

Electronic supplementary information for
Aromatic character and relative stability of neo-confused porphyrin
tautomers and related compounds.

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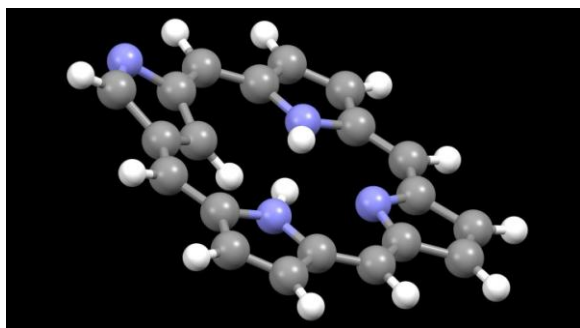
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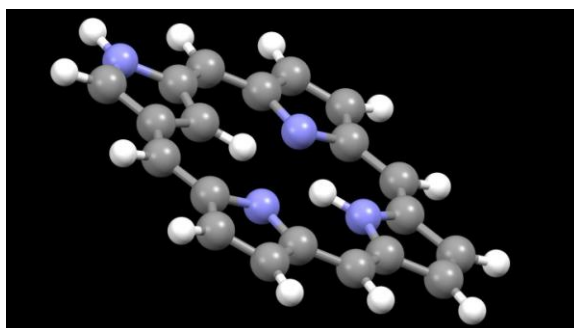
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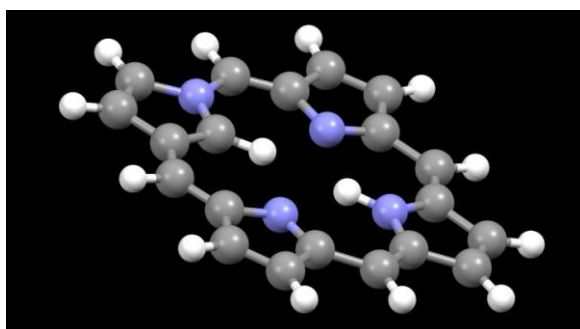
2-5	Selected conformations of N-confused porphyrin, neo-confused porphyrin, benzo-neo-confused porphyrin, benzoporphyrin and benzocarbaporphyrin tautomers (Figures S1-S4)
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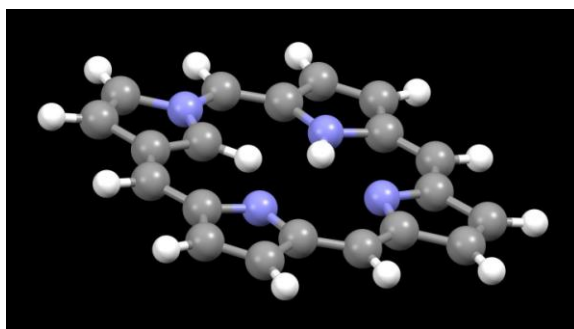
NCP-22,24-H



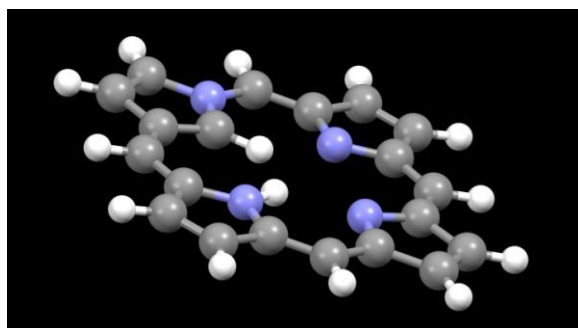
NCP-2,23-H



neo-CP-23-H

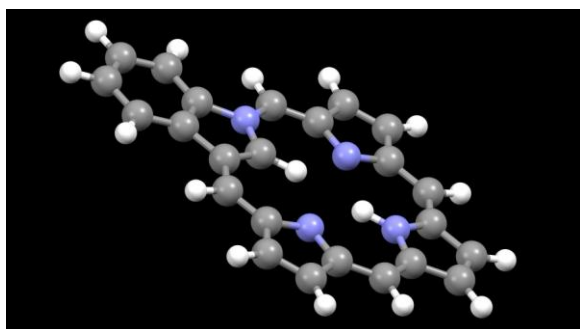


neo-CP-24-H

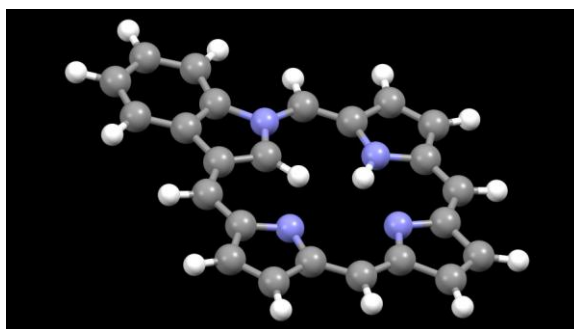


neo-CP-22-H

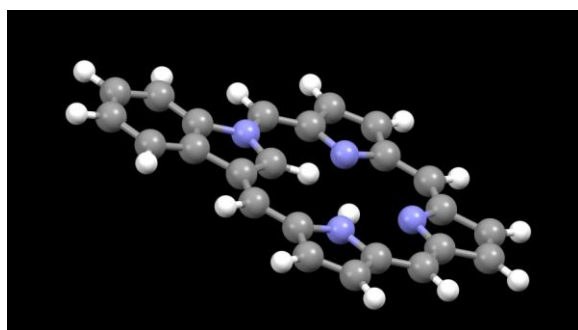
Figure S1. Mercury 3.1 renderings of the minimized conformations for selected N-confused porphyrins and neo-confused porphyrins.



B-neo-CP-23-H

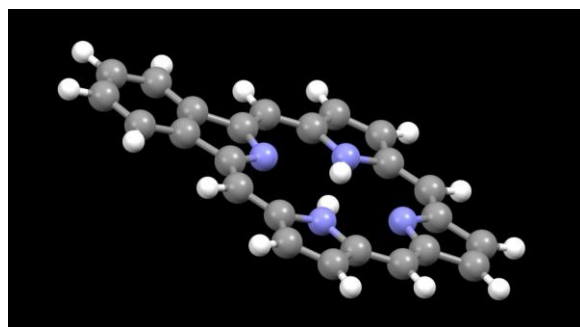


B-neo-CP-24-H

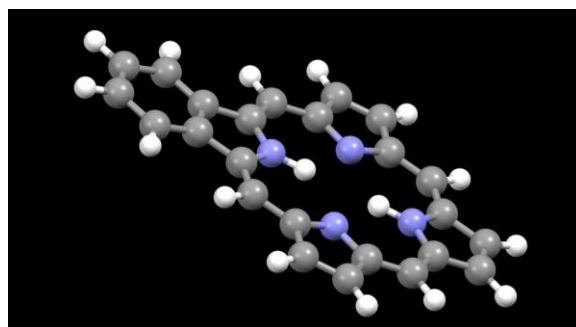


B-neo-CP-22-H

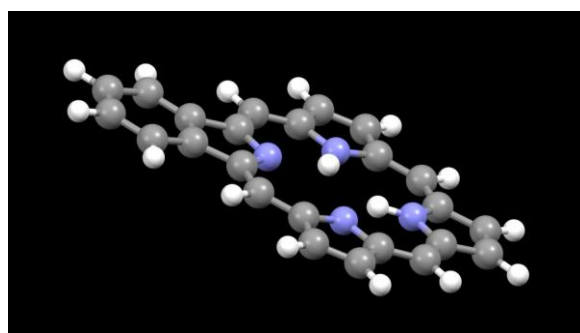
Figure S2. Mercury 3.1 renderings of the minimized conformations for selected benzo-neo-confused porphyrins.



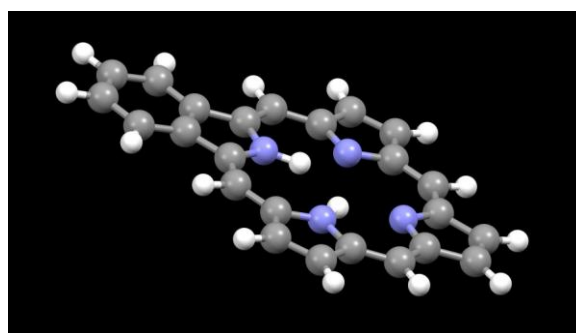
BP-22,24-H



BP-21,23-H

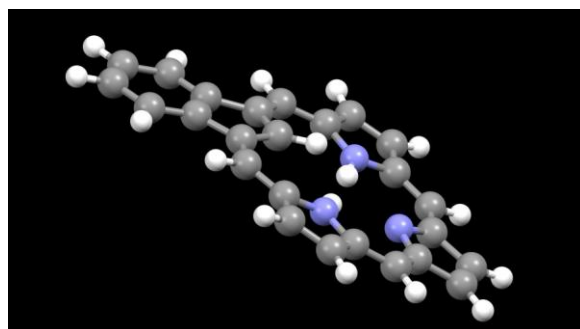


BP-22,23-H

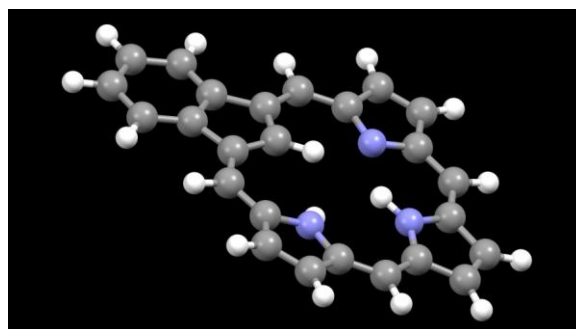


BP-21,22-H

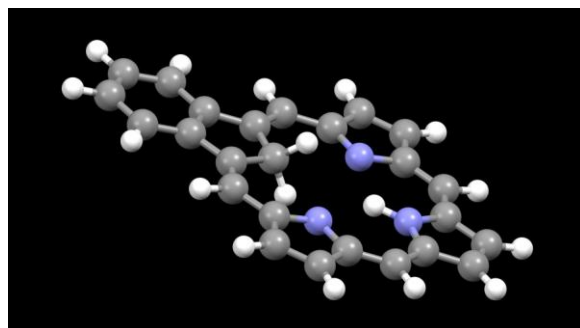
Figure S3. Mercury 3.1 renderings of the minimized conformations for selected benzoporphyrins.



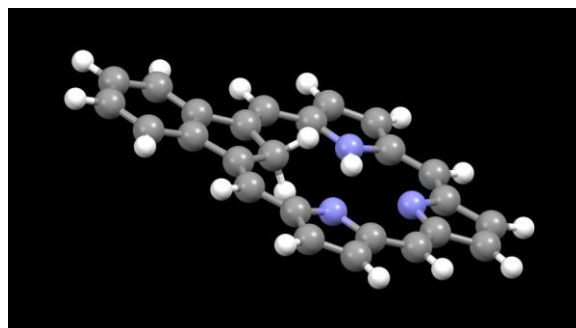
BCP-22,24-H



BCP-22,23-H



BCP-21,23-H



BCP-21,22-H

Figure S4. Mercury 3.1 renderings of the minimized conformations for selected benzocarbaporphyrins.

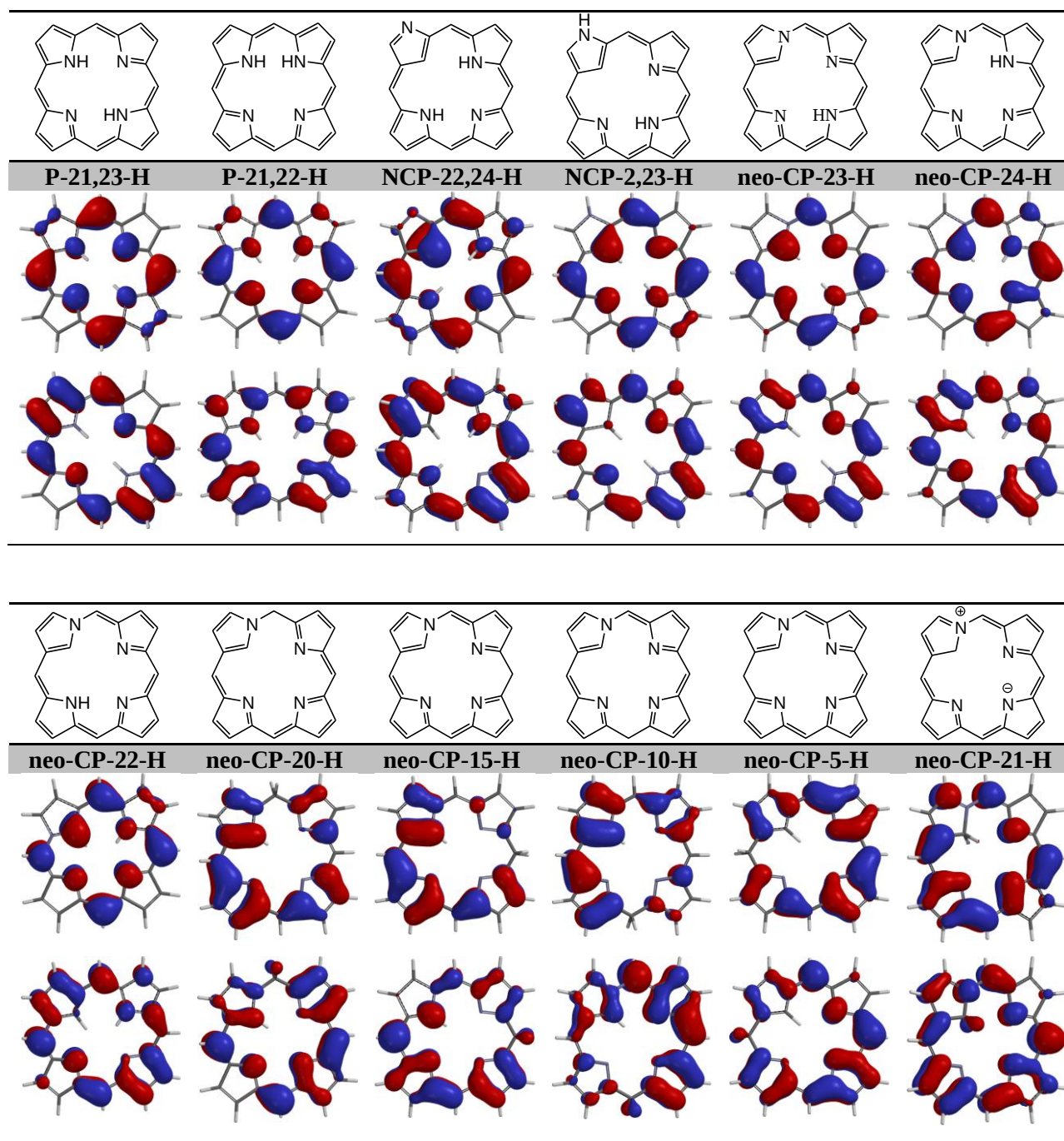


Figure S5. HOMO and LUMO surfaces for porphyrin, N-confused porphyrin and neo-confused porphyrin tautomers.

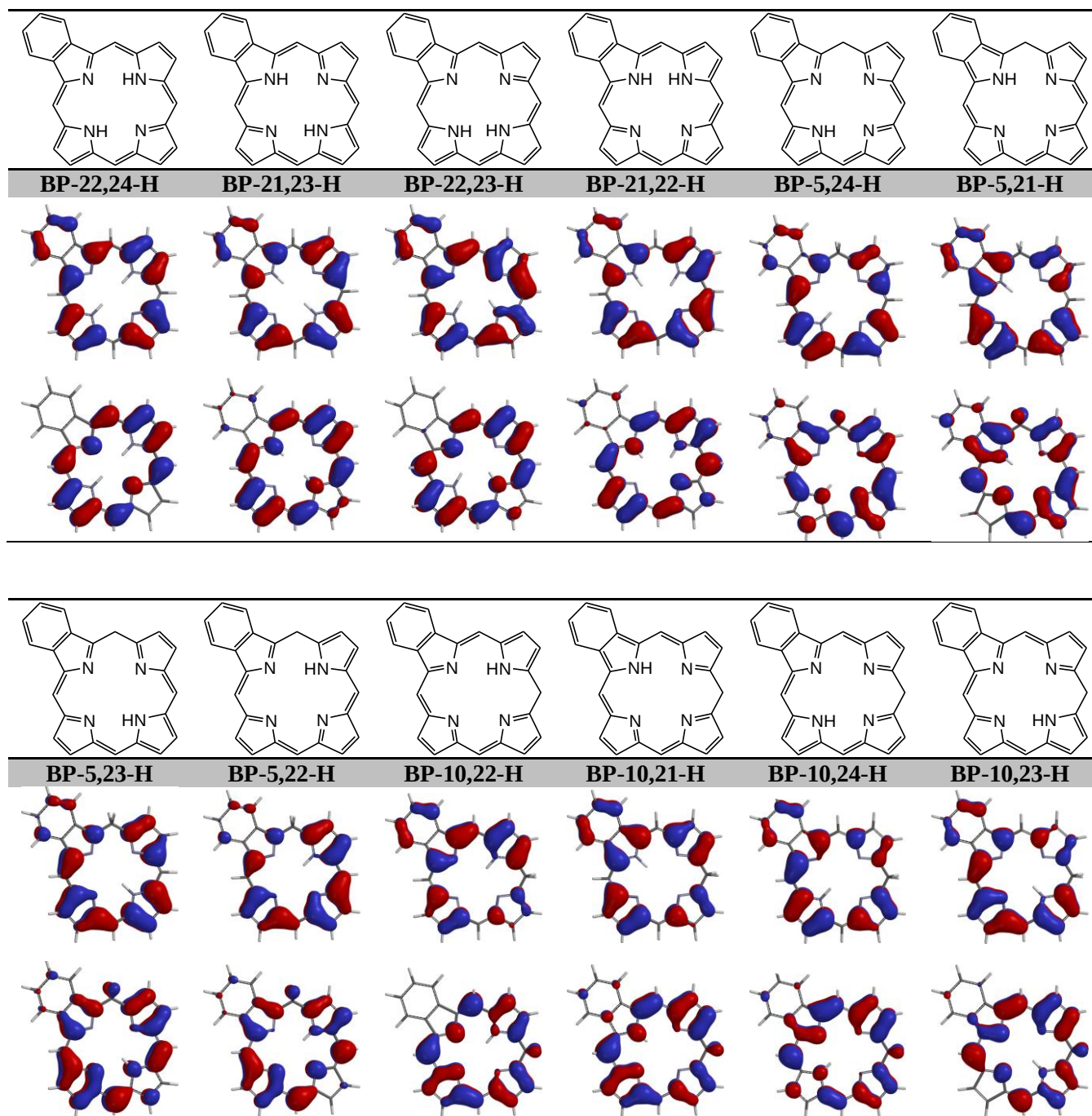


Figure S6. HOMO and LUMO surfaces for benzoporphyrin tautomers.

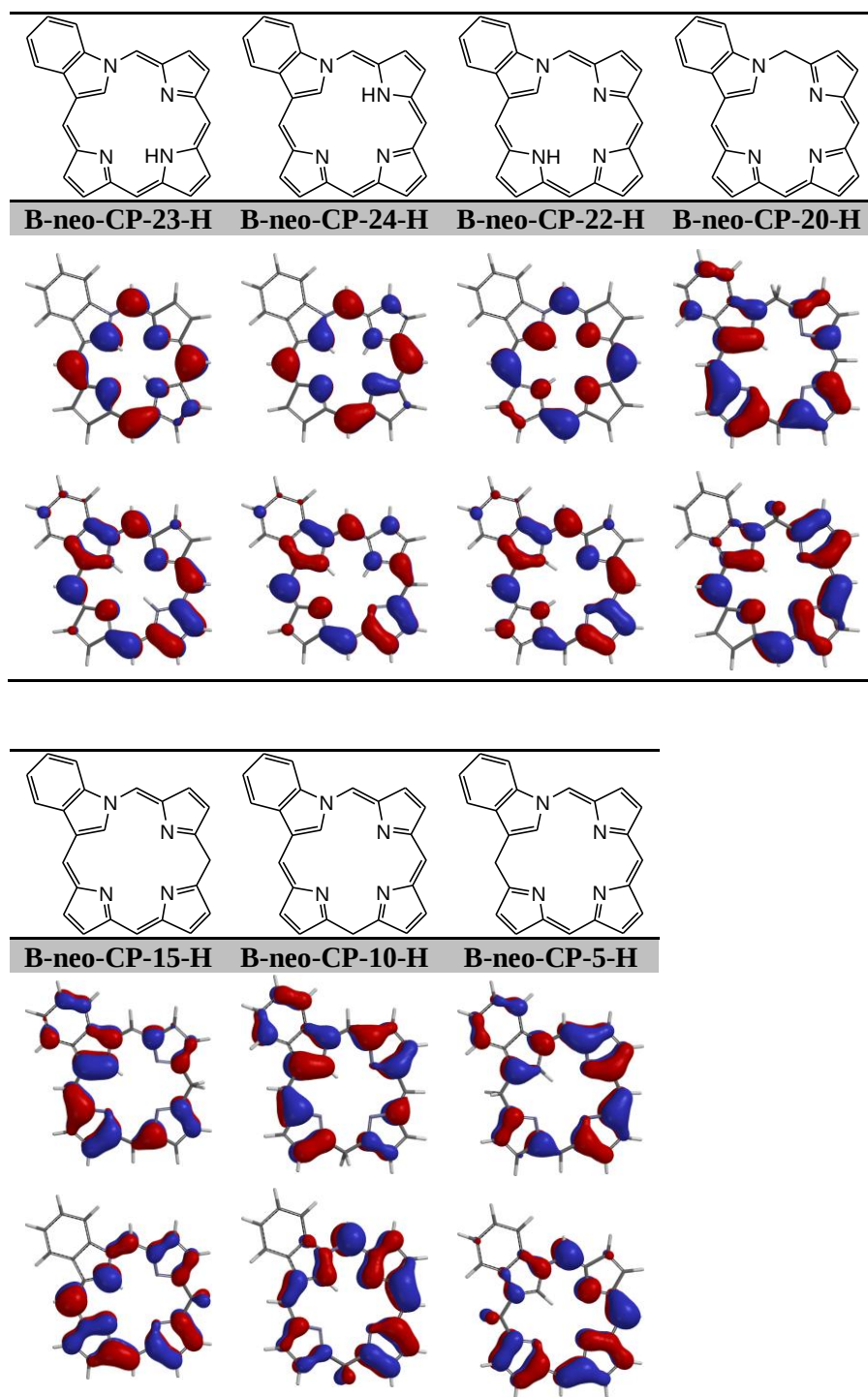


Figure S7. HOMO and LUMO surfaces for benzo-neo-confused porphyrin tautomers.

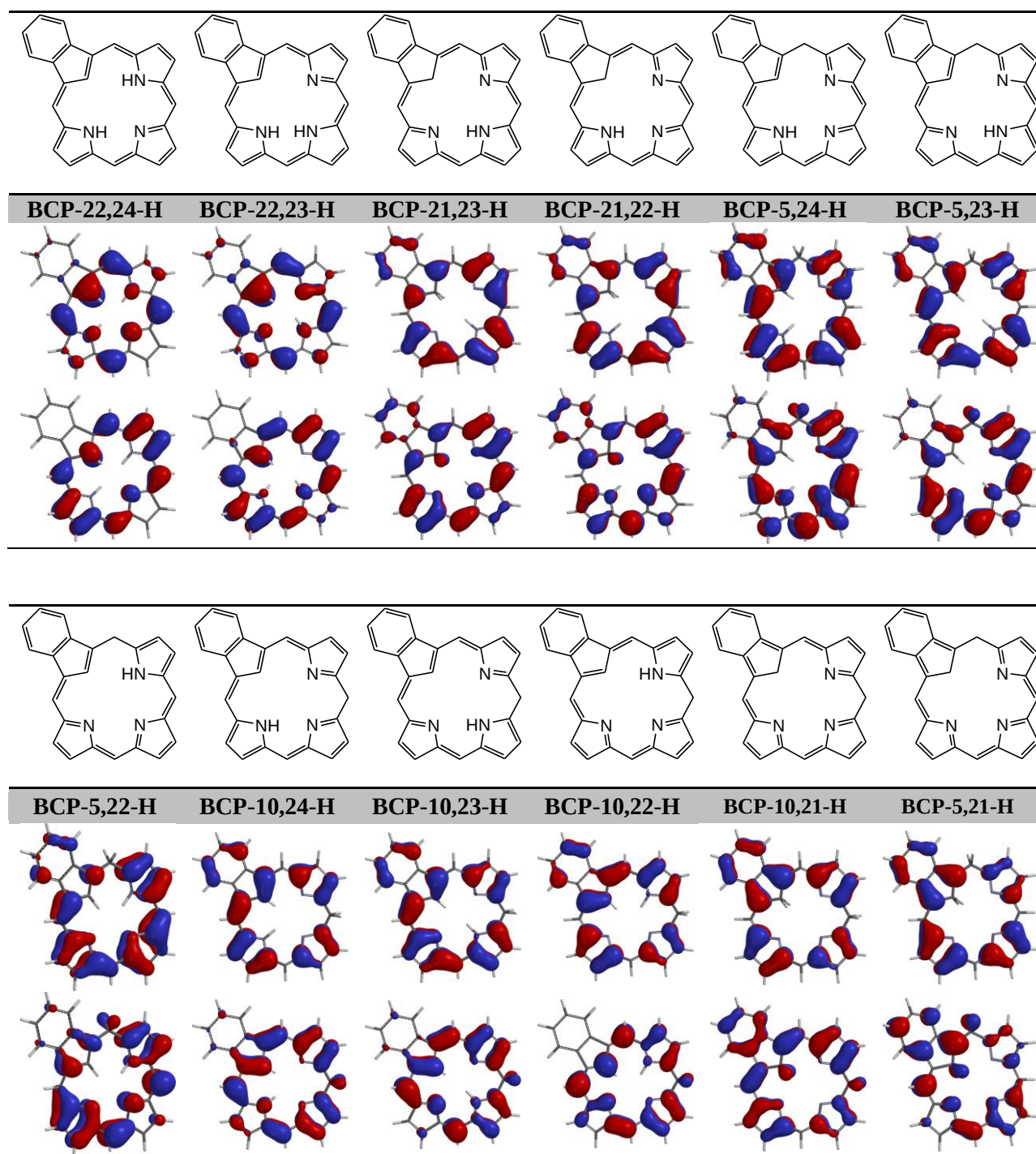


Figure S8. HOMO and LUMO surfaces for benzocarba porphyrin tautomers.

Cartesian Coordinates

The following pages contain Cartesian coordinates for all of the N-confused porphyrin, neo-confused porphyrin, benzo-neo-confused porphyrin, benzoporphyrin and benzocarbaporphyrin tautomers examined in this study.

P-21,23-H				P-21,22-H			
	X	Y	Z		X	Y	Z
C1	-4.25760	0.00000	0.67327	C1	4.02716	1.70357	-0.00730
C2	-4.25758	0.00000	-0.68171	C2	3.22684	2.79847	-0.00515
C3	-2.85655	0.00000	-1.08959	C3	1.84716	2.30869	-0.00239
N4	-2.03490	0.00000	-0.00421	N4	1.83015	0.95307	-0.00252
C5	-2.85656	0.00000	1.08116	C5	3.13011	0.55446	-0.00553
C6	0.68532	0.00000	4.24986	C6	1.66543	-3.91029	-0.00449
C7	-0.68532	0.00000	4.24986	C7	2.87517	-3.26681	-0.00625
C8	-1.12914	0.00000	2.88666	C8	2.62016	-1.85979	-0.00559
N9	0.00000	0.00000	2.10837	N9	1.25234	-1.70038	-0.00370
C10	1.12914	0.00000	2.88666	C10	0.62371	-2.92116	-0.00240
C11	-2.43947	0.00000	2.41593	C11	3.51462	-0.79220	-0.00651
C12	4.25758	0.00000	-0.68171	C12	-4.02093	-1.65994	0.00727
C13	4.25760	0.00000	0.67327	C13	-3.22010	-2.77220	0.00545
C14	2.85656	0.00000	1.08116	C14	-1.84836	-2.34543	0.00256
N15	2.03490	0.00000	-0.00421	N15	-1.87292	-0.97284	0.00269
C16	2.85655	0.00000	-1.08959	C16	-3.16984	-0.51048	0.00543
C17	2.43947	0.00000	2.41593	C17	-0.74327	-3.19589	0.00026
C18	-0.68532	0.00000	-4.25826	C18	-1.64939	3.93431	0.00383
C19	0.68532	0.00000	-4.25826	C19	-2.85134	3.30649	0.00576
C20	1.12914	0.00000	-2.89506	C20	-2.55534	1.87944	0.00514
N21	0.00000	0.00000	-2.11676	N21	-1.21282	1.66120	0.00327
C22	-1.12914	0.00000	-2.89506	C22	-0.62857	2.88499	0.00217
C23	-2.43945	0.00000	-2.42435	C23	0.74210	3.16730	-0.00019
C24	2.43945	0.00000	-2.42435	C24	-3.49757	0.84309	0.00603
H25	-5.10567	0.00000	1.34322	H25	5.10714	1.66263	-0.00972
H26	-5.10566	0.00000	-1.35166	H26	3.52095	3.83872	-0.00551
H27	1.34419	0.00000	5.10496	H27	1.48792	-4.97514	-0.00427
H28	-1.34419	0.00000	5.10496	H28	3.85839	-3.71234	-0.00774
H29	0.00000	0.00000	1.09466	H29	0.88911	-0.74043	-0.00326
H30	-3.21482	0.00000	3.17387	H30	4.57189	-1.02945	-0.00790
H31	5.10566	0.00000	-1.35166	H31	-5.09984	-1.62579	0.00958
H32	5.10567	0.00000	1.34322	H32	-3.53169	-3.80598	0.00606
H33	3.21482	0.00000	3.17387	H33	-1.12232	-0.27291	0.00129
H34	-1.34423	0.00000	-5.11333	H34	-0.99009	-4.25135	0.00068
H35	1.34423	0.00000	-5.11333	H35	-1.45320	4.99727	0.00357
H36	0.00000	0.00000	-1.10305	H36	-3.83824	3.74702	0.00731
H37	-3.21479	0.00000	-3.18230	H37	0.98919	4.22498	-0.00052
H38	3.21479	0.00000	-3.18230	H38	-4.55005	1.10087	0.00731

NCP-22,24-H				NCP-2,23-H			
	X	Y	Z		X	Y	Z
C1	4.37545	-0.12379	-0.10103	C1	4.22921	-1.21253	0.00322
C2	4.19237	1.23712	-0.09797	C2	4.38183	0.13366	0.00139
C3	2.78309	1.49351	-0.06667	C3	3.02734	0.69729	0.00242
N4	2.16781	0.27149	-0.07377	N4	2.10211	-0.26734	0.00510
C5	3.08933	-0.75602	-0.08192	C5	2.78842	-1.46703	0.00540
N6	-0.17827	-4.20190	0.36171	N6	-1.19228	-3.99846	0.00319
C7	1.10871	-4.01963	0.34508	C7	0.14169	-4.20672	0.00290
C8	1.49004	-2.65488	-0.04755	C8	0.79169	-2.95456	0.00769
C9	0.26430	-2.02590	-0.31022	C9	-0.23464	-1.98432	0.01130
C10	-0.74820	-2.95827	-0.02045	C10	-1.46396	-2.61643	0.00784
C11	2.78334	-2.11512	-0.03545	C11	2.19944	-2.71450	0.00649
C12	-4.36984	0.09813	-0.07814	C12	-4.20611	1.22527	0.00300
C13	-4.18652	-1.26486	-0.06616	C13	-4.38201	-0.11949	0.00445
C14	-2.78152	-1.53364	-0.03928	C14	-3.04471	-0.71023	0.00581
N15	-2.16383	-0.30077	-0.03815	N15	-2.09229	0.28279	0.00519
C16	-3.07984	0.71561	-0.04733	C16	-2.75752	1.44572	0.00332
C17	-2.13058	-2.76876	0.01277	C17	-2.76868	-2.06729	0.00674
C18	0.11854	4.23935	0.03745	C18	1.20799	4.09650	-0.00243
C19	-1.22306	4.06171	0.03902	C19	-0.14110	4.27429	-0.00220
C20	-1.45031	2.62109	0.00961	C20	-0.77163	2.97341	0.00016
N21	-0.25929	1.94493	-0.00488	N21	0.25295	2.05239	0.00116
C22	0.71247	2.90681	0.00639	C22	1.48173	2.67658	-0.00028
C23	2.09946	2.70801	-0.02339	C23	2.73056	2.08433	0.00023
C24	-2.73557	2.06862	-0.01485	C24	-2.13078	2.71559	0.00113
H25	5.31401	-0.65690	-0.12363	H25	5.00115	-1.96970	0.00309
H26	4.95507	2.00104	-0.10968	H26	5.30270	0.70006	-0.00071
H27	1.16686	0.19972	0.04329	H27	-1.88902	-4.72695	-0.00087
H28	1.79937	-4.80657	0.63050	H28	0.55416	-5.20464	-0.00106
H29	0.12682	-1.08335	-0.80969	H29	-0.09252	-0.92918	0.01605
H30	3.62570	-2.79016	0.07611	H30	2.86158	-3.57512	0.00542
H31	-5.30718	0.63279	-0.10082	H31	-4.96423	1.99610	0.00157
H32	-4.94998	-2.02805	-0.08562	H32	-5.31359	-0.66828	0.00464
H33	-1.18051	-0.10477	0.08675	H33	-3.61514	-2.74806	0.00578
H34	-2.74969	-3.64788	0.15095	H34	1.97317	4.85851	-0.00379
H35	0.67124	5.16794	0.05214	H35	-0.68282	5.20828	-0.00336
H36	-1.99820	4.81479	0.05472	H36	0.11465	1.04966	0.00169
H37	2.71497	3.59994	-0.01491	H37	3.57279	2.76703	-0.00138
H38	-3.56214	2.76977	-0.01038	H38	-2.77665	3.58617	-0.00010

neo-CP-23-H				neo-CP-24-H			
	X	Y	Z		X	Y	Z
C1	4.18062	-1.22718	0.00309	C1	3.44933	2.74814	-0.00607
C2	4.35879	0.11751	0.00201	C2	2.40105	3.61018	-0.02009
C3	3.01844	0.70236	0.00220	C3	1.18830	2.78171	-0.01635
N4	2.07135	-0.25305	0.00344	N4	1.50298	1.48243	-0.00103
C5	2.73749	-1.45228	0.00387	C5	2.86740	1.40659	0.00613
C6	-1.24919	-4.05386	0.00505	C6	2.58633	-3.31863	0.05939
C7	0.08882	-4.26763	0.00549	C7	3.56741	-2.38232	0.05273
C8	0.74683	-2.96890	0.00502	C8	2.93346	-1.07681	0.03460
C9	-0.26769	-2.01956	0.00514	C9	1.56007	-1.31226	0.02963
N10	-1.47383	-2.65582	0.00501	N10	1.33544	-2.65604	0.04455
C11	2.13558	-2.70426	0.00455	C11	3.55184	0.19690	0.02339
C12	-4.15058	1.20123	0.00152	C12	-3.40866	-2.69221	0.02431
C13	-4.31415	-0.14395	0.00265	C13	-2.35232	-3.55325	0.03683
C14	-2.96907	-0.71714	0.00359	C14	-1.12884	-2.78036	0.03574
N15	-2.02533	0.28142	0.00318	N15	-1.51908	-1.45478	0.02283
C16	-2.70672	1.44071	0.00185	C16	-2.88877	-1.34892	0.01534
C17	-2.71595	-2.07159	0.00445	C17	0.13247	-3.32398	0.04610
C18	1.23379	4.11541	-0.00186	C18	-2.62911	3.35216	-0.03643
C19	-0.11839	4.28992	-0.00190	C19	-3.60510	2.41477	-0.02892
C20	-0.74224	2.98839	0.00026	C20	-2.91933	1.12282	-0.01163
N21	0.28218	2.07191	0.00146	N21	-1.57758	1.28261	-0.00858
C22	1.50719	2.69921	0.00033	C22	-1.35021	2.63273	-0.02356
C23	2.74975	2.08943	0.00084	C23	-0.12936	3.29764	-0.02720
C24	-2.10137	2.71546	0.00061	C24	-3.55860	-0.13413	-0.00027
H25	4.93732	-1.99946	0.00328	H25	4.50460	2.98283	-0.00400
H26	5.28907	0.66796	0.00113	H26	2.42935	4.69096	-0.03198
H27	-2.08381	-4.73570	0.00483	H27	2.62446	-4.39543	0.07312
H28	0.57444	-5.23163	0.00571	H28	4.62861	-2.57950	0.06078
H29	-0.21381	-0.95428	0.00516	H29	0.80450	-0.55361	0.01586
H30	2.80295	-3.56102	0.00455	H30	4.63707	0.23159	0.02891
H31	-4.91730	1.96328	0.00056	H31	-4.45855	-2.94299	0.02185
H32	-5.23943	-0.70281	0.00276	H32	-2.38516	-4.63255	0.04609
H33	-3.54195	-2.77013	0.00458	H33	-0.98121	-0.58320	0.01522
H34	1.99641	4.87991	-0.00312	H34	0.21832	-4.40095	0.05683
H35	-0.66232	5.22252	-0.00322	H35	-2.73761	4.42763	-0.04968
H36	0.15711	1.06665	0.00263	H36	-4.67596	2.56108	-0.03453
H37	3.60380	2.75724	-0.00006	H37	-0.19960	4.38146	-0.04016
H38	-2.75918	3.57679	-0.00032	H38	-4.64137	-0.16057	-0.00451

neo-CP-22-H				neo-CP-20-H			
	X	Y	Z		X	Y	Z
C1	-2.76786	-3.30995	0.00734	C1	3.62843	-2.52634	-0.00182
C2	-3.71139	-2.32193	0.02112	C2	4.20504	-1.29357	-0.00339
C3	-3.02560	-1.05814	0.02010	C3	3.10246	-0.33086	0.00005
N4	-1.68340	-1.33622	0.00557	N4	1.92099	-0.95329	0.00348
C5	-1.46158	-2.70038	-0.00302	C5	2.19002	-2.28905	0.00251
C6	3.31996	-2.65451	-0.05594	C6	-2.43728	-3.42399	0.01655
C7	2.30421	-3.55038	-0.04917	C7	-1.23094	-4.05183	0.01272
C8	1.05146	-2.80751	-0.02993	C8	-0.21260	-3.02877	0.00996
C9	1.39918	-1.46076	-0.02540	C9	-0.89080	-1.78856	0.01247
N10	2.76565	-1.35523	-0.04139	N10	-2.21652	-2.03894	0.01643
C11	-0.24809	-3.36599	-0.01881	C11	1.18107	-3.24720	0.00550
C12	2.76469	3.31047	-0.02038	C12	-3.50607	2.57169	0.02150
C13	3.70374	2.33176	-0.03416	C13	-4.13890	1.37029	0.02234
C14	2.96189	1.07051	-0.03156	C14	-3.06686	0.36780	0.01975
N15	1.61584	1.30922	-0.01611	N15	-1.87986	0.90263	0.01745
C16	1.45867	2.63663	-0.00939	C16	-2.07325	2.28506	0.01821
C17	3.50479	-0.19721	-0.04372	C17	-3.34475	-1.10624	0.02027
C18	-3.33823	2.76573	0.03905	C18	2.54990	3.50783	0.00413
C19	-2.27474	3.60031	0.03165	C19	1.33347	4.10703	0.00858
C20	-1.07338	2.75400	0.01613	C20	0.34981	3.01541	0.01077
N21	-1.43156	1.43511	0.01426	N21	0.93567	1.82562	0.00781
C22	-2.78459	1.40940	0.02797	C22	2.28890	2.06613	0.00375
C23	-3.55072	0.23116	0.03092	C23	3.26293	1.08482	0.00024
C24	0.20883	3.29579	0.00577	C24	-1.07157	3.21877	0.01542
H25	-2.93440	-4.37689	0.00403	H25	4.11712	-3.49053	-0.00336
H26	-4.78474	-2.43612	0.03141	H26	5.25925	-1.05364	-0.00657
H27	-1.02762	-0.55414	0.00177	H27	-3.44186	-3.81561	0.01934
H28	4.38951	-2.78635	-0.07006	H28	-1.06874	-5.11882	0.01183
H29	2.40666	-4.62490	-0.05721	H29	-0.49474	-0.78543	0.01177
H30	0.83718	-0.54486	-0.01261	H30	1.50231	-4.28644	0.00435
H31	-0.31775	-4.44857	-0.02370	H31	-3.95198	3.55623	0.02277
H32	2.92481	4.37968	-0.01788	H32	-5.20317	1.17939	0.02439
H33	4.77915	2.44052	-0.04528	H33	-3.96605	-1.33757	-0.85437
H34	4.57670	-0.34107	-0.05690	H34	-3.96043	-1.33784	0.89882
H35	-4.38913	3.01816	0.05083	H35	3.52468	3.97511	0.00133
H36	-2.27393	4.68141	0.03602	H36	1.11207	5.16538	0.01033
H37	-4.62996	0.32401	0.04247	H37	4.29140	1.43719	-0.00269
H38	0.25205	4.38073	0.00982	H38	-1.39252	4.25741	0.01668

neo-CP-15-H				neo-CP-10-H			
	X	Y	Z		X	Y	Z
C1	4.36067	0.80373	0.01799	C1	4.36067	0.80373	0.01799
C2	3.87242	2.07115	0.01748	C2	3.87242	2.07115	0.01748
C3	2.40856	1.94373	0.01235	C3	2.40856	1.94373	0.01235
N4	2.03528	0.67574	0.00983	N4	2.03528	0.67574	0.00983
C5	3.19148	-0.07220	0.01273	C5	3.19148	-0.07220	0.01273
C6	0.72735	-4.15004	0.00867	C6	0.72735	-4.15004	0.00867
C7	2.01840	-3.73543	0.00843	C7	2.01840	-3.73543	0.00843
C8	2.01655	-2.28495	0.00818	C8	2.01655	-2.28495	0.00818
C9	0.68536	-1.88149	0.00828	C9	0.68536	-1.88149	0.00828
N10	-0.10040	-3.00940	0.00876	N10	-0.10040	-3.00940	0.00876
C11	3.17400	-1.44906	0.01076	C11	3.17400	-1.44906	0.01076
C12	-4.26425	-0.86172	0.03243	C12	-4.26425	-0.86172	0.03243
C13	-3.81266	-2.14089	0.03204	C13	-3.81266	-2.14089	0.03204
C14	-2.35581	-2.04206	0.01457	C14	-2.35581	-2.04206	0.01457
N15	-1.96838	-0.70241	0.00270	N15	-1.96838	-0.70241	0.00270
C16	-3.06818	-0.00242	0.01327	C16	-3.06818	-0.00242	0.01327
C17	-1.48166	-3.08379	0.01495	C17	-1.48166	-3.08379	0.01495
C18	-0.70686	4.25820	-0.00947	C18	-0.70686	4.25820	-0.00947
C19	-1.98677	3.82113	-0.01374	C19	-1.98677	3.82113	-0.01374
C20	-1.90817	2.34505	0.00060	C20	-1.90817	2.34505	0.00060
N21	-0.67965	1.91397	0.01156	N21	-0.67965	1.91397	0.01156
C22	0.13262	3.05540	0.00490	C22	0.13262	3.05540	0.00490
C23	1.49863	3.06064	0.00755	C23	1.49863	3.06064	0.00755
C24	-3.14663	1.49520	0.00266	C24	-3.14663	1.49520	0.00266
H25	5.39421	0.48675	0.02186	H25	5.39421	0.48675	0.02186
H26	4.43022	2.99746	0.02081	H26	4.43022	2.99746	0.02081
H27	0.29306	-5.13631	0.00864	H27	0.29306	-5.13631	0.00864
H28	2.88892	-4.37363	0.00819	H28	2.88892	-4.37363	0.00819
H29	0.25143	-0.89438	0.00882	H29	0.25143	-0.89438	0.00882
H30	4.13588	-1.95533	0.01231	H30	4.13588	-1.95533	0.01231
H31	-5.29199	-0.52487	0.04442	H31	-5.29199	-0.52487	0.04442
H32	-4.39240	-3.05294	0.04452	H32	-4.39240	-3.05294	0.04452
H33	-1.86198	-4.09794	0.02217	H33	-1.86198	-4.09794	0.02217
H34	-0.34726	5.27767	-0.01721	H34	-0.34726	5.27767	-0.01721
H35	-2.89195	4.41345	-0.02480	H35	-2.89195	4.41345	-0.02480
H36	1.96966	4.04022	0.00435	H36	1.96966	4.04022	0.00435
H37	-3.76217	1.80389	0.86190	H37	-3.76217	1.80389	0.86190
H38	-3.75593	1.79099	-0.86571	H38	-3.75593	1.79099	-0.86571

neo-CP-5-H				neo-CP-21-H			
	X	Y	Z		X	Y	Z
C1	4.38899	0.40874	0.01329	C1	4.37653	-0.63699	0.00750
C2	4.04202	1.71646	0.01675	C2	4.32663	0.71719	0.00562
C3	2.57419	1.75073	0.00868	C3	2.90167	1.07830	0.00323
N4	2.08048	0.44272	0.00022	N4	2.13386	-0.05064	0.00348
C5	3.11827	-0.34315	0.00284	C5	2.97781	-1.08500	0.00614
C6	0.17626	-4.19295	-0.02662	C6	-0.70024	-4.06719	0.00619
C7	1.50848	-3.93870	-0.01898	C7	0.66523	-4.11410	0.00788
C8	1.69135	-2.49894	-0.01295	C8	1.19010	-2.78992	0.00652
C9	0.45149	-1.92635	-0.01688	C9	0.01429	-1.84940	0.00324
N10	-0.49980	-2.95892	-0.02533	N10	-1.16039	-2.76775	0.00371
C11	3.03968	-1.83943	-0.00391	C11	2.51697	-2.42836	0.00760
C12	-4.35508	-0.29590	-0.03422	C12	-4.29988	0.67686	-0.00184
C13	-4.06509	-1.62481	-0.03826	C13	-4.32841	-0.68321	-0.00098
C14	-2.60918	-1.70497	-0.03109	C14	-2.93014	-1.09731	0.00030
N15	-2.05510	-0.45344	-0.02335	N15	-2.09976	-0.02406	-0.00005
C16	-3.06857	0.40435	-0.02490	C16	-2.88736	1.06241	-0.00120
C17	-1.85655	-2.85939	-0.03181	C17	-2.45629	-2.40439	0.00215
C18	-0.32525	4.30754	0.00378	C18	0.67339	4.23840	-0.00299
C19	-1.64619	4.01582	-0.00387	C19	-0.68015	4.24450	-0.00436
C20	-1.73542	2.54983	-0.00979	C20	-1.08939	2.83258	-0.00098
N21	-0.46993	1.99572	-0.00563	N21	0.00252	2.01627	0.00166
C22	0.37573	3.00921	0.00235	C22	1.07104	2.81994	0.00023
C23	1.81220	2.88370	0.00938	C23	2.41915	2.37887	0.00174
C24	-2.90677	1.82931	-0.01844	C24	-2.40933	2.39479	-0.00185
H25	5.38354	-0.01611	0.01712	H25	5.25063	-1.27311	0.00954
H26	4.69167	2.58026	0.02400	H26	5.15328	1.41406	0.00590
H27	-0.37680	-5.11801	-0.03288	H27	-1.40562	-4.88578	0.00676
H28	2.29079	-4.68351	-0.01781	H28	1.24889	-5.02316	0.01004
H29	0.14310	-0.89546	-0.01460	H29	-0.02524	-1.17713	-0.85520
H30	3.61755	-2.19821	-0.86936	H30	-0.02756	-1.17231	0.85776
H31	3.60954	-2.20570	0.86368	H31	3.26046	-3.21989	0.00980
H32	-5.33266	0.16568	-0.03726	H32	-5.14250	1.35433	-0.00284
H33	-4.75495	-2.45687	-0.04507	H33	-5.19312	-1.33181	-0.00116
H34	-2.36785	-3.81557	-0.03815	H34	-3.16183	-3.22815	0.00283
H35	0.14100	5.28317	0.00968	H35	1.34468	5.08614	-0.00449
H36	-2.48232	4.70090	-0.00542	H36	-1.34492	5.09711	-0.00708
H37	2.35770	3.82375	0.01636	H37	3.17080	3.16371	0.00165
H38	-3.82725	2.40689	-0.02090	H38	-3.17098	3.16996	-0.00363

B-neo-CP-23-H				H39	-4.15887	-3.11506	0.02941
				H40	-3.94488	3.29990	0.00171
				H41	4.55880	2.44347	-0.03024
				H42	6.69534	1.19628	-0.03072
				H43	6.71849	-1.27213	-0.02020
				H44	4.60450	-2.55918	-0.00955
				B-neo-CP-24-H			
					X	Y	Z
	X	Y	Z	C1	-0.20551	-4.37295	-0.00160
C1	-0.31826	-4.30386	0.01369	C2	-1.55958	-4.28722	-0.01138
C2	-1.67367	-4.26823	0.02075	C3	-1.88078	-2.85496	-0.01033
C3	-2.04075	-2.85339	0.01621	N4	-0.76014	-2.11822	-0.00037
N4	-0.94506	-2.06695	0.00676	C5	0.28399	-2.99497	0.00473
C5	0.13035	-2.91339	0.00533	C6	3.33956	0.67094	0.02646
C6	3.38151	0.62249	-0.01993	C7	3.41930	-0.73622	0.02617
C7	3.36847	-0.78632	-0.01419	C8	2.05106	-1.24660	0.01792
C8	1.96606	-1.20665	-0.00824	C9	1.22493	-0.12695	0.01408
C9	1.21497	-0.03985	-0.01046	N10	1.96019	1.02656	0.01885
N10	2.02837	1.06328	-0.01736	C11	1.61617	-2.58858	0.01368
C11	1.46620	-2.52408	-0.00159	C12	-1.51839	4.26202	-0.00079
C12	-1.38421	4.29152	-0.01519	C13	-0.15747	4.16763	0.00754
C13	-0.02961	4.24044	-0.02143	C14	0.20595	2.76954	0.00994
C14	0.32333	2.82303	-0.01771	N15	-0.98278	2.06710	0.00320
N15	-0.80708	2.04767	-0.00989	C16	-2.05491	2.92846	-0.00364
C16	-1.84740	2.90533	-0.00799	C17	1.50727	2.31937	0.01700
C17	1.62843	2.37039	-0.02115	C18	-5.06940	-0.68372	-0.02908
C18	-5.12423	-0.55097	0.02521	C19	-5.14866	0.66780	-0.02754
C19	-5.07484	0.81284	0.01937	C20	-3.76855	1.14907	-0.01703
C20	-3.69083	1.21459	0.00859	N21	-2.89255	0.11753	-0.01245
N21	-2.95346	0.05470	0.00865	C22	-3.64284	-1.02406	-0.01955
C22	-3.77291	-1.04981	0.01852	C23	-3.19546	-2.34265	-0.01861
C23	-3.36629	-2.37522	0.02171	C24	-3.37659	2.50089	-0.01287
C24	-3.20022	2.51203	0.00064	C25	4.46510	1.48405	0.03291
C25	4.55655	1.36053	-0.02592	C26	5.70978	0.85521	0.03942
C26	5.75844	0.65183	-0.02607	C27	5.81279	-0.54154	0.03934
C27	5.76980	-0.74794	-0.02021	C28	4.67527	-1.34487	0.03273
C28	4.58126	-1.47542	-0.01426	H29	0.40685	-5.26384	0.00092
H29	0.32649	-5.17154	0.01425	H30	-2.27758	-5.09562	-0.01844
H30	-2.36451	-5.09951	0.02821				
H31	0.15298	0.08550	-0.00747				
H32	2.19583	-3.32808	-0.00137				
H33	-2.01675	5.16786	-0.01539				
H34	0.66893	5.06537	-0.02761				
H35	2.43191	3.09271	-0.02683				
H36	-6.00236	-1.17899	0.03373				
H37	-5.90556	1.50241	0.02197				
H38	-1.94092	0.00833	0.00229				

H31	0.15317	-0.16587	0.00768
H32	2.37369	-3.36605	0.01691
H33	-2.11393	5.16223	-0.00456
H34	0.55692	4.97743	0.01160
H35	-1.19103	1.06263	0.00080
H36	2.28361	3.06879	0.02129
H37	-5.87973	-1.39932	-0.03588
H38	-6.03354	1.28831	-0.03280
H39	-3.98175	-3.09215	-0.02514
H40	-4.14729	3.26219	-0.01722
H41	4.39920	2.56497	0.03309
H42	6.60913	1.45960	0.04460
H43	6.79408	-1.00183	0.04445
H44	4.76787	-2.42480	0.03265

B-neo-CP-22-H

	X	Y	Z
C1	-0.35556	-4.25799	0.00673
C2	-1.72211	-4.26955	0.01781
C3	-2.17320	-2.90606	0.01416
N4	-1.04950	-2.11647	0.00101
C5	0.09410	-2.88913	-0.00405
C6	3.39948	0.62897	-0.04462
C7	3.33884	-0.77767	-0.03772
C8	1.92293	-1.15393	-0.02546
C9	1.20932	0.03681	-0.02535
N10	2.06481	1.11614	-0.03653
C11	1.41536	-2.46941	-0.01585
C12	-1.36192	4.28769	-0.02197
C13	-0.00512	4.30044	-0.03276
C14	0.40370	2.89718	-0.03070
N15	-0.68899	2.07924	-0.01917
C16	-1.76628	2.87754	-0.01369
C17	1.70736	2.43597	-0.03894
C18	-5.16654	-0.50802	0.02637
C19	-5.03769	0.83873	0.01953
C20	-3.59795	1.12479	0.00711
N21	-2.88940	-0.04217	0.00661
C22	-3.80359	-1.04064	0.01810

C23	-3.47146	-2.40609	0.02200
C24	-3.10296	2.42675	-0.00178
C25	4.59986	1.32573	-0.05705
C26	5.77615	0.57612	-0.06242
C27	5.73959	-0.82336	-0.05542
C28	4.52661	-1.50898	-0.04316
H29	0.30828	-5.10966	0.00586
H30	-2.37393	-5.12989	0.02775
H31	-1.17507	-1.10245	-0.00346
H32	0.15635	0.26035	-0.01799
H33	2.14296	-3.27366	-0.01781
H34	-2.03119	5.13668	-0.01976
H35	0.65380	5.15725	-0.04115
H36	2.52993	3.13647	-0.04780
H37	-6.07383	-1.09536	0.03614
H38	-5.82076	1.58421	0.02234
H39	-4.27867	-3.12885	0.03176
H40	-3.85837	3.20703	0.00091
H41	4.63917	2.40793	-0.06252
H42	6.73133	1.08772	-0.07213
H43	6.66951	-1.38008	-0.05969
H44	4.51271	-2.59292	-0.03785

B-neo-CP-20-H

	X	Y	Z
C1	-0.80530	-4.30587	-0.11277
C2	-2.14907	-4.08935	-0.11027
C3	-2.32503	-2.63768	-0.08548
N4	-1.14324	-2.00974	-0.07425
C5	-0.19328	-2.98317	-0.09004
C6	3.38651	0.22187	-0.02840
C7	3.22174	-1.17850	-0.05264
C8	1.78895	-1.43304	-0.06177
C9	1.16459	-0.16794	-0.04310
N10	2.10493	0.80497	-0.02356
C11	1.17044	-2.69517	-0.08333
C12	-1.00734	4.44419	0.04215
C13	0.34283	4.29413	0.03741
C14	0.56965	2.84645	0.00931

N15	-0.53822	2.16166	-0.00234	C7	3.38183	-0.67549	0.02146
C16	-1.57397	3.09886	0.01741	C8	2.00165	-1.15063	0.02059
C17	1.94818	2.25689	-0.00472	C9	1.19103	-0.02571	0.02474
C18	-5.19058	-0.02649	-0.03249	N10	1.97225	1.11405	0.02813
C19	-5.00102	1.31646	-0.00719	C11	1.58901	-2.51437	0.01628
C20	-3.54591	1.51428	-0.00737	C12	-1.49997	4.26769	0.03781
N21	-2.89218	0.35957	-0.03092	C13	-0.14311	4.27942	0.03793
C22	-3.85210	-0.62153	-0.04699	C14	0.26013	2.87726	0.03368
C23	-3.58577	-1.97906	-0.07278	N15	-0.86476	2.05498	0.03150
C24	-2.91086	2.79961	0.01501	C16	-1.89894	2.85224	0.03374
C25	4.63903	0.82946	-0.01313	C17	1.54468	2.42451	0.03221
C26	5.75512	-0.00417	-0.02244	C18	-5.10775	-0.80874	0.02633
C27	5.61425	-1.39919	-0.04686	C19	-5.13295	0.54346	0.02958
C28	4.35650	-1.99423	-0.06200	C20	-3.71791	0.97189	0.02935
H29	-0.28391	-5.25270	-0.12845	N21	-2.89453	-0.03645	0.02616
H30	-2.94030	-4.82620	-0.12288	C22	-3.69076	-1.18774	0.02420
H31	0.10970	0.06610	-0.04246	C23	-3.22618	-2.47220	0.02050
H32	1.83742	-3.55375	-0.09602	C24	-3.33520	2.42255	0.03249
H33	-1.57181	5.36569	0.06103	C25	4.48629	1.51490	0.02893
H34	1.09836	5.06770	0.05120	C26	5.71346	0.85425	0.02631
H35	2.48734	2.63355	0.87376	C27	5.78049	-0.54529	0.02125
H36	2.47962	2.65589	-0.87830	C28	4.62241	-1.31721	0.01887
H37	-6.12606	-0.56815	-0.04038	H29	0.52099	-5.25115	0.00832
H38	-5.75146	2.09498	0.00946	H30	-2.16828	-5.19885	0.01098
H39	-4.45386	-2.63319	-0.08370	H31	0.11358	0.04656	0.02540
H40	-3.58566	3.65159	0.03262	H32	2.38071	-3.25866	0.01327
H41	4.75696	1.90612	0.00553	H33	-2.16762	5.11840	0.04034
H42	6.74643	0.43357	-0.01099	H34	0.51764	5.13467	0.04047
H43	6.50114	-2.02231	-0.05399	H35	2.34840	3.14833	0.03424
H44	4.26559	-3.07446	-0.08081	H36	-5.94384	-1.49381	0.02547
B-neo-CP-15-H				H37	-5.99768	1.19334	0.03180
	X	Y	Z	H38	-3.98300	-3.25243	0.01935
C1	-0.12906	-4.38762	0.01167	H39	-3.82657	2.89529	0.89736
C2	-1.48634	-4.35975	0.01295	H40	-3.82606	2.89882	-0.83077
C3	-1.86482	-2.94013	0.01779	H41	4.45040	2.59732	0.03289
N4	-0.79848	-2.15631	0.01935	H42	6.62822	1.43515	0.02826
C5	0.29615	-2.98992	0.01572	H43	6.74924	-1.03137	0.01926
C6	3.33717	0.73248	0.02635	H44	4.68889	-2.39927	0.01500

B-neo-CP-10-H			
	X	Y	Z
C1	-0.24981	-4.36531	0.01528
C2	-1.60468	-4.31195	0.01209
C3	-1.95593	-2.88031	0.01716
N4	-0.89810	-2.11832	0.02303
C5	0.20406	-2.97716	0.02197
C6	3.35866	0.65613	0.03322
C7	3.34957	-0.75210	0.03250
C8	1.95209	-1.17611	0.02854
C9	1.18301	-0.03199	0.02760
N10	2.00758	1.08920	0.03029
C11	1.49667	-2.53603	0.02508
C12	-1.38936	4.31577	0.01618
C13	-0.03062	4.30256	0.02117
C14	0.34484	2.89259	0.02417
N15	-0.77357	2.09413	0.02092
C16	-1.81445	2.91243	0.01616
C17	1.62770	2.40300	0.02856
C18	-5.14472	-0.50365	0.00538
C19	-5.09851	0.84711	0.00321
C20	-3.67465	1.20322	0.00982
N21	-2.89644	0.03884	0.01498
C22	-3.73514	-0.95618	0.01253
C23	-3.38090	-2.41329	0.01585
C24	-3.18804	2.47855	0.01065
C25	4.53552	1.39448	0.03596
C26	5.73782	0.68821	0.03800
C27	5.75180	-0.71222	0.03729
C28	4.56472	-1.44004	0.03467
H29	0.38444	-5.24050	0.01287
H30	-2.30120	-5.13952	0.00642
H31	0.10956	0.08002	0.02497
H32	2.26918	-3.30001	0.02426
H33	-2.04200	5.17760	0.01254
H34	0.64471	5.14639	0.02266
H35	2.45130	3.10460	0.03054
H36	-6.01947	-1.13998	0.00176
H37	-5.92346	1.54557	-0.00213
H38	-3.88422	-2.87814	-0.84666

H39	-3.88444	-2.87419	0.88048
H40	-3.92769	3.27472	0.00648
H41	4.54055	2.47757	0.03659
H42	6.67362	1.23452	0.04012
H43	6.70127	-1.23494	0.03879
H44	4.59029	-2.52382	0.03410

B-neo-CP-5-H			
	X	Y	Z
C1	-0.04079	-4.39589	-0.00006
C2	-1.39429	-4.41763	0.00128
C3	-1.82694	-3.01679	0.01215
N4	-0.70218	-2.18359	0.01715
C5	0.33534	-2.97011	0.01004
C6	3.27616	0.93237	0.03060
C7	3.38710	-0.47204	0.01939
C8	2.03597	-1.01890	0.02066
C9	1.16863	0.02985	0.03153
N10	1.89481	1.24338	0.03799
C11	1.75457	-2.49041	0.01209
C12	-1.75213	4.19062	0.06714
C13	-0.39380	4.27692	0.06567
C14	0.08144	2.90006	0.05425
N15	-0.96579	2.02240	0.04930
C16	-2.07167	2.76361	0.05660
C17	1.40563	2.50609	0.04837
C18	-5.08297	-0.93379	0.02714
C19	-5.16254	0.41757	0.03819
C20	-3.77719	0.90191	0.04335
N21	-2.89925	-0.16272	0.03574
C22	-3.64391	-1.25320	0.02611
C23	-3.12659	-2.59736	0.01599
C24	-3.39796	2.22457	0.05343
C25	4.38662	1.76604	0.03212
C26	5.64501	1.16298	0.02176
C27	5.77782	-0.23065	0.01012
C28	4.65539	-1.05659	0.00897
H29	0.63861	-5.23724	-0.00702
H30	-2.04875	-5.27776	-0.00443

H31	0.09110	0.05020	0.03509
H32	2.25973	-2.95007	0.87574
H33	2.25887	-2.93969	-0.85745
H34	-2.46558	5.00292	0.07443
H35	0.21755	5.16826	0.07163
H36	2.16560	3.27736	0.05195
H37	-5.89405	-1.64905	0.02030
H38	-6.04945	1.03542	0.04218
H39	-3.87899	-3.38187	0.01037
H40	-4.20113	2.95675	0.05920
H41	4.30142	2.84606	0.04086
H42	6.53119	1.78663	0.02261
H43	6.76851	-0.67044	0.00201
H44	4.76979	-2.13468	-0.00011

BP-22,24-H

	X	Y	Z
C1	-0.18268	-4.24151	-0.00778
C2	-1.55354	-4.24531	-0.00868
C3	-2.00081	-2.88456	-0.00792
N4	-0.87063	-2.10226	-0.00671
C5	0.25851	-2.87736	-0.00678
C6	3.42877	0.70866	-0.00270
C7	3.42890	-0.69706	-0.00438
C8	2.01457	-1.09331	-0.00496
N9	1.21246	0.00553	-0.00391
C10	2.01433	1.10461	-0.00241
C11	1.57437	-2.41588	-0.00620
C12	-1.55445	4.25589	0.00351
C13	-0.18359	4.25231	0.00421
C14	0.25786	2.88826	0.00012
N15	-0.87114	2.11297	-0.00288
C16	-2.00143	2.89509	-0.00132
C17	1.57382	2.42704	-0.00030
C18	-5.12840	-0.67335	-0.00829
C19	-5.12853	0.68304	-0.00683
C20	-3.72969	1.09044	-0.00568
N21	-2.90733	0.00513	-0.00654
C22	-3.72944	-1.08032	-0.00794

C23	-3.30969	-2.41561	-0.00853
C24	-3.31025	2.42587	-0.00323
C25	4.62720	1.42217	-0.00186
C26	5.82278	0.70741	-0.00279
C27	5.82290	-0.69516	-0.00450
C28	4.62746	-1.41026	-0.00526
H29	0.47855	-5.09474	-0.00792
H30	-2.20995	-5.10230	-0.00968
H31	-0.88154	-1.08950	-0.00561
H32	2.33588	-3.18710	-0.00666
H33	-2.21103	5.11276	0.00584
H34	0.47750	5.10564	0.00733
H35	-0.88193	1.10021	-0.00562
H36	2.33514	3.19844	0.00142
H37	-5.97663	-1.34309	-0.00935
H38	-5.97690	1.35259	-0.00650
H39	-4.08436	-3.17438	-0.00942
H40	-4.08510	3.18446	-0.00243
H41	4.64108	2.50670	-0.00055
H42	6.76714	1.24002	-0.00222
H43	6.76739	-1.22757	-0.00527
H44	4.64161	-2.49479	-0.00660

BP-21,23-H

	X	Y	Z
C1	-0.18610	-4.25110	-0.00934
C2	-1.54141	-4.25395	-0.00879
C3	-1.95184	-2.85545	-0.00607
N4	-0.85978	-2.02972	-0.00488
C5	0.21823	-2.84915	-0.00687
C6	3.42887	0.70872	-0.00234
C7	3.42968	-0.70493	-0.00516
C8	2.04583	-1.14244	-0.00479
N9	1.28506	0.00066	-0.00197
C10	2.04453	1.14463	-0.00038
C11	1.56289	-2.43683	-0.00687
C12	-1.54653	4.25169	0.00568
C13	-0.19122	4.25055	0.00553
C14	0.21488	2.84911	0.00320

N15	-0.86210	2.02832	0.00210	C7	3.51441	-0.58491	0.00022
C16	-1.95519	2.85267	0.00350	C8	2.15150	-1.12591	0.00053
C17	1.56004	2.43844	0.00212	N9	1.23885	-0.11956	0.00063
C18	-5.11941	-0.69056	-0.00155	C10	1.90660	1.06067	0.00030
C19	-5.12020	0.68400	0.00074	C11	1.79780	-2.47668	0.00045
C20	-3.76095	1.12516	0.00094	C12	-1.71002	4.22819	-0.00021
N21	-2.98148	-0.00204	-0.00126	C13	-0.35580	4.17816	-0.00001
C22	-3.75965	-1.13013	-0.00282	C14	0.01205	2.75994	0.00028
C23	-3.28148	-2.44281	-0.00516	N15	-1.09840	1.98592	0.00053
C24	-3.28433	2.43840	0.00293	C16	-2.16033	2.84179	0.00022
C25	4.63348	1.42081	-0.00188	C17	1.34936	2.33897	0.00022
C26	5.82296	0.70703	-0.00427	C18	-5.04265	-0.86632	-0.00055
C27	5.82376	-0.70053	-0.00716	C19	-5.18817	0.49835	-0.00039
C28	4.63509	-1.41565	-0.00761	C20	-3.88094	1.07398	0.00006
H29	0.48566	-5.09776	-0.01119	N21	-2.98343	0.03193	0.00019
H30	-2.20998	-5.10307	-0.01011	C22	-3.64195	-1.17326	-0.00031
H31	0.26915	0.00014	-0.00127	C23	-3.09830	-2.45823	-0.00048
H32	2.30886	-3.22302	-0.00877	C24	-3.49028	2.41402	0.00012
H33	-2.21616	5.09997	0.00710	C25	4.47583	1.64980	-0.00033
H34	0.47948	5.09806	0.00681	C26	5.74125	1.06652	-0.00052
H35	2.30507	3.22553	0.00319	C27	5.89328	-0.32755	-0.00031
H36	-5.97436	-1.34954	-0.00236	C28	4.78128	-1.16686	0.00007
H37	-5.97591	1.34201	0.00215	H29	0.64939	-5.17408	0.00011
H38	-1.96730	-0.00151	-0.00170	H30	-2.03637	-5.10344	-0.00094
H39	-4.03767	-3.22007	-0.00637	H31	-0.47396	-1.12732	0.00045
H40	-4.04144	3.21476	0.00417	H32	2.58728	-3.21849	0.00024
H41	4.64446	2.50478	0.00033	H33	-2.34956	5.09936	-0.00048
H42	6.76776	1.23842	-0.00394	H34	0.34196	5.00381	-0.00017
H43	6.76916	-1.23084	-0.00905	H35	2.07151	3.14967	-0.00008
H44	4.64730	-2.49962	-0.00983	H36	-5.82507	-1.61042	-0.00089
BP-22,23-H				H37	-6.10882	1.06171	-0.00049
	X	Y	Z	H38	-1.98517	0.26969	0.00045
C1	0.01375	-4.30174	0.00005	H39	-3.83293	-3.25534	-0.00087
C2	-1.35634	-4.26487	-0.00049	H40	-4.27489	3.16133	0.00006
C3	-1.77538	-2.89264	-0.00023	H41	4.37427	2.72948	-0.00050
N4	-0.62245	-2.13946	0.00035	H42	6.62277	1.69785	-0.00084
C5	0.48679	-2.95236	0.00036	H43	6.88993	-0.75443	-0.00046
C6	3.35989	0.81388	0.00003	H44	4.90919	-2.24389	0.00025

BP-21,22-H				H39	-3.77750	-3.26421	0.00028
				H40	-4.36046	3.07037	0.00120
				H41	4.34172	2.73992	0.00064
				H42	6.59194	1.72439	0.00203
				H43	6.87716	-0.72811	0.00224
				H44	4.91076	-2.23178	0.00111
				BP-5,24-H			
				X	Y	Z	
C1	0.01523	-4.32736	-0.00014	C1	-0.55927	-4.16922	-0.08427
C2	-1.34047	-4.28823	0.00002	C2	-1.93812	-4.06023	-0.08858
C3	-1.71899	-2.87599	-0.00027	C3	-2.26165	-2.68156	-0.07063
N4	-0.60300	-2.09117	-0.00066	N4	-1.07397	-1.98227	-0.05628
C5	0.45311	-2.93766	-0.00053	C5	-0.02367	-2.85756	-0.06378
C6	3.33504	0.81746	0.00011	C6	3.49588	0.37253	0.00335
C7	3.49951	-0.58633	0.00027	C7	3.39963	-1.03243	-0.01666
C8	2.17685	-1.17313	-0.00066	C8	1.96143	-1.31700	-0.03255
N9	1.28285	-0.12407	-0.00105	N9	1.24323	-0.11531	-0.02357
C10	1.90711	1.10011	-0.00082	C10	2.10482	0.86506	-0.00324
C11	1.79202	-2.50070	-0.00052	C11	1.36565	-2.54232	-0.05172
C12	-1.78670	4.19208	-0.00022	C12	-1.24947	4.38854	0.02016
C13	-0.41359	4.16040	-0.00057	C13	0.10121	4.29128	0.02273
C14	0.00732	2.79090	-0.00089	C14	0.39724	2.84667	0.01012
N15	-1.13390	2.03423	-0.00039	N15	-0.68026	2.11608	0.00038
C16	-2.25114	2.84372	0.00001	C16	-1.75218	3.01385	0.00566
C17	1.34273	2.36357	-0.00108	C17	1.80099	2.32908	0.00990
C18	-5.04581	-0.93016	0.00128	C18	-5.25386	-0.24442	-0.04311
C19	-5.21569	0.41714	0.00146	C19	-5.09155	1.10449	-0.02429
C20	-3.87657	0.98615	0.00080	C20	-3.64671	1.34394	-0.01914
N21	-2.93160	0.00378	0.00018	N21	-2.96653	0.20061	-0.03368
C22	-3.60379	-1.16901	0.00043	C22	-3.90800	-0.79968	-0.04866
C23	-3.04848	-2.45895	0.00008	C23	-3.56111	-2.13591	-0.06665
C24	-3.55355	2.34673	0.00068	C24	-3.07072	2.65699	-0.00219
C25	4.45137	1.66148	0.00072	C25	4.73661	1.00558	0.02427
C26	5.71437	1.08805	0.00152	C26	5.88425	0.21146	0.02456
C27	5.87689	-0.31029	0.00165	C27	5.78881	-1.18572	0.00391
C28	4.77786	-1.15607	0.00104	C28	4.54672	-1.82157	-0.01674
H29	0.66159	-5.19348	0.00003	H29	0.03067	-5.07297	-0.09427
H30	-2.03189	-5.11911	0.00037	H30	-2.66212	-4.86086	-0.10232
H31	0.28387	-0.36970	-0.00116				
H32	2.57447	-3.24994	-0.00037				
H33	-2.42509	5.06248	0.00001				
H34	0.26308	5.00154	-0.00078				
H35	-1.28780	1.01873	-0.00025				
H36	2.06024	3.17542	-0.00118				
H37	-5.80750	-1.69739	0.00164				
H38	-6.14110	0.97534	0.00203				

H31	-1.00598	-0.96135	-0.04181
H32	2.01644	-3.41063	-0.05789
H33	-1.85619	5.28301	0.02671
H34	0.82649	5.09388	0.03199
H35	2.31862	2.76447	0.87904
H36	2.32385	2.77993	-0.84835
H37	-6.17606	-0.80778	-0.05219
H38	-5.85872	1.86644	-0.01496
H39	-4.36491	-2.86514	-0.07878
H40	-3.78810	3.47333	0.00475
H41	4.82173	2.08678	0.04032
H42	6.86229	0.67889	0.04075
H43	6.69499	-1.78104	0.00419
H44	4.48925	-2.90459	-0.03236

BP-5,21-H

	X	Y	Z
C1	-0.18192	-4.32192	-0.00109
C2	-1.54338	-4.29931	-0.00020
C3	-1.92852	-2.89274	0.00184
N4	-0.84046	-2.09511	0.00230
C5	0.22764	-2.92781	0.00084
C6	3.37495	0.69721	0.00641
C7	3.37477	-0.72195	0.00620
C8	2.00321	-1.14802	0.00380
N9	1.23533	0.02283	0.00328
C10	2.01037	1.11900	0.00447
C11	1.54477	-2.45541	0.00203
C12	-1.66774	4.24904	-0.00289
C13	-0.31097	4.31935	-0.00242
C14	0.14564	2.93234	0.00098
N15	-0.83636	2.06897	0.00229
C16	-2.01051	2.83313	-0.00014
C17	1.58808	2.54844	0.00336
C18	-5.15745	-0.75607	0.00686
C19	-5.16430	0.60164	0.00603
C20	-3.75462	1.00582	0.00235
N21	-2.94083	-0.04498	0.00099
C22	-3.74804	-1.14827	0.00372

C23	-3.27209	-2.44944	0.00337
C24	-3.29707	2.35719	0.00042
C25	4.58283	1.41923	0.00862
C26	5.76967	0.71196	0.01067
C27	5.77061	-0.70162	0.01038
C28	4.59063	-1.42397	0.00821
H29	0.47325	-5.18155	-0.00272
H30	-2.22271	-5.14026	-0.00109
H31	0.20622	0.04072	0.00221
H32	2.32680	-3.20855	0.00185
H33	-2.37723	5.06445	-0.00501
H34	0.31307	5.20221	-0.00404
H35	2.06683	3.02797	0.87029
H36	2.06969	3.02724	-0.86237
H37	-6.00408	-1.42821	0.00947
H38	-6.01871	1.26429	0.00786
H39	-4.02283	-3.23558	0.00431
H40	-4.07543	3.11616	-0.00054
H41	4.58995	2.50349	0.00901
H42	6.71457	1.24266	0.01259
H43	6.71861	-1.22756	0.01197
H44	4.61407	-2.50775	0.00804

BP-5,23-H

	X	Y	Z
C1	-0.16018	-4.27877	-0.01176
C2	-1.51511	-4.33933	-0.00871
C3	-1.96938	-2.95383	-0.00531
N4	-0.89737	-2.08867	-0.00573
C5	0.18876	-2.85267	-0.00952
C6	3.43608	0.68894	-0.00083
C7	3.44286	-0.71899	-0.00740
C8	2.02413	-1.11528	-0.00731
N9	1.22192	0.03189	-0.00156
C10	2.00735	1.06806	0.00205
C11	1.54863	-2.39209	-0.01088
C12	-1.64085	4.29933	-0.01288
C13	-0.28448	4.29484	-0.00787
C14	0.11918	2.88131	0.00030

N15	-0.91093	2.07549	0.00041	C7	3.44685	-0.72363	-0.01548
C16	-2.03990	2.89937	-0.00734	C8	2.02575	-1.10215	-0.01741
C17	1.56660	2.49520	0.00952	N9	1.24387	0.06568	-0.01170
C18	-5.08476	-0.75990	-0.00362	C10	2.05466	1.08483	-0.00678
C19	-5.09402	0.62437	-0.00500	C11	1.55393	-2.38176	-0.02291
C20	-3.74825	1.06319	-0.00510	C12	-1.67773	4.18068	0.00684
N21	-2.95074	-0.05055	-0.00330	C13	-0.29151	4.21920	0.00720
C22	-3.73258	-1.18036	-0.00230	C14	0.16812	2.88783	0.00139
C23	-3.27550	-2.51897	-0.00307	N15	-0.90592	2.06521	-0.00229
C24	-3.31939	2.41839	-0.00873	C16	-2.07369	2.82492	0.00067
C25	4.62548	1.41234	0.00145	C17	1.61680	2.51038	-0.00043
C26	5.83011	0.70530	-0.00306	C18	-5.16655	-0.76443	-0.01452
C27	5.83800	-0.69400	-0.00999	C19	-5.22534	0.59448	-0.00927
C28	4.64469	-1.41982	-0.01222	C20	-3.84202	1.04339	-0.00662
H29	0.54297	-5.10014	-0.01505	N21	-2.98040	-0.01570	-0.01007
H30	-2.14773	-5.21543	-0.00904	C22	-3.74695	-1.11249	-0.01487
H31	2.29468	-3.18179	-0.01455	C23	-3.26419	-2.45274	-0.01984
H32	-2.30837	5.14908	-0.01992	C24	-3.39481	2.35606	-0.00143
H33	0.38293	5.14583	-0.01003	C25	4.67099	1.38871	-0.00389
H34	2.03071	2.98136	0.88225	C26	5.86107	0.66122	-0.00685
H35	2.04676	2.99640	-0.84546	C27	5.84261	-0.73957	-0.01427
H36	-5.93513	-1.42462	-0.00345	C28	4.63866	-1.44453	-0.01855
H37	-5.95329	1.27749	-0.00619	H29	0.50275	-5.10907	-0.02842
H38	-1.92712	-0.05073	-0.00301	H30	-2.18848	-5.15163	-0.02646
H39	-4.05702	-3.27202	-0.00290	H31	2.30894	-3.16321	-0.02618
H40	-4.12408	3.14695	-0.01320	H32	-2.35862	5.01837	0.01060
H41	4.63107	2.49719	0.00670	H33	0.34213	5.09303	0.01123
H42	6.77054	1.24473	-0.00126	H34	-0.87695	1.04151	-0.00704
H43	6.78542	-1.22128	-0.01364	H35	2.08282	2.99806	0.86800
H44	4.66805	-2.50430	-0.01762	H36	2.08227	3.00546	-0.86498
BP-5,22-H				H37	-5.98953	-1.46560	-0.01791
	X	Y	Z	H38	-6.10191	1.22665	-0.00740
C1	-0.17864	-4.26942	-0.02651	H39	-4.02988	-3.22406	-0.02185
C2	-1.53342	-4.29184	-0.02549	H40	-4.14990	3.13661	0.00139
C3	-1.95755	-2.88931	-0.02234	H41	4.69538	2.47335	0.00201
N4	-0.86279	-2.05663	-0.02155	H42	6.81137	1.18279	-0.00339
C5	0.19773	-2.84751	-0.02388	H43	6.78057	-1.28346	-0.01658
C6	3.46829	0.68448	-0.00842	H44	4.64410	-2.52907	-0.02411

BP-10,22-H			
	X	Y	Z
C1	-0.12683	-4.28358	-0.01003
C2	-1.48223	-4.28380	-0.01118
C3	-1.88140	-2.86951	-0.01117
N4	-0.83014	-2.06029	-0.01021
C5	0.27314	-2.87379	-0.00948
C6	3.48791	0.70628	-0.00881
C7	3.46948	-0.70461	-0.00889
C8	2.04768	-1.08006	-0.00813
N9	1.26872	0.00789	-0.00738
C10	2.07819	1.10378	-0.00793
C11	1.57753	-2.41828	-0.00856
C12	-1.55329	4.20948	-0.00416
C13	-0.16742	4.18710	-0.00557
C14	0.24669	2.83473	-0.00620
N15	-0.91123	2.06244	-0.00521
C16	-1.99663	2.87232	-0.00409
C17	1.57828	2.39612	-0.00758
C18	-5.13956	-0.79483	-0.01000
C19	-5.20856	0.55958	-0.00722
C20	-3.81780	1.02020	-0.00573
N21	-2.95737	0.03660	-0.00727
C22	-3.72000	-1.13733	-0.00996
C23	-3.23884	-2.41933	-0.01166
C24	-3.43405	2.46162	-0.00215
C25	4.69641	1.40308	-0.00948
C26	5.88213	0.67265	-0.01006
C27	5.86490	-0.73040	-0.00998
C28	4.66123	-1.43082	-0.00943
H29	0.54236	-5.13244	-0.00957
H30	-2.14974	-5.13434	-0.01189
H31	2.34736	-3.18478	-0.00836
H32	-2.19740	5.07560	-0.00335
H33	0.50374	5.03264	-0.00617
H34	-0.95106	1.03908	-0.00599
H35	2.30642	3.20153	-0.00834
H36	-5.95450	-1.50480	-0.01188
H37	-6.09077	1.18450	-0.00625
H38	-3.99147	-3.20352	-0.01320

H39	-3.91308	2.93590	0.86714
H40	-3.91725	2.94196	-0.86567
H41	4.72499	2.48762	-0.00952
H42	6.83335	1.19307	-0.01056
H43	6.80288	-1.27421	-0.01038
H44	4.66346	-2.51555	-0.00939

BP-10,21-H			
	X	Y	Z
C1	-0.15049	-4.32947	0.00318
C2	-1.50823	-4.29149	0.00205
C3	-1.87942	-2.87478	0.00065
N4	-0.79853	-2.09162	0.00086
C5	0.27798	-2.93750	0.00227
C6	3.38045	0.70885	-0.00051
C7	3.39814	-0.71044	0.00036
C8	2.03161	-1.15235	0.00114
N9	1.24837	-0.02107	0.00067
C10	2.00443	1.11694	-0.00028
C11	1.58564	-2.48108	0.00227
C12	-1.52639	4.27714	0.00211
C13	-0.17067	4.30556	0.00096
C14	0.25033	2.91098	0.00032
N15	-0.85877	2.06854	0.00086
C16	-1.90652	2.85560	0.00184
C17	1.54206	2.45347	-0.00045
C18	-5.13490	-0.77299	-0.00349
C19	-5.15945	0.58108	-0.00241
C20	-3.74609	1.00560	0.00056
N21	-2.92334	-0.00463	0.00137
C22	-3.71974	-1.14909	-0.00096
C23	-3.23933	-2.42969	-0.00094
C24	-3.34344	2.44320	0.00236
C25	4.58355	1.43654	-0.00154
C26	5.77552	0.73777	-0.00165
C27	5.79279	-0.67602	-0.00066
C28	4.61902	-1.40585	0.00030
H29	0.49640	-5.19513	0.00445
H30	-2.19772	-5.12421	0.00219

H31	0.22128	-0.04100	0.00098	C23	-3.32621	-2.44121	0.00019
H32	2.36980	-3.23083	0.00307	C24	-3.34417	2.43932	0.00098
H33	-2.20932	5.11566	0.00294	C25	4.62692	1.44679	0.00196
H34	0.48287	5.16609	0.00065	C26	5.84619	0.77066	0.00213
H35	2.32590	3.20347	-0.00097	C27	5.89129	-0.63018	0.00133
H36	-5.97123	-1.45771	-0.00583	C28	4.71920	-1.38523	0.00027
H37	-6.02353	1.23174	-0.00376	H29	0.50722	-5.06707	-0.00098
H38	-3.98347	-3.22171	-0.00222	H30	-2.19453	-5.07672	0.00056
H39	-3.82689	2.93061	-0.85976	H31	-0.86454	-1.05538	-0.00227
H40	-3.82554	2.92797	0.86678	H32	2.34933	-3.23307	-0.00117
H41	4.58462	2.52056	-0.00237	H33	-2.15954	5.12012	-0.00384
H42	6.71529	1.27791	-0.00252	H34	0.53000	5.10184	-0.00199
H43	6.74591	-1.19241	-0.00069	H35	2.30811	3.15979	-0.00092
H44	4.64808	-2.48952	0.00106	H36	-6.05245	-1.40070	0.00221

BP-10,24-H

	X	Y	Z
C1	-0.15479	-4.21459	-0.00098
C2	-1.53865	-4.21954	-0.00011
C3	-1.97348	-2.87321	-0.00036
N4	-0.85473	-2.07813	-0.00190
C5	0.27219	-2.86389	-0.00127
C6	3.45221	0.69562	0.00097
C7	3.49852	-0.71330	0.00003
C8	2.09591	-1.14144	-0.00083
N9	1.26347	-0.04448	-0.00099
C10	2.02055	1.04382	0.00027
C11	1.61938	-2.43022	-0.00122
C12	-1.49717	4.26507	-0.00234
C13	-0.14522	4.25791	-0.00117
C14	0.24942	2.84530	0.00061
N15	-0.88684	2.03360	0.00213
C16	-1.90618	2.84419	0.00014
C17	1.53808	2.39389	0.00021
C18	-5.19483	-0.74325	0.00167
C19	-5.17440	0.61359	0.00189
C20	-3.75679	1.00103	0.00102
N21	-2.96387	-0.04020	0.00022
C22	-3.79969	-1.15792	0.00060

H37	-6.01769	1.29073	0.00270
H38	-4.05768	-3.24327	0.00039
H39	-3.82611	2.92476	0.86483
H40	-3.82732	2.92507	-0.86200
H41	4.60685	2.53118	0.00255
H42	6.77267	1.33370	0.00290
H43	6.85254	-1.13174	0.00147
H44	4.76958	-2.46884	-0.00039

BP-10,23-H

	X	Y	Z
C1	-0.12745	-4.29079	0.00339
C2	-1.48619	-4.33677	0.00283
C3	-1.92280	-2.94911	0.00017
N4	-0.85619	-2.09651	-0.00054
C5	0.23406	-2.87396	0.00127
C6	3.44577	0.69736	-0.00123
C7	3.46779	-0.71219	-0.00181
C8	2.05340	-1.12297	0.00023
N9	1.24269	-0.01349	0.00186
C10	2.01662	1.05888	0.00118
C11	1.58207	-2.41630	0.00071
C12	-1.49705	4.30420	0.00249
C13	-0.14272	4.26175	0.00480
C14	0.22736	2.84778	0.00232

N15	-0.93200	2.06196	-0.00142	C7	3.40415	-0.70847	-0.01052
C16	-1.93137	2.90370	-0.00142	C8	2.01778	-1.16163	-0.24557
C17	1.52078	2.40051	0.00289	C9	1.24065	0.00046	-0.41356
C18	-5.06255	-0.78221	-0.00666	C10	2.01865	1.16185	-0.24390
C19	-5.09891	0.60376	-0.00771	C11	1.58622	-2.48971	-0.24191
C20	-3.76566	1.06086	-0.00580	C12	-1.55893	4.30881	-0.11598
N21	-2.94624	-0.01502	-0.00391	C13	-0.18873	4.30480	-0.21990
C22	-3.70622	-1.18085	-0.00423	C14	0.26722	2.94729	-0.19739
C23	-3.23587	-2.50058	-0.00194	N15	-0.86720	2.17393	-0.08568
C24	-3.36830	2.50205	-0.00547	C16	-1.99706	2.95119	-0.02155
C25	4.63054	1.43087	-0.00333	C17	1.58794	2.49018	-0.23889
C26	5.84012	0.73609	-0.00599	C18	-5.05651	-0.67679	0.30454
C27	5.86267	-0.66458	-0.00655	C19	-5.05614	0.67842	0.30368
C28	4.67806	-1.40145	-0.00448	C20	-3.66565	1.09095	0.17790
H29	0.56644	-5.11993	0.00529	N21	-2.84141	0.00009	0.11207
H30	-2.12694	-5.20710	0.00406	C22	-3.66628	-1.09021	0.17901
H31	2.33299	-3.20157	0.00063	C23	-3.28616	-2.43792	0.11595
H32	-2.13941	5.17376	0.00331	C24	-3.28490	2.43842	0.11397
H33	0.55177	5.08984	0.00795	C25	4.58317	1.41047	0.21381
H34	2.27965	3.17796	0.00459	C26	5.76749	0.69658	0.41679
H35	-5.90135	-1.46179	-0.00745	C27	5.76686	-0.70024	0.41594
H36	-5.97164	1.23894	-0.00950	C28	4.58195	-1.41289	0.21199
H37	-1.92255	0.02180	-0.00235	H29	0.46216	-5.15970	-0.30945
H38	-4.01508	-3.25702	-0.00190	H30	-2.21450	-5.16679	-0.09714
H39	-3.85252	2.97957	0.85904	H31	-0.93630	-1.17419	0.04385
H40	-3.84707	2.97868	-0.87356	H32	0.22963	0.00116	-0.78054
H41	4.62650	2.51568	-0.00305	H33	2.33995	-3.26973	-0.21537
H42	6.77527	1.28471	-0.00770	H34	-2.21367	5.16688	-0.10260
H43	6.81570	-1.18171	-0.00866	H35	0.46320	5.16052	-0.31106
H44	4.71207	-2.48571	-0.00504	H36	-0.93301	1.17536	0.04968
BCP-22,24-H				H37	2.34205	3.26974	-0.21120
	X	Y	Z	H38	-5.90219	-1.34588	0.37604
C1	-0.19006	-4.30412	-0.21928	H39	-5.90141	1.34809	0.37460
C2	-1.56008	-4.30854	-0.11334	H40	-4.08509	-3.16869	0.16982
C3	-1.99856	-2.95087	-0.02078	H41	-4.08371	3.16949	0.16617
N4	-0.86913	-2.17329	-0.08761	H42	4.59488	2.49509	0.23102
C5	0.26544	-2.94637	-0.19978	H43	6.69579	1.23241	0.58072
C6	3.40473	0.70731	-0.00953	H44	6.69467	-1.23709	0.57926
				H45	4.59276	-2.49753	0.22783

BCP-22,23-H							
	X	Y	Z				
C1	-0.09762	-4.30804	-0.29184	H39	-1.96177	0.20868	-0.08439
C2	-1.47208	-4.29249	-0.20935	H40	-3.97444	-3.21727	0.14125
C3	-1.89617	-2.94729	0.01310	H41	-4.14017	3.20652	0.08286
N4	-0.74398	-2.18737	0.04581	H42	4.54776	2.60344	0.14557
C5	0.38214	-2.97514	-0.12865	H43	6.70722	1.41763	0.40515
C6	3.40815	0.77403	0.00622	H44	6.79192	-1.04976	0.43761
C7	3.45793	-0.64217	0.02110	H45	4.71958	-2.38621	0.21060
C8	2.07633	-1.14790	-0.14079	BCP-21,23-H			
C9	1.25116	-0.01461	-0.26734		X	Y	Z
C10	1.99432	1.17144	-0.16255	C1	-0.18549	-4.33225	-0.00312
C11	1.69308	-2.49338	-0.15565	C2	-1.54219	-4.33090	-0.00343
C12	-1.62751	4.27967	-0.11846	C3	-1.94214	-2.92817	-0.00276
C13	-0.27141	4.26888	-0.17827	N4	-0.83562	-2.11300	-0.00196
C14	0.13680	2.86854	-0.18224	C5	0.22800	-2.92765	-0.00222
N15	-0.95752	2.05716	-0.13157	C6	3.37796	0.71158	-0.00035
C16	-2.03953	2.88439	-0.07893	C7	3.37799	-0.71140	-0.00070
C17	1.48606	2.47006	-0.18303	C8	2.01404	-1.19885	-0.00114
C18	-5.03965	-0.75882	0.29378	C9	1.11163	0.00004	-0.00095
C19	-5.11785	0.61047	0.26938	C10	2.01398	1.19897	-0.00051
C20	-3.79327	1.12550	0.12729	C11	1.59120	-2.49792	-0.00169
N21	-2.94981	0.03435	0.07963	C12	-1.54238	4.33087	0.00025
C22	-3.66464	-1.14422	0.16638	C13	-0.18568	4.33227	0.00024
C23	-3.19896	-2.46059	0.11987	C14	0.22787	2.92769	-0.00024
C24	-3.36644	2.44840	0.04082	N15	-0.83571	2.11300	-0.00052
C25	4.57228	1.51892	0.14943	C16	-1.94227	2.92811	-0.00020
C26	5.79064	0.84801	0.29911	C17	1.59109	2.49802	-0.00027
C27	5.83876	-0.54698	0.31749	C18	-5.04362	-0.69004	-0.00178
C28	4.66922	-1.30272	0.18517	C19	-5.04365	0.68985	-0.00091
H29	0.53346	-5.16282	-0.48312	C20	-3.69128	1.12748	-0.00088
H30	-2.14223	-5.13158	-0.31942	N21	-2.90668	-0.00005	-0.00172
H31	-0.68493	-1.27106	0.45852	C22	-3.69123	-1.12761	-0.00210
H32	0.20732	0.00933	-0.51135	C23	-3.24445	-2.46498	-0.00283
H33	2.46889	-3.25153	-0.17873	C24	-3.24456	2.46487	-0.00034
H34	-2.28984	5.13313	-0.08896	C25	4.59521	1.41441	0.00009
H35	0.40080	5.11472	-0.21311	C26	5.78357	0.70530	0.00019
H36	2.20357	3.28512	-0.15425	C27	5.78360	-0.70501	-0.00015
H37	-5.85446	-1.46022	0.39184	C28	4.59527	-1.41418	-0.00059
H38	-6.00642	1.21892	0.34368	H29	0.47988	-5.18423	-0.00342

H30	-2.21234	-5.17883	-0.00407
H31	0.43544	-0.00018	0.85809
H32	0.43560	0.00022	-0.86010
H33	2.33617	-3.28855	-0.00181
H34	-2.21256	5.17877	0.00055
H35	0.47965	5.18428	0.00048
H36	2.33602	3.28868	-0.00006
H37	-5.89926	-1.34803	-0.00209
H38	-5.89932	1.34780	-0.00036
H39	-1.89051	-0.00002	-0.00191
H40	-4.03346	-3.20987	-0.00348
H41	-4.03360	3.20973	0.00000
H42	4.60735	2.49855	0.00035
H43	6.72884	1.23634	0.00052
H44	6.72889	-1.23601	-0.00004
H45	4.60746	-2.49832	-0.00084

BCP-21,22-H

	X	Y	Z
C1	-0.35089	-4.25007	-0.00121
C2	-1.73169	-4.24206	-0.00026
C3	-2.15468	-2.88713	-0.00018
N4	-1.01409	-2.11031	-0.00073
C5	0.10446	-2.90141	-0.00105
C6	3.41677	0.62302	0.00000
C7	3.33839	-0.79797	-0.00003
C8	1.95063	-1.20932	-0.00069
C9	1.11407	0.03873	-0.00083
C10	2.08462	1.18953	-0.00067
C11	1.46609	-2.48609	-0.00095
C12	-1.40559	4.35522	-0.00049
C13	-0.04955	4.37978	-0.00091
C14	0.37779	2.97608	-0.00106
N15	-0.67018	2.15095	-0.00095
C16	-1.78895	2.93994	-0.00036
C17	1.72978	2.50966	-0.00099
C18	-5.15496	-0.48924	0.00146
C19	-5.02461	0.86292	0.00099
C20	-3.59044	1.14391	0.00079

N21	-2.87997	-0.00018	0.00091
C22	-3.80024	-1.01587	0.00089
C23	-3.45364	-2.36514	0.00030
C24	-3.09046	2.47404	0.00063
C25	4.67130	1.25717	0.00085
C26	5.81847	0.48375	0.00166
C27	5.74084	-0.92451	0.00161
C28	4.51528	-1.56696	0.00075
H29	0.29988	-5.11120	-0.00175
H30	-2.39375	-5.09461	0.00008
H31	-1.10927	-1.09320	-0.00092
H32	0.44478	0.10469	-0.86506
H33	0.44500	0.10455	0.86362
H34	2.17543	-3.30782	-0.00100
H35	-2.08764	5.19398	-0.00025
H36	0.60170	5.24275	-0.00109
H37	2.51032	3.26498	-0.00102
H38	-6.06299	-1.07531	0.00203
H39	-5.80883	1.60717	0.00113
H40	-4.25968	-3.09114	0.00008
H41	-3.86054	3.24080	0.00158
H42	4.74267	2.33890	0.00098
H43	6.79165	0.96167	0.00244
H44	6.65523	-1.50703	0.00230
H45	4.46908	-2.65023	0.00077

BCP-5,24-H

	X	Y	Z
C1	-0.20873	-4.25958	0.00863
C2	-1.59287	-4.31290	0.01226
C3	-2.07016	-2.97991	0.01189
N4	-0.96554	-2.15663	0.00791
C5	0.18289	-2.89474	0.00591
C6	3.44430	0.69380	-0.00842
C7	3.41151	-0.72342	-0.00572
C8	1.99032	-1.13156	-0.00160
C9	1.22221	0.09796	-0.00205
C10	2.05011	1.17856	-0.00583
C11	1.53026	-2.41691	0.00174

C12	-1.62141	4.30364	-0.00235
C13	-0.26755	4.38580	-0.00612
C14	0.21916	2.99846	-0.00420
N15	-0.76312	2.13597	0.00040
C16	-1.94393	2.87711	0.00173
C17	1.67358	2.62605	-0.00746
C18	-5.16213	-0.69871	0.01519
C19	-5.08137	0.65878	0.01277
C20	-3.65987	0.98959	0.00924
N21	-2.90761	-0.11682	0.00942
C22	-3.79168	-1.17504	0.01304
C23	-3.39202	-2.50431	0.01426
C24	-3.20649	2.35205	0.00574
C25	4.65876	1.36853	-0.01269
C26	5.84601	0.62410	-0.01421
C27	5.81322	-0.76943	-0.01146
C28	4.59042	-1.45404	-0.00720
H29	0.47881	-5.09152	0.00790
H30	-2.21666	-5.19375	0.01498
H31	-1.09826	-1.14598	0.00696
H32	0.15352	0.20619	0.00036
H33	2.26698	-3.21461	0.00133
H34	-2.33894	5.11203	-0.00224
H35	0.34500	5.27692	-0.00991
H36	2.14782	3.11884	0.85605
H37	2.14297	3.11558	-0.87546
H38	-6.04804	-1.31743	0.01797
H39	-5.89260	1.37330	0.01324
H40	-4.16946	-3.26127	0.01717
H41	-4.01114	3.08291	0.00613
H42	4.69988	2.45271	-0.01490
H43	6.80079	1.13804	-0.01756
H44	6.74147	-1.32937	-0.01263
H45	4.58019	-2.53909	-0.00512

BCP-5,23-H

	X	Y	Z
C1	-0.15497	-4.31996	0.00297
C2	-1.51054	-4.35696	0.00179

C3	-1.94765	-2.96582	0.00043
N4	-0.85689	-2.11951	0.00140
C5	0.22074	-2.90309	0.00264
C6	3.42475	0.70515	-0.00173
C7	3.44271	-0.71272	-0.00261
C8	2.03591	-1.16816	0.00328
C9	1.22442	0.03314	0.00874
C10	2.01058	1.13995	0.00559
C11	1.58950	-2.45690	0.00192
C12	-1.66361	4.30563	0.00218
C13	-0.30666	4.33681	0.00640
C14	0.13536	2.93931	0.00623
N15	-0.87954	2.10576	0.00275
C16	-2.03225	2.89844	-0.00017
C17	1.59145	2.57223	0.00903
C18	-5.08041	-0.77724	-0.00879
C19	-5.09079	0.60927	-0.00945
C20	-3.74741	1.05247	-0.00628
N21	-2.95461	-0.06556	-0.00408
C22	-3.72948	-1.19834	-0.00529
C23	-3.25464	-2.53312	-0.00285
C24	-3.30901	2.40432	-0.00461
C25	4.61411	1.42176	-0.00802
C26	5.82781	0.71896	-0.01512
C27	5.84453	-0.67402	-0.01595
C28	4.64566	-1.40130	-0.00978
H29	0.53419	-5.15276	0.00409
H30	-2.15758	-5.22245	0.00159
H31	0.15567	0.02889	0.01371
H32	2.32928	-3.25273	-0.00098
H33	-2.35222	5.13846	0.00067
H34	0.33854	5.20438	0.00932
H35	2.05013	3.07309	0.87671
H36	2.05486	3.07882	-0.85266
H37	-5.93166	-1.44070	-0.01046
H38	-5.95226	1.25947	-0.01180
H39	-1.93949	-0.06952	-0.00192
H40	-4.02899	-3.29336	-0.00390
H41	-4.11293	3.13388	-0.00673
H42	4.61825	2.50680	-0.00774
H43	6.76359	1.26680	-0.02012

H44	6.79200	-1.20083	-0.02153
H45	4.67190	-2.48604	-0.01074

H35	-1.09696	1.11743	0.00778
H36	1.98274	3.03955	0.86203
H37	1.96531	3.01603	-0.86879
H38	-5.84201	-1.60768	-0.00383
H39	-6.08938	1.07605	0.01548
H40	-3.89725	-3.25075	-0.01594
H41	-4.28807	3.07721	0.02784
H42	4.48755	2.59758	0.05064
H43	6.69044	1.46824	0.08244
H44	6.84422	-0.99471	0.09204
H45	4.79292	-2.38660	0.06893

BCP-5,22-H

	X	Y	Z
C1	-0.08137	-4.38003	0.00485
C2	-1.43721	-4.36596	-0.00671
C3	-1.82924	-2.95350	-0.00283
N4	-0.70938	-2.15759	0.00996
C5	0.33683	-2.97204	0.01472
C6	3.38529	0.73659	0.04094
C7	3.47477	-0.67816	0.04550
C8	2.09685	-1.20409	0.02904
C9	1.22168	-0.04120	0.01406
C10	1.95165	1.10311	0.02165
C11	1.70234	-2.51066	0.02794
C12	-1.78056	4.24734	0.03156
C13	-0.39056	4.26835	0.02915
C14	0.06522	2.93355	0.01804
N15	-1.02572	2.13358	0.01371
C16	-2.18593	2.89606	0.02204
C17	1.51094	2.53088	0.00837
C18	-5.05562	-0.86585	0.00047
C19	-5.18257	0.48818	0.01034
C20	-3.82900	1.00963	0.01259
N21	-2.90937	-0.01214	0.00510
C22	-3.62412	-1.14804	-0.00171
C23	-3.12398	-2.48712	-0.00805
C24	-3.47826	2.35441	0.02126
C25	4.53710	1.51372	0.05404
C26	5.78366	0.87383	0.07222
C27	5.87087	-0.51759	0.07759
C28	4.71233	-1.30474	0.06438
H29	0.57620	-5.23812	0.00641
H30	-2.11341	-5.20913	-0.01633
H31	0.15670	-0.18326	-0.00105
H32	2.46669	-3.28280	0.03738
H33	-2.44896	5.09487	0.03992
H34	0.24970	5.13735	0.03485

BCP-5,24-H

	X	Y	Z
C1	-0.18647	-4.26041	-0.04158
C2	-1.57453	-4.30774	-0.03568
C3	-2.04225	-2.97638	-0.02581
N4	-0.94242	-2.15724	-0.02598
C5	0.21107	-2.90097	-0.03526
C6	3.46790	0.70008	-0.01823
C7	3.43737	-0.71699	-0.02894
C8	2.01807	-1.13441	-0.03113
C9	1.24730	0.07118	-0.02307
C10	2.07028	1.17932	-0.01476
C11	1.55234	-2.42635	-0.03712
C12	-1.47324	4.32025	0.01889
C13	-0.11610	4.36711	0.01479
C14	0.33704	2.98181	0.00279
N15	-0.77104	2.12813	-0.00008
C16	-1.82767	2.89366	0.00924
C17	1.63734	2.54123	-0.00386
C18	-5.15428	-0.71459	0.00278
C19	-5.08501	0.64068	0.01042
C20	-3.65956	0.98279	0.00499
N21	-2.90029	-0.08977	-0.00513
C22	-3.78048	-1.18345	-0.00699
C23	-3.37612	-2.49465	-0.01655
C24	-3.24824	2.42656	0.01062
C25	4.68187	1.37669	-0.01237

C26	5.86911	0.63613	-0.01770	C17	1.54221	2.45655	-0.00401
C27	5.83915	-0.75885	-0.02875	C18	-5.05960	-0.78344	-0.00325
C28	4.61983	-1.44547	-0.03424	C19	-5.10743	0.60524	-0.00555
H29	0.49645	-5.09624	-0.04947	C20	-3.78036	1.07367	-0.00763
H30	-2.20176	-5.18599	-0.03791	N21	-2.95787	-0.00036	-0.00732
H31	-1.07095	-1.14752	-0.01870	C22	-3.70237	-1.17437	-0.00547
H32	0.17774	0.17892	-0.02303	C23	-3.21514	-2.49099	-0.00508
H33	2.28927	-3.22410	-0.04304	C24	-3.36985	2.51218	-0.01088
H34	-2.16625	5.15041	0.02769	C25	4.62925	1.42725	-0.00116
H35	0.52094	5.24019	0.01937	C26	5.84791	0.73802	-0.00049
H36	2.40716	3.30830	0.00021	C27	5.87832	-0.65660	-0.00194
H37	-6.03478	-1.34096	0.00364	C28	4.68940	-1.39504	-0.00391
H38	-5.90294	1.34798	0.01880	H29	0.53587	-5.17721	-0.00694
H39	-4.14957	-3.25578	-0.01711	H30	-2.15882	-5.19748	-0.00574
H40	-3.74497	2.89373	0.87585	H31	0.18380	-0.05075	-0.00671
H41	-3.74918	2.90155	-0.84798	H32	2.36420	-3.28600	-0.00731
H42	4.72095	2.46079	-0.00357	H33	-2.16939	5.17592	-0.00825
H43	6.82279	1.15200	-0.01320	H34	0.52390	5.13624	-0.00461
H44	6.76894	-1.31635	-0.03299	H35	2.29180	3.24402	-0.00250
H45	4.61179	-2.53052	-0.04256	H36	-5.89461	-1.46768	-0.00096

BCP-10,23-H

	X	Y	Z
C1	-0.13649	-4.33083	-0.00671
C2	-1.49781	-4.34248	-0.00618
C3	-1.90621	-2.94886	-0.00622
N4	-0.81146	-2.12378	-0.00731
C5	0.26043	-2.92874	-0.00730
C6	3.44604	0.69945	-0.00320
C7	3.47693	-0.71816	-0.00446
C8	2.07684	-1.19321	-0.00598
C9	1.25371	-0.02331	-0.00581
C10	2.02543	1.11843	-0.00429
C11	1.62482	-2.48930	-0.00699
C12	-1.51460	4.31586	-0.00745
C13	-0.15503	4.29535	-0.00568
C14	0.23869	2.89708	-0.00543
N15	-0.90926	2.09059	-0.00720
C16	-1.92889	2.91820	-0.00818

C17	1.54221	2.45655	-0.00401
C18	-5.05960	-0.78344	-0.00325
C19	-5.10743	0.60524	-0.00555
C20	-3.78036	1.07367	-0.00763
N21	-2.95787	-0.00036	-0.00732
C22	-3.70237	-1.17437	-0.00547
C23	-3.21514	-2.49099	-0.00508
C24	-3.36985	2.51218	-0.01088
C25	4.62925	1.42725	-0.00116
C26	5.84791	0.73802	-0.00049
C27	5.87832	-0.65660	-0.00194
C28	4.68940	-1.39504	-0.00391
H29	0.53587	-5.17721	-0.00694
H30	-2.15882	-5.19748	-0.00574
H31	0.18380	-0.05075	-0.00671
H32	2.36420	-3.28600	-0.00731
H33	-2.16939	5.17592	-0.00825
H34	0.52390	5.13624	-0.00461
H35	2.29180	3.24402	-0.00250
H36	-5.89461	-1.46768	-0.00096
H37	-5.98661	1.23134	-0.00522
H38	-1.94362	0.05772	-0.00785
H39	-3.99126	-3.25068	-0.00360
H40	-3.85128	2.99413	0.85226
H41	-3.84600	2.98870	-0.88006
H42	4.62288	2.51221	0.00002
H43	6.77826	1.29494	0.00116
H44	6.83141	-1.17331	-0.00147
H45	4.72646	-2.47943	-0.00494

BCP-10,22-H

	X	Y	Z
C1	-0.35306	-4.37735	-0.06874
C2	-1.70873	-4.24420	-0.05080
C3	-1.97074	-2.80817	-0.00664
N4	-0.83460	-2.11131	0.00185
C5	0.18293	-3.02381	-0.03473
C6	3.48837	0.48550	0.04389
C7	3.45522	-0.93135	-0.00669

C8	2.03914	-1.34675	-0.00035
C9	1.26738	-0.18341	0.05185
C10	2.09041	0.96587	0.07907
C11	1.53089	-2.65982	-0.03753
C12	-1.30542	4.36648	0.21245
C13	0.07849	4.21961	0.20005
C14	0.38039	2.83984	0.15206
N15	-0.84446	2.18060	0.13679
C16	-1.85821	3.07628	0.17221
C17	1.67575	2.28630	0.12536
C18	-5.07485	-0.51811	0.08896
C19	-5.10264	0.83915	0.12992
C20	-3.70761	1.25844	0.12935
N21	-2.87245	0.24262	0.09126
C22	-3.67301	-0.90963	0.06433
C23	-3.27125	-2.22413	0.02230
C24	-3.30450	2.70228	0.16502
C25	4.70385	1.16048	0.05192
C26	5.88936	0.42140	0.00888
C27	5.85705	-0.97413	-0.04278
C28	4.63950	-1.66008	-0.05069
H29	0.22547	-5.28987	-0.10117
H30	-2.45353	-5.02780	-0.06546
H31	0.19326	-0.23417	0.06810
H32	2.24805	-3.47584	-0.07142
H33	-1.86679	5.28755	0.24664
H34	0.81862	5.00548	0.22196
H35	-1.05723	1.18188	0.10389
H36	2.45499	3.04381	0.14319
H37	-5.91197	-1.20159	0.07651
H38	-5.96485	1.49043	0.15768
H39	-4.08716	-2.94264	0.00879
H40	-3.78029	3.20260	-0.69070
H41	-3.77936	3.16198	1.04340
H42	4.74516	2.24418	0.09151
H43	6.84349	0.93625	0.01523
H44	6.78673	-1.53106	-0.07698
H45	4.62978	-2.74427	-0.09105

BCP-10,21-H

	X	Y	Z
C1	-0.14126	-4.40706	-0.00132
C2	-1.49925	-4.36404	-0.00052
C3	-1.86127	-2.94058	-0.00004
N4	-0.77334	-2.17032	-0.00059
C5	0.29816	-3.01262	-0.00130
C6	3.32034	0.72518	0.00185
C7	3.33271	-0.71744	0.00090
C8	2.00007	-1.20173	-0.00090
C9	1.08693	-0.01343	-0.00184
C10	1.98368	1.18451	0.00043
C11	1.61400	-2.54486	-0.00130
C12	-1.52064	4.34348	0.00024
C13	-0.16392	4.38544	0.00106
C14	0.27582	2.99355	0.00037
N15	-0.82466	2.14527	-0.00078
C16	-1.88279	2.91348	-0.00075
C17	1.57851	2.53373	0.00101
C18	-5.07127	-0.77562	0.00384
C19	-5.09407	0.57819	0.00315
C20	-3.67995	1.00208	0.00030
N21	-2.85754	-0.01221	-0.00070
C22	-3.65692	-1.15636	0.00143
C23	-3.20354	-2.45341	0.00138
C24	-3.30344	2.45128	-0.00121
C25	4.54843	1.44025	0.00424
C26	5.72774	0.74098	0.00549
C27	5.73909	-0.68580	0.00440
C28	4.57220	-1.40773	0.00218
H29	0.49895	-5.27796	-0.00190
H30	-2.19069	-5.19534	-0.00017
H31	0.38755	-0.01686	-0.84397
H32	0.38304	-0.01797	0.83646
H33	2.39907	-3.29630	-0.00110
H34	-2.21054	5.17646	0.00049
H35	0.47783	5.25496	0.00204
H36	2.35922	3.28956	0.00225
H37	-5.90877	-1.45901	0.00592
H38	-5.95732	1.23002	0.00454

H39	-3.97335	-3.22098	0.00270	H31	0.35123	0.02148	-0.78044
H40	-3.80468	2.92370	0.85982	H32	0.39157	0.01854	0.88879
H41	-3.80339	2.92147	-0.86428	H33	2.35441	-3.29988	0.01099
H42	4.55494	2.52407	0.00511	H34	-2.36414	5.13902	-0.00472
H43	6.67265	1.27249	0.00736	H35	0.32060	5.29037	0.03000
H44	6.69298	-1.20131	0.00541	H36	2.08259	3.08154	0.91882
H45	4.59957	-2.49123	0.00144	H37	2.11883	3.11410	-0.81023

BCP-5,21-H

C1	-0.18754	-4.40704	0.01830	H38	-5.93862	-1.41139	-0.03722
C2	-1.54797	-4.36381	0.01248	H39	-5.94911	1.28028	-0.04775
C3	-1.90930	-2.94567	0.00869	H40	-4.01466	-3.21256	-0.00846
N4	-0.81036	-2.17312	0.01416	H41	-4.05820	3.12097	-0.02854
C5	0.25000	-3.01547	0.01915	H42	4.56319	2.49775	-0.03062
C6	3.31149	0.70356	-0.00552	H43	6.67174	1.22621	-0.06698
C7	3.30829	-0.74425	-0.00448	H44	6.66363	-1.24738	-0.06480
C8	1.97064	-1.21132	0.01839	H45	4.56742	-2.52303	-0.02747
C9	1.08225	-0.00231	0.03698				
C10	1.99868	1.17022	0.01975				
C11	1.57266	-2.54436	0.01772				
C12	-1.65244	4.32535	0.00033				
C13	-0.29559	4.40171	0.01796				
C14	0.17372	3.01279	0.01622				
N15	-0.80848	2.15322	0.00086				
C16	-1.98437	2.90325	-0.00896				
C17	1.61882	2.61510	0.03453				
C18	-5.09119	-0.74018	-0.03082				
C19	-5.09587	0.61612	-0.03602				
C20	-3.68452	1.02117	-0.02273				
N21	-2.87110	-0.03254	-0.01051				
C22	-3.68139	-1.13731	-0.01442				
C23	-3.23669	-2.45300	-0.00438				
C24	-3.25575	2.38728	-0.02108				
C25	4.55035	1.41361	-0.02892				
C26	5.72074	0.70647	-0.04917				
C27	5.71438	-0.72328	-0.04800				
C28	4.54375	-1.43946	-0.02700				
H29	0.45141	-5.27904	0.02189				
H30	-2.23885	-5.19555	0.00956				