
12	-0.489679	-2.008420	-0.142662	
6	1.620620	-2.231574	-0.624993	

6	0.264967	1.874259	-0.264448	
6	-3.014650	-0.800005	-0.813300	
6	-2.071476	1.275765	0.358816	
6	3.806976	0.804712	0.136917	
8	-1.001086	-0.912328	1.486990	
6	-2.470347	-1.903847	-1.061706	
6	-3.044879	0.456495	-0.246170	
8	-0.093672	0.258029	1.231815	
6	2.864872	1.565425	-0.177077	
6	-3.448465	1.641899	0.461410	
16				
328.961658	Kcal/mol	14.265146	eV	-100.859446 H MutD_9_74.log
6	-3.812584	-1.399651	-0.342729	
6	-2.452723	-1.479351	-0.273820	
6	-1.061616	2.104915	-0.109247	
6	2.642432	2.238971	0.254706	
12	-3.058993	0.608561	-0.116644	
6	1.572172	-0.067170	0.029746	
6	0.946754	-1.212160	-0.125696	
8	1.004785	-2.171531	1.061993	
6	2.080069	0.989838	0.432452	
6	-1.277975	-1.908121	-0.090852	
12	5.495165	-1.463195	-0.522105	
6	0.024000	-2.260107	-0.085521	
6	-2.291775	2.608335	-0.267969	
8	2.441688	3.375985	-0.159126	
6	-1.018363	1.109107	0.774084	
6	-4.818032	-0.621277	-0.121477	
16				
329.363377	Kcal/mol	14.282566	eV	-100.858806 H
	Original2D_13_2.log			
6	1.865751	1.480191	0.000000	
6	3.272171	1.547095	0.000000	
12	0.000000	0.618672	0.000000	
6	0.418254	-1.694765	-0.000000	
8	-1.767791	-2.630555	-0.000000	
6	-2.084028	0.946928	-0.000000	
6	-3.310165	3.237588	-0.000000	
6	2.758760	-0.989041	0.000000	
12	-2.667840	-0.962837	-0.000000	
6	1.863316	-2.081282	0.000000	
6	2.257787	-3.372499	0.000000	
8	-0.319286	-2.791947	-0.000000	
6	3.292601	0.114894	0.000000	
6	-2.695324	2.071887	-0.000000	
6	-3.932718	4.357332	-0.000000	
6	4.412044	2.300008	0.000000	
16				
332.742348	Kcal/mol	14.429092	eV	-100.853422 H MutI_2_77.log
8	-2.150883	-1.922375	-0.009389	
6	1.753222	2.105744	-2.259122	
6	3.487951	-0.207095	0.726661	
8	-0.837713	1.741635	-1.066807	
6	-2.714933	3.661179	1.128257	
6	0.364095	-2.260790	-0.201985	

6	0.273788	1.401268	-1.225191	
6	-0.182963	-3.624666	-0.127138	
6	4.524445	0.234234	1.335434	
6	5.535338	0.843007	1.934511	
6	-3.220152	1.074131	0.881723	
6	-0.980098	-2.483641	-0.095942	
6	-2.910198	2.341098	1.006211	
6	1.531126	0.928453	-1.565767	
12	-3.639871	-0.996252	0.435589	
12	1.901458	-0.889715	-0.486951	
16				
333.863046 Kcal/mol 14.477690 eV -100.851636 H				Child_7_19.log
12	-2.201377	2.269937	-0.096888	
6	-0.499892	-2.324781	0.118790	
12	1.761224	1.966357	-0.144208	
6	0.836128	-1.641527	-0.005394	
6	-0.246608	1.645834	-0.504728	
6	-1.766538	-2.221463	0.103798	
6	3.816070	0.333038	-0.124082	
6	2.165226	-1.622804	0.183168	
6	-0.961419	0.311333	-0.192852	
8	-4.124935	-1.556282	0.014031	
6	3.219018	-0.858736	0.083717	
6	-2.915870	-1.255654	0.038775	
6	-2.336904	0.113572	0.001117	
6	-0.174767	-0.813345	-0.316295	
6	5.287218	-1.310809	-0.000518	
8	-0.031082	2.435847	0.808492	
16				
335.054007 Kcal/mol 14.529335 eV -100.849738 H				
OriginalD_13_0.log				
12	0.000000	0.000000	-0.183995	
6	0.000000	0.000000	1.853997	
6	0.000000	0.000000	-2.246806	
6	0.000000	0.000000	-3.525505	
12	0.000000	0.000000	3.927827	
6	0.000000	0.000000	-4.806207	
6	0.000000	0.000000	5.936890	
8	0.000000	0.000000	-6.028402	
6	0.000000	0.000000	7.200414	
6	0.000000	0.000000	8.517037	
6	0.000000	0.000000	-7.293251	
6	0.000000	0.000000	9.784278	
6	0.000000	0.000000	-8.535524	
8	0.000000	0.000000	10.989719	
6	0.000000	0.000000	-9.849924	
6	0.000000	0.000000	-11.138152	
16				
335.246353 Kcal/mol 14.537676 eV -100.849431 H				Child_9_19.log
6	2.792912	3.570147	0.052251	
6	-4.687751	-1.261793	0.227651	
8	1.638293	3.642399	0.029617	
6	-3.406623	-1.609396	-0.049652	
8	2.354330	1.264034	-0.164596	
6	4.023545	-2.103206	-0.017177	

12	-1.311837	-2.045024	-0.046455	
6	1.932099	0.154779	-0.079630	
6	-3.089593	-0.208019	-0.404258	
6	-1.592701	3.040452	0.102376	
6	-3.135340	1.016586	-0.031112	
6	2.746948	-1.780007	0.053779	
6	-2.581456	2.154093	0.127879	
6	-0.222972	2.569779	0.078919	
6	1.491707	-1.117092	-0.033214	
12	1.514701	-3.439091	0.122535	
16				
336.976069 Kcal/mol 14.612684 eV -100.846675 H				Child_12_54.log
6	-1.591812	2.735483	0.446393	
12	3.685683	-2.298474	2.366021	
6	-0.270723	2.804024	0.339072	
6	-4.658183	-2.595485	-0.447270	
6	-2.738038	2.259890	0.480189	
6	-3.436505	-2.217256	-0.610353	
6	0.934926	2.489578	0.176494	
6	-2.087785	-1.905025	-0.755121	
8	-3.811354	1.567234	0.431212	
6	-0.889960	-1.563649	-0.854114	
6	2.008207	1.754433	-0.048333	
6	0.424185	-1.190502	-0.875013	
6	2.933005	0.833678	-0.265483	
6	1.636850	-0.817348	-0.921893	
12	-3.302830	-0.218946	-0.030861	
8	9.038948	0.268030	-1.432377	
16				
338.386720 Kcal/mol 14.673856 eV -100.844427 H				MutD_14_36.log
6	-0.460220	-0.054335	-0.875836	
6	-0.881499	-1.373264	-1.799619	
6	-2.188684	-0.628373	0.406861	
12	-0.447761	-2.162114	0.106841	
6	-1.243337	0.257852	0.189685	
6	0.805675	0.511258	-0.509352	
8	1.548920	-1.694900	-0.302640	
6	-0.304046	2.810360	-0.761574	
8	-0.224194	0.712712	3.054111	
6	3.202905	0.048755	-0.166654	
6	0.550271	1.882357	-0.692514	
12	-2.083199	1.738000	-0.679953	
6	4.335352	0.635775	0.005278	
6	-0.173596	0.268391	1.984879	
6	-2.266410	-1.790209	0.015402	
6	1.919208	-0.410756	-0.318963	
16				
340.845773 Kcal/mol 14.780490 eV -100.840508 H				
Original3D_12_5.log				
6	3.279096	-0.428251	0.360420	
6	2.733001	0.939403	0.827677	
6	1.921679	-0.399484	-0.154964	
6	4.329126	-0.188810	-1.277150	
12	0.632285	0.877558	0.921716	
6	-4.068354	-1.335395	0.705124	

6	3.003045	0.316989	-1.073016	
8	-1.249778	0.961861	0.850938	
6	-2.378802	0.440110	0.578386	
6	4.380783	-1.261368	-0.213048	
8	2.925565	1.698549	-0.536446	
6	-5.718194	-0.661515	-1.146000	
6	-3.023242	-0.701524	1.035985	
6	5.078614	-2.296038	0.211416	
6	-5.074089	-1.210534	-0.186195	
12	-3.980808	0.742044	-0.965695	
16				
341.817091 Kcal/mol 14.822611 eV -100.838960 H				MutD_16_54.log
6	4.737452	-0.356963	-0.431092	
8	-3.861477	2.011507	0.241299	
6	-6.674120	-0.946279	0.341467	
6	10.550514	0.023489	0.236596	
12	1.572516	-0.067769	-0.527930	
8	-10.599405	-0.845130	-0.210706	
6	-8.135989	-0.562301	0.149181	
6	-9.398486	-0.747847	-0.127401	
6	-1.632683	0.990303	-0.063488	
6	9.779345	-0.550638	1.088823	
6	-0.421004	0.647842	-0.194886	
6	-2.873700	1.430027	0.134342	
6	6.068245	-0.266800	-0.607876	
6	-5.542971	-0.345890	0.777804	
6	3.530065	0.183246	-0.362524	
12	8.074738	-0.458910	0.037062	
16				
343.107093 Kcal/mol 14.878550 eV -100.836904 H				Child_3_61.log
6	-2.120725	1.334271	-1.319702	
6	5.158771	-3.232590	-0.601947	
6	-1.451605	2.376495	0.942900	
6	4.589677	-3.344808	0.522672	
6	-2.859089	0.865184	-0.188388	
12	4.456288	-1.226034	0.022601	
6	-1.156646	2.167579	-1.136131	
6	3.795189	0.708267	0.057990	
6	-2.492060	1.629334	0.980415	
6	3.272157	1.840435	0.154303	
6	-0.518551	2.729794	-0.036751	
12	1.583269	2.895740	0.118362	
6	-3.565228	-0.326866	-0.100063	
8	-4.078117	-2.686466	0.577171	
6	-3.926111	-1.469443	0.128521	
8	-4.025552	-3.776332	-0.341481	
16				
343.551130 Kcal/mol 14.897806 eV -100.836197 H				Child_16_20.log
12	-0.486142	3.045646	-0.073961	
6	-1.113709	-2.330833	0.348859	
6	-2.390629	1.833360	-0.456785	
6	0.042336	-2.406146	-0.285197	
6	-1.414231	0.993244	-0.255831	
8	1.021658	-2.270602	-1.025211	
6	0.841737	1.445338	0.015998	

6	-2.270742	-1.568263	0.565410		
6	2.355228	1.186656	0.101388		
6	4.219269	-0.524636	0.966184		
8	-4.804208	-0.195870	0.355996		
6	-3.510746	-0.984096	0.480363		
6	-0.215262	0.459152	-0.056479		
6	2.813882	-0.449805	1.338359		
6	3.572441	0.664447	0.035671		
12	1.543054	-0.560541	-0.878866		
16					
343.738521 Kcal/mol 14.905932 eV -100.835898 H				Child_12_48.log	
6	-6.219157	1.595735	-0.058725		
6	2.310991	-2.577407	-0.193301		
6	-4.789486	1.619335	-0.313964		
6	3.480749	-2.020976	-0.246333		
6	1.628184	4.542812	0.131936		
6	4.636638	-1.463426	-0.318134		
6	-5.507616	0.277490	0.063690		
6	1.067453	-2.835908	0.062045		
8	1.662480	3.416285	0.522264		
6	-0.181355	-2.903333	0.268463		
6	-4.103902	0.359801	-0.200876		
12	-2.094774	-2.382933	0.506055		
6	-2.893548	-0.248174	-0.279217		
12	4.477873	0.598329	0.098262		
6	-1.605273	-0.279893	-0.486340		
8	3.895114	2.211079	-0.250673		
16					
347.090156 Kcal/mol 15.051273 eV -100.830557 H				Child_7_31.log	
8	6.524925	-0.942160	0.831119		
6	-5.326620	-1.625709	0.986813		
6	5.534782	-0.419736	0.411731		
6	-2.994597	1.946265	0.849559		
6	4.466137	0.118442	-0.014603		
6	-0.763380	-1.176969	0.001522		
6	3.340079	0.559334	-0.489955		
6	-4.677145	-1.621738	-0.211445		
6	2.193768	0.946015	-0.894126		
6	-1.814993	1.786827	1.451011		
6	0.894995	1.065261	-1.223437		
6	-4.269059	1.902616	0.499463		
6	-0.324749	0.833772	-1.382959		
12	-2.813282	-1.078678	-0.562385		
12	1.141624	-0.370857	0.691274		
8	-1.211851	-0.119322	-1.012132		
16					
350.846511 Kcal/mol 15.214164 eV -100.824571 H				Child_7_42.log	
6	-2.913004	-2.373071	1.647459		
12	3.982516	1.775575	0.121712		
6	-3.250007	-1.680737	0.634794		
6	2.402723	3.034719	0.119385		
6	-3.920140	-0.801380	-0.095188		
6	4.173051	-0.243654	0.214623		
12	-5.529576	1.769683	-0.147983		
6	1.116268	2.883086	0.205561		

6	-0.380809	-1.539044	-0.548636	
6	3.440438	-1.343957	0.029941	
6	-4.550584	0.110080	-0.749528	
6	-0.227792	2.733128	0.259657	
6	0.892905	-1.769040	-0.280706	
6	2.127093	-1.735284	-0.084878	
8	-1.539206	-1.359521	-0.641696	
8	4.677187	-1.914501	-0.333260	
16				
351.089316	Kcal/mol	15.224693	eV	-100.824184 H MutD_1_68.log
6	4.112388	-1.620813	0.582296	
12	0.267242	1.703831	0.647856	
12	5.094882	-1.000676	-1.482026	
8	-1.395604	3.525703	-1.751427	
6	-1.411791	-0.889434	-1.076781	
6	-1.333364	3.233234	-0.597327	
6	2.590725	0.214994	1.490283	
6	1.829875	1.144644	1.790653	
6	-1.168480	0.406839	-0.239665	
6	-2.036454	-0.127768	0.781236	
6	-3.460768	-2.192666	0.025491	
6	-4.391137	-3.087388	0.142591	
6	3.373488	-0.795689	1.046460	
6	-2.476801	-1.305568	-0.060868	
8	-2.227184	0.232405	1.941890	
6	-1.521546	-1.397508	-2.469980	
16				
351.230608	Kcal/mol	15.230820	eV	-100.823959 H MutD_16_78.log
6	0.431523	-2.032273	0.465757	
6	-3.427196	-1.379513	-0.580491	
6	3.645939	3.699004	-0.123742	
6	2.370574	1.416309	0.395968	
6	2.737370	2.772448	-0.048879	
6	4.256197	-2.084478	0.064515	
8	-1.752889	2.085438	0.068443	
8	3.547292	0.731373	-0.145406	
12	-3.178619	0.608821	0.062991	
6	-2.140909	-1.731184	-0.068147	
6	-4.666105	-0.907435	0.053323	
6	-1.970597	3.224195	-0.146436	
12	2.384368	-2.695256	-0.111245	
6	-0.761926	-1.928610	0.041391	
6	-5.375072	0.184137	0.189174	
6	4.096166	-0.815477	-0.043307	
16				
354.267583	Kcal/mol	15.362516	eV	-100.819119 H
	Original2D_7_1.log			
8	1.788692	2.904683	0.000000	
6	1.207345	-1.712951	-0.000000	
6	2.476848	-2.279106	-0.000000	
6	0.000000	-1.414835	-0.000000	
6	3.051862	-3.484262	-0.000000	
6	5.110858	-2.310877	-0.000000	
6	1.041746	3.801582	0.000000	
12	-1.994107	-1.277553	-0.000000	

6	3.898664	-1.905432	-0.000000	
12	5.039554	-4.532547	-0.000000	
6	-4.944381	0.063710	0.000000	
8	-2.891942	3.939002	0.000000	
6	-3.065205	5.132373	0.000000	
6	-3.495960	6.420798	0.000000	
6	-5.852922	1.030057	0.000000	
6	-4.048750	-0.845772	0.000000	
16				
354.535254	Kcal/mol	15.374123	eV	-100.818692 H Child_9_51.log
6	-1.122681	3.285291	0.080663	
6	-3.149103	-3.365394	-0.049074	
6	-2.099472	2.484784	0.017397	
12	1.705853	-2.113212	-0.376044	
12	0.587344	2.103920	0.019551	
6	-3.675123	-2.216673	0.168850	
6	-3.020226	1.505679	0.031522	
6	3.639476	-1.072078	-0.088333	
6	-3.618998	0.387753	0.081899	
6	1.597688	0.249817	0.029958	
6	-0.198768	-1.012450	-0.210419	
8	-0.462021	0.237327	-0.183544	
6	-3.831656	-0.903316	0.126219	
6	3.449393	-1.832858	0.930687	
6	4.035867	0.535361	0.122255	
8	3.017427	1.242174	-0.212933	
16				
354.843171	Kcal/mol	15.387476	eV	-100.818202 H MutI_10_73.log
12	1.490999	2.157365	0.065816	
6	1.294047	-1.902974	1.287799	
6	-0.359722	3.209496	-0.042427	
6	2.514814	1.075539	-1.498374	
6	-1.579559	2.860597	0.213876	
6	-1.169281	-1.202241	0.691003	
8	2.716074	-0.106628	-1.368688	
12	-5.316703	-1.091770	-0.945645	
6	-2.142498	1.638601	0.382247	
6	-3.585105	-0.763587	-0.178851	
6	3.746754	-1.383007	-1.251204	
6	1.697462	0.587525	1.566784	
8	3.261725	-2.213053	-0.529898	
6	1.690356	-0.678730	1.853463	
6	-0.026355	-1.623083	0.992167	
6	-2.399903	-0.856416	0.274622	
16				
355.506279	Kcal/mol	15.416231	eV	-100.817145 H Child_10_32.log
6	-0.179472	-0.965434	2.552064	
12	1.598016	-2.650160	-0.997795	
6	-6.002877	2.565597	-0.622819	
6	3.050304	-1.552499	-2.192062	
8	-6.994253	2.510762	-1.020988	
6	2.701748	-0.598086	-1.455134	
6	0.671410	-0.884888	1.663252	
12	-1.671193	-1.938488	1.455153	
6	2.050044	-0.021594	-0.280454	

6	-2.721259	-3.011650	-0.092688	
6	2.978115	3.850165	0.330182	
6	1.898771	1.294375	0.042025	
6	1.426880	-1.018213	0.533941	
6	-2.096098	-2.067204	-0.757181	
6	3.416947	5.003420	0.247613	
8	1.708131	2.426717	0.358396	
16				
359.185933	Kcal/mol	15.575796	eV	-100.811281 H MutD_14_42.log
12	-3.483662	-1.926796	0.142400	
8	0.682448	-0.478723	-0.766216	
6	-1.291374	-0.285874	2.103487	
6	0.752413	3.977529	-0.506233	
6	-0.265303	0.093096	1.315897	
6	-0.294673	-0.686789	0.049833	
6	-1.515664	-2.933928	-0.515672	
6	4.573859	-2.698267	-0.644996	
6	-1.249463	-1.712871	-0.232246	
6	-3.395891	1.187788	-1.042969	
6	1.362271	2.865144	-0.235719	
12	1.655467	0.800856	0.418938	
8	-2.317533	1.372149	-0.693246	
6	4.006253	-1.600703	-0.161566	
6	-0.161629	3.482682	0.394893	
6	3.315705	-0.627162	0.298565	
16				
359.417805	Kcal/mol	15.585851	eV	-100.810911 H Child_8_57.log
6	-2.361834	4.195924	-0.120586	
6	6.323290	1.195655	-1.211888	
6	-2.305220	2.884871	0.088584	
6	5.369036	0.661068	-0.516951	
6	-2.845729	1.387071	0.038024	
6	4.434749	0.023088	0.130438	
6	-1.560554	1.638563	0.358966	
12	2.555311	-1.295995	0.224293	
8	-5.709210	-1.440323	-0.101689	
6	0.640212	-1.988884	-0.075720	
6	-4.700501	-0.800857	0.002898	
6	-0.634667	-2.214143	-0.313321	
6	-3.428385	-0.287703	-0.127588	
6	-1.922578	-2.494063	-0.585662	
8	4.027853	-0.413242	1.267509	
12	0.061684	0.431410	0.164896	
16				
360.465848	Kcal/mol	15.631298	eV	-100.809241 H Child_12_8.log
6	0.461967	-1.187428	-1.068719	
6	-0.219646	4.331883	2.245953	
8	-3.260053	-1.311838	-0.223591	
6	-0.114328	3.538053	1.226725	
12	-1.451921	-1.309415	-0.230540	
6	0.064713	2.770695	0.201261	
6	1.701791	-1.067376	-0.878585	
8	0.954679	1.731090	-1.735748	
6	-4.495935	-0.970645	-0.059679	
6	1.604338	1.272508	-2.610161	

6	2.912237	-1.116336	-0.216764	
6	-0.003182	1.873684	-0.738045	
6	-5.744422	-0.518278	0.188336	
6	4.253498	-0.959174	0.333649	
6	3.173149	-1.600721	1.052616	
12	1.191748	-2.153519	1.698473	
16				
361.284190 Kcal/mol 15.666785 eV -100.807937 H				MutD_4_64.log
6	-2.483204	4.261848	0.545029	
6	-3.483471	3.821160	0.054355	
8	0.586221	-0.442891	1.256197	
6	-2.792475	-3.500481	-1.112714	
6	7.020560	0.147250	-0.785485	
8	-2.922538	-4.243864	-0.382860	
6	-3.405859	-0.151777	-1.401989	
6	5.688007	0.089553	-0.368774	
12	-0.907926	-0.488292	1.611920	
6	8.258814	0.528855	-1.000100	
6	3.101012	-0.043175	0.468948	
12	-3.662110	1.933894	-1.212427	
6	1.893819	-0.181812	0.822844	
6	4.455346	0.067253	0.047350	
6	-3.155819	-0.572888	-0.196540	
6	-2.841569	-1.107982	0.963641	
16				
361.739202 Kcal/mol 15.686516 eV -100.807212 H				MutD_18_60.log
8	3.489132	0.313960	-0.163964	
8	-1.920885	2.690804	-0.023101	
6	4.395496	-0.189937	-0.929120	
6	2.577385	0.890464	0.505335	
6	-3.383415	-0.334809	-0.546428	
6	-1.356652	-1.988532	0.467217	
12	0.503688	0.854006	0.738554	
6	-2.664153	-2.531421	-0.039431	
6	-3.840016	1.151627	-0.827222	
6	-3.558134	-1.669163	-0.500547	
6	-2.586766	1.462671	-0.300015	
6	-1.622313	-3.356825	0.497719	
6	-0.697805	2.781403	0.410456	
12	6.387010	-0.711985	-0.214815	
6	-2.079668	0.138539	-0.015191	
6	-1.056352	-0.644410	0.479170	
16				
362.911526 Kcal/mol 15.737353 eV -100.805344 H				Child_9_44.log
8	4.422815	0.579293	-0.829194	
6	-4.583234	0.708265	0.622392	
6	3.499523	-0.012514	-0.443452	
6	2.185426	0.537005	1.315350	
6	-0.900720	-1.950214	-0.593812	
6	0.921719	0.428038	1.563675	
6	0.308145	-1.779006	-0.322414	
6	-3.129345	1.293690	0.091963	
6	2.507466	-0.571306	0.240870	
6	-2.159182	2.021843	-0.276946	
6	1.697498	-1.677300	0.028500	

6	-3.632519	-0.203137	0.332806	
6	2.647554	-2.320414	0.718677	
12	-2.997319	-1.755467	-0.747026	
12	-0.486218	0.947666	0.204679	
8	1.280742	3.276196	-0.815492	
16				
363.248091	Kcal/mol	15.751948	eV	-100.804807 H Child_16_12.log
6	0.386893	5.615833	-1.185584	
6	-5.611407	-0.578001	2.283449	
6	3.944320	-0.066202	0.664129	
12	-5.237793	-0.148388	0.164967	
6	0.653714	4.431609	-0.653459	
8	-3.713258	-0.691191	-0.961475	
8	2.804870	0.132016	0.781676	
6	-2.611453	-1.237688	-0.863747	
12	2.199482	2.241780	1.019922	
6	-1.458594	-1.691583	-0.700860	
6	0.791198	3.226514	-0.196132	
6	4.829699	-2.888519	-0.202538	
6	2.201525	-2.768053	-0.244805	
6	-0.272685	-2.165946	-0.498173	
6	0.941771	-2.507546	-0.296154	
6	3.492826	-2.811635	-0.236172	
16				
363.804655	Kcal/mol	15.776083	eV	-100.803921 H Child_15_31.log
12	3.352218	2.876521	0.179732	
6	-5.008076	-1.118128	1.665848	
8	3.789386	-2.827584	-0.150968	
6	-4.703983	-0.215546	0.814028	
6	2.622091	-1.149046	1.146327	
6	-4.019875	-2.406800	-0.691309	
6	3.002251	-1.869930	-0.073367	
8	-4.439351	0.902710	-0.053053	
6	2.088065	-0.358810	1.975046	
6	-3.277848	0.962997	-0.586341	
6	2.229812	-1.244505	-1.145680	
6	-2.080428	1.085196	-0.896420	
12	1.188116	1.110236	0.844018	
6	-0.842992	0.786594	-1.228088	
6	1.379080	-0.409958	-1.477416	
6	0.397855	0.530920	-1.278101	
16				
363.972708	Kcal/mol	15.783370	eV	-100.803653 H Child_11_40.log
8	3.415173	0.133746	-0.714312	
6	-6.331247	-2.945540	0.221878	
8	4.137525	-2.041971	-0.874359	
12	2.511200	1.686197	-0.353921	
12	-3.282013	1.882644	-0.223331	
6	3.375192	-1.181090	-0.423599	
6	-3.552032	-0.118590	-0.345007	
6	2.309309	-1.486038	0.572929	
6	-1.703862	3.038461	0.024020	
6	0.580479	1.735457	0.520778	
6	-3.287046	-1.364969	-0.521031	
6	1.296521	-0.652833	1.155458	

6	-0.622435	2.560996	0.217949	
6	0.759418	0.528470	1.007574	
6	-2.964894	-2.666376	-0.702500	
6	1.611960	-2.041332	1.544283	
16				
365.090153 Kcal/mol 15.831827 eV -100.801872 H				MutI_15_41.log
6	5.786524	0.149804	-0.069894	
6	-2.322695	0.427055	-0.307381	
6	-4.219271	-1.650382	0.071333	
12	1.492953	-0.574937	-0.168268	
6	-2.635744	3.019625	0.229529	
6	-1.465013	-0.578830	-0.186235	
6	-4.778747	-0.529352	-0.286266	
8	-3.155744	-2.258129	0.653981	
6	-1.884125	-1.907990	0.588137	
6	8.387681	0.294449	0.083714	
6	4.493166	0.047927	-0.105092	
12	-4.062453	1.347683	-0.795173	
6	-2.159058	3.045562	1.369833	
6	7.079674	0.230283	0.008134	
8	-0.187765	-0.677190	-0.140721	
6	3.314619	-0.179883	-0.153275	
16				
371.654016 Kcal/mol 16.116464 eV -100.791412 H				Child_9_10.log
12	6.446533	-0.038915	0.318212	
8	-6.287168	-0.536467	0.168425	
8	1.945965	2.121204	-0.218313	
6	1.322964	-2.540666	-0.170476	
6	0.651715	2.132471	-0.060182	
12	-0.676113	-1.805341	-0.033854	
6	2.793141	1.001013	0.141827	
6	-5.098710	-0.402252	0.150945	
6	-0.576294	2.114052	0.030139	
6	2.603833	-2.274667	-0.240048	
6	-1.921047	1.974900	-0.035154	
6	-2.515912	-0.785350	0.082610	
6	-3.792827	-0.261465	0.129503	
6	-3.117518	1.681223	-0.182095	
6	1.237744	-0.859530	-0.072718	
6	2.660342	-0.204202	-0.276550	
16				
372.974511 Kcal/mol 16.173726 eV -100.789307 H				MutI_17_33.log
12	0.694100	-0.964500	-0.035085	
8	3.560942	0.500793	0.126360	
6	4.683757	1.029081	-0.258341	
6	2.460164	0.068920	0.546003	
6	-2.145492	-0.220585	-0.242028	
8	-1.952853	-2.752510	0.047082	
6	-3.556191	0.252024	-0.064295	
12	6.431981	-0.238070	-0.080618	
6	-2.699456	2.404157	0.087051	
6	-2.734404	-1.536595	-0.145105	
6	-1.327494	1.919666	-0.127543	
6	-0.661011	-2.721055	0.184623	
6	-1.571332	3.273158	0.179763	

6	-1.019929	0.574554	-0.287064	
6	-3.740897	1.586581	0.078408	
6	-4.083997	-1.222476	0.048679	
16				
373.896622	Kcal/mol	16.213713	eV	-100.787838 H MutI_13_49.log
12	-1.772415	-1.090378	0.428001	
6	1.184542	3.323288	0.020834	
6	3.453542	-0.812998	-0.539527	
6	0.660766	-0.199256	1.109670	
6	-4.495632	2.638383	-0.903597	
6	0.479462	1.112624	0.497075	
8	2.330965	-1.126164	-0.554591	
8	-0.814435	1.410746	0.233943	
6	-0.088112	-0.975586	1.795107	
6	-1.524042	-3.062120	-0.642564	
6	1.519704	2.064229	0.092037	
6	-3.813444	1.581001	-0.436098	
12	3.740346	1.371994	-0.381683	
6	0.357104	-3.258698	0.081184	
6	-0.595788	-3.937944	-0.714637	
6	-3.096006	0.584402	-0.024590	
16				
374.042819	Kcal/mol	16.220052	eV	-100.787605 H Child_3_56.log
12	1.893579	-2.692188	-0.083722	
8	-0.350894	3.968061	-0.853941	
6	-3.640108	-1.294082	0.780397	
12	0.397953	2.744249	0.314081	
6	-2.420157	-1.728914	0.559361	
6	2.059714	1.772175	1.291865	
6	-1.214872	-2.058663	0.345193	
6	0.387125	0.479839	-1.269967	
6	-0.030920	-1.976279	-0.220496	
6	-4.682617	0.876127	-0.357625	
6	3.281849	-1.334475	-0.678646	
6	1.025426	0.707124	1.334511	
6	3.007911	-0.171913	-0.271567	
6	2.347508	0.536757	0.723196	
6	-4.227605	-0.374678	-0.094464	
8	-0.006344	-0.620916	-1.097915	
16				
374.695857	Kcal/mol	16.248371	eV	-100.786564 H Original3D_2_3.log
6	-1.260903	-3.034118	0.841006	
6	-0.103358	-2.677588	1.094380	
12	-2.132763	-1.549008	-0.457719	
8	-2.342627	3.022436	1.466419	
6	2.222758	-1.524585	1.106874	
6	-2.432957	0.305952	-1.184782	
8	0.994476	2.198834	1.513355	
6	-2.175195	-3.601421	-1.072288	
6	1.142757	-2.104658	1.263163	
6	3.204142	-0.686927	0.657298	
6	1.098611	2.373495	0.371772	
6	3.942202	0.076770	-0.020140	
6	-2.547985	1.593609	-0.627027	

6	-2.430959	2.406985	0.474538	
6	-2.856573	1.245903	-2.064327	
12	4.130260	0.881454	-1.949032	
16				
376.978209 Kcal/mol 16.347343 eV -100.782927 H				Child_17_12.log
6	0.259106	5.046554	0.313582	
6	8.625044	-1.379385	1.056025	
6	-0.463843	3.986265	0.133508	
6	9.244010	-0.845266	0.053431	
8	-5.774359	-1.819624	0.126655	
12	6.941943	-1.184252	-0.043028	
6	-6.959231	-2.220107	0.185389	
6	4.865335	-0.948661	-0.520894	
6	-1.168651	2.921229	-0.016173	
6	3.606730	-0.734170	-0.562898	
6	-8.157660	-2.798831	0.236824	
6	2.300853	-0.480889	-0.581084	
12	-4.150473	-0.902713	-0.004269	
6	-1.850665	1.868536	-0.149371	
6	-2.768519	0.793375	-0.124019	
8	-4.062227	1.043585	-0.073951	
16				
377.440767 Kcal/mol 16.367401 eV -100.782190 H				Child_17_25.log
6	-1.195743	-4.009749	-0.478735	
6	-1.441433	3.435527	0.239996	
6	-1.886165	-2.790817	-0.158654	
6	-0.111215	3.166715	0.044173	
6	-0.445295	-2.837374	-0.229060	
6	1.125068	2.992158	0.002283	
6	-2.862964	-1.929544	0.114726	
12	2.842255	1.993868	-0.118963	
6	0.680501	-2.057047	-0.080720	
8	-2.199626	2.280462	-0.174989	
6	-3.524950	-0.929458	0.406886	
6	4.075549	0.247192	-0.375662	
6	1.564301	-1.159439	0.103223	
6	-3.047740	1.616148	-0.798148	
8	-4.067741	0.184017	0.662476	
12	4.871033	-1.509009	0.398818	
16				
378.768844 Kcal/mol 16.424992 eV -100.780074 H				Child_11_54.log
6	1.786303	-2.253122	0.883624	
8	-4.476898	0.863440	-0.084920	
8	1.982535	2.274590	0.663003	
6	-2.339647	2.031233	0.175366	
12	3.507446	-1.109995	0.532184	
6	-3.071259	0.947689	-0.029260	
6	2.738882	1.828407	-0.152730	
6	-1.657066	3.093426	0.438289	
6	3.605206	1.298232	-0.932587	
6	-4.422781	-0.578343	-0.200964	
6	4.561997	0.343475	-0.858198	
6	-2.890729	-0.545379	-0.193450	
6	5.423310	-0.501386	-0.369693	
6	-5.382126	-1.499960	-0.224115	

6	-1.896241	-1.400530	-0.271396	
12	-0.072463	-2.363896	-0.050016	
16				
381.787915 Kcal/mol 16.555912 eV -100.775262 H				Child_13_12.log
8	4.099777	2.796468	0.298608	
6	-7.328758	-1.295364	-0.440634	
6	3.272945	1.925556	0.027225	
6	-6.132670	-1.186764	-0.014497	
12	5.631879	-3.213531	0.781525	
8	-4.915774	-1.145467	0.581754	
6	3.522101	0.559957	-0.400836	
6	-3.799067	-0.695184	0.253531	
6	3.390210	-0.630939	-0.755759	
6	-4.099963	3.598311	0.693272	
6	1.821436	2.021793	0.078733	
6	-2.630339	-0.302058	0.063213	
12	1.363054	-0.956206	-0.884647	
6	-1.433511	0.165222	-0.116295	
6	0.707248	1.504659	-0.055903	
6	-0.191502	0.472950	-0.299622	
16				
381.803365 Kcal/mol 16.556582 eV -100.775238 H				MutD_14_58.log
12	-5.336815	-3.480630	-0.674248	
6	-1.702078	2.013415	-0.359454	
8	-3.842268	3.131148	-0.164629	
6	3.993035	3.603209	-0.587930	
6	-3.103924	2.163766	0.014978	
8	4.936913	-1.301451	-0.477800	
6	0.087065	0.165487	-0.158145	
6	7.105501	-0.667514	0.870381	
6	1.322228	-0.198524	-0.255606	
6	3.734511	-0.996681	-0.340965	
6	2.541515	-0.639436	-0.293555	
6	-3.490398	-0.229093	1.186038	
6	-0.715651	1.272582	-0.395237	
12	-1.582892	-0.915254	0.816470	
6	6.039899	-1.024016	0.271923	
6	-3.431816	0.888980	0.619702	
16				
385.984739 Kcal/mol 16.737904 eV -100.768574 H				MutI_15_65.log
8	0.801118	1.451769	0.509384	
12	3.196627	1.474410	-0.573612	
6	-4.262991	0.984120	-0.505483	
6	1.529897	0.153335	0.551413	
6	-0.210102	-1.827390	0.562448	
6	4.894793	-1.145596	-0.311039	
8	4.126474	-0.112918	-0.266980	
6	-1.072498	3.146930	0.309701	
6	5.532972	-2.290927	-0.231757	
6	-0.167247	2.260315	0.398289	
6	0.581159	-0.850534	0.530875	
6	-1.371838	-2.498602	0.429186	
6	-5.151494	0.109201	-0.744284	
6	-2.541771	-3.007944	0.207256	
12	-4.167763	-1.629483	-0.280534	

6	-2.388730	3.492104	0.188479	
16				
390.489999	Kcal/mol	16.933270	eV	-100.761395 H MutI_15_73.log
6	-1.101718	3.383388	0.815942	
6	3.660441	-0.476541	-0.053765	
6	2.687486	-0.084254	-0.806120	
12	-2.756614	-0.704091	0.386829	
6	-0.824818	1.513497	-1.831269	
6	-0.719318	0.397315	-0.938912	
6	-0.681683	0.066819	0.436663	
8	-1.544318	2.452563	1.268944	
6	-6.631154	-2.322940	0.219214	
6	0.339045	0.585818	-1.711095	
6	1.647954	0.315099	-1.466794	
12	-4.839748	-1.161238	-0.047173	
8	0.393928	0.061911	1.101580	
6	7.387198	-1.227087	0.606851	
6	4.855279	-0.755561	0.302684	
6	6.107864	-1.017527	0.586588	
16				
391.833384	Kcal/mol	16.991525	eV	-100.759254 H OriginalID_11_0.log
6	0.000000	0.000000	8.598351	
12	0.000000	0.000000	10.502546	
6	0.000000	0.000000	7.299133	
6	0.000000	0.000000	5.993999	
12	0.000000	0.000000	4.052634	
6	0.000000	0.000000	1.971168	
8	0.000000	0.000000	0.698465	
6	0.000000	0.000000	-0.577471	
6	0.000000	0.000000	-1.813028	
6	0.000000	0.000000	-3.153602	
6	0.000000	0.000000	-4.396500	
6	0.000000	0.000000	-5.727236	
6	0.000000	0.000000	-6.962461	
8	0.000000	0.000000	-8.186387	
6	0.000000	0.000000	-9.543057	
6	0.000000	0.000000	-10.815762	
16				
392.208988	Kcal/mol	17.007813	eV	-100.758655 H Child_12_47.log
6	-0.420835	2.109930	-0.442633	
6	-7.199369	-2.786296	-0.126294	
6	2.602855	1.071175	1.129865	
8	-6.473906	-2.775726	0.766106	
12	0.540119	1.731762	1.474213	
6	1.233071	-2.060467	-0.377317	
6	-1.414290	3.187842	-0.367597	
6	0.318324	-1.624010	-1.094728	
12	2.034869	0.608842	-1.586523	
6	2.221847	-1.486819	0.457517	
6	-0.473407	0.719262	-0.600277	
6	2.096299	-0.107727	0.960534	
6	-5.138504	4.282146	0.020831	
6	-0.236832	-0.333368	-1.334161	
6	3.581783	-1.561637	0.360297	

8	4.733216	-1.792705	0.462832	
16				
	396.449810 Kcal/mol	17.191713 eV	-100.751897 H	Child_7_47.log
6	-0.185689	-3.068701	0.250770	
6	0.191887	4.858094	0.414164	
8	-4.402446	-1.447109	-0.178074	
6	0.196177	3.592243	0.073926	
6	-1.100135	-2.207189	0.254506	
6	0.927525	2.252805	-0.021430	
12	1.826843	-3.024860	0.029319	
6	-0.343906	2.304812	-0.490612	
6	-3.370693	-0.823726	0.032269	
6	1.637231	1.085814	0.473144	
6	-1.924347	-1.116610	0.203183	
6	3.739916	-0.245471	-0.157389	
6	-3.102512	0.656169	0.112835	
6	2.502238	0.181774	-0.110891	
8	4.818727	-0.774419	-0.181185	
12	-1.688210	0.770872	-0.307050	
16				
	398.348036 Kcal/mol	17.274028 eV	-100.748872 H	MutI_16_39.log
6	5.018483	1.371716	-0.668769	
6	-5.872377	1.213427	-0.065719	
6	7.395256	2.102230	-1.338690	
6	14.643474	-2.098158	0.565720	
8	-4.350830	3.139548	0.722726	
6	-5.123005	2.118119	0.300218	
6	-7.976699	-2.192272	-0.167585	
6	-3.003926	3.046638	0.731067	
6	-1.738587	2.966164	0.639400	
6	6.210401	1.753397	-1.016791	
12	-7.994861	-4.218131	-0.242218	
8	3.928480	1.042687	-0.382678	
6	-9.127294	-1.610246	-0.086326	
12	-6.559978	-0.683009	0.043713	
6	13.597104	-1.663205	-0.034065	
6	15.649980	-2.781845	1.085152	
16				
	399.392850 Kcal/mol	17.319335 eV	-100.747207 H	Child_12_26.log
8	-6.924519	1.661805	0.026949	
6	3.600704	2.075573	0.039562	
6	-5.830142	1.211549	0.011810	
6	3.441713	3.314750	0.433233	
6	-4.652145	0.693570	0.014864	
6	3.754672	0.857928	-0.352470	
6	-3.544003	0.089952	-0.076619	
12	4.548810	-1.124715	-0.256229	
12	-1.126349	-3.469900	0.619502	
6	2.830235	4.420599	0.732216	
6	-2.426204	-0.592594	-0.260590	
8	2.942665	-0.124453	-0.916437	
6	-1.751066	-1.764804	-0.612820	
6	3.813791	-2.803125	0.817582	
6	-0.984989	-0.401722	-0.244465	
6	0.211651	0.037752	-0.042865	

16

402.623437 Kcal/mol 17.459427 eV -100.742059 H

Original3D_7_7.log

6	-0.343843	-1.359160	0.428682
6	-2.581613	1.052386	-1.024529
8	-0.370924	1.656363	-1.692433
6	0.404267	-0.466179	0.558557
6	-2.651067	1.138687	0.385075
6	2.533829	0.593618	-0.126253
6	-2.862807	0.829822	1.645929
6	3.682863	0.769947	-0.708945
12	3.450837	-1.485295	-0.812621
6	-1.322621	-2.402715	0.252509
6	-0.934195	-3.543151	0.618830
6	-1.490220	1.613919	-1.626987
8	0.978561	1.966819	1.264870
12	-2.619819	-0.953237	-0.547787
6	1.396458	0.556585	0.737592
6	1.696732	1.262397	2.150440

16

404.287414 Kcal/mol 17.531584 eV -100.739407 H

Child_10_10.log

8	5.671795	-1.411522	-0.304876
6	-0.041234	4.799865	-0.583984
6	4.553010	-1.744916	-0.242716
12	-1.194798	2.933445	-0.331671
6	3.340597	-2.120934	-0.146036
6	0.851027	4.174441	-0.158852
6	2.107629	-2.391858	0.036579
6	-2.310071	1.104250	-0.365524
6	0.854517	-2.572792	0.214449
6	1.338115	2.909823	0.535319
6	-0.419532	-2.414292	0.267431
6	-2.657692	-0.096468	-0.222061
6	-1.693973	-2.150453	0.208052
6	-2.665967	-1.445155	-0.000908
8	0.439583	2.624511	1.236476
12	-4.507668	-2.767861	-0.060270

16

404.451305 Kcal/mol 17.538691 eV -100.739146 H

MutI_16_63.log

12	5.776796	-0.970907	-0.039182
6	2.168624	2.811912	0.080983
6	2.092628	-0.788627	0.016833
6	2.118755	0.455574	0.009175
12	-5.348960	-0.314801	-0.041113
6	4.384074	-2.503113	0.061855
8	-6.993299	-0.566801	0.022743
6	-8.177634	-0.749324	0.055845
6	-1.223098	0.766377	-0.009247
6	-2.473950	0.406800	-0.052836
6	1.261634	1.611129	0.035643
6	-3.670751	0.063120	-0.049768
6	4.576456	0.410509	-0.044174
6	-0.061077	1.166832	0.011112
6	2.739975	-1.831897	0.048620
8	3.549819	1.130894	-0.025331

16
405.851070 Kcal/mol 17.599390 eV -100.736915 H
Original1D_16_0.log

6	0.000000	0.000000	0.901632
6	0.000000	0.000000	2.215708
6	0.000000	0.000000	-0.334540
6	0.000000	0.000000	3.387709
6	0.000000	0.000000	-1.589785
8	0.000000	0.000000	-2.796446
12	0.000000	0.000000	5.051973
8	0.000000	0.000000	-4.590991
6	0.000000	0.000000	-5.802106
6	0.000000	0.000000	-7.047347
12	0.000000	0.000000	7.632196
6	0.000000	0.000000	-8.312925
6	0.000000	0.000000	10.125446
6	0.000000	0.000000	11.470254
6	0.000000	0.000000	-9.615125
6	0.000000	0.000000	-10.917344

16
409.643098 Kcal/mol 17.763828 eV -100.730872 H
Original3D_0_45.log

6	0.802996	0.891055	-0.313265
12	0.479328	-1.373752	-0.206865
12	-2.906670	0.862243	0.647815
6	3.763984	-1.582315	0.759496
8	-2.220074	2.252552	1.934331
6	1.682794	1.769247	-0.824095
6	-3.210162	-1.943323	-0.197025
6	4.285474	-0.627499	0.051348
6	-1.139140	2.667394	-0.043297
6	-4.276610	-1.491853	-1.560116
6	-4.044023	-0.792523	-0.430968
6	-0.323162	1.679900	0.034425
6	3.911639	-2.636249	1.539423
6	2.602566	2.663002	-1.473376
6	-2.451900	-2.966790	-0.232265
8	4.657745	0.292177	-0.578471

16
409.941580 Kcal/mol 17.776772 eV -100.730397 H Child_14_24.log

12	4.119598	-0.811339	-0.112763
8	-6.323407	-0.433956	0.014051
8	3.879360	0.966761	-0.079638
6	-5.193891	-0.108496	-0.176162
12	2.249056	1.725417	-0.032549
6	-3.833157	0.026380	-0.317905
6	2.597132	-2.168297	-0.086430
6	1.340612	-2.171868	-0.019836
6	0.323774	1.140020	-0.014153
6	-1.397285	2.694942	0.159730
6	-0.632836	-1.318629	-0.055905
6	-1.214149	-2.687518	0.159819
6	-0.593126	0.087737	-0.031182
6	0.015069	2.941827	0.273623
6	-1.161315	1.455866	0.031019

6	0.270591	-2.430528	0.455454	
16				
410.321570 Kcal/mol 17.793250 eV -100.729791 H				Child_15_29.log
6	8.841972	0.320001	-0.529833	
6	-3.648887	2.864162	-0.556762	
6	7.571287	0.158428	-0.317308	
6	-3.998273	1.804007	-1.148350	
6	6.289693	-0.003700	-0.098471	
12	-2.178482	2.402263	0.825872	
6	5.080617	-0.152854	0.123004	
6	-4.098345	0.530714	-1.540778	
8	3.876094	-0.299541	0.355100	
6	-3.823214	-0.689943	-1.587281	
12	1.672054	-0.729008	0.623879	
6	-0.258189	-0.468017	0.917516	
6	-3.305258	-1.891555	-1.416327	
6	-1.523947	-0.343128	1.111132	
6	-2.641784	-2.959775	-1.087008	
8	-6.480706	-1.586598	2.068121	
16				
410.620513 Kcal/mol 17.806213 eV -100.729315 H				Child_1_47.log
12	3.461971	0.243883	-0.738133	
6	-6.167751	1.208000	0.093196	
6	2.874241	-1.354125	0.582691	
6	-4.947984	0.671086	-0.052272	
6	1.301916	3.535637	1.831631	
6	-3.775557	0.207385	-0.188995	
8	1.381288	4.187753	0.845974	
12	-1.831610	-0.665912	-0.552999	
6	1.661254	-1.844345	0.412541	
6	1.627828	1.225331	-1.721032	
8	-0.596477	-1.796856	0.264531	
6	0.705697	-0.534970	-0.155983	
6	0.515214	0.147782	-1.448949	
6	1.231762	0.792841	-0.323285	
6	0.412216	-2.573502	0.791531	
6	0.254028	-3.824924	1.280517	
16				
413.563645 Kcal/mol 17.933840 eV -100.724624 H				Child_4_16.log
6	-8.166932	0.403060	-0.700072	
8	4.448123	2.302526	0.865981	
6	-6.895686	0.291663	-0.423921	
6	3.486445	-1.570292	0.366417	
6	-5.632469	0.180724	-0.148761	
6	3.833436	1.726347	-0.022776	
6	-4.398321	0.072404	0.124702	
12	3.414934	-0.998796	-1.588319	
6	-3.142019	-0.038450	0.415873	
6	3.165813	1.021180	-0.962163	
6	-1.927724	-0.143400	0.711668	
6	2.568773	-1.841643	1.214730	
8	-0.754108	-0.238932	0.996997	
6	2.003529	0.538585	-1.081921	
12	1.122306	-0.464252	1.205984	
6	1.105322	-0.465541	-1.213075	

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16
413.571243 Kcal/mol 17.934169 eV -100.724612 H      Child_8_37.log
12   5.838667   -1.138823   -0.532623
6    -4.634798   -1.011548   -0.121830
6    2.689732    2.400253    0.199612
12  -4.208985    0.983762    -0.130430
6    2.475952    1.083705    0.344580
6   -3.709849   -1.809743   -0.316301
6    1.908189    0.013739    0.100697
6   -2.692933    2.271466   -0.234669
6    1.214571   -1.091474   -0.040982
6   -2.376588   -2.110801   -0.235799
6    0.482992   -2.322045   -0.223241
6   -1.414498    2.446219   -0.119936
6   -1.100992   -1.916711   -0.188089
6   -1.078677    0.488454    1.017712
8    1.462933   -2.038560    1.031476
8    2.270219    3.440017   -0.173213
16
415.849718 Kcal/mol 18.032973 eV -100.720981 H
Original3D_0_77.log
6    2.149702   -0.923502   -0.410963
6   -1.150992    0.027453    1.352585
6   -1.991846    0.974680    0.891978
6    5.823423    0.288522   -0.820386
12  -3.375586    2.351830    0.075207
6    2.535080   -3.398837    0.151905
6    5.834952    1.473441   -0.279531
6   -0.840681    1.269657    1.904344
8    2.036164    0.239872   -0.501514
6    2.301526   -2.188042   -0.229907
12  -3.547261   -0.452116   -0.944429
8   -0.869023   -1.301327    1.198033
6   -2.628681   -2.248654   -0.448607
6    5.905421    2.671848    0.195844
6   -3.899806    1.560290   -1.846998
6   -1.748589   -1.891010    0.349489
16
416.454478 Kcal/mol 18.059198 eV -100.720018 H      MutD_14_32.log
8    5.982023   -1.735528   -0.718117
12  -4.893369   -4.010010   -0.619975
8   -4.757571    2.469644   -0.209022
6   -0.139444    0.703785   -0.085811
6    3.539633    0.970965    1.038671
6   -3.837469    0.342176    0.489656
6    3.813267    3.747327   -1.117674
6   -1.217781    1.539720   -0.298125
6   -3.526156   -0.802881    0.889291
6    2.412901    0.779149    0.417993
6    1.147249    0.780107    0.084798
12  -1.512356   -0.905446    0.527488
6    6.995426   -1.521035   -0.141219
6    8.183559   -1.319189    0.503847
6   -2.392208    1.929568   -0.323350
6   -3.800132    1.702398   -0.036918

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16
416.633966 Kcal/mol 18.066982 eV -100.719732 H Child_11_34.log
6 -2.216502 -3.133938 0.103966
8 2.791888 3.827048 -0.258859
6 -0.994208 -3.597797 0.155163
6 2.471008 2.703716 -0.165966
6 -3.297693 -2.559612 -0.256466
6 4.708977 0.094590 0.132595
6 0.306193 -3.469957 0.204561
6 2.204300 1.393332 -0.050829
8 -3.652467 3.665644 0.419927
6 3.328061 0.506136 0.056378
6 -3.908205 2.504172 0.186079
6 3.573680 -0.828905 0.125760
12 -4.125978 -0.672462 -0.280703
6 0.864501 0.901780 -0.040368
6 -4.169036 1.270945 -0.071524
12 3.264160 -2.214896 -0.016351

16
418.888034 Kcal/mol 18.164727 eV -100.716140 H Child_4_32.log
8 -4.065906 -1.327609 -1.091940
6 4.662950 2.483576 0.048947
6 0.997897 -2.452751 -0.536108
6 3.751457 1.604766 -0.322814
6 -3.526284 -0.290284 -0.759990
12 -2.266600 2.389789 0.770308
6 -0.182728 -1.146016 1.328457
8 0.592847 -1.206545 2.311463
6 0.119460 -1.898165 0.267193
6 -3.429943 0.659320 0.264391
6 -2.385028 0.460537 -1.234610
6 2.383907 1.200325 -0.958236
6 -0.999502 -0.013613 1.434813
6 -1.302819 1.269786 -1.066162
12 2.902572 -1.754158 -0.576501
6 3.269432 0.230127 -0.479526

16
418.914893 Kcal/mol 18.165892 eV -100.716097 H Child_11_26.log
8 -0.671972 3.651832 -0.108362
12 -2.839035 -0.511183 -1.483766
8 4.505883 1.554441 0.173202
6 -0.382710 -2.232379 -0.147073
6 -1.152432 2.557777 -0.011718
6 3.435637 -1.974976 -0.969915
6 3.629750 0.736830 0.120077
6 -0.563504 -0.412992 -1.441485
6 -1.569537 1.342151 -0.022003
6 0.966800 -2.020104 -0.101440
6 2.703340 -0.164454 -0.072549
6 -0.531281 -0.645362 -0.104406
12 -0.999444 -0.993157 1.865343
6 -2.474233 0.467795 0.491365
6 -3.227350 -0.621711 0.976012
6 1.730598 -0.965592 0.433526

419.075724 Kcal/mol 18.172866 eV -100.715840 H

Original3D_16_5.log

6	3.106149	0.301985	-0.282514
8	1.995053	-2.508412	-0.436396
6	1.931273	2.504649	-0.924931
8	-0.823399	-2.338720	0.768985
6	1.333266	-1.577890	-0.192615
6	4.187556	-0.345198	-0.563976
6	1.475776	0.614810	1.076320
6	0.748775	2.448600	-0.391866
6	0.564914	-0.521399	0.579192
6	-0.337192	2.439824	0.398103
6	-0.230263	-1.504443	1.450170
12	-1.191682	-0.983369	-0.730440
6	-3.476333	-1.130264	-0.313272
6	2.133242	1.249770	-0.091533
6	-1.164733	2.705024	1.346616
12	-4.725636	0.622057	-0.536134

16

420.299629 Kcal/mol 18.225940 eV -100.713890 H

Child_7_11.log

6	-3.745911	-0.824442	1.901294
6	2.493494	2.250395	0.221616
6	-3.167548	-0.963746	0.771300
12	3.605633	0.534648	0.031042
8	-2.516575	-1.653034	-1.457846
6	1.346652	2.778894	0.154790
6	-2.483411	-0.990241	-0.412359
6	3.874102	-1.438609	-0.021600
6	-1.320191	0.127667	-0.352051
6	0.092641	3.108007	0.047998
6	0.462061	-1.619253	-0.072508
6	-1.158877	3.254119	-0.136497
6	1.474665	-2.325525	0.159709
6	3.008041	-2.312307	0.243050
8	-2.330037	3.422191	-0.336816
12	-0.812417	-2.236567	-0.086971

16

422.812990 Kcal/mol 18.334930 eV -100.709885 H

MutI_18_59.log

6	-4.895280	-0.087987	0.188304
6	3.767151	-1.581631	0.401433
12	-1.918393	-0.433910	-0.002480
6	0.992798	-0.478105	-0.377034
6	1.758832	2.458192	-0.299363
6	3.208777	0.914034	0.241445
6	1.808981	1.013908	-0.179501
6	-3.652152	-0.196027	0.160407
6	3.542218	-2.810561	0.182661
8	-6.099027	0.204161	0.114958
8	-0.258465	-0.521510	-0.298956
6	-7.353508	0.395500	0.105184
6	3.806055	-0.230496	0.512462
6	1.982379	3.766115	-0.376509
12	1.823374	-2.454330	-0.355614
6	3.700443	3.036668	0.402031

16

424.502551 Kcal/mol 18.408196 eV -100.707192 H Child_14_9.log

6	-4.651020	-1.593211	-0.075231
6	2.591167	1.751329	1.448820
6	-4.444285	-0.332399	-0.217843
12	3.849419	1.801223	-0.622510
12	-2.637004	-1.823744	0.235018
6	2.854994	0.597166	0.919106
6	-4.042136	0.945199	-0.338055
6	2.773968	-0.733070	0.366645
6	-3.614055	2.147488	-0.520934
6	2.744946	-2.047178	-0.341001
6	-0.865925	-0.861517	0.789050
6	-1.055546	2.339414	0.132403
8	3.135206	-2.730572	-1.296249
6	0.271442	-1.455960	0.550825
6	1.728489	-1.614815	0.398207
8	-0.672858	3.407519	-0.456507

16

426.054911 Kcal/mol 18.475513 eV -100.704718 H

Original3D_0_71.log

6	-0.677806	0.653934	0.684476
6	0.432252	0.472023	1.518247
6	1.638159	0.331903	1.737520
6	4.179420	0.186789	1.220664
8	-1.882978	0.811312	0.967845
6	-0.822930	-1.315232	-1.324350
6	2.972563	0.211980	1.590655
6	-2.879610	1.804133	-0.713509
6	-1.245542	-3.475155	-0.117660
6	-5.037958	1.761788	0.689762
6	-1.287919	-4.611882	0.483527
12	0.233544	0.744810	-1.340887
6	-4.006788	2.013649	-0.077264
12	3.958066	0.540289	-0.824047
6	2.252743	1.435370	-1.686319
8	-1.041877	-2.340936	-0.724756

16

431.258316 Kcal/mol 18.701154 eV -100.696426 H

Original3D_14_7.log

6	0.295657	-0.885716	0.270389
6	-0.167325	-0.491270	-0.971807
8	-1.421289	-0.146510	-1.269770
6	1.435205	1.642891	-0.183789
6	-3.510992	-2.849240	0.301387
6	0.829308	2.830655	0.109661
8	2.468020	-1.993831	0.960616
12	-0.996616	1.555596	0.008598
6	-3.230797	-1.560051	0.066142
6	-2.824052	-0.298048	-0.124546
12	2.869098	-1.483306	-0.873604
6	-3.273559	0.917439	0.299807
6	3.121190	0.841798	-0.419060
6	1.441256	-1.183814	1.049592
6	0.876634	0.064280	1.309214
6	-0.133130	3.680284	0.435228

16
431.302777 Kcal/mol 18.703082 eV -100.696355 H MutD_18_78.log
6 -0.365299 -0.703288 -0.016556
6 1.213252 2.272596 1.396937
6 0.540669 0.557631 -0.100123
6 1.933435 -0.758687 0.547393
6 -0.431211 1.434055 -0.687821
6 3.194339 -0.587058 0.086922
8 4.500299 -2.606933 -0.642653
6 -6.699114 -1.244469 0.341995
12 3.035902 1.586036 -0.255794
6 0.480374 -1.249312 0.953946
12 -2.470089 0.044394 -0.293011
6 -1.183508 2.225197 -1.549250
6 -5.484259 -0.781690 0.121412
8 -4.300391 -0.368199 -0.096152
6 3.884385 -1.660252 -0.297623
6 1.518767 1.201258 1.285452

16
431.522474 Kcal/mol 18.712609 eV -100.696005 H Child_2_10.log
6 3.163155 -2.766036 0.911527
6 -8.331176 0.160402 0.628548
6 3.326306 -1.563788 1.549287
12 -6.170970 0.176456 0.278764
6 2.788722 -3.454263 -0.101045
6 -4.170179 0.139829 -0.057794
6 3.207513 -0.333508 1.316569
8 -2.951031 0.025867 -0.265800
8 3.020189 4.005024 0.652752
6 -1.704935 -0.303218 -0.536488
6 2.918324 3.043967 -0.081411
6 -0.515028 -0.724735 -0.767132
6 2.838696 0.439553 0.298993
6 2.645488 2.181295 -1.029363
6 2.491379 0.728290 -0.946468
12 1.795732 -1.637611 -1.129344

16
433.753359 Kcal/mol 18.809350 eV -100.692450 H MutI_8_79.log
6 -0.423959 0.355552 -1.116864
6 2.344527 1.817414 0.298665
6 1.841735 -0.319969 0.041708
12 -2.604439 -0.244802 -0.362729
8 2.662923 -2.541186 0.470171
6 -4.205178 1.376065 2.001367
8 1.263149 1.863662 -0.439914
6 3.496442 2.079968 1.061395
6 -3.598674 0.825268 1.000321
12 -0.311841 -2.857484 -0.190602
6 -0.863998 2.561633 -0.861191
6 0.901796 0.492873 -0.604662
6 1.749034 -1.781880 0.085293
6 2.800549 0.625718 0.736299
6 -2.344040 -2.335969 0.021545
6 -1.100438 1.411263 -1.597558

16

434.147705 Kcal/mol 18.826450 eV -100.691822 H Child_4_43.log

12	1.033927	-1.998180	0.274488
6	-0.053482	3.067308	-0.616784
6	2.292415	-1.012771	-1.250682
6	-5.657953	-0.046008	0.281115
6	2.920508	-0.439123	-0.056907
6	-1.224900	1.553384	-0.520037
6	3.839248	0.576040	-0.012573
6	-4.513605	-0.517534	-0.029005
6	-0.951970	-1.077731	0.586113
12	-2.690902	-0.265550	-0.790944
6	1.331694	-1.181240	-2.012435
6	0.087929	2.032749	0.246760
6	4.016186	1.870753	0.315197
6	-0.691070	0.897012	0.578340
8	2.408775	-0.914233	1.068594
8	-0.969562	0.017699	1.574263

16

434.183273 Kcal/mol 18.827992 eV -100.691765 H MutD_16_66.log

6	-11.292864	-0.450573	0.520052
6	10.078158	0.139437	0.511660
6	-5.757892	0.565766	-0.444212
6	-10.006997	-0.511089	-0.096125
12	-3.133146	0.768895	0.179616
6	-7.122846	-0.035843	-0.076003
6	-8.436679	-0.107356	-0.059110
6	7.228641	-0.112151	-0.057501
8	5.918205	-0.116809	-0.075760
6	11.143871	-0.150713	-0.118129
6	3.405265	-0.108404	-0.070876
6	2.124970	-0.107615	-0.069980
12	0.046375	-0.076804	-0.057118
6	8.493270	-0.095876	-0.012341
8	-4.694497	-0.106189	-0.073186
6	4.685035	-0.112436	-0.073837

16

434.595329 Kcal/mol 18.845861 eV -100.691108 H Child_18_9.log

6	-4.700999	-2.385248	-0.454837
12	3.906851	-2.157644	-0.838858
6	-2.407578	0.699109	-0.734214
6	3.982536	-0.194384	-0.055309
6	-1.399709	1.599584	-0.437676
6	1.644325	-1.336230	-0.021044
6	-3.901672	-1.418783	-0.670935
6	-1.457084	-1.332858	1.124901
8	-1.173230	4.070510	-0.051329
6	3.428371	2.274693	0.730088
6	-3.126640	-0.345292	-0.798864
6	3.480949	1.035262	0.268224
6	-1.381322	2.926386	-0.293397
6	2.541718	-0.688171	0.143802
8	-2.202574	-1.614233	1.862472
12	-0.007763	0.103092	0.231059

16

435.270844 Kcal/mol 18.875154 eV -100.690032 H MutI_9_65.log

6	2.062113	-4.451433	-0.085487	
8	-7.155656	1.600157	-0.213927	
12	5.214821	3.688818	0.124166	
6	0.644581	0.609482	-0.018698	
6	-3.477718	0.400004	-0.003712	
6	2.539544	0.008902	-0.135555	
6	3.075233	1.267647	-0.237315	
12	2.365653	-2.033834	-0.118097	
6	-4.735624	0.775525	-0.234634	
6	3.792866	2.293258	-0.016720	
6	1.014015	-3.709277	0.149780	
6	-0.479475	-1.574482	0.177289	
6	-0.785623	-0.197917	-0.013426	
6	0.128123	-2.658850	0.212267	
6	-2.178968	0.170200	-0.026283	
8	-5.414356	1.217573	0.379193	
16				
435.871140	Kcal/mol	18.901185	eV	-100.689075 H Child_12_61.log
8	4.168761	0.482411	-0.367206	
6	-3.739713	0.342021	-0.495335	
6	3.639636	-0.696959	-0.216351	
6	-2.187707	3.995040	-0.476718	
6	3.050329	-1.701593	-0.063440	
6	-2.615130	2.829595	-0.169676	
12	3.260027	1.981919	-0.224271	
6	-3.387438	-0.899012	-0.170346	
6	1.978690	-2.555152	0.141827	
6	-2.623995	1.471141	0.038898	
6	1.239045	2.965445	0.951566	
6	-2.917845	-2.109897	-0.077178	
6	0.921246	-3.038089	0.360799	
6	-1.473794	0.612756	1.022848	
12	-1.511821	-3.209293	-0.138988	
8	-0.703562	0.447179	0.276924	
16				
438.444977	Kcal/mol	19.012798	eV	-100.684974 H Child_11_19.log
6	-4.242551	0.853978	-0.403677	
12	3.356710	-1.617422	-0.162177	
6	-3.278320	1.686618	-0.303659	
6	4.647413	-0.278718	0.841389	
6	-2.227710	2.484138	-0.191868	
6	3.836684	0.608999	0.471205	
12	-3.919435	-1.126429	0.397175	
6	2.059112	-0.135324	-0.897584	
6	2.594267	0.903711	-0.144149	
8	1.316537	1.660263	0.824220	
6	-2.313363	-2.124076	-0.501010	
6	0.701391	0.295439	-1.115727	
6	-0.263866	-0.572209	-1.082904	
6	1.257021	1.830404	-0.474904	
6	-1.230776	-1.482193	-0.774838	
8	-1.626926	-0.597563	2.256577	
16				
439.729592	Kcal/mol	19.068504	eV	-100.682926 H Original3D_9_3.log

6	1.412985	-0.571572	0.131017	
6	0.794248	-1.824659	0.556645	
6	0.045461	-0.024728	-0.287708	
6	-0.645015	-1.263702	0.472136	
6	-0.681237	-0.747749	-1.310242	
6	-2.461855	1.178003	0.635109	
8	-1.296010	1.837301	0.730023	
6	-0.240827	1.427773	-0.124458	
12	-2.831181	-1.207378	0.003334	
8	0.954251	2.244798	0.153028	
12	3.217897	0.416114	0.122024	
6	-1.575205	-1.539441	-1.756438	
6	1.114103	-3.075657	0.883196	
6	0.292367	2.482552	-1.053440	
6	-3.568002	0.599836	0.573365	
6	5.195223	-0.500927	-0.147300	
16				
441.883137	Kcal/mol	19.161891	eV	-100.679494 H Child_9_46.log
8	-5.097010	-0.945494	0.417250	
6	3.927360	0.826893	0.864010	
6	-3.926802	-0.673401	0.449014	
12	2.002763	1.158554	1.751683	
12	-1.987310	2.121366	-1.301089	
6	3.656552	-0.106709	-0.011139	
6	-2.650657	-0.327191	0.578449	
6	3.183346	-1.141434	-0.744573	
6	-1.284043	-0.614795	0.255156	
6	-0.035898	-0.407734	1.626519	
6	-1.552196	0.849313	0.450617	
6	2.305665	-2.045091	-0.864981	
6	-0.360221	-1.367624	-0.294380	
6	1.332135	-3.122792	-1.196792	
6	0.760983	-1.809907	-0.828969	
8	1.056661	3.480967	-1.305339	
16				
443.107128	Kcal/mol	19.214968	eV	-100.677544 H
	Original3D_14_6.log			
6	0.860452	2.721610	0.193961	
6	-0.320621	1.042342	0.256242	
8	-0.480297	2.436610	-0.118090	
6	-1.821879	-1.151137	0.657339	
6	-1.785697	-1.613959	1.834998	
6	1.204882	1.191642	0.717285	
12	2.635293	0.023293	-0.904216	
6	1.740271	0.826657	1.867081	
6	-2.781474	-0.681665	-0.366027	
6	-0.591488	0.702586	-1.876757	
6	-2.138970	-1.386228	-1.497292	
8	-3.445734	0.322373	-0.171144	
6	2.956126	-1.947852	-0.017221	
6	3.910918	-1.584854	-0.865040	
6	-1.242553	-0.442698	-1.870319	
12	-0.012923	-0.700838	1.579915	
16				
443.390179	Kcal/mol	19.227242	eV	-100.677093 H Child_3_44.log

6	-3.374277	3.276953	-0.100821	
6	4.176309	-0.728993	-0.358529	
6	-4.151070	-2.198097	-0.953769	
6	3.231736	-1.463888	0.005511	
6	-2.354235	2.508328	0.101864	
6	1.961659	-1.668931	0.516821	
8	-3.461918	-1.668002	-0.190893	
12	3.658761	1.294330	-0.510410	
6	-1.632662	1.223848	0.516048	
6	1.003554	-1.386000	1.597093	
6	-0.861762	2.279086	0.256887	
6	2.101166	2.365872	0.475467	
12	-1.697855	-0.830212	0.652837	
6	0.631990	-1.708434	0.215361	
6	-0.362836	-1.076065	-0.598971	
8	0.243379	-0.095934	-1.277467	
16				
443.551059	Kcal/mol	19.234219	eV	-100.676836 H MutD_8_70.log
6	-2.612623	-0.317360	0.463422	
6	2.262547	3.073414	-0.793866	
6	0.858494	-2.125104	-1.228113	
6	0.311895	1.772874	0.184193	
6	-1.175695	0.021201	2.561789	
12	-3.840884	1.055560	-1.218889	
8	-0.759419	-1.085664	2.022820	
6	-1.325817	-0.040631	1.017257	
12	2.649138	0.697722	-0.324135	
6	2.734074	-1.403801	0.232074	
6	-0.361466	0.772491	0.323596	
8	-0.228124	-2.611726	-1.801017	
6	3.514265	-0.838952	1.081547	
6	-3.756517	-0.538424	0.058654	
6	1.459075	2.572677	-0.331627	
6	1.791984	-1.525098	-0.778616	
16				
445.030027	Kcal/mol	19.298353	eV	-100.674480 H MutI_5_65.log
8	1.476060	2.089854	0.002700	
6	1.082055	-3.157273	0.171690	
6	1.552390	-1.959894	0.097159	
6	-2.527298	1.422142	0.105083	
6	1.500793	0.877501	-0.217013	
6	5.106180	1.212072	0.241833	
6	-4.661697	-0.307477	0.285089	
6	-3.795800	0.618242	0.234409	
6	0.049203	1.002379	-0.261818	
12	-0.657333	-1.702994	-0.247292	
8	2.687912	-1.179264	0.180639	
6	-3.098326	2.652162	0.021317	
6	2.655951	0.400199	-0.097286	
12	-2.374311	-1.184857	-0.093053	
6	-1.211239	0.816283	-0.140583	
6	3.859113	0.985247	-0.003642	
16				
445.298858	Kcal/mol	19.310010	eV	-100.674051 H MutI_18_43.log
6	0.596507	-0.661788	-0.267204	

12	3.165993	-2.299200	-0.931301	
6	1.694885	-1.209327	-0.047484	
6	-5.017894	-1.578141	0.578724	
6	-3.639437	1.270200	0.034037	
6	-5.121343	-0.317869	0.626522	
6	-2.364943	1.218733	-0.386686	
6	-1.776370	0.009337	-0.430461	
8	4.843137	1.189511	0.800945	
6	-4.787174	0.983586	0.521048	
6	0.197802	6.103411	-0.831263	
8	-0.339055	0.074446	-0.670172	
6	5.909500	1.563904	0.878435	
12	3.845522	-0.845931	0.434625	
6	-2.271604	-1.258341	-0.137430	
6	-3.448402	-1.518721	0.280750	
16				
449.034460	Kcal/mol	19.472002	eV	-100.668098 H MutI_16_53.log
12	3.001095	0.155361	-0.055975	
6	0.988656	-0.418666	-0.392823	
6	-4.915486	-0.991703	0.112850	
6	-6.190381	-0.848827	0.413477	
6	-7.443144	-0.717905	0.708849	
12	-1.786427	-1.168731	-0.577981	
6	2.063580	2.108385	0.364656	
6	-0.177266	0.072536	-0.390328	
6	-1.118682	1.241351	-0.158078	
8	5.961718	-1.232524	0.244995	
6	7.078101	-1.771768	0.392807	
6	-3.681270	-1.159173	-0.181700	
8	0.902032	2.320830	-0.034003	
6	-2.538709	1.296737	-0.037002	
6	4.777205	-0.730120	0.128173	
6	-0.423606	2.494818	0.025710	
16				
451.323249	Kcal/mol	19.571253	eV	-100.664451 H Child_11_20.log
12	-6.066582	-1.983721	-0.238209	
8	2.804445	-1.058511	2.045178	
6	-4.679537	-0.592839	0.286270	
6	2.667346	-1.263211	0.969610	
6	-3.696607	0.262977	0.265787	
6	2.865041	-1.890201	-0.255630	
8	-2.367077	2.115201	0.258273	
6	3.668461	-1.012015	-1.042045	
6	-1.222388	2.719575	-0.012397	
6	2.316528	-3.105925	-0.481897	
6	-0.154565	3.220937	-0.258421	
6	3.620666	0.256282	-0.443840	
6	-2.463209	0.804313	-0.077773	
6	1.549527	-4.124743	-0.676314	
12	1.856233	2.912359	-0.336286	
6	3.366277	1.458652	-0.195629	
16				
451.673725	Kcal/mol	19.586451	eV	-100.663892 H MutI_3_77.log
12	-4.105879	-0.326061	-0.012491	
6	1.504212	1.008479	1.147422	

12	1.805007	-2.041170	-0.014375
6	1.303244	1.097257	-1.077264
6	-0.770720	-0.290567	-0.030497
6	0.680170	1.930598	0.176929
6	-1.532861	1.044601	0.060870
8	-2.834925	1.078133	0.069276
6	-1.391249	-1.497461	-0.044844
6	0.662578	-0.238579	-0.129056
6	3.063423	0.625107	0.504875
6	-0.609249	2.012425	0.157245
6	3.813179	-1.711162	0.027176
8	2.667751	1.010276	-0.828432
6	-5.528428	-1.481991	-0.028671
6	3.630343	-0.548790	0.301756
16			
452.847430 Kcal/mol 19.637348 eV -100.662022 H MutI_15_35.log			
6	-1.658677	2.896362	-0.134457
6	-0.507191	1.460183	-0.190996
6	-0.378041	3.252624	-0.261306
6	0.703242	2.174285	-0.322373
6	3.848684	-0.736241	0.522300
6	-3.867286	-0.582756	0.277705
12	1.468280	-2.522630	0.115145
6	-1.327763	-1.138351	-0.521396
8	-0.051024	-1.764035	-0.594034
6	-3.857995	-1.928430	-0.088565
6	-3.372197	0.556862	0.534140
6	2.089163	2.147109	-0.338979
12	3.438756	1.034422	-0.037985
6	-2.797773	1.749393	0.982788
8	2.994095	-1.669573	0.461099
6	-2.612334	-2.296479	-0.435934
16			
453.461039 Kcal/mol 19.663957 eV -100.661044 H			
OriginalD_0_0.log			
6	0.000000	0.000000	5.818438
8	0.000000	0.000000	7.054462
6	0.000000	0.000000	8.369403
12	0.000000	0.000000	10.155663
6	0.000000	0.000000	4.617108
6	0.000000	0.000000	3.296101
6	0.000000	0.000000	2.011444
12	0.000000	0.000000	0.169760
6	0.000000	0.000000	-2.151385
8	0.000000	0.000000	-3.422363
6	0.000000	0.000000	-4.703303
6	0.000000	0.000000	-5.941790
6	0.000000	0.000000	-7.278583
6	0.000000	0.000000	-8.532182
6	0.000000	0.000000	-9.857561
6	0.000000	0.000000	-11.141335
16			
457.859082 Kcal/mol 19.854674 eV -100.654035 H Child_6_53.log			
8	-4.288447	0.963263	-0.040532
8	5.350275	1.482265	0.789519

12	-2.821027	2.582840	-0.006287	
12	4.591405	-1.458312	-0.303141	
6	-3.873181	-0.282665	0.057667	
6	4.384398	0.920255	0.352135	
6	3.130548	0.768465	-0.068877	
6	-3.273686	-1.393264	0.044468	
6	1.946045	0.491026	-0.503663	
6	-1.298637	3.760885	-0.425873	
6	-2.285329	-2.477788	0.112078	
6	0.065456	-2.906851	-1.297958	
6	-0.074368	4.470878	-0.097968	
6	-0.943681	-2.758439	-0.230673	
6	-0.291947	-3.681372	0.264250	
6	-2.442148	-2.420890	1.414620	
16				
457.905849	Kcal/mol	19.856702	eV	-100.653961 H Child_17_22.log
8	4.804912	-2.449154	0.524516	
6	-0.168071	4.208343	-0.235410	
6	3.866455	-1.729219	0.106041	
6	0.384882	2.998107	0.032772	
6	-2.991347	-1.179344	0.166754	
6	-3.702442	1.167520	-0.148922	
6	2.527778	-2.006539	-0.419182	
8	2.743331	1.930812	0.471674	
12	-0.134808	-0.093963	-0.803880	
6	0.823289	1.806406	-0.035401	
6	1.411949	-1.649634	-0.867895	
6	-6.407381	-2.510779	0.093838	
6	3.400746	0.829882	0.402688	
6	-2.496983	0.025471	-0.192276	
6	3.863873	-0.317942	0.259813	
12	-5.153728	-0.381611	0.558343	
16				
458.371130	Kcal/mol	19.876879	eV	-100.653219 H
	Original3D_10_7.log			
6	2.346535	-1.984197	-0.545135	
12	1.842271	0.316366	1.137933	
6	-1.238177	-0.743069	-0.741510	
6	-0.123134	-1.312120	-0.679179	
8	2.430316	1.830331	-0.523316	
6	-2.444574	-0.999172	-1.180150	
6	3.517183	-1.599660	-0.126459	
6	4.203186	-0.512428	0.481110	
12	-1.826020	0.630281	1.658886	
8	-3.476899	-1.359305	-1.460258	
6	-1.920443	-1.740508	2.317248	
6	-3.510302	1.370525	0.388060	
6	-2.055482	1.809851	-0.605701	
6	2.396768	2.858735	-1.108590	
6	-0.891163	2.130872	-0.544439	
6	1.082543	-1.800156	-0.604130	
16				
462.830674	Kcal/mol	20.070263	eV	-100.646112 H
	Original2D_18_1.log			
12	2.516070	0.602283	-0.000000	

12	0.791632	3.926335	-0.000000	
6	-0.478230	-0.657033	0.000000	
6	0.511569	1.728040	-0.000000	
6	-1.537071	-1.420715	0.000000	
6	0.000000	0.651527	-0.000000	
6	0.622526	-2.339184	-0.000000	
6	1.501062	-1.496777	-0.000000	
6	3.011061	2.634619	-0.000000	
8	1.714699	5.477523	-0.000000	
6	0.105695	-3.723464	0.000000	
6	-1.666153	-2.749578	0.000000	
8	-3.478684	0.201657	0.000000	
6	-1.492939	-4.044886	0.000000	
6	-0.251615	-5.046270	0.000000	
6	-4.589330	-0.165755	0.000000	
16				
462.884681	Kcal/mol	20.072605	eV	-100.646026 H
				Child_12_15.log
6	0.593296	3.082693	1.498317	
8	-3.019827	-1.647693	0.012802	
6	-0.017741	2.383633	0.515234	
6	-0.673456	-2.252948	-0.167539	
6	1.183206	2.606741	-0.315024	
6	-1.747416	-1.901538	0.090197	
6	2.214798	2.655469	-1.046608	
8	0.583135	-2.285623	-0.161148	
6	-6.254693	-0.183046	0.024769	
6	-1.182057	1.467453	0.269572	
6	-4.928465	-0.315592	0.043386	
6	10.652659	-2.255752	0.794301	
6	-3.614762	-0.476830	0.066451	
12	2.984555	0.766018	-0.919640	
12	1.612300	-0.801617	0.074180	
6	-2.170156	0.505336	0.115658	
16				
463.368463	Kcal/mol	20.093584	eV	-100.645255 H
				Original2D_11_1.log
6	-2.319562	0.393987	-0.000000	
6	-0.945920	0.327338	-0.000000	
6	0.090975	1.298357	0.000000	
12	-3.929032	1.415345	-0.000000	
6	1.351677	0.642195	0.000000	
6	-3.174375	-0.259830	-0.000000	
6	2.218269	-0.344984	0.000000	
12	-2.115467	-2.220364	-0.000000	
6	-0.000000	-0.874091	-0.000000	
8	3.684259	0.338730	0.000000	
6	1.755477	-1.618473	0.000000	
6	3.565352	1.643168	0.000000	
6	-0.114276	-2.331828	-0.000000	
6	1.272619	-2.866822	-0.000000	
8	2.161981	1.889232	0.000000	
6	0.593778	2.630404	0.000000	
16				
463.436593	Kcal/mol	20.096538	eV	-100.645147 H
				Child_3_31.log
6	-0.660624	2.941235	-0.002220	

6	-4.236068	-1.623600	0.000646
6	0.404192	2.216205	-0.002785
6	-2.992583	-1.839788	0.000552
6	2.743246	1.105072	0.012345
6	-1.655310	-1.902382	0.000411
6	4.098665	0.324796	0.009171
12	1.726295	-2.085783	-0.000650
8	5.295546	0.116974	-0.008608
6	-0.681885	-1.050574	0.001302
6	1.378729	1.192671	0.002401
12	-4.643506	0.369979	0.001438
6	-0.618922	0.481430	-0.001025
6	-3.671832	2.370558	-0.002359
6	0.630240	-0.187885	-0.009919
8	3.026885	-0.564071	0.001035
16			
464.228823 Kcal/mol 20.130892 eV -100.643884 H MutI_18_49.log			
6	-2.085722	-2.651820	0.148314
6	6.563302	-0.645579	-0.477587
6	0.385950	-0.988109	0.339738
12	2.161044	-0.471556	0.122709
8	-1.002962	-2.342138	0.061778
6	-0.191719	0.076377	-0.187528
6	-3.825176	1.234981	-0.181360
6	5.276204	-0.593182	-0.207439
6	-1.860223	2.914662	-0.161904
6	-2.921022	2.212944	-0.183234
6	-4.392328	0.091554	-0.134853
12	-3.770821	-1.660260	-0.010674
8	-0.232546	1.628546	-0.026893
6	2.536484	2.427714	0.559627
6	3.956328	-0.648577	-0.005720
6	1.424821	1.784125	0.221363
16			
465.220410 Kcal/mol 20.173892 eV -100.642304 H			
OriginalID_17_0.log			
6	0.000000	0.000000	3.715608
12	0.000000	0.000000	1.961962
6	0.000000	0.000000	4.909252
6	0.000000	0.000000	6.175311
6	0.000000	0.000000	7.432491
6	0.000000	0.000000	8.625937
12	0.000000	0.000000	10.358594
6	0.000000	0.000000	-0.507009
8	0.000000	0.000000	-1.780530
6	0.000000	0.000000	-3.092070
6	0.000000	0.000000	-4.346821
6	0.000000	0.000000	-5.717446
6	0.000000	0.000000	-7.012170
6	0.000000	0.000000	-8.362897
6	0.000000	0.000000	-9.658182
8	0.000000	0.000000	-10.821805
16			
467.410969 Kcal/mol 20.268884 eV -100.638813 H MutI_18_47.log			
6	-3.099958	-2.238695	0.298085

6	-1.601312	2.215962	-0.248706	
8	3.881614	-0.743836	-0.258934	
6	1.149003	4.166631	0.653985	
12	-4.590254	-1.186020	-0.489247	
6	0.104449	-0.678216	0.573171	
6	5.145946	-1.099261	-0.460065	
6	1.494970	-0.169894	0.172144	
6	2.709172	-0.405299	-0.120041	
8	-2.407859	1.164823	-0.501666	
6	0.268071	0.622534	0.289214	
6	-3.338885	0.478506	-0.913311	
12	-1.132383	-2.331853	0.922049	
6	-0.261315	1.984879	0.135274	
6	6.372446	-1.471980	-0.598354	
6	0.537680	3.069263	0.367132	
16				
467.792983 Kcal/mol 20.285449 eV -100.638204 H				Child_3_29.log
6	-2.027269	2.807134	0.791834	
6	5.368291	2.775106	-0.017187	
6	-2.402594	1.446141	0.671410	
6	4.716433	0.253531	0.011803	
6	-3.196101	-2.653850	-0.189166	
6	5.016577	1.492687	-0.030897	
6	-2.054386	3.836041	-0.042388	
12	3.827083	-1.587794	-0.109151	
6	-3.718057	-1.766710	-0.898443	
6	2.098850	-2.606374	0.062531	
6	-2.871867	1.291004	-0.566159	
6	0.998100	-1.930678	-0.016860	
12	-2.263349	-0.865447	0.773670	
6	-0.143706	-1.277191	-0.040569	
8	-1.854373	4.850813	-0.632985	
8	-1.829431	-3.921084	-0.165724	
16				
467.895791 Kcal/mol 20.289907 eV -100.638041 H				MutD_13_70.log
6	7.907664	-0.749231	1.565460	
8	6.404077	0.101054	0.073450	
8	-2.522069	3.510469	0.742662	
6	-2.980269	-3.517193	0.769727	
6	1.679639	0.058729	-0.908897	
6	2.939793	0.470475	-0.761971	
12	-2.635160	1.066617	-0.343904	
6	5.542573	0.236853	-0.069472	
6	0.354393	0.052281	-0.808193	
6	-3.242385	4.403864	0.539201	
6	-4.219294	-1.285151	0.308190	
12	-1.619591	-2.096424	-0.247885	
6	-4.297511	-0.061618	0.025303	
6	4.266974	0.323316	-0.446564	
6	-3.689251	-2.578443	0.521066	
6	-0.928834	-0.109632	-0.638419	
16				
470.642738 Kcal/mol 20.409026 eV -100.633663 H				Child_10_41.log
6	-0.388876	-3.397600	-0.009354	
8	3.224136	4.485908	-0.504085	

6	0.866791	-3.319064	-0.105032	
6	3.718393	3.411634	-0.238258	
12	-2.291717	-2.714903	0.074869	
6	4.232686	2.268891	0.053180	
6	-4.167182	-1.965455	-0.162037	
8	-4.974661	3.639508	0.700869	
6	2.164314	-3.166795	-0.049083	
12	4.601018	0.366714	0.314782	
6	3.260021	-2.453041	-0.007599	
6	-4.591969	2.647206	0.244722	
6	-3.882726	-0.723804	-0.315567	
6	-4.121338	1.558124	-0.206375	
6	4.191855	-1.653166	0.339748	
6	-3.566537	0.655560	-0.586026	
16				
476.016328	Kcal/mol	20.642048	eV	-100.625100 H Child_15_26.log
12	7.617425	1.340549	0.001602	
6	-3.960273	3.504130	0.451242	
6	5.791087	0.591380	0.048207	
8	-3.701149	4.448530	1.199020	
6	4.593695	0.094430	0.022893	
6	-4.072674	2.429902	-0.249987	
6	3.405458	-0.390515	0.029340	
6	-4.093012	-1.144497	-1.318863	
8	2.272149	-0.849425	0.046851	
12	-3.239948	0.767014	-1.029312	
6	1.135391	-1.319607	0.054101	
6	-3.092574	-1.915369	-1.157202	
6	0.021707	-1.829915	0.039219	
6	-3.387880	-3.723428	3.419001	
6	-1.149396	-2.473276	-0.018716	
6	-2.041150	-2.837168	-0.924977	
16				
479.332442	Kcal/mol	20.785848	eV	-100.619815 H Child_13_17.log
8	-4.046321	1.306537	-0.425736	
6	3.074799	-3.016023	-0.589899	
6	-4.396206	0.084976	-0.401032	
6	3.266098	-1.785996	-0.297471	
6	-4.203549	-1.148652	-0.276991	
6	3.839451	0.878011	-0.662478	
12	-2.052007	1.021399	0.027550	
6	3.004250	-0.453645	-0.084416	
6	-2.875362	-1.465218	-0.023447	
6	3.253712	2.021673	-0.317849	
6	-0.201628	1.610448	0.833954	
6	1.745790	0.154837	0.951792	
6	-1.638144	-1.315032	0.182107	
6	2.549438	3.110506	-0.199905	
8	0.926397	0.154427	0.240741	
12	0.422632	-1.333318	0.538597	
16				
482.215812	Kcal/mol	20.910883	eV	-100.615220 H Child_7_61.log
6	0.814801	1.179705	2.205344	
6	-3.901252	-0.018332	-0.192711	
12	4.211891	-1.132217	-0.311277	

6	-3.722935	-1.372731	-0.267131	
6	1.112582	0.814484	0.913664	
6	-3.419754	1.154141	-0.123303	
6	0.454519	-0.219349	1.565513	
6	-3.245612	-2.553593	-0.294063	
6	1.738820	-1.830348	0.589044	
6	-2.407564	2.132928	-0.154370	
6	3.331866	0.538914	-0.722166	
6	-1.163751	2.625166	-0.296572	
6	1.799978	0.862995	-0.183251	
12	-1.138674	-2.427734	0.018870	
8	0.247929	2.966542	-0.520467	
8	1.598472	-0.112101	-1.320922	
16				
482.228276 Kcal/mol 20.911424 eV -100.615200 H				MutI_18_79.log
12	-3.492810	-1.661000	-0.059159	
8	2.569571	0.740357	0.504837	
6	-1.639818	-2.402432	-0.282985	
6	3.385590	3.075485	-0.149612	
6	-3.317966	0.823347	0.007259	
6	2.971459	1.815311	0.190829	
6	-2.644987	3.485260	0.212641	
6	2.326494	-1.999245	-0.069543	
12	3.834039	-3.238758	-0.073624	
8	-1.129726	-1.145932	-0.318380	
6	0.471537	-0.484191	0.617376	
6	-4.297238	0.006844	0.343033	
6	1.126642	-1.607274	0.153319	
6	-1.962132	1.140471	-0.588802	
6	-2.877888	2.209994	0.055383	
6	3.856054	4.276712	-0.471941	
16				
485.691003 Kcal/mol 21.061582 eV -100.609682 H				Child_10_59.log
8	-5.349096	-0.559328	-0.129789	
6	7.557543	-0.770549	0.090450	
6	-4.310491	-1.202059	-0.056362	
6	6.280985	-0.473051	-0.090215	
6	-3.207429	-1.709013	0.010425	
6	5.065485	-0.186758	-0.213782	
8	-3.285653	1.870390	0.156495	
6	3.783980	0.124365	-0.304719	
6	-1.907564	-2.668919	0.138155	
6	2.576763	0.374090	-0.213260	
6	-1.664761	1.374410	0.460857	
6	1.003924	0.726373	0.154642	
6	-0.670620	-2.794715	0.060641	
6	0.929733	0.879142	1.604590	
12	-0.959492	2.487730	-0.443608	
12	-1.002783	-0.198429	-0.394906	
16				
488.456634 Kcal/mol 21.181511 eV -100.605275 H				Child_4_21.log
6	4.137369	-0.426248	-0.860109	
6	-4.490727	-0.132511	-0.062826	
8	3.643736	-1.464781	0.026961	
6	-3.886069	-1.238060	-0.091290	

12	2.719312	1.224558	-0.496194	
6	-2.414423	-2.126667	-0.464885	
6	3.385546	-2.408945	0.735279	
12	-2.315078	0.621116	0.240623	
6	0.917781	0.884271	0.585341	
6	-1.535950	2.809420	-0.136758	
8	-1.445248	-1.057536	-0.617717	
6	0.735151	-0.512022	1.323566	
6	-0.249102	2.804422	-0.158451	
6	-1.083287	-2.759022	-0.478922	
6	-0.273944	0.436850	1.084761	
6	1.017871	2.340252	-0.176889	
16				
489.893438	Kcal/mol	21.243817	eV	-100.602985 H Child_3_32.log
6	5.341094	-0.918867	0.121793	
6	-2.575957	-3.043314	-0.569648	
6	2.504437	2.957258	-0.231458	
6	-2.869810	-1.851529	-0.292046	
6	4.545798	-2.237259	0.247791	
6	-3.455783	0.580414	0.288626	
6	1.281021	3.336256	-0.253626	
6	-2.619060	-0.478888	0.048968	
12	2.028687	0.858807	-0.019879	
8	-4.039673	1.557621	0.534765	
6	-0.075743	3.534778	-0.257631	
12	-0.582094	-2.310981	-0.228722	
8	0.840656	-1.138093	0.170687	
6	-1.328011	0.003293	0.227808	
6	-0.889211	2.472955	-0.163247	
6	1.513395	-2.010118	0.389270	
16				
490.092566	Kcal/mol	21.252452	eV	-100.602668 H MutD_1_66.log
8	-3.253275	0.490279	-0.026476	
6	4.435567	0.288475	-0.189356	
6	3.105263	0.485087	-0.201637	
12	9.756703	-1.205034	0.096922	
6	8.081890	0.454254	0.236401	
6	-8.175958	-0.491507	-0.005500	
6	-4.447318	0.277720	0.415164	
8	6.946699	-0.365528	-0.129457	
6	5.665982	0.018982	-0.060565	
6	-5.653340	0.019663	0.163496	
12	-0.095888	0.932007	-0.192090	
6	-6.945803	-0.236693	0.093772	
6	-10.711265	-1.029818	-0.226643	
6	1.901127	0.720780	-0.123890	
6	-2.043585	0.636542	0.411177	
6	-9.458754	-0.763766	-0.114173	
16				
493.730452	Kcal/mol	21.410206	eV	-100.596870 H Child_1_11.log
6	1.997496	-2.337722	0.351539	
6	-1.568314	3.612968	-0.692451	
6	0.734056	-2.824815	0.547211	
6	-0.427654	3.106800	0.041276	
6	3.010958	-1.570222	0.226111	

6	-4.622534	0.111741	1.513954	
6	-0.249816	-2.170726	-0.139795	
6	-3.724605	0.513965	0.712587	
12	0.976504	-0.591845	-1.000635	
6	4.185892	3.067187	0.822884	
6	-1.563950	-2.081553	-0.232502	
8	-0.261696	1.668551	-0.291219	
12	4.066322	0.277838	0.273693	
6	-2.508900	0.551758	0.069274	
8	-2.660842	-1.758382	-0.469372	
6	-1.451564	0.768408	-0.752083	
16				
495.058991	Kcal/mol	21.467817	eV	-100.594753 H Child_16_29.log
6	-2.317975	-1.847159	-0.931319	
6	4.131122	0.918609	0.121847	
6	-2.752204	-0.831657	-0.351541	
6	3.290740	2.063095	0.034315	
6	-2.752186	1.502860	-0.208088	
8	2.938834	0.075981	0.258607	
6	-3.175869	0.342132	0.377343	
6	2.040366	2.525847	-0.169452	
6	-2.041886	2.561403	-0.574149	
6	2.040966	-2.976344	0.076542	
8	-3.816089	0.363254	1.497488	
6	2.318126	-1.478156	-0.374805	
6	-1.166042	3.481999	-0.905088	
6	1.603809	1.100581	-0.054576	
12	-0.521259	-2.671683	-1.031907	
12	0.496612	-1.302745	1.340663	
16				
496.244149	Kcal/mol	21.519210	eV	-100.592865 H Child_7_59.log
6	2.723408	3.838269	0.778127	
12	-6.533983	-0.317025	-0.100806	
6	2.525136	2.580393	1.137828	
6	-1.722804	-2.192133	-0.090963	
6	2.379845	1.339503	1.441396	
6	-2.014662	-0.973135	-0.325481	
6	2.057464	0.062470	1.604101	
12	-0.108472	-2.666471	1.433024	
6	-2.336144	0.273198	-0.537501	
8	3.207299	0.406263	-1.371627	
6	-2.740927	1.484073	-0.640846	
6	1.359465	-1.023151	1.245830	
6	-3.109493	2.740756	-0.695206	
6	2.006539	0.250238	-1.433825	
8	5.457156	-2.562149	-1.493074	
6	0.604477	0.461026	-1.328292	
16				
497.848587	Kcal/mol	21.588785	eV	-100.590308 H Child_1_34.log
6	0.183144	1.313994	1.623279	
6	-1.696652	-2.163864	-1.227243	
6	1.912596	3.655211	-0.875177	
6	-2.647548	-1.184362	-1.104696	
6	-4.927200	2.471594	0.696118	
6	-0.615165	-2.069973	-0.364550	

8	-0.658311	1.566380	0.764478	
6	0.578101	-2.532599	-0.151150	
6	1.543954	2.403833	-1.193140	
8	1.709875	-2.690512	0.245701	
12	1.195566	-0.799116	1.378224	
6	-3.264263	-0.056712	-0.977539	
6	3.822231	0.370973	-0.386270	
6	1.366902	1.123377	-0.948769	
12	-1.318275	-0.192831	0.535430	
6	2.587234	0.151265	-0.265076	
16				
503.354056 Kcal/mol 21.827525 eV -100.581534 H				Child_1_58.log
8	2.529149	-2.543826	1.712804	
12	-2.250935	2.248843	0.681097	
6	4.119228	0.608669	-0.541250	
8	-4.041866	-0.295118	-0.097724	
12	2.372974	-1.352350	0.180310	
6	-0.166361	2.782158	0.890306	
6	1.468997	0.819264	0.642735	
6	-0.804388	0.766834	-0.257593	
6	-2.033765	-3.292753	0.057711	
6	-2.955407	-0.818470	-0.369851	
6	1.018576	-0.105454	-1.580947	
6	0.289438	1.599858	0.369850	
6	3.136626	1.333582	-1.059945	
6	-1.608092	-0.383703	-0.236569	
6	1.762268	0.804874	-0.898575	
6	-2.454241	-2.122588	-0.892127	
16				
505.045785 Kcal/mol 21.900886 eV -100.578838 H				MutI_14_79.log
6	3.238851	0.953234	-0.454546	
6	3.194041	-3.830497	-1.153731	
6	-3.379186	-1.284107	-0.466435	
6	-1.746423	0.520449	-1.197922	
6	-2.614649	-0.452597	-0.848963	
6	0.615829	0.077018	2.232211	
6	2.817834	-1.463842	-0.316786	
6	-0.708934	2.900624	-0.731485	
12	-4.635753	-2.439727	0.326665	
12	1.258444	2.057493	-0.107890	
6	-1.637167	4.109983	-0.587957	
6	-1.180443	1.581101	-1.035713	
8	2.824102	-0.316951	-0.038310	
6	-0.063328	0.285564	3.368269	
6	2.936752	-2.673503	-0.653296	
8	1.136979	0.347731	1.094914	
16				
506.719092 Kcal/mol 21.973447 eV -100.576172 H				
Original3D_0_60.log				
6	-1.824161	-0.865734	-0.297414	
6	-0.646457	-0.209701	-0.717041	
6	-2.700324	0.857809	0.982954	
6	-3.230773	0.038786	1.911339	
6	0.005832	-1.461446	-0.588046	
6	-3.886958	-0.872970	-0.845263	

12	0.792539	1.334727	-1.013552	
6	2.475525	0.287462	-0.118932	
6	1.944950	0.541668	1.153908	
6	-0.379879	3.544496	-0.378503	
12	3.436000	-1.187324	1.148355	
8	1.017097	-2.060935	-0.761376	
6	-3.145873	0.026090	-0.224917	
8	-1.455645	-2.160322	0.049799	
6	3.775070	0.630853	-0.859442	
6	-0.259299	2.816224	0.660519	
16				
509.690895	Kcal/mol	22.102317	eV	-100.571436 H Child_6_10.log
8	3.018653	4.404970	-0.419932	
12	-7.359226	0.527648	-0.014620	
6	2.961467	3.280561	-0.159500	
8	-5.540691	0.194286	0.020527	
6	2.878934	2.083057	0.219364	
6	-4.344420	-0.062702	0.077384	
12	-2.440185	-0.395133	0.122158	
6	2.811005	0.903768	-0.230477	
6	2.694586	-0.339592	0.211409	
6	0.194512	-0.957891	0.107142	
6	1.966527	-2.262539	-1.197656	
6	1.473347	-1.305922	0.051812	
6	3.336832	-1.609037	0.154865	
6	2.823379	-0.919003	1.652673	
6	4.649477	-1.802432	0.132941	
6	1.515891	-3.405639	-0.702494	
16				
510.185664	Kcal/mol	22.123772	eV	-100.570647 H Child_9_50.log
8	0.073736	-1.997876	1.209163	
6	-1.487602	2.822326	0.179308	
8	2.882259	-2.134678	-1.194420	
6	-0.225824	2.980423	0.061707	
6	1.815525	-1.925788	-0.716657	
6	1.063144	2.660397	-0.213253	
6	0.625448	-1.794752	-0.185502	
12	-2.969319	1.339000	-0.036820	
6	4.103500	-0.341577	1.502894	
6	-0.702117	-1.297454	0.130468	
6	-5.381836	-0.209536	0.140314	
6	4.812177	0.337703	0.643441	
6	2.167130	2.121989	-0.500508	
12	-3.125638	-1.699333	-0.177548	
6	3.267001	1.402128	-0.671827	
6	-1.807960	-0.525120	0.038692	
16				
516.127905	Kcal/mol	22.381452	eV	-100.561178 H Child_4_26.log
6	-6.977372	-0.774622	-1.099857	
8	5.521911	-1.112950	-0.536652	
6	-5.957034	-0.661082	-0.357409	
6	4.378522	-1.002997	-0.286759	
12	-4.318404	0.229811	0.130138	
6	2.155652	-1.849952	0.262195	
8	-2.740386	1.494466	-0.034128	

6	3.089510	-0.816933	0.041463	
6	-1.747737	0.766989	-0.320115	
6	2.217480	1.105775	1.408993	
6	-0.600760	0.135386	-0.872911	
6	0.920123	-1.664853	0.562609	
6	-1.453737	-0.685583	-0.242368	
6	2.560387	0.584309	0.274658	
6	6.072876	2.472766	-1.721986	
12	0.135101	0.711244	1.426125	
16				
516.205653	Kcal/mol	22.384824	eV	-100.561054 H Child_2_29.log
8	0.187242	3.929494	-1.174120	
6	-4.057726	-2.359230	-0.039856	
12	0.891335	2.735486	0.052651	
6	-2.629280	-2.891872	-0.259600	
6	-4.478863	1.668664	0.505912	
6	2.278840	-2.187576	0.199999	
6	2.461758	1.597210	0.804895	
12	4.468115	-2.197330	-0.497756	
6	-4.135352	0.442301	0.143680	
6	2.609180	-0.926805	0.279152	
6	1.360073	0.785616	1.391955	
6	-3.922273	-0.843158	0.084476	
6	2.212658	0.300932	0.848320	
6	-2.692855	-1.522713	-0.071885	
6	0.249426	0.407813	-0.899369	
8	-0.168108	-0.590116	-0.398982	
16				
516.930742	Kcal/mol	22.416267	eV	-100.559898 H Child_4_36.log
6	1.584690	-1.579045	1.299608	
8	-3.929258	3.117467	-0.031586	
6	-0.434860	-2.206201	-0.309451	
6	8.215137	2.432138	-0.362560	
6	0.914345	-1.870827	-0.195388	
6	-3.921763	1.892860	-0.011872	
8	2.874232	-0.975646	1.036957	
6	7.321567	1.485541	-0.272637	
6	-1.304934	1.314473	0.354766	
6	-1.666695	-1.965739	-0.359895	
6	-2.563334	1.021783	0.268755	
6	3.142814	-1.118412	-0.320367	
6	6.377725	0.631789	0.044394	
6	1.955461	-1.799996	-1.129730	
12	-5.569728	-0.020930	-0.254317	
12	-3.536999	-0.526132	0.081259	
16				
516.998500	Kcal/mol	22.419205	eV	-100.559790 H Child_16_30.log
12	-8.681104	0.740074	-0.057676	
6	9.003859	-0.327130	-0.101690	
8	-6.870610	0.043234	0.236946	
6	7.714604	-0.135175	-0.087717	
6	-5.609420	-0.206267	0.097444	
6	6.463987	0.214135	-0.094730	
6	-4.401127	-0.483229	-0.040790	
6	5.242076	0.607781	-0.099271	

6	-3.064787	-0.634650	-0.172806	
6	4.032637	1.054122	-0.102810	
6	1.736318	-0.404624	1.305946	
6	2.757884	1.371953	-0.061674	
6	-1.810477	-0.717319	-0.374804	
6	1.462280	1.099248	0.067679	
12	0.233100	-0.854262	-0.687279	
8	1.896742	-0.951086	0.629403	
16				
519.883396 Kcal/mol 22.544306 eV -100.555193 H				Child_2_21.log
8	-4.975273	0.656019	-0.542692	
6	5.351953	-1.025961	0.227068	
6	-3.986561	0.109886	-0.277006	
6	4.096135	-0.678595	0.310216	
6	-2.809718	-0.486453	0.055987	
6	1.974701	1.274522	-1.921427	
12	-0.164097	1.158207	1.566913	
6	2.340354	1.047229	-0.853469	
6	-1.626158	0.286584	0.451118	
6	2.831770	-0.263441	0.317623	
6	-2.697727	-1.929767	0.224247	
12	1.010803	-0.624061	-0.949950	
6	-1.054747	-1.170231	0.770774	
8	-0.093654	-1.741247	0.210878	
6	1.603676	2.343116	0.928550	
6	-0.958521	0.871789	-1.025188	
16				
523.692997 Kcal/mol 22.709506 eV -100.549122 H				MutI_18_39.log
6	2.517723	-1.622729	-0.085272	
6	0.148817	1.210903	0.358373	
6	3.381872	2.029150	-0.260543	
12	-4.389762	-0.339729	-0.036676	
6	0.742872	2.579382	0.179204	
8	-2.868058	-0.259892	0.194070	
8	0.889441	-1.357463	0.212222	
6	4.281343	1.092361	-0.217285	
6	0.451046	-0.179915	0.333447	
6	-7.424620	-0.275172	-0.435481	
6	-6.000710	-0.444124	-0.301065	
6	2.066922	2.511204	-0.188834	
6	5.039560	-2.682702	-0.049196	
6	4.169307	-0.272334	-0.291399	
6	4.823502	-1.387609	-0.104351	
12	-1.389977	0.138759	0.297016	
16				
528.243155 Kcal/mol 22.906820 eV -100.541871 H				MutI_17_65.log
12	4.672267	4.528777	0.000000	
6	-3.383271	-3.390117	0.000000	
6	1.129897	-2.361208	0.000000	
12	-1.786739	0.335999	0.000000	
6	0.000000	1.169690	0.000000	
6	1.356013	1.422421	0.000000	
6	-4.084263	-2.324051	0.000000	
6	-2.200130	-2.664190	0.000000	
6	-0.103119	-2.402620	0.000000	

6	-1.328271	-1.832322	0.000000
6	3.210339	3.321774	0.000000
6	2.198085	2.588035	0.000000
6	-4.262714	-1.081952	0.000000
6	-3.928342	0.125421	0.000000
8	2.255884	-2.015695	0.000000
8	1.962658	0.290370	0.000000
16			
528.509669 Kcal/mol 22.918377 eV -100.541446 H MutD_18_58.log			
6	-1.083473	2.363598	-1.690185
8	-4.336260	-0.222679	-0.194782
6	0.392358	-0.496131	-0.685177
6	1.156985	-1.331137	0.190321
6	2.774290	-0.841482	0.779041
8	4.315660	-2.462127	-0.813529
6	-6.736393	-1.019590	0.456851
6	-5.506702	-0.551452	0.237908
6	-0.553519	1.114983	-0.976624
6	1.737521	-0.203680	0.912954
6	1.799385	2.191595	1.549956
6	3.770177	-1.503964	-0.392995
6	-0.617819	-0.985678	0.475948
12	3.161492	1.740089	-0.317902
6	1.672540	0.986624	1.357071
12	-2.550434	0.187939	-0.117425
16			
529.068420 Kcal/mol 22.942607 eV -100.540556 H			
Original3D_0_54.log			
6	0.153084	-0.197502	1.830705
6	1.631734	-0.748151	1.093492
6	2.510710	0.891768	-0.414754
6	2.193972	1.620042	-1.486821
6	0.460635	-0.601560	0.306388
12	-1.253783	-1.177171	-1.086029
12	-0.193462	1.748029	0.749376
6	2.602201	0.446187	1.047945
6	2.880200	-0.857611	-0.802555
6	-0.521220	2.721803	-1.118101
6	-3.116171	-1.851809	-0.656758
6	-3.073560	0.658555	0.683846
8	2.394633	-1.825143	-1.233325
6	0.769180	-1.377077	2.245990
6	-3.414293	-0.920959	0.124834
8	-2.531117	1.131091	-0.402354
16			
532.115973 Kcal/mol 23.074762 eV -100.535699 H			
Original3D_15_6.log			
6	-0.133194	0.113050	2.167586
6	0.293131	-0.740004	1.162243
6	-1.914886	1.523053	0.921334
8	1.955429	-0.836075	-0.854459
6	3.090938	-0.002251	-0.407978
6	0.987159	-1.106185	0.007546
6	-0.457160	-1.457848	0.084505
12	-2.345815	-0.797402	-0.406073

6	3.478297	0.874714	-1.364243
6	-1.072086	0.943703	1.710332
6	-2.884629	2.194751	0.301897
6	-4.130560	-1.942113	-0.599368
12	3.720185	-0.581820	1.543595
6	-4.009034	-1.475234	-1.819982
8	3.862908	1.505261	-2.251618
6	-3.754498	2.940560	-0.297480

16

532.227670 Kcal/mol 23.079605 eV -100.535521 H

Original2D_0_18.log

12	0.000000	0.423569	0.000000
12	2.785677	1.369998	0.000000
6	0.238956	3.566594	0.000000
6	3.220941	-0.907373	0.000000
6	1.729013	-1.017251	0.000000
6	-1.383052	-1.485525	-0.000000
8	-1.568243	2.973226	-0.000000
6	1.142095	2.717043	0.000000
6	-2.711531	-2.160206	-0.000000
6	-3.981392	-1.519636	-0.000000
6	-1.785317	-3.466180	-0.000000
6	2.532526	-2.138708	0.000000
6	-2.928110	2.267990	-0.000000
8	2.777611	-3.370004	0.000000
6	-0.641887	-2.769265	-0.000000
6	-2.616088	3.854420	-0.000000

16

533.042045 Kcal/mol 23.114920 eV -100.534223 H

Child_3_63.log

6	3.960405	1.114112	0.008561
8	-3.313895	-0.694515	-1.433209
12	3.582794	-0.794320	-0.474123
6	-2.737535	0.165739	-0.743957
6	2.759571	1.464194	0.198057
6	-1.892113	-0.133371	0.509613
6	1.850168	-2.003923	-0.648872
6	-1.282345	-1.387713	0.563579
12	0.697968	1.682219	0.320054
6	-2.412715	1.561660	-1.007009
6	0.805056	-1.357303	-0.300936
6	-1.234685	0.993908	1.091341
6	-1.100312	2.569163	-0.352060
6	-0.403895	-2.255758	0.350763
6	-0.103644	-0.501288	0.180125
8	-1.763216	-0.809398	1.777408

16

533.652685 Kcal/mol 23.141400 eV -100.533250 H

MutI_14_63.log

6	3.901172	0.309173	0.249106
6	-3.383599	1.540420	0.378496
6	2.744519	0.421241	-0.103926
6	-2.826466	-2.153649	0.421157
12	-0.586766	-3.593022	-0.345779
8	0.678452	-2.343816	-0.698593
6	-0.808178	4.108343	-0.604880
6	-2.851258	2.590238	0.129600

8	1.504066	-0.310166	-0.594637	
12	5.377850	0.184714	0.710142	
6	0.310662	2.632813	-0.173572	
6	1.470851	1.063728	-0.373621	
6	-1.942740	3.490214	-0.268278	
6	-3.450303	-0.952545	0.580779	
6	-3.619534	0.234543	0.580383	
6	-2.037321	-2.929260	0.180336	
16				
534.795298	Kcal/mol	23.190948	eV	-100.531429 H MutI_5_77.log
6	-1.638690	1.759838	-0.276725	
6	-2.194378	0.760398	-0.334839	
8	-2.268577	-1.665237	-0.270404	
6	3.025108	3.222245	0.044604	
8	-2.520382	-0.447532	-0.357036	
6	0.005901	-3.927445	0.082831	
6	-0.629455	2.713167	-0.224622	
12	2.660211	-1.979583	0.262015	
6	-7.975613	2.461922	0.864753	
6	0.460283	3.224033	-0.157930	
12	-1.388365	-2.942791	-0.153302	
6	1.033507	-3.333569	0.220842	
6	3.360345	2.031060	0.102683	
6	3.382859	0.657111	0.160365	
6	1.776593	3.497936	-0.073710	
6	3.235126	-0.404923	0.210909	
16				
537.160554	Kcal/mol	23.293516	eV	-100.527660 H MutD_1_78.log
6	4.945612	0.368025	0.493564	
6	10.836548	0.153928	0.381673	
6	-2.098864	0.064704	0.256725	
6	2.399935	-0.225270	0.618612	
12	0.053279	1.505934	-0.206061	
6	-3.074307	-0.114428	0.090990	
6	5.951277	-0.382715	-0.236357	
6	-8.341552	-0.305292	-0.110212	
6	8.465504	-0.379244	-0.240824	
6	7.210967	-0.434844	-0.288724	
6	-5.828730	-0.211922	-0.035226	
8	3.321889	-0.311765	-0.234930	
6	9.745858	-0.327794	-0.177807	
12	-10.413529	-0.149291	0.024205	
8	-7.090141	-0.211092	-0.034874	
6	-4.467414	-0.221292	-0.028965	
16				
537.859063	Kcal/mol	23.323806	eV	-100.526547 H MutI_18_33.log
6	-1.933307	-2.843820	-0.000000	
12	-4.462018	2.891540	0.000000	
6	-6.466987	3.795797	0.000000	
6	0.585860	-2.103377	-0.000000	
6	-2.721060	2.208633	0.000000	
6	2.515036	1.170256	0.000000	
6	-0.647960	-2.663764	-0.000000	
6	3.565322	0.445698	-0.000000	
8	-1.779955	1.342759	0.000000	

6	-1.992540	-0.092567	0.000000	
12	4.068780	-2.454315	-0.000000	
6	1.255139	0.641407	0.000000	
6	1.248781	-0.841778	-0.000000	
6	0.000000	0.493611	0.000000	
6	1.993619	-2.062280	-0.000000	
8	4.318383	-0.609459	-0.000000	
16				
540.908426 Kcal/mol 23.456039 eV -100.521687 H				Child_15_19.log
12	-7.377399	-1.322379	-0.515625	
12	4.335295	-2.206218	-0.989657	
6	-5.580628	-0.701750	-0.137562	
6	4.302069	-3.925693	1.321538	
6	-4.361164	-0.337489	0.068069	
8	4.519672	-0.383598	0.227603	
6	-3.166006	0.052960	0.298551	
6	3.505804	-0.283219	-0.647347	
8	-2.025354	0.435898	0.537358	
6	2.277016	0.316514	-0.286876	
6	-0.879139	0.807679	0.794911	
6	1.799373	1.515427	-0.531836	
6	0.267799	1.156925	1.064649	
6	1.545765	2.803577	-0.792094	
6	1.571893	1.546123	1.265897	
6	1.475665	4.036408	-0.427284	
16				
546.050398 Kcal/mol 23.679016 eV -100.513493 H				Child_14_31.log
6	-3.017217	2.448513	-0.096771	
12	5.199438	-0.263195	-0.217405	
6	-2.670647	2.900715	1.045937	
6	-0.016923	-2.287035	0.806052	
6	-3.105416	1.616471	-1.161639	
6	3.025365	-0.857414	-0.022161	
6	-2.630951	0.441936	-1.155697	
6	0.952796	-1.419605	0.861419	
12	-1.498526	1.077276	1.253495	
6	-1.222942	-2.558243	0.417755	
6	-2.019051	-0.473206	-0.435022	
6	1.978236	-0.547754	0.720311	
6	5.434953	2.782363	-0.136817	
6	-2.339852	-2.081548	-0.085425	
8	2.959853	0.141365	-1.267903	
8	-4.287485	-1.336382	-0.854688	
16				
547.374024 Kcal/mol 23.736414 eV -100.511384 H				MutI_17_41.log
6	-4.261508	-3.520784	-0.000000	
8	1.957556	-1.404887	0.000000	
6	-5.280872	-4.269683	-0.000000	
6	0.000000	1.055649	-0.000000	
8	0.599926	-2.561427	0.000000	
6	-0.777107	-2.669017	-0.000000	
6	1.815085	4.006062	0.000000	
12	-2.931765	-2.183529	-0.000000	
6	-1.040775	0.266749	-0.000000	
6	1.418942	1.002298	0.000000	

6	3.298754	4.753480	0.000000
12	-0.154582	3.261482	-0.000000
6	3.730419	2.799813	0.000000
6	-1.177192	-1.244777	-0.000000
6	2.151910	-0.189593	0.000000
6	2.885064	1.142314	0.000000
16			
547.970095 Kcal/mol 23.762262 eV -100.510434 H			
Original1D_14_0.log			
8	0.000000	0.000000	4.616886
6	0.000000	0.000000	3.336600
6	0.000000	0.000000	2.058567
6	0.000000	0.000000	5.918201
6	0.000000	0.000000	0.744764
6	0.000000	0.000000	-0.576107
6	0.000000	0.000000	-1.765419
12	0.000000	0.000000	-3.531495
8	0.000000	0.000000	-5.978050
6	0.000000	0.000000	-7.231014
6	0.000000	0.000000	7.169070
6	0.000000	0.000000	-8.479010
6	0.000000	0.000000	-9.843588
6	0.000000	0.000000	-11.147309
6	0.000000	0.000000	8.408704
12	0.000000	0.000000	10.142209
16			
551.129809 Kcal/mol 23.899281 eV -100.505399 H			
Child_1_17.log			
6	4.154729	-2.945585	-0.974900
8	-3.945099	3.315038	-0.206429
6	3.308097	-2.051607	-0.595890
6	-3.100849	2.482697	-0.201550
6	1.371293	-1.316680	2.242743
6	-2.295509	1.440722	-0.203115
6	2.323422	-1.212650	-0.287197
12	4.173457	2.454856	1.047766
12	-5.110281	-2.642307	0.689492
6	-0.952299	1.194210	-0.115781
6	1.485090	-0.913616	0.977472
6	1.541911	-0.137242	-0.934932
6	-0.389707	-0.123652	-0.034725
6	-4.337053	-1.344850	-0.632343
6	2.174076	0.246819	0.313873
8	1.387933	0.477214	-2.064700
16			
556.922438 Kcal/mol 24.150473 eV -100.496168 H			
Child_2_61.log			
6	-6.301415	-1.868074	-0.163225
6	3.425041	-3.144613	-0.318391
6	0.712178	4.820497	0.006114
6	3.632808	-1.932635	-0.206593
6	-5.051321	-1.382378	-0.139543
6	3.406937	-0.623137	-0.135080
6	0.106994	3.816512	-0.006574
12	1.533793	-2.580041	0.103739
12	-1.987173	0.966630	-0.087900
6	2.709886	0.622417	-0.017967

6	-3.874019	-0.862519	-0.088565
6	-0.398833	-1.508639	0.803083
6	-0.386820	2.479965	-0.040839
6	-0.313920	-0.153386	0.281180
8	1.373796	2.895959	0.001174
8	1.055638	-0.673852	-0.005133
16			
557.933606 Kcal/mol 24.194322 eV -100.494556 H Child_8_39.log			
6	4.250506	1.099618	0.440328
6	-5.077205	-0.545299	0.019825
6	2.955775	1.167840	0.107660
6	-3.735952	-0.881927	-0.030720
12	0.935053	2.131557	0.133998
6	-2.641153	-1.527491	-0.034456
6	3.343027	-0.229986	-0.100433
6	-4.143344	0.618211	0.046815
6	3.922376	-1.652849	-0.149765
6	-1.464722	-1.816403	0.005917
6	-0.469001	2.865510	-1.460069
8	-0.262972	-2.211545	0.049381
8	-0.262564	1.477983	1.096291
6	-3.545077	1.851044	-0.029641
6	2.641584	-1.201465	-0.767210
12	1.396896	-1.515918	0.078096
16			
560.038363 Kcal/mol 24.285593 eV -100.491202 H			
OriginalID_5_0.log			
8	0.000000	0.000000	8.367857
12	0.000000	0.000000	9.687857
6	0.000000	0.000000	7.047857
12	0.000000	0.000000	5.727857
8	0.000000	0.000000	3.087857
6	0.000000	0.000000	1.767857
6	0.000000	0.000000	0.447857
6	0.000000	0.000000	-0.872143
6	0.000000	0.000000	-2.192143
6	0.000000	0.000000	-3.512143
6	0.000000	0.000000	-4.832143
6	0.000000	0.000000	-6.152143
6	0.000000	0.000000	-7.472143
6	0.000000	0.000000	-8.792143
6	0.000000	0.000000	-10.112143
6	0.000000	0.000000	-11.432143
16			
560.358175 Kcal/mol 24.299461 eV -100.490692 H Child_10_11.log			
12	-2.753500	2.010154	-0.151113
6	2.432544	0.093328	1.177557
6	-2.653034	-0.046464	-0.018116
6	3.428985	-0.207297	0.202107
6	-0.723704	1.515919	-0.214068
6	1.274095	0.191514	1.732155
6	-3.407855	-1.083690	0.114736
6	3.119384	-1.354166	-0.450464
8	-4.205672	-1.968816	0.232123
6	2.153953	-2.020350	-0.717555

8	0.519168	1.848647	-0.292473	
6	-1.225132	0.154836	-0.112114	
6	0.798895	-2.206102	-0.413155	
12	2.359059	1.621077	-0.362523	
6	-0.340688	-0.810154	-0.095284	
6	0.846779	-1.329611	-0.098060	
16				
560.851622	Kcal/mol	24.320859	eV	-100.489906 H Child_18_26.log
6	-0.105765	-1.786535	-0.168507	
6	-1.982467	2.709557	0.261265	
6	-1.401573	-1.497232	-0.461022	
6	-0.632573	2.414143	0.077548	
12	-3.469440	-1.488165	-0.251783	
6	0.611425	2.237303	0.059898	
6	0.866967	-1.872281	0.500879	
8	-2.686188	1.522491	-0.224595	
6	-5.667896	-1.294936	0.056902	
12	2.517897	1.225720	0.029228	
6	7.946671	-0.890269	0.066658	
8	-5.126758	-0.626393	0.879607	
6	6.600409	-0.685041	0.038244	
6	-3.393568	0.756852	-0.770700	
6	4.213239	-0.355044	-0.134835	
6	5.265478	-0.406426	0.045432	
16				
562.808418	Kcal/mol	24.405714	eV	-100.486788 H Child_11_56.log
8	-1.273437	4.856338	-0.004328	
6	-3.189676	-2.559977	-0.405124	
6	3.995014	-0.355841	0.452208	
12	-5.058246	-1.829808	0.050452	
6	-1.632132	3.673871	0.044179	
6	-1.955928	-2.370169	-0.376035	
6	2.734213	-0.729496	0.587992	
12	-0.173483	-1.571281	-0.215897	
6	1.525309	-1.290724	1.013814	
6	-3.775746	0.554197	0.080172	
6	-2.111905	2.458612	-0.063313	
6	-2.810046	1.416027	-0.064157	
6	5.125137	0.006577	-0.330520	
6	1.267691	-0.038645	0.265215	
6	4.907688	-1.473041	-0.102434	
8	6.061315	0.776751	-0.574002	
16				
572.431995	Kcal/mol	24.823032	eV	-100.471451 H Child_5_47.log
6	-3.150434	2.437473	0.170889	
12	0.351851	-2.970450	-0.003713	
6	-1.698084	2.346489	-0.035297	
12	3.437137	-0.457004	-0.307219	
6	-0.413822	2.644174	-0.175528	
6	1.607093	-1.281185	-0.151730	
6	-2.497083	1.329131	0.003696	
6	4.390046	1.373299	-0.338068	
6	0.867136	2.746106	-0.235298	
6	-0.716655	-1.348429	0.021979	
6	0.445352	-0.653033	-0.097911	

6	-2.108854	0.114590	-0.207720	
6	-1.920996	-1.177096	0.110626	
6	-2.875300	-1.812059	-0.015883	
8	3.915237	0.757258	0.987520	
8	-3.545018	-0.655672	0.191563	
16				
573.884496	Kcal/mol	24.886018	eV	-100.469137 H MutI_5_67.log
6	4.522746	-0.809481	0.069327	
6	2.480854	2.182710	-0.014361	
6	-2.955022	2.263922	0.013666	
6	-3.699993	1.265624	0.034539	
6	3.441258	-1.408947	-0.008138	
6	-2.418169	-2.538255	-0.003768	
6	-2.132419	3.307528	-0.009094	
8	-3.680209	0.079888	0.026614	
8	1.501328	2.946568	-0.060674	
6	4.445678	0.503926	0.083544	
12	-3.598483	-1.433855	0.025019	
6	-0.250848	3.544757	-0.048779	
6	3.421415	1.318682	0.035239	
12	2.174584	-2.263192	-0.043919	
6	0.313881	-3.089850	-0.051440	
6	-1.416410	-3.181798	-0.017522	
16				
580.724275	Kcal/mol	25.182620	eV	-100.458237 H MutI_15_39.log
6	-4.205686	-0.800804	0.000000	
6	-2.038132	4.552682	-0.000000	
8	-1.215401	-3.410071	0.000000	
6	-0.000000	0.784062	-0.000000	
8	-3.015981	-0.508056	0.000000	
6	3.336269	1.196041	-0.000000	
6	0.861422	2.078588	-0.000000	
6	4.658291	0.924359	-0.000000	
6	2.245006	0.336264	-0.000000	
12	-1.318882	2.529891	-0.000000	
6	1.078266	-0.058370	-0.000000	
6	2.146454	1.941966	-0.000000	
6	5.689435	0.163610	-0.000000	
6	1.531653	-2.574652	0.000000	
12	-3.358389	-2.905140	0.000000	
6	-0.306593	-2.569079	0.000000	
16				
581.678024	Kcal/mol	25.223978	eV	-100.456717 H MutI_4_71.log
6	-2.001747	-0.211050	-0.270627	
8	-4.069362	0.905170	0.481979	
6	4.527640	-0.282012	0.552584	
6	-1.252911	0.708757	-0.413926	
6	-3.390663	-0.222049	-0.012888	
6	4.058310	0.889905	0.267467	
12	0.969278	-2.219566	-0.014974	
8	1.815359	2.412693	-0.340530	
6	-4.781042	1.784765	0.961642	
12	-0.015023	1.839354	-0.497698	
6	-3.462498	-2.063264	-0.159708	
6	2.645539	-1.647692	0.160161	

6	3.591261	-1.169919	0.462905	
6	3.406391	2.056734	-0.015682	
6	-1.629196	-1.572832	-0.341872	
6	-0.614257	-1.934740	-0.353312	
16				
581.759917	Kcal/mol	25.227530	eV	-100.456586 H Child_9_13.log
6	5.011031	-0.467974	-0.060872	
6	-3.419334	0.839866	-0.511785	
6	3.824470	-1.001428	0.099339	
6	-3.659649	-0.407200	-0.624363	
12	3.400670	1.170600	-0.244578	
8	-4.150189	2.297011	1.024428	
6	2.152187	2.869000	0.016560	
6	-2.738021	2.415089	-0.152223	
6	2.357638	-0.918532	0.164896	
6	-3.493272	-1.789376	-0.483027	
8	1.721604	-2.148803	0.383732	
6	-2.927025	-2.905339	-0.234464	
6	0.873407	3.096435	0.142474	
6	-0.295552	3.072079	-0.348377	
12	-0.836902	-2.539732	0.537782	
6	0.424700	-2.261966	-0.472114	
16				
582.765726	Kcal/mol	25.271146	eV	-100.454984 H Child_12_45.log
8	-5.977963	1.744594	0.060460	
6	6.574349	0.450899	1.299339	
6	-4.888279	2.446730	-0.372381	
6	6.776528	1.210291	0.159888	
6	-5.774119	0.449062	0.429104	
8	7.135813	1.934333	-0.682262	
6	-5.158786	-0.596914	0.686947	
6	5.464105	0.158962	0.619474	
6	-3.691546	1.839175	-0.387366	
6	4.304242	-0.351081	0.212886	
6	-2.668059	1.103080	-0.349725	
6	3.238169	-0.841214	-0.207081	
12	-3.268620	-1.379778	0.428635	
12	1.369155	-1.661880	-0.708807	
6	-0.454533	-2.412143	-0.722371	
6	-1.466941	-2.278765	0.020698	
16				
583.929897	Kcal/mol	25.321629	eV	-100.453128 H Child_8_32.log
6	-3.493650	2.882418	-0.672534	
8	4.901028	-1.458645	0.772071	
12	-6.890278	0.179415	0.522842	
6	2.613820	-1.580085	-0.417038	
6	-3.348649	1.623416	-0.444779	
6	1.444177	-1.861320	-0.243171	
6	3.296405	3.102084	-0.194405	
6	3.820496	-1.004889	-0.158255	
6	2.779181	2.269022	0.672749	
6	0.104288	-2.004996	-0.128686	
6	-3.212306	0.340465	-0.202925	
6	-1.129517	-2.006639	-0.179698	
6	2.343651	1.282488	1.459428	

12	4.248052	1.007834	-0.656971	
6	-3.252803	-0.870458	0.177901	
8	-2.411509	-1.950856	-0.322318	
16				
584.087591	Kcal/mol	25.328467	eV	-100.452877 H Child_2_20.log
6	-3.659772	-2.200996	0.227428	
8	2.588653	1.991404	-1.050924	
8	-2.124019	-1.959623	-1.189434	
6	1.817510	1.359359	-0.305062	
6	-3.099146	-1.225744	-0.618158	
6	0.513540	1.706740	0.143417	
6	-3.564047	-0.302174	0.649893	
12	-2.655236	2.318705	-0.113833	
12	-0.096686	-0.646356	0.327350	
6	-0.685677	1.238378	0.148347	
6	3.056606	-1.644346	0.038474	
6	2.049225	-0.038955	0.173678	
6	3.291920	-0.551875	0.458035	
6	-1.444491	0.624526	1.589843	
6	4.392702	-1.206772	0.793843	
6	2.215963	-1.145214	-0.739629	
16				
585.661418	Kcal/mol	25.396715	eV	-100.450369 H Child_7_29.log
6	3.817336	-3.872817	-0.059791	
6	-4.869259	1.582957	-0.138155	
6	4.658113	-2.894477	-0.003579	
6	-4.432337	0.390403	-0.070837	
12	2.506274	-2.059796	-0.068018	
6	-4.928863	-2.207418	-0.143146	
6	2.804871	1.432874	0.273365	
6	-4.075843	-1.080648	0.010301	
6	2.093499	0.221588	0.108860	
12	-2.209135	0.749832	0.154360	
6	0.936006	-0.439859	-0.071389	
6	0.207421	2.047276	0.120877	
8	-0.199260	0.601463	-0.065271	
6	-2.923795	-1.852921	0.096446	
6	1.432828	2.292047	0.129765	
8	3.713569	4.649230	-0.253781	
16				
586.315764	Kcal/mol	25.425090	eV	-100.449326 H Child_7_36.log
6	-2.100503	-4.224415	1.507714	
8	-0.849738	4.351669	0.347404	
6	-1.748279	-3.133691	0.884438	
6	0.136082	3.682237	0.386027	
6	-7.178899	0.473719	-0.403824	
6	1.143255	2.947201	0.505148	
6	-1.426457	-2.080915	0.144494	
6	2.118961	2.027292	0.433095	
8	-6.107364	0.897514	-0.319047	
6	2.921096	1.182283	0.383772	
6	-0.357208	-1.601088	-0.901929	
6	3.687829	-0.017800	0.364122	
6	-1.621541	-0.870417	-0.565170	
12	3.533915	-2.104425	-0.034033	

6	0.829372	-1.478260	-1.285393	
12	2.902299	0.151896	-0.711119	
16				
589.596584 Kcal/mol 25.567360 eV -100.444098 H				Child_4_58.log
6	1.181696	-3.594880	-0.127511	
6	-1.612582	3.044510	-0.181058	
6	0.002449	-4.318148	-0.198839	
6	-0.409756	3.634834	-0.160011	
6	4.427152	0.454263	0.192674	
6	0.898916	3.943377	-0.094400	
12	2.588904	-0.663172	0.068212	
6	-1.932342	1.849719	-0.115221	
8	1.016886	-2.135890	-0.037960	
8	-4.582158	-0.372250	0.337819	
6	3.590469	1.440548	0.180774	
6	-3.547707	-0.786683	0.065153	
12	-0.318995	-0.809976	-0.060406	
6	-1.432109	0.067527	0.137080	
6	1.319982	1.561761	0.012724	
6	-2.272292	-1.006345	-0.126790	
16				
592.358504 Kcal/mol 25.687128 eV -100.439697 H				MutI_13_57.log
6	3.467825	-1.993173	0.506287	
6	1.138891	-2.634491	-0.195993	
6	4.693723	1.717359	0.177387	
12	-3.581247	-0.116168	0.150570	
6	3.475228	2.351138	0.174551	
6	-1.873478	-0.563828	-0.519914	
6	-0.060949	-2.273768	-0.540664	
6	2.364886	-2.529944	0.086573	
6	4.517665	0.327847	0.282379	
6	-1.152869	-1.573437	-0.571225	
8	-1.557345	0.863154	-0.561066	
12	-3.240154	1.472558	0.076063	
6	0.049974	2.125671	-0.426006	
6	1.614057	3.052586	-0.055336	
8	-5.013589	-0.689183	0.926256	
6	4.169093	-0.950700	0.141777	
16				
594.120027 Kcal/mol 25.763515 eV -100.436889 H				MutI_1_73.log
6	-4.197046	-0.049131	-1.396353	
6	-3.213709	-1.731013	-0.480877	
6	-1.327705	1.157795	0.341143	
6	-0.490038	0.219080	1.024827	
6	-2.153701	-0.920429	0.122536	
8	-2.352178	0.425342	-0.246899	
12	4.072767	1.755400	-1.053670	
6	0.991121	-1.329316	1.554763	
6	4.140005	-2.454623	-1.108902	
6	-4.322833	-1.459802	-1.232033	
8	-1.137886	-1.109429	0.917184	
6	1.002867	-0.051198	1.550432	
6	2.320178	-1.729108	0.697212	
6	2.643903	1.050411	-0.380142	
6	3.179951	-2.242858	-0.211861	

12	-1.032554	3.470754	0.366440	
16				
595.754743 Kcal/mol 25.834403 eV -100.434284 H				MutD_4_66.log
8	0.328148	-0.065540	-1.166129	
6	-3.492012	-3.244404	-0.053107	
6	8.329973	-0.249294	1.578373	
6	-3.585875	-0.029657	1.886935	
12	-0.181226	1.086110	-1.831908	
6	1.918856	0.007081	-0.848867	
6	5.596264	-0.438021	0.215699	
12	-3.729895	-1.845014	1.200317	
6	-2.867303	1.011474	-1.069165	
6	-3.163915	0.520352	0.129232	
8	-2.849446	4.122094	0.267086	
6	6.868423	-0.579690	0.600355	
6	-3.466501	-4.483097	-0.679663	
6	4.387384	-0.294941	-0.137975	
6	-2.450288	4.031446	1.344217	
6	3.108966	-0.142178	-0.504129	
16				
596.558200 Kcal/mol 25.869245 eV -100.433004 H				
Original3D_11_5.log				
6	-0.838511	-1.132378	-0.630839	
12	-1.389825	0.959765	-0.034657	
6	-3.919184	1.319610	-0.679007	
6	1.784685	0.188296	-0.480775	
6	0.150534	2.459920	-1.096758	
6	-3.580617	0.046956	-0.778850	
8	2.660440	-0.506949	1.518261	
6	-0.151758	-2.190530	-0.775264	
6	1.314111	-0.660658	0.834044	
8	-3.820261	-0.960280	0.620391	
6	1.125322	-1.853664	-0.283271	
12	1.440227	2.213102	0.657648	
6	-3.359620	-1.006870	1.575521	
6	3.355969	0.247754	0.227894	
6	2.169978	-1.166620	-1.049648	
6	3.394714	-0.641247	-0.960565	
16				
596.965857 Kcal/mol 25.886922 eV -100.432354 H				Child_7_63.log
6	-1.213524	3.161407	0.299039	
6	2.331227	-3.471860	0.300836	
6	-1.850181	2.090245	0.293555	
6	2.277007	-2.485900	-0.512217	
12	0.685269	3.153255	-0.093755	
6	2.337486	-1.364064	-1.240292	
8	-2.454717	0.909210	0.286497	
12	1.046801	-1.817153	1.492671	
6	-1.736792	-0.287707	0.601425	
6	2.230221	-0.149037	-1.669087	
6	1.799791	1.247546	0.288954	
8	-6.383548	-2.170607	-1.036209	
6	-2.111139	-1.504343	0.027297	
6	1.523939	1.272888	-1.035105	
6	3.355706	0.355286	-0.049735	

6	-0.623530	0.145198	0.897117	
16				
606.800897	Kcal/mol	26.313411	eV	-100.416681 H Child_11_24.log
8	-6.645425	-0.581263	0.610321	
6	4.975772	-0.075936	-0.585897	
6	1.745727	-1.843860	0.882007	
6	-0.812618	2.797752	-0.524973	
6	1.980077	-0.636168	1.179753	
6	-2.121715	2.851685	-0.440509	
6	-5.529247	-0.439936	0.197586	
6	-0.176539	1.727404	-0.479064	
6	2.159063	0.715777	1.467962	
12	2.792720	0.124541	-0.419987	
6	1.439739	1.768785	1.017601	
8	0.876152	1.025710	-0.433144	
6	-4.258364	-0.164822	-0.246180	
6	-1.760887	-2.605337	-1.220313	
12	0.006180	-1.867882	-0.222975	
6	4.453556	-1.201258	-0.198283	
16				
613.188654	Kcal/mol	26.590410	eV	-100.406502 H Child_10_54.log
12	-5.275101	0.375535	0.009429	
6	4.433941	-0.083369	-0.211456	
8	-3.343157	0.128738	-0.426421	
12	2.958496	-1.772093	-0.340517	
6	-2.048768	0.072108	-0.031807	
6	-1.212975	1.158904	-0.207754	
6	0.895993	-2.570665	-0.482031	
6	-0.091473	1.775568	-0.219343	
8	1.005683	0.058680	1.632611	
6	0.251130	-0.667294	0.802024	
6	1.128600	2.103509	-0.196655	
6	-0.685231	-2.456137	-0.339843	
6	2.421061	2.347541	-0.158279	
6	2.885742	3.428184	-0.269718	
6	0.929921	-1.487102	0.207313	
6	-1.158100	-1.078019	0.161471	
16				
614.818062	Kcal/mol	26.661068	eV	-100.403905 H MutD_4_78.log
6	0.264067	-2.719347	-1.118179	
6	3.016521	1.298092	0.029205	
8	1.224664	-0.535946	2.070477	
6	-4.305262	0.200782	-0.511340	
8	2.613870	-1.695226	-1.107797	
12	-2.241716	-0.922409	-0.053939	
6	-5.554583	2.375679	-1.178973	
6	3.591599	2.783908	-0.825390	
12	2.346420	-0.464650	0.222677	
6	-0.985653	0.440518	2.924366	
6	1.816989	-2.353857	-1.634304	
6	4.006253	4.041665	-0.973513	
6	-1.079496	-1.639928	-1.314080	
6	-1.386247	-0.205683	1.819247	
6	-4.753004	1.649258	-0.922344	
6	0.041362	-0.122072	2.084254	

16
615.930789 Kcal/mol 26.709321 eV -100.402132 H Child_8_47.log
6 -1.897112 2.598043 -0.004014
6 4.252316 -1.207305 -1.014940
6 -2.972079 1.915260 -0.064621
6 4.698796 -0.138026 -0.493638
6 -5.539638 0.102935 -0.230635
12 2.300890 -1.309178 -0.448543
6 -3.856802 0.882012 -0.136452
6 5.074451 1.010799 0.052874
12 0.062518 1.816498 0.173361
6 5.384592 2.136969 0.688726
6 -3.365280 -0.498410 -0.138762
6 0.794258 -2.556367 1.230029
6 -2.295027 -1.276999 -0.191243
6 1.112177 0.387247 0.198395
8 0.010846 -2.208200 0.586453
8 -4.598947 -1.069897 -0.095469

16
616.062276 Kcal/mol 26.715022 eV -100.401922 H Child_11_52.log
8 3.220213 1.997019 -0.100906
6 -2.514717 -3.058439 -0.272431
12 5.773947 -1.136791 -0.200227
6 -3.290786 -2.058253 -0.155933
6 -0.975346 4.128125 -0.179998
6 -3.898237 -0.825867 -0.037897
6 3.889432 -0.285084 0.326074
6 -4.845817 0.157812 0.084627
6 3.026513 0.793041 -0.023275
6 -3.476331 0.596162 0.068183
6 -1.697905 3.133885 -0.058804
12 -0.958167 -1.698709 -0.019061
6 1.578892 0.194219 0.114512
8 -2.446743 1.266382 0.091934
6 0.246382 -0.207222 0.097501
6 1.295066 -1.248581 0.487981

16
618.223662 Kcal/mol 26.808749 eV -100.398478 H MutD_9_70.log
6 4.745981 7.058253 4.797890
6 -1.500558 -2.265769 2.015070
6 2.639822 -0.910840 -1.222880
6 -2.267922 -1.578697 2.520273
6 4.047541 0.060234 -1.980126
6 1.044996 -3.306740 1.440757
6 -3.241881 -0.732857 1.517926
8 5.136877 -0.366654 -1.681809
8 -2.846659 2.547546 -1.907251
6 -3.601527 0.319195 0.823777
6 0.463362 0.083548 -2.205293
6 -0.197559 -2.914234 1.929481
6 -3.297513 1.974946 -0.908450
12 -1.249842 1.472719 -2.193596
12 2.104220 -2.405003 0.210097
6 -3.597122 1.169674 0.023986

621.763157 Kcal/mol 26.962236 eV -100.392837 H Child_10_24.log
6 4.304079 -0.569022 0.175389
12 -5.928861 -1.682778 0.169878
12 3.582369 1.343924 0.175679
6 -4.026814 -1.037552 -0.091402
6 4.019028 -1.765666 0.046177
6 -3.138020 -0.117217 -0.202767
8 3.527407 -2.996357 -0.156056
6 -1.777292 0.411621 -0.045882
6 2.048487 2.908860 -0.152425
6 2.175809 -3.073863 -0.128039
6 -0.776998 0.282206 0.007508
6 0.905726 -2.936117 0.013048
6 -0.109273 4.734900 0.011994
6 0.885898 3.649583 -0.096621
6 0.533422 -0.135020 0.013677
8 -3.790708 1.740103 -0.025270

16

624.417196 Kcal/mol 27.077327 eV -100.388608 H Child_17_11.log
6 -4.700578 1.657154 -1.734270
6 2.075991 -3.018956 -1.708388
6 -2.682622 -0.952477 1.789928
6 2.625749 -1.912209 -0.908193
6 -3.547461 1.573043 -1.097702
12 3.812521 -0.257427 -0.525611
6 -2.954832 -0.176057 0.841810
6 1.400128 -2.426983 -0.588808
6 -2.222566 2.446847 -0.945468
6 3.919992 1.694659 -0.018473
6 -2.772558 0.644899 -0.264590
6 0.250928 -2.290015 0.291966
8 3.083000 6.663731 1.114503
8 -0.237318 -3.266267 0.902133
6 -1.546363 1.223493 -0.640761
12 -0.632546 -1.239248 1.672661

16

626.216241 Kcal/mol 27.155341 eV -100.385741 H Child_3_47.log
12 -0.082527 1.408728 1.700828
6 -2.665169 -1.628039 -0.913094
6 0.105895 2.457669 -0.667936
12 -0.995256 -2.563952 -0.283072
6 1.242908 2.137309 -0.985858
6 -1.205755 2.305881 -0.159578
6 -3.073690 -0.810663 -0.168068
6 2.050392 1.069142 -0.999014
8 0.793837 -2.204111 0.177701
6 1.447937 0.534636 0.911023
6 -3.240365 0.392357 0.600680
6 2.387296 -0.130897 -0.654995
6 0.947700 -0.689490 0.203667
6 -0.655988 -0.844961 0.966921
6 -2.386974 1.843086 -1.132443
8 4.607197 -1.040077 -0.055313

16

628.489393 Kcal/mol 27.253914 eV -100.382118 H Child_1_33.log

6	-3.266028	-2.600181	-0.089298	
12	5.458038	0.821078	0.737435	
6	-0.670209	-2.635299	-0.464944	
6	-1.023629	2.017669	2.111424	
8	-1.816241	-2.415878	-0.887783	
6	-2.727086	4.648740	-1.080140	
6	0.606056	-2.427035	-0.491891	
6	-2.251451	3.482757	-0.743659	
6	-2.998637	-1.171992	0.211968	
6	-1.225231	1.762415	0.834977	
12	2.488758	-1.535552	-0.533994	
6	-1.700474	2.307662	-0.391214	
6	3.756502	0.232006	-0.536896	
6	2.799314	0.774480	-0.520319	
6	-1.133854	0.882288	-0.348390	
8	-2.727909	-1.967544	1.713908	
16				
631.442636	Kcal/mol	27.381979	eV	-100.377412 H Child_9_32.log
6	2.013538	2.954031	-0.277308	
6	-5.046448	-0.254159	0.748146	
6	2.543499	1.723620	-0.136938	
6	-4.346594	-1.321956	0.292264	
6	3.069964	0.520361	-0.132386	
6	-3.537020	-2.143492	-0.291649	
6	3.887349	-2.599118	0.709689	
8	-4.786917	0.949234	0.585125	
6	2.261458	-0.700656	-0.142527	
12	-2.313475	-0.215853	-0.623693	
6	1.420666	2.609722	0.885381	
8	-3.426201	1.331362	-0.312251	
6	2.727131	-1.966258	0.276237	
6	0.893090	-0.653008	-0.455930	
6	-0.299418	-0.456185	-0.691933	
12	4.995280	-0.160996	0.050253	
16				
631.708354	Kcal/mol	27.393501	eV	-100.376988 H MutD_17_68.log
6	-1.785224	0.156081	0.179837	
6	-4.307830	1.761875	-0.403269	
8	-3.714325	-2.480735	-0.281046	
6	0.783796	-1.890069	0.647300	
6	-1.170814	-2.036885	-0.257149	
6	-2.478394	-1.438239	-0.158922	
6	2.425710	-2.130574	1.017042	
6	1.547288	1.224978	-1.231952	
6	-0.375053	2.491140	0.869624	
6	2.818262	1.035705	-1.083632	
12	-0.436010	0.956887	-0.910760	
12	3.922873	-0.898110	0.233005	
6	4.127546	0.941903	-0.849255	
8	-0.184242	3.189783	1.753445	
6	-0.139267	-2.147101	0.732438	
6	-3.221656	0.968234	-0.069751	
16				
635.676919	Kcal/mol	27.565595	eV	-100.370664 H Child_11_13.log
6	5.434960	-0.467462	-0.008604	

6	-4.431660	2.225840	-0.732377	
6	4.722308	0.589243	-0.011619	
6	-3.667503	1.205689	-0.534298	
12	3.918493	-1.781209	-0.179108	
8	-4.204112	-1.785082	0.008559	
6	3.806183	1.491925	-0.028112	
6	-2.916384	0.306781	0.071182	
6	2.642883	2.063428	-0.045927	
6	-3.436436	-0.921937	0.023282	
6	1.234716	-1.653200	-0.203638	
12	-1.279776	1.479185	0.757983	
6	1.376068	2.351392	-0.060525	
6	-1.059964	-2.147559	0.081376	
6	-0.084495	-0.075504	-0.034866	
8	-2.469473	-1.488359	0.236222	
16				
637.728110 Kcal/mol 27.654543 eV -100.367395 H				
Original3D_6_5.log				
6	0.073857	1.078604	1.125668	
6	0.700528	0.780078	-0.234067	
6	2.220911	-0.304715	-1.159156	
6	-0.738263	1.695558	-0.907061	
8	0.864269	-0.429331	-1.504264	
6	0.784530	-1.632680	1.135251	
6	-2.008596	0.695689	-0.848576	
8	-0.857239	2.802701	-0.906251	
6	-2.038350	0.657959	0.621332	
6	2.166118	0.668880	-0.129320	
6	-1.157238	0.116625	1.662613	
6	-0.209733	1.667387	2.283752	
12	-0.699149	-0.897570	-0.144501	
12	3.685557	-0.995729	0.292891	
6	-2.659095	-1.801331	-0.648440	
6	-3.116858	-2.999948	0.015248	
16				
639.781207 Kcal/mol 27.743574 eV -100.364124 H				
Child_3_54.log				
6	2.818737	4.063894	-0.394825	
6	0.179456	-3.394468	0.023441	
6	1.819263	3.349396	-0.160648	
6	1.470424	-3.384195	0.034556	
6	0.854079	2.661865	0.122519	
6	2.774898	-2.995900	0.042199	
6	-0.055478	1.918740	0.445576	
6	-0.517719	-2.267761	0.011368	
12	-3.672230	1.626193	-0.302608	
12	-2.804997	-2.051606	-0.103411	
8	4.286420	0.444826	0.254716	
6	-0.160458	-0.907507	0.054590	
6	-1.929963	1.403733	0.936453	
6	-1.661489	-0.269529	0.031226	
6	3.208157	-1.573632	-0.461414	
8	-1.170509	1.239817	-0.159468	
16				
640.658514 Kcal/mol 27.781618 eV -100.362725 H				
Child_7_16.log				
6	-5.349818	-0.046142	-1.270515	

6	13.804906	-0.876501	-0.785206
12	-4.394534	-1.796114	-0.908093
8	12.864966	-1.008557	-0.470997
6	-4.359267	0.703058	-1.111011
6	1.734925	3.197211	1.236811
6	-3.222655	1.385530	-0.863760
6	1.105113	3.825930	0.309638
8	-1.848636	-2.247665	-0.316642
6	-1.056450	-1.244784	2.419495
6	-2.105275	1.748777	-0.530100
12	-0.351566	2.443433	-0.040234
6	-0.897327	-1.561479	0.418037
6	-2.051628	-1.139007	1.478182
6	0.125801	-0.880588	0.943021
6	-2.924565	-2.065015	0.702248
16			
645.638448 Kcal/mol 27.997568 eV -100.354789 H Child_9_56.log			
6	3.181765	-3.493999	0.540870
6	0.100954	2.861869	0.014734
6	3.024922	-2.238317	0.184547
6	-1.089586	2.443840	-0.030340
6	2.834469	-0.971256	-0.140335
6	1.424673	3.143912	0.099212
12	4.235345	0.424894	-0.443451
8	-4.403958	0.994193	0.682238
8	-0.951251	-1.189859	-0.178746
6	-3.533018	1.218578	-0.275119
12	0.779346	-0.479439	-0.057645
6	-4.639324	-1.879853	-0.233548
6	-3.890213	-0.159819	-0.246765
6	-3.316997	-1.470701	-0.119046
6	5.096944	1.671794	0.456249
6	-2.083690	-0.756070	0.080413
16			
649.241798 Kcal/mol 28.153824 eV -100.349047 H			
Original3D_13_7.log			
6	1.558972	0.226003	0.880241
6	1.741659	-0.604545	-1.876819
12	-0.487308	0.428781	0.240646
6	-2.543375	2.317119	-0.510458
8	-1.976132	3.019850	0.633201
6	1.773665	0.831210	-1.193956
6	1.716783	-1.859845	-2.051176
6	-2.786658	1.898706	0.823306
6	1.542152	-0.484118	2.005117
6	1.055444	2.901199	0.077870
6	-2.952762	-1.871983	-0.748264
6	1.468041	2.091515	-1.386592
12	2.844027	-1.176477	-0.165691
6	-4.010340	-2.448907	-0.283191
6	-4.482006	-3.240219	0.342768
8	2.879872	-1.715406	2.195231
16			
652.788316 Kcal/mol 28.307616 eV -100.343395 H Child_6_63.log			
6	-1.888389	2.654839	1.491366

6	-4.496980	-0.980407	-0.457350	
8	3.724282	0.543940	-0.129649	
6	-3.444697	-1.692722	-0.278295	
12	2.541268	1.711147	-0.771613	
8	-2.256104	-2.329743	-0.116501	
12	3.355549	-0.705518	0.859462	
6	-1.152024	-1.610577	-0.055368	
6	-2.830480	2.160048	0.781516	
6	0.554216	1.590475	-1.042834	
6	-1.262283	-0.242171	-0.169138	
6	-0.380042	0.643729	-0.927154	
6	1.493175	-1.973715	0.704665	
6	0.297278	0.153116	0.353742	
6	-3.793347	1.674569	-0.005033	
6	3.152370	-2.007372	-0.243611	
16				
663.286047	Kcal/mol	28.762842	eV	-100.326666 H Child_5_13.log
6	2.540070	3.610486	-1.061317	
6	-1.110106	0.612330	1.386777	
6	3.354096	0.126216	-0.935218	
6	0.102679	-0.110927	1.270939	
8	2.694454	4.387511	-0.189700	
6	-1.033992	-0.802265	0.707814	
12	3.356333	-2.014685	-0.746382	
6	-3.640153	2.331828	0.504272	
6	2.855477	0.662255	0.135140	
6	-1.058248	-2.191015	0.015671	
6	2.341319	1.263749	1.231604	
6	0.122091	-2.747577	-0.033922	
6	3.205221	-3.734151	0.522447	
8	-3.835518	1.401567	-0.114423	
6	-7.157626	-0.250938	-1.097335	
12	-2.856039	-1.229697	-0.374306	
16				
663.358106	Kcal/mol	28.765966	eV	-100.326551 H
	Original3D_0_39.log			
6	1.053331	-1.138880	-0.993086	
6	-1.539967	0.198318	0.040484	
6	0.160353	-2.022153	0.470508	
8	1.167822	1.750281	-0.783592	
6	1.566364	2.802606	-0.605033	
6	3.435937	0.686986	-1.026199	
8	3.111553	0.463043	-2.075130	
6	-0.896846	-1.033671	0.440091	
6	-2.012191	-2.139042	-0.026870	
12	-3.910198	-1.080276	-0.398890	
6	5.018320	0.167691	1.479496	
6	1.384622	-1.839636	-0.163298	
12	-3.574209	1.503254	0.715602	
6	-1.116302	-3.110973	0.266799	
6	5.769649	-0.143429	2.412030	
6	-3.560289	3.775127	0.883282	
16				
665.944793	Kcal/mol	28.878136	eV	-100.322429 H Child_1_9.log
6	3.776304	-2.431423	-1.197405	

6	-8.228587	-0.584184	-0.729925	
6	3.603516	-3.009279	-0.023256	
8	-7.028187	-0.401248	-0.463242	
6	3.479571	-1.260630	-0.664868	
6	-5.774680	-0.210219	-0.184762	
6	3.355627	0.488018	-1.306481	
12	-3.826153	0.086727	0.248126	
6	3.306783	-1.838487	0.509281	
12	-1.118011	0.499436	0.849770	
6	3.182839	-0.089838	-0.132331	
6	0.862283	0.801223	1.289714	
6	3.010051	-0.667695	1.041818	
6	2.067705	0.984924	1.557512	
6	2.934950	3.407459	-1.415556	
8	2.762162	2.829602	-0.241407	
16				
668.100624	Kcal/mol	28.971622	eV	-100.318994 H Child_10_60.log
8	4.634155	0.507300	-0.867025	
6	-4.876385	-0.897117	-0.151943	
6	3.705001	-0.036324	-0.389484	
6	-3.790767	-1.629897	-0.443071	
6	2.644145	-2.616531	0.459198	
12	-3.018120	0.427150	-0.040055	
6	2.663455	-0.613213	0.284341	
6	-2.406209	2.591227	-0.223126	
6	1.662707	-1.974611	-0.202868	
6	-2.474582	-1.886807	-0.425425	
8	1.302258	3.095118	-0.464147	
6	-1.015888	0.983115	1.091061	
6	2.325967	0.216797	1.300432	
6	-0.940108	1.925402	0.093856	
6	0.392376	-1.606892	-0.583671	
12	0.115656	-0.056335	0.522854	
16				
672.436668	Kcal/mol	29.159651	eV	-100.312084 H Child_9_35.log
6	-14.055529	-0.801280	-0.741210	
6	2.307512	8.560110	0.275900	
8	-0.955200	-2.298693	2.783829	
6	2.046951	7.261924	0.117735	
6	-12.755025	-0.597369	-1.006050	
12	1.550002	4.793334	-0.185360	
6	-1.357473	-1.392632	2.331218	
6	1.266109	3.373693	-0.359389	
6	0.528041	-2.948831	1.062350	
6	1.017204	2.138830	-0.510267	
6	1.529145	-3.425882	0.565888	
6	0.759729	0.847235	-0.663120	
12	2.929318	-4.126699	-0.047989	
6	0.503471	-0.417418	-0.826888	
8	4.202380	-4.585457	-1.134952	
6	4.921650	-4.752785	-1.977972	
16				
672.954659	Kcal/mol	29.182113	eV	-100.311258 H Child_6_37.log
6	-1.942203	-2.458688	-1.197894	
6	-0.304600	2.265085	-0.197036	

6	-0.766457	-2.134984	-1.484709
6	2.141380	2.238982	-0.533360
6	-2.626493	-2.275698	-0.034861
6	-2.857023	1.824430	-0.340403
6	0.325396	-1.549215	-0.940037
8	3.152359	1.705556	-0.421322
6	-2.874751	-1.914931	1.171054
6	-1.669891	1.914472	-0.478553
6	0.973478	-1.098746	0.064162
6	-4.041187	1.396323	0.021311
12	7.901458	-0.838728	0.361864
6	-5.065500	0.574993	0.440987
12	-0.994820	-0.761108	1.321295
8	0.518572	1.607682	0.528588

16

673.623930 Kcal/mol 29.211135 eV -100.310192 H

Original3D_11_7.log

6	-1.205890	0.945245	0.576799
6	-0.716588	-1.078490	0.907529
6	0.878560	-0.874568	1.118322
6	2.217583	-0.903178	0.687618
6	-0.986255	-0.151913	-0.453807
8	3.326392	-0.917992	0.676520
12	-2.624289	2.624698	0.430102
6	-3.079644	-1.194011	-0.911100
6	4.838487	0.038778	-0.767028
6	5.782310	0.690893	-1.068581
6	-4.056914	4.362663	-0.531767
6	6.908291	0.833012	-0.582313
6	0.936957	-0.222643	2.323567
12	-4.037099	-3.050991	-0.533100
6	-2.850861	-0.184298	-0.148390
8	0.166163	-0.138685	-1.385159

16

674.451294 Kcal/mol 29.247013 eV -100.308873 H

Child_11_17.log

12	5.719740	-0.773879	0.752479
6	-4.181469	0.812051	0.149672
6	3.845147	-0.616833	0.122984
6	-3.264655	-1.700138	-0.239160
6	2.260356	2.099782	-0.976826
6	-3.528452	-0.409266	0.189259
6	1.587199	2.976923	-0.163212
6	-2.579867	-2.745833	-0.445286
6	2.693226	-0.857836	-0.266519
6	-2.787197	1.293793	0.333129
6	0.377100	3.418687	-0.086602
8	-1.961657	1.944253	-0.075713
6	1.462932	-1.133251	-0.776210
12	-1.010694	-1.308561	0.256512
6	0.373909	-1.422730	-1.333526
8	-2.295585	-0.107104	1.181450

16

677.384894 Kcal/mol 29.374226 eV -100.304198 H

Child_5_26.log

6	7.306605	-1.870273	-0.258149
12	-0.983060	2.399209	-0.050425

6	-0.748870	-1.205000	1.367810	
6	-6.321952	0.934645	0.077599	
6	6.221798	-1.127136	-0.257612	
6	-5.054370	0.774208	-0.093832	
6	5.081234	-0.548058	-0.158738	
6	-3.771216	0.685450	-0.308222	
6	-1.879615	-1.226457	0.741548	
6	-2.487337	0.757250	-0.398091	
6	3.887840	-0.024928	0.038376	
8	4.707619	2.966873	0.244231	
12	-3.617386	-2.392426	-0.194417	
6	-0.035197	0.523667	-0.360816	
6	2.672232	0.253615	0.253378	
8	-1.460312	-1.422285	-0.359405	
16				
680.386737	Kcal/mol	29.504399	eV	-100.299414 H Child_17_10.log
8	-5.718707	-2.387716	-0.517914	
6	8.632897	-4.744565	0.017098	
12	-6.665705	-4.051922	0.287793	
6	7.702311	-3.773629	0.010075	
6	-4.768412	-1.602356	-0.491439	
12	5.977174	-1.973691	-0.002946	
6	-3.857648	-0.735654	-0.124792	
6	-2.956431	0.231997	0.143209	
6	3.040248	1.090580	-0.025113	
6	-2.218139	1.247030	0.208518	
6	2.229297	1.936692	-0.031234	
6	1.320023	2.885392	-0.038097	
6	-1.566573	2.245825	0.864423	
6	0.464720	3.777781	-0.044552	
6	2.631390	5.268923	-0.290691	
8	-1.238760	5.555123	-0.057409	
16				
681.756886	Kcal/mol	29.563814	eV	-100.297231 H Child_17_30.log
6	5.826079	-0.885394	-0.220469	
6	-9.416354	0.142363	-0.594340	
6	5.481934	0.345362	-0.288389	
6	-8.220700	0.038355	-0.205859	
8	5.247324	1.736721	-0.294692	
6	-6.869857	-0.157273	-0.026604	
6	4.606177	-2.005566	-0.287470	
6	-5.643792	-0.141483	0.056729	
6	3.786339	1.664552	-0.115264	
8	-4.354860	-0.133162	0.189975	
6	3.416142	-2.432162	-0.292373	
6	-3.044123	-0.135076	0.358661	
6	2.506788	1.648684	-0.027006	
6	-1.794991	-0.014737	0.473791	
12	0.253171	0.337765	0.191085	
12	3.835032	-0.440618	0.463022	
16				
694.448984	Kcal/mol	30.114196	eV	-100.277005 H Child_1_50.log
12	-3.342665	0.698924	0.334280	
6	2.869048	1.414917	-0.640302	
6	-3.927282	2.913382	0.920835	

6	1.874552	2.368407	-0.601234
12	-2.791416	-2.070559	-0.473123
6	0.921440	3.352697	-0.517815
6	-0.846236	-2.956660	-0.185915
6	2.692441	-1.175427	-0.093090
6	0.463786	-2.991614	-0.121576
6	0.267208	-0.690816	0.067050
6	2.455371	-0.223405	-1.320562
6	-0.360952	0.366124	-0.038931
6	3.610035	-1.100602	2.256126
6	1.145276	-1.810277	0.197741
8	2.169790	1.350916	0.452100
8	-1.342183	1.106492	-0.185579

16

694.614015 Kcal/mol 30.121353 eV -100.276742 H

Original1D_0_7.log

6	0.000000	0.000000	3.347143
6	0.000000	0.000000	2.027143
6	0.000000	0.000000	0.707143
6	0.000000	0.000000	4.667143
6	0.000000	0.000000	-0.612857
6	0.000000	0.000000	5.987143
6	0.000000	0.000000	7.307143
6	0.000000	0.000000	-1.932857
6	0.000000	0.000000	-3.252857
6	0.000000	0.000000	-4.572857
6	0.000000	0.000000	-5.892857
8	0.000000	0.000000	8.627143
6	0.000000	0.000000	-7.212857
12	0.000000	0.000000	9.947143
12	0.000000	0.000000	-8.532857
8	0.000000	0.000000	-11.172857

16

694.870898 Kcal/mol 30.132492 eV -100.276332 H

Original1D_0_6.log

6	0.000000	0.000000	-10.844980
6	0.000000	0.000000	-9.532825
6	0.000000	0.000000	-8.249155
6	0.000000	0.000000	-6.945521
6	0.000000	0.000000	-5.709261
12	0.000000	0.000000	-3.684622
8	0.000000	0.000000	-2.050899
6	0.000000	0.000000	-0.800799
6	0.000000	0.000000	0.443383
6	0.000000	0.000000	1.736784
6	0.000000	0.000000	3.022419
6	0.000000	0.000000	4.278258
8	0.000000	0.000000	5.505809
12	0.000000	0.000000	7.465627
6	0.000000	0.000000	9.574470
6	0.000000	0.000000	10.858668

16

695.128750 Kcal/mol 30.143674 eV -100.275922 H

Original2D_1_2.log

8	-0.171907	1.627213	0.000000
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6	-1.301091	2.528061	0.000000	
6	0.804949	2.741591	0.000000	
12	1.910292	1.051150	0.000000	
6	2.449273	-1.172020	-0.000000	
6	3.327143	-2.399463	-0.000000	
6	3.987668	0.058687	0.000000	
6	1.391752	-2.132016	-0.000000	
6	-2.390515	1.503815	0.000000	
6	-1.065426	-1.908800	-0.000000	
6	-1.898608	-2.871260	-0.000000	
12	-3.406000	3.287706	0.000000	
6	-0.000000	-1.183591	-0.000000	
6	-2.606565	0.366911	-0.000000	
8	-2.675600	-3.841640	-0.000000	
6	4.089512	-1.257056	-0.000000	
16				
701.329976	Kcal/mol	30.412585	eV	-100.266039 H Child_8_17.log
8	5.385944	-1.193230	0.396589	
12	-5.619810	1.109902	-0.051368	
6	5.745101	-0.089566	0.973565	
6	-3.534253	1.568155	0.161879	
12	3.089651	0.069380	-0.605000	
6	-4.330720	-0.826088	0.071548	
6	0.980427	-0.118323	-0.758525	
6	5.063324	1.051776	0.535565	
6	-3.507101	0.229378	-0.090144	
6	-0.157101	0.346394	-0.474013	
6	-2.149676	1.667925	0.322706	
6	3.950925	1.876495	0.285712	
6	-4.343557	-2.133866	0.284845	
6	-1.267584	0.976856	-0.028163	
6	-4.368623	-3.442036	0.437270	
8	4.348424	-1.406019	-0.703723	
16				
703.134759	Kcal/mol	30.490847	eV	-100.263163 H Child_15_22.log
8	2.918351	2.929845	0.116616	
12	-5.932636	-0.047981	0.448192	
6	2.909533	1.680384	0.388385	
6	-4.058208	-0.156116	-0.065167	
8	1.657227	3.344239	-0.765383	
6	-2.871740	-0.269590	-0.385223	
6	2.753674	0.486336	0.668210	
6	-1.593753	-0.567118	-0.555925	
12	2.183095	-1.407163	0.757859	
6	-0.009432	-2.092464	-0.111624	
6	0.023222	3.060500	-0.195419	
6	2.002858	-3.642802	-0.519772	
6	-1.188098	2.889531	0.103358	
6	-0.367003	-0.760019	-0.335186	
6	3.036044	-2.973793	-0.231218	
6	0.761213	-3.110008	-0.307498	
16				
703.754644	Kcal/mol	30.517728	eV	-100.262175 H
	Original2D_0_29.log			
12	1.423929	1.360256	0.000000	

12	-0.979838	2.680925	-0.000000
6	-0.000000	-0.836145	0.000000
8	-2.056907	-1.495114	-0.000000
6	-1.301808	-0.088408	-0.000000
6	-0.698767	-2.175576	-0.000000
6	1.386033	-1.616809	0.000000
6	0.574726	-2.924906	0.000000
8	-2.216565	0.906094	-0.000000
6	-0.194391	-4.178628	0.000000
6	-0.863487	-5.161006	0.000000
6	-2.632249	-2.763211	-0.000000
6	1.582690	4.216000	0.000000
6	1.843792	-3.592183	0.000000
6	2.217593	5.349244	0.000000
6	2.895647	6.474623	0.000000

16

705.735378 Kcal/mol 30.603621 eV -100.259019 H

Original3D_11_4.log

6	1.663252	1.074737	0.039011
12	1.952199	3.262234	0.205213
12	-0.267341	1.489488	-0.983692
6	2.688218	0.601244	-0.453202
6	-2.362349	-0.245214	-0.554258
6	-3.143942	0.924397	-0.270429
6	-3.541127	2.408636	0.710298
8	-2.375988	1.781961	0.908353
6	2.812154	-0.686646	0.125561
8	-3.114190	-2.638139	-0.320737
6	-2.270275	-3.511750	1.332709
6	-3.605592	-1.585251	-0.748643
6	3.892364	-1.907399	0.121125
6	2.876367	-1.093078	1.480604
6	3.097434	-2.377824	-0.931889
6	1.844019	-1.963725	-0.077414

16

706.311076 Kcal/mol 30.628586 eV -100.258101 H

MutI_3_75.log

6	-3.904693	-0.871522	0.858573
6	4.593016	-1.792612	-0.168355
6	-1.827649	3.506328	-0.229463
8	2.125041	-1.904557	0.096170
6	-0.442883	3.543834	-0.170126
8	-1.194753	2.397742	0.536453
6	2.151336	1.354345	0.750525
6	-2.820606	-1.510568	0.600345
6	1.565330	2.157770	0.062916
6	0.829229	3.767503	-0.576715
6	3.307352	-1.879105	-0.030479
12	-5.044764	-1.931932	-0.608492
12	0.962573	-0.088559	-0.310981
6	-0.854225	-1.329377	-0.456497
6	-1.534654	-2.027101	0.437723
6	5.862445	-1.536093	-0.082998

16

706.468991 Kcal/mol 30.635434 eV -100.257850 H

MutI_14_57.log

8	-1.476764	2.638555	0.207713
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6	-4.450359	-1.196285	-0.620906	
6	0.929163	-1.923825	0.434634	
12	-1.871230	0.989144	-0.324746	
6	-3.422638	2.063339	1.465833	
8	2.053417	-1.427351	0.190570	
12	5.465169	-0.021829	-0.234727	
6	-2.888171	-0.731383	0.240594	
6	2.008406	0.956413	-0.262253	
6	-5.684704	-1.516874	-1.145412	
6	-0.263263	-2.186966	0.608036	
6	0.883164	1.557136	-0.370976	
6	4.066484	-0.136170	-0.088254	
6	-0.339332	1.866922	-0.286440	
6	-1.613204	-2.174615	0.717752	
6	2.817707	-0.127260	-0.104706	
16				
710.547986	Kcal/mol	30.812316	eV	-100.251349 H Child_14_25.log
12	6.441027	1.388599	0.096493	
12	-2.579595	-2.572793	-0.394217	
6	4.924615	0.385529	0.076693	
6	-0.486928	-3.058223	-0.189288	
6	3.970815	-0.314920	0.033170	
6	-2.997073	-0.473581	-0.025336	
8	-2.578378	2.997996	0.171277	
6	0.635531	-2.510892	0.018458	
6	-3.718849	2.568488	0.613811	
6	-2.223118	0.752985	-0.281511	
6	-1.184470	3.036701	-0.799480	
6	1.732412	-1.732509	0.039701	
6	2.890989	-1.141425	-0.001515	
6	-3.377280	1.047560	0.263631	
6	-1.446806	1.761122	-0.554029	
8	-2.253649	-1.462331	0.879580	
16				
717.137854	Kcal/mol	31.098080	eV	-100.240848 H
	Original2D_12_1.log			
6	0.000000	-0.841756	0.000000	
12	0.710604	1.241956	0.000000	
6	-2.111115	1.324967	0.000000	
6	-2.489007	0.142799	0.000000	
8	-2.318342	2.651929	0.000000	
6	1.224039	-1.747704	0.000000	
6	-1.681068	3.904183	0.000000	
6	-1.360620	-1.422968	0.000000	
6	2.585865	-1.088634	0.000000	
8	1.198221	-3.052438	0.000000	
6	-0.244024	3.821850	0.000000	
6	2.730110	0.280367	0.000000	
6	0.136986	5.099011	0.000000	
12	-0.309627	-4.143903	0.000000	
6	-2.084938	-2.590043	0.000000	
6	3.985313	-0.544167	0.000000	
16				
722.271205	Kcal/mol	31.320683	eV	-100.232667 H Child_6_39.log
8	5.723901	-1.958815	0.452317	

8	-3.907036	1.827524	1.440471
6	-3.561023	-2.787100	0.082240
6	-2.855771	1.244867	1.262347
6	4.649522	-1.469233	0.249849
12	3.207415	2.397576	-0.646574
6	3.422942	-1.125708	0.032853
6	-3.121387	-1.553697	-0.063412
6	-1.703733	0.748138	1.017657
12	0.272182	-0.866768	-0.372281
6	-9.585705	0.240287	-1.669081
6	2.366262	-0.334673	-0.198174
6	1.533598	1.254097	-0.173960
6	-1.841051	-0.782264	-0.176836
6	5.158583	1.831233	-0.698996
6	-3.843919	-0.152507	-0.150496

16
727.052675 Kcal/mol 31.528028 eV -100.225048 H

Original3D_0_43.log

6	0.051849	-1.796913	-0.567146
12	2.287699	-0.569811	-0.764080
6	0.203997	1.806054	-1.127345
6	0.477476	-1.150578	0.471356
12	-1.101829	0.040368	-0.871813
6	2.614763	2.085013	-1.494167
6	3.232844	-2.946519	-0.077862
6	-1.408370	1.845690	1.747260
6	0.727336	1.185244	0.417540
6	-4.256356	-0.884115	-0.302557
8	0.104237	1.965328	2.010532
8	-5.190484	-1.094869	-1.061260
6	-3.243339	0.054976	1.547799
6	2.980759	-1.463536	1.293381
6	1.526485	-1.610984	1.282517
6	1.502480	2.773940	-1.184687

16
727.463728 Kcal/mol 31.545853 eV -100.224392 H

Original2D_0_12.log

6	-1.323492	0.216856	-0.000000
12	-3.484017	0.568766	-0.000000
6	-3.606576	2.400462	-0.000000
8	0.000000	-0.741757	-0.000000
6	-4.895696	2.482749	-0.000000
6	-1.141857	1.347176	-0.000000
6	0.043726	2.076218	0.000000
6	1.700164	1.098663	0.000000
6	-0.302457	-2.007529	-0.000000
6	1.566349	-0.206181	0.000000
12	3.791070	-0.307540	0.000000
6	-0.508806	-3.258110	-0.000000
6	-0.035191	-4.570023	-0.000000
6	1.108347	-3.796247	0.000000
6	1.456694	2.519756	0.000000
8	3.993518	1.622075	0.000000

16
727.917557 Kcal/mol 31.565533 eV -100.223669 H

Child_11_35.log

6	5.275830	4.032616	-0.526299
6	-4.018192	-0.761321	-0.137095
8	4.645928	3.418417	0.211854
12	-3.996490	1.170520	0.317298
6	4.348816	-2.408340	-0.256795
6	-3.511921	-1.860781	-0.417625
6	3.980448	-1.101436	-0.117398
6	-2.800514	-3.058546	-0.508575
6	2.918480	-2.528749	-0.087054
6	-2.543939	2.504307	0.743412
6	1.472673	-2.974358	0.019159
6	-1.715353	-3.632755	-0.295326
6	0.202783	-3.061119	0.227783
6	-1.246580	2.587599	0.766878
12	-1.826052	3.992448	-0.654619
8	2.315987	-1.965706	0.735828

16

728.905750 Kcal/mol 31.608385 eV -100.222094 H

Original3D_12_6.log

6	-0.592215	1.214690	1.083950
6	-1.608696	1.685551	0.149402
8	-0.156418	0.203818	0.295399
6	-2.200754	2.705556	-0.156543
6	0.894214	-2.476438	0.731539
12	1.091938	-0.822520	-0.728287
6	-1.658081	-2.599349	-1.350822
12	4.219011	-0.720195	-0.722778
6	-1.912805	0.327603	-0.196145
6	-3.037053	4.012374	0.115240
6	5.907262	0.922630	0.090272
6	6.250146	1.794539	1.143949
8	-2.461791	-2.516820	-0.485589
6	-3.265089	3.249535	-0.997059
6	-3.263441	-2.194083	0.712339
6	-2.644441	-2.473178	1.829593

16

729.680876 Kcal/mol 31.641997 eV -100.220859 H

Child_11_42.log

8	-5.643173	-1.917078	-0.592576
6	2.253377	1.992202	-0.822510
6	-5.023805	-0.933479	-0.350762
8	3.252099	1.056614	-0.720121
6	-4.447723	0.191586	0.090003
6	1.048226	1.488634	-0.276037
6	3.978679	-1.855103	-0.503263
6	2.703375	-0.172535	-0.069381
6	0.282976	-0.686171	0.558811
12	-1.000206	1.118518	0.022069
6	2.803281	-1.552345	-0.920643
6	-4.707212	1.347294	0.789132
6	-0.870901	-0.996036	0.949151
6	1.320523	0.149804	0.115310
6	-3.293955	1.105586	0.167834
12	4.570836	-0.584594	0.989239

16

733.029786 Kcal/mol 31.787220 eV -100.215522 H

MutI_3_71.log

6	3.098230	-1.925383	-0.952055		
6	0.444633	-0.987741	-1.099301		
6	-4.448808	-2.793252	0.918581		
6	0.884893	1.284683	-0.600417		
6	1.561137	-1.585993	-1.221424		
6	-2.128765	1.731633	0.169412		
6	3.684554	-1.029250	-0.243059		
6	-0.201158	0.266170	-0.750695		
6	4.189044	-0.465743	0.954534		
8	-3.774138	-1.988768	0.527722		
6	-2.926248	2.575911	0.726770		
6	-1.492215	0.565798	-0.372112		
8	4.904580	-0.079936	1.911206		
12	-0.459276	2.742495	-0.152727		
6	2.133440	1.084873	-0.543951		
12	-2.693720	-0.724211	0.033634		
16					
733.865775	Kcal/mol	31.823472	eV	-100.214190 H	Child_16_14.log
12	2.912729	0.176397	-0.838666		
6	-3.284672	-1.066274	1.561316		
8	4.480247	-0.337761	-0.113040		
6	-3.420433	-2.117093	0.830966		
12	5.756450	-0.864646	1.026326		
6	-2.691905	0.044795	1.866129		
6	0.851751	0.516081	-0.997372		
8	-3.261628	-2.741212	-0.161174		
6	-0.089142	-0.364961	-1.309778		
6	0.163143	1.598439	-0.283806		
6	-2.643237	2.478125	0.291001		
6	-1.235289	-0.928748	-1.460754		
6	-3.526843	2.335951	-0.588157		
6	-0.858292	2.260624	0.410108		
6	-2.527459	-1.072816	-1.471022		
6	0.299196	1.797675	1.141668		
16					
736.239964	Kcal/mol	31.926427	eV	-100.210407 H	Child_17_24.log
8	-8.306982	1.205031	-0.205467		
6	8.956857	0.304551	-0.111195		
6	-7.359229	0.505674	-0.137199		
6	8.477584	-0.351418	0.869756		
6	-6.311482	-0.251657	-0.043647		
12	6.728795	-0.439714	-0.103759		
6	-5.298533	-0.995304	-0.061156		
6	4.619433	-0.654795	-0.443271		
6	-4.170504	-1.691375	-0.069154		
6	3.445288	-0.247894	-0.387413		
12	-2.458370	-0.235274	0.600839		
6	2.461062	0.686918	-0.446009		
6	-1.063557	1.314973	1.127292		
6	-3.120700	-2.428981	-0.211543		
6	-1.087128	1.137746	-0.187902		
8	2.239526	1.811122	-0.464072		
16					
736.635008	Kcal/mol	31.943558	eV	-100.209777 H	Child_2_55.log
6	1.840247	-0.942018	1.792422		

6	-0.278844	1.313976	-1.567763	
6	0.666418	-1.087054	1.376615	
6	0.870618	0.748263	-1.290071	
6	-1.816593	-0.825696	0.828833	
6	-1.550787	0.902462	-1.045951	
6	-0.509925	-1.160231	0.635432	
12	2.764805	-0.090107	-1.074881	
6	-3.072262	-0.534265	0.674777	
6	-1.103590	-0.631246	-0.912061	
12	3.309048	-0.569832	0.401286	
6	-1.968393	-1.676460	-1.169591	
6	-4.304736	-0.226653	0.403676	
8	-1.626246	1.525795	0.263022	
8	0.663318	3.021667	1.442557	
6	0.364046	-0.624484	-0.653234	
16				
742.317682	Kcal/mol	32.189982	eV	-100.200721 H MutD_17_72.log
12	4.830912	3.065440	-1.305019	
6	-6.815432	0.820786	-0.872454	
6	2.314523	-0.358164	1.908845	
6	-8.325206	0.617516	-0.652708	
6	-1.291759	3.005606	1.581002	
6	2.930141	0.623889	0.851095	
6	-0.037413	-2.642443	0.765039	
8	-5.258521	1.127328	-0.084590	
6	1.653917	-1.389549	-0.142201	
12	0.587249	-2.110595	-1.758231	
8	-0.898461	1.384702	1.410531	
6	1.079899	-1.775856	1.097721	
6	1.627433	-1.023571	2.157558	
6	2.394977	-0.221836	-0.353503	
6	2.466680	0.173093	-1.715569	
6	-0.624772	-3.088534	-0.266247	
16				
743.253445	Kcal/mol	32.230561	eV	-100.199230 H MutI_8_65.log
6	-0.069638	0.884613	-0.534730	
8	-2.505998	-0.893342	0.831276	
6	-5.738447	1.195985	-0.009023	
6	0.406817	-2.149816	-0.059913	
6	2.029730	0.805462	-2.015574	
6	0.654644	0.939771	-1.739811	
8	-2.139985	-2.022026	-0.137342	
6	4.807239	2.218426	0.548864	
6	-0.810854	-2.065862	-0.159752	
6	1.738459	-2.145891	0.024354	
6	-5.104297	2.351653	-0.037186	
6	1.520455	0.732453	-0.547615	
12	-3.789741	0.485094	0.566854	
12	3.602790	0.139342	0.353635	
6	2.980865	-1.945974	0.166936	
6	4.153574	1.817466	1.597225	
16				
744.938933	Kcal/mol	32.303650	eV	-100.196544 H Child_8_40.log
6	-2.979075	3.223364	-0.137250	
12	3.149414	-2.318580	-0.268035	

6	-3.741543	2.253665	0.081982
6	4.639706	-0.909865	-0.369616
6	-4.271779	1.015629	0.274382
6	1.240349	-2.926564	0.066213
12	-1.092932	2.495713	-0.387532
6	0.004051	-2.839643	0.177213
6	-4.298864	-0.211718	0.378435
6	4.002763	0.110898	0.002147
6	-3.861087	-1.497973	0.406856
6	-1.319907	-2.543277	0.250463
6	0.027903	0.792743	-0.400625
6	3.404465	1.243613	0.403095
8	6.938676	2.881644	0.422318
8	-4.658635	-1.430496	-0.288938

16

748.825953 Kcal/mol 32.472208 eV -100.190350 H

Original2D_6_1.log

6	1.764164	-3.170082	0.000000
6	0.403170	-2.553074	0.000000
6	0.955149	-1.281687	0.000000
8	0.000000	-0.268603	0.000000
6	-1.630291	1.159766	-0.000000
8	-0.845945	-2.882559	0.000000
12	-1.937348	-1.175371	0.000000
6	-2.905133	1.205353	-0.000000
6	2.331866	-1.702149	0.000000
6	-0.221751	1.107203	-0.000000
12	-0.976721	3.376421	-0.000000
6	-2.371590	4.911224	-0.000000
6	3.456877	-0.995647	0.000000
6	4.116539	0.127569	0.000000
6	-1.186989	5.401066	-0.000000
6	2.244053	-4.410092	0.000000

16

754.909942 Kcal/mol 32.736035 eV -100.180654 H

MutD_16_56.log

8	8.845498	0.619704	0.292911
12	-10.561411	0.442021	0.385987
6	-4.921086	0.239638	-0.140914
6	12.135455	-0.251336	-0.232038
6	-6.244057	-0.014563	-0.067342
6	7.721103	0.269170	0.199081
6	2.593195	-0.276243	0.086896
8	-8.734945	-0.380475	-0.164383
6	-2.516560	0.937557	-0.629272
6	5.206357	-0.098904	0.197971
6	3.867788	-0.166772	0.150168
6	6.462573	0.014637	0.264752
12	-1.506974	-0.867742	0.016649
6	-3.685079	0.292832	-0.362530
6	-7.505226	-0.367737	-0.073654
6	10.874903	-0.045810	-0.369763

16

757.023310 Kcal/mol 32.827679 eV -100.177286 H

Child_18_16.log

6	-7.457067	-0.644843	0.226165
6	4.737791	-0.287300	0.120716

6	-6.104782	-0.790618	0.104554
6	4.149449	0.810032	-0.102546
8	-4.922388	-0.919309	0.049251
6	4.447661	-1.597412	0.358026
6	-1.302414	-1.989535	-0.914832
6	3.523860	-2.453566	0.572270
8	-0.999967	-1.140734	-1.587728
6	2.217304	-1.970136	0.574250
6	0.008682	2.672360	-0.672082
12	2.052022	0.752138	-0.387537
6	-0.917177	3.128132	0.191792
6	1.361449	-1.048113	0.483155
6	0.976147	2.382431	-1.490489
12	-0.924238	1.515507	1.687699

16

758.680573 Kcal/mol 32.899545 eV -100.174645 H

Original1D_12_0.log

6	0.000000	0.000000	-0.695493
8	0.000000	0.000000	0.581641
6	0.000000	0.000000	1.891843
6	0.000000	0.000000	-1.902249
6	0.000000	0.000000	-3.277520
6	0.000000	0.000000	3.108888
6	0.000000	0.000000	-4.580809
6	0.000000	0.000000	4.433467
8	0.000000	0.000000	5.649124
6	0.000000	0.000000	6.911025
12	0.000000	0.000000	-6.467794
12	0.000000	0.000000	8.777683
6	0.000000	0.000000	10.987510
6	0.000000	0.000000	-8.629573
6	0.000000	0.000000	-9.916082
6	0.000000	0.000000	-11.258475

16

760.392484 Kcal/mol 32.973781 eV -100.171917 H

MutI_13_51.log

6	2.316495	1.453469	1.651631
12	0.182258	-0.207927	0.964074
6	-1.605615	-1.051686	0.526545
12	-3.220079	-0.356031	-0.774214
8	-0.431367	1.768737	-0.782675
6	9.740717	-2.582610	-0.376582
6	1.673520	0.591847	1.603731
6	-3.243826	-1.846116	0.252552
8	-4.280025	-2.456640	0.351706
6	-5.214037	-3.142916	0.587448
6	1.883380	3.371177	0.134558
6	-3.272864	1.219879	-1.835783
6	-2.047316	1.110475	-1.216234
6	8.891446	-3.124116	-1.393144
6	0.832838	3.386254	-0.710605
6	2.402761	2.659463	0.970788

16

760.458564 Kcal/mol 32.976646 eV -100.171812 H

Original3D_17_5.log

6	1.435992	-2.063072	0.396301
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8	-0.366533	0.226454	0.477415
12	-1.566784	-0.585266	-1.035701
6	1.192952	-0.224074	0.787264
6	2.592497	-0.096360	-0.240077
6	1.125696	-1.581924	1.664252
6	3.562469	1.070676	0.197793
6	1.235578	-1.490422	-1.338255
6	2.747198	1.559225	-1.290861
12	-1.484057	-0.696876	2.171378
6	-0.330358	1.680075	1.161750
6	2.654691	-0.898518	-1.470134
6	-2.802840	1.928128	-1.181438
6	-1.543069	1.979892	-1.013230
6	-3.767910	-2.682511	-1.488843
8	-1.134377	2.310924	0.680679

16

761.132850 Kcal/mol 33.005886 eV -100.170737 H
Original3D_18_6.log

8	-2.135912	0.319574	-2.117402
6	-0.665021	0.172298	0.623646
12	0.692919	-0.262496	-1.118852
6	1.273947	2.357876	-0.141455
6	3.292679	-0.734709	-1.343871
6	2.387783	-2.031481	-0.601764
8	-2.735995	-1.399948	0.532094
12	1.438691	2.325035	1.901488
6	2.609709	-3.272593	0.039571
6	-1.945330	-2.122448	0.972932
6	-0.348233	-0.326556	2.129189
6	0.251425	-2.057742	1.324835
6	-1.710040	1.655875	-1.155854
6	2.111006	2.174807	-1.074940
6	-3.009798	0.063542	-0.489050
6	-2.015470	1.436551	0.265233

16
762.677605 Kcal/mol 33.072873 eV -100.168276 H
Original3D_1_5.log

6	2.994864	0.259533	1.324190
8	1.889201	0.793586	-1.409186
6	1.035340	0.880267	-1.767310
6	3.199300	-0.174792	-0.940039
6	3.168387	-2.135149	-0.600062
6	1.345717	2.082699	0.581814
12	-0.316139	-0.401399	-0.525637
6	0.380849	2.852189	0.077450
8	1.710739	-1.946416	0.848138
6	-1.863526	-0.092698	1.494607
6	-2.634246	-0.887492	0.522592
6	1.850887	1.078516	1.178355
6	2.687315	-1.179892	0.330432
6	-2.356657	1.039397	0.913186
6	-3.456783	-1.234375	-0.240186
12	-5.259544	-0.074149	-0.537846

16
767.366697 Kcal/mol 33.276211 eV -100.160803 H Child_5_23.log

6	1.904391	-2.910737	0.194187
6	-7.356448	1.168263	-0.764401
6	-0.450473	-2.137755	1.122776
6	2.883159	1.906496	-1.601170
6	3.112400	-2.696682	-0.377170
12	3.325263	3.548673	0.792024
6	0.833681	-2.425998	0.575933
6	2.779213	1.718185	-0.265027
8	4.271964	-2.515036	-0.919723
6	2.549403	1.613693	0.797022
6	0.112276	-1.158584	0.521068
6	-6.213613	0.671350	-0.484791
6	-3.535849	0.133336	0.067846
6	-5.018280	0.240899	-0.125470
12	0.978320	0.601463	-0.466543
8	-4.427234	-0.802018	0.685901

16

768.468176 Kcal/mol 33.323976 eV -100.159048 H

Original2D_10_2.log

6	-1.961783	0.139105	0.000000
6	-0.000000	0.735734	0.000000
6	-1.115112	1.397539	0.000000
8	-2.016764	2.520065	0.000000
6	-3.037270	3.018645	0.000000
6	2.135558	1.125943	0.000000
6	0.243135	-1.264801	-0.000000
6	1.192167	-0.104983	-0.000000
6	3.358469	0.198449	-0.000000
8	2.490031	-1.054738	-0.000000
6	1.349805	-2.138018	-0.000000
6	1.001503	1.984311	0.000000
12	2.907145	-3.054648	-0.000000
6	-3.231166	0.094374	0.000000
12	-5.383003	-0.215154	0.000000
6	4.385387	-0.600464	-0.000000

16

771.005131 Kcal/mol 33.433989 eV -100.155005 H

Child_6_45.log

6	-3.337592	-1.597432	-0.577951
8	5.604914	2.205724	0.459440
6	-2.061152	-1.983038	-0.350668
6	-0.380388	3.573476	0.187504
6	2.134317	-2.637196	-0.416661
6	4.860694	1.507032	-0.095825
12	0.054637	-2.312681	0.005504
8	0.163144	2.776659	-0.500221
6	-2.373111	-0.562323	-0.188436
6	0.328017	-1.349266	1.953176
6	3.072145	-1.816081	-0.528967
6	4.014228	0.775658	-0.741323
6	-1.695277	0.434655	0.139329
6	-0.493581	-0.440664	1.537479
6	3.694558	-0.726160	-0.596528
12	-7.781438	1.401761	-0.138881

16

775.654439 Kcal/mol 33.635602 eV -100.147596 H

MutI_15_69.log

6	0.000000	0.000000	-6.836812	
6	0.000000	0.000000	-0.526731	
6	0.000000	0.000000	-1.779273	
6	0.000000	0.000000	-8.157571	
6	0.000000	0.000000	10.213844	
6	0.000000	0.000000	-9.494067	
6	0.000000	0.000000	7.643009	
6	0.000000	0.000000	-4.280605	
6	0.000000	0.000000	8.908103	
12	0.000000	0.000000	1.046782	
12	0.000000	0.000000	3.156800	
6	0.000000	0.000000	-10.703279	
6	0.000000	0.000000	-3.059537	
8	0.000000	0.000000	6.454817	
8	0.000000	0.000000	4.974906	
6	0.000000	0.000000	-5.573876	
16				
779.240551	Kcal/mol	33.791111	eV	-100.141881 H MutD_15_66.log
6	-0.617803	-2.042314	1.141937	
8	2.650152	-1.027759	0.500500	
6	2.496157	-0.900789	-0.706966	
6	-3.514039	2.718600	1.822343	
6	1.176886	1.871007	-0.690617	
6	3.908327	-0.173247	-0.005173	
12	5.588122	-0.013434	-0.143526	
6	0.805564	-2.028482	0.536458	
6	-0.323847	1.834793	-0.380320	
6	-4.397890	-1.297418	-0.658892	
12	-1.983312	0.846698	-0.419023	
6	-1.784768	-2.155073	0.684911	
6	-3.010159	-0.911526	0.121005	
6	2.020415	0.961290	-0.300384	
8	-1.430251	2.587328	0.077406	
6	-5.594996	-1.622793	-1.209747	
16				
779.450529	Kcal/mol	33.800217	eV	-100.141546 H
	OriginalID_4_0.log			
6	0.000000	0.000000	-9.617143	
8	0.000000	0.000000	-10.937143	
6	0.000000	0.000000	-8.297143	
6	0.000000	0.000000	-6.977143	
6	0.000000	0.000000	-5.657143	
6	0.000000	0.000000	-4.337143	
6	0.000000	0.000000	-3.017143	
12	0.000000	0.000000	-1.697143	
6	0.000000	0.000000	0.942857	
6	0.000000	0.000000	2.262857	
8	0.000000	0.000000	3.582857	
6	0.000000	0.000000	4.902857	
6	0.000000	0.000000	6.222857	
12	0.000000	0.000000	7.542857	
6	0.000000	0.000000	10.182857	
6	0.000000	0.000000	11.502857	
16				
782.871731	Kcal/mol	33.948574	eV	-100.136094 H MutD_8_68.log

12	3.645489	1.895414	-0.151562	
6	3.121895	-1.430260	-1.798620	
8	0.589165	-3.357637	0.162881	
12	0.042721	2.561428	0.328702	
6	-2.422334	-0.747054	-1.650548	
6	1.105772	-0.348411	0.468937	
6	0.213625	-1.036151	-0.399654	
6	-1.059407	-0.774735	-0.743172	
8	-2.731515	-1.438879	1.742140	
6	-1.575381	1.452252	0.203738	
6	-1.398448	2.677869	0.554589	
6	2.284829	-1.198111	0.421558	
6	-2.704244	-0.553414	0.947361	
6	-3.631093	0.567688	-1.911996	
6	-1.863489	0.193522	0.002159	
6	3.408319	-1.321523	1.011341	
16				
786.266975	Kcal/mol	34.095806	eV	-100.130683 H MutI_1_75.log
6	-3.658173	3.909673	0.000000	
6	-1.104431	-2.715917	0.000000	
6	1.247984	1.197378	-0.000000	
6	-3.164176	-1.382824	0.000000	
6	0.000000	1.431756	0.000000	
6	3.711843	0.598208	-0.000000	
6	-3.903234	-2.709317	0.000000	
12	-2.242440	3.101389	0.000000	
8	-1.576692	-0.206020	0.000000	
6	4.933755	1.073519	-0.000000	
6	-0.748520	2.157107	0.000000	
6	2.427279	0.870806	-0.000000	
8	0.026130	-2.434721	-0.000000	
12	3.682059	-1.253827	-0.000000	
6	1.886249	-1.953401	-0.000000	
6	-2.440398	-2.651126	0.000000	
16				
795.482776	Kcal/mol	34.495442	eV	-100.115997 H MutI_12_65.log
6	-0.189543	2.626838	0.137420	
6	-1.868891	2.480278	0.974453	
6	2.582655	-0.809761	-0.053902	
6	1.945570	-1.895834	0.168352	
6	-4.899951	0.146228	-0.677887	
6	5.352017	1.735013	-0.223295	
6	4.222910	1.093539	-0.227905	
6	2.746239	0.724836	-0.173444	
6	-4.071590	-0.771364	-1.113367	
8	1.846476	1.527404	-0.194927	
6	-1.926429	-2.162294	0.987540	
8	-5.629937	0.929781	-0.190179	
12	4.566146	-0.893468	-0.123882	
6	-3.558727	1.467704	0.713050	
6	1.318603	-2.995607	0.424867	
12	-2.870270	-1.564443	-0.087321	
16				
806.377599	Kcal/mol	34.967886	eV	-100.098635 H Original3D_0_65.log

6	-0.809017	-1.542140	-0.451367
6	1.937023	-1.739782	-0.355344
6	2.590419	-1.349030	-1.332878
6	-1.906910	-0.135080	0.801654
6	1.978488	0.368952	1.934087
8	0.280802	0.993660	0.491250
6	-2.912833	-0.289371	-0.114610
8	-0.503706	2.084856	0.262571
12	0.707528	-0.838159	0.742599
12	-2.241892	-2.302330	0.180632
6	-1.537096	1.642658	-0.677672
6	2.928128	0.101280	-0.750513
6	3.722990	0.389457	-1.825460
6	1.178455	1.439297	2.912410
6	-2.474929	0.757672	-1.256453
6	-1.328785	2.532379	-1.735411

16

811.272821 Kcal/mol 35.180164 eV -100.090834 H

Original2D_11_2.log

6	-3.070716	1.807668	0.000000
6	-1.952074	0.755678	0.000000
6	-2.752431	-0.295404	0.000000
12	-0.933317	2.325467	-0.000000
6	-0.000000	-0.326636	0.000000
6	2.220209	0.227276	-0.000000
8	2.865541	-2.320172	-0.000000
6	2.882996	1.322718	-0.000000
6	-0.592700	-1.486004	0.000000
6	3.334136	-0.807554	-0.000000
6	4.498690	-1.469914	-0.000000
8	-2.074051	-1.850747	0.000000
6	-4.066315	2.462180	0.000000
12	1.395426	-1.391801	-0.000000
6	-4.241474	-0.433376	0.000000
6	1.760141	1.937261	-0.000000

16

812.614977 Kcal/mol 35.238365 eV -100.088695 H

Child_17_9.log

8	6.347303	0.741702	0.770339
6	-5.066822	-0.920106	0.828781
6	5.257755	0.693614	0.281638
6	-4.586760	0.250999	0.805834
6	4.204389	-2.081206	0.188243
8	-3.777872	1.305698	0.709434
6	4.263258	-0.805595	0.259481
6	-3.750406	-1.888341	-0.056091
12	2.215085	-1.664553	-0.236724
6	-2.643681	1.686898	0.289123
6	0.410767	-0.872240	-0.474354
6	-1.567558	1.272519	-0.247170
6	1.165691	5.986681	-0.777148
12	-1.889823	-1.471245	-0.764673
6	-0.310761	0.183778	-0.486162
6	-1.452304	0.034727	-0.582411

16

813.338532 Kcal/mol 35.269741 eV -100.087542 H

MutI_16_69.log

6	8.005120	2.114076	0.124694	
6	-3.725967	2.035526	-0.408198	
6	-1.161530	-2.990472	-1.106744	
6	-3.362598	-1.504601	-1.528359	
6	6.262460	1.185788	0.114144	
6	3.988356	-0.028819	0.020578	
6	-3.738495	3.103653	0.310947	
8	-2.515884	-4.079463	3.188499	
6	2.906532	-0.598764	0.002801	
6	-2.294146	-2.174427	-1.352353	
6	-0.332537	-2.554665	-0.172959	
6	1.822807	-1.180105	-0.025616	
6	0.766503	-1.798674	-0.076115	
8	5.121816	0.572273	0.051314	
12	-3.593112	4.056513	1.078542	
12	-2.712427	0.477356	-1.189827	
16				
814.195123 Kcal/mol 35.306887 eV -100.086177 H				MutI_7_67.log
6	1.258173	0.366528	0.279686	
6	1.754326	-0.694833	0.128452	
12	-0.483683	0.782574	0.168039	
8	-0.952616	-3.222422	0.091463	
6	0.358308	-2.289560	0.579377	
6	4.978496	0.291782	-0.475298	
6	-2.917359	-2.787625	-0.316225	
6	-2.167774	2.174065	-0.075648	
6	-1.900982	3.536587	0.050766	
12	3.453090	-0.193114	-0.207027	
6	-0.048594	3.619190	0.004119	
6	-2.631686	-1.485884	-0.249087	
8	-2.824634	-0.245332	-0.244883	
6	1.579514	-1.985974	0.149709	
6	-2.263746	0.910710	-0.076944	
6	1.098841	1.789766	0.283628	
16				
814.784414 Kcal/mol 35.332441 eV -100.085238 H				
Original2D_17_1.log				
6	0.918927	-0.585922	0.000000	
6	-1.448272	0.543617	-0.000000	
6	1.167907	1.372341	0.000000	
6	0.000000	0.594064	-0.000000	
6	2.123049	0.039741	0.000000	
6	-1.738003	-0.878100	-0.000000	
12	3.329120	-1.684717	0.000000	
8	-1.423607	2.800345	-0.000000	
6	-2.212180	-2.294959	-0.000000	
12	0.507835	3.403432	-0.000000	
6	-1.545100	4.147732	-0.000000	
6	-2.388979	1.617109	-0.000000	
6	-2.586769	-3.598468	-0.000000	
6	-0.835836	-1.843279	0.000000	
6	2.093859	-3.686754	0.000000	
8	0.506723	-1.948758	0.000000	
16				
822.973650 Kcal/mol 35.687560 eV -100.072188 H				MutI_13_69.log

12	1.446150	0.317827	-0.855872	
8	-2.729095	1.182300	-0.186392	
6	7.782115	-0.420079	1.028502	
12	-4.357427	-0.720999	0.368444	
6	-1.705973	-2.036446	-0.230090	
6	3.139861	0.330057	-0.589912	
6	-2.978447	4.245198	0.743916	
6	-3.893761	-2.498658	0.460648	
6	-0.268029	-0.043079	-0.772375	
6	6.603041	-0.243554	0.563485	
6	4.292757	0.140812	-0.253938	
6	-3.540337	0.902863	-0.058671	
8	5.460790	-0.056405	0.092356	
6	-2.750371	3.034163	0.253002	
6	-1.410419	-0.578114	-0.408190	
6	-3.090145	-3.528011	0.363860	
16				
824.961600	Kcal/mol	35.773766	eV	-100.069020 H MutI_8_73.log
6	12.882322	-0.973900	-0.548371	
6	-5.190188	-0.260699	-1.261015	
12	-0.563543	-1.677424	0.192725	
6	-0.382005	2.201785	-0.025735	
6	-1.957755	-1.347275	1.596358	
12	-2.970847	1.398640	-0.805293	
6	-4.149311	-1.899261	-0.967576	
6	-1.470443	1.826433	-0.342954	
8	-4.395559	0.482472	-1.137324	
6	-1.964630	-2.542919	-0.617042	
6	-0.815862	-1.395720	2.284949	
6	14.232654	-0.748557	-1.000656	
6	0.664913	-0.866627	1.103211	
6	-2.657718	-2.165212	0.517378	
6	1.892807	3.146088	1.270013	
8	1.383558	3.705103	0.549756	
16				
825.630229	Kcal/mol	35.802760	eV	-100.067954 H
	Original3D_13_5.log			
6	1.618403	-0.711242	-0.007492	
12	-0.094916	0.305802	-0.826490	
6	1.695029	2.989603	-1.307267	
6	2.402122	2.049538	0.356257	
6	-3.073548	-1.001417	-0.362849	
6	-2.364979	0.837817	0.328891	
6	-1.707243	1.164777	1.509687	
6	1.524246	-1.983568	0.560750	
6	-3.586952	1.119900	1.029455	
6	-2.990782	1.562548	-1.030254	
6	1.161690	2.240231	0.911402	
6	2.319939	-1.661984	1.632602	
8	-3.082128	-1.947798	0.151977	
6	2.436241	3.374450	-0.242860	
8	-0.785539	-2.503063	-1.058604	
12	2.956277	-2.328887	-0.258253	
16				
829.237894	Kcal/mol	35.959204	eV	-100.062205 H MutI_15_53.log

6	0.802890	2.077808	0.617147	
6	3.010687	-0.762617	-0.023534	
6	-4.587937	-1.878862	0.107057	
6	-0.463818	1.432817	0.107791	
6	1.819207	-0.959461	-0.090864	
6	-2.019105	-1.195716	0.085254	
6	-0.656113	-1.241484	-0.019426	
6	0.570933	-1.077069	-0.064586	
6	-4.795206	0.685732	-0.186595	
6	6.797192	0.160036	-0.078465	
12	4.949502	-0.340094	-0.044382	
8	-1.570699	1.241024	0.105160	
6	7.994990	0.431610	-0.090607	
12	-3.301888	2.160273	-0.244885	
6	-3.233567	-2.223877	0.154325	
8	-4.830837	-0.557980	-0.059382	
16				
833.077720 Kcal/mol 36.125715 eV -100.056086 H				MutI_16_33.log
6	-5.233227	-1.470864	0.711415	
6	1.311682	1.662841	-0.381885	
6	-2.660260	1.026261	0.496820	
8	-3.805644	0.664884	0.871192	
6	4.388141	-0.014886	-0.039917	
12	-2.007992	-1.866239	-0.948394	
6	-3.880379	-2.372538	-0.350495	
6	-1.607094	0.646819	-0.084210	
12	-0.282851	1.548162	-0.213670	
6	2.981165	0.700048	-0.368740	
6	6.559810	-1.275027	0.411412	
6	-1.507103	-0.508685	-0.579757	
8	0.511615	2.953950	-0.288404	
6	7.673461	-1.904242	0.670418	
6	-4.690552	-0.332937	0.841578	
6	5.638080	-0.345750	0.220439	
16				
836.497547 Kcal/mol 36.274013 eV -100.050636 H				MutI_9_67.log
12	4.583273	-1.187635	-0.434660	
6	2.927703	3.035697	0.515193	
6	-6.525378	2.938124	-0.765286	
8	0.154149	-2.235399	-0.805768	
6	-5.913371	4.239184	-0.890549	
6	4.339440	0.845623	-0.001329	
6	-0.988155	-2.160615	-0.485748	
6	-2.202357	-2.035907	-0.146153	
8	-4.609474	-1.711825	0.668781	
6	4.517570	2.062770	0.150400	
6	-5.838383	-1.609042	1.019538	
6	-3.435385	-1.871743	0.264945	
12	1.689645	0.821859	0.508646	
6	2.332963	-1.695319	-0.411100	
6	3.170148	-0.159051	0.151290	
6	1.009801	2.404796	0.633477	
16				
839.025001 Kcal/mol 36.383613 eV -100.046608 H				Child_1_39.log
6	-1.680103	-2.883775	0.055888	

6	-0.469731	3.488601	-0.016247
6	-4.504245	-2.919295	-0.926136
6	0.421144	2.572203	-0.086558
6	-2.767718	-2.444593	0.077435
6	-4.149544	2.853276	0.374209
6	-4.038567	-2.078854	0.017587
8	-2.803964	2.423631	0.401044
12	0.660552	-1.608190	-0.164087
12	2.111990	1.583153	-0.261498
6	4.329827	-2.145883	1.294888
6	-3.718657	1.327516	0.377416
6	3.597931	-1.282824	0.598594
6	2.269569	-0.694529	0.015493
6	3.562225	-0.100096	-0.205824
8	4.006055	0.845112	-0.945224

16

839.556146 Kcal/mol 36.406646 eV -100.045762 H

Original3D_0_68.log

8	-0.123104	-1.033729	-0.547179
6	0.360063	-0.864041	2.078677
6	0.970345	-2.097568	2.001295
6	2.175822	0.690592	-1.009278
6	-0.717431	0.018664	0.613124
12	-2.507988	-0.137887	1.291782
6	0.564573	0.076205	-1.629266
6	0.841532	-2.280879	-1.367617
8	1.349759	1.379353	0.287375
12	1.722571	-0.839536	0.460445
6	-4.706166	1.294229	-0.162736
6	-1.282672	0.753952	-1.050287
6	-0.394838	-2.358773	-1.935014
6	2.519516	1.945622	-0.231008
6	2.250513	3.048491	0.566650
6	-2.645962	1.267520	-1.032588

16

840.167508 Kcal/mol 36.433157 eV -100.044787 H

Original3D_14_5.log

6	-0.143630	-0.071520	-0.600356
6	-1.470013	-0.025214	-0.700699
6	1.284091	-1.157427	1.541690
8	1.248414	0.032415	-0.775703
6	1.228400	-1.560137	-0.150557
12	3.150254	-1.072181	0.033878
6	-1.716864	1.501239	-0.866816
6	0.000737	-1.260648	1.439587
6	3.785328	0.979153	-0.299162
8	-1.779016	-1.562516	-0.507734
6	-0.555883	1.840410	0.056554
12	-3.444664	-0.080684	-0.562624
6	3.741902	2.316414	-0.015358
6	-0.212856	-1.527612	-0.194167
6	-4.265701	0.526893	1.608887
6	-0.379222	2.784314	0.949139

16

840.477747 Kcal/mol 36.446611 eV -100.044293 H

Child_18_25.log

12	-7.864818	-0.965053	0.131874
12	4.891827	0.659620	0.540362
6	-2.187794	-0.037551	1.118070
6	-1.499510	0.746928	0.191979
6	3.640308	-1.868851	0.248477
6	-1.082956	-0.535464	0.215588
8	2.891405	-2.654520	-0.183002
6	-1.292482	3.300550	-0.721365
6	1.946696	0.845839	-0.174719
8	-0.876681	1.952380	-0.202620
6	1.435061	2.232584	-0.298024
6	-0.084766	-1.386735	-0.206399
6	0.596463	0.445423	0.034276
6	0.428751	-2.572805	-0.837329
6	0.089428	1.862932	0.012685
6	1.270486	-1.485798	-0.413548
16			
849.329816	Kcal/mol	36.830473 eV	-100.030186 H
			MutI_16_57.log
6	-0.554262	-2.062036	0.109616
6	2.746626	1.841849	0.108241
6	-0.598618	-0.649832	0.024196
12	1.599053	-0.852789	-0.236327
6	-3.659725	-0.486232	-0.190164
6	-3.354758	-1.666250	-0.108259
6	0.185923	1.558486	0.127924
6	-0.827817	0.617918	-0.003628
8	-1.935937	-2.197104	0.256530
6	-1.791370	3.717926	0.095541
12	2.855396	-1.339316	-0.260152
6	1.028336	-2.937063	0.426720
6	1.375425	1.902376	0.109329
6	-2.335243	2.408401	-0.088791
8	-2.026497	1.104283	-0.097362
6	4.159828	1.595763	0.170009
16			
849.485919	Kcal/mol	36.837242 eV	-100.029938 H
			Original3D_0_46.log
6	0.094088	1.984736	-0.849046
6	0.514579	0.402207	-1.134154
8	1.546517	-1.713911	0.466315
6	-1.449761	-0.473550	-0.491288
6	2.479998	-1.453300	0.994713
6	4.616837	-0.743207	0.555565
6	-2.969445	-1.927377	-0.234688
6	-4.599411	-1.437224	0.638603
6	-2.116857	-1.411461	-1.267296
8	-0.127827	-0.660158	0.218944
12	2.827872	-0.542074	-1.049362
12	0.847675	1.100044	1.310651
6	-1.809363	1.259564	0.046794
6	-2.310571	1.530215	1.413001
6	-3.129400	1.124336	-0.483496
6	1.436628	3.194548	-0.624965
16			
849.869223	Kcal/mol	36.853864 eV	-100.029327 H
			Child_2_54.log

6	-4.696883	-2.573806	0.109570
12	0.334318	3.325229	-0.707786
6	2.789738	-3.199922	0.045515
8	0.828298	2.825019	1.178242
8	1.361748	-2.207358	0.028417
6	0.896287	1.595225	0.935687
6	3.765530	-2.124831	-0.078996
12	-5.565677	-0.479020	-0.008945
6	0.846643	1.261675	-0.547963
6	0.344717	-1.021279	-0.021365
6	0.724190	0.327855	1.790480
6	2.778891	-1.263475	0.005337
6	-0.208905	0.836071	-1.249832
6	-3.571426	-0.032252	-0.058228
6	2.145126	-0.206363	-1.274283
6	1.728748	-0.114865	0.168663

16

852.773410 Kcal/mol 36.979802 eV -100.024699 H

Original3D_0_66.log

6	-0.195315	-1.454937	-0.302425
8	1.529951	0.058299	0.135522
6	-1.722855	-1.660749	0.416398
6	-1.147019	0.958379	0.853988
6	-2.694191	0.090533	0.188041
6	-1.529168	-2.895740	-0.106274
6	-0.292896	1.049985	-1.729342
12	3.403898	0.194717	0.296005
6	2.242984	-2.223873	2.130816
6	4.998210	1.254105	-1.096924
6	-4.214675	0.753051	0.434746
6	-1.263242	2.268847	1.226208
8	0.627262	1.006976	-0.914428
12	-1.555906	-0.835337	-1.619553
6	-1.447550	3.382848	1.011146
6	0.693450	-1.661575	0.659259

16

853.376706 Kcal/mol 37.005963 eV -100.023737 H

MutI_18_45.log

6	-0.745268	0.471098	-0.026589
6	4.021260	-0.960403	-0.028730
8	-0.092612	-0.519137	-0.029837
6	2.192751	2.411881	-0.659884
6	-3.780276	-1.869860	-0.312298
12	1.368994	-0.995547	-0.085815
8	-5.034015	0.538540	-0.550271
12	-2.826643	-2.748133	0.201864
6	-3.318444	2.028831	1.010791
6	5.233830	-0.604251	0.182970
6	-0.271166	1.859861	-0.028022
6	6.363395	0.009251	0.345917
6	-2.122868	0.880576	0.208411
6	2.937155	-1.236878	-0.173205
6	-1.687119	2.183193	0.321380
6	0.927551	2.288188	-0.299361

16

856.308653 Kcal/mol 37.133105 eV -100.019065 H

Original1D_8_0.log

6	0.000000	0.000000	-5.704286
6	0.000000	0.000000	-4.384286
8	0.000000	0.000000	-3.064286
8	0.000000	0.000000	-1.744286
6	0.000000	0.000000	-7.024286
12	0.000000	0.000000	-0.424286
6	0.000000	0.000000	2.215714
6	0.000000	0.000000	3.535714
6	0.000000	0.000000	4.855714
6	0.000000	0.000000	6.175714
6	0.000000	0.000000	-8.344286
12	0.000000	0.000000	7.495714
6	0.000000	0.000000	-9.664286
6	0.000000	0.000000	10.135714
6	0.000000	0.000000	-10.984286
6	0.000000	0.000000	11.455714

16

864.445828 Kcal/mol 37.485966 eV -100.006097 H

MutI_10_69.log

8	1.601687	-2.180939	-0.397952
12	3.064997	1.138772	-0.206204
6	0.711411	2.068836	0.056742
6	-3.776291	-2.018426	0.142992
6	-3.860582	-0.713533	0.121566
6	3.346262	-2.022772	0.907798
6	-3.587869	0.558773	0.096859
6	-3.309306	-3.207850	-0.088395
6	-2.932131	1.657700	0.063175
6	1.554423	0.179114	0.042993
6	3.611643	-1.206225	-0.090732
6	4.104972	0.261290	0.137213
6	-0.927008	3.314284	0.135187
6	-1.979130	2.573295	0.058786
8	-0.211966	-1.062222	-0.222801
12	-0.469674	0.301092	-0.172054

16

867.102178 Kcal/mol 37.601157 eV -100.001864 H

MutI_6_73.log

6	1.813443	-1.506155	-0.174849
8	-13.837926	-0.193882	0.914635
8	-13.346167	-0.223586	-0.245171
6	0.488940	-1.432504	-0.316000
6	-2.974385	-0.105553	-0.629942
6	3.441221	2.712010	0.170978
6	0.169821	1.129790	-0.246437
12	5.456652	0.265404	0.303605
6	1.801794	1.513144	-0.037665
6	6.921995	-1.236933	0.402548
12	4.969563	-1.218973	0.188773
6	-1.967490	1.326808	-0.449065
6	4.343296	1.945572	0.247351
6	-0.141853	-0.233733	-0.331751
6	3.085260	-1.583243	-0.034950
6	-1.589012	-0.065442	-0.477590

16

868.026047 Kcal/mol 37.641219 eV -100.000392 H MutI_6_65.log

6	-2.378820	-2.450133	0.735419
8	1.955777	-1.148710	0.115090
6	-0.705100	4.250411	0.319317
6	3.183776	-1.345814	-0.312975
6	-3.467823	-1.768491	0.289940
6	-1.719045	0.695430	-0.975254
6	-3.603861	-0.685121	-0.330574
6	1.867168	2.176634	-0.234744
6	-1.090495	-2.701213	0.939884
12	-0.115548	0.154996	-0.594291
8	2.862919	1.487168	1.071909
6	4.304300	-1.956767	-0.565790
6	-1.894435	3.874365	0.762405
12	1.342512	0.416117	-0.328905
6	-0.174436	-2.098260	0.542348
6	-3.200088	0.415457	-0.906249

16

872.176114 Kcal/mol 37.821184 eV -99.993778 H Child_13_23.log

8	5.527798	-2.838397	0.004219
8	-8.125582	-1.358600	-0.242231
6	4.720510	-1.981714	-0.024715
6	-6.995125	-1.113984	0.147121
6	3.758390	-1.048005	-0.039813
6	-0.604620	2.663161	-0.008898
12	1.545315	-1.438289	-0.074706
6	-1.788941	2.068885	0.026973
6	-5.706982	-1.096650	0.499895
6	-2.752695	1.189165	-0.313389
6	4.066868	0.362146	0.057586
6	0.628066	2.333054	0.152588
6	3.116785	1.366299	0.314175
6	3.220687	2.541183	-0.346229
12	-1.466189	-0.183257	-0.113779
6	1.642518	1.555548	0.229025

16

877.068367 Kcal/mol 38.033332 eV -99.985982 H Child_10_44.log

6	-5.306330	-1.421471	-0.128247
12	5.809956	-1.959500	-0.130505
6	-4.762760	-0.297641	-0.127422
6	4.059033	-1.018217	0.049361
6	-3.931968	0.753081	-0.105696
6	2.566141	0.178694	0.175808
12	-3.690037	-2.523412	0.100918
6	1.531952	0.956486	0.211862
6	-2.929628	1.444358	-0.068391
6	-1.710414	1.889460	-0.027960
6	0.144645	-0.262069	0.019005
6	-1.040148	-2.081406	0.194439
6	-0.091255	4.731214	0.013143
6	-0.320243	2.316621	0.026557
8	3.152478	2.811015	-0.025381
8	2.510875	-1.478483	-0.104583

16

902.520957 Kcal/mol 39.137062 eV -99.945421 H Original3D_7_3.log

12	1.546792	1.015983	-0.447043
8	-0.554560	-1.116663	-0.858083
6	-0.209418	-0.684705	1.552012
6	3.491947	-1.480671	-0.616448
6	-0.072190	3.690911	-0.724225
6	-1.675379	0.542454	-1.688979
6	1.378838	-0.535926	1.612856
6	2.405620	-1.913464	-1.106502
6	2.310285	0.758940	2.737028
6	0.098065	-1.612785	0.291707
12	-2.496126	-0.746263	-0.111837
8	0.251250	3.584955	-1.720961
6	1.692343	-2.674751	-1.698237
6	0.916937	0.788843	2.509066
6	-3.189950	0.859162	1.934285
6	-4.844016	-1.568507	-0.246077
16			
903.830677 Kcal/mol 39.193857 eV -99.943334 H MutI_1_77.log			
8	-5.132426	-0.800260	0.006774
6	-3.286105	1.895815	2.716349
12	1.260529	-0.716955	-0.694255
6	-2.800954	0.876708	-0.255272
8	-0.279247	-1.481583	0.319499
6	2.978632	0.630930	-0.280860
6	5.565883	-1.873648	0.644727
12	1.457202	3.050466	0.373427
6	-0.406861	1.280240	-1.018886
6	-2.081359	0.957724	-1.323777
6	2.577743	1.259690	-1.796255
6	3.091757	-0.860973	0.871208
6	4.329451	-1.423282	0.788701
6	-2.512300	-1.320198	1.194576
6	-1.653881	-1.418432	-0.306073
6	-4.021906	-1.629138	-1.027813
16			
904.014932 Kcal/mol 39.201847 eV -99.943040 H Child_5_44.log			
8	6.464849	-0.972776	-0.221674
6	-0.990535	-1.239270	1.184975
6	5.458990	-0.365255	-0.151320
6	-2.146226	-1.039464	0.618862
6	4.372354	0.311072	-0.076835
12	-4.066883	-1.829826	-0.352864
6	3.243147	0.857371	-0.010949
6	-4.103861	0.373854	-0.272878
6	2.096785	1.476454	0.062115
6	-2.787292	0.300414	0.171339
6	0.906222	1.892159	0.116044
6	-4.934032	1.309449	-0.603148
8	1.494010	-1.383930	-0.218260
6	0.352809	-1.014512	-0.180252
6	-1.548219	0.695475	0.270011
12	-1.199094	1.622090	0.082173
16			
906.278222 Kcal/mol 39.299993 eV -99.939433 H Child_15_16.log			
12	-2.336998	-2.616004	0.006851

6	1.950370	3.199504	0.116447
6	-0.336335	-2.023016	0.122099
6	-3.451619	3.739489	-0.019283
6	0.906298	-1.872857	0.105346
6	5.365964	0.242365	-0.086451
6	2.242340	-1.683844	0.074607
6	-3.137120	2.486493	-0.018178
6	-4.238377	-2.186337	-0.184245
12	3.128577	0.603123	-0.039138
6	-2.242479	1.290735	0.070214
6	4.704209	-0.842005	-0.044723
6	-4.268237	-0.913239	-0.059353
8	-3.561733	0.883276	0.070556
6	3.452228	-1.399733	0.007509
8	1.663933	2.107878	-0.085117
16			
913.622214 Kcal/mol 39.618459 eV -99.927730 H MutI_15_49.log			
6	3.739601	-0.748208	0.000000
6	0.451907	-2.790441	0.000000
6	1.010598	2.041102	0.000000
12	-4.318934	1.341245	0.000000
6	0.209477	3.330671	0.000000
6	0.000000	-1.247063	0.000000
6	-3.190675	-0.347480	0.000000
6	-0.524451	2.273377	0.000000
6	1.816146	0.744870	0.000000
6	1.171147	-0.590121	0.000000
12	-1.269505	0.198782	0.000000
8	-2.210015	1.988676	0.000000
6	3.570550	-2.116485	0.000000
6	3.164015	0.394256	0.000000
8	2.137064	-2.005221	0.000000
6	-0.144169	-4.002474	0.000000
16			
916.758000 Kcal/mol 39.754440 eV -99.922733 H Child_18_22.log			
6	-1.589161	3.968356	0.464579
6	6.749664	1.027088	-0.423423
6	-1.953141	2.731606	0.195922
6	5.479860	0.696514	-0.186831
6	-2.540639	1.453533	0.082191
6	4.244031	0.402806	0.025167
6	-3.742443	0.786156	0.010275
8	1.832877	-2.202364	0.406184
6	-1.078351	1.372369	-0.029458
12	2.026911	-0.151363	0.234051
6	-3.918820	-0.496734	-0.155905
6	0.587979	-2.540120	0.315930
8	-4.026684	-1.699554	-0.284436
6	-0.663876	-2.815307	0.301012
12	-1.137682	-0.975384	-0.365891
6	-0.428486	0.869784	-0.498108
16			
917.749727 Kcal/mol 39.797445 eV -99.921152 H MutI_11_77.log			
6	3.643553	-2.229463	-0.159377
6	2.039195	-1.708575	0.188048

6	-2.169449	-0.526729	-0.392362
8	-7.111639	0.745237	0.015846
6	5.781856	0.149694	-0.260851
12	1.175811	2.508041	0.118846
6	1.426203	-0.053626	-0.539773
6	-4.639356	0.109796	-0.341087
6	3.677320	1.351065	-0.024254
6	-5.845206	0.423275	-0.191614
6	-3.368297	-0.233116	-0.460120
6	4.763953	0.816823	-0.134038
6	2.408316	2.338038	0.182463
12	-0.537732	-1.223860	1.375188
6	1.298746	-2.724972	-0.798704
8	-0.608105	-0.955664	-0.058144

16

921.556368 Kcal/mol 39.962517 eV -99.915086 H MutI_17_75.log

6	-4.417749	-0.166402	-0.913368
8	-3.486115	1.743941	-0.563046
6	1.972162	-1.442343	1.153101
6	-0.237913	1.312416	0.050513
6	-0.680267	-1.465274	0.931954
6	2.999033	2.133583	0.304444
6	4.870603	-2.791127	-0.785094
6	4.149321	2.308042	0.152310
6	-1.682912	-0.649633	0.418753
6	-1.332301	0.853498	0.052496
6	-2.402143	1.593770	-0.265810
6	0.577691	-1.407168	1.068916
6	-3.000525	-0.845490	0.068402
12	1.321415	1.846284	0.150749
8	-6.777155	-2.037026	-0.155385
12	5.113265	-1.367829	-0.790103

16

921.572705 Kcal/mol 39.963225 eV -99.915060 H Original3D_5_3.log

6	-0.019920	0.390256	-0.849511
12	1.274094	-1.339254	-0.522311
6	1.667774	0.937485	0.953598
6	-1.259106	-1.630571	0.235016
6	4.029448	-1.612327	-0.061163
6	-0.029534	1.691208	-0.032076
8	1.600608	1.862476	-0.346917
6	-0.047661	2.887611	0.899444
6	0.662519	-1.583626	2.652118
6	-2.638798	-1.507207	0.491668
6	-3.937817	0.209379	0.277757
6	0.181156	0.825169	1.398049
8	-3.194378	-0.709547	-0.734523
12	-1.784257	0.405701	-0.335748
6	0.627915	0.069789	-2.460980
6	3.909378	-0.347300	-0.345880

16

923.446314 Kcal/mol 40.044473 eV -99.912074 H Original1D_1_0.log

6	0.000000	0.000000	8.655127
12	0.000000	0.000000	10.109839
6	0.000000	0.000000	7.380494

6	0.000000	0.000000	6.060454
6	0.000000	0.000000	4.760602
6	0.000000	0.000000	3.430429
6	0.000000	0.000000	2.124368
6	0.000000	0.000000	0.780548
6	0.000000	0.000000	-0.517245
8	0.000000	0.000000	-1.834519
6	0.000000	0.000000	-3.170603
6	0.000000	0.000000	-4.448842
8	0.000000	0.000000	-5.741867
6	0.000000	0.000000	-7.066159
12	0.000000	0.000000	-8.523882
6	0.000000	0.000000	-11.059237
16			
923.561061 Kcal/mol 40.049449 eV -99.911891 H MutI_16_47.log			
6	3.855376	0.053340	-0.668895
12	5.237603	0.375237	-0.873969
8	-4.967871	0.315982	-0.421173
6	0.929400	0.105454	2.884319
12	-1.319741	2.197412	-0.221652
6	-3.353721	2.562674	-0.534463
6	1.406750	-0.655820	-0.428544
6	-0.470160	1.125270	-0.314485
6	2.675052	-0.276303	-0.562948
6	-1.610513	-2.008921	0.028381
6	-2.886313	-1.715613	0.053334
6	-4.163733	-1.460199	0.040774
8	-0.464347	-1.392132	-0.222749
6	0.937432	-2.006116	-0.328437
6	1.987981	0.603280	3.229910
6	0.099682	-0.037479	-0.349140
16			
923.765729 Kcal/mol 40.058324 eV -99.911565 H Child_11_61.log			
6	7.394759	1.766361	0.299323
6	-3.135043	2.407026	-0.506460
8	6.507473	1.035178	0.327683
6	-3.433138	1.099120	-0.642463
12	1.519948	-1.870824	-0.749391
6	-2.060711	2.981982	-0.031395
8	0.550620	-3.343460	0.108160
6	-3.605709	-0.161506	-0.744147
6	1.388505	0.084168	-1.202358
6	-0.378012	-2.498470	0.492078
6	-0.952754	3.468823	0.359276
6	0.432539	0.440088	-0.480351
6	-2.503467	-0.030224	2.280922
6	-1.086658	-1.522249	0.658844
12	-1.892154	-1.038318	0.108060
6	-0.726691	0.860873	0.218269
16			
932.335323 Kcal/mol 40.429937 eV -99.897909 H MutI_11_73.log			
6	2.718492	-2.851285	-0.068896
12	4.126901	-1.913648	0.225927
6	1.469129	3.562061	0.120381
6	3.190226	0.800215	0.161449

6	-4.620154	-1.701003	-0.260424
6	-0.942373	5.418514	-0.188487
6	1.523964	-3.073197	-0.300969
12	3.791534	-0.682084	0.231846
6	-0.312649	-3.270478	-0.440098
8	-2.371339	-2.735327	-0.533123
8	-1.935428	6.081795	-0.351236
6	-6.793208	-1.056747	1.071273
6	0.192260	4.685489	0.001696
6	-5.683823	-1.413291	0.430513
6	2.651917	1.869783	0.167405
6	-3.488295	-2.240552	-0.430244

16

939.338334 Kcal/mol 40.733617 eV -99.886749 H MutI_18_77.log

8	-0.551807	-1.288812	-0.223290
8	-1.732317	0.701497	2.762481
6	0.208072	3.746462	0.019564
6	1.954208	-1.650069	-0.020650
6	-0.283154	2.683619	-0.179861
12	3.056187	-0.045075	-0.310174
6	-2.809105	-1.751777	-1.074470
6	0.251250	-0.343425	-0.428868
6	-1.041760	-2.401351	0.017390
6	4.425228	0.856489	-0.329000
6	-2.459531	0.767888	-1.173309
6	-0.872665	-0.050933	2.817389
12	-0.788694	1.159855	-0.630469
6	1.051785	-2.748209	0.768506
6	-3.209511	-0.068731	-1.536038
6	1.295695	-0.486434	-0.384953

16

946.348730 Kcal/mol 41.037617 eV -99.875577 H Child_12_32.log

12	8.365407	-0.288791	-0.048411
6	-1.741955	6.427647	-0.621939
6	6.477047	-0.524751	0.014980
6	-2.129272	5.164676	-0.295287
6	5.188488	-0.685762	0.058237
6	-2.464286	3.908050	-0.029999
6	3.894177	-0.847493	0.101686
6	-2.724478	2.739050	0.330283
12	1.968826	-1.088075	0.166319
6	-0.095368	-1.346006	0.235613
6	-3.319390	-1.627244	-2.101944
8	-1.357547	-1.503721	0.277983
6	-3.361096	-2.889465	-2.209412
6	-2.622999	-1.661845	0.320464
6	-2.400605	-0.425158	2.825821
8	-10.168999	-2.604755	0.573779

16

947.340419 Kcal/mol 41.080620 eV -99.873996 H Original3D_0_36.log

6	1.823708	-2.130468	-0.093380
6	1.246941	-0.563250	0.736161
12	-0.248883	-1.623103	-0.417714
8	3.250060	-1.778998	-0.386851
6	-2.157607	-0.175237	-0.891803

6	-2.952000	-0.766732	-0.197261
6	2.475396	-0.626346	-0.947868
8	-1.063348	1.145429	-0.345965
6	-1.605547	2.664230	0.114947
6	-4.045787	-0.865422	0.277018
6	4.245654	-0.563362	0.405422
12	1.880865	1.372254	-0.218601
6	-3.188979	2.718189	-1.070604
6	0.430694	-0.404710	1.573524
6	2.624770	3.807847	1.075431
6	-5.076821	-1.748281	1.268132
16			
951.548475 Kcal/mol 41.263099 eV -99.867290 H Original3D_8_5.log			
6	-1.182664	-1.055498	0.147153
6	-1.526090	-1.046303	-1.235674
8	-2.090260	0.747047	-1.049347
6	-2.657710	-1.648955	0.521117
6	0.644545	-0.195549	-0.182724
8	0.107364	-1.595727	-0.079367
6	1.009797	-0.030746	1.158824
6	1.724322	1.040439	2.015591
6	-2.540279	2.448009	0.388158
12	1.532886	-0.774210	-1.854632
6	3.055716	1.738990	0.462153
12	1.662336	-1.979285	0.981519
6	-1.523462	0.838956	1.587121
6	4.390667	2.393791	-1.189088
6	-3.319403	1.335788	-0.734303
6	-1.822024	0.819642	0.312850
16			
951.648461 Kcal/mol 41.267435 eV -99.867131 H Original2D_12_2.log			
6	1.375225	-0.839527	-0.000000
8	0.133396	0.720348	-0.000000
6	-0.000000	-0.647277	0.000000
6	2.826855	-2.358485	-0.000000
6	-1.327227	0.821653	0.000000
6	-1.427245	-0.523498	0.000000
6	1.579629	0.836943	-0.000000
8	1.370634	-2.453400	-0.000000
6	1.775237	2.147123	-0.000000
6	-1.387017	-1.763268	0.000000
6	-2.522158	2.067898	0.000000
12	-1.417901	-3.561849	0.000000
6	-1.268458	2.244442	0.000000
6	2.907613	-0.856467	-0.000000
6	3.039052	0.642774	-0.000000
12	-2.370539	3.831061	0.000000
16			
951.925944 Kcal/mol 41.279468 eV -99.866689 H MutI_14_67.log			
6	1.876243	2.931670	0.000000
6	2.745712	1.776739	0.000000
6	3.708249	-1.720266	0.000000
8	1.354354	-1.133247	0.000000
6	0.169835	-3.283995	0.000000
6	2.659151	-0.842009	0.000000

8	2.979278	0.517688	0.000000
6	1.115043	-2.570381	0.000000
6	2.426520	4.225804	-0.000000
6	-3.560311	0.486410	-0.000000
6	-5.784726	1.633354	-0.000000
12	-1.915838	-0.271743	-0.000000
12	-1.662357	-2.577283	-0.000000
6	0.000000	0.909792	-0.000000
6	-4.624587	1.009373	-0.000000
6	0.647085	1.962305	-0.000000

16

956.477270 Kcal/mol 41.476832 eV -99.859436 H MutI_7_71.log

6	4.037711	-1.945621	0.000000
6	1.791684	2.202105	0.000000
6	1.372221	0.854383	0.000000
8	-3.118019	-0.344748	0.000000
12	-0.142897	3.153063	0.000000
6	-2.032663	-3.503688	0.000000
8	-0.625435	-0.742287	0.000000
6	0.000000	0.496425	0.000000
12	-3.709187	-2.028612	0.000000
6	-1.096481	1.414283	0.000000
6	3.379029	-0.854186	0.000000
6	3.216089	1.779489	0.000000
6	4.344816	2.466654	0.000000
6	-3.174896	-4.236756	0.000000
6	-1.880721	0.218040	0.000000
6	2.738651	0.309351	0.000000

16

958.896787 Kcal/mol 41.581753 eV -99.855580 H Original3D_7_5.log

6	2.892407	1.262759	0.867462
6	1.220804	0.870029	0.027393
6	0.946309	-0.038245	0.973096
6	-0.402416	0.452011	-0.810790
8	1.831693	-1.404388	-0.023787
12	1.966704	-1.411805	1.828244
12	-2.263268	-0.855025	-0.721983
6	-2.724404	1.286638	1.206598
6	-1.270491	1.719130	0.195592
8	1.741292	-1.287522	-1.990894
6	-5.356130	-1.721514	-0.548813
6	-0.978112	2.630775	-0.724226
6	-4.602182	-0.017104	1.298886
6	2.506576	0.408672	-0.080242
6	2.119815	-0.514640	-1.010269
6	1.476970	1.784363	-0.920968

16

965.835687 Kcal/mol 41.882652 eV -99.844522 H Original2D_0_23.log

12	-0.754286	0.141429	0.000000
8	-2.074286	2.781429	0.000000
6	1.885714	-1.178571	0.000000
6	1.885714	0.141429	0.000000
6	3.205714	0.141429	0.000000
8	-0.754286	-2.498571	0.000000
6	4.525714	-1.178571	0.000000

6	1.885714	-2.498571	0.000000
12	-3.394286	4.101429	0.000000
6	4.525714	0.141429	0.000000
6	3.205714	-1.178571	0.000000
6	-3.394286	1.461429	0.000000
6	-2.074286	-3.818571	0.000000
6	-0.754286	5.421429	0.000000
6	-0.754286	-3.818571	0.000000
6	-2.074286	-2.498571	0.000000
16			
967.632795 Kcal/mol 41.960582 eV -99.841658 H Original3D_0_61.log			
6	-0.712922	-0.450543	-0.910446
6	-2.632677	-1.618136	-0.895948
12	-0.656613	1.326446	0.243222
6	-1.622110	0.273961	-2.475933
12	2.234619	1.488826	-1.184318
8	2.886373	-1.278967	-0.421558
6	0.953554	3.428284	-0.982841
6	-1.767736	-0.781034	-1.931493
6	-1.246427	-1.062857	1.684066
6	-1.878380	3.271734	1.998880
6	-3.571949	0.696720	1.240029
6	-0.562030	-0.542442	2.708961
8	4.041858	-0.764082	0.716277
6	-0.768997	-1.972627	0.221637
6	-1.787335	-2.829546	-0.637826
6	3.203356	-1.319995	1.470147
16			
974.190749 Kcal/mol 42.244962 eV -99.831208 H Original3D_10_4.log			
12	3.160422	0.474204	1.721397
6	0.737041	-0.419263	1.175010
6	1.008907	-0.367372	-0.115648
6	0.561364	0.873650	-0.160023
6	0.244759	-2.055128	-0.344465
6	1.456450	-1.608394	-0.071272
6	-1.414474	-1.260840	-0.662035
6	-2.133883	-0.071709	0.584247
6	-1.142608	-1.208949	-1.952692
6	-2.450488	-3.000487	0.399804
6	1.280773	-0.315481	-1.406305
8	3.256612	1.819009	-0.904293
12	-2.309560	1.221204	-0.750786
6	-4.688203	3.204624	0.177926
8	-2.405750	-0.123600	1.874904
6	3.704154	0.577987	-0.859917
16			
974.727902 Kcal/mol 42.268256 eV -99.830352 H MutI_7_73.log			
6	-0.678180	-1.161477	-0.028686
6	3.912116	1.201553	0.015003
6	5.448324	-1.479848	0.019260
6	3.157674	2.292579	0.020026
6	-5.659273	-0.682802	0.027812
6	0.556879	-1.650962	-0.022308
6	-1.707655	-0.550480	-0.032710
8	4.400433	-0.032123	0.015787

6	-6.820627	-1.102034	0.051912
12	3.425388	-1.561306	0.001344
6	1.940055	3.167388	0.012816
12	-4.076184	-0.049889	0.005830
6	-1.016034	2.628507	-0.018381
6	1.692969	-1.962048	-0.015585
8	-2.412636	0.511993	-0.031043
6	-2.175052	1.882187	-0.023166
16			
975.403259 Kcal/mol 42.297542 eV -99.829275 H Child_17_29.log			
6	8.902209	0.158343	0.654500
6	-8.710789	-0.964688	0.116556
6	7.703763	-0.353029	0.353639
6	-8.077405	-0.504859	1.132404
6	-0.178077	1.920998	0.111386
12	-6.358329	-0.330178	0.051445
6	1.114081	1.803808	-0.033401
6	-4.286651	-0.334248	-0.488442
8	6.538548	-0.666019	-0.010112
6	-1.777535	-0.267995	-0.376273
6	2.307351	1.236126	-0.169257
6	-3.033344	-0.252694	-0.444074
6	-1.533321	1.750656	0.221051
12	0.270406	-0.210103	-0.476667
6	3.480364	0.629928	-0.229628
8	5.660351	-2.140317	0.011600
16			
975.773363 Kcal/mol 42.313591 eV -99.828686 H MutI_18_71.log			
6	2.425968	4.907462	-0.442928
6	2.362526	2.954947	-0.257199
6	-1.613869	-1.143357	-0.594842
12	0.686475	-1.861720	-0.148634
6	0.972865	-0.227845	-0.244219
6	3.290757	-0.500397	0.226710
6	-0.212841	-2.982143	-0.217369
6	-4.881786	-0.440319	-0.865220
6	5.381182	-1.916199	0.802007
6	4.322566	-1.198389	0.509825
6	-3.601896	-0.700024	-0.655882
8	-0.128092	0.338250	-0.496605
12	-4.318381	0.427402	0.439019
8	-4.182908	1.253968	1.528556
6	2.335616	1.695479	-0.160911
6	2.230726	0.296463	-0.056675
16			
978.903553 Kcal/mol 42.449329 eV -99.823697 H Child_12_13.log			
8	-3.390459	-3.849896	0.118700
12	-0.541798	3.954064	-0.075128
6	-2.874559	-2.726498	0.040145
6	3.552187	1.246747	-0.408730
6	-1.695873	-1.902179	-0.123554
6	4.624057	0.605175	-0.379335
6	-2.969448	-1.314861	-0.089429
8	5.550647	-0.379604	-0.230936
6	-3.427732	-0.022297	-0.157142

6	-1.591002	2.267084	0.840315
12	0.126563	-0.818006	-0.486293
6	8.964400	-2.327944	0.741976
6	-2.398670	1.284712	0.263563
6	-3.313194	1.206463	-0.080132
6	-1.016317	0.827633	0.371084
6	0.096368	0.223180	0.253729
16			
979.769433 Kcal/mol 42.486877 eV -99.822317 H Original1D_0_3.log			
6	0.000000	0.000000	-3.121315
8	0.000000	0.000000	-4.377981
6	0.000000	0.000000	-1.913237
8	0.000000	0.000000	-0.577588
6	0.000000	0.000000	0.761250
6	0.000000	0.000000	2.017931
6	0.000000	0.000000	3.389873
6	0.000000	0.000000	4.690811
6	0.000000	0.000000	-5.681731
6	0.000000	0.000000	5.984323
12	0.000000	0.000000	-7.433656
6	0.000000	0.000000	7.287522
6	0.000000	0.000000	-9.741635
6	0.000000	0.000000	8.479316
12	0.000000	0.000000	10.203080
6	0.000000	0.000000	-11.084530
16			
981.183866 Kcal/mol 42.548213 eV -99.820063 H MutI_14_77.log			
8	2.147021	-2.627825	-0.795284
6	-4.539890	2.492600	-0.262323
6	-2.292977	-1.032381	1.378821
6	0.587652	-3.315812	0.912137
6	9.484498	2.655460	0.382940
6	1.411033	-0.577076	-1.473940
12	-1.864402	1.087548	-0.418242
12	-0.077733	0.235844	-0.845432
6	-3.470470	0.421364	0.908096
6	-5.476243	3.171703	-0.509266
6	-3.514888	-1.128413	2.007852
6	1.633433	-3.319761	0.060856
6	-3.502225	1.886104	-0.154356
8	2.055053	-1.438801	-1.504604
6	-0.678561	-1.698676	0.952211
6	8.640141	3.220273	1.390836
16			
997.056213 Kcal/mol 43.236504 eV -99.794769 H MutI_13_65.log			
6	3.689871	0.346110	0.008066
12	-0.280680	-0.274612	-0.632416
8	-1.779342	-1.550856	-0.686631
6	-2.742562	-1.702937	-0.385059
6	-3.946449	1.117609	0.165207
6	6.982225	-0.148459	0.332402
6	-3.952184	-1.399946	0.296998
6	-1.517463	1.056209	-0.201695
6	-4.596067	-0.121206	0.526197
8	-2.583366	1.266217	0.085767

6	-4.507185	2.348957	-0.188206
12	5.331700	0.120878	0.164298
6	-5.727456	-1.118646	1.171339
6	2.490187	0.300523	-0.149979
6	1.343660	0.348457	-0.291153
6	8.198328	-0.339688	0.453270
16			
999.627521 Kcal/mol 43.348007 eV -99.790672 H MutI_12_67.log			
6	2.122701	5.654533	0.363234
6	2.958601	1.811955	-0.041739
6	0.840039	3.096383	-0.091803
6	3.159883	0.602663	-0.044713
6	2.719041	-1.592374	0.055852
6	1.818654	4.275526	0.182056
12	1.398729	-2.838644	0.401997
6	-0.597718	1.872336	-0.505584
6	-9.487556	1.335280	0.369573
12	0.136903	-2.911134	-0.474416
6	-1.386343	-1.170789	-1.062171
6	2.198139	2.896423	0.015159
6	-1.251323	-2.700263	-1.488561
8	0.399045	-3.649187	1.634736
6	-10.857923	0.937245	0.258139
8	3.120362	-0.490333	-0.033189
16			
1002.154501 Kcal/mol 43.457587 eV -99.786645 H MutI_16_73.log			
6	-1.065521	1.125430	-1.098630
12	2.619308	-0.556123	1.123462
6	2.791539	3.529159	0.456219
6	-3.511388	0.915714	-0.475806
6	1.892660	-0.387571	-1.581203
8	0.979552	0.338678	-1.708870
6	4.523566	-2.560942	-0.202801
12	3.218073	-1.329533	-0.174726
8	1.001804	1.376114	1.050664
6	-4.614971	0.595283	0.205254
6	-3.885396	-2.473441	-0.794422
6	-4.992345	-1.662260	1.480403
6	-4.833421	-0.522061	0.734149
6	-2.258124	1.228014	-0.800351
6	0.199657	1.035034	-1.079338
6	1.437174	0.662563	2.136660
16			
1006.006102 Kcal/mol 43.624608 eV -99.780507 H			
Original3D_0_49.log			
6	-0.100293	-0.559080	-0.136075
12	1.390157	-1.512759	1.311770
6	3.042628	-0.439527	-0.885845
6	2.728696	0.932153	0.340834
6	-1.890855	-0.499766	-0.660641
6	-2.190967	-1.394131	0.262639
6	-0.538497	-0.320898	-1.934977
8	-1.138721	-2.109628	-0.088418
6	2.290493	1.170335	-1.458068
12	-0.114113	1.706964	0.167325

6	-0.714337	-0.081765	2.013883	
6	-0.838609	-1.215263	-1.011697	
8	-1.766583	0.633732	2.364940	
6	-1.918494	4.032323	-0.053841	
6	-2.329059	-0.261584	-2.459542	
6	3.780943	0.216656	-0.010223	
16				
1009.313475	Kcal/mol	43.768030	eV	-99.775236 H MutD_15_44.log
6	2.267579	0.064521	-0.221778	
6	10.412321	0.228754	0.315128	
6	-4.787027	-0.443315	0.165887	
6	-1.747063	1.738757	-0.051731	
6	6.526954	-0.061966	0.172954	
6	12.282149	-0.044684	-0.112570	
12	-1.522281	-0.481345	-0.104383	
6	5.370300	-0.058222	0.071639	
8	8.948164	-0.113027	-0.031583	
6	3.659619	0.051247	-0.116692	
12	-10.739902	0.103485	0.045263	
6	7.750351	-0.081499	-0.078095	
6	-7.564409	-0.063900	0.001590	
6	-3.607958	-0.315318	0.007556	
6	-6.201653	-0.141189	-0.017404	
8	-8.825762	0.024928	0.017900	
16				
1012.340450	Kcal/mol	43.899292	eV	-99.770412 H Child_10_16.log
6	6.135758	-0.252647	-0.117433	
6	-4.461152	2.030426	0.003409	
6	5.617737	-1.254776	0.403090	
12	-4.244173	-0.224704	-0.189611	
12	3.890550	-0.046780	-0.024125	
8	2.117938	0.771837	-0.182523	
6	-2.803540	-2.054827	-0.247798	
6	1.101959	1.422486	-0.351072	
6	-1.651674	-2.746051	-0.482923	
6	-0.272763	0.351015	0.397992	
6	-0.913199	2.503475	-0.663427	
6	-1.347780	-0.653053	0.596167	
6	-0.369124	-2.893200	-0.604025	
6	0.420629	2.553442	-0.668106	
6	-2.582098	-0.983123	0.754940	
8	-0.743569	1.118013	1.237518	
16				
1012.519605	Kcal/mol	43.907061	eV	-99.770127 H MutI_7_75.log
6	-3.180256	2.921831	-0.083073	
6	5.852791	1.173644	0.313279	
6	4.892304	0.410678	0.139804	
12	1.472511	-1.826674	-0.376907	
8	-1.478993	-2.206608	-0.269647	
6	6.964253	2.040998	0.521529	
6	4.149577	-0.152979	0.007720	
6	-3.604785	0.453903	0.064902	
6	-4.332964	-0.812654	0.333977	
6	-3.469129	1.739847	-0.024690	
12	2.704134	-1.246502	-0.237511	

8	-3.893926	-3.770623	0.701455	
6	-2.305303	5.544795	-0.125994	
6	-3.059647	-0.923286	0.019749	
6	-2.806770	4.118090	-0.109411	
6	-0.289469	-2.398872	-0.404699	
16				
1019.877198 Kcal/mol 44.226117 eV -99.758402 H				
OriginalID_10_0.log				
8	0.000000	0.000000	0.895714	
6	0.000000	0.000000	-0.424286	
6	0.000000	0.000000	-1.744286	
6	0.000000	0.000000	-3.064286	
6	0.000000	0.000000	2.215714	
6	0.000000	0.000000	3.535714	
6	0.000000	0.000000	-4.384286	
8	0.000000	0.000000	-5.704286	
6	0.000000	0.000000	-7.024286	
12	0.000000	0.000000	4.855714	
6	0.000000	0.000000	7.495714	
6	0.000000	0.000000	-8.344286	
12	0.000000	0.000000	8.815714	
6	0.000000	0.000000	-9.664286	
6	0.000000	0.000000	11.455714	
6	0.000000	0.000000	-10.984286	
16				
1031.797531 Kcal/mol 44.743032 eV -99.739405 H				
Child_6_48.log				
8	3.390934	-2.290945	-0.015307	
6	-5.462414	-0.921031	0.641847	
8	4.466163	0.330334	0.048012	
6	2.625948	-1.329851	0.004226	
6	-2.779692	1.636553	-0.057724	
6	3.251952	0.104514	0.056086	
6	-4.409814	-1.304398	-0.007728	
12	0.486819	-1.293119	-0.050732	
6	-1.625243	1.069168	-0.098672	
6	2.218560	1.114523	0.063485	
6	-3.344575	-1.683978	-0.666900	
6	1.192148	1.827058	0.017761	
6	-0.314068	0.679937	-0.034320	
6	-1.645193	-1.063188	-0.138283	
6	0.087070	-0.504099	0.468881	
12	-0.622222	2.787589	-0.095401	
16				
1034.579107 Kcal/mol 44.863653 eV -99.734973 H				
Child_10_9.log				
8	-2.885816	4.338525	0.507335	
6	2.721487	-2.805765	0.985003	
6	-3.429350	3.267629	0.276145	
6	1.769505	-2.209406	0.256492	
6	-4.062539	2.177340	0.047614	
6	0.382578	-2.341594	-0.094029	
8	5.065147	2.969541	-0.884546	
6	-0.823572	-2.537326	-0.360594	
12	-4.213705	0.166944	-0.157215	
6	2.569745	-1.086823	0.410998	
6	5.056395	1.833650	-0.495358	

12	-2.920922	-2.368456	-0.532977	
6	5.078708	0.647400	-0.046764	
6	3.560422	-0.558479	-0.299028	
6	-3.693860	-1.803980	-0.218619	
6	2.233960	0.076288	1.421468	
16				
1042.327936	Kcal/mol	45.199674	eV	-99.722624 H
	Original2D_0_15.log			
6	2.370469	-1.336884	-0.000000	
6	1.179175	-1.076236	-0.000000	
8	0.000000	-0.709645	0.000000	
6	2.756329	0.423183	-0.000000	
6	0.348434	1.059137	-0.000000	
6	3.710636	-1.982876	-0.000000	
6	-1.759291	0.169831	0.000000	
12	-2.193563	-2.061008	0.000000	
8	-3.421879	-3.728392	0.000000	
6	4.798641	-1.352090	-0.000000	
12	-1.017878	2.652423	0.000000	
6	4.077762	-0.053737	-0.000000	
6	-3.177405	4.108149	0.000000	
6	1.698181	1.271188	-0.000000	
6	-0.902016	4.823506	-0.000000	
6	-4.115526	-1.318619	0.000000	
16				
1046.255948	Kcal/mol	45.370009	eV	-99.716364 H
				MutD_13_38.log
6	-1.598765	5.214457	-0.851369	
6	-3.005299	-0.570031	2.873962	
6	-1.820989	6.342425	-0.300182	
6	-0.142817	-0.806025	0.703467	
6	-3.060729	2.687801	0.740875	
12	2.003023	-1.106707	0.135921	
6	-2.402981	3.901961	-0.254324	
6	-3.260379	-1.685555	-2.179667	
8	-10.146027	-2.556124	0.439886	
6	-2.593033	-1.654953	0.250951	
8	-1.326360	-1.503868	0.219247	
6	3.930208	-0.876779	0.087744	
6	-3.306960	-2.950183	-2.252071	
6	6.515401	-0.568396	0.023076	
6	5.225708	-0.722255	0.055285	
12	8.405552	-0.342864	-0.024217	
16				
1046.585947	Kcal/mol	45.384319	eV	-99.715838 H
				MutI_2_69.log
6	5.722537	-1.440502	0.221637	
6	4.575126	-1.179418	0.456197	
6	-0.767092	1.633966	-0.923306	
6	2.411163	1.783605	-1.503307	
8	-2.427070	-1.340144	0.856605	
6	-4.820205	-0.828127	-0.271853	
12	2.890541	-0.512570	0.692563	
6	1.341716	-0.019026	-0.840476	
6	2.660748	1.184971	-0.465789	
6	-2.891788	1.098045	-0.115034	
6	-1.928453	1.328774	-1.074399	

8	-1.902194	-1.269310	-0.586295	
12	-0.161822	-1.263850	0.105148	
6	1.287299	3.251933	0.746560	
6	-3.924395	-1.314867	-1.130096	
6	-3.351742	1.532759	2.944031	
16				
1046.610470	Kcal/mol	45.385383	eV -99.715799	H Child_4_48.log
8	5.904589	0.775110	-0.653980	
6	-5.716764	-0.223245	-0.247000	
6	4.806327	0.395137	-0.365334	
6	-5.039818	-1.611561	-0.217340	
6	3.646834	-0.080687	-0.112883	
6	-2.553731	3.408346	-0.188815	
6	2.370638	-0.326719	0.219856	
12	-2.262803	1.265918	-0.177396	
6	1.571770	0.421781	1.157362	
6	-1.996829	-1.663448	-0.285297	
6	1.508072	-1.326838	-0.339899	
6	-1.302169	3.680193	-0.165806	
6	0.528272	0.862789	1.634333	
8	-1.254003	-0.835418	-0.132750	
6	0.404390	-1.825497	-0.535086	
12	0.048917	-2.080837	0.424837	
16				
1054.553336	Kcal/mol	45.729818	eV -99.703142	H MutI_12_79.log
6	-3.833745	-1.501704	-1.462108	
6	1.944357	1.672916	-0.446536	
6	-0.717918	-2.003515	1.024157	
6	-0.293573	-0.690127	1.389026	
6	-1.183415	0.389350	1.069372	
6	-0.058750	3.088558	-0.901173	
12	-2.548592	-1.091074	-0.617753	
6	0.963623	0.924525	1.511549	
6	2.479612	0.796302	-0.533623	
12	3.158982	-0.901787	-0.365512	
6	-1.610648	2.376421	-0.160298	
6	1.058204	2.498732	-0.790443	
8	3.567718	-2.531153	-0.271343	
6	-0.758057	1.602760	1.432349	
6	-1.243262	-2.454956	0.001221	
8	-2.043125	0.495997	0.146120	
16				
1056.114953	Kcal/mol	45.797537	eV -99.700653	H MutI_18_41.log
6	-2.535475	2.879416	-0.398288	
6	-0.430485	3.928858	-0.140737	
6	-2.874230	1.596789	-0.592087	
6	-2.886609	-2.654425	-0.058675	
12	-0.900295	-1.972312	0.385788	
6	1.180353	2.776747	0.632674	
6	-2.873739	0.160532	-0.431636	
6	0.910232	1.637501	0.764095	
6	-4.113596	-3.216076	0.119493	
6	7.748146	-1.140968	0.140223	
8	-1.107645	4.922855	-0.159705	
6	1.044907	-1.215415	0.761481	

6	-2.928021	-1.086897	-0.063518
6	0.644496	0.099983	0.694406
8	-1.787855	-3.646747	-0.504249
12	6.387638	-0.761448	-0.656868
16			
1059.928214 Kcal/mol 45.962895 eV -99.694576 H			
Original2D_16_1.log			
6	1.404167	0.969496	0.000000
8	1.792519	-0.419422	0.000000
6	-0.000000	0.761218	-0.000000
12	0.298040	-0.802909	0.000000
8	2.166093	-3.044331	0.000000
6	-0.216816	1.873666	-0.000000
6	-2.199742	-1.260612	-0.000000
12	-0.492616	3.439239	-0.000000
6	-3.483013	-1.512426	-0.000000
6	-4.787676	-1.883076	-0.000000
6	-5.715785	-3.269774	-0.000000
6	0.273436	6.045798	-0.000000
6	0.994522	-3.228844	0.000000
6	2.354558	2.358664	0.000000
6	3.377171	-1.383688	0.000000
6	3.110179	-0.124745	0.000000
16			
1060.780567 Kcal/mol 45.999857 eV -99.693218 H			
Original2D_3_1.log			
6	-2.687143	-3.559286	0.000000
8	-1.367143	-2.239286	0.000000
12	-1.367143	-0.919286	0.000000
6	-1.367143	-3.559286	0.000000
6	1.272857	0.400714	0.000000
12	1.272857	-2.239286	0.000000
6	-0.047143	1.720714	0.000000
6	-2.687143	1.720714	0.000000
6	-1.367143	1.720714	0.000000
6	1.272857	3.040714	0.000000
6	-2.687143	3.040714	0.000000
6	3.912857	-0.919286	0.000000
8	3.912857	0.400714	0.000000
6	3.912857	-2.239286	0.000000
6	-1.367143	4.360714	0.000000
6	-1.367143	3.040714	0.000000
16			
1071.535225 Kcal/mol 46.466224 eV -99.676079 H			
Child_1_19.log			
6	-1.515182	4.101801	0.805128
6	-1.480983	-2.713098	0.038396
6	2.289118	1.222470	-1.407282
6	2.576063	-2.376158	1.435378
12	0.092547	1.600870	0.447190
6	-1.606008	-1.490759	0.561990
6	2.851057	0.888725	-0.226097
6	1.082631	-1.725130	0.515195
6	-2.871709	0.400606	-2.087796
6	-0.063233	-1.433858	-0.183699
6	4.043089	0.229907	-0.663841

6	-2.266593	-0.026061	0.993940	
6	-0.465725	0.189986	-1.899514	
12	-1.660492	-0.759502	-1.140412	
8	1.535438	0.274040	-0.038139	
8	-1.112915	0.512586	2.666625	
16				
1083.497119 Kcal/mol 46.984941 eV -99.657017 H				
Original3D_0_48.log				
6	0.164621	-0.938376	-0.226558	
6	-0.804587	-0.419110	-2.126718	
6	-1.400643	1.128708	-1.555987	
6	1.409020	0.505691	-0.327180	
6	2.478333	-0.245424	-0.174929	
6	1.874375	-1.207799	-1.111542	
6	-1.958031	0.583859	-0.485803	
6	1.242755	-1.820348	-0.071768	
6	3.537125	-1.018133	0.012396	
6	0.760161	2.372546	0.494554	
6	4.413068	-1.540261	1.903166	
8	-2.002267	-1.696711	-0.171238	
12	0.108170	1.348673	-0.554920	
6	-3.573454	-1.663449	0.542712	
12	-3.016049	-0.581850	1.543110	
8	0.257028	3.743050	1.034695	
16				
1098.166469 Kcal/mol 47.621065 eV -99.633640 H				
MutD_12_74.log				
6	8.300110	-0.780675	0.885752	
6	0.087687	-2.776600	-1.009568	
12	1.680082	1.580010	-0.532656	
6	1.800707	1.988995	0.398634	
12	-2.425381	-1.991049	-0.086572	
6	6.723699	-1.027957	0.804119	
8	-3.772314	0.705077	-0.468226	
6	-1.912756	1.640433	-0.260635	
6	0.161763	2.708996	-0.330192	
6	-5.248955	-0.592371	1.458575	
6	-1.122749	2.673750	-0.268245	
6	-1.067367	-2.518660	-1.519325	
6	5.517701	-0.746612	0.313783	
8	-6.382873	-0.588146	1.243285	
6	-2.532800	0.403767	-0.134588	
6	4.323809	-0.306896	-0.133266	
16				
1112.219902 Kcal/mol 48.230481 eV -99.611244 H				
MutI_5_79.log				
6	0.887105	-1.340435	-0.331680	
6	-1.619075	-1.182071	-0.611321	
6	-3.092218	-1.650932	-0.592946	
12	-2.496519	1.594819	-0.031080	
6	1.768346	1.477417	1.257407	
6	1.929515	-0.927615	1.911458	
6	-0.296474	-1.353993	-0.594930	
8	4.415620	0.828935	-1.937124	
6	-4.101294	2.490203	0.155007	
12	3.150155	0.057576	-0.788012	
6	1.402241	-1.859963	2.409000	

6	0.636200	1.845203	0.817158
6	-0.529180	2.172483	0.371381
6	-2.592201	-0.347633	-0.482241
8	1.922975	-0.979726	0.360409
6	-4.151698	-2.426399	-0.567822

16

1116.406306 Kcal/mol 48.412020 eV -99.604573 H

Original2D_2_2.log

6	-0.000000	-0.825143	0.000000
6	1.562242	-2.494400	0.000000
12	-1.313654	0.692067	-0.000000
6	1.663722	0.357597	-0.000000
6	-2.674448	-1.923337	0.000000
6	1.559140	-0.940176	0.000000
6	-2.825976	2.206384	-0.000000
6	1.390918	-3.972414	0.000000
6	1.168018	-5.222185	0.000000
6	2.936918	-2.685902	0.000000
6	-2.001498	3.044910	-0.000000
6	-0.098330	-2.221159	0.000000
12	0.995329	3.077666	-0.000000
8	3.458075	3.919277	-0.000000
6	-1.576952	4.354881	-0.000000
8	-3.808404	-1.833167	0.000000

16

1117.586844 Kcal/mol 48.463214 eV -99.602691 H

Child_9_52.log

6	2.143275	2.731464	-0.057866
8	-3.048010	-1.977751	-0.065399
6	2.424463	1.512285	-0.208029
6	-4.296053	0.328390	0.170160
12	3.926849	-1.365301	0.455499
6	-3.295648	-0.665639	-0.011779
6	2.700819	0.166872	-0.318500
6	-1.760411	-2.388081	-0.010374
12	0.191356	3.032792	0.088968
6	-0.560898	-2.661999	0.079227
6	1.804576	-0.900761	-0.369519
6	-2.875051	0.608226	0.059240
8	2.281960	-2.168524	-0.206759
6	-1.909644	1.578729	0.136406
6	-1.141647	1.579945	0.044780
6	-0.448791	0.303952	-0.239802

16

1123.417323 Kcal/mol 48.716047 eV -99.593400 H

Original1D_9_0.log

6	0.000000	0.000000	-4.572857
8	0.000000	0.000000	-3.252857
6	0.000000	0.000000	-1.932857
6	0.000000	0.000000	-5.892857
6	0.000000	0.000000	-0.612857
8	0.000000	0.000000	0.707143
12	0.000000	0.000000	-7.212857
6	0.000000	0.000000	2.027143
6	0.000000	0.000000	-9.852857
6	0.000000	0.000000	3.347143

6	0.000000	0.000000	-11.172857	
6	0.000000	0.000000	4.667143	
6	0.000000	0.000000	5.987143	
6	0.000000	0.000000	7.307143	
6	0.000000	0.000000	8.627143	
12	0.000000	0.000000	9.947143	
16				
1125.060723 Kcal/mol 48.787312 eV -99.590781 H				Child_3_21.log
8	5.102374	2.099287	-0.435080	
12	-4.678304	0.456967	0.461443	
6	3.534024	-2.177211	-0.273738	
8	-3.061018	1.597952	0.950701	
6	5.793600	3.025187	-0.077191	
6	-7.345865	0.329007	-1.078850	
6	3.320417	-1.078800	1.187613	
6	2.212071	-2.411607	-0.268330	
6	-2.087126	1.085369	0.333436	
12	3.737250	0.523090	-0.319705	
6	0.906152	-2.686269	-0.111506	
6	-1.777772	-0.209262	-0.352241	
6	-6.319066	0.010405	-0.395891	
6	2.258126	-0.765182	0.416628	
6	-0.354697	-2.788170	0.114479	
6	-0.979562	0.776767	-0.465380	
16				
1128.272042 Kcal/mol 48.926568 eV -99.585663 H				Child_10_46.log
6	0.456115	2.034478	-0.201433	
12	-5.457537	-1.145788	-0.621381	
6	-0.781224	2.133799	0.009946	
6	2.762621	-2.057334	0.193795	
6	1.700913	1.726899	-0.512021	
12	0.869737	-1.416264	0.708639	
6	-2.051884	1.902434	0.316640	
6	-3.462320	-0.747070	-0.204313	
6	2.783266	1.130006	-0.733724	
6	-2.163056	-0.611428	-0.210506	
6	3.884256	0.416908	-1.081015	
6	-0.855264	-0.506068	-0.189173	
6	-3.178446	1.405123	0.580798	
6	3.256704	-1.121277	-0.465644	
8	4.025401	-0.768781	-0.303841	
8	1.092540	0.332006	2.045442	
16				
1129.134401 Kcal/mol 48.963964 eV -99.584289 H				Child_7_13.log
6	3.642730	-3.067154	-0.051157	
6	5.410449	3.435810	0.701739	
6	0.318693	-2.841586	-0.403556	
6	0.493695	2.683332	-0.098795	
6	4.412693	-2.118611	0.458325	
6	-0.766991	2.356173	-0.037176	
8	-0.819889	-3.012388	0.955985	
6	1.754208	2.628728	0.014398	
12	-0.285478	-1.109037	-0.273962	
6	-1.950648	1.940717	0.072855	
6	2.326064	0.525982	-0.886485	

6	-3.097887	1.354812	0.253035
12	0.731114	-0.018124	-0.476012
8	-4.090853	0.785792	0.426790
6	-4.082510	-0.905328	-0.283546
6	-2.804110	-0.769759	-0.083388

16

1140.889496 Kcal/mol 49.473713 eV -99.565556 H Child_4_14.log

8	7.875965	0.391594	0.187499
8	-5.775775	-0.874738	-0.175587
6	6.718471	0.297586	0.091879
6	-4.662324	-0.566327	0.092260
12	4.653479	0.130287	-0.083078
6	2.717467	-0.044018	-0.266925
6	-3.393489	-0.378648	0.261105
6	1.500350	-0.160986	-0.446783
6	0.084807	-2.380168	1.237407
6	0.191116	-0.264646	-0.635516
6	-2.548860	0.530270	0.871350
6	-3.752605	3.090344	-0.315854
12	-1.470749	-1.169293	-0.613347
6	-1.035981	-0.287522	-0.780469
6	-1.368101	1.012855	1.144681
6	-3.616568	1.873463	0.123832

16

1142.614667 Kcal/mol 49.548524 eV -99.562807 H Child_13_31.log

12	-6.321396	-2.702909	-0.927731
6	4.320577	0.670683	-0.106277
8	-3.045565	-0.125983	1.723466
6	4.306716	-0.833396	-0.158667
6	-2.511530	0.661732	1.001522
6	4.343683	-2.336138	-0.212673
6	-1.925850	1.473375	0.194330
6	2.943663	2.069110	-0.012083
6	-1.334764	2.303378	-0.601381
6	2.851155	0.748336	-0.055459
6	-0.705218	3.122367	-1.418960
6	2.778495	-0.937957	-0.112326
6	-0.433567	-2.524089	0.562489
8	2.900034	-2.546144	-0.172805
6	0.840944	-2.284900	0.357784
12	-1.318736	3.418076	0.174807

16

1143.753342 Kcal/mol 49.597902 eV -99.560992 H

Original2D_0_16.log

6	0.000000	-0.380872	0.000000
6	0.660461	0.980959	-0.000000
6	-0.755146	1.483372	-0.000000
6	1.362937	-1.041567	0.000000
6	0.815241	-2.157040	0.000000
8	-1.384011	0.168485	-0.000000
6	0.007989	2.751463	-0.000000
6	2.029531	0.232966	0.000000
6	-1.219120	-2.534566	0.000000
8	1.265126	2.333264	-0.000000
12	0.187822	-3.816305	0.000000

12	-1.702764	3.359965	-0.000000	
6	-4.203235	3.014628	-0.000000	
6	2.612906	-1.556885	0.000000	
6	-1.832270	-1.211101	0.000000	
6	3.709105	-2.004342	0.000000	
16				
1156.584432 Kcal/mol 50.154311 eV -99.540545 H				
Original2D_15_2.log				
8	2.308504	1.117735	-0.000000	
6	2.174565	-1.371350	-0.000000	
6	-0.000000	0.869177	0.000000	
6	-0.945575	1.676790	0.000000	
6	4.094125	0.919632	-0.000000	
12	2.244457	-3.288388	-0.000000	
6	-0.546246	-2.101170	0.000000	
12	-2.102476	0.212241	0.000000	
6	-2.820000	3.345770	0.000000	
6	1.617198	-5.716896	-0.000000	
6	3.120960	-0.180723	-0.000000	
6	-4.770850	3.148824	0.000000	
6	-3.875181	4.103349	0.000000	
6	0.433984	-1.161833	-0.000000	
6	-3.221987	-1.462141	0.000000	
8	1.032780	1.944414	-0.000000	
16				
1159.578666 Kcal/mol 50.284154 eV -99.535773 H				
Child_2_43.log				
6	3.460229	1.210847	-0.000000	
6	-2.772793	-3.643402	0.000000	
6	2.636169	2.196183	-0.000000	
6	-2.673698	-2.182803	0.000000	
6	1.626825	3.091767	-0.000000	
6	-1.426141	-2.941797	0.000000	
6	0.314816	2.573563	-0.000000	
6	-2.701102	-0.845513	0.000000	
12	1.899469	-0.324597	0.000000	
8	-2.388390	0.276679	-0.000000	
12	-1.571444	3.609531	-0.000000	
8	-0.205396	-1.387835	0.000000	
6	-0.000000	1.265358	-0.000000	
6	-1.855247	2.122588	-0.000000	
6	2.342802	-4.351473	0.000000	
6	3.850470	-3.583645	0.000000	
16				
1197.934922 Kcal/mol 51.947440 eV -99.474648 H				
Original2D_9_1.log				
6	-0.094286	-0.212143	0.000000	
6	-0.094286	1.107857	0.000000	
12	-1.414286	2.427857	0.000000	
6	1.225714	1.107857	0.000000	
6	-2.734286	5.067857	0.000000	
6	-1.414286	-0.212143	0.000000	
8	-2.734286	-0.212143	0.000000	
6	-0.094286	-1.532143	0.000000	
6	1.225714	-2.852143	0.000000	
6	1.225714	-0.212143	0.000000	

6	2.545714	-0.212143	0.000000	
6	1.225714	-4.172143	0.000000	
12	-1.414286	5.067857	0.000000	
6	2.545714	-4.172143	0.000000	
6	3.865714	-2.852143	0.000000	
8	-0.094286	-4.172143	0.000000	
16				
1202.907856	Kcal/mol	52.163087	eV	-99.466723 H MutI_10_77.log
6	-0.716420	0.199634	-0.024689	
6	-4.697735	0.414790	-0.246862	
6	2.882583	2.236194	-0.207902	
12	-0.148936	-1.175575	0.169090	
6	4.562245	4.972785	0.170879	
8	0.590976	1.172751	-0.010515	
6	-5.540517	0.742521	0.373901	
6	0.691206	-2.197683	0.199382	
8	-3.403826	0.259767	-0.012812	
6	-7.240940	0.817767	-0.216358	
6	2.559884	0.905775	-0.117813	
12	2.911233	-3.587847	-0.115708	
6	2.739203	-1.118269	-0.132475	
6	-2.099437	0.269825	-0.030510	
6	3.428250	3.388269	0.013680	
6	1.657549	-3.014788	0.143104	
16				
1205.514315	Kcal/mol	52.276114	eV	-99.462570 H
	Original2D_0_21.log			
6	1.232815	0.003594	-0.000000	
8	0.255916	1.044573	-0.000000	
12	-0.000000	-1.012605	0.000000	
6	-0.739605	2.137238	-0.000000	
6	-2.454563	2.119457	-0.000000	
6	2.863258	0.138554	-0.000000	
6	1.308852	2.004623	-0.000000	
12	-2.361257	4.073800	-0.000000	
6	-3.490093	1.252895	0.000000	
6	-1.009657	-3.665625	0.000000	
6	1.844219	-2.881547	0.000000	
6	-4.483593	0.433801	0.000000	
6	2.986467	1.786850	-0.000000	
8	2.832000	-1.948323	0.000000	
6	3.679483	-2.992823	0.000000	
6	-1.132289	-5.254405	0.000000	
16				
1207.672121	Kcal/mol	52.369686	eV	-99.459131 H MutI_13_33.log
6	-1.465162	-3.791745	-0.000000	
6	2.999072	0.463307	0.000000	
6	1.590452	0.905672	0.000000	
12	-2.723773	2.050066	-0.000000	
6	-2.261598	3.890598	-0.000000	
6	2.931274	-0.956367	0.000000	
6	2.766896	-2.445193	0.000000	
6	-1.496596	-0.441891	-0.000000	
8	1.853382	2.181481	0.000000	
6	0.194395	0.688600	0.000000	

6	0.000000	-0.644926	0.000000
6	-1.203786	2.238423	-0.000000
6	-1.283252	0.878551	-0.000000
8	1.304027	-1.018257	0.000000
6	1.410690	-2.590350	0.000000
12	-1.472359	-1.922889	-0.000000
16			
1212.933960 Kcal/mol 52.597861 eV -99.450746 H MutI_13_59.log			
8	-2.873406	-2.312700	-0.556271
6	-1.696153	-2.768464	-0.113416
6	4.507326	-0.445509	-0.425010
6	0.284421	2.441471	-0.097487
8	-2.291306	2.410163	-0.250113
12	5.447702	-1.185697	-0.553840
6	0.272565	0.740188	1.533946
6	3.520686	0.352070	-0.274682
12	-0.628235	-1.040163	1.445669
6	-4.296362	0.151459	-0.788376
6	2.547792	1.186145	-0.131566
6	-0.949180	2.629695	-0.124265
6	-3.967555	-1.833094	-0.887132
6	-1.031968	-1.921401	0.698631
6	1.493255	1.862901	0.191862
6	-3.437479	1.926308	-0.290983
16			
1213.340069 Kcal/mol 52.615472 eV -99.450099 H MutI_14_35.log			
6	0.000000	0.000000	-0.165705
6	0.000000	0.000000	7.218695
6	0.000000	0.000000	-2.228505
6	0.000000	0.000000	5.955195
8	0.000000	0.000000	-4.787905
6	0.000000	0.000000	-6.010105
6	0.000000	0.000000	-3.507205
6	0.000000	0.000000	9.802595
6	0.000000	0.000000	-9.831605
8	0.000000	0.000000	-11.119905
6	0.000000	0.000000	11.007995
12	0.000000	0.000000	1.872295
6	0.000000	0.000000	3.946095
6	0.000000	0.000000	-8.517205
6	0.000000	0.000000	-7.275005
12	0.000000	0.000000	8.535295
16			
1218.035165 Kcal/mol 52.819070 eV -99.442617 H MutI_16_59.log			
6	0.000000	0.736961	0.000000
12	-0.235903	3.570928	0.000000
6	1.782966	-4.802989	0.000000
6	-1.453225	0.443044	0.000000
6	-1.989378	1.728460	0.000000
6	-1.427776	2.877906	0.000000
6	2.187151	1.495208	0.000000
6	3.512931	1.753723	0.000000
6	-2.540488	-2.400437	0.000000
6	-1.254562	-2.345370	0.000000
8	1.231565	0.201824	0.000000

8	0.542524	2.362179	0.000000		
6	-0.008304	-3.515330	0.000000		
6	2.445245	-2.883112	0.000000		
12	-1.998154	-0.982444	0.000000		
6	0.848100	-1.683703	0.000000		
16					
1238.787682	Kcal/mol	53.718986	eV	-99.409545 H	Child_18_19.log
8	-3.033502	6.545319	-0.142248		
12	4.770636	-1.057099	-0.487237		
6	-3.630445	-3.114806	-0.443546		
6	2.041548	0.073099	-0.798941		
6	-2.795338	-0.528643	-0.420759		
6	2.109104	0.963228	0.101251		
6	-2.839021	-2.099602	-0.152001		
6	1.640187	1.951763	0.984123		
6	-1.543724	-1.810176	0.475959		
6	1.380406	3.167694	0.301367		
6	-1.377148	-0.620679	-0.256993		
6	0.972043	1.490572	2.129263		
6	-0.838941	-2.135701	1.628640		
12	0.278346	-0.161458	-1.978262		
6	0.064502	-2.122168	2.500071		
8	-0.927352	-1.128420	-0.695827		
16					
1262.717677	Kcal/mol	54.756690	eV	-99.371410 H	Child_1_43.log
12	-0.777475	4.382074	0.000000		
6	2.436190	-6.800943	0.000000		
6	-3.375907	0.855569	0.000000		
6	1.872348	-5.615593	0.000000		
6	-1.978991	1.493636	0.000000		
6	1.342043	-4.427079	0.000000		
6	-0.985154	2.337502	0.000000		
12	1.460662	-1.582035	0.000000		
6	-2.314194	0.174762	0.000000		
8	0.384892	1.971269	0.000000		
6	1.778292	1.443211	0.000000		
6	-1.166119	-1.026690	0.000000		
6	0.000000	0.797624	0.000000		
6	1.067930	0.361124	0.000000		
6	2.344506	3.305929	0.000000		
8	-2.175380	-0.845616	0.000000		
16					
1265.839777	Kcal/mol	54.892077	eV	-99.366435 H	Original3D_0_64.log
6	1.305225	0.326015	0.497418		
12	-0.690279	-0.056831	0.093540		
8	1.008946	-2.053006	-1.179856		
6	2.434565	-0.552200	-0.449138		
6	-3.735119	0.354632	0.999572		
6	1.810567	1.936518	0.166085		
6	1.259734	-1.462920	1.848300		
6	0.375370	2.181227	-1.955839		
8	3.704537	2.243420	0.542472		
6	3.987284	1.121985	0.215150		
6	-4.155418	-0.782375	-0.573633		

6	4.543300	-1.393380	-0.447865	
6	2.448189	-2.224208	0.938114	
12	-4.645982	0.723859	-0.343206	
6	-4.013010	-0.043613	2.413274	
6	-1.872809	-1.049620	-2.302261	
16				
1269.926273	Kcal/mol	55.069285	eV	-99.359923 H MutI_13_79.log
12	-3.707723	-1.433771	0.250644	
6	2.499978	1.387374	-0.524869	
8	-0.841264	-0.084732	-0.769146	
6	0.414194	2.853967	1.609333	
6	1.780565	2.306093	1.093539	
6	4.733200	-0.719608	0.050561	
6	-0.743812	2.514685	-0.109901	
8	0.494383	1.633901	-0.818439	
12	-4.905766	-1.632563	0.654013	
6	5.314857	-3.635939	0.518362	
6	-0.746115	1.188857	-0.890076	
6	-2.110286	2.580655	-0.120114	
6	-1.881742	-1.106658	-0.438529	
6	-0.895822	-1.722140	-1.015160	
6	5.503616	-1.920838	0.243204	
6	3.820853	0.340659	-0.108883	
16				
1290.027702	Kcal/mol	55.940966	eV	-99.327889 H Child_15_14.log
8	4.014101	-0.703152	1.822570	
8	-7.798924	-3.037645	1.367249	
6	3.146439	-0.389674	1.092188	
6	-2.572572	2.317297	0.864111	
6	2.202149	-0.061385	0.213043	
6	-2.070717	1.885352	-0.451990	
6	1.608782	2.254206	-0.001606	
6	-1.757151	0.620510	-0.952629	
6	1.300458	3.550744	0.117420	
6	-1.292709	3.012921	0.616406	
6	1.123583	-0.877777	-0.113245	
6	-1.571071	3.227024	-0.815159	
6	0.146403	-1.565315	-0.402617	
6	-1.296942	-0.484770	-1.270497	
12	0.232543	-1.877220	-1.342571	
12	2.807347	-2.373483	-0.231687	
16				
1294.885933	Kcal/mol	56.151639	eV	-99.320147 H
	Original2D_14_1.log			
6	2.036996	0.986184	0.000000	
12	0.000000	0.648854	0.000000	
6	-2.397082	-1.655721	-0.000000	
8	1.055398	-1.602803	-0.000000	
6	2.395221	-1.521253	-0.000000	
12	-2.942069	0.366249	0.000000	
6	-1.495167	2.941079	0.000000	
8	3.424934	1.770729	0.000000	
6	2.904933	3.048795	0.000000	
6	3.320625	0.052381	0.000000	
6	3.137080	4.313560	0.000000	

6	-4.324544	-1.251377	-0.000000
6	-4.095409	-2.577936	-0.000000
6	-4.957840	0.632578	0.000000
6	1.500629	-2.999598	-0.000000
6	1.884920	-4.222800	-0.000000

16

1306.740236 Kcal/mol 56.665691 eV -99.301256 H

Original3D_4_5.log

6	-1.494842	1.006529	0.521147
12	0.107632	0.318891	-0.957512
6	-0.163566	2.778945	-0.038716
6	2.684499	-1.248655	0.207373
12	2.848660	-0.774556	-1.013561
6	-1.088044	-2.683552	-0.857047
6	0.839387	3.603163	1.843290
6	-1.387804	-1.927624	0.823285
6	-1.466281	2.710655	-0.240390
6	-2.469234	1.886438	-2.122397
6	5.318489	0.592051	-0.150815
8	-2.690518	-1.995914	0.621611
6	-0.356289	0.600720	1.943755
6	0.050509	-3.089361	0.565562
6	-2.497796	0.182312	-1.360860
8	-0.220690	-0.629307	1.484357

16

1308.992797 Kcal/mol 56.763372 eV -99.297666 H

MutI_1_67.log

6	-4.379036	1.007168	0.000000
6	-0.557231	-1.688791	0.000000
6	1.068674	3.657506	0.000000
12	-2.275067	-2.286705	0.000000
12	3.304688	4.494908	0.000000
8	-0.000000	0.996623	0.000000
6	-2.612031	0.222092	0.000000
6	1.769154	-4.020733	0.000000
6	0.714040	-1.059479	0.000000
6	-0.086258	-3.085722	0.000000
6	-3.049931	1.749067	0.000000
6	0.245719	-4.415702	0.000000
8	1.391925	-2.431314	0.000000
6	1.873156	2.989016	0.000000
6	4.968133	2.655565	0.000000
6	-3.869531	-0.513472	0.000000

16

1315.809160 Kcal/mol 57.058958 eV -99.286804 H

MutI_18_51.log

6	7.853828	-1.315184	1.164435
6	-0.449088	4.965293	0.320191
12	8.698444	-0.664223	0.009807
6	-4.806089	-1.132664	0.026501
6	-7.493139	-2.474409	0.201003
8	-3.291189	0.692398	-0.112828
8	-4.716284	0.805506	-0.055081
6	-6.274812	-1.971988	0.139590
6	4.576689	-0.965494	-0.424515
6	1.520359	-0.487873	-0.542146
6	-2.511302	1.717120	-0.127966

6	-8.673942	-3.072490	0.255986	
12	3.061052	-0.749508	-0.512372	
6	6.424058	-1.102789	0.071963	
6	-1.856632	2.780914	-0.003415	
6	-1.152291	3.889821	0.147381	
16				
1318.254474	Kcal/mol	57.164996	eV	-99.282907 H MutI_7_77.log
6	-0.201034	-2.522300	-1.480902	
6	-3.278350	-0.083898	0.046056	
12	-0.956760	-3.144236	0.261717	
6	-1.549274	3.699893	-0.006462	
12	-1.290375	-2.048722	-0.273498	
6	4.340903	-2.254338	-0.291032	
8	-3.479272	1.157959	0.034645	
6	5.892302	0.354771	0.845114	
6	2.363068	0.334408	-0.468364	
8	3.470765	0.300485	-0.060792	
6	-3.550508	2.462225	-0.066130	
6	-2.736728	-1.301135	0.108892	
6	-2.752063	-1.260759	1.454131	
6	4.700918	0.063451	0.351291	
6	1.270438	4.660255	-0.089370	
6	0.005939	4.288752	-0.344798	
16				
1330.478196	Kcal/mol	57.695068	eV	-99.263427 H MutI_2_67.log
6	1.447275	0.559105	-0.036354	
12	2.143167	-2.886604	0.027528	
6	-2.647954	0.549089	1.795215	
6	0.758226	1.726443	-0.184447	
6	-2.842148	2.333415	1.298079	
6	4.658641	1.780105	0.748056	
8	-2.375746	-1.175331	0.922454	
6	4.987333	2.661813	-0.286955	
6	-2.268728	1.370245	-1.650494	
6	-1.385199	-1.915803	-0.052684	
6	1.796620	-0.720799	0.019138	
6	-2.024623	-1.024352	-0.649315	
12	0.617913	-2.387641	-0.003537	
6	-1.757215	2.185481	-0.108271	
8	-2.175627	0.009130	-1.369546	
6	-0.175889	2.598682	-0.343827	
16				
1331.998955	Kcal/mol	57.761014	eV	-99.261004 H
	Original2D_4_2.log			
6	3.399245	-1.997743	0.000000	
6	2.191507	-2.487868	-0.000000	
12	0.097427	-2.077112	-0.000000	
6	-0.000000	1.186794	0.000000	
12	-1.661370	0.199250	-0.000000	
8	-3.544936	1.848385	-0.000000	
6	-1.260293	-4.374067	-0.000000	
6	2.675905	-0.642361	0.000000	
6	1.955479	0.753465	0.000000	
6	0.468334	2.983561	0.000000	
8	-4.009448	0.004438	-0.000000	

6	3.975399	-0.044500	0.000000	
6	-4.386252	-1.513152	-0.000000	
6	3.176711	1.574698	0.000000	
6	1.185528	1.841735	0.000000	
6	-0.181165	4.004732	0.000000	
16				
1333.514367	Kcal/mol	57.826729	eV	-99.258589 H MutI_7_65.log
6	3.597135	0.931859	0.768334	
12	-2.229344	1.686936	-0.444851	
6	0.718643	1.850390	-0.269450	
8	-7.848119	-2.860974	0.574348	
6	5.477903	0.158445	1.986036	
6	2.612427	1.589291	0.432877	
12	3.950724	-2.129341	-0.378325	
6	2.111174	-2.078064	-1.248179	
8	0.434227	-0.936607	-1.331921	
6	-8.337676	-2.176750	1.350923	
6	-4.019109	3.421883	0.271593	
6	-3.168266	2.533665	-0.095921	
6	-0.445575	-0.080371	-1.132296	
6	4.449836	-1.216668	0.297484	
6	-1.182493	1.041143	-0.808682	
6	4.628429	-0.026573	1.103730	
16				
1341.864866	Kcal/mol	58.188841	eV	-99.245281 H MutI_16_65.log
8	3.330784	0.261883	0.178098	
6	2.170149	-0.042999	0.432222	
6	1.004339	-0.335296	0.704240	
6	-1.517701	-2.297740	-0.769005	
12	-1.515816	-3.506102	-0.324430	
6	7.613793	1.353760	-0.690337	
12	-1.484975	-0.909096	1.202783	
6	-4.031971	2.830672	-1.313329	
8	4.546313	0.571956	-0.067806	
6	-4.319782	1.103845	0.018185	
6	5.784478	0.856144	-0.287064	
6	-1.702578	-0.983578	-0.594862	
6	-3.916222	4.693008	0.881604	
6	-0.160905	-0.604245	0.986962	
6	-3.308937	0.892446	-0.840317	
6	-2.115876	0.252593	-0.432061	
16				
1349.816770	Kcal/mol	58.533669	eV	-99.232609 H MutI_13_77.log
6	3.436237	1.279230	0.137115	
8	0.915355	1.993677	-0.028795	
6	2.319998	-1.720840	-0.417837	
6	1.415014	-2.382667	-1.226691	
12	-3.281206	-1.392056	-0.038594	
6	5.043728	0.653689	0.277649	
6	-1.656825	2.524745	-0.215877	
6	2.135928	1.709659	0.046169	
12	-3.924200	-0.497711	-0.778284	
6	-7.480849	2.676362	1.692019	
6	-0.392346	2.272207	-0.152551	
8	7.186361	-0.242735	0.686611	

6	-4.691544	0.534133	-1.563050	
6	-1.808872	-3.321653	1.581405	
6	-2.420151	-2.556404	0.890045	
6	7.708207	-0.223516	-0.291726	
16				
1368.297408	Kcal/mol	59.335066	eV	-99.203158 H MutI_14_61.log
6	0.000000	0.000000	-2.952520	
6	0.000000	0.000000	-7.035420	
6	0.000000	0.000000	-10.882820	
8	0.000000	0.000000	8.751380	
6	0.000000	0.000000	4.929880	
12	0.000000	0.000000	10.039680	
6	0.000000	0.000000	-5.026320	
6	0.000000	0.000000	3.707680	
6	0.000000	0.000000	6.194780	
12	0.000000	0.000000	2.426980	
6	0.000000	0.000000	-0.914520	
6	0.000000	0.000000	7.436980	
6	0.000000	0.000000	-8.298920	
6	0.000000	0.000000	1.148280	
8	0.000000	0.000000	-9.615520	
6	0.000000	0.000000	-12.088220	
16				
1388.448051	Kcal/mol	60.208882	eV	-99.171046 H Child_15_25.log
6	-3.269581	2.773075	-0.291090	
12	6.671358	0.890050	0.073217	
6	-3.825397	1.615822	-0.210595	
6	5.030848	0.050613	-0.010425	
6	-4.365011	0.382391	-0.201483	
6	3.978471	-0.549846	-0.099778	
8	-0.217777	3.669641	-0.153095	
6	2.817061	-1.239676	-0.188069	
6	-4.710806	-0.852835	-0.172475	
6	1.646466	-1.695312	-0.184511	
6	-0.687973	2.657592	0.316839	
6	0.451662	-2.339418	-0.252419	
12	-2.762609	-1.349099	0.040019	
6	-0.735452	-2.741113	-0.486133	
6	-0.854071	-0.618836	0.691718	
8	-2.252508	-1.062910	0.799555	
16				
1392.649967	Kcal/mol	60.391094	eV	-99.164350 H MutD_13_68.log
6	-0.241525	0.065025	-0.651022	
6	1.350909	-0.726445	-0.226936	
6	3.016106	-0.279247	0.540961	
6	-3.339386	0.909721	0.278655	
6	5.867399	0.813072	0.025867	
6	-3.602070	3.285289	-0.358443	
6	-3.738009	2.044297	0.038139	
6	-3.010992	4.400856	-0.662195	
12	1.080992	-3.420285	-0.552586	
8	-3.038078	-0.142339	0.995248	
8	6.792702	1.811385	0.004766	
12	-4.629652	-1.171244	0.344042	
6	-3.870665	-2.838825	-0.729929	

6	1.681833	-1.702346	0.673783
6	3.440205	0.181948	0.126199
6	4.537352	0.804317	0.028659

16

1405.158402 Kcal/mol 60.933512 eV -99.144416 H

Original3D_0_32.log

6	-0.700520	0.064300	0.966526
6	0.064763	0.214770	-0.098416
6	-0.771894	1.119356	-0.571838
6	-3.049665	0.924008	-0.600134
6	0.901420	-0.689816	0.375006
6	0.669219	2.219290	-1.016965
8	-0.611067	-0.734695	-0.718231
6	0.225590	-1.639281	-0.244809
6	1.505876	1.314704	-0.543542
6	1.577251	0.259648	0.994821
6	0.990873	-1.488811	-1.309750
8	0.740593	1.164235	0.521399
6	0.811967	0.109179	2.059763
6	-0.096064	2.068821	0.047977
12	-3.654121	-1.080512	0.318415
12	2.503361	-1.443933	-0.216513

16

1425.804247 Kcal/mol 61.828802 eV -99.111515 H

Original2D_0_28.log

6	-0.565714	-0.330000	0.000000
6	0.754286	-1.650000	0.000000
8	-0.565714	-1.650000	0.000000
12	0.754286	0.990000	0.000000
6	-1.885714	0.990000	0.000000
6	-0.565714	-2.970000	0.000000
6	-1.885714	2.310000	0.000000
6	-1.885714	-1.650000	0.000000
6	-1.885714	-2.970000	0.000000
6	2.074286	-2.970000	0.000000
8	-0.565714	3.630000	0.000000
6	3.394286	2.310000	0.000000
6	0.754286	-2.970000	0.000000
6	3.394286	-0.330000	0.000000
12	-3.205714	0.990000	0.000000
6	4.714286	3.630000	0.000000

16

1434.003217 Kcal/mol 62.184343 eV -99.098449 H

Child_4_38.log

8	4.156062	-1.252781	-0.300006
6	-3.245063	1.953932	-0.136033
12	2.384505	-1.602102	-0.246959
6	-1.824944	1.792641	0.051578
6	0.481974	-1.295061	-0.264931
6	-2.745972	0.649099	-0.135492
6	2.341144	1.825344	-0.113601
8	-0.163498	-1.363358	1.877815
6	-3.111971	-0.709391	-0.171358
6	2.740551	2.895687	-0.058010
6	-3.835268	-1.418017	-0.669163
6	0.424974	-0.091386	-0.213383

6	-0.631775	-2.003489	-0.283209	
12	0.163701	1.900236	0.239103	
6	1.121981	0.948315	-0.118202	
6	-2.135461	-1.655757	0.023770	
16				
1436.762909 Kcal/mol 62.304015 eV -99.094051 H				
Original3D_1_3.log				
12	0.259819	0.745568	-0.067897	
6	1.039109	-1.342640	-0.852423	
6	1.061007	3.832574	-0.735198	
6	-1.387164	-1.063861	1.517960	
12	2.990330	-1.736923	-1.876364	
8	2.444071	-1.638822	1.028218	
6	-2.303460	-1.249480	0.630876	
6	1.190447	-1.793411	0.721936	
6	-0.154309	-0.471512	1.902949	
6	-2.590350	-0.373227	-0.812624	
6	-2.395585	2.000560	-0.799450	
8	1.324318	2.673769	0.123838	
6	-0.051038	3.446709	0.158304	
6	-3.588619	-1.652254	-0.022282	
6	-3.401008	-1.009823	-1.699779	
6	1.056154	0.279146	2.342179	
16				
1444.209777 Kcal/mol 62.626942 eV -99.082184 H				
Child_2_22.log				
6	5.294258	-0.526912	-0.265916	
6	-4.169044	3.095685	-0.076443	
6	4.157585	-1.088975	-0.217131	
6	-4.198964	-2.827508	-0.309663	
8	3.688833	2.722333	0.830019	
6	-3.751456	-1.805376	0.444399	
6	2.940109	-1.617059	-0.061887	
6	-3.639958	1.622571	0.175878	
6	2.792973	3.122138	0.170011	
8	-2.798419	2.755118	-0.042792	
6	-2.458052	-2.081383	0.502930	
6	1.761740	-2.071677	0.096667	
6	-1.345897	-2.454670	0.504047	
12	0.097407	-1.155392	-0.566104	
6	-0.557194	3.858237	-0.762012	
12	0.895935	-1.108777	-0.059154	
16				
1448.608098 Kcal/mol 62.817672 eV -99.075175 H				
Original3D_0_78.log				
6	-2.202883	0.920336	-1.753589	
12	-0.102532	1.275509	-0.923181	
6	-1.358785	-1.693224	-0.672475	
6	1.676985	-0.608991	-0.421603	
6	2.841917	-0.982877	0.988341	
6	1.383234	3.141296	0.815595	
12	-2.863129	0.759640	-0.014897	
8	2.887578	0.688432	0.158016	
6	4.667094	-1.196068	0.659594	
6	6.492272	-1.409258	0.330846	
6	-2.019032	-1.853919	1.066217	

8	-3.248203	1.167308	2.882952	
6	0.741566	-1.338050	0.157933	
6	-5.009141	-1.266843	-0.014979	
6	-3.459136	-2.048397	-1.502883	
6	2.658066	1.791378	-1.831465	
16				
1449.585636	Kcal/mol	62.860062	eV	-99.073617 H Child_16_11.log
6	-0.279730	-2.421209	-0.320702	
8	-3.525108	1.843212	-0.582335	
12	8.656634	-0.534862	0.049641	
12	-1.597009	2.125577	-0.138043	
8	6.741334	-0.511422	0.007416	
6	0.312066	1.845845	0.398112	
6	5.477976	-0.459360	-0.014907	
6	4.113753	-0.421502	-0.042297	
6	1.382752	1.201120	0.476758	
6	2.688770	-0.182281	0.153753	
6	-3.010719	-0.717055	-0.474067	
6	1.515773	-0.328855	-0.030849	
6	-6.347747	-0.339897	0.747945	
6	-12.482993	-1.322411	0.051699	
6	-7.434551	-0.951883	0.365972	
6	-4.342902	-0.859664	-0.368054	
16				
1463.387661	Kcal/mol	63.458575	eV	-99.051622 H MutI_16_77.log
6	-0.022238	0.309036	1.635393	
6	3.029797	-1.469604	-0.382822	
12	3.186525	-2.853023	-0.522076	
6	-2.326903	-0.106568	2.581661	
6	-0.325188	0.562351	2.842777	
12	-5.937543	0.266863	-1.517779	
6	2.396556	0.375592	-0.459215	
8	-0.277840	-0.118533	0.309278	
8	-5.255321	0.752782	-0.628242	
6	0.504087	0.146873	-0.722544	
6	-1.546624	-0.757121	0.279625	
6	3.590578	3.536373	-0.431913	
6	3.113420	-4.256082	-0.603827	
6	3.975363	4.801964	-0.522798	
6	3.145767	2.316671	-0.462598	
6	-2.655030	-1.132831	0.751258	
16				
1490.579226	Kcal/mol	64.637714	eV	-99.008290 H Child_7_12.log
12	3.470254	1.415142	0.915987	
8	-5.384060	-1.474621	1.448076	
6	-0.514028	4.651785	-0.842021	
6	-6.130470	-1.020240	0.697517	
8	4.294711	-2.597258	-0.498796	
6	-3.416900	-0.378263	-1.111950	
6	3.691019	-1.647946	-0.105125	
6	-2.055040	-0.854464	-0.946380	
6	3.151545	-0.552388	0.328288	
6	-2.317623	0.492947	-0.733348	
12	-0.099966	-1.466981	-0.636857	
6	1.384181	1.212981	0.822302	

6	-1.621110	1.619535	-0.362066
6	1.776199	-0.057001	0.556606
6	-0.808102	2.510026	-0.002845
6	1.572220	-0.444120	-0.124945
16			
1497.610459 Kcal/mol 64.942618 eV -98.997085 H MutI_17_73.log			
6	-4.972868	-0.451790	-0.828097
6	2.292023	2.775699	-0.228510
6	3.224429	-0.624955	0.239700
12	0.872211	-0.509023	-0.261158
6	-1.642922	-1.255220	-0.631533
6	2.149451	0.130488	-0.050869
6	-0.120983	-2.926894	-0.264602
8	2.255202	1.544886	-0.144424
6	-0.187577	0.189597	-0.531775
6	0.615418	-1.902898	-0.199261
6	-3.657701	-0.720963	-0.630255
6	4.263266	-1.308395	0.525700
6	5.316022	-2.019190	0.830803
8	-4.370462	0.235559	0.289477
12	-4.279717	0.958500	1.253256
6	2.356802	4.841641	-0.408900
16			
1504.976459 Kcal/mol 65.262038 eV -98.985346 H MutI_17_63.log			
8	1.151305	-0.040132	0.007132
6	-6.095169	-1.553784	0.022957
6	0.268019	1.061765	0.064300
6	6.103944	-0.129434	-1.042902
12	5.096682	-0.176089	-0.188827
8	-2.648223	2.464383	0.000823
6	4.768297	-0.353280	1.243349
12	2.459316	-0.070571	0.092824
6	-0.527207	-1.343117	-0.109087
6	3.737679	-0.145874	0.208934
6	-2.504005	-1.808386	-0.050774
6	-5.022914	-0.929478	-0.027714
6	-0.735796	1.799325	0.087530
6	-4.507664	1.685717	-0.104271
6	-4.893352	0.509253	-0.082953
6	-3.707937	-1.531720	-0.027970
16			
1529.847652 Kcal/mol 66.340557 eV -98.945711 H			
Original2D_0_24.log			
6	1.390714	-0.942857	0.000000
6	0.070714	-0.942857	0.000000
6	-1.249286	-2.262857	0.000000
6	0.070714	0.377143	0.000000
12	1.390714	0.377143	0.000000
8	-1.249286	1.697143	0.000000
6	2.710714	-2.262857	0.000000
6	-1.249286	-0.942857	0.000000
6	-2.569286	-0.942857	0.000000
6	-2.569286	-2.262857	0.000000
6	-2.569286	0.377143	0.000000
6	-1.249286	0.377143	0.000000

8	-2.569286	1.697143	0.000000
12	4.030714	1.697143	0.000000
6	2.710714	4.337143	0.000000
6	-1.249286	-3.582857	0.000000
16	1538.470459 Kcal/mol 66.714477 eV -98.931970 H Child_7_15.log		
8	5.585022	1.902168	-0.264568
8	-4.089382	-0.836271	0.043005
6	4.501873	1.410717	-0.122042
12	-2.629176	-1.911468	0.023182
6	3.268218	1.065472	0.046743
6	-4.136144	0.452199	-0.047706
6	4.956219	-1.971030	0.517800
6	-4.514986	1.705929	-0.093702
6	2.198647	0.271049	0.189570
6	-0.570890	-2.015313	-0.033534
12	0.109361	0.813552	0.387749
6	-2.980099	1.520469	-0.160906
6	0.696787	-1.406219	-0.437928
6	1.346174	-1.296684	0.005819
6	1.972322	-1.783247	-0.460491
6	-3.692679	2.821294	0.069933
16	1559.842864 Kcal/mol 67.641274 eV -98.897911 H Original3D_18_5.log		
6	-0.502966	-0.521196	0.401945
6	-0.181221	-0.577580	-1.436016
6	-2.741287	-0.280871	0.002742
6	-1.131847	0.630222	0.256534
12	0.125914	-1.672615	0.547357
6	2.072067	0.817251	-0.136348
8	-2.127375	-3.067447	-0.752311
6	1.428219	0.333513	-1.182224
6	3.008082	-1.429202	1.992436
6	3.666540	0.093187	-0.783021
6	-3.706880	-0.708226	0.794827
12	-0.487999	1.113961	1.302410
6	5.904861	-0.147138	-0.383818
6	-2.404575	1.297903	-0.934754
6	-0.810102	0.573838	-1.581427
8	-0.780167	3.844153	0.219503
16	1563.458895 Kcal/mol 67.798080 eV -98.892148 H MutD_13_76.log		
6	1.862621	-0.465476	-1.701977
6	2.611994	0.672543	-0.245158
6	-0.591179	2.995896	0.812450
8	8.783521	-0.085879	-1.274530
6	-2.608066	-2.266097	-0.679479
6	-1.612304	2.750524	0.197238
8	-3.780350	1.496662	0.335751
12	-3.204552	-0.302366	0.028642
6	0.545216	-1.195675	-0.800988
6	-3.263404	-2.349539	-0.362409
6	-4.465004	-2.760341	-0.139725
6	2.017000	1.874893	-0.281000

12	3.905911	-1.866104	2.458672
6	-2.736577	2.233936	0.298532
6	0.917536	2.583532	-0.102006
6	-0.751446	-1.618300	-0.718399
16			
1568.089254 Kcal/mol 67.998872 eV -98.884769 H MutI_17_51.log			
8	-2.324844	0.092660	1.804813
6	4.927599	-0.687479	0.289659
6	0.773115	1.680928	1.153547
6	-3.081223	-2.103068	0.865330
12	0.711450	1.394558	-0.262251
8	3.427273	-0.162978	-0.560057
6	-2.891352	-2.795938	-0.074382
6	-0.720059	-1.149366	-1.360577
6	1.394817	0.242975	-0.863726
6	-2.944543	-1.012826	1.535126
6	-2.014369	-1.245104	-1.439612
6	-2.084533	2.414755	0.085981
6	-2.920996	2.249094	-0.834248
6	-0.320031	2.138465	0.325893
12	0.437860	-0.620560	-1.176401
6	6.113050	-1.186676	1.534638
16			
1581.468103 Kcal/mol 68.579034 eV -98.863449 H			
Original3D_12_4.log			
8	-1.075753	1.798159	-0.066304
6	1.084984	1.298890	-0.679749
6	-2.132338	-0.130202	0.467758
6	0.046276	2.230628	0.532400
6	-3.829261	-0.863790	1.030435
6	1.574511	0.067852	-0.753161
6	-4.428828	-1.033843	-0.792487
12	-3.258066	-0.563535	-0.223309
6	1.139792	4.132768	0.037196
6	3.199952	-0.742888	-0.177381
6	2.632174	-2.373318	-0.857980
6	-0.067118	-0.653226	-0.175052
6	-0.578848	0.557859	-0.105545
6	2.688078	0.514523	-0.138988
8	2.687447	-1.009017	1.029692
12	1.518916	-1.465187	0.387328
16			
1587.677836 Kcal/mol 68.848314 eV -98.853553 H			
Original2D_17_2.log			
6	1.107857	-1.791429	0.000000
6	-0.212143	-1.791429	-0.000000
6	-1.532143	-0.471429	-0.000000
6	1.107857	-3.111429	0.000000
6	-1.532143	0.848571	-0.000000
6	-0.212143	2.168571	-0.000000
6	1.107857	3.488571	0.000000
6	1.107857	-0.471429	0.000000
6	2.427857	-0.471429	0.000000
6	-2.852143	-1.791429	-0.000000
6	-0.212143	3.488571	-0.000000

8	-1.532143	-3.111429	-0.000000	
8	-2.852143	0.848571	-0.000000	
6	1.107857	2.168571	0.000000	
12	2.427857	0.848571	0.000000	
12	-0.212143	-0.471429	-0.000000	
16				
1627.581719 Kcal/mol 70.578712 eV -98.789962 H				
Original3D_9_7.log				
8	-1.599759	-1.538753	0.027118	
12	-0.224364	0.287338	0.056770	
8	2.945941	-0.185276	-0.367738	
6	2.144966	0.392288	1.216452	
6	-3.394668	0.759952	0.481278	
6	4.130605	-0.132801	0.212103	
6	3.138900	-1.328854	2.346483	
6	-4.274211	-0.468112	-0.615563	
6	-0.338754	3.236544	0.023581	
6	-0.834607	2.638517	1.090771	
6	2.066398	-1.413340	-1.464580	
12	-3.089546	-0.415638	-0.035722	
6	2.755210	-1.958892	0.182451	
6	-5.954728	-1.118613	-0.128214	
6	3.441794	0.412750	-1.434928	
6	1.952007	1.535865	-1.497769	
16				
1639.152519 Kcal/mol 71.080470 eV -98.771523 H				
MutD_17_78.log				
6	-1.372994	2.152004	1.467505	
12	0.670943	1.378102	-1.673952	
12	-3.847157	-2.516014	-0.731316	
6	-2.678582	0.327651	1.978910	
6	-2.739635	-0.178409	-1.677550	
6	0.533520	3.144907	-0.150045	
6	6.284706	-0.693917	-0.007589	
6	-2.442949	0.309168	-0.816133	
6	1.079887	-2.391707	0.554843	
6	-1.734624	1.448686	-0.419719	
6	7.587201	-0.315966	-0.109298	
8	5.154311	-1.082476	0.085844	
6	-2.686851	-0.077417	1.391257	
8	0.668507	-1.470607	1.105001	
6	-0.150927	2.602690	0.769233	
6	-3.090081	-0.647756	0.241329	
16				
1657.563656 Kcal/mol 71.878854 eV -98.742183 H				
MutD_15_36.log				
6	-1.922946	-1.428289	-0.531236	
6	3.026225	0.168019	1.484722	
12	-2.004116	3.092114	-0.635503	
6	-2.063774	0.829106	0.229399	
6	-1.975795	-1.805143	0.064255	
12	-2.637398	0.008567	1.378613	
6	1.082525	1.132127	-1.588104	
6	1.873672	0.432475	-0.796071	
8	4.237402	-0.179250	-0.587302	
8	2.889218	0.002233	2.431405	
6	-2.989236	-1.986459	0.938144	

6	0.433373	-0.074376	-0.671408	
6	-0.533758	0.604392	0.134915	
6	-0.208864	-2.541210	-1.968554	
6	3.068658	0.055559	-0.091765	
6	-0.009212	-1.351539	-1.149321	
16				
1662.516499	Kcal/mol	72.093630	eV	-98.734290 H MutI_16_49.log
6	1.185711	-0.648684	2.688696	
6	2.396167	0.514488	0.033560	
6	6.369802	-1.174162	-2.122688	
6	-2.054710	2.069098	-0.209583	
12	-1.985958	3.358537	-0.327136	
6	-1.737405	0.016144	-0.360429	
6	1.051271	0.081938	0.168145	
6	3.580322	0.703041	0.396049	
12	-3.412246	-2.904651	-0.235343	
6	3.265219	-0.304180	2.262251	
8	-2.790538	-1.779495	-0.304043	
6	0.178681	-0.040597	-0.758403	
6	-3.999839	-4.088716	-0.303241	
8	-1.719400	4.651108	-0.402934	
6	5.739276	-1.538625	-1.234010	
6	0.835164	-0.326333	1.507247	
16				
1694.810838	Kcal/mol	73.494047	eV	-98.682826 H MutI_8_67.log
6	2.622097	0.127048	0.005415	
6	2.018844	1.425843	-0.229387	
6	-3.479762	-0.805843	-0.671068	
12	1.907854	-1.069617	0.266916	
6	2.621094	3.369730	0.806849	
12	-0.324228	-2.313509	0.318603	
6	-2.529178	1.027872	-0.717563	
6	-5.265570	1.920763	0.827504	
6	-1.544348	-2.306881	0.128728	
8	0.645778	1.517675	-0.383807	
6	5.126792	0.140449	-0.320636	
6	3.964329	0.131513	-0.174980	
8	-2.706603	-1.696533	-0.248918	
6	-4.289402	2.134773	0.233936	
6	0.924194	-1.800902	0.379541	
6	-0.588576	1.640363	-0.595743	
16				
1757.627146	Kcal/mol	76.218023	eV	-98.582721 H
	Original2D_8_1.log			
6	2.341974	-0.661572	-0.000000	
6	-0.015911	-1.363025	0.000000	
6	3.573437	0.230810	-0.000000	
6	0.840577	-0.288342	-0.000000	
6	0.000000	0.824055	-0.000000	
12	-1.856410	1.699147	0.000000	
6	4.520425	-0.702921	-0.000000	
6	-3.706094	2.908270	0.000000	
6	1.231900	-4.114264	0.000000	
6	-4.389746	1.719170	0.000000	
6	-2.782884	4.006147	-0.000000	

8	0.210846	-3.542895	0.000000	
12	2.105516	1.490880	-0.000000	
6	-1.087856	-2.160579	0.000000	
8	2.615142	-1.905049	-0.000000	
6	-4.792016	0.486122	0.000000	
16				
1764.211755	Kcal/mol	76.503559	eV	-98.572228 H MutI_7_79.log
6	-3.188870	-0.189236	-0.365508	
6	-5.253389	-1.262500	0.048824	
6	6.046182	-1.021445	-1.597200	
6	-2.779582	0.753743	0.149182	
6	2.486924	-2.281267	2.007158	
6	1.140152	3.045400	0.325901	
8	-5.745438	-0.356149	-0.371735	
6	3.625413	3.500355	-0.104233	
6	-0.040553	-2.090347	-0.527905	
8	3.058323	-3.094436	1.508258	
6	4.694688	-0.692701	-1.465370	
12	-1.668570	-1.433580	-0.947043	
6	1.032838	-2.388667	0.220380	
6	0.040780	2.746261	0.475646	
6	2.296871	3.308889	0.143416	
12	-1.590747	2.019728	0.534216	
16				
1805.009679	Kcal/mol	78.272727	eV	-98.507212 H Child_9_36.log
8	7.134413	1.841172	0.424978	
6	-5.322150	-2.304364	0.371050	
6	3.452725	0.569379	0.383785	
8	-5.577162	-1.238539	-0.025984	
6	3.937530	-0.624148	0.006650	
6	-0.303328	-1.833670	-0.131649	
12	-0.885225	2.258096	-0.482148	
12	-1.616578	-0.296255	0.740090	
6	4.471755	-1.709819	-0.342288	
6	2.015337	-3.254693	-0.401003	
6	-2.690583	3.176840	-0.266532	
6	0.057111	0.450355	-0.456639	
6	1.060442	-2.392015	-0.255414	
6	-3.549851	2.292835	-0.043245	
6	0.788757	-0.964802	-0.146930	
6	-0.990473	1.866912	0.234340	
16				
1805.549011	Kcal/mol	78.296114	eV	-98.506353 H Child_5_36.log
6	5.333852	3.850544	0.172465	
6	2.939233	-4.060866	-0.221931	
6	4.716775	2.933937	0.049335	
6	-3.649217	-1.308418	-0.251024	
6	4.607659	1.381993	-0.167628	
6	-2.389227	-1.375687	-0.198616	
6	-4.352302	3.245651	0.375247	
8	2.274232	-3.117011	-0.098361	
6	-3.659360	2.107747	0.344004	
6	-1.008331	-1.027949	-0.211659	
6	1.933285	-1.034188	1.035800	
12	-3.650362	0.729552	-0.408949	

12	2.850814	-0.231408	-0.366806	
6	-2.781289	0.698954	-0.372221	
6	-0.925819	0.359180	-0.293559	
8	-1.648855	-1.958379	1.066832	
16				
1810.366395	Kcal/mol	78.505016	eV	-98.498676 H MutD_6_70.log
6	-1.882883	-0.941082	0.614773	
8	-2.183418	1.046789	-0.507069	
6	-0.153703	4.485672	-0.730430	
6	-2.064579	-1.602109	0.852456	
12	-1.785148	2.833035	0.984114	
8	-2.471362	0.457929	0.214099	
6	-7.861750	-2.477595	-1.164310	
6	0.554970	-3.186823	0.089913	
6	1.083940	3.382141	-0.302943	
6	3.116764	-3.167794	-0.042996	
6	1.864345	-3.449653	0.042955	
6	-0.549547	-2.680167	0.123625	
12	2.722560	2.041068	-0.292632	
6	3.310073	0.472382	-0.219440	
6	3.448635	-1.970187	-0.097094	
6	3.465283	-0.619283	-0.158846	
16				
1814.507172	Kcal/mol	78.684577	eV	-98.492077 H
	Original3D_6_6.log			
6	-2.662232	0.566755	-0.513572	
6	-1.339063	-0.750012	-0.525670	
6	-3.018841	-1.121375	0.199061	
8	0.340715	-0.378648	-1.250401	
6	-2.132347	-2.887615	1.348724	
8	-3.905335	0.644865	-0.950603	
12	1.503751	0.781900	-0.364243	
12	4.070023	-0.612976	0.060690	
6	-3.178975	1.355941	1.097317	
6	-0.532636	-1.277593	1.073121	
6	2.100561	-1.245943	-2.424260	
6	-4.502145	2.672708	1.109414	
6	2.150042	2.731634	2.132805	
6	-2.938773	-2.360033	-0.250067	
6	6.119552	-1.218667	2.096511	
6	3.540137	2.841394	-1.801606	
16				
1819.059715	Kcal/mol	78.881995	eV	-98.484822 H MutI_16_61.log
8	2.961072	0.002349	0.103583	
6	-5.362656	0.557511	0.054792	
6	1.782803	0.646814	-0.158212	
6	1.827890	-1.697267	1.469804	
6	-0.706212	0.233257	0.539704	
6	0.905964	4.629396	-0.911093	
6	0.534107	-0.116682	-0.095116	
6	2.988184	-1.118540	0.780727	
12	-0.498427	-2.865508	-1.906361	
6	-0.924615	-1.133991	-0.834590	
6	-4.133506	0.501245	0.421753	
6	0.259062	-1.146279	-0.855113	

6	-1.696809	0.820350	1.181936	
6	-2.979670	0.802509	0.900294	
12	1.655268	2.759482	-0.494666	
8	0.932762	-2.077053	1.626794	
16				
1838.022616	Kcal/mol	79.704305	eV	-98.454603 H Child_7_23.log
6	3.776290	-1.929998	-0.150862	
6	0.142695	3.470567	0.353413	
12	1.770317	-2.189005	-0.372506	
8	-5.505474	-0.085691	0.047745	
6	4.014200	-0.714524	0.009265	
6	-4.275506	-0.119917	0.024907	
6	-0.016072	-1.220297	-0.446076	
6	-3.359525	0.938758	-0.317076	
6	3.943013	0.644032	0.137800	
6	-2.239000	1.430911	-0.444565	
6	-0.872806	-0.316838	-0.424472	
6	0.314129	2.261330	-0.159695	
6	3.429082	1.767769	0.202631	
8	-4.125862	-2.326876	0.939218	
6	-1.679642	0.846841	-0.385311	
12	3.062145	0.268066	0.514552	
16				
1888.546836	Kcal/mol	81.895245	eV	-98.374087 H MutD_15_38.log
12	2.022949	2.075116	-1.377380	
6	-3.894463	-0.427239	0.090963	
6	0.001223	-0.218678	-0.327978	
6	-3.235774	-2.816467	-0.378454	
6	-3.471754	-0.561066	-0.484723	
6	-4.011561	2.562392	1.055831	
6	3.625372	0.592356	-0.036833	
12	3.077553	-1.182285	1.038015	
6	1.481619	-0.554798	-0.461103	
6	-3.520902	-3.517829	-0.920927	
6	3.482908	-2.599589	2.709263	
8	4.438308	1.562088	-0.367669	
6	2.328773	0.523393	-0.646682	
6	-4.013153	1.324587	0.681878	
6	-3.912859	3.784031	1.465650	
8	-0.733631	-1.469654	-1.183447	
16				
1890.103157	Kcal/mol	81.962734	eV	-98.371607 H MutD_15_68.log
6	2.222989	-0.403268	-1.284494	
6	4.717734	0.894009	0.180907	
6	6.903342	0.189174	2.489276	
6	6.130018	0.926215	0.175497	
6	-5.270241	-0.733044	1.061965	
8	4.235388	0.952451	-0.929821	
6	-1.046922	-2.535320	-0.594007	
8	-4.217798	3.870976	-0.535753	
6	3.074775	0.320675	-1.208334	
6	-4.603810	2.842951	-0.055167	
6	-5.192053	0.445658	0.770846	
6	-5.065639	1.750293	0.462142	
6	-2.063689	-2.782290	0.078914	

12	0.520736	-1.601022	-1.384887	
12	-3.816858	-2.211947	0.734022	
6	6.762287	0.279651	1.178282	
16				
1922.175282 Kcal/mol 83.353514 eV -98.320497 H				MutD_13_78.log
6	-3.134580	1.017931	0.039617	
6	-6.595272	-0.192341	1.176984	
6	1.514259	2.953629	-0.328367	
6	3.779578	-2.073386	-0.227009	
12	3.222781	1.908871	0.254478	
8	5.876237	-1.738990	0.185840	
6	-4.224858	0.301691	0.260801	
8	-7.142019	-1.930493	-0.689624	
6	-5.413548	-0.213678	0.556633	
6	-6.770702	-1.159228	0.127775	
6	4.940374	0.552314	0.650329	
6	2.513080	-1.957298	-0.389710	
6	5.544189	-0.487308	0.477400	
6	4.866934	-2.560195	-0.293550	
12	-1.222462	1.434140	-0.626388	
6	0.667619	2.024491	-0.635370	
16				
2008.317582 Kcal/mol 87.089003 eV -98.183220 H				Child_1_10.log
8	5.321441	-1.107480	0.033913	
6	-4.980960	2.332660	0.899406	
6	4.211349	-0.654937	-0.007402	
12	-3.745616	0.684515	-0.267570	
6	3.095945	-0.035612	-0.078024	
8	-1.958730	0.116687	-0.066383	
6	1.775480	0.158575	-0.066318	
6	-3.280114	-2.227923	-1.633156	
12	1.940982	3.225430	-0.614406	
6	0.560852	-0.657870	0.120409	
6	0.115206	0.933045	1.611789	
6	0.082362	-1.869195	0.351294	
6	-1.590282	-1.821206	-0.268790	
6	0.949582	1.397794	-0.256652	
6	-0.645492	-1.677816	0.650105	
6	-1.168275	-2.376349	0.484584	
16				
2016.295811 Kcal/mol 87.434972 eV -98.170506 H				MutI_17_59.log
6	1.422522	3.808338	-0.064299	
8	5.283695	-0.703214	0.348860	
6	-5.412969	0.028796	0.128431	
6	4.348304	-1.636880	0.121715	
12	0.453541	0.600857	-0.099062	
8	1.338794	-2.632879	-0.471132	
6	6.176598	0.041218	0.706040	
6	-0.640445	-1.088166	-0.261541	
6	-7.664930	-1.215448	0.620830	
6	-6.587651	-0.522892	0.415665	
6	0.388165	-1.879680	-0.392804	
6	1.708019	5.108834	-0.076982	
6	1.239460	2.539135	-0.075599	
6	3.933662	-2.833318	0.015369	

12 -2.210755 0.258764 -0.313063
6 -4.226292 0.378947 -0.149544
16

2055.226788 Kcal/mol 89.123181 eV -98.108466 H
Original2D_18_2.log

6 0.495000 -0.259286 0.000000
6 1.815000 -1.579286 0.000000
6 0.495000 -1.579286 0.000000
8 -0.825000 1.060714 -0.000000
6 1.815000 -2.899286 0.000000
6 0.495000 1.060714 -0.000000
6 -0.825000 2.380714 -0.000000
6 0.495000 2.380714 -0.000000
12 -0.825000 -1.579286 0.000000
6 -3.465000 -2.899286 0.000000
6 0.495000 3.700714 -0.000000
8 1.815000 1.060714 -0.000000
6 -4.785000 -2.899286 0.000000
12 1.815000 -0.259286 -0.000000
6 -2.145000 1.060714 -0.000000
6 1.815000 2.380714 -0.000000

16

2056.707847 Kcal/mol 89.187406 eV -98.106106 H
Original3D_0_69.log

12 1.392137 -0.918772 0.023012
6 4.017241 -0.486924 0.501980
8 -1.441502 -2.111345 0.498018
6 -0.093973 1.621422 0.604379
6 -2.761389 -2.732963 0.331756
12 3.246139 1.434165 -0.490326
8 -3.192551 -1.848384 -0.648822
6 -3.335514 0.961705 -0.689020
6 0.598692 1.220074 1.739974
6 -1.030866 2.189014 0.014813
6 3.299534 -2.768775 -0.362642
6 -1.575996 4.352917 -0.206621
6 4.803875 -0.542320 -0.469736
6 -2.136205 -0.726402 -0.136159
6 -1.797902 0.969652 -0.631260
6 -3.085312 0.191455 0.438236

16

2070.606471 Kcal/mol 89.790108 eV -98.083957 H MutI_1_71.log

6 0.533897 2.981345 -0.442970
6 -0.447964 0.139418 0.183170
12 4.364723 -1.927616 0.316833
6 -1.531847 1.914432 0.333874
6 -3.209214 -1.547501 -1.155643
6 -2.405645 -0.761521 -0.360165
6 0.955514 1.803696 -0.250213
8 1.059329 0.401847 0.017372
12 -3.622015 -0.024076 1.753312
6 1.883639 4.483727 -0.837763
6 -4.017055 -2.129893 -1.956532
6 2.195938 -0.390122 0.002385
8 2.579535 -1.765812 0.271913

6	-0.949525	-0.795274	-0.533200	
6	-2.801875	0.310282	0.482689	
6	3.456901	-0.286587	0.008366	
16				
2086.676191	Kcal/mol	90.486958	eV	-98.058348 H MutI_16_45.log
6	1.619932	0.853329	0.650452	
6	-5.558201	-2.680750	0.640701	
6	-3.466701	0.765970	-1.139358	
8	-2.492096	0.613376	-0.154687	
8	6.854815	-1.576781	-1.228856	
6	1.448680	-0.527227	0.175227	
6	3.968750	-0.307418	0.516738	
6	-4.336790	0.710858	-2.050677	
6	0.250729	3.114410	0.912246	
6	0.993739	2.084083	0.829785	
6	2.681161	-0.026412	0.646309	
6	-4.401641	-2.569419	1.226194	
6	6.116037	-1.119750	-0.425353	
12	-4.118113	-0.963268	-0.112152	
12	-1.058313	1.791464	-0.152346	
6	5.220200	-0.669525	0.391456	
16				
2122.561197	Kcal/mol	92.043081	eV	-98.001161 H Child_1_13.log
6	-0.820557	4.299454	-0.000000	
6	0.630824	-5.407440	0.000000	
6	-0.499821	3.020437	-0.000000	
6	-3.607375	-2.197156	0.000000	
12	2.758371	1.631475	-0.000000	
6	0.840367	-3.827754	0.000000	
6	0.734185	2.175978	-0.000000	
6	-1.788891	-2.468871	0.000000	
6	4.448217	0.510371	-0.000000	
8	-2.561695	-1.351112	0.000000	
6	-1.332450	1.657066	-0.000000	
12	0.402783	-1.023040	0.000000	
6	0.000000	1.021431	-0.000000	
6	-2.159542	0.696913	0.000000	
6	3.976084	-0.654033	-0.000000	
8	-2.495817	1.318663	-0.000000	
16				
2139.063757	Kcal/mol	92.758701	eV	-97.974863 H Original1D_6_0.log
6	0.000000	0.000000	-8.328804	
6	0.000000	0.000000	-9.628353	
6	0.000000	0.000000	-7.000773	
6	0.000000	0.000000	-5.727803	
12	0.000000	0.000000	-4.268361	
6	0.000000	0.000000	-1.687803	
6	0.000000	0.000000	-0.393287	
6	0.000000	0.000000	0.960541	
8	0.000000	0.000000	-10.903483	
6	0.000000	0.000000	2.245456	
8	0.000000	0.000000	3.570609	
6	0.000000	0.000000	4.877621	
6	0.000000	0.000000	6.181203	

6	0.000000	0.000000	7.469939
12	0.000000	0.000000	8.931347
6	0.000000	0.000000	11.483256

16

2149.801963 Kcal/mol 93.224354 eV -97.957751 H MutI_17_49.log

6	1.353447	-1.236387	0.304402
6	4.862547	0.544056	-0.140982
12	-3.307561	-0.556501	-0.306983
6	-0.303434	-0.784650	-0.736983
6	3.577241	1.012770	-0.095623
6	8.585555	-0.486531	-0.261223
6	2.420717	1.346194	-0.034590
12	1.270118	-0.489864	1.192780
6	-8.813715	0.869300	-0.004470
6	7.310398	-0.259955	-0.219553
6	-1.533767	-0.623826	-0.650192
6	-5.207365	-0.310798	-0.115915
6	6.044238	0.125403	-0.182848
8	-6.266311	-0.000420	0.025237
6	-7.454433	0.276113	0.168616
8	1.191403	1.216200	0.123087

16

2154.400161 Kcal/mol 93.423751 eV -97.950423 H Child_15_30.log

8	-5.287301	0.153354	-0.141254
6	4.229493	2.073918	0.138054
6	-4.067930	0.244473	-0.162151
6	4.161256	0.912865	-0.274341
6	-2.855453	-0.534738	-0.098458
12	3.492959	-0.878130	-0.314847
6	-2.816642	0.901148	-0.239969
6	1.526836	-1.206406	1.325990
6	-1.975398	-1.484453	-0.016692
6	0.286194	2.914815	1.282470
12	-0.975867	1.918974	-0.343955
8	1.479556	0.049222	-0.940946
6	-0.795055	-1.921260	0.108044
6	1.527841	-1.091243	-0.791925
6	0.672858	-1.937057	-0.039557
6	0.148809	-1.223851	1.529073

16

2169.647341 Kcal/mol 94.084932 eV -97.926125 H

Original2D_5_2.log

6	0.000000	-0.073551	0.000000
6	1.779218	1.278563	-0.000000
6	0.138226	1.363075	-0.000000
6	0.437700	3.137050	-0.000000
6	1.979673	2.717301	-0.000000
6	-0.223846	-1.535538	0.000000
8	1.659191	-0.311456	-0.000000
6	2.641153	4.089313	-0.000000
12	-1.897261	-2.413696	0.000000
6	1.368184	-1.980690	0.000000
8	3.853367	3.665149	-0.000000
6	-1.318709	1.834841	-0.000000
12	-4.503096	-2.990965	0.000000

6	3.212916	-0.791022	-0.000000	
6	-2.348784	-4.607818	0.000000	
6	-2.215096	0.906207	0.000000	
16				
2205.878033	Kcal/mol	95.656046	eV	-97.868388 H MutD_16_46.log
12	8.211893	1.645124	-0.852904	
6	3.057436	-0.056187	0.766623	
6	4.561330	-0.451085	0.516431	
6	-4.375522	3.874692	0.957840	
6	-2.019575	-1.529842	-0.470360	
6	5.360373	0.402756	0.235348	
6	-0.443912	-1.288479	1.002418	
6	-1.747856	-1.626850	1.092498	
6	-1.631978	-3.955451	-0.912275	
6	-1.720086	-2.670225	-1.088078	
6	-2.389941	-0.216095	-0.393344	
8	-4.604894	0.523027	0.204532	
12	-4.345692	2.425364	-0.733352	
8	1.951889	-0.582625	0.673544	
6	-3.564523	0.435500	-0.527380	
6	0.719194	-0.980247	0.822022	
16				
2266.650832	Kcal/mol	98.291407	eV	-97.771540 H MutI_18_61.log
6	-0.911951	-1.976975	0.136567	
6	1.841082	-0.892429	0.069340	
6	6.352963	-0.836026	-0.354633	
8	-3.927252	-1.019895	0.003932	
8	-0.340265	-0.123585	0.070203	
6	2.961067	3.016279	0.555772	
6	-1.759441	2.959814	-0.265895	
6	2.862007	-0.891330	0.002407	
12	4.691413	-0.833726	-0.141672	
6	-0.280696	1.804598	-0.090185	
6	0.463610	-1.137668	0.100977	
6	1.623867	2.484293	0.287340	
6	-4.067757	0.103101	-0.085479	
6	-2.907463	2.295827	-0.249666	
6	-3.764028	1.281906	-0.192460	
12	-3.053031	-2.509649	0.135206	
16				
2291.728499	Kcal/mol	99.378879	eV	-97.731576 H MutI_15_47.log
12	-2.394265	-3.153102	-0.439303	
8	1.023610	1.396029	-0.177496	
12	1.102103	3.080250	-0.295452	
6	-0.393501	-1.964009	-0.539164	
6	4.744380	-1.397004	0.649414	
6	-3.772687	-0.236116	0.456809	
6	0.192965	-0.247165	-0.760483	
6	3.554695	-0.906517	0.412910	
6	1.117656	-0.984853	-0.307478	
6	5.814235	-1.974417	0.766415	
6	-3.210160	-1.237358	0.221373	
6	2.235273	-0.534348	0.147764	
6	-1.062841	-0.012547	-1.037381	
6	-4.094448	1.935295	1.029106	

6	1.408173	4.717219	-0.382667	
8	-3.985672	0.844613	0.787166	
16				
2344.678693 Kcal/mol 101.675019 eV -97.647194 H				MutI_11_79.log
6	-5.095972	-2.134287	0.005976	
6	-2.618557	-1.942742	-0.225328	
12	-0.921078	-1.557065	-0.270207	
6	2.614643	-1.580607	3.587150	
6	-3.816159	-2.046310	-0.112986	
6	1.736303	-0.749705	-0.331432	
6	-6.380930	-2.184817	-0.013183	
6	6.985337	1.428328	-0.274335	
6	0.685173	-1.110688	-0.321859	
12	5.470855	0.633084	-0.287340	
6	-7.617389	-2.041314	-0.474769	
6	-6.781040	5.943641	-0.160454	
8	4.025726	0.033874	-0.400943	
6	8.067459	1.984495	-0.254808	
8	2.925000	-0.363484	-0.347669	
6	-6.146059	6.721449	0.689272	
16				
2378.052375 Kcal/mol 103.122241 eV -97.594010 H				
Original2D_7_2.log				
6	-2.352813	-0.893982	-0.000000	
6	-1.690748	0.268060	0.000000	
6	-0.000000	1.022999	0.000000	
8	1.275329	-0.328340	-0.000000	
12	-0.460966	-1.469500	-0.000000	
6	-2.129623	1.696291	0.000000	
6	-1.258473	3.899615	0.000000	
12	-3.875138	0.651500	0.000000	
6	-1.033022	2.521289	0.000000	
6	1.857227	-1.437348	-0.000000	
6	1.031696	1.862583	0.000000	
6	1.544265	-3.129049	-0.000000	
8	4.336874	-2.303244	-0.000000	
6	2.736501	-2.386729	-0.000000	
6	3.780038	-3.545228	-0.000000	
6	-1.295777	5.266278	0.000000	
16				
2394.315153 Kcal/mol 103.827463 eV -97.568094 H				MutI_14_43.log
12	5.526381	-0.214007	-0.283458	
8	3.225843	0.848758	-0.158289	
6	-8.910009	0.639991	-0.231848	
6	-6.349522	0.139723	-0.133830	
6	2.367152	-1.308680	0.271092	
6	-5.181887	-0.097569	-0.090217	
6	-4.160653	-0.265231	-0.048596	
6	-7.528775	0.369298	-0.176064	
6	3.744959	-1.708008	0.159473	
6	4.905533	-1.914068	0.079667	
8	5.328935	1.503053	-0.558873	
6	2.163494	2.348431	0.247330	
12	-2.415355	-0.780138	0.083975	
6	0.528460	-1.656914	0.317324	

6	-0.804923	-1.257838	0.244762		
6	1.597749	3.563407	0.716089		
16					
2575.941611	Kcal/mol	111.703541	eV	-97.278653	H MutI_12_69.log
12	-0.463124	-0.789067	-1.229025		
6	-4.050166	-0.926287	0.741000		
6	0.865085	0.308370	-1.358696		
8	-3.367690	1.638757	0.166184		
6	1.214666	1.695276	0.823608		
6	2.121114	-0.498327	-0.741767		
6	4.357076	-1.355912	0.759543		
6	2.436460	0.987915	-0.146176		
8	-1.603752	-1.779019	-0.626108		
6	-1.732995	-0.569838	2.442890		
6	1.078726	1.825589	-0.543973		
12	3.994582	0.573527	0.583308		
6	3.251429	-1.562875	0.089180		
6	-3.973655	0.062710	0.466865		
6	-2.802366	2.970035	-0.549019		
6	-3.199699	-2.318560	-0.078788		
16					
2606.441935	Kcal/mol	113.026162	eV	-97.230048	H MutI_15_37.log
6	-5.716323	0.233560	0.919677		
8	5.282761	0.611581	0.701274		
6	-4.761165	3.882829	-0.286996		
6	-2.620215	-2.623135	0.096520		
6	-5.274495	2.553866	0.261688		
6	-5.623588	1.419177	0.703377		
6	-5.551549	-1.070845	1.068754		
12	2.248095	0.315724	-1.294411		
8	-0.244505	-1.843654	-1.058022		
6	3.843206	1.611984	-0.838681		
6	4.489332	1.091844	-0.114783		
6	-1.275661	-2.392468	-0.506279		
6	6.965178	-0.363284	2.399191		
12	1.216350	-0.446011	-1.509034		
6	-4.249862	-2.558009	0.827244		
6	6.128576	0.117818	1.552840		
16					
2664.896430	Kcal/mol	115.560992	eV	-97.136895	H Child_9_9.log
8	3.523962	0.105875	1.523219		
8	-4.890050	-0.180843	-0.681719		
6	2.664689	-0.014769	0.688291		
6	-3.893384	-0.275667	-0.077636		
6	2.080645	-1.031088	-0.005007		
6	-2.736442	-0.378215	0.618833		
6	1.891476	0.728910	-0.366716		
12	-0.895378	-2.964750	0.051059		
12	0.513186	2.342144	-0.103852		
6	-2.001540	-1.287476	1.020007		
6	-1.233736	3.168524	0.294442		
6	1.933703	-3.180879	-0.755204		
6	1.938666	-0.233222	-1.428788		
6	-2.335051	2.543500	0.515845		
6	2.213726	3.246373	-1.103372		

6	2.063085	-1.940820	-0.417108	
16				
2682.386332 Kcal/mol 116.319427 eV -97.109023 H				MutI_3_67.log
6	-1.536830	-0.594056	-1.010326	
6	2.566289	-1.441873	-0.578825	
12	0.087527	2.422150	0.249064	
12	1.939917	-1.247682	1.476546	
6	0.273941	-2.196126	-0.699881	
8	3.212009	0.886412	-0.719424	
6	-0.673280	-1.565265	-0.895379	
6	-1.896164	1.589990	-0.601189	
6	-4.664296	-1.429785	1.329956	
6	1.947682	0.752965	1.586745	
6	1.500468	-2.323340	-0.419462	
6	1.968083	1.692291	0.744506	
6	-1.996480	2.804168	-0.228457	
8	-2.456245	0.402441	-1.113886	
6	-5.636499	-1.042398	0.620733	
6	3.084515	-0.313976	-0.855230	
16				
2691.303478 Kcal/mol 116.706112 eV -97.094812 H				Child_5_55.log
6	0.934156	-1.668991	-1.084831	
6	-11.266916	1.286539	0.097059	
12	2.959753	-1.738279	-0.409900	
8	-10.852360	0.525988	0.851074	
8	-0.167589	-1.869919	-0.306673	
6	1.542913	2.859386	-1.419785	
6	-1.322489	-1.318866	-0.706992	
6	3.736208	1.248307	0.703213	
6	2.310436	2.095212	-0.695541	
6	-2.400447	-0.743777	-1.055698	
6	3.988503	2.106330	-0.409647	
6	4.272693	-0.247708	0.225521	
6	-5.644902	-1.185268	-0.042990	
6	2.440005	0.945774	0.174592	
6	3.504566	0.680093	0.559591	
12	3.339517	-0.394282	1.874721	
16				
2733.559909 Kcal/mol 118.538526 eV -97.027472 H				Child_7_49.log
12	-4.305558	0.403285	-0.245297	
8	4.159609	-0.655309	-0.246260	
6	-4.469848	-1.618845	-0.122861	
6	3.304823	-1.735953	-0.170866	
6	-2.425466	0.804179	0.085139	
6	3.678812	0.459720	-0.159171	
6	-3.084432	-1.625614	-0.080533	
6	2.231267	-2.404731	-0.078787	
6	-1.869348	-0.383926	0.101556	
6	3.159532	1.611123	-0.075530	
6	-0.051261	4.283572	-0.553365	
6	1.108812	-2.996111	0.038220	
6	-0.985788	0.914702	0.280537	
6	-0.229557	-3.247297	0.270054	
12	0.150177	2.030006	0.493012	
8	1.797802	1.459758	0.223892	

16
 2768.109353 Kcal/mol 120.036734 eV -96.972414 H Child_3_34.log
 6 -5.789239 -1.670960 0.129760
 6 3.003282 0.645042 -0.793364
 6 -4.498592 -1.520611 -0.169366
 6 3.735529 -0.419255 -0.868198
 12 -2.724953 -0.895152 -0.603989
 12 1.060276 1.129431 -1.301598
 8 4.435571 -1.429409 -0.954964
 6 -1.298246 0.197461 0.703352
 6 -2.607796 1.080601 -0.286782
 6 0.802789 1.738956 1.398794
 6 -2.527555 2.274417 0.622745
 6 -0.257950 1.485174 0.698530
 8 2.158185 -0.973564 1.232714
 6 -0.987359 0.961709 -0.578871
 6 1.043822 -1.335412 0.945523
 6 3.918990 -0.701715 1.638719

16
 2796.356981 Kcal/mol 121.261669 eV -96.927399 H Child_3_60.log
 6 -7.573826 1.217225 0.238287
 12 3.365809 -1.304387 -0.659511
 12 -5.443396 0.807278 0.074091
 6 -3.478602 0.395499 -0.078812
 6 -1.549570 -2.079562 -0.608486
 8 4.264267 3.081228 0.307319
 6 0.928584 -1.159060 -0.156328
 8 -2.298894 0.072936 -0.161133
 6 1.577677 -0.207164 -1.000382
 6 4.009450 2.032334 -0.173478
 6 -0.433633 -1.112975 -0.600257
 6 -1.236993 -0.459326 -0.263201
 6 2.228128 -1.169995 2.374664
 6 3.645909 0.944865 -0.904830
 6 -0.029413 -1.315365 1.142859
 6 3.446964 -0.297811 1.005892

16
 2887.060330 Kcal/mol 125.194943 eV -96.782854 H
 Original3D_0_35.log
 8 -0.593097 -1.069216 0.663458
 6 1.952826 -0.440988 1.751831
 8 -0.165509 1.164074 0.029759
 6 -2.160850 -0.691477 0.909094
 6 2.648291 -0.578893 0.405578
 6 -0.559474 1.431547 -1.003893
 6 -2.799760 -0.948103 -0.181491
 6 -1.302820 -1.046587 1.932670
 6 3.369835 -0.041746 1.348986
 12 -2.564898 1.475054 -0.061016
 6 -2.072283 -2.921541 -1.343232
 6 2.308779 -0.382647 -0.985336
 6 -2.495255 4.260855 -0.028774
 12 4.293957 0.546880 -0.588886
 6 1.633813 -0.604084 -1.770274
 6 -2.969745 -2.206681 -0.659645

16
 2984.118610 Kcal/mol 129.403794 eV -96.628181 H MutI_8_77.log
 8 1.232942 1.397163 0.492112
 12 7.001334 -2.253813 -0.577216
 6 -0.872120 -1.541039 0.913320
 6 3.794325 3.924325 -0.167694
 6 -3.579604 0.880631 -0.316814
 6 2.104931 2.124938 0.218686
 8 -4.174874 -1.444398 -0.251948
 6 -5.787522 0.076637 -0.721816
 6 5.165475 -2.352226 0.186886
 6 -4.517519 -0.154694 -0.434929
 6 -0.246938 -0.650460 0.495287
 6 -0.206172 0.781315 0.078066
 6 2.972212 3.004196 0.038573
 12 -2.586730 -2.407861 0.306879
 6 -1.286791 1.925712 0.038032
 6 -2.446909 1.366991 -0.107140

16
 2988.859415 Kcal/mol 129.609375 eV -96.620626 H
 Original3D_12_3.log

6 2.021271 0.296730 -2.051166
 6 2.428547 0.499833 -0.691636
 6 0.882163 0.868316 -2.216524
 6 3.060164 0.995717 -0.104937
 12 0.190399 0.189996 -0.285561
 8 2.482384 -1.386203 1.163854
 6 -2.297662 2.171749 0.202473
 6 3.372406 1.969377 0.928542
 8 -3.083152 2.575097 -1.041394
 6 -0.635826 -2.693736 -0.576769
 6 2.536667 -1.355292 -0.050240
 6 -2.365500 0.894357 1.134295
 6 -2.267741 1.641270 2.243157
 6 0.837965 -0.737338 2.471332
 6 -1.079655 -1.932383 0.100839
 12 -3.036286 -2.291892 -0.490761

16
 3029.550347 Kcal/mol 131.373903 eV -96.555781 H MutD_13_58.log

12 -1.742509 0.795377 -1.285267
 8 5.941166 -2.944754 -0.533230
 6 1.335602 0.993452 0.122711
 6 1.034809 0.445078 1.758844
 8 -5.001590 -1.859468 -0.663301
 6 1.672895 3.221939 0.017840
 6 0.650966 2.191018 0.235550
 6 -0.167398 -1.458171 1.198469
 6 -2.168769 -1.353543 -0.228075
 6 -2.508633 1.165434 -1.052677
 6 -3.520431 -1.368732 -0.034625
 6 7.220549 -2.974551 -0.188397
 6 5.395984 4.141911 -0.696493
 6 -1.144328 -1.906823 0.576879
 6 -2.031836 -0.017908 -0.834709
 12 -1.768581 0.867885 1.645295

16
 3043.984709 Kcal/mol 131.999837 eV -96.532779 H MutI_15_59.log
 6 4.711963 1.750826 0.000000
 6 -1.852963 0.342119 0.000000
 12 -3.039684 2.628111 0.000000
 6 3.201679 1.189535 0.000000
 6 -4.076098 4.265959 0.000000
 6 -3.014039 -0.605944 0.000000
 6 2.994613 -0.261350 0.000000
 6 -0.415801 -4.660027 0.000000
 6 4.607309 0.258754 0.000000
 8 4.860117 -0.984548 0.000000
 6 -3.363879 0.523266 0.000000
 6 0.909145 3.225836 0.000000
 8 -0.229584 -3.487968 0.000000
 6 0.132896 -1.764872 0.000000
 12 -1.964752 -2.172512 0.000000
 6 0.000000 0.788053 0.000000

16
 3049.496874 Kcal/mol 132.238867 eV -96.523994 H Child_14_15.log
 8 -9.533817 -2.416464 -0.956777
 6 4.953233 -0.382002 -0.826894
 6 -0.772562 6.059183 -0.293080
 6 3.628152 -0.905696 -0.570449
 6 -2.284188 2.422688 0.390833
 6 1.650522 -2.135792 -1.411155
 6 -2.606683 -0.946922 2.316493
 6 4.178173 0.006716 0.333389
 6 -1.468989 3.653995 -0.455694
 6 2.304441 -1.399466 -0.450678
 6 -0.545889 4.953504 -0.885909
 8 0.108007 -2.117187 -0.496009
 6 -1.969645 -1.904791 -0.311056
 6 3.349764 0.336347 1.363504
 12 2.633169 -1.593449 0.081710
 12 -1.557460 -0.262999 1.287161

16
 3107.465823 Kcal/mol 134.752642 eV -96.431615 H Child_2_19.log
 8 -8.992162 -2.491788 -0.004933
 6 0.888674 3.255769 -0.818592
 6 -9.076872 -2.332650 -1.127881
 6 4.854356 -0.654256 -1.436889
 6 1.695872 -1.572955 1.186945
 6 -0.184389 2.445508 -0.652740
 12 3.374675 -2.605679 0.709561
 6 1.125447 1.795605 -0.494372
 6 -2.903087 2.153401 2.277279
 8 5.937538 -0.817598 -0.002744
 6 1.317253 -0.594355 0.619744
 6 -1.464659 1.809144 -0.569298
 6 1.390626 0.659206 -0.270681
 12 -1.322367 1.835863 0.882773
 6 -2.376990 1.020832 -1.075127
 6 4.701984 -2.033101 -0.812819

3148.777607 Kcal/mol 136.544093 eV -96.365780 H MutI_3_69.log

6	1.251510	4.500573	-0.157730
8	-0.497468	1.645477	-0.254635
12	3.194210	-3.618198	0.248153
6	5.162312	-0.813743	0.154633
12	-4.889594	-3.551405	0.044232
6	-3.983587	1.300607	-0.034411
6	3.967339	-1.916692	0.045986
6	-1.574790	1.999125	-0.051074
6	2.994219	-0.836081	-0.122092
6	-4.646791	-1.467430	-0.132063
6	-2.762306	2.453777	0.162167
6	2.251063	0.284670	-0.257239
6	3.653907	0.436256	-0.335367
6	-4.202222	-0.116164	0.084802
6	0.489997	5.286142	0.657762
8	1.090056	0.775647	-0.195473

16

3192.809528 Kcal/mol 138.453500 eV -96.295611 H Child_1_41.log

6	-4.715323	0.775644	1.349446
12	5.053758	-1.305458	0.263232
6	-4.079722	-0.041400	0.640177
6	3.472058	-3.783884	0.264846
6	-3.946838	-1.145452	-0.027962
8	3.254196	-0.805612	0.176267
8	-3.798011	-2.257517	-0.698466
6	3.701495	0.909218	0.147264
12	-1.052848	1.398281	-0.256530
6	0.683241	4.555320	-0.411260
6	-1.529754	-0.623971	-0.020033
6	1.865520	3.781205	-0.205027
6	0.450849	3.394388	0.056559
6	-0.137617	-0.710723	-0.295630
6	-2.593867	-1.284876	-0.046313
6	-0.446777	-1.926942	-0.769207

16

3325.703292 Kcal/mol 144.216326 eV -96.083831 H

Original3D_10_3.log

12	2.731002	1.059734	0.173104
6	5.443019	1.054004	0.357158
8	0.748969	-0.389116	-0.664437
6	-0.728493	-0.342861	-0.934485
6	1.107397	3.810365	0.072369
6	-0.503946	-2.600562	0.168505
6	-1.172240	-1.709299	-0.810627
6	-2.422424	2.197502	-0.090043
12	-2.927833	-0.697355	-0.588309
6	-3.256728	2.768667	-0.077442
6	-3.232574	3.958905	0.603642
6	0.647436	-2.890555	-0.705019
8	0.093171	-1.813758	1.351430
6	1.113382	-1.623206	0.168135
6	-2.737643	-2.596144	1.489020
6	5.013623	0.185592	-0.326792

16

3438.846845 Kcal/mol 149.122701 eV -95.903525 H MutD_14_74.log

6	-4.097834	-0.362011	0.325017
6	5.432380	0.326351	-0.427997
12	-3.099671	1.050247	-1.166283
6	7.915220	-0.690837	1.668488
6	-0.861398	0.415965	-1.002569
6	1.745916	0.059134	-0.763600
6	-3.006673	4.437737	0.970597
6	-3.699475	-2.560366	0.668804
8	6.502251	-0.094050	0.074129
12	-1.593869	-2.046023	-0.143805
6	-2.929913	-3.535467	0.843289
8	-2.324796	3.530728	1.112544
6	2.928908	0.345535	-0.642072
6	0.349126	0.097128	-0.705517
6	4.208657	0.238463	-0.422750
6	-4.167775	-1.362319	0.526254

16

3503.404449 Kcal/mol 151.922187 eV -95.800646 H MutD_15_62.log

6	-4.000014	0.367945	-0.684519
6	-2.996779	-2.731076	0.512121
8	2.615363	3.030662	0.049737
6	2.415784	3.773046	1.300668
6	4.458995	-2.147647	-0.573138
6	-2.930983	0.206732	0.014973
12	1.325374	1.396534	-0.342763
6	-1.799045	-1.910752	0.861570
6	-1.839591	1.012578	-0.273376
12	0.192097	-1.421586	0.515986
6	2.061018	-0.521055	0.133668
6	-0.711698	1.455986	-0.426339
6	3.121622	-1.144247	-0.152049
6	-2.825591	-1.138877	0.556439
6	5.552855	-2.298204	-0.698867
8	-5.271500	0.813594	-0.737935

16

3682.598018 Kcal/mol 159.692766 eV -95.515083 H

Original3D_0_37.log

6	-2.142495	-1.208232	-0.814380
6	-1.560337	-1.094223	0.076826
8	-4.418245	-0.585548	-1.162548
6	-4.287452	0.572073	-0.462129
12	0.177880	-0.260494	1.091223
12	3.465704	0.450271	1.151813
8	4.120419	-1.794545	-0.606145
6	1.795431	2.836866	-0.824598
6	2.877338	-1.360238	-0.758758
6	1.234494	2.795611	-1.549484
6	2.588182	2.736207	0.151676
6	3.295918	-2.077957	-1.770695
6	-4.475856	1.287907	0.345342
6	-2.979839	-0.698422	-1.833257
6	-1.264302	-2.270775	2.937428
6	-1.971148	1.275087	2.374214

16

3687.093438 Kcal/mol 159.887706 eV -95.507919 H Child_4_23.log

6	8.364755	-0.020391	-0.393908
6	-6.045806	-2.970580	-0.860204
6	7.059237	-0.136966	-0.315234
6	-3.528865	2.873414	-0.108471
6	5.727001	-0.253044	-0.216559
8	-4.692996	2.706184	-0.779827
6	4.483224	-0.149307	-0.100280
6	-4.818918	-2.500760	-0.278708
8	3.229074	-0.551116	0.011896
12	-1.158090	1.636839	0.546174
6	2.216863	0.382276	-0.035874
6	-3.784558	-2.174085	0.179303
6	0.977441	-0.185079	0.197769
6	-2.850136	2.975437	0.258483
6	-0.290712	-0.296772	0.391696
12	-1.620725	-1.845622	0.606774

16

3738.800678 Kcal/mol 162.129947 eV -95.425518 H Child_4_31.log

6	4.030980	-1.102668	-0.026716
6	-2.586781	3.689847	-0.436927
12	3.673458	0.846410	0.336790
6	-1.184945	3.625800	-0.400672
6	2.828357	-1.442305	-0.223549
6	-2.743908	-1.524626	-0.137706
6	1.966913	2.085528	0.403144
8	-1.246103	2.284618	-0.341016
12	0.820719	-1.577454	-0.383883
6	-2.808745	-2.952363	-0.066680
6	0.916922	1.422525	0.070230
6	-0.644122	-2.350356	0.705208
6	-1.301110	-1.371156	-0.235141
6	0.009435	0.599180	-0.376633
6	-1.497736	-3.440613	-0.244905
8	-3.234106	0.882854	1.139415

16

3750.522143 Kcal/mol 162.638238 eV -95.406839 H

Original3D_0_76.log

6	-1.451735	0.682994	-0.582532
6	1.151887	-0.135830	-0.853677
6	0.708985	-1.738658	0.950617
6	0.588702	0.885234	0.124806
12	-3.238748	0.358506	-1.047982
6	1.305264	2.689929	0.511379
6	2.272781	-1.312301	1.122066
6	1.960250	-1.771714	-0.534183
6	-0.362676	1.397926	-0.978271
8	-1.699197	-1.937627	0.199222
8	1.752744	3.976021	0.841582
6	-4.109727	1.109258	1.905054
12	-0.351421	-1.002744	-0.419704
6	0.270539	-2.576342	1.851914
6	2.579134	-0.127191	-0.212217
6	2.195537	-0.532688	-1.757325

16

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3821.173729 Kcal/mol 165.701985 eV -95.294248 H      Child_18_29.log
6      -4.272285   2.817355   -0.062639
6      3.296128    -0.191712  -0.194421
12     -1.605730    1.346222  -0.273650
12     1.333382    -2.279299 -0.364995
6      0.318257    3.259674  -0.459051
6      1.860651    -0.719601 -0.218319
6      -1.709544   -1.408313 -1.328870
6      3.074631    1.301487  -0.119138
6      0.753135    1.983323  -0.583971
6      -0.562372   -2.761205 -0.092916
6      1.372436    0.769678  0.026167
6      -2.274297   -2.576669 1.042920
6      -0.607503   -1.105479 0.146351
8      -0.466378   -0.044774 0.780854
6      -2.095737   -1.513978 0.201842
8      1.509775    1.553470  1.408647
16
3862.482975 Kcal/mol 167.493326 eV -95.228418 H      Child_2_47.log
6      -1.233909   -0.803200 -2.056787
8      -2.010392   -3.478892  1.610161
6      -0.395071   -0.261296 -1.284468
6      -1.674380   -3.137057  0.603030
12     -3.071653    -0.257261 -1.213299
6      0.499345    1.281902  0.647413
8      4.384119    -0.024392 -0.667735
6      10.004982   -0.084564  1.108754
12     2.520498    1.040491  -0.125966
6      -3.599720    1.552982  1.254685
6      0.662348    0.278948  -0.550706
6      -2.112701    1.572360  1.163450
6      -4.790368    0.630374  -0.310980
6      -0.780707    1.546388  1.123747
6      5.278375    -0.774577 -0.696504
6      -3.920851    1.302323  0.420326
16
3922.148501 Kcal/mol 170.080671 eV -95.133334 H      MutD_16_64.log
6      -3.562097    0.764948  -1.114586
6      -2.255755    0.502178  0.925527
6      8.196406     0.049807  -0.277971
6      -3.906939    -1.140145 -1.830241
12     -1.465194     4.126101  0.300960
6      -3.869563    -1.415620 -1.331935
6      -0.314572    -0.196580 0.883571
6      -2.730190    -3.272398 0.100775
6      5.033003     -0.320947 0.095356
8      -6.561459    -0.635893 2.325120
6      -3.373398    -2.437116 -0.659691
8      3.824940     -0.338721 0.353136
6      6.245654     -0.296372 -0.153881
12     1.612462     -0.583492 0.752345
6      -3.639391    2.236455  -1.909257
6      7.531001     -0.259944 -0.405283
16
4212.502980 Kcal/mol 182.671649 eV -94.670625 H      Child_12_58.log

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8	-3.323962	4.386967	-0.053086
6	-2.456464	-2.742687	-0.102671
6	-2.875317	3.267600	-0.003294
6	-3.554283	-2.381050	-0.297132
6	8.751568	1.306628	-0.265474
6	-1.097354	-2.820510	0.078112
8	9.876812	1.081435	-0.183274
6	-4.686086	-1.607454	-0.670770
6	-1.882754	2.294798	0.082827
6	0.079923	-2.573168	0.153356
6	-3.304643	1.770207	-0.090813
6	1.157658	-2.173885	-0.310341
12	-0.252976	0.964120	0.427381
6	-3.864298	0.628827	-0.169883
6	3.388055	-1.042538	-0.526331
12	1.056408	-1.573106	0.791400

16

4410.929288 Kcal/mol 191.276239 eV -94.354412 H

Original3D_3_7.log

12	-2.318762	-1.103864	0.441226
8	0.114747	-0.163159	-0.340901
8	2.389433	-0.758991	-0.907766
6	-5.577931	-0.868167	0.687631
6	0.524779	-0.008111	-1.474189
6	0.963611	2.055868	0.158305
6	3.162864	1.454281	-0.849410
6	2.978138	-1.840036	-0.753995
6	1.191360	0.858808	1.412528
6	-5.167697	0.553381	0.797453
6	4.677258	0.717842	-0.273832
6	-6.764853	-0.491406	-0.793909
6	-5.089376	1.752898	-0.225521
6	0.293840	-2.860134	-0.121800
6	0.350049	3.092188	-0.174378
12	4.878289	-0.490075	1.196778

16

4540.637253 Kcal/mol 196.900915 eV -94.147709 H

Child_18_12.log

12	2.583443	-1.579931	-0.271422
6	-1.869913	4.468520	-1.377423
6	0.469326	-1.619197	-0.489183
12	-0.975522	1.226776	1.980429
6	-1.070381	-2.119452	-0.691713
6	-2.512316	-0.910965	1.014064
6	3.870376	0.150620	0.091326
8	-0.292031	0.171866	0.236711
8	2.582356	0.443078	-0.001389
6	-2.962593	-0.886373	-0.302208
6	0.061693	-0.301538	-0.389707
6	2.222085	2.149758	-0.986831
6	-1.394485	-0.808742	-0.562641
6	1.084250	-0.428861	0.948818
6	-4.607700	-0.979005	-0.874286
6	0.440050	1.171619	-0.111995

16

4559.434909 Kcal/mol 197.716060 eV -94.117753 H

MutD_15_46.log

12	0.059729	-0.777857	-0.819948
6	6.194117	-0.241591	0.959174
12	-4.541288	-2.169182	0.073215
6	-2.394603	-2.708660	-0.119885
8	-3.336571	4.090765	-0.111927
6	-4.896945	1.635106	0.708315
8	4.242623	1.247610	-0.970995
6	-4.401095	2.730474	0.283181
6	5.938135	0.383389	0.605149
6	7.653117	-0.796496	2.322052
6	5.140953	0.822872	-0.150880
6	3.202778	0.454444	-1.294624
6	-0.861862	-2.653773	-0.681200
6	-5.033216	0.326073	0.867018
6	-5.016586	-0.921224	0.989422
6	2.230257	-0.254370	-1.550361

16

4582.458127 Kcal/mol 198.714442 eV -94.081063 H

Original3D_6_3.log

12	-0.212099	-1.205666	1.029637
6	2.113136	0.809379	0.285714
6	4.326135	0.387727	0.523361
8	-1.237320	1.815151	0.187400
6	2.484329	-1.263653	-0.250288
6	3.100170	0.120937	-0.391521
8	0.760821	-2.288501	-1.465921
6	1.220585	-1.354204	-1.105836
12	-2.689119	3.294146	-0.489254
6	-2.844951	-2.009059	0.083738
6	-3.673989	-0.986604	-0.945841
6	-3.328877	-2.084781	-0.847156
6	-0.954389	2.159724	0.677749
6	0.544392	0.386965	-1.505594
6	-1.330492	-1.267169	3.971459
6	4.781718	1.554912	0.128145

16

4708.837298 Kcal/mol 204.194769 eV -93.879665 H

Child_1_15.log

6	4.603185	-2.008149	-0.175238
6	-2.469759	3.119593	-0.538948
6	3.303650	-2.343924	-0.137539
6	-1.554017	2.945213	-0.168572
6	2.116781	-1.532709	-0.052919
8	-1.056107	1.557335	-0.112719
6	4.090503	-0.696502	-0.114102
6	-1.940607	0.563750	-0.688754
6	0.846898	-1.143054	0.013012
6	3.207205	3.426464	1.060141
8	-3.904856	-2.806001	0.173345
6	-4.307674	-0.095367	0.573842
6	2.924633	-0.079655	0.007315
6	-3.053948	0.146632	0.047402
12	-2.350769	-1.868875	0.160935
12	1.774654	1.550173	-0.114173

16

4824.591406 Kcal/mol 209.214348 eV -93.695199 H

MutI_15_63.log

6	2.695219	-0.165933	0.000000	
12	-4.754963	4.280691	-0.000000	
6	-0.000000	1.241673	-0.000000	
6	-3.549820	2.768384	-0.000000	
6	-1.688692	1.105419	-0.000000	
6	-2.012323	-0.210245	-0.000000	
6	-5.696764	5.795363	-0.000000	
6	0.738377	-2.509034	0.000000	
8	-2.772467	1.888058	-0.000000	
6	6.671661	-4.246114	0.000000	
6	-0.546488	-2.188372	0.000000	
8	2.162022	0.846254	-0.000000	
12	3.873106	-3.159912	0.000000	
6	2.015323	-2.341214	0.000000	
6	-1.511951	-1.372155	0.000000	
6	5.463102	-3.765080	0.000000	
16				
4970.142458 Kcal/mol 215.526047 eV -93.463248 H				Child_6_20.log
8	7.126982	3.026852	-0.210775	
12	-3.869291	-2.052693	-0.260612	
6	6.242401	3.618244	-0.639682	
6	-2.065851	-2.800650	-0.134225	
6	-3.289049	5.020639	0.696572	
6	-4.632853	-0.158365	-0.556543	
6	5.825734	-2.496945	0.205943	
6	-0.860511	-2.524631	-0.051822	
6	-2.660871	3.912947	0.264954	
6	-3.981633	1.178302	-0.380973	
6	4.593471	-2.257458	0.316777	
6	-3.134920	2.236044	-0.405368	
6	3.408709	-1.630189	0.405759	
12	0.846349	-1.734277	-0.090826	
6	2.421997	-0.955104	0.380981	
8	-3.992537	0.296478	0.661152	
16				
5006.781613 Kcal/mol 217.114874 eV -93.404860 H				MutI_18_57.log
6	-2.037527	-1.700250	0.189123	
6	0.762062	1.574615	-0.954566	
6	-1.386344	0.674900	-0.458776	
6	0.323693	-1.309494	-0.052234	
8	-4.278752	-0.217168	0.859877	
6	-3.253568	-1.936427	0.490730	
8	-0.946899	-0.908619	-0.070942	
6	-6.715423	1.533293	0.085356	
6	-0.566330	1.482248	-0.848157	
12	-3.051273	0.713396	-0.038698	
6	5.138969	1.898492	1.016191	
12	4.562272	-1.840054	-0.058276	
6	1.652665	-1.599295	-0.143853	
6	4.816371	3.179793	1.052449	
6	3.183501	-1.774896	-0.221683	
6	2.027469	1.731385	-1.012548	
16				
5104.058026 Kcal/mol 221.333183 eV -93.249840 H				Child_6_51.log
6	2.993301	1.387152	0.252139	

12	-4.571264	-0.889951	-0.031728		
6	3.558146	0.250405	0.004472		
6	-4.006445	1.050693	-0.515299		
6	4.361891	-1.176661	-0.313487		
6	-2.834296	1.482061	-0.550068		
6	2.031451	2.179480	0.439190		
12	-2.283494	-2.449525	0.491175		
6	-1.498448	1.708404	-0.526552		
6	2.821509	-0.973749	-0.261380		
6	-0.335693	-1.845557	0.417728		
6	-1.017687	4.228251	0.916717		
6	-0.262295	1.678945	-0.457694		
8	1.586469	-1.196126	-0.299774		
6	0.542363	-0.996007	0.214034		
8	3.930321	-0.524723	-0.104246		
16					
5250.375688 Kcal/mol 227.678126 eV -93.016668 H MutI_13_37.log					
6	4.176618	1.886361	-0.072950		
6	-1.455932	-1.313625	-0.248570		
8	0.051332	-0.926347	-0.446618		
6	-7.194714	1.293828	-0.017406		
6	4.779953	-2.565860	0.714387		
6	-0.636865	-2.364927	-0.350546		
6	3.989651	3.146028	0.165321		
8	1.116281	-0.097506	0.169435		
6	4.158754	-0.377407	-0.772511		
12	-4.167061	0.408867	0.109702		
6	-0.291327	-3.668425	0.661919		
6	-2.496228	-0.503330	-0.000823		
6	3.460763	4.297201	0.433020		
12	-5.513124	0.821178	0.014123		
6	5.079492	-1.556581	-0.089930		
6	4.233388	0.631785	-0.299986		
16					
5348.234475 Kcal/mol 231.921690 eV -92.860720 H Child_14_14.log					
8	6.023967	-0.659689	0.702553		
6	-7.307325	0.533646	1.507216		
6	4.829980	-0.500514	0.389822		
8	-5.870077	-0.224901	0.095707		
6	3.556640	-0.994948	0.099344		
6	-4.767130	-0.325097	-0.145763		
6	2.462314	-1.772642	-0.095181		
6	-3.715870	-0.339264	-0.464229		
6	3.711976	0.418115	0.171689		
6	-2.211028	-0.436832	-0.811659		
6	1.215859	-2.136215	-0.190387		
6	-0.887642	0.123233	-0.901332		
6	3.034031	1.397153	0.157788		
6	0.312617	0.197201	-0.736876		
12	2.017731	2.591986	-0.193973		
12	-2.237536	-0.084177	0.171584		
16					
5571.369854 Kcal/mol 241.597768 eV -92.505131 H MutI_13_53.log					
8	0.086686	-1.952863	-0.941399		
6	-3.480916	2.167034	-0.672693		

12	0.348737	1.340778	-0.087973
6	-2.100517	0.563079	1.019363
6	-1.780644	-2.501429	0.369232
6	8.582983	0.262318	0.607953
6	-3.271077	0.180448	1.688388
6	-2.784496	-2.350224	1.139048
6	-0.882906	-1.553839	-0.149927
6	1.907809	0.723140	-1.235746
8	-4.511813	1.841037	-1.373678
6	9.803964	0.176398	0.906067
6	-1.240065	-0.128259	0.352792
6	-3.262887	-1.151532	1.612894
12	1.614245	-1.099116	-1.755000
6	0.482958	3.278645	1.135344

16

5638.031889 Kcal/mol 244.488511 eV -92.398898 H

Original3D_17_6.log

6	-4.010723	-0.117744	0.790270
6	-4.064188	0.176499	-0.961837
6	-4.277833	1.327810	0.397093
6	-1.203986	1.214177	-0.531272
6	-0.331230	0.206301	-0.518333
12	2.010363	-0.000031	-0.650184
6	-3.162836	-1.097379	0.485648
6	-1.207037	2.478610	-0.396833
8	2.310134	-2.912466	-1.551076
6	-5.415599	0.498616	0.130957
6	-3.962478	-1.425651	-0.701700
8	0.101893	-0.780087	1.379889
6	1.369301	-1.311870	1.898668
12	4.520199	-0.063547	0.971252
6	5.008945	1.052086	-1.030168
6	4.980503	2.049105	0.023620

16

6651.493749 Kcal/mol 288.436432 eV -90.783843 H

Child_10_28.log

6	-5.797448	-1.067650	-0.212284
6	3.596345	0.548308	-0.307869
12	-3.881095	0.092996	-0.365542
6	3.452180	-0.764873	-0.310156
6	-1.313474	2.398729	0.798109
6	3.210338	1.758759	-0.277244
6	0.004444	-0.625693	1.213271
6	2.734878	-1.806641	-0.343576
6	0.981897	-1.311498	1.705732
6	2.284611	2.692663	-0.211917
6	-1.894021	-0.725830	-0.377658
8	1.849722	-2.704728	-0.366103
8	-1.862028	2.195049	-0.114940
6	1.156328	3.338589	-0.143929
6	-0.878635	-0.145451	0.120420
12	0.120577	-1.897915	-0.140211

16

6684.982840 Kcal/mol 289.888658 eV -90.730474 H

Original1D_0_2.log

6	0.000000	0.000000	-9.752148
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6	0.000000	0.000000	-8.478796
12	0.000000	0.000000	-7.013548
6	0.000000	0.000000	-11.074450
6	0.000000	0.000000	-4.442061
8	0.000000	0.000000	-3.131038
6	0.000000	0.000000	-1.827251
6	0.000000	0.000000	-0.494015
6	0.000000	0.000000	0.805852
8	0.000000	0.000000	2.142076
6	0.000000	0.000000	3.456504
6	0.000000	0.000000	4.736830
6	0.000000	0.000000	6.083547
6	0.000000	0.000000	7.343737
12	0.000000	0.000000	8.811932
6	0.000000	0.000000	11.364099
16			
6967.118943 Kcal/mol 302.123253 eV -90.280861 H MutI_6_67.log			
6	-6.643827	3.251745	0.812957
6	-1.978159	-1.084783	-0.485274
6	-7.511597	-2.563115	0.069557
6	5.073856	-2.551573	0.792400
6	4.192101	4.030877	-0.547407
12	0.938803	0.784655	-0.897023
8	5.282985	-3.568036	1.168604
6	4.692475	0.084933	-0.042127
6	2.735940	1.762545	-0.214786
6	5.013634	-1.187926	0.401215
6	-0.904931	-0.386724	-0.617380
12	-5.174666	-2.751443	-0.420099
6	3.800353	1.184812	-0.065535
6	-3.101672	-1.733652	-0.495322
6	3.694286	2.875279	-0.246768
8	-5.726035	3.756406	1.285931
16			
7274.851817 Kcal/mol 315.467830 eV -89.790458 H			
OriginalID_0_1.log			
8	0.000000	0.000000	-6.804192
8	0.000000	0.000000	-8.165177
6	0.000000	0.000000	-9.506002
6	0.000000	0.000000	-10.795947
6	0.000000	0.000000	-5.508607
6	0.000000	0.000000	-4.233727
6	0.000000	0.000000	-2.892916
6	0.000000	0.000000	-1.630861
12	0.000000	0.000000	-0.166601
6	0.000000	0.000000	2.402788
6	0.000000	0.000000	3.707385
6	0.000000	0.000000	5.027270
6	0.000000	0.000000	6.336532
6	0.000000	0.000000	7.611261
12	0.000000	0.000000	9.076004
6	0.000000	0.000000	11.623175
16			
7748.879703 Kcal/mol 336.023651 eV -89.035045 H MutI_14_73.log			
6	-0.079093	-2.897314	-0.134037

6	-4.659159	2.175200	0.020653		
6	-3.546978	-2.372803	-0.421097		
6	-1.040077	-2.069957	0.064851		
6	-4.353941	0.063980	0.186653		
12	6.161143	0.961027	0.475760		
6	-2.143522	1.555759	-0.060151		
6	-3.545135	1.319792	0.025445		
6	-2.118897	-1.261823	0.175624		
6	2.991724	0.114716	-0.155359		
6	-3.545897	-1.113460	0.097491		
12	1.824284	-1.811434	0.163092		
8	1.650327	0.157081	-0.217714		
8	-5.591229	2.887712	0.018871		
6	7.571926	2.259788	-0.568726		
6	3.752730	-0.132787	-0.243929		
16					
8355.321673 Kcal/mol 362.321497 eV -88.068618 H MutD_1_72.log					
6	1.126964	2.101533	-1.681929		
6	-0.221785	-0.160851	-0.962064		
6	-0.073405	-1.124146	1.521355		
8	-0.882367	-0.265866	2.246160		
12	2.844807	-2.028266	0.990458		
6	-1.791898	-2.029175	0.150801		
6	-2.776002	-0.095798	-1.847659		
8	-0.674992	-2.329980	-0.699620		
6	-1.078504	0.395573	-1.889482		
6	-2.077787	-0.735978	-0.422074		
6	2.548687	1.015056	-1.390347		
6	-0.822766	-0.983660	-1.230147		
6	-2.890361	3.030649	1.894883		
6	3.368201	1.479880	-0.410672		
6	2.270690	1.667029	0.389960		
12	-0.597584	1.478774	0.917203		
16					
8632.377436 Kcal/mol 374.335787 eV -87.627101 H MutD_2_78.log					
8	2.388915	1.294035	0.925394		
6	0.695756	3.296034	-1.330564		
6	0.718050	-0.617380	0.082733		
12	-4.065296	-0.191031	1.329382		
12	-3.293507	-1.013236	-1.467572		
6	0.785302	-2.940955	-0.205490		
6	-0.481156	-3.174228	-0.342740		
8	-1.205600	0.929816	-0.104942		
6	1.497537	-1.754899	-0.055778		
6	2.581642	1.287673	-0.119080		
6	2.864496	-1.124205	-0.185932		
6	2.742248	0.036006	-0.921755		
6	-0.272997	0.164285	0.015518		
6	-3.766547	2.759737	1.045966		
6	3.859884	-1.004292	2.049889		
6	1.915637	2.515624	-0.850321		
16					
10241.170539 Kcal/mol 444.099747 eV -85.063324 H Child_2_37.log					
6	-4.251322	-0.729929	-0.527340		
12	3.880566	-1.654259	1.363207		

6	-2.978649	-0.870262	-0.609523	
8	3.394070	0.200665	-0.566971	
12	-3.198408	0.197743	1.455759	
6	2.102373	-0.378023	1.034296	
6	-1.554076	-0.826175	-0.588330	
6	2.058444	0.217757	-0.202021	
8	0.233160	3.924460	-0.963279	
6	-0.441711	-0.560911	-1.288512	
6	-1.676660	1.233862	2.728554	
6	0.570621	-0.010782	-2.190064	
6	-0.635940	-0.632332	0.412520	
6	-0.913590	-4.037429	-1.298272	
6	0.772437	3.373761	-0.093674	
6	0.747448	0.633329	-0.975232	
16				
10402.779092	Kcal/mol	451.107766	eV	-84.805784 H Child_2_62.log
6	8.394469	0.719837	-0.364906	
12	-4.697645	-2.058419	-0.158519	
6	7.148471	0.398953	-0.275250	
6	-2.620989	-1.599112	-0.069931	
6	5.895806	0.114764	-0.213142	
6	0.054738	-1.738699	-0.100640	
6	4.671742	-0.124237	-0.153799	
6	-3.415268	-0.358987	0.133366	
6	3.417143	-0.192164	-0.057240	
8	-1.302133	-1.218551	-0.029083	
12	-1.216738	1.126066	0.705573	
6	-3.373722	1.099549	0.355449	
6	2.197037	-0.138353	0.085778	
6	0.323598	1.680601	0.429864	
6	0.832014	-0.217442	0.285009	
8	-7.470073	2.883550	-0.832414	
16				
11579.273498	Kcal/mol	502.125456	eV	-82.930920 H Child_8_25.log
6	1.611518	-3.166600	-0.244155	
6	0.518771	2.981781	-0.054884	
6	0.681608	-2.265285	-0.160108	
6	-0.816625	2.870596	-0.012464	
6	2.265903	-1.737346	-0.169658	
6	1.747948	2.736879	-0.108283	
12	4.419012	-0.716012	0.532057	
6	-1.978680	2.392065	0.007738	
6	-0.515379	-1.513177	-0.075885	
6	2.908132	2.111014	-0.169004	
6	2.311430	-0.443285	-0.101461	
12	-3.095716	0.540611	0.000210	
6	-1.737097	-1.260841	-0.135702	
6	3.583533	0.990862	-0.160678	
8	-7.549196	-0.207919	0.261498	
8	-2.371545	-2.301476	-0.021493	
16				
12033.187622	Kcal/mol	521.809060	eV	-82.207561 H MutI_18_37.log
6	-5.375702	-1.932019	-0.272600	
6	1.231346	-0.113279	0.482386	
6	-5.841096	-0.697197	-0.233115	

6	-4.095391	-1.879504	-0.131087	
6	6.140899	0.263330	0.110772	
6	9.591273	-0.039958	-0.711537	
6	-3.490528	2.304179	-0.118869	
6	5.015175	0.188400	0.158005	
12	8.044528	0.031276	-0.108432	
6	-4.228525	0.281385	0.579182	
6	-6.413643	0.472945	-0.122854	
8	-2.985561	-1.895242	-0.066341	
6	3.820874	0.123537	0.267954	
6	2.610129	0.063613	0.391925	
12	-5.199277	2.011339	-0.215827	
8	-0.505924	-0.445252	0.252608	
16				
12208.670167	Kcal/mol	529.418713	eV	-81.927912 H Child_3_17.log
12	-4.284311	-1.807482	0.168965	
12	3.988847	0.302564	-0.510930	
6	-3.175052	-0.259250	-0.424268	
8	3.988787	-1.571467	0.010386	
8	-0.018110	4.057156	1.305548	
6	2.279025	1.297948	-0.509811	
6	-2.314527	-1.211684	0.101928	
6	2.774103	-1.875672	0.212501	
6	-2.256748	2.178757	-1.156095	
6	1.220149	1.083683	0.086294	
6	-0.405303	0.499333	0.476002	
6	1.535609	-1.987622	0.347744	
6	-2.780128	1.018959	-0.647531	
6	0.254510	-1.691063	0.411432	
6	-0.869763	-1.004206	0.325874	
6	-0.965180	1.646401	-0.294718	
16				
22726.870256	Kcal/mol	985.531614	eV	-65.166080 H MutI_17_71.log
6	-1.361118	1.959846	0.638201	
6	-0.934977	-0.389240	-0.033655	
6	1.557113	3.071286	-1.243599	
6	6.661897	-0.693789	-0.175698	
6	-2.949981	-1.682898	-0.766722	
6	-1.683232	0.756267	0.492105	
12	5.459481	-1.072430	1.237786	
8	-3.426701	0.887253	1.060593	
6	1.748064	-0.336697	0.218982	
6	-5.482736	-1.101117	-0.169023	
6	-4.196439	-1.669002	-0.688186	
6	0.460258	-0.419378	-0.079399	
12	0.348083	2.273343	-0.229416	
6	-5.915685	-0.416427	0.437988	
6	7.260948	-0.729458	-1.231922	
8	-1.657728	-1.450666	-0.622452	