

Computational Study on the Mechanisms of Inhibition of SARS-CoV-2 M^{pro} by Aldehyde Warhead Based on DFT

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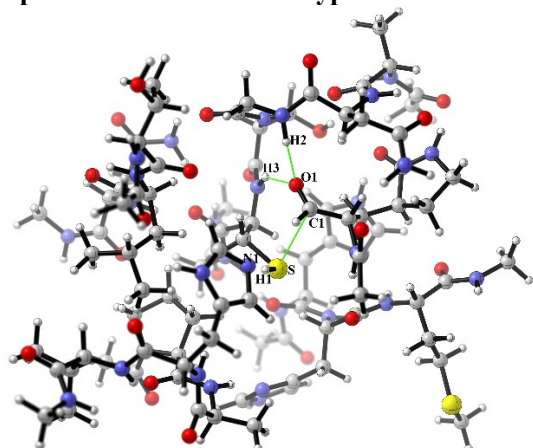
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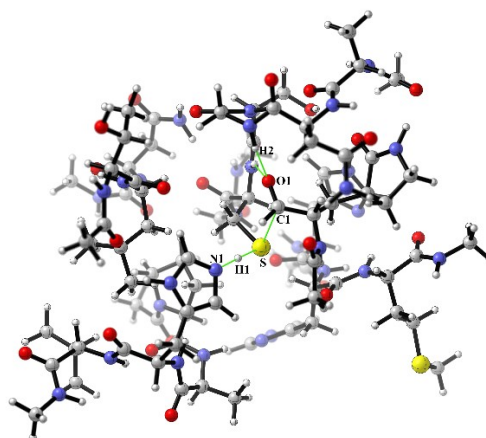
Reference for Gaussian 09 program:

Gaussian 09, Revision E.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Petersson, G. A.; Nakatsuji, H.; Li, X.; Caricato, M.; Marenich, A. V.; Bloino, J.; Janesko, B. G.; Gomperts, R.; Mennucci, B.; Hratchian, H. P.; Ortiz, J. V.; Izmaylov, A. F.; Sonnenberg, J. L.; Williams-Young, D.; Ding, F.; Lipparini, F.; Egidi, F.; Goings, J.; Peng, B.; Petrone, A.; Henderson, T.; Ranasinghe, D.; Zakrzewski, V. G.; Gao, J.; Rega, N.; Zheng, G.; Liang, W.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Throssell, K.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M. J.; Heyd, J. J.; Brothers, E. N.; Kudin, K. N.; Staroverov, V. N.; Keith, T. A.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A. P.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Millam, J. M.; Klene, M.; Adamo, C.; Cammi, R.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Farkas, O.; Foresman, J. B.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2013.

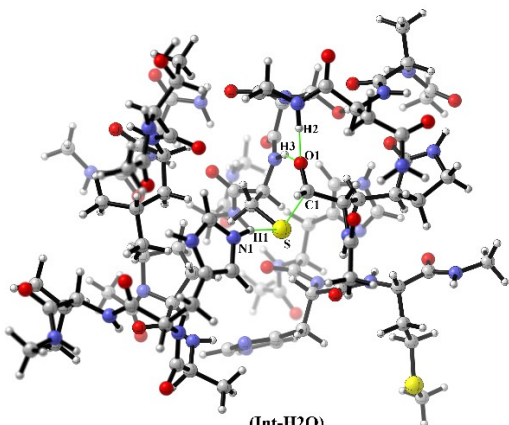
Optimized Structures in Hypothetical Calculation:



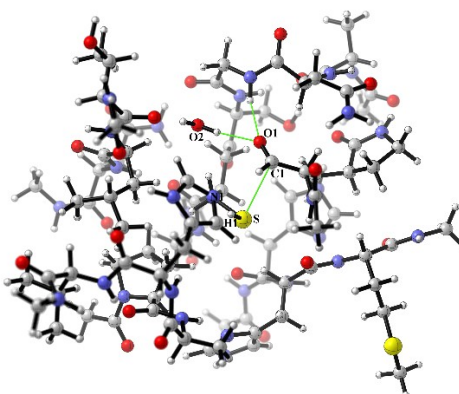
(Reac-H2O)



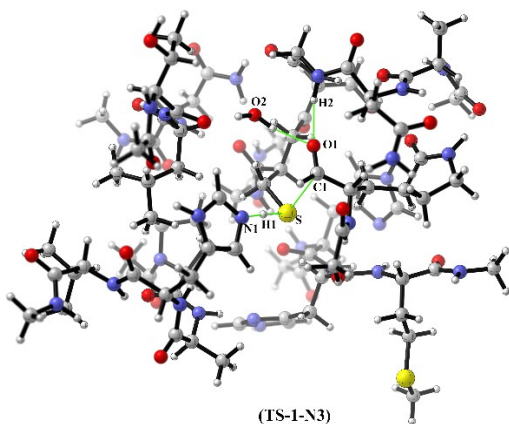
(TS-1-H2O)



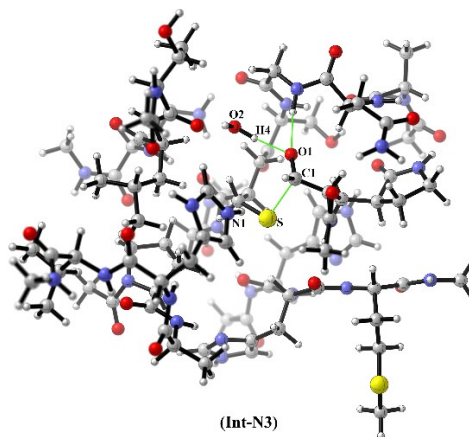
(Int-H2O)



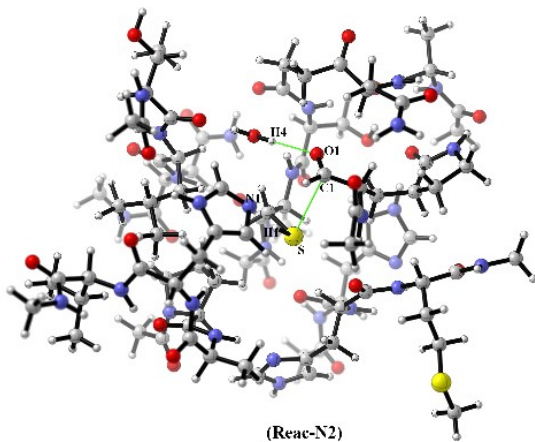
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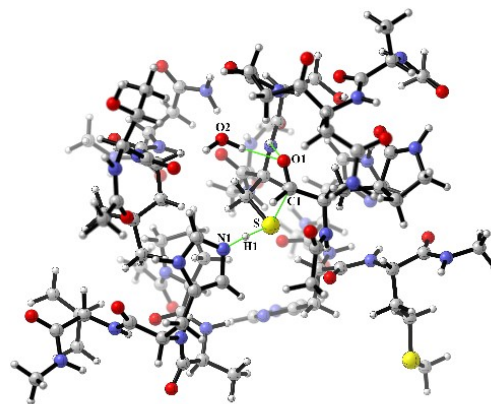
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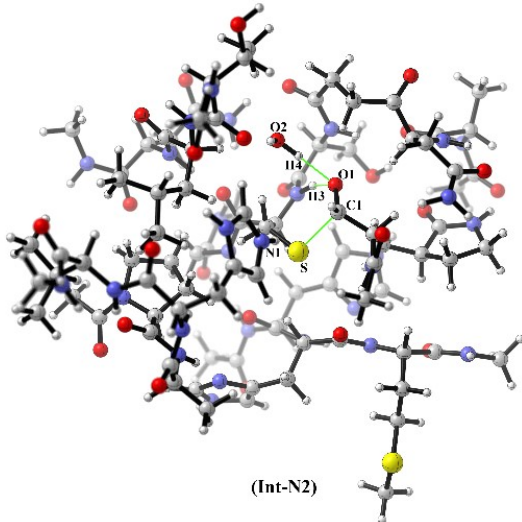
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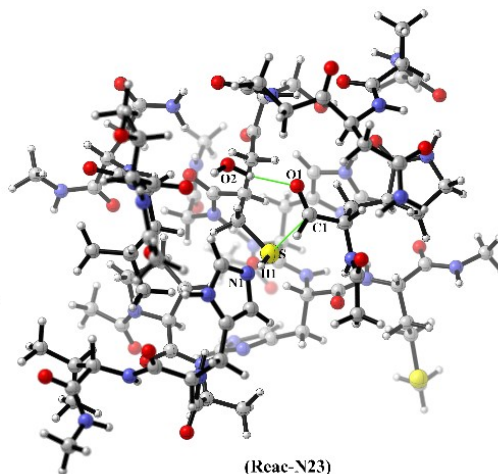
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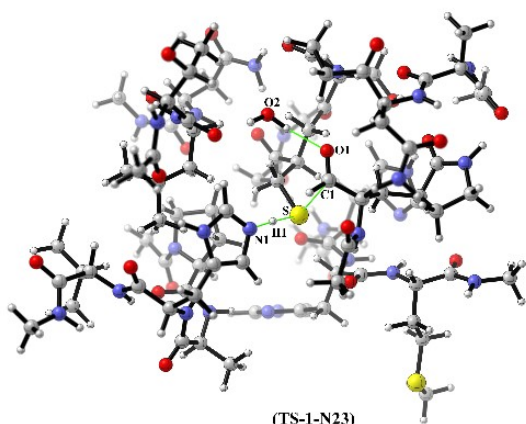
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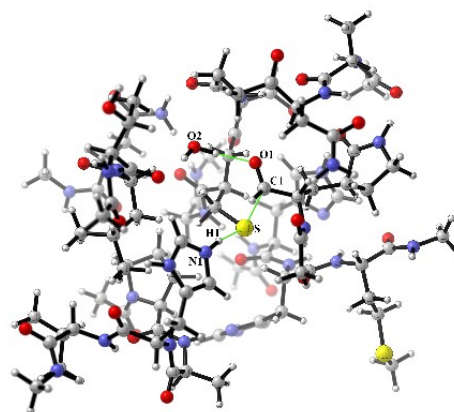
(Int-N2)



(Reac-N23)



(TS-1-N23)



(Int-N23)

Coordinates for All Optimized Compounds and Transition States:

R-Com							
C	-5.63679	-5.21094	-4.41469	C	4.96833	-3.85606	-4.30391
C	-4.80354	-4.97286	-3.16331	O	6.17471	-3.68371	-4.10227
O	-4.63483	-3.83280	-2.72702	N	4.26147	-3.12654	-5.20231
N	-4.29917	-6.08285	-2.56120	N	2.05208	-4.93639	-0.91760
C	-3.77803	-6.17932	-1.19994	C	1.13214	-5.56468	0.00361
C	-3.06368	-4.92145	-0.69047	O	1.02801	-4.83384	1.34926
O	-2.01137	-4.52794	-1.22517	C	0.01858	-4.96971	2.04737
C	-2.77820	-7.34856	-1.12719	N	2.10057	-4.07950	1.69297
O	-3.48966	-8.47299	-1.66010	C	2.23353	-3.40338	2.97306
C	-2.29364	-7.61465	0.29681	C	1.70049	-1.96201	3.00690
N	-3.59501	-4.40915	0.41929	O	1.83438	-1.29486	4.04166
C	-3.07455	-3.27771	1.16799	C	3.69436	-3.40579	3.47424
C	-3.82621	-3.30094	2.51519	O	4.56082	-2.53879	2.75829
O	-4.69262	-4.14955	2.74091	N	1.09697	-1.47601	1.90227
C	-3.21828	-1.95101	0.39349	C	0.56032	-0.12980	1.93411
C	-4.58458	-1.67203	-0.25379	C	-0.39287	0.04638	3.13629
C	-5.75584	-1.66878	0.74046	O	-1.03340	-0.90265	3.61782
C	-4.53410	-0.34654	-1.02911	C	-0.23151	0.20989	0.67142
N	-3.46667	-2.33664	3.38852	S	0.80525	0.52047	-0.81679
C	-3.92341	-2.35139	4.76483	N	-0.49102	1.30226	3.58534
C	-4.63675	-1.03562	5.09443	C	-1.23275	1.67227	4.77862
O	-4.25770	0.04333	4.63197	C	-0.25788	1.79093	5.95374
C	-2.73570	-2.55231	5.74258	O	0.02275	2.88585	6.45863
C	-2.02827	-3.86030	5.37313	N	0.29620	0.62927	6.36499
O	-2.46785	-4.93872	5.75277	C	1.33036	0.63013	7.38769
N	-0.94489	-3.71361	4.56244	C	1.00556	6.26148	6.17566
C	-6.08713	3.64435	3.89752	C	1.55208	5.91697	4.79231
C	-5.31709	4.14520	2.68595	O	1.98495	6.77768	4.02431
O	-4.98409	5.32517	2.57421	N	1.59070	4.58389	4.50082
N	-5.02027	3.20338	1.73182	C	2.44807	4.04483	3.45735
C	-3.99449	3.52472	0.74532	C	1.71743	3.80004	2.12543
C	-4.52760	3.63728	-0.68422	O	0.59725	3.27226	2.07808
O	-5.66377	3.31867	-1.02986	C	3.05885	2.72046	3.96039
C	-2.91355	2.40851	0.88345	C	3.94878	2.03491	2.97040
C	-3.44919	1.50741	2.01119	N	4.80101	2.71573	2.11402
C	-4.95803	1.76284	2.00657	C	4.10770	0.67689	2.81742
N	-3.58263	4.10820	-1.55711	C	5.46447	1.76571	1.46705
C	-3.97653	4.67777	-2.84346	N	5.07812	0.52460	1.86055
C	-4.70478	3.71730	-3.79165	N	2.39330	4.14527	1.00659
O	-5.46203	4.17097	-4.64395	C	1.82700	3.95690	-0.31771
C	-2.73205	5.22663	-3.55336	C	2.80285	3.51489	-1.41162
N	-4.40721	2.38860	-3.69660	O	2.32262	3.23753	-2.52102
C	-4.96157	1.42456	-4.63015	C	1.10850	5.25149	-0.83845
C	-6.09211	0.55703	-4.03505	C	0.12459	5.81630	0.13761
O	-6.20992	-0.63138	-4.33298	N	-1.24673	5.61378	0.04843
C	-3.86834	0.56443	-5.29288	C	0.41468	6.54826	1.26550
C	-2.99550	-0.20897	-4.35605	C	-1.76600	6.21807	1.10662
N	-3.29343	-1.47303	-3.88381	N	-0.79621	6.78903	1.87011
C	-1.76425	0.08538	-3.81316	N	4.15035	3.55535	-1.22338
C	-2.26536	-1.88574	-3.09916	C	5.01899	3.58942	-2.40120
N	-1.31245	-0.96332	-3.03211	C	6.47938	3.31003	-2.02896
N	-6.97521	1.22521	-3.24143	O	6.89204	3.37635	-0.87472
C	-8.03060	0.51202	-2.51474	C	4.89664	4.95690	-3.12261
C	-9.32711	0.27262	-3.32306	C	5.35324	6.12609	-2.24901
O	-10.08978	-0.62527	-2.97741	S	5.06075	7.71197	-3.12176
C	-8.30949	1.24119	-1.17038	C	5.63209	8.85652	-1.81711
C	-8.89508	2.64757	-1.36931	N	7.27177	3.01947	-3.09990
C	-9.19633	0.40409	-0.24039	C	8.72528	2.90385	-3.02415
C	8.65356	-2.35969	2.99575	C	3.54173	2.28071	-5.59379
C	8.49504	-3.01300	1.63260	C	3.77270	0.89635	-5.01510
O	9.26957	-2.77104	0.69919	O	4.27524	-0.00784	-5.68706
N	7.49058	-3.92677	1.53590	C	6.13461	-1.53641	0.31297
C	7.20654	-4.63854	0.30149	O	6.51941	-1.15373	-0.79962
C	5.76260	-4.41275	-0.14503	N	7.71199	-1.44881	-1.34719
O	4.85158	-4.27817	0.68894	C	7.91990	-0.85490	-2.66135
C	7.41098	-6.15577	0.47825	C	6.48132	-0.52402	-3.10568
N	5.52733	-4.50861	-1.46201	C	5.72564	-0.28204	-1.78246
C	4.17443	-4.48228	-2.00417	C	4.20454	-0.57206	-1.71157
C	3.26968	-5.45976	-1.22202	C	3.48955	-0.56515	-3.07335
O	3.63909	-6.59149	-0.94044	N	3.41127	0.73762	-3.70718
C	4.18414	-4.87906	-3.49326	C	2.12290	-1.23692	-3.06930
				O	1.94348	-2.38318	-2.70106

H	-5.53437	-6.21642	-4.83118	H	1.39350	-0.36361	7.83462
H	-1.93152	-7.08390	-1.77656	H	0.21045	-0.18853	5.77077
H	-1.62374	-8.48109	0.30354	H	1.85391	6.34833	6.86257
H	-3.14124	-7.83732	0.95207	H	2.25438	2.03123	4.24441
H	-1.74031	-6.76807	0.71503	H	3.60679	2.96091	4.88066
H	-2.87504	-9.21464	-1.72506	H	3.65071	-0.16326	3.31226
H	-4.61229	-6.41786	-0.52526	H	5.40159	-0.35956	1.46138
H	-4.49751	-6.98975	-2.96281	H	6.22547	1.94150	0.72156
H	-2.45927	-1.95221	-0.39023	H	3.24900	4.76849	3.28448
H	-2.95162	-1.13944	1.07435	H	1.16774	3.93872	5.16399
H	-4.76195	-2.46642	-0.98223	H	0.61102	4.99426	-1.77551
H	-5.37939	-0.28334	-1.71447	H	1.87653	6.00127	-1.06634
H	-4.59163	0.51431	-0.36393	H	1.33964	6.86022	1.72342
H	-3.61597	-0.25031	-1.61377	H	-0.92416	7.27805	2.74302
H	-6.66605	-1.31042	0.24968	H	-2.81416	6.27336	1.37111
H	-5.96367	-2.66606	1.13436	H	1.07670	3.16940	-0.23765
H	-5.55517	-1.01482	1.59574	H	3.32796	4.50933	1.13068
H	-2.01207	-3.44977	1.38772	H	3.84845	5.08274	-3.40790
H	-4.40447	-4.83644	0.86215	H	5.47840	4.93240	-4.05095
H	-3.11672	-2.64583	6.76263	H	6.41659	6.03813	-2.00057
H	-2.07291	-1.68598	5.68206	H	4.79160	6.13058	-1.30898
H	-0.63553	-4.51767	4.02881	H	5.51387	9.87114	-2.20320
H	-0.75869	-2.80877	4.14455	H	5.02898	8.75017	-0.91117
H	-4.59544	-3.20570	4.85323	H	6.68607	8.68789	-1.57972
H	-2.68412	-1.71966	3.18748	H	4.69278	2.80890	-3.08989
H	-5.46594	2.98002	4.50858	H	4.58027	3.59975	-0.30367
H	-1.94330	2.85489	1.11533	H	9.06770	2.10221	-3.68213
H	-2.80713	1.85619	-0.05399	H	6.84997	3.02702	-4.01685
H	-3.06297	1.82896	2.97687	H	4.50563	2.69697	-5.90393
H	-3.19311	0.45643	1.90240	H	1.38403	0.58208	2.06234
H	-5.47267	1.23212	1.20283	H	-0.79468	1.11780	0.86123
H	-5.42192	1.48599	2.94856	H	-0.91361	-0.60342	0.43572
H	-3.58186	4.49276	1.01124	H	8.40482	-1.56253	-3.33890
H	-3.02134	5.68168	-4.50282	H	3.72123	0.14262	-1.04142
H	-2.24003	5.97964	-2.93061	H	4.04425	-1.55088	-1.25165
H	-2.01724	4.42041	-3.74896	H	4.06407	-1.18859	-3.76118
H	-4.69657	5.49019	-2.68844	H	2.93780	1.50602	-3.23020
H	-2.73134	4.50093	-1.14208	N	-5.67245	-1.11294	5.96690
H	-3.23363	1.23911	-5.87463	H	-6.10282	-0.22096	6.17079
H	-4.35800	-0.11955	-5.99081	C	-6.28116	-2.32280	6.51052
H	-1.17679	0.98308	-3.95296	H	-7.02938	-2.02802	7.24799
H	-2.27095	-2.84603	-2.60511	H	-6.77594	-2.91777	5.73506
H	-5.43691	2.03012	-5.41060	H	-5.54223	-2.95216	7.01473
H	-3.81515	2.06450	-2.94333	H	0.89228	-2.06526	1.09580
H	-7.32582	1.36037	-0.69813	H	1.29183	-0.65734	-3.51510
H	-9.27585	0.89514	0.73533	N	-9.59093	1.12266	-4.35526
H	-10.19962	0.28013	-0.65424	H	-8.86924	1.78491	-4.60266
H	-8.78525	-0.59810	-0.08612	C	-10.76338	0.99028	-5.19718
H	-9.01808	3.13804	-0.39924	H	-11.28489	1.94863	-5.28867
H	-9.87531	2.60107	-1.85570	H	-10.50240	0.63372	-6.20094
H	-8.24228	3.29203	-1.96493	H	-11.42600	0.26273	-4.72694
H	-7.66910	-0.49909	-2.30209	H	6.43368	0.32216	-3.79194
H	-6.65918	2.10749	-2.85062	H	5.90040	0.75297	-1.46160
H	9.31432	-1.49931	2.89587	H	6.08996	-1.40191	-3.62000
H	7.19280	-6.68814	-0.45150	H	8.54829	0.04230	-2.58443
H	6.73760	-6.53680	1.25143	H	8.43083	-1.90892	-0.78313
H	7.89977	-4.25728	-0.45121	H	7.68295	-2.04075	3.39029
H	6.74660	-3.89758	2.22212	H	9.09454	-3.07271	3.69966
H	3.14755	-4.96226	-3.82973	H	0.50604	7.23072	6.13206
H	4.65899	-5.85950	-3.59491	H	0.32717	5.49539	6.56020
H	4.67478	-2.30249	-5.62662	H	-6.37385	4.51166	4.49204
H	3.25646	-3.19763	-5.23783	H	-6.98327	3.08948	3.60522
H	3.76281	-3.47605	-1.91809	H	-6.68581	-5.03823	-4.15585
H	6.28440	-4.45117	-2.13600	H	-5.36017	-4.47148	-5.16875
H	1.48046	-6.58494	0.18856	H	2.93657	2.18022	-6.49840
H	0.12430	-5.60385	-0.41476	H	3.05136	2.96256	-4.89634
H	1.81931	-3.98748	-1.18758	H	2.31020	0.89341	6.97116
H	4.05819	-4.44239	3.45720	H	1.07104	1.36282	8.15257
H	3.67990	-3.04868	4.50557	H	9.21867	3.83949	-3.30993
H	4.74418	-2.93836	1.88762	H	8.99164	2.66762	-1.99320
H	1.63364	-3.94994	3.70910	H	8.44323	-6.35452	0.77617
H	2.90878	-4.08632	1.07729	H	-4.19097	-1.94469	-3.95240
H	-2.01984	0.93635	4.96218	H	-0.05903	-0.04977	-1.70091
H	-1.68198	2.65590	4.63348	O	-0.01289	-2.77823	-0.53968
H	0.01392	2.05756	3.10309	H	0.08789	-2.31991	-1.38707

H	-0.75382	-3.40691	-0.68055	O	6.52528	-3.01831	-4.65367
				N	4.63450	-2.11659	-5.52231
				N	2.77846	-4.93243	-1.18173
TS-1				C	2.20152	-5.78543	-0.16224
C	-5.35595	-4.78230	-5.07512	C	2.18541	-5.14414	1.23476
C	-4.80123	-4.64762	-3.66590	O	1.45866	-5.61011	2.10678
O	-4.74808	-3.54744	-3.10747	N	3.00874	-4.06927	1.41232
N	-4.39070	-5.80305	-3.08883	C	3.15538	-3.40465	2.69697
C	-3.97071	-6.01210	-1.70988	C	2.40721	-2.06262	2.80518
C	-3.21467	-4.82478	-1.10547	O	2.42582	-1.43403	3.87179
O	-2.25411	-4.32124	-1.70916	C	4.63458	-3.19256	3.07449
C	-3.02819	-7.23545	-1.68304	O	5.29840	-2.23777	2.26295
O	-3.76842	-8.27940	-2.32760	N	1.74716	-1.64110	1.70924
C	-2.60565	-7.63455	-0.27259	C	0.93331	-0.43576	1.70023
N	-3.60562	-4.49549	0.13050	C	0.07112	-0.36963	2.96750
C	-3.04928	-3.42504	0.94616	O	-0.49420	-1.38051	3.42052
C	-3.51438	-3.69436	2.38927	C	-0.03672	-0.43611	0.49599
O	-4.44149	-4.47588	2.63010	S	0.52725	0.56752	-0.93190
C	-3.47889	-2.01480	0.44942	N	-0.08316	0.84921	3.48620
C	-4.87464	-1.91358	-0.18838	C	-0.83648	1.12480	4.70059
C	-6.02317	-2.25179	0.77339	C	0.10456	1.13838	5.89587
C	-5.09760	-0.52459	-0.80319	O	0.30174	2.15700	6.57324
N	-2.84570	-2.99563	3.32700	N	0.72361	-0.03143	6.13958
C	-3.11950	-3.14440	4.75176	C	1.76108	-0.08535	7.14155
C	-3.94082	-1.93821	5.23104	C	0.93991	5.61299	6.76530
O	-3.50572	-0.78717	5.13260	C	1.40550	5.49801	5.31317
C	-1.81139	-3.24771	5.55779	O	1.64735	6.48509	4.61569
C	-1.02035	-4.45745	5.04381	N	1.60640	4.22128	4.87950
O	-1.36550	-5.59525	5.34492	C	2.42570	3.90352	3.72354
N	0.02251	-4.16011	4.22764	C	1.61883	3.75235	2.41998
C	-6.04183	2.75562	4.43392	O	0.48466	3.25676	2.40404
C	-5.40365	3.31230	3.16586	C	3.19104	2.59761	4.02855
O	-5.34842	4.52184	2.94378	C	4.10735	2.12405	2.94275
N	-4.87542	2.39870	2.29042	N	4.81613	2.97710	2.10920
C	-3.98999	2.90655	1.23628	C	4.45476	0.81911	2.68502
C	-4.71873	3.28926	-0.05188	C	5.58525	2.18159	1.37555
O	-5.86803	2.94308	-0.32390	N	5.40134	0.87357	1.69301
C	-2.92029	1.80383	1.02489	N	2.24707	4.16240	1.29062
C	-3.00671	1.02714	2.34067	C	1.61092	4.01215	-0.01107
C	-4.49723	1.02500	2.65518	C	2.52727	3.70801	-1.19947
N	-3.94171	4.01990	-0.90821	O	1.98389	3.35892	-2.25939
C	-4.55389	4.77179	-2.00224	C	0.78533	5.28865	-0.40828
C	-5.24148	3.91806	-3.07681	C	-0.20199	5.71431	0.63278
O	-6.08029	4.42467	-3.81432	N	-1.55635	5.41576	0.56418
C	-3.49163	5.65216	-2.67206	C	0.06776	6.37715	1.80741
N	-4.82483	2.62408	-3.20230	C	-2.08583	5.89060	1.68165
C	-5.39259	1.73027	-4.19318	N	-1.13719	6.47401	2.46192
C	-6.46067	0.76426	-3.63318	N	3.86427	3.94848	-1.15436
O	-6.58904	-0.37082	-4.09061	C	4.62148	4.03563	-2.40453
C	-4.30446	0.96173	-4.97062	C	6.13099	4.07173	-2.09354
C	-3.32984	0.23754	-4.09866	O	6.55075	4.14117	-0.94142
N	-3.44943	-1.08039	-3.69343	C	4.19083	5.28496	-3.21579
C	-2.17264	0.68907	-3.51006	C	4.48004	6.59290	-2.47819
C	-2.39813	-1.38934	-2.90209	S	3.85203	8.01304	-3.45327
N	-1.60384	-0.32900	-2.77379	C	4.26624	9.35698	-2.28683
N	-7.28294	1.29223	-2.68802	N	6.94133	4.04755	-3.18898
C	-8.31929	0.47616	-2.05056	C	8.39340	4.23188	-3.13644
C	-9.55485	0.23246	-2.94095	C	1.45572	1.68585	-5.27718
O	-10.30045	-0.71169	-2.69589	C	2.15652	0.50675	-4.63191
C	-8.69246	1.10636	-0.68133	O	2.24582	-0.58474	-5.20927
C	-9.38734	2.46798	-0.83521	O	6.40593	-1.08840	-0.09051
C	-9.52911	0.14701	0.17331	C	6.49229	-0.57409	-1.21214
C	9.04782	-1.80856	2.06307	N	7.49491	-0.77649	-2.08220
C	8.97072	-2.42636	0.68246	C	7.38957	-0.00232	-3.31014
O	9.47537	-1.90969	-0.31788	C	5.91634	0.47610	-3.29735
N	8.31982	-3.62566	0.64997	C	5.49596	0.42896	-1.81119
C	7.91942	-4.25150	-0.59479	C	4.02652	0.11591	-1.41606
C	6.42722	-4.02245	-0.82672	C	3.11011	-0.36304	-2.54211
O	5.63519	-4.03147	0.13212	N	2.65191	0.72928	-3.38720
C	8.16543	-5.76877	-0.56260	C	1.93633	-1.22406	-2.07665
N	6.03146	-3.93150	-2.09990	O	2.10738	-2.13855	-1.24709
C	4.62035	-3.94243	-2.44653	H	-5.33718	-5.80217	-5.46638
C	3.97353	-5.18694	-1.77117	H	-2.14528	-6.96440	-2.28065
O	4.53900	-6.27165	-1.78284	H	-2.00387	-8.54823	-0.31053
C	4.44002	-4.01329	-3.97435	H	-3.48068	-7.83003	0.35450
C	5.29062	-2.99954	-4.73611				

H	-1.99739	-6.86036	0.20283	H	3.75503	2.78191	4.95194
H	-3.18425	-9.04060	-2.43602	H	4.13974	-0.10813	3.13020
H	-4.85043	-6.24941	-1.09596	H	5.80587	0.06059	1.22044
H	-4.51063	-6.67081	-3.59415	H	6.27981	2.52111	0.62229
H	-2.73734	-1.68552	-0.28248	H	3.14046	4.72022	3.58890
H	-3.40289	-1.32771	1.29336	H	1.28321	3.45964	5.47242
H	-4.90634	-2.62881	-1.01389	H	0.26987	5.06581	-1.34500
H	-5.90875	-0.58254	-1.52545	H	1.49461	6.10275	-0.60255
H	-5.36578	0.23393	-0.06330	H	0.98215	6.71360	2.26969
H	-4.21311	-0.16739	-1.33952	H	-1.26558	6.86988	3.38093
H	-6.98589	-2.13063	0.26581	H	-3.12922	5.83934	1.96646
H	-5.96647	-3.27339	1.15348	H	0.91582	3.17265	0.05512
H	-6.02262	-1.58400	1.64331	H	3.23888	4.35897	1.38732
H	-1.95650	-3.48474	0.92406	H	3.12122	5.19118	-3.41759
H	-4.37270	-4.98523	0.58165	H	4.69568	5.28343	-4.18868
H	-2.06408	-3.43367	6.60516	H	5.55575	6.71821	-2.30949
H	-1.26272	-2.30818	5.48467	H	3.98627	6.58635	-1.50097
H	0.44763	-4.90482	3.68223	H	3.94013	10.29329	-2.74447
H	0.10939	-3.21901	3.86270	H	3.74119	9.22586	-1.33667
H	-3.66089	-4.08207	4.86752	H	5.34403	9.40602	-2.10877
H	-2.06239	-2.39583	3.07587	H	4.40047	3.14697	-3.00646
H	-5.27147	2.39709	5.12556	H	4.38281	4.07970	-0.29130
H	-1.93751	2.24785	0.84768	H	8.90000	3.41835	-3.66324
H	-3.16988	1.16696	0.17240	H	6.50595	4.03463	-4.09930
H	-2.51252	1.60950	3.11296	H	1.81884	1.80069	-6.30105
H	-2.55938	0.03535	2.33767	H	1.58317	0.44728	1.67414
H	-5.04401	0.30478	2.03887	H	-0.98935	-0.00566	0.80093
H	-4.68984	0.79634	3.70053	H	-0.22966	-1.46672	0.19075
H	-3.50215	3.80332	1.61616	H	7.60778	-0.63144	-4.17732
H	-3.95281	6.23676	-3.47026	H	3.56827	0.99368	-0.95316
H	-3.04024	6.32840	-1.94092	H	4.03833	-0.65404	-0.63860
H	-2.69671	5.03263	-3.10091	H	3.65655	-1.06031	-3.18948
H	-5.35984	5.40337	-1.61008	H	2.42326	1.61463	-2.93393
H	-3.05999	4.39624	-0.54070	N	-5.15277	-2.19265	5.77967
H	-3.75121	1.68576	-5.57497	H	-5.64101	-1.36227	6.08805
H	-4.80149	0.26138	-5.64464	C	-5.87174	-3.46703	5.78574
H	-1.71787	1.66743	-3.56621	H	-6.91355	-3.26898	6.04389
H	-2.26432	-2.36401	-2.45180	H	-5.84087	-3.93978	4.79989
H	-5.92442	2.38038	-4.89744	H	-5.46288	-4.16148	6.52756
H	-4.20296	2.24847	-2.49937	H	1.76885	-2.21917	0.87994
H	-7.73740	1.27836	-0.16936	H	1.10724	-1.27239	-2.79793
H	-9.72217	0.59505	1.15381	N	-9.77657	1.12752	-3.94128
H	-10.48454	-0.08110	-0.30452	H	-9.09287	1.85963	-4.06873
H	-9.00599	-0.80168	0.33123	C	-10.89950	1.02429	-4.85142
H	-9.55434	2.91575	0.14887	H	-11.51241	1.93200	-4.82561
H	-10.35902	2.36167	-1.32951	H	-10.56388	0.85527	-5.88114
H	-8.78715	3.17741	-1.41377	H	-11.50475	0.17525	-4.53139
H	-7.92246	-0.52994	-1.88228	H	5.81532	1.46982	-3.73722
H	-6.94422	2.09802	-2.17085	H	5.76667	1.38268	-1.34172
H	9.63924	-0.89497	2.01532	H	5.31384	-0.21014	-3.89189
H	7.82099	-6.23354	-1.49012	H	8.09026	0.84420	-3.29576
H	7.60637	-6.22125	0.26194	H	8.33907	-1.24772	-1.75209
H	8.50853	-3.78702	-1.38866	H	8.03167	-1.57481	2.40223
H	7.73077	-3.84715	1.44299	H	9.49726	-2.50273	2.77978
H	3.37690	-3.90643	-4.20658	H	0.33928	6.51681	6.87917
H	4.76150	-5.00643	-4.30670	H	0.37801	4.73353	7.09078
H	5.21068	-1.44598	-6.01169	H	-6.59449	3.56457	4.91133
H	3.64814	-1.87888	-5.42353	H	-6.71766	1.92284	4.22039
H	4.14986	-3.03755	-2.05071	H	-6.38546	-4.41467	-5.06755
H	6.69368	-3.82501	-2.86438	H	-4.78267	-4.13218	-5.74155
H	2.78237	-6.71082	-0.12460	H	0.38805	1.44924	-5.33335
H	1.16089	-6.02391	-0.38641	H	1.58272	2.61576	-4.71891
H	2.42700	-3.98325	-1.22741	H	2.66479	0.44570	6.81746
H	5.13821	-4.16850	3.04654	H	1.40650	0.37850	8.06368
H	4.65886	-2.80925	4.09732	H	8.68205	5.18825	-3.58366
H	5.51024	-2.64026	1.40140	H	8.69077	4.22105	-2.08772
H	2.70266	-4.04778	3.45926	H	9.23014	-5.97140	-0.42438
H	3.72602	-3.90179	0.71200	H	-4.24549	-1.70877	-3.82486
H	-1.62418	0.37782	4.83347	H	-0.58264	0.04375	-1.89555
H	-1.26754	2.12295	4.62498	O	-0.00027	-3.64685	-0.30118
H	0.31227	1.67421	3.02564	H	0.59414	-3.11222	-0.85503
H	2.01939	-1.12811	7.33230	H	-0.74763	-3.91218	-0.87206
H	0.70354	-0.76008	5.43546				
H	1.82726	5.71017	7.39950	Intl			
H	2.47678	1.79718	4.25551	C	-5.22068	-5.03785	-5.08484

C	-4.58655	-4.80168	-3.72309	C	2.45119	-4.99411	1.36205
O	-4.61383	-3.68104	-3.20219	O	1.80392	-5.51555	2.26741
N	-4.02711	-5.89486	-3.15145	N	3.21718	-3.87831	1.51070
C	-3.46771	-6.04769	-1.81305	C	3.36359	-3.19062	2.78070
C	-2.92398	-4.75924	-1.20163	C	2.55243	-1.88396	2.90533
O	-2.06026	-4.09770	-1.80544	O	2.49576	-1.30733	4.00237
C	-2.29011	-7.04490	-1.89611	C	4.84044	-2.91985	3.12122
O	-2.86065	-8.22195	-2.47959	O	5.45371	-1.96891	2.26575
C	-1.64884	-7.32739	-0.54042	N	1.91820	-1.45086	1.80225
N	-3.34139	-4.51177	0.04103	C	1.01238	-0.31745	1.80121
C	-2.86638	-3.42564	0.88910	C	0.11980	-0.33163	3.04899
C	-3.34366	-3.75422	2.31294	O	-0.39098	-1.38340	3.47527
O	-4.24699	-4.57492	2.51482	C	0.06133	-0.40887	0.58636
C	-3.34739	-2.03032	0.40509	S	0.66828	0.32754	-0.97297
C	-4.72367	-1.97756	-0.27859	N	-0.13720	0.86610	3.58160
C	-5.88506	-2.41068	0.62760	C	-0.92391	1.05770	4.79239
C	-4.99941	-0.57904	-0.85203	C	0.02030	1.09468	5.98610
N	-2.70596	-3.07306	3.28411	O	0.22845	2.13559	6.62649
C	-3.00154	-3.29013	4.69482	N	0.64293	-0.07276	6.22686
C	-3.90313	-2.15867	5.20330	C	1.76160	-0.15189	7.13544
O	-3.56475	-0.97497	5.10701	C	0.71534	5.51226	6.80440
C	-1.71215	-3.34554	5.53239	C	1.10855	5.45205	5.32723
C	-0.85010	-4.50710	5.02050	O	1.22995	6.46375	4.63194
O	-1.17603	-5.66475	5.26499	N	1.39114	4.20047	4.86670
N	0.22525	-4.14547	4.28066	C	2.21824	3.94859	3.69895
C	-6.15919	2.39913	4.48192	C	1.41680	3.75962	2.39450
C	-5.56915	3.04598	3.23525	O	0.28526	3.25594	2.38240
O	-5.59799	4.26277	3.05773	C	3.07472	2.69785	3.99970
N	-4.98297	2.20327	2.32282	C	4.01853	2.28080	2.91480
C	-4.12304	2.81378	1.30446	N	4.64673	3.16895	2.05310
C	-4.84978	3.18219	0.01155	C	4.46836	1.00389	2.67988
O	-5.98236	2.79992	-0.28369	C	5.46783	2.42055	1.32452
C	-2.95898	1.81081	1.08424	N	5.39466	1.11156	1.67432
C	-3.01616	0.97197	2.36272	N	2.05007	4.15390	1.26142
C	-4.50892	0.84781	2.64129	C	1.41407	3.98127	-0.03744
N	-4.08615	3.95191	-0.82394	C	2.33509	3.71263	-1.22946
C	-4.70800	4.72507	-1.89746	O	1.80367	3.31769	-2.27905
C	-5.33810	3.90177	-3.02883	C	0.54791	5.23454	-0.43583
O	-6.10417	4.44021	-3.81940	C	-0.39122	5.67544	0.64029
C	-3.67213	5.68167	-2.50191	N	-1.73766	5.33894	0.67517
N	-4.96051	2.59099	-3.13872	C	-0.05605	6.35867	1.78516
C	-5.51531	1.72695	-4.16088	C	-2.19340	5.80703	1.82860
C	-6.51693	0.68341	-3.62079	N	-1.20725	6.42715	2.52955
O	-6.55554	-0.45555	-4.09041	N	3.65401	4.02910	-1.19541
C	-4.41704	1.04158	-5.00046	C	4.41402	4.11021	-2.44258
C	-3.44680	0.26089	-4.17660	C	5.91035	4.27340	-2.11506
N	-3.59782	-1.07481	-3.82897	O	6.29492	4.51236	-0.97303
C	-2.28746	0.66979	-3.57270	C	3.91983	5.29287	-3.31600
C	-2.57748	-1.46604	-3.05634	C	4.11312	6.64821	-2.63448
N	-1.77071	-0.41510	-2.89344	S	3.39886	7.97840	-3.67522
N	-7.37103	1.13333	-2.66723	C	3.72587	9.39914	-2.57389
C	-8.31596	0.22191	-2.01095	N	6.74366	4.18044	-3.18797
C	-9.52190	-0.17110	-2.88846	C	8.17231	4.49626	-3.13883
O	-10.14397	-1.19659	-2.62912	C	1.37127	1.55864	-5.20226
C	-8.74604	0.83205	-0.64920	C	2.04564	0.39227	-4.50115
C	-9.58428	2.10820	-0.81985	O	2.09224	-0.72613	-5.03321
C	-9.47137	-0.19719	0.22579	O	6.53544	-0.78172	-0.05806
C	9.08731	-1.55075	2.01351	C	6.53137	-0.34037	-1.21305
C	9.06117	-2.14653	0.62215	N	7.50428	-0.53736	-2.11853
O	9.55035	-1.59116	-0.36454	C	7.28562	0.13586	-3.39039
N	8.46518	-3.37445	0.56400	C	5.78356	0.50798	-3.33112
C	8.05072	-3.96719	-0.69186	C	5.44037	0.54897	-1.82615
C	6.54808	-3.75592	-0.87914	C	4.01553	0.17075	-1.33441
O	5.78753	-3.74426	0.10386	C	3.04434	-0.37965	-2.37744
C	8.32525	-5.47974	-0.71520	N	2.57281	0.66647	-3.28417
N	6.11140	-3.70122	-2.14132	C	1.84494	-1.14398	-1.75177
C	4.69163	-3.77191	-2.44703	O	2.15921	-2.07769	-0.87994
C	4.10527	-5.01172	-1.71794	H	-5.07712	-6.04777	-5.47594
O	4.69258	-6.08716	-1.74071	H	-1.54947	-6.59698	-2.57451
C	4.47492	-3.90673	-3.96485	H	-0.88294	-8.10220	-0.64819
C	5.26974	-2.89542	-4.78446	H	-2.39218	-7.68309	0.17927
O	6.50742	-2.88534	-4.75462	H	-1.15868	-6.43781	-0.13398
N	4.55734	-2.04425	-5.55673	H	-2.14860	-8.85358	-2.64261
N	2.93937	-4.75953	-1.07966	H	-4.23090	-6.48665	-1.15652
C	2.42444	-5.62475	-0.03864	H	-4.06088	-6.77253	-3.65308

H	-2.59551	-1.65436	-0.29555	H	2.87483	4.81283	3.56251
H	-3.32832	-1.35840	1.26380	H	1.15182	3.41641	5.47069
H	-4.69330	-2.66701	-1.12643	H	-0.00049	4.97787	-1.34495
H	-5.77138	-0.65237	-1.61492	H	1.23597	6.05229	-0.68267
H	-5.34332	0.13394	-0.09855	H	0.87850	6.72554	2.17497
H	-4.11113	-0.14760	-1.32653	H	-1.25073	6.79591	3.46849
H	-6.83191	-2.34686	0.08115	H	-3.21218	5.73398	2.18655
H	-5.77057	-3.43341	0.99053	H	0.74918	3.11736	0.02653
H	-5.96585	-1.76193	1.50783	H	3.05500	4.30122	1.35930
H	-1.77087	-3.43517	0.88800	H	2.86191	5.12256	-3.52856
H	-4.03425	-5.10287	0.49246	H	4.44512	5.27867	-4.27777
H	-1.98341	-3.56327	6.56913	H	5.17567	6.85458	-2.46401
H	-1.20990	-2.37893	5.49256	H	3.61230	6.65107	-1.66083
H	0.71709	-4.85497	3.74213	H	3.34370	10.29103	-3.07486
H	0.29843	-3.19112	3.94912	H	3.20790	9.28064	-1.61817
H	-3.48555	-4.26301	4.76408	H	4.79813	9.52289	-2.39881
H	-1.93072	-2.44909	3.06842	H	4.26059	3.18287	-3.00554
H	-5.36322	2.05241	5.15006	H	4.15867	4.25067	-0.34290
H	-2.01200	2.34196	0.95955	H	8.75965	3.67247	-3.55396
H	-3.13288	1.19185	0.19940	H	6.33190	4.01342	-4.09413
H	-2.58014	1.55229	3.17091	H	1.82729	1.69284	-6.18688
H	-2.49566	0.01730	2.32316	H	1.57045	0.62684	1.77339
H	-4.98777	0.11650	1.98343	H	-0.84120	0.16410	0.80175
H	-4.70813	0.55924	3.67004	H	-0.22191	-1.45272	0.43522
H	-3.72331	3.73856	1.72009	H	7.50526	-0.53620	-4.22451
H	-4.14117	6.27805	-3.28618	H	3.55276	1.03566	-0.85103
H	-3.26999	6.34362	-1.73056	H	4.11011	-0.58563	-0.54992
H	-2.83866	5.11847	-2.93554	H	3.54072	-1.13266	-2.99529
H	-5.54777	5.30448	-1.49460	H	2.37102	1.58279	-2.88415
H	-3.22114	4.34712	-0.43248	N	-5.07017	-2.51982	5.78763
H	-3.86756	1.81966	-5.53603	H	-5.61643	-1.73745	6.12306
H	-4.89533	0.38921	-5.73338	C	-5.68211	-3.84884	5.78871
H	-1.79445	1.62848	-3.56995	H	-6.71874	-3.74605	6.11423
H	-2.45061	-2.45718	-2.62942	H	-5.67211	-4.28601	4.78596
H	-6.08396	2.39249	-4.82053	H	-5.17399	-4.52976	6.47964
H	-4.42062	2.18756	-2.38613	H	2.10576	-1.87111	0.88484
H	-7.81166	1.11163	-0.14594	H	1.19672	-1.47669	-2.58231
H	-9.70937	0.24561	1.19853	N	-9.86504	0.68521	-3.88899
H	-10.39796	-0.53607	-0.24313	H	-9.27660	1.49247	-4.03346
H	-8.84772	-1.07980	0.39892	C	-10.97831	0.43869	-4.78444
H	-9.78967	2.55422	0.15757	H	-11.68434	1.27597	-4.77240
H	-10.54313	1.88933	-1.30171	H	-10.63573	0.28069	-5.81361
H	-9.06993	2.86708	-1.41863	H	-11.48564	-0.46220	-4.43749
H	-7.81273	-0.73235	-1.82756	H	5.58069	1.45168	-3.84253
H	-7.09093	1.96021	-2.14677	H	5.67190	1.55098	-1.44188
H	9.65662	-0.62198	1.99718	H	5.20472	-0.26531	-3.83391
H	7.97071	-5.92089	-1.65024	H	7.92204	1.02883	-3.47090
H	7.79087	-5.97050	0.10385	H	8.38353	-0.95224	-1.80637
H	8.61166	-3.46603	-1.48398	H	8.05593	-1.34811	2.32543
H	7.88388	-3.62954	1.35292	H	9.53418	-2.24522	2.73177
H	3.40325	-3.84079	-4.17049	H	0.08742	6.38833	6.97351
H	4.82138	-4.90144	-4.26578	H	0.20685	4.60239	7.13279
H	5.09468	-1.36018	-6.07102	H	-6.75137	3.15326	4.99990
H	3.57282	-1.82878	-5.39426	H	-6.78947	1.53950	4.23719
H	4.19590	-2.87496	-2.06570	H	-6.29159	-4.83447	-4.99778
H	6.75078	-3.62605	-2.92801	H	-4.80815	-4.31611	-5.79453
H	3.02368	-6.53900	-0.02481	H	0.32321	1.29083	-5.36924
H	1.37989	-5.88278	-0.21762	H	1.42064	2.48970	-4.63419
H	2.58025	-3.80015	-1.11197	H	2.64360	-0.50666	6.59359
H	5.37695	-3.87855	3.11142	H	1.94858	0.84079	7.54491
H	4.87524	-2.50551	4.13218	H	8.38893	5.41303	-3.69635
H	5.66110	-2.38790	1.41036	H	8.44378	4.63843	-2.09272
H	2.95592	-3.84614	3.55743	H	9.39606	-5.66639	-0.60370
H	3.85308	-3.63584	0.75769	H	-4.41371	-1.66729	-3.99498
H	-1.66890	0.26301	4.89067	H	-0.93655	-0.34044	-2.26625
H	-1.41310	2.03026	4.74202	O	0.09006	-3.65648	-0.11643
H	0.19371	1.72457	3.13117	H	0.81348	-3.06867	-0.43517
H	1.55314	-0.84076	7.96122	H	-0.50857	-3.78116	-0.87217
H	0.54812	-0.81608	5.54457				
H	1.63140	5.62652	7.39352	Int2			
H	2.41921	1.85041	4.23395	C	-5.55160	-5.24195	-4.64089
H	3.62798	2.92410	4.92018	C	-5.04774	-5.05822	-3.21770
H	4.23100	0.06488	3.14647	O	-5.19268	-3.97355	-2.64679
H	5.85332	0.32254	1.20636	N	-4.41693	-6.11531	-2.64982
H	6.12170	2.79699	0.55240	C	-3.94871	-6.18956	-1.26859

C	-3.27345	-4.90124	-0.78606	C	2.08193	-2.00225	2.77016
O	-2.34181	-4.41666	-1.45102	C	2.03986	-1.48609	3.89936
C	-2.89416	-7.31244	-1.18415	O	4.09750	-3.46271	3.12831
O	-3.56270	-8.47806	-1.68109	O	4.95500	-2.53338	2.48626
C	-2.34923	-7.51603	0.22755	N	1.63059	-1.40365	1.65797
N	-3.68594	-4.45656	0.40192	C	0.94857	-0.12707	1.71339
C	-3.14381	-3.31735	1.13208	C	-0.05097	-0.12067	2.88456
C	-3.69103	-3.44933	2.56941	O	-0.74341	-1.11462	3.16535
O	-4.55767	-4.28498	2.84913	C	0.11058	0.11770	0.44572
C	-3.50128	-1.95354	0.48441	S	0.94386	0.71140	-1.07035
C	-4.90440	-1.83722	-0.13261	N	-0.15743	1.05823	3.50523
C	-6.05118	-2.02860	0.87029	C	-0.96397	1.30505	4.68515
C	-5.05711	-0.49426	-0.86752	C	-0.03889	1.37506	5.89535
N	-3.16221	-2.58118	3.45455	O	0.13182	2.42275	6.53259
C	-3.41030	-2.69390	4.88684	N	0.59838	0.22143	6.18931
C	-4.20771	-1.47206	5.35624	C	1.57513	0.19804	7.25776
O	-3.76583	-0.32821	5.21369	C	1.03066	5.87148	6.36190
C	-2.07711	-2.80530	5.65611	C	1.56377	5.64566	4.95555
C	-1.37577	-4.07033	5.15078	O	1.94619	6.56790	4.23349
O	-1.74527	-5.17889	5.52350	N	1.65216	4.33681	4.58739
N	-0.40282	-3.85647	4.22917	C	2.51545	3.89874	3.50355
C	-6.03858	3.13869	4.14777	C	1.76110	3.75061	2.17225
C	-5.39484	3.65223	2.86789	O	0.64643	3.21340	2.11581
O	-5.36524	4.85076	2.58754	C	3.15484	2.56189	3.92281
N	-4.83100	2.71491	2.04162	C	4.10160	1.98153	2.92284
C	-3.96871	3.20774	0.96733	N	4.89953	2.75737	2.09659
C	-4.70102	3.57261	-0.31934	C	4.40104	0.64916	2.76076
O	-5.85008	3.22398	-0.59250	C	5.67594	1.88838	1.46140
C	-2.91818	2.09797	0.73528	N	5.41292	0.60874	1.83631
C	-2.94672	1.34457	2.06512	N	2.38468	4.21025	1.06411
C	-4.42282	1.36101	2.45276	C	1.76211	4.09372	-0.24520
N	-3.90980	4.26864	-1.18998	C	2.69792	3.75544	-1.40735
C	-4.48606	4.95337	-2.34146	O	2.18497	3.56567	-2.51848
C	-5.11300	4.03324	-3.39564	C	0.96418	5.37968	-0.64714
O	-5.86996	4.50145	-4.23855	C	-0.04882	5.81486	0.36748
C	-3.41465	5.82207	-3.01202	N	-1.41448	5.59292	0.23124
N	-4.75059	2.71337	-3.37988	C	0.19920	6.46038	1.55632
C	-5.28746	1.78436	-4.35141	C	-1.97023	6.10150	1.32063
C	-6.39831	0.86055	-3.80210	N	-1.03036	6.62793	2.15002
O	-6.56766	-0.27092	-4.27253	N	4.05212	3.77883	-1.26353
C	-4.17746	0.98225	-5.06305	C	4.86861	3.84182	-2.47535
C	-3.45242	-0.00487	-4.20433	C	6.34278	3.56704	-2.15655
N	-3.98499	-1.25591	-3.92179	O	6.77354	3.53146	-1.00743
C	-2.22928	0.02587	-3.58060	C	4.70995	5.22390	-3.16293
C	-3.12871	-1.94632	-3.16246	C	5.21135	6.37348	-2.28803
N	-2.05495	-1.19156	-2.95272	S	4.88754	7.97860	-3.11373
N	-7.20101	1.39498	-2.85471	C	5.54065	9.09260	-1.82106
C	-8.22025	0.58747	-2.17076	N	7.12269	3.40291	-3.26171
C	-9.40509	0.15569	-3.05778	C	8.57437	3.27288	-3.22171
O	-10.05475	-0.83578	-2.74065	C	2.73527	1.76108	-5.45175
C	-8.67461	1.33907	-0.89019	C	3.02162	0.51538	-4.63106
C	-9.41993	2.64328	-1.21172	O	3.20520	-0.57900	-5.17911
C	-9.50332	0.43418	0.02914	O	6.40583	-1.46632	0.24389
C	8.85582	-2.30247	2.50423	C	6.56540	-1.02601	-0.90255
C	8.71772	-3.00648	1.16469	N	7.56122	-1.38566	-1.73018
O	9.37429	-2.68520	0.17046	C	7.56923	-0.66571	-2.99640
N	7.85370	-4.06460	1.17090	C	6.14096	-0.07396	-3.06206
C	7.50709	-4.78542	-0.04197	C	5.69826	0.03685	-1.58659
C	6.10105	-4.40057	-0.50357	C	4.19555	-0.06291	-1.20571
O	5.19263	-4.25196	0.33215	C	3.22239	-0.39627	-2.33607
C	7.52817	-6.30424	0.19374	N	3.09140	0.70446	-3.29076
N	5.89362	-4.33476	-1.82263	C	1.82457	-0.85039	-1.83932
C	4.57029	-4.06687	-2.36352	O	1.86472	-1.91252	-1.01478
C	3.56151	-5.09226	-1.78188	H	-5.47178	-6.26575	-5.01505
O	3.83881	-6.28334	-1.71418	H	-2.07546	-7.02330	-1.85972
C	4.57283	-4.18636	-3.89837	H	-1.69545	-8.39442	0.24386
C	5.69355	-3.40498	-4.57433	H	-3.16097	-7.68513	0.94151
O	6.88023	-3.65035	-4.32191	H	-1.75327	-6.66056	0.56101
N	5.32045	-2.47441	-5.48274	H	-2.91749	-9.19500	-1.73050
N	2.39142	-4.52655	-1.40140	H	-4.78635	-6.45231	-0.60889
C	1.43924	-5.20932	-0.55325	H	-4.40638	-7.00664	-3.12754
C	1.37382	-4.63051	0.87193	H	-2.75670	-1.76176	-0.28908
O	0.34388	-4.76671	1.54127	H	-3.36076	-1.17944	1.24115
N	2.49827	-4.01448	1.30614	H	-4.99480	-2.62663	-0.88157
C	2.63899	-3.43034	2.63088	H	-5.83707	-0.57698	-1.62335

H	-5.33237	0.32637	-0.19855	H	1.10878	6.75340	2.05723
H	-4.13509	-0.20190	-1.38086	H	-1.19071	7.05084	3.05156
H	-7.01597	-1.88558	0.37219	H	-3.02732	6.11615	1.55286
H	-6.04924	-3.02618	1.31408	H	1.05539	3.26642	-0.18069
H	-5.98908	-1.30449	1.69144	H	3.31932	4.57881	1.17655
H	-2.05085	-3.40769	1.17780	H	3.65007	5.35377	-3.39505
H	-4.42200	-4.93806	0.91248	H	5.24521	5.22100	-4.11914
H	-2.28891	-2.92845	6.72137	H	6.28559	6.27836	-2.09374
H	-1.48813	-1.89747	5.50944	H	4.69525	6.35945	-1.32254
H	-0.13583	-4.62475	3.62595	H	5.41146	10.11567	-2.18046
H	-0.28422	-2.93261	3.82829	H	4.98736	8.97370	-0.88538
H	-3.95839	-3.62273	5.03601	H	6.60441	8.91031	-1.64507
H	-2.39826	-1.96558	3.17957	H	4.51753	3.07301	-3.17132
H	-5.27344	2.81611	4.86260	H	4.52207	3.71696	-0.36412
H	-1.94757	2.54227	0.50412	H	8.89582	2.40119	-3.79854
H	-3.20534	1.44304	-0.09199	H	6.68278	3.47698	-4.16679
H	-2.39314	1.92494	2.79989	H	3.59888	1.96215	-6.09372
H	-2.51488	0.34719	2.03146	H	1.66745	0.68792	1.85016
H	-4.99223	0.60883	1.89751	H	-0.56369	0.94647	0.65920
H	-4.57064	1.18066	3.51586	H	-0.48796	-0.76655	0.22784
H	-3.46561	4.10441	1.32722	H	7.77855	-1.35220	-3.82105
H	-3.85404	6.35291	-3.85820	H	3.87422	0.87117	-0.73790
H	-3.01024	6.54530	-2.29885	H	4.07658	-0.83196	-0.43667
H	-2.58797	5.20120	-3.37289	H	3.58690	-1.24994	-2.91243
H	-5.31937	5.58645	-2.01377	H	2.79394	1.60909	-2.93295
H	-3.01109	4.62378	-0.84578	N	-5.40698	-1.70496	5.94416
H	-3.45862	1.69846	-5.46794	H	-5.88433	-0.86408	6.24089
H	-4.63016	0.44973	-5.90373	C	-6.12124	-2.97874	6.02366
H	-1.47542	0.79609	-3.53268	H	-7.15106	-2.77406	6.32141
H	-3.29249	-2.92994	-2.75286	H	-6.13471	-3.48641	5.05485
H	-5.77527	2.41602	-5.10344	H	-5.67767	-3.64892	6.76773
H	-4.18888	2.37186	-2.61252	H	1.80357	-1.78009	0.71332
H	-7.74873	1.60536	-0.36391	H	1.21610	-1.02628	-2.74539
H	-9.75227	0.97105	0.95033	H	0.36930	-2.36442	-1.07374
H	-10.43015	0.11597	-0.45376	N	-9.70612	0.94097	-4.12641
H	-8.94873	-0.46908	0.30204	H	-9.08944	1.71455	-4.32695
H	-9.64917	3.18049	-0.28686	C	-10.77788	0.62618	-5.05105
H	-10.36293	2.44128	-1.73071	H	-11.35316	-0.19449	-4.62123
H	-8.82552	3.31697	-1.83734	H	-11.43377	1.49099	-5.19437
H	-7.77318	-0.36633	-1.87601	H	-10.38742	0.31251	-6.02642
H	-6.86505	2.22206	-2.36721	H	6.12270	0.88583	-3.58096
H	9.28884	-2.97874	3.24782	H	6.08324	0.98401	-1.18957
H	7.24498	-6.83885	-0.71729	H	5.49243	-0.75513	-3.61093
H	6.81064	-6.57060	0.97566	H	8.33473	0.12305	-2.98592
H	8.24771	-4.50690	-0.79491	H	8.34010	-1.92899	-1.35632
H	7.15534	-4.08375	1.90406	H	9.50085	-1.43330	2.38118
H	3.58981	-3.88437	-4.26912	H	7.86882	-1.98564	2.85867
H	4.72343	-5.24158	-4.15112	H	0.49517	6.82186	6.39767
H	6.07169	-1.93186	-5.88639	H	0.38745	5.05510	6.70166
H	4.40466	-2.02767	-5.45962	H	-6.61125	3.95549	4.58650
H	4.26411	-3.05826	-2.06353	H	-6.69606	2.28551	3.95757
H	6.66244	-4.34751	-2.48921	H	-6.59479	-4.92019	-4.67526
H	1.72726	-6.26344	-0.48948	H	-4.97950	-4.58018	-5.29796
H	0.42343	-5.15788	-0.95757	H	1.88938	1.55350	-6.11217
H	2.29865	-3.49657	-1.42225	H	2.51712	2.63881	-4.83931
H	4.47264	-4.49076	3.03112	H	2.50237	0.71266	6.97533
H	4.07722	-3.18901	4.18560	H	1.16428	0.69844	8.13623
H	5.15361	-2.85817	1.58960	H	9.06358	4.16810	-3.61974
H	2.04577	-4.02358	3.33379	H	8.86734	3.14080	-2.17971
H	3.31181	-4.00443	0.69596	H	8.52687	-6.61998	0.50486
H	-1.72607	0.52961	4.79666	O	-0.63502	-2.37303	-1.19491
H	-1.44986	2.27879	4.60210	H	-1.28869	-1.55914	-2.28164
H	0.29984	1.87802	3.08982	H	-1.04705	-3.25683	-1.14108
H	1.81029	-0.83903	7.50269	H	-4.95560	-1.50458	-4.11017
H	0.65693	-0.50499	5.48203				
H	1.88582	5.94086	7.04257	TS-2			
H	2.37381	1.82528	4.14337	C	-5.55991	-5.31771	-4.55201
H	3.67136	2.75811	4.87182	C	-5.03417	-5.13330	-3.13620
H	4.00743	-0.24064	3.22240	O	-5.22397	-4.07186	-2.53835
H	5.79625	-0.24345	1.41495	N	-4.32628	-6.15979	-2.59948
H	6.43055	2.15172	0.73662	C	-3.85522	-6.21636	-1.21846
H	3.30016	4.64951	3.37829	C	-3.20863	-4.90986	-0.74332
H	1.27754	3.63721	5.22265	O	-2.26674	-4.42785	-1.39853
H	0.47244	5.17057	-1.59897	C	-2.77788	-7.31573	-1.12535
H	1.68470	6.18894	-0.81963	O	-3.42131	-8.49956	-1.61193

C	-2.22903	-7.49449	0.28826	N	1.60002	-1.39521	1.66114
N	-3.65075	-4.44898	0.42647	C	0.93291	-0.11138	1.72155
C	-3.13885	-3.29312	1.15212	C	-0.09783	-0.09766	2.89253
C	-3.70040	-3.42232	2.58427	O	-0.76289	-1.08858	3.17667
O	-4.55169	-4.27252	2.86357	C	0.10112	0.15609	0.45518
C	-3.51157	-1.94051	0.49011	S	0.94469	0.76289	-1.04780
C	-4.91191	-1.84554	-0.13567	N	-0.16987	1.08537	3.50559
C	-6.06255	-2.03007	0.86380	C	-0.97716	1.34377	4.68258
C	-5.06657	-0.51559	-0.89297	C	-0.04864	1.43705	5.88902
N	-3.19956	-2.53307	3.46646	O	0.13033	2.49876	6.50004
C	-3.44756	-2.64576	4.89820	N	0.58400	0.28727	6.20826
C	-4.22660	-1.41292	5.37036	C	1.56645	0.28188	7.27261
O	-3.77573	-0.27493	5.21021	C	1.03237	5.94267	6.29426
C	-2.11381	-2.77410	5.66598	C	1.58007	5.69806	4.89762
C	-1.42245	-4.04400	5.15911	O	1.98387	6.60825	4.17204
O	-1.78876	-5.14968	5.54229	N	1.65473	4.38486	4.54247
N	-0.45894	-3.83811	4.22463	C	2.52524	3.92755	3.47290
C	-6.03972	3.19008	4.11402	C	1.77987	3.76306	2.13940
C	-5.38891	3.69066	2.83228	O	0.67830	3.19967	2.07966
O	-5.34675	4.88764	2.54659	C	3.15371	2.59351	3.91485
N	-4.83487	2.74356	2.01089	C	4.09772	1.99330	2.92453
C	-3.97246	3.22114	0.92971	N	4.90211	2.75339	2.09033
C	-4.70714	3.58122	-0.35722	C	4.38487	0.65649	2.77654
O	-5.86020	3.24033	-0.62081	C	5.67034	1.87106	1.46403
C	-2.93273	2.10069	0.70296	N	5.39568	0.59769	1.85219
C	-2.95998	1.36159	2.04094	N	2.39524	4.23616	1.03268
C	-4.43609	1.38912	2.42933	C	1.77457	4.11731	-0.27641
N	-3.91442	4.26387	-1.23686	C	2.71184	3.76157	-1.43200
C	-4.49067	4.93961	-2.39385	O	2.20294	3.56949	-2.54463
C	-5.13522	4.01160	-3.43058	C	0.98183	5.40310	-0.68467
O	-5.90912	4.47525	-4.26097	C	-0.04101	5.83348	0.32266
C	-3.41361	5.78590	-3.08345	N	-1.40457	5.60726	0.17329
N	-4.76830	2.69433	-3.41520	C	0.19399	6.48018	1.51370
C	-5.30623	1.75977	-4.38203	C	-1.97245	6.11609	1.25598
C	-6.41889	0.84267	-3.82476	N	-1.04227	6.64562	2.09458
O	-6.60776	-0.28281	-4.30063	N	4.06556	3.76679	-1.27987
C	-4.19552	0.95312	-5.08782	C	4.88710	3.81831	-2.48880
C	-3.47852	-0.04151	-4.23001	C	6.35534	3.51394	-2.17216
N	-4.02066	-1.28803	-3.95859	O	6.78888	3.47217	-1.02442
C	-2.25512	-0.03313	-3.60123	C	4.75542	5.20531	-3.17242
C	-3.15937	-1.98280	-3.19863	C	5.27674	6.34300	-2.29363
N	-2.07494	-1.25110	-2.97340	S	4.98777	7.95564	-3.11743
N	-7.20581	1.37870	-2.86373	C	5.65798	9.05428	-1.82038
C	-8.21967	0.57632	-2.16675	N	7.12817	3.33000	-3.27971
C	-9.39844	0.11685	-3.04704	C	8.57939	3.19287	-3.24444
O	-10.04092	-0.87368	-2.71212	C	2.85786	1.75092	-5.45439
C	-8.68313	1.34950	-0.90247	C	3.08973	0.50126	-4.62347
C	-9.43777	2.64097	-1.25211	O	3.28374	-0.59559	-5.16146
C	-9.50605	0.45624	0.03328	O	6.38673	-1.48135	0.28487
C	8.84672	-2.29948	2.56184	C	6.54136	-1.05051	-0.86579
C	8.70044	-3.00237	1.22173	N	7.54749	-1.40000	-1.68490
O	9.36072	-2.68736	0.22801	C	7.54087	-0.70206	-2.96333
N	7.82679	-4.05295	1.22637	C	6.09877	-0.14789	-3.04101
C	7.48849	-4.78193	0.01596	C	5.65289	-0.01761	-1.56814
C	6.08868	-4.39938	-0.46689	C	4.15148	-0.14077	-1.18477
O	5.16873	-4.24165	0.35427	C	3.17341	-0.41987	-2.32730
C	7.50284	-6.29906	0.26449	N	3.10252	0.68840	-3.27979
N	5.89731	-4.34667	-1.78966	C	1.74595	-0.79520	-1.85730
C	4.58224	-4.07818	-2.35003	O	1.70855	-1.89533	-1.06196
C	3.55859	-5.08540	-1.76366	H	-5.44445	-6.33195	-4.94280
O	3.82443	-6.27738	-1.67762	H	-1.96516	-7.01565	-1.80335
C	4.59908	-4.22403	-3.88270	H	-1.55505	-8.35742	0.31238
C	5.72767	-3.45532	-4.56002	H	-3.03726	-7.67651	1.00303
O	6.91080	-3.69715	-4.28922	H	-1.65331	-6.62234	0.61434
N	5.36564	-2.54065	-5.48929	H	-2.76159	-9.20380	-1.65090
N	2.38752	-4.50798	-1.40197	H	-4.68664	-6.49039	-0.55528
C	1.41404	-5.17859	-0.56732	H	-4.28809	-7.04919	-3.07922
C	1.34304	-4.60675	0.85993	H	-2.77059	-1.74284	-0.28474
O	0.30669	-4.73309	1.52105	H	-3.38436	-1.15825	1.24063
N	2.46901	-4.00044	1.30519	H	-4.99061	-2.64701	-0.87237
C	2.60136	-3.42580	2.63525	H	-5.84232	-0.61472	-1.65108
C	2.05592	-1.99397	2.77338	H	-5.34894	0.31434	-0.23783
O	2.02518	-1.47084	3.89833	H	-4.14411	-0.23075	-1.40901
C	4.05410	-3.47207	3.14835	H	-7.02548	-1.90340	0.35775
O	4.92517	-2.54536	2.52133	H	-6.05568	-3.02065	1.32347

H	-6.01131	-1.29183	1.67329	H	3.31047	4.64888	1.14754
H	-2.04536	-3.36713	1.21399	H	3.69843	5.35543	-3.40593
H	-4.39492	-4.93006	0.92524	H	5.29183	5.19539	-4.12797
H	-2.32436	-2.89717	6.73148	H	6.34813	6.22592	-2.09557
H	-1.51659	-1.87150	5.51911	H	4.75720	6.33754	-1.32985
H	-0.19622	-4.61275	3.62837	H	5.55062	10.08024	-2.17873
H	-0.33843	-2.91698	3.81792	H	5.09872	8.94515	-0.88707
H	-4.00831	-3.56738	5.04547	H	6.71720	8.85054	-1.64059
H	-2.44050	-1.91104	3.19386	H	4.52233	3.05949	-3.18811
H	-5.27905	2.86297	4.83162	H	4.52780	3.70722	-0.37624
H	-1.96079	2.53529	0.45950	H	8.89573	2.34048	-3.85171
H	-3.23043	1.43896	-0.11503	H	6.68809	3.42084	-4.18324
H	-2.40207	1.94605	2.76968	H	3.75718	1.94800	-6.04695
H	-2.53325	0.36183	2.01567	H	1.66183	0.69306	1.86459
H	-5.00985	0.63778	1.87704	H	-0.56334	0.98993	0.67707
H	-4.58535	1.21576	3.49338	H	-0.51086	-0.71530	0.22357
H	-3.46043	4.11614	1.28112	H	7.76899	-1.39670	-3.77601
H	-3.85291	6.31103	-3.93331	H	3.83239	0.77100	-0.67361
H	-2.99473	6.51385	-2.38337	H	4.03654	-0.94256	-0.44868
H	-2.59777	5.14987	-3.44263	H	3.50161	-1.28662	-2.90581
H	-5.31429	5.58669	-2.06941	H	2.80400	1.59701	-2.93287
H	-3.01299	4.61675	-0.89992	N	-5.41783	-1.62811	5.98087
H	-3.47301	1.66839	-5.48854	H	-5.88258	-0.77984	6.27647
H	-4.64779	0.42734	-5.93331	C	-6.13931	-2.89523	6.09072
H	-1.50111	0.73838	-3.55909	H	-7.15616	-2.68079	6.42380
H	-3.34567	-2.96540	-2.79949	H	-6.19204	-3.40740	5.12558
H	-5.79545	2.38694	-5.13681	H	-5.67535	-3.56611	6.82148
H	-4.17750	2.35827	-2.66733	H	1.74221	-1.78849	0.72318
H	-7.76072	1.63354	-0.37929	H	1.14385	-0.92133	-2.77401
H	-9.76349	1.00987	0.94223	H	0.38219	-2.26704	-1.15209
H	-10.42803	0.11864	-0.44578	N	-9.70431	0.87902	-4.13054
H	-8.94322	-0.43547	0.32682	H	-9.08781	1.64762	-4.34976
H	-9.67291	3.19588	-0.33915	C	-10.76080	0.52752	-5.05918
H	-10.37815	2.42086	-1.76851	H	-11.34698	-0.27184	-4.60461
H	-8.84685	3.30473	-1.89142	H	-11.40980	1.38796	-5.25114
H	-7.76685	-0.36777	-1.85051	H	-10.35527	0.16983	-6.01322
H	-6.85992	2.20337	-2.37943	H	6.05716	0.80041	-3.57903
H	9.28288	-2.97770	3.30177	H	6.01791	0.94512	-1.19033
H	7.22841	-6.84087	-0.64495	H	5.46676	-0.85464	-3.57655
H	6.77641	-6.55714	1.04097	H	8.28569	0.10607	-2.96482
H	8.23777	-4.51185	-0.73147	H	8.33289	-1.92855	-1.30339
H	7.12718	-4.06794	1.95832	H	9.49298	-1.43173	2.43568
H	3.62006	-3.92729	-4.26806	H	7.86280	-1.98070	2.92293
H	4.75005	-5.28364	-4.11572	H	0.50352	6.89728	6.31396
H	6.12191	-2.00336	-5.89077	H	0.37945	5.13484	6.63575
H	4.45296	-2.08888	-5.47697	H	-6.60442	4.01500	4.54783
H	4.28327	-3.06043	-2.07352	H	-6.70586	2.34302	3.92666
H	6.67403	-4.36705	-2.44698	H	-6.61587	-5.03933	-4.55988
H	1.68443	-6.23738	-0.50663	H	-5.02943	-4.62286	-5.20991
H	0.40435	-5.10745	-0.98354	H	2.04825	1.55108	-6.16079
H	2.28996	-3.48342	-1.44504	H	2.61201	2.62831	-4.85200
H	4.42243	-4.50244	3.04933	H	2.50310	0.76499	6.96670
H	4.02392	-3.20456	4.20688	H	1.17022	0.82389	8.13274
H	5.13155	-2.86688	1.62524	H	9.07369	4.09885	-3.61108
H	1.99476	-4.01720	3.32839	H	8.87239	3.02353	-2.20781
H	3.29236	-4.00617	0.70798	H	8.49736	-6.61440	0.58894
H	-1.73426	0.56519	4.80457	O	-0.68484	-2.33455	-1.26166
H	-1.47037	2.31268	4.58676	H	-1.24504	-1.72914	-2.14794
H	0.29648	1.89833	3.08562	H	-1.11683	-3.21536	-1.16812
H	1.78020	-0.75009	7.55595	H	-4.99221	-1.52466	-4.14855
H	0.62969	-0.45715	5.51937				
H	1.87993	6.01371	6.98422	Pro-Cov			
H	2.36649	1.86603	4.14342	C	-5.60349	-5.19944	-4.62204
H	3.66873	2.79989	4.86249	C	-5.09275	-5.03798	-3.19860
H	3.98342	-0.22505	3.24751	O	-5.25414	-3.97620	-2.59602
H	5.77375	-0.26146	1.44067	N	-4.43190	-6.09589	-2.65864
H	6.42741	2.11956	0.73647	C	-3.99401	-6.18027	-1.26982
H	3.31471	4.67252	3.34382	C	-3.29596	-4.90690	-0.77745
H	1.26821	3.69540	5.18187	O	-2.31531	-4.47120	-1.40494
H	0.49806	5.19498	-1.64081	C	-2.97325	-7.33026	-1.15913
H	1.70297	6.21344	-0.84949	O	-3.66229	-8.48242	-1.65903
H	1.09815	6.77837	2.02174	C	-2.46041	-7.53793	0.26413
H	-1.21499	7.07276	2.99182	N	-3.74228	-4.42809	0.38531
H	-3.03171	6.12817	1.47849	C	-3.19644	-3.29054	1.11347
H	1.06255	3.29566	-0.20572	C	-3.74165	-3.41357	2.55147

O	-4.63554	-4.21826	2.83174	C	0.13797	0.11813	0.52244
C	-3.54385	-1.92587	0.45949	S	1.01304	0.80592	-0.92753
C	-4.94215	-1.80185	-0.16603	N	-0.16992	1.08027	3.54100
C	-6.09832	-1.97322	0.82938	C	-0.97143	1.34250	4.72335
C	-5.07263	-0.46613	-0.91632	C	-0.02474	1.41349	5.91569
N	-3.17721	-2.57224	3.44401	O	0.22778	2.47797	6.49572
C	-3.43901	-2.68212	4.87366	N	0.55485	0.23955	6.24377
C	-4.20543	-1.44178	5.34799	C	1.60068	0.21029	7.24375
O	-3.74129	-0.30766	5.19715	C	1.09181	5.88591	6.34080
C	-2.11859	-2.83103	5.65873	C	1.64359	5.65152	4.94265
C	-1.42770	-4.10060	5.15130	O	2.05771	6.56588	4.22821
O	-1.81872	-5.20763	5.50449	N	1.70804	4.34145	4.57191
N	-0.42912	-3.89209	4.25403	C	2.57698	3.89071	3.49803
C	-6.00339	3.19795	4.15503	C	1.83173	3.73808	2.16314
C	-5.33963	3.68969	2.87491	O	0.74485	3.14788	2.09153
O	-5.26331	4.88809	2.60156	C	3.20108	2.54953	3.92547
N	-4.81639	2.73388	2.04314	C	4.13852	1.95205	2.92575
C	-3.94328	3.19199	0.96088	N	4.93384	2.71417	2.08484
C	-4.67177	3.54727	-0.33275	C	4.42474	0.61557	2.77063
O	-5.83272	3.22924	-0.58592	C	5.69468	1.83460	1.44670
C	-2.90803	2.06150	0.75481	N	5.42517	0.55932	1.83399
C	-2.96653	1.32340	2.09333	N	2.43171	4.24881	1.06478
C	-4.44919	1.36854	2.45370	C	1.80536	4.15489	-0.24268
N	-3.86924	4.20716	-1.22184	C	2.73237	3.79107	-1.40353
C	-4.44201	4.90260	-2.37054	O	2.21404	3.58678	-2.51049
C	-5.15369	4.00066	-3.38655	C	1.02771	5.45477	-0.62952
O	-5.97315	4.49043	-4.15697	C	-0.00817	5.85466	0.37735
C	-3.34168	5.69249	-3.08970	N	-1.36660	5.61467	0.20741
N	-4.78909	2.68547	-3.42922	C	0.20674	6.47739	1.58510
C	-5.37731	1.77614	-4.39397	C	-1.95302	6.09467	1.29299
C	-6.48031	0.86786	-3.80847	N	-1.03864	6.61674	2.15401
O	-6.69616	-0.25252	-4.27957	N	4.08673	3.80062	-1.26237
C	-4.30892	0.95613	-5.14294	C	4.89920	3.85160	-2.47759
C	-3.54321	-0.01103	-4.29751	C	6.36811	3.53649	-2.17382
N	-4.02950	-1.26632	-3.97594	O	6.80587	3.46712	-1.02899
C	-2.29576	0.04543	-3.71593	C	4.76459	5.23991	-3.15721
C	-3.09523	-1.90366	-3.23381	C	5.30005	6.37462	-2.28314
N	-2.02595	-1.14018	-3.06148	S	5.01176	7.98851	-3.10439
N	-7.23733	1.41465	-2.82650	C	5.69824	9.08433	-1.81352
C	-8.26380	0.63059	-2.13273	N	7.13452	3.37023	-3.28856
C	-9.45961	0.23171	-3.01936	C	8.58492	3.22109	-3.26429
O	-10.15394	-0.72757	-2.69617	C	2.82663	1.78951	-5.48512
C	-8.69612	1.39403	-0.85210	C	3.06392	0.54995	-4.64246
C	-9.41335	2.71365	-1.17485	O	3.25516	-0.55423	-5.16326
C	-9.54042	0.51037	0.07366	O	6.35120	-1.52648	0.19831
C	8.84791	-2.34716	2.46943	C	6.51753	-1.07603	-0.94290
C	8.69953	-3.04867	1.13046	N	7.51043	-1.43461	-1.77417
O	9.32859	-2.71170	0.12413	C	7.51721	-0.70719	-3.03657
N	7.85672	-4.12401	1.14979	C	6.08750	-0.11955	-3.09833
C	7.50413	-4.85032	-0.05701	C	5.66075	0.00078	-1.61962
C	6.10121	-4.45900	-0.52123	C	4.16323	-0.06663	-1.21619
O	5.19070	-4.30616	0.31125	C	3.15931	-0.34546	-2.33994
C	7.51495	-6.36747	0.18901	N	3.08129	0.75416	-3.29916
N	5.89722	-4.39289	-1.84195	C	1.73900	-0.67737	-1.83760
C	4.57721	-4.11959	-2.38451	O	1.75864	-1.83899	-1.06455
C	3.56289	-5.12857	-1.78345	H	-5.50170	-6.21181	-5.02149
O	3.82206	-6.32067	-1.70650	H	-2.13448	-7.06806	-1.82083
C	4.57338	-4.25778	-3.91774	H	-1.82916	-8.43218	0.29985
C	5.68554	-3.46952	-4.60048	H	-3.28947	-7.68055	0.96371
O	6.87372	-3.70295	-4.34648	H	-1.85058	-6.69404	0.60142
N	5.30369	-2.54568	-5.51218	H	-3.03371	-9.21475	-1.69394
N	2.40083	-4.54631	-1.39482	H	-4.85065	-6.41548	-0.62354
C	1.42843	-5.20188	-0.54521	H	-4.42630	-6.98332	-3.14296
C	1.38537	-4.64337	0.88900	H	-2.80155	-1.74084	-0.31803
O	0.37154	-4.79848	1.57282	H	-3.40001	-1.15048	1.21468
N	2.50689	-4.00446	1.31174	H	-5.03076	-2.59557	-0.90958
C	2.65979	-3.46574	2.65728	H	-5.86254	-0.54434	-1.66174
C	2.10833	-2.03902	2.84203	H	-5.32564	0.36843	-0.25491
O	2.10168	-1.52917	3.96983	H	-4.15165	-0.20792	-1.44849
C	4.12396	-3.51333	3.13458	H	-7.05702	-1.82576	0.32098
O	4.97615	-2.58483	2.48406	H	-6.11139	-2.96582	1.28451
N	1.62471	-1.43128	1.74381	H	-6.03857	-1.24111	1.64397
C	0.95903	-0.14705	1.79744	H	-2.10447	-3.39031	1.15882
C	-0.04134	-0.11980	2.96793	H	-4.52214	-4.87161	0.86180
O	-0.70698	-1.11712	3.29371	H	-2.34871	-2.96400	6.71905

H	-1.51371	-1.93125	5.53192	H	4.78969	6.37162	-1.31441
H	-0.16121	-4.66234	3.65438	H	5.59256	10.11050	-2.17171
H	-0.29828	-2.96809	3.85765	H	5.14624	8.97854	-0.87551
H	-4.01406	-3.59608	5.01270	H	6.75801	8.87583	-1.64273
H	-2.39918	-1.97512	3.17308	H	4.52606	3.09537	-3.17524
H	-5.25158	2.84195	4.86822	H	4.55423	3.74535	-0.36108
H	-1.92826	2.48956	0.53036	H	8.89030	2.36194	-3.86797
H	-3.19298	1.40227	-0.06914	H	6.69114	3.48411	-4.18787
H	-2.41926	1.90275	2.83385	H	3.70883	1.96251	-6.10943
H	-2.54955	0.31877	2.07900	H	1.69009	0.65559	1.93746
H	-5.02369	0.63428	1.88056	H	-0.56466	0.91905	0.74522
H	-4.62088	1.18649	3.51262	H	-0.43450	-0.76718	0.24120
H	-3.42850	4.08755	1.30628	H	7.73002	-1.38832	-3.86453
H	-3.77540	6.23802	-3.92979	H	3.87925	0.86706	-0.72569
H	-2.86904	6.40056	-2.40313	H	4.04222	-0.84250	-0.45339
H	-2.56915	5.01488	-3.46809	H	3.46175	-1.22366	-2.91548
H	-5.22639	5.58979	-2.03212	H	2.79061	1.66958	-2.96011
H	-2.96893	4.55782	-0.88332	N	-5.39868	-1.64709	5.95689
H	-3.61001	1.66259	-5.59891	H	-5.85485	-0.79474	6.25433
H	-4.80972	0.41391	-5.94973	C	-6.14449	-2.90287	6.03852
H	-1.57751	0.85271	-3.74381	H	-7.16298	-2.67432	6.35689
H	-3.23693	-2.88948	-2.82296	H	-6.18864	-3.40153	5.06593
H	-5.88497	2.42208	-5.11991	H	-5.70484	-3.59019	6.76905
H	-4.15161	2.32404	-2.73252	H	1.77157	-1.83819	0.82514
H	-7.76234	1.64137	-0.33050	H	1.09751	-0.82154	-2.71576
H	-9.77559	1.05540	0.99397	H	0.79016	-2.19642	-1.08202
H	-10.47475	0.20962	-0.40593	N	-9.71402	1.01245	-4.10317
H	-9.00356	-0.40328	0.34793	H	-9.06227	1.75601	-4.30561
H	-9.62897	3.25868	-0.25103	C	-10.77699	0.71981	-5.04380
H	-10.36190	2.53051	-1.69095	H	-11.39767	-0.06320	-4.60664
H	-8.80540	3.37062	-1.80490	H	-11.39068	1.60814	-5.22588
H	-7.83790	-0.33374	-1.83839	H	-10.37898	0.36240	-6.00116
H	-6.86483	2.22464	-2.33856	H	6.06412	0.83704	-3.62295
H	9.29380	-3.02151	3.20704	H	6.06769	0.94192	-1.22985
H	7.22871	-6.90648	-0.71839	H	5.43532	-0.80550	-3.63783
H	6.79565	-6.62437	0.97253	H	8.27899	0.08488	-3.02108
H	8.24599	-4.58127	-0.81222	H	8.28957	-1.97972	-1.40312
H	7.17943	-4.16540	1.90113	H	9.48443	-1.47245	2.34176
H	3.58603	-3.97059	-4.28910	H	7.86219	-2.03891	2.83530
H	4.73338	-5.31389	-4.15983	H	0.56956	6.84397	6.36723
H	6.04824	-1.99731	-5.92029	H	0.43290	5.07870	6.67131
H	4.38560	-2.10781	-5.49371	H	-6.54125	4.03671	4.59631
H	4.28493	-3.10023	-2.10178	H	-6.69614	2.37396	3.96181
H	6.66718	-4.40263	-2.50743	H	-6.65414	-4.90166	-4.64089
H	1.68361	-6.26473	-0.49749	H	-5.05228	-4.50720	-5.26532
H	0.41534	-5.10896	-0.94701	H	1.99014	1.59264	-6.16048
H	2.32987	-3.53251	-1.45674	H	2.61261	2.67938	-4.88870
H	4.49073	-4.54296	3.02399	H	2.54735	0.60501	6.85379
H	4.12086	-3.24778	4.19407	H	1.30088	0.82080	8.09665
H	5.17551	-2.91319	1.58912	H	9.08252	4.12070	-3.64148
H	2.06946	-4.07941	3.34566	H	8.88486	3.05660	-2.22889
H	3.33140	-4.02856	0.71588	H	8.51155	-6.68753	0.50208
H	-1.73633	0.57133	4.84383	O	-0.64802	-2.42384	-1.16306
H	-1.45044	2.31865	4.63305	H	-1.04910	-1.87175	-1.90066
H	0.30013	1.88798	3.11256	H	-1.18206	-3.25148	-1.14053
H	1.75846	-0.81985	7.56763	H	-4.99186	-1.55777	-4.11521
H	0.52330	-0.52350	5.57606				
H	1.93739	5.94457	7.03431	Reac-H₂O			
H	2.40979	1.82531	4.15068	C	-5.45954	-5.08680	-4.69728
H	3.72029	2.74411	4.87310	C	-4.59273	-4.85052	-3.46368
H	4.03205	-0.26682	3.24704	O	-4.51358	-3.72962	-2.95554
H	5.79446	-0.29776	1.41332	N	-3.96744	-5.94744	-2.96169
H	6.44393	2.08634	0.71217	C	-3.38159	-6.12280	-1.63224
H	3.36870	4.63427	3.37486	C	-2.78352	-4.85363	-0.99783
H	1.31626	3.64731	5.20431	O	-1.81044	-4.27073	-1.48649
H	0.55459	5.27460	-1.59682	C	-2.26213	-7.17644	-1.71685
H	1.75398	6.26654	-0.76150	O	-2.85238	-8.29855	-2.38808
H	1.10213	6.77639	2.10863	C	-1.73131	-7.57389	-0.34073
H	-1.22970	7.02665	3.05557	N	-3.33673	-4.54146	0.18642
H	-3.01464	6.09005	1.50489	C	-2.92613	-3.41806	1.00605
H	1.07828	3.34731	-0.17472	C	-3.53548	-3.64702	2.40385
H	3.32556	4.70322	1.18744	O	-4.34632	-4.55134	2.61340
H	3.70539	5.39406	-3.37839	C	-3.33715	-2.06580	0.37219
H	5.28889	5.23043	-4.11949	C	-4.75458	-1.99326	-0.21959
H	6.37275	6.25146	-2.09560	C	-5.87790	-2.23679	0.79883

C	-4.96821	-0.65092	-0.93625	C	0.03305	1.36248	5.85679
N	-3.11904	-2.76424	3.33928	O	0.17151	2.41641	6.49316
C	-3.46331	-2.89386	4.74350	N	0.70489	0.23506	6.16253
C	-4.17970	-1.62141	5.20899	C	1.65682	0.24840	7.25492
O	-3.73548	-0.50097	4.94470	C	0.97920	5.92660	6.48949
C	-2.20259	-3.09587	5.61994	C	1.55203	5.69013	5.09558
C	-1.46917	-4.34988	5.13855	O	1.94990	6.60978	4.37831
O	-1.84278	-5.46674	5.47598	N	1.65485	4.37983	4.73577
N	-0.43510	-4.10892	4.28837	C	2.51073	3.93988	3.64741
C	-6.04858	3.08656	4.27839	C	1.75149	3.76734	2.32332
C	-5.34814	3.56849	3.01063	O	0.67054	3.16750	2.27382
O	-5.15869	4.76680	2.79507	C	3.15038	2.59581	4.04924
N	-4.92876	2.60222	2.13422	C	4.04976	2.00717	3.00890
C	-3.97653	2.98947	1.08719	N	4.86554	2.78139	2.19993
C	-4.64391	3.30442	-0.25271	C	4.27056	0.67019	2.76865
O	-5.79605	2.98008	-0.53645	C	5.57516	1.91056	1.49674
C	-2.95814	1.81812	0.99531	N	5.25335	0.62615	1.81028
C	-3.20610	1.06653	2.30649	N	2.34109	4.25660	1.20664
C	-4.71236	1.19479	2.49840	C	1.69811	4.12414	-0.08976
N	-3.81443	3.94673	-1.13073	C	2.59845	3.74423	-1.26697
C	-4.36605	4.64771	-2.28966	O	2.04198	3.42203	-2.32810
C	-5.12118	3.76174	-3.28990	C	0.90566	5.41252	-0.49262
O	-5.98895	4.25529	-4.00343	C	-0.13378	5.80056	0.51375
C	-3.23442	5.37714	-3.02447	N	-1.48102	5.50256	0.35632
N	-4.72579	2.46055	-3.39299	C	0.06478	6.44045	1.71544
C	-5.32280	1.55555	-4.35864	C	-2.08017	5.96293	1.44335
C	-6.38488	0.60809	-3.75682	N	-1.18163	6.53015	2.29266
O	-6.51832	-0.54401	-4.16759	N	3.95106	3.88519	-1.20130
C	-4.25820	0.77624	-5.15674	C	4.72094	3.89668	-2.44819
C	-3.24440	0.06538	-4.31915	C	6.22718	3.76330	-2.14648
N	-3.36948	-1.22607	-3.84320	O	6.65273	3.64035	-1.00102
C	-2.02494	0.49576	-3.84715	C	4.39981	5.17624	-3.26108
C	-2.25655	-1.52401	-3.12286	C	4.83179	6.45440	-2.54182
N	-1.41428	-0.49681	-3.10589	S	4.33793	7.92284	-3.52236
N	-7.20332	1.17441	-2.82903	C	4.91878	9.22808	-2.38349
C	-8.22963	0.38752	-2.14159	N	7.02747	3.78208	-3.24985
C	-9.49479	0.12640	-2.98678	C	8.48821	3.70668	-3.21579
O	-10.24059	-0.80164	-2.68622	C	1.61559	1.59970	-5.39090
C	-8.55982	1.06153	-0.78164	C	2.32452	0.46616	-4.68024
C	-9.23964	2.42835	-0.95578	O	2.51299	-0.62679	-5.22737
C	-9.38657	0.14033	0.12309	O	6.16647	-1.38138	0.03390
C	8.94596	-1.98506	2.38285	C	6.38571	-0.84075	-1.05805
C	8.74558	-2.66135	1.03482	N	7.42650	-1.11245	-1.86199
O	9.31941	-2.27942	0.01054	C	7.47865	-0.29506	-3.06673
N	7.93562	-3.75889	1.06225	C	6.05241	0.30301	-3.14389
C	7.59629	-4.50770	-0.13634	C	5.54718	0.28096	-1.68572
C	6.13658	-4.27146	-0.52084	C	4.03644	0.15216	-1.37316
O	5.25867	-4.25156	0.35994	C	3.14439	-0.34108	-2.51622
C	7.78660	-6.01737	0.08492	N	2.71571	0.72692	-3.40335
N	5.85683	-4.19930	-1.82659	C	1.95553	-1.17266	-2.05531
C	4.48691	-4.04455	-2.28693	O	2.06101	-1.98646	-1.14221
C	3.61193	-5.18324	-1.69078	H	-5.25845	-6.03409	-5.20446
O	4.02342	-6.33024	-1.60268	H	-1.46026	-6.73864	-2.32843
C	4.41373	-4.09699	-3.82443	H	-0.95895	-8.34308	-0.44892
C	5.39637	-3.15762	-4.51719	H	-2.53894	-7.98979	0.26928
O	6.61397	-3.25456	-4.31986	H	-1.28526	-6.73251	0.19751
N	4.87135	-2.25363	-5.37456	H	-2.15619	-8.94376	-2.56375
N	2.37756	-4.76072	-1.31041	H	-4.16086	-6.52506	-0.96932
C	1.50955	-5.49780	-0.41880	H	-4.08669	-6.83046	-3.44065
C	1.49119	-4.93654	1.01545	H	-2.62489	-1.86368	-0.43131
O	0.52351	-5.16656	1.74154	H	-3.20471	-1.28180	1.11882
N	2.56622	-4.18866	1.38580	H	-4.81794	-2.77168	-0.98248
C	2.70784	-3.59422	2.70966	H	-5.77402	-0.75317	-1.66117
C	2.06619	-2.19985	2.84705	H	-5.23873	0.15662	-0.25032
O	2.07647	-1.62117	3.93911	H	-4.07653	-0.33637	-1.48727
C	4.18243	-3.50404	3.15220	H	-6.85287	-2.06828	0.32932
O	4.93175	-2.51876	2.45879	H	-5.86820	-3.25507	1.19233
N	1.49668	-1.69855	1.73368	H	-5.79864	-1.55429	1.65325
C	0.77374	-0.43931	1.69389	H	-1.83357	-3.44040	1.11378
C	-0.11117	-0.31193	2.94408	H	-4.08824	-5.09188	0.58774
O	-0.74911	-1.28276	3.38089	H	-2.51141	-3.25662	6.65647
C	-0.14402	-0.40813	0.44302	H	-1.58249	-2.19787	5.56302
S	0.37262	0.86779	-0.77296	H	-0.11516	-4.86601	3.69610
N	-0.17527	0.91516	3.46143	H	-0.31845	-3.17688	3.90822
C	-0.91263	1.25884	4.66469	H	-4.09228	-3.77986	4.82590

H	-2.36033	-2.12088	3.12930	H	4.41906	3.02991	-3.04860
H	-5.33216	2.60801	4.95526	H	4.46123	3.90042	-0.32234
H	-1.93801	2.19566	0.89147	H	8.84247	2.85648	-3.80616
H	-3.17116	1.18071	0.13277	H	6.59041	3.91460	-4.14934
H	-2.73108	1.60325	3.12403	H	2.01493	1.69436	-6.40296
H	-2.84658	0.04177	2.34174	H	1.48395	0.39702	1.68007
H	-5.26943	0.54458	1.81744	H	-1.17167	-0.19667	0.73085
H	-5.01562	0.97109	3.51682	H	-0.13862	-1.38341	-0.04903
H	-3.46185	3.88686	1.42406	H	7.71517	-0.91675	-3.93396
H	-3.64471	5.93175	-3.87086	H	3.64220	1.10829	-1.02073
H	-2.72801	6.07247	-2.34882	H	3.92908	-0.54309	-0.53568
H	-2.49575	4.65903	-3.39600	H	3.69648	-1.06233	-3.13317
H	-5.11833	5.37417	-1.96060	H	2.42029	1.60483	-2.97650
H	-2.94150	4.33106	-0.75627	N	-5.29370	-1.78003	5.96164
H	-3.73119	1.49456	-5.79130	H	-5.70864	-0.91062	6.26896
H	-4.77845	0.06826	-5.80581	C	-5.97292	-3.03239	6.28222
H	-1.55772	1.45898	-4.00356	H	-6.85548	-2.79880	6.87969
H	-2.11413	-2.48272	-2.64144	H	-6.29767	-3.55907	5.37925
H	-5.87128	2.20038	-5.05502	H	-5.33408	-3.70087	6.86804
H	-4.05043	2.09778	-2.73313	H	1.64748	-2.18122	0.85813
H	-7.58942	1.23561	-0.30013	H	1.06003	-1.13972	-2.69822
H	-9.54070	0.61733	1.09696	N	-9.74418	0.98956	-4.00945
H	-10.36054	-0.08175	-0.31877	H	-9.05093	1.70066	-4.19322
H	-8.87702	-0.81408	0.28968	C	-10.88986	0.85605	-4.88627
H	-9.37971	2.90256	0.02019	H	-11.48144	1.77791	-4.90257
H	-10.22284	2.32289	-1.42702	H	-10.58384	0.61595	-5.91131
H	-8.64202	3.11545	-1.56290	H	-11.50533	0.04224	-4.50078
H	-7.83528	-0.61584	-1.95362	H	6.05874	1.30295	-3.57930
H	-6.86566	2.00803	-2.35810	H	5.90797	1.18707	-1.18603
H	9.54949	-1.08943	2.24135	H	5.43192	-0.33105	-3.77760
H	7.51097	-6.57523	-0.81440	H	8.24126	0.48960	-2.96774
H	7.14382	-6.35876	0.90171	H	8.21252	-1.64558	-1.48600
H	8.26321	-4.15367	-0.92526	H	7.97506	-1.71361	2.81250
H	7.29549	-3.85297	1.84078	H	9.45077	-2.66302	3.07775
H	3.38249	-3.90076	-4.13071	H	0.42286	6.86555	6.49487
H	4.67043	-5.11367	-4.14182	H	0.34431	5.10264	6.82611
H	5.52924	-1.63496	-5.82779	H	-6.47618	3.95847	4.77293
H	3.89589	-1.95805	-5.36834	H	-6.83898	2.36390	4.05731
H	4.10577	-3.08396	-1.92245	H	-6.50595	-5.07043	-4.37758
H	6.58576	-4.08424	-2.52736	H	-5.31591	-4.25870	-5.39382
H	1.83838	-6.54028	-0.39027	H	0.55872	1.32628	-5.47701
H	0.47604	-5.45552	-0.77353	H	1.69284	2.55037	-4.85816
H	2.16576	-3.77195	-1.38442	H	1.18970	0.67259	8.14605
H	4.63541	-4.49948	3.05249	H	1.97573	-0.77466	7.45921
H	4.18207	-3.21503	4.20542	H	8.93414	4.62716	-3.60438
H	5.13372	-2.85878	1.56813	H	8.78950	3.57264	-2.17647
H	2.17448	-4.22226	3.43144	H	8.82811	-6.22905	0.33828
H	3.37316	-4.15060	0.76661	H	-4.19090	-1.82569	-3.88711
H	-1.69451	0.51619	4.84618	H	-0.41270	0.36430	-1.78923
H	-1.36223	2.24427	4.53727				
H	0.29983	1.70075	3.00229				
H	2.53937	0.85400	7.01513	TS-1-H₂O			
H	0.73582	-0.53211	5.49885	C	-5.34356	-5.14368	-4.77417
H	1.81593	6.02628	7.18875	C	-4.52700	-4.86220	-3.51339
H	2.36372	1.87151	4.28866	O	-4.49630	-3.73105	-3.01906
H	3.70124	2.77979	4.98066	N	-3.89151	-5.93426	-2.97548
H	3.85414	-0.22208	3.20622	C	-3.32050	-6.08532	-1.63585
H	5.59948	-0.21999	1.35241	C	-2.77565	-4.79925	-0.99168
H	6.32472	2.17421	0.76617	O	-1.83989	-4.16339	-1.48709
H	3.29416	4.69025	3.51404	C	-2.16282	-7.10007	-1.70532
H	1.23871	3.67687	5.34262	O	-2.71209	-8.24421	-2.37381
H	0.43080	5.21718	-1.45646	C	-1.62400	-7.47110	-0.32527
H	1.62269	6.23128	-0.63243	N	-3.32154	-4.53063	0.20689
H	0.95077	6.77883	2.23133	C	-2.93610	-3.40824	1.04037
H	-1.38419	6.93298	3.19485	C	-3.48695	-3.68851	2.45301
H	-3.13787	5.90645	1.66916	O	-4.30468	-4.58752	2.66411
H	0.97186	3.31770	0.00917	C	-3.43201	-2.05591	0.46358
H	3.22441	4.73493	1.31295	C	-4.83344	-2.05862	-0.16827
H	3.32263	5.18628	-3.44330	C	-5.96254	-2.39378	0.81700
H	4.87617	5.12073	-4.24687	C	-5.11706	-0.71622	-0.85682
H	5.91768	6.46925	-2.39242	N	-3.00986	-2.84828	3.39511
H	4.35576	6.50587	-1.55710	C	-3.29275	-2.99930	4.81293
H	4.68507	10.18837	-2.84787	C	-4.05372	-1.75863	5.29489
H	4.40308	9.16596	-1.42126	O	-3.59355	-0.62469	5.13255
H	5.99924	9.16344	-2.22783	C	-1.98727	-3.14725	5.62631
				C	-1.24811	-4.38876	5.11982

O	-1.60336	-5.51186	5.45882	N	1.56382	4.36322	4.75740
N	-0.23762	-4.13281	4.24811	C	2.41192	3.95969	3.64941
C	-6.09735	2.90878	4.29791	C	1.63538	3.77213	2.33617
C	-5.44668	3.39362	3.00466	O	0.54024	3.19730	2.31037
O	-5.37780	4.59146	2.72548	C	3.10568	2.63740	4.03669
N	-4.92690	2.43536	2.17386	C	4.01185	2.07482	2.98812
C	-4.04390	2.88399	1.08999	N	4.80410	2.86813	2.17379
C	-4.78118	3.22365	-0.20455	C	4.27123	0.74382	2.75365
O	-5.92794	2.85818	-0.46086	C	5.53861	2.01387	1.47460
C	-2.99777	1.75365	0.91254	N	5.25367	0.72303	1.79445
C	-3.07047	1.04937	2.26821	N	2.23102	4.22367	1.20672
C	-4.55888	1.07482	2.59635	C	1.59680	4.05238	-0.09119
N	-4.01543	3.93551	-1.08663	C	2.52302	3.73174	-1.26725
C	-4.63923	4.64270	-2.20379	O	1.98794	3.42695	-2.34397
C	-5.32090	3.74398	-3.24552	C	0.75018	5.30514	-0.50700
O	-6.17606	4.21309	-3.98910	C	-0.27754	5.70595	0.50632
C	-3.58900	5.51137	-2.90660	N	-1.62772	5.40892	0.37119
N	-4.88017	2.45564	-3.33543	C	-0.06445	6.36981	1.69248
C	-5.43951	1.51870	-4.29093	C	-2.21214	5.88913	1.45804
C	-6.47596	0.54629	-3.68517	N	-1.30242	6.47106	2.28463
O	-6.59567	-0.60001	-4.11569	N	3.87127	3.90898	-1.18693
C	-4.34572	0.75401	-5.06449	C	4.64430	3.98811	-2.42962
C	-3.32616	0.09981	-4.18914	C	6.15341	3.89345	-2.13007
N	-3.38175	-1.20621	-3.73395	O	6.58489	3.78611	-0.98542
C	-2.17835	0.61977	-3.64061	C	4.29111	5.28934	-3.19448
C	-2.30350	-1.44163	-2.95196	C	4.68215	6.54929	-2.42154
N	-1.55269	-0.34504	-2.87981	S	4.13694	8.04124	-3.33736
N	-7.28937	1.08255	-2.73728	C	4.67588	9.31465	-2.14311
C	-8.31620	0.27249	-2.07883	N	6.95066	3.93816	-3.23520
C	-9.54130	-0.01798	-2.96936	C	8.41354	3.93000	-3.20254
O	-10.28257	-0.95692	-2.69271	C	1.65175	1.65542	-5.38392
C	-8.70703	0.94187	-0.73362	C	2.34628	0.50472	-4.68306
C	-9.43442	2.27953	-0.93791	O	2.53334	-0.57938	-5.25013
C	-9.52003	-0.00760	0.15414	O	6.25177	-1.24656	0.02161
C	9.00052	-1.81612	2.32807	C	6.43178	-0.70016	-1.07464
C	8.84901	-2.48352	0.97049	N	7.47298	-0.92937	-1.89141
O	9.41055	-2.06080	-0.04433	C	7.47714	-0.11093	-3.09628
N	8.09248	-3.61908	0.97852	C	6.02628	0.42673	-3.15697
C	7.77004	-4.34843	-0.23606	C	5.53503	0.38004	-1.69394
C	6.29955	-4.14895	-0.59999	C	4.03396	0.17508	-1.36969
O	5.43337	-4.16001	0.29266	C	3.15347	-0.32386	-2.51540
C	8.01218	-5.85600	-0.05581	N	2.72354	0.74582	-3.40069
N	6.00335	-4.07133	-1.90132	C	1.97325	-1.18133	-2.06342
C	4.62479	-3.95993	-2.34826	O	2.11353	-2.03756	-1.17929
C	3.79712	-5.13473	-1.75469	H	-5.10656	-6.09871	-5.24987
O	4.25261	-6.26645	-1.67768	H	-1.37333	-6.63849	-2.31590
C	4.54116	-3.99975	-3.88556	H	-0.83887	-8.22812	-0.42672
C	5.49045	-3.02602	-4.57754	H	-2.42209	-7.89384	0.29259
O	6.71217	-3.08982	-4.39142	H	-1.18805	-6.61707	0.20131
N	4.93264	-2.13119	-5.42373	H	-1.99619	-8.87166	-2.53414
N	2.55306	-4.75886	-1.35975	H	-4.09486	-6.51656	-0.98596
C	1.73199	-5.52998	-0.45362	H	-3.96868	-6.82424	-3.45048
C	1.69085	-4.94668	0.97191	H	-2.71369	-1.75072	-0.30073
O	0.72098	-5.18094	1.69419	H	-3.38407	-1.30985	1.25732
N	2.75533	-4.18502	1.34019	H	-4.83127	-2.82031	-0.95177
C	2.87940	-3.57258	2.65671	H	-5.91869	-0.84792	-1.58063
C	2.19583	-2.19806	2.78401	H	-5.42250	0.06581	-0.15524
O	2.15459	-1.63640	3.88586	H	-4.24592	-0.34722	-1.40696
C	4.35050	-3.43538	3.09819	H	-6.93411	-2.31493	0.31735
O	5.06797	-2.42774	2.40369	H	-5.87378	-3.40251	1.22493
N	1.65238	-1.69704	1.65984	H	-5.96956	-1.69678	1.66424
C	0.86815	-0.47446	1.61309	H	-1.84119	-3.38085	1.10872
C	-0.02004	-0.38126	2.86020	H	-4.04729	-5.11465	0.60830
O	-0.66292	-1.36400	3.26396	H	-2.24094	-3.30515	6.67808
C	-0.05834	-0.49735	0.36706	H	-1.39820	-2.23200	5.53179
S	0.46271	0.65736	-0.95839	H	0.08476	-4.88500	3.65082
N	-0.09265	0.83258	3.40617	H	-0.14228	-3.19949	3.86519
C	-0.85719	1.16401	4.59502	H	-3.87208	-3.91521	4.92165
C	0.05414	1.27779	5.80898	H	-2.26349	-2.19662	3.16297
O	0.12244	2.31677	6.48052	H	-5.33344	2.57594	5.00932
N	0.77023	0.17511	6.10126	H	-2.01072	2.16559	0.68793
C	1.67098	0.20233	7.23325	H	-3.28004	1.07662	0.10217
C	0.87040	5.87324	6.53556	H	-2.56175	1.66743	3.00347
C	1.41370	5.66667	5.12452	H	-2.63035	0.05628	2.30877
O	1.75364	6.60509	4.40167	H	-5.11571	0.33275	2.01412

H	-4.74735	0.89560	3.65200	H	-0.09797	-1.51432	-0.03468
H	-3.53383	3.78459	1.42779	H	7.72928	-0.72198	-3.96679
H	-4.05933	6.06412	-3.72201	H	3.60196	1.10178	-0.98427
H	-3.14230	6.21694	-2.20055	H	3.96341	-0.54879	-0.55268
H	-2.78903	4.88650	-3.31790	H	3.71762	-1.03437	-3.13344
H	-5.45115	5.27777	-1.83028	H	2.42553	1.62128	-2.97133
H	-3.13461	4.32809	-0.73810	N	-5.23586	-1.95992	5.92287
H	-3.83217	1.46987	-5.71222	H	-5.68565	-1.10805	6.23089
H	-4.83696	0.01154	-5.69639	C	-5.96280	-3.22115	6.05494
H	-1.76828	1.61413	-3.74341	H	-6.95598	-3.00245	6.45051
H	-2.11349	-2.39223	-2.46797	H	-6.07843	-3.71854	5.08734
H	-5.99894	2.13411	-5.00493	H	-5.46417	-3.90786	6.74685
H	-4.23677	2.11610	-2.63341	H	1.84530	-2.15308	0.77588
H	-7.75744	1.15591	-0.22725	H	1.15257	-1.25005	-2.79493
H	-9.73185	0.47188	1.11579	N	-9.75712	0.83048	-4.01050
H	-10.46537	-0.28219	-0.31927	H	-9.08334	1.56832	-4.15564
H	-8.96903	-0.93311	0.35102	C	-10.86969	0.68066	-4.92658
H	-9.61360	2.75974	0.02865	H	-11.49927	1.57741	-4.93373
H	-10.40273	2.13130	-1.42810	H	-10.52101	0.48717	-5.94754
H	-8.85012	2.98021	-1.54278	H	-11.46295	-0.16909	-4.58654
H	-7.90713	-0.72150	-1.87412	H	5.98740	1.42747	-3.58923
H	-6.95899	1.90662	-2.24386	H	5.85608	1.30247	-1.19712
H	9.58330	-0.90352	2.20995	H	5.42656	-0.22993	-3.78706
H	7.74694	-6.39939	-0.96697	H	8.20741	0.70508	-3.00596
H	7.38853	-6.23975	0.75704	H	8.28276	-1.43317	-1.52582
H	8.41732	-3.95180	-1.02113	H	8.01123	-1.57455	2.73308
H	7.45411	-3.75047	1.75314	H	9.50414	-2.48685	3.03082
H	3.50230	-3.83009	-4.18148	H	0.28794	6.79564	6.56550
H	4.82498	-5.00535	-4.21516	H	0.26724	5.02815	6.87853
H	5.56972	-1.48730	-5.87169	H	-6.64182	3.74763	4.73086
H	3.95047	-1.85781	-5.39942	H	-6.78165	2.07400	4.12265
H	4.21098	-3.01809	-1.97132	H	-6.40121	-5.13815	-4.49378
H	6.72182	-3.93232	-2.60854	H	-5.18797	-4.33014	-5.48529
H	2.11941	-6.55202	-0.41208	H	0.59244	1.39644	-5.48462
H	0.69534	-5.55483	-0.79957	H	1.73226	2.59756	-4.83704
H	2.30578	-3.77372	-1.42286	H	1.14060	0.55406	8.12075
H	4.83485	-4.41625	3.00038	H	2.05038	-0.80542	7.40885
H	4.34166	-3.14482	4.15104	H	8.81660	4.87254	-3.58530
H	5.27661	-2.75724	1.51087	H	8.72121	3.80302	-2.16421
H	2.36514	-4.20815	3.38556	H	9.06235	-6.03923	0.18371
H	3.55873	-4.12912	0.71758	H	-4.14941	-1.87262	-3.82978
H	-1.63455	0.41364	4.76544	H	-0.56275	0.10691	-1.97209
H	-1.31198	2.14575	4.46155				
H	0.34941	1.63452	2.94737				
H	2.51939	0.87576	7.05984	Int-H2O			
H	0.86490	-0.56885	5.41700	C	-5.35145	-5.23563	-4.75885
H	1.72179	5.98815	7.21447	C	-4.54612	-4.91075	-3.50383
H	2.34925	1.88587	4.28863	O	-4.54155	-3.76369	-3.04107
H	3.66330	2.84050	4.96010	N	-3.89266	-5.95538	-2.94063
H	3.87879	-0.15718	3.19558	C	-3.30781	-6.07097	-1.60294
H	5.62473	-0.11477	1.33987	C	-2.78799	-4.76436	-0.98840
H	6.28064	2.29549	0.74328	O	-1.89458	-4.09828	-1.52760
H	3.16632	4.73788	3.50678	C	-2.12593	-7.05972	-1.66544
H	1.17555	3.64202	5.36095	O	-2.65678	-8.22467	-2.31255
H	0.26146	5.06817	-1.45409	C	-1.56752	-7.39454	-0.28427
H	1.44093	6.13831	-0.68860	N	-3.29795	-4.49876	0.22160
H	0.82735	6.71528	2.19305	C	-2.89507	-3.37718	1.05009
H	-1.48844	6.88655	3.18467	C	-3.47070	-3.65052	2.45558
H	-3.26757	5.83662	1.69500	O	-4.28753	-4.55497	2.65335
H	0.91496	3.20461	-0.00141	C	-3.35708	-2.01587	0.46571
H	3.14632	4.64201	1.29950	C	-4.74172	-2.00081	-0.20323
H	3.21501	5.27590	-3.38289	C	-5.89552	-2.35676	0.74559
H	4.77600	5.28674	-4.17751	C	-5.01291	-0.64414	-0.87059
H	5.76716	6.59422	-2.27217	N	-3.01125	-2.81002	3.40220
H	4.20688	6.54307	-1.43517	C	-3.30060	-2.97669	4.81666
H	4.40848	10.28585	-2.56468	C	-4.10539	-1.76660	5.29777
H	4.16518	9.19278	-1.18394	O	-3.69067	-0.61547	5.13164
H	5.75829	9.28001	-1.99159	C	-1.99506	-3.09287	5.63361
H	4.36724	3.13677	-3.06260	C	-1.24642	-4.33045	5.13081
H	4.37841	3.92338	-0.30623	O	-1.61556	-5.45488	5.45209
H	8.80585	3.10065	-3.79833	N	-0.22313	-4.06972	4.27873
H	6.50708	4.05360	-4.13394	C	-6.13835	2.84598	4.28444
H	2.06090	1.75992	-6.39113	C	-5.51876	3.36896	2.99224
H	1.53308	0.39696	1.58311	O	-5.49249	4.57097	2.72805
H	-1.07408	-0.22298	0.65033	N	-4.97386	2.43867	2.14147
				C	-4.09485	2.93909	1.07872

C	-4.80885	3.25108	-0.23486	C	4.28999	0.75545	2.75985
O	-5.94790	2.87742	-0.51471	C	5.51858	2.05975	1.47921
C	-2.98178	1.87093	0.91708	N	5.28274	0.76371	1.81246
C	-3.05947	1.12727	2.25076	N	2.18169	4.17724	1.18339
C	-4.55396	1.08806	2.54954	C	1.56060	4.00983	-0.12257
N	-4.02342	3.95214	-1.11030	C	2.49843	3.72096	-1.29724
C	-4.62048	4.66111	-2.24044	O	1.97223	3.44821	-2.38624
C	-5.26306	3.77016	-3.31195	C	0.70869	5.26125	-0.53639
O	-6.04510	4.25755	-4.11984	C	-0.30284	5.68529	0.48261
C	-3.55863	5.54678	-2.90461	N	-1.65943	5.40724	0.36954
N	-4.87417	2.45882	-3.35353	C	-0.06430	6.36118	1.65654
C	-5.44373	1.53212	-4.31179	C	-2.22067	5.90965	1.45921
C	-6.46178	0.54599	-3.70145	N	-1.29116	6.48790	2.26521
O	-6.53343	-0.61576	-4.10564	N	3.84493	3.89151	-1.20094
C	-4.36318	0.77263	-5.10768	C	4.62903	3.98360	-2.43423
C	-3.38434	0.05107	-4.24141	C	6.13168	3.88651	-2.11925
N	-3.51518	-1.26091	-3.80563	O	6.55660	3.84494	-0.96781
C	-2.22054	0.50905	-3.68504	C	4.29649	5.29916	-3.18458
C	-2.47595	-1.59200	-3.02758	C	4.68165	6.54341	-2.38352
N	-1.68020	-0.52326	-2.94813	C	4.14355	8.05380	-3.27335
N	-7.29862	1.07455	-2.77354	C	4.68521	9.30287	-2.05483
C	-8.29831	0.24080	-2.09941	N	6.93221	3.86893	-3.22140
C	-9.52058	-0.09451	-2.97943	C	8.39238	3.85669	-3.17892
O	-10.22769	-1.05443	-2.68824	C	2.00136	1.71722	-5.42233
C	-8.69885	0.90982	-0.75673	C	2.55576	0.52687	-4.65848
C	-9.47191	2.22074	-0.96614	O	2.73311	-0.56157	-5.22199
C	-9.47407	-0.05732	0.14576	O	6.34067	-1.21186	0.11237
C	8.96954	-1.87057	2.37226	C	6.50038	-0.71423	-1.01037
C	8.83695	-2.56073	1.02402	N	7.51691	-0.99934	-1.84137
O	9.43672	-2.17390	0.01675	C	7.51746	-0.21975	-3.07165
N	8.05159	-3.67679	1.03574	C	6.07768	0.34791	-3.12284
C	7.72415	-4.40910	-0.17658	C	5.61012	0.35804	-1.65116
C	6.26666	-4.15766	-0.56429	C	4.10901	0.18846	-1.30199
O	5.39240	-4.11574	0.31937	C	3.19529	-0.30873	-2.41924
C	7.90817	-5.92164	0.02610	N	2.84051	0.75496	-3.35395
N	5.99031	-4.08784	-1.86910	C	1.93649	-1.04578	-1.89357
C	4.62476	-3.91818	-2.34213	O	2.15026	-1.97413	-1.01610
C	3.72531	-5.04210	-1.75810	H	-5.11949	-6.21074	-5.19412
O	4.11114	-6.20324	-1.69490	H	-1.35172	-6.59091	-2.28974
C	4.57136	-3.97894	-3.87941	H	-0.76886	-8.13763	-0.38151
C	5.58334	-3.06987	-4.56745	H	-2.35107	-7.82197	0.34897
O	6.79810	-3.20169	-4.36738	H	-1.14071	-6.52356	0.22207
N	5.08586	-2.15333	-5.42822	H	-1.92968	-8.84100	-2.46600
N	2.51263	-4.58209	-1.37017	H	-4.06744	-6.50902	-0.94099
C	1.62913	-5.31796	-0.49714	H	-3.94551	-6.85562	-3.40002
C	1.60816	-4.76939	0.94178	H	-2.61096	-1.71302	-0.27365
O	0.61239	-4.95670	1.64854	H	-3.32047	-1.27506	1.26476
N	2.71867	-4.10571	1.34630	H	-4.72523	-2.74819	-1.00042
C	2.85198	-3.49396	2.65980	H	-5.79925	-0.76065	-1.61390
C	2.19094	-2.10860	2.78760	H	-5.33517	0.12322	-0.16155
O	2.08447	-1.59336	3.91225	H	-4.12860	-0.25817	-1.38981
C	4.32239	-3.39408	3.11219	H	-6.85323	-2.27942	0.21979
O	5.06924	-2.39233	2.44034	H	-5.80900	-3.37042	1.14100
N	1.73976	-1.55292	1.65411	H	-5.93125	-1.67284	1.60219
C	0.91014	-0.36394	1.61401	H	-1.80092	-3.37313	1.13570
C	-0.03011	-0.33775	2.82469	H	-3.98803	-5.10168	0.65990
O	-0.68590	-1.34145	3.15036	H	-2.24651	-3.24543	6.68673
C	0.03312	-0.40526	0.33569	H	-1.41681	-2.17089	5.53337
S	0.70645	0.46986	-1.12289	H	0.09140	-4.81125	3.66395
N	-0.13174	0.84887	3.42767	H	-0.11628	-3.13401	3.90510
C	-0.91227	1.12045	4.61976	H	-3.85012	-3.91143	4.91860
C	-0.00448	1.22726	5.83803	H	-2.26614	-2.15217	3.17781
O	0.04238	2.25672	6.52589	H	-5.35759	2.51716	4.97910
N	0.73149	0.13224	6.11151	H	-2.01240	2.34510	0.74411
C	1.62445	0.15683	7.25039	H	-3.19580	1.20058	0.08013
C	0.82024	5.82466	6.53167	H	-2.58689	1.74203	3.01265
C	1.33168	5.62252	5.10942	H	-2.58199	0.15085	2.26690
O	1.65341	6.56436	4.38278	H	-5.06939	0.33387	1.94629
N	1.47800	4.32034	4.73454	H	-4.75599	0.88116	3.59748
C	2.33036	3.92529	3.62602	H	-3.64628	3.86604	1.43168
C	1.55960	3.74702	2.30643	H	-4.00965	6.09930	-3.73065
O	0.44506	3.20894	2.27245	H	-3.14264	6.25114	-2.17928
C	3.03961	2.61210	4.01419	H	-2.73821	4.93434	-3.29375
C	3.97417	2.07656	2.97684	H	-5.44894	5.28653	-1.88658
N	4.74298	2.89273	2.16134	H	-3.15060	4.34895	-0.74289

H	-3.81511	1.49977	-5.71211	H	-5.75938	-1.18440	6.24021
H	-4.85972	0.06966	-5.77887	C	-5.94673	-3.30769	6.07063
H	-1.73645	1.46975	-3.75410	H	-6.94263	-3.13117	6.48021
H	-2.32338	-2.55289	-2.54137	H	-6.05405	-3.81027	5.10472
H	-6.00673	2.15790	-5.01379	H	-5.40940	-3.97176	6.75552
H	-4.32020	2.10304	-2.58692	H	1.98693	-1.93340	0.73145
H	-7.75241	1.15870	-0.26029	H	1.31504	-1.32412	-2.76741
H	-9.69233	0.42405	1.10482	N	-9.77300	0.73672	-4.02724
H	-10.41453	-0.36506	-0.31676	H	-9.13008	1.49910	-4.18284
H	-8.89300	-0.96326	0.34611	C	-10.89609	0.54863	-4.92425
H	-9.65758	2.70354	-0.00231	H	-11.56300	1.41786	-4.91092
H	-10.43938	2.03637	-1.44543	H	-10.55811	0.37948	-5.95284
H	-8.91764	2.93608	-1.58233	H	-11.44688	-0.32809	-4.58153
H	-7.85541	-0.73779	-1.89017	H	6.05082	1.33681	-3.58362
H	-6.99796	1.92031	-2.29686	H	5.95688	1.29057	-1.19026
H	9.55460	-0.96031	2.24671	H	5.45171	-0.31316	-3.72090
H	7.64060	-6.46628	-0.88370	H	8.26791	0.58180	-3.01926
H	7.25545	-6.27219	0.83116	H	8.31878	-1.51627	-1.47777
H	8.39822	-4.04582	-0.95531	H	7.97522	-1.62285	2.76025
H	7.38179	-3.76360	1.79034	H	9.46510	-2.52980	3.09161
H	3.54930	-3.75674	-4.19728	H	0.24074	6.74817	6.57887
H	4.80708	-5.00445	-4.18506	H	0.22319	4.97945	6.88529
H	5.76319	-1.54015	-5.85991	H	-6.69654	3.66352	4.73998
H	4.12184	-1.81990	-5.39385	H	-6.80512	1.99817	4.10358
H	4.24450	-2.95485	-1.98536	H	-6.41164	-5.20877	-4.48977
H	6.72546	-4.00137	-2.56746	H	-5.18147	-4.45386	-5.50202
H	1.93990	-6.36700	-0.47316	H	1.01281	1.44736	-5.80568
H	0.59672	-5.25895	-0.85379	H	1.91970	2.61971	-4.81262
H	2.34220	-3.55980	-1.38060	H	1.07948	0.47541	8.14154
H	4.78626	-4.38368	3.00339	H	2.02710	-0.84523	7.40566
H	4.31253	-3.11896	4.16950	H	8.80306	4.76833	-3.62370
H	5.26260	-2.70549	1.53791	H	8.69298	3.80071	-2.13232
H	2.32345	-4.11709	3.38859	H	8.94616	-6.14018	0.28845
H	3.51151	-4.04300	0.71174	H	-4.32357	-1.87762	-3.91586
H	-1.67236	0.34732	4.76256	H	-0.83250	-0.38436	-2.35059
H	-1.39527	2.09259	4.51795				
H	0.29470	1.67427	2.99786				
H	2.45736	0.85462	7.09880	Reac-N3			
H	0.87186	-0.57987	5.39946	C	-5.54718	-4.48773	-5.12113
H	1.68719	5.93450	7.19153	C	-5.07107	-4.45156	-3.67853
H	2.29626	1.84305	4.25217	O	-4.99780	-3.38557	-3.06283
H	3.57947	2.82087	4.94710	N	-4.74094	-5.64931	-3.13393
H	3.92530	-0.15642	3.20240	C	-4.42767	-5.90073	-1.73551
H	5.68166	-0.06478	1.35971	C	-3.52103	-4.82508	-1.11903
H	6.25469	2.36207	0.75027	O	-2.50871	-4.44047	-1.72058
H	3.07788	4.71089	3.48743	C	-3.68959	-7.25434	-1.65237
H	1.11593	3.59762	5.35155	O	-4.52425	-8.17829	-2.36264
H	0.20990	5.01777	-1.47642	C	-3.44726	-7.71475	-0.21850
H	1.40133	6.08870	-0.73484	N	-3.86840	-4.45511	0.12114
H	0.83926	6.69574	2.14213	C	-3.21495	-3.42408	0.91606
H	-1.45385	6.91270	3.16550	C	-3.69140	-3.62548	2.36688
H	-3.27385	5.88209	1.70820	O	-4.67443	-4.32829	2.62558
H	0.89157	3.14976	-0.05294	C	-3.51842	-1.99559	0.38139
H	3.13793	4.49311	1.28556	C	-4.92258	-1.77496	-0.20787
H	3.22371	5.29532	-3.39141	C	-6.06817	-2.00229	0.78945
H	4.80229	5.30835	-4.15672	C	-5.03801	-0.37873	-0.83808
H	5.76522	6.58562	-2.22446	N	-2.97027	-2.96851	3.30073
H	4.19903	6.51817	-1.40108	C	-3.27091	-3.09033	4.72361
H	4.42192	10.28295	-2.45811	C	-4.02628	-1.83970	5.19911
H	4.17325	9.16454	-1.09854	O	-3.53051	-0.71387	5.09864
H	5.76728	9.26126	-1.90267	C	-1.98850	-3.26354	5.55810
H	4.35838	3.14212	-3.08220	C	-1.23426	-4.49793	5.04997
H	4.34817	3.89722	-0.31805	O	-1.64745	-5.62485	5.29804
H	8.78571	2.98594	-3.71190	N	-0.13281	-4.22708	4.30119
H	6.49168	3.91860	-4.12771	C	-5.91491	2.96677	4.47093
H	2.63905	1.90700	-6.29019	C	-5.21047	3.49436	3.22542
H	1.52749	0.54212	1.61561	O	-5.03980	4.70000	3.03920
H	-0.92586	0.07553	0.53504	N	-4.76155	2.55786	2.33293
H	-0.15915	-1.45086	0.07783	C	-3.82133	2.99533	1.29509
H	7.74254	-0.86343	-3.92608	C	-4.50479	3.41247	-0.00854
H	3.71024	1.12911	-0.91363	O	-5.66679	3.12741	-0.29470
H	4.02913	-0.52986	-0.48126	C	-2.82826	1.81690	1.11049
H	3.70377	-1.07994	-3.00548	C	-3.03303	1.01980	2.40178
H	2.54786	1.64867	-2.96224	C	-4.52883	1.14372	2.65971
N	-5.27667	-2.01648	5.92788	N	-3.67740	4.09737	-0.85516
				C	-4.23674	4.87614	-1.95883

C	-5.02414	4.06070	-2.99281	C	0.04463	5.79643	0.77262
O	-5.91403	4.59915	-3.64485	N	-1.31002	5.51718	0.65134
C	-3.10635	5.62977	-2.67080	C	0.28994	6.39003	1.98935
N	-4.63446	2.76973	-3.19822	C	-1.86690	5.94083	1.77543
C	-5.26542	1.93793	-4.20783	N	-0.93400	6.46903	2.61261
C	-6.37785	1.01418	-3.66177	N	4.04123	3.87558	-1.08257
O	-6.55941	-0.11014	-4.12866	C	4.80039	3.92401	-2.33480
C	-4.23069	1.14499	-5.02912	C	6.31102	3.85730	-2.02901
C	-3.29560	0.30707	-4.21811	O	6.73653	3.85990	-0.87721
N	-3.55464	-0.98184	-3.79346	C	4.44763	5.20471	-3.13416
C	-2.03839	0.58989	-3.73264	C	4.82791	6.48599	-2.39127
C	-2.47762	-1.41776	-3.08817	S	4.30173	7.95041	-3.36096
N	-1.53254	-0.48677	-3.03026	C	4.80430	9.25758	-2.18757
N	-7.17979	1.57237	-2.71631	N	7.11753	3.81518	-3.12742
C	-8.25365	0.80629	-2.08121	C	8.57958	3.89660	-3.07297
O	-9.52029	0.66298	-2.95133	C	1.60835	1.99006	-5.34837
O	-10.31942	-0.23828	-2.71275	C	2.21862	0.73777	-4.75361
C	-8.56191	1.42351	-0.68959	O	2.28389	-0.31894	-5.39191
C	-9.14986	2.83939	-0.79473	O	6.23634	-1.36397	-0.18999
C	-9.46195	0.50974	0.15046	C	6.39253	-0.79427	-1.27699
C	8.96426	-2.22404	2.05926	N	7.42918	-0.98093	-2.10939
C	8.86531	-2.75359	0.64310	C	7.39264	-0.15227	-3.30549
O	9.34489	-2.16657	-0.33009	C	5.92900	0.35006	-3.33735
N	8.21776	-3.95081	0.54341	C	4.55504	0.26853	-1.86969
C	7.77702	-4.49141	-0.72798	C	3.96240	0.00003	-1.53247
C	6.27708	-4.24452	-0.89093	C	3.05224	-0.32895	-2.71994
O	5.52764	-4.29540	0.10121	N	2.67437	0.85260	-3.47608
C	8.02559	-6.00616	-0.80693	C	1.81939	-1.15164	-2.36727
N	5.83714	-4.08555	-2.14110	O	1.88299	-2.13361	-1.63561
C	4.41749	-4.01643	-2.44837	H	-5.58046	-5.48993	-5.55523
C	3.72458	-5.24817	-1.79740	H	-2.73150	-7.12308	-2.17715
O	4.22490	-6.36141	-1.88246	H	-2.96806	-8.69907	-0.21968
C	4.19444	-4.04246	-3.97333	H	-4.39426	-7.79836	0.32328
C	5.07548	-3.06581	-4.74928	H	-2.79173	-7.02828	0.32318
O	6.30899	-3.10320	-4.65266	H	-4.04955	-9.01595	-2.43620
N	4.45105	-2.19719	-5.57704	H	-5.35961	-5.98026	-1.15848
N	2.57160	-4.95782	-1.14573	H	-4.90426	-6.49474	-3.66381
C	1.95088	-5.84729	-0.18385	H	-2.78042	-1.77866	-0.39535
C	1.99781	-5.28571	1.24629	H	-3.33405	-1.28796	1.19175
O	1.16345	-5.63504	2.07877	H	-5.04245	-2.49263	-1.02158
N	2.99503	-4.39686	1.49576	H	-5.85798	-0.37707	-1.55388
C	3.14394	-3.70751	2.76331	H	-5.24046	0.40637	-0.10538
C	2.37031	-2.37153	2.83884	H	-4.13173	-0.10250	-1.38555
O	2.42766	-1.70898	3.86511	H	-7.02684	-1.76253	0.31793
C	4.62711	-3.44882	3.09213	H	-6.11689	-3.03214	1.14761
O	5.22770	-2.49142	2.23386	H	-5.96590	-1.36115	1.67268
C	0.87225	-0.60271	1.70980	H	-2.13168	-3.57767	0.88763
C	0.05868	-0.45383	2.98852	H	-4.69051	-4.84837	0.56776
O	-0.52859	-1.42897	3.50155	H	-2.27684	-3.44898	6.59653
C	-0.10329	-0.43114	0.51003	H	-1.39978	-2.34729	5.51012
S	0.45399	0.85395	-0.67916	H	0.26722	-4.97037	3.73506
N	-0.03503	0.78293	3.48313	H	-0.00601	-3.28028	3.96399
C	-0.76512	1.12199	4.69648	H	-3.86667	-3.99483	4.83396
C	0.17122	1.11555	5.89565	H	-2.14951	-2.42180	3.05055
O	0.42773	2.14263	6.53981	H	-5.19287	2.50638	5.15443
N	0.71610	-0.08571	6.16104	H	-1.80797	2.18611	0.98296
C	1.75373	-0.24145	7.15184	H	-3.08434	1.21859	0.23250
C	1.18205	5.49108	6.83861	H	-2.52705	1.53388	3.21304
C	1.70793	5.40050	5.40604	H	-2.67312	-0.00696	2.39238
O	2.03797	6.39316	4.75411	H	-5.11453	0.50329	1.99463
N	1.85173	4.12848	4.94093	H	-4.78330	0.90028	3.68811
C	2.66899	3.79366	3.79052	H	-3.28132	3.85939	1.67934
C	1.86111	3.68780	2.48698	H	-3.52194	6.24052	-3.47505
O	0.74176	3.16279	2.45481	H	-2.57653	6.27551	-1.96473
C	3.36552	2.44643	4.07747	H	-2.38677	4.92345	-3.09800
C	4.23624	1.93115	2.97365	H	-4.97091	5.59324	-1.57332
N	5.00682	2.74817	2.16182	H	-2.79322	4.44668	-0.47058
C	4.47169	0.61008	2.67156	H	-3.63635	1.86618	-5.59743
C	5.70107	1.91646	1.39588	H	-4.77684	0.52075	-5.74021
N	5.41175	0.61705	1.67157	H	-1.47249	1.50372	-3.85852
N	2.46515	4.16344	1.37107	H	-2.44116	-2.40456	-2.64826
C	1.80937	4.08895	0.07671	H	-5.77664	2.63749	-4.87939
C	2.68982	3.73349	-1.12401	H	-3.95687	2.35353	-2.57286
O	2.11273	3.43220	-2.18126	H	-7.59016	1.50639	-0.18716
C	1.04881	5.41436	-0.27073	H	-9.59611	0.93775	1.14965

H	-10.44292	0.38211	-0.31283	C	-10.84982	1.58148	-4.81540
H	-9.02227	-0.48629	0.26393	H	-11.51285	0.78033	-4.48636
H	-9.27847	3.26496	0.20492	H	-11.38992	2.53381	-4.77737
H	-10.12848	2.82457	-1.28657	H	-10.54691	1.38985	-5.85149
H	-8.49885	3.52090	-1.35126	H	5.85849	1.35564	-3.75440
H	-7.91576	-0.22607	-1.94615	H	5.74698	1.19395	-1.35792
H	-6.81332	2.36864	-2.20530	H	5.34081	-0.31314	-3.97165
H	9.60534	-1.34338	2.07046	H	8.10465	0.68039	-3.22236
H	7.66168	-6.40588	-1.75703	H	8.25109	-1.47816	-1.76049
H	7.48697	-6.51760	-0.00341	H	7.95748	-1.95213	2.39954
H	8.33930	-3.97316	-1.50767	H	9.36278	-2.98210	2.74025
H	7.65949	-4.23707	1.33769	H	0.63219	6.42582	6.96032
H	3.13223	-3.87535	-4.17191	H	0.55437	4.63695	7.10432
H	4.44946	-5.04604	-4.33211	H	-6.38378	3.81352	4.97193
H	5.04806	-1.55469	-6.07920	H	-6.67339	2.21832	4.22536
H	3.47429	-1.92413	-5.50392	H	-6.54367	-4.04018	-5.15838
H	4.00211	-3.09745	-2.02395	H	-4.88438	-3.85897	-5.72211
H	6.47678	-3.94110	-2.91990	H	0.54246	1.79873	-5.50761
H	2.47262	-6.80728	-0.22371	H	1.72262	2.86655	-4.70699
H	0.89454	-5.99407	-0.41053	H	2.63494	-0.70479	6.69707
H	2.24521	-4.00148	-1.14927	H	2.01314	0.74472	7.53658
H	5.16133	-4.40824	3.06870	H	8.93301	4.85429	-3.46789
H	4.67467	-3.04041	4.10436	H	8.87783	3.80712	-2.02826
H	5.43736	-2.91021	1.37891	H	9.09351	-6.21494	-0.70833
H	2.71642	-4.33934	3.55170	H	-4.43458	-1.49084	-3.86362
H	3.70842	-4.25380	0.78621	H	-0.41081	0.46584	-1.65860
H	-1.58705	0.41607	4.84702	O	-0.19706	-3.62890	-0.48945
H	-1.14902	2.13728	4.59824	H	0.29961	-3.08353	-1.11923
H	0.41063	1.57547	3.01183	H	-0.99302	-3.94090	-0.96670
H	1.41827	-0.86811	7.98561	C	1.55435	-1.97248	1.63756
H	0.53308	-0.85132	5.52380	H	0.80976	-2.76061	1.47199
H	2.04184	5.51132	7.51650	H	2.19513	-2.01724	0.75101
H	2.60558	1.68948	4.30529				
H	3.94935	2.58888	4.99562	TS-1-N3			
H	4.09496	-0.30405	3.09396	C	-5.34968	-4.68750	-5.18875
H	5.75117	-0.21102	1.17688	C	-4.79360	-4.57362	-3.77720
H	6.41677	2.22091	0.64743	O	-4.74111	-3.48324	-3.19924
H	3.42135	4.57874	3.67584	N	-4.38322	-5.73809	-3.21876
H	1.44699	3.37168	5.48928	C	-3.96788	-5.97222	-1.84237
H	0.54949	5.26641	-1.23087	C	-3.20776	-4.79945	-1.21352
H	1.78857	6.21481	-0.39595	O	-2.25071	-4.28027	-1.80843
H	1.19510	6.69388	2.49253	C	-3.03147	-7.20084	-1.83517
H	-1.09366	6.83099	3.54051	O	-3.77343	-8.22840	-2.50378
H	-2.91792	5.88615	2.03131	C	-2.61841	-7.63079	-0.43107
H	1.06180	3.29878	0.14886	N	-3.59272	-4.50223	0.03321
H	3.41332	4.50080	1.47096	C	-3.03484	-3.45168	0.87384
H	3.37304	5.18411	-3.32990	C	-3.47495	-3.77074	2.31417
H	4.94362	5.17612	-4.11125	O	-4.41452	-4.54251	2.53822
H	5.90983	6.53449	-2.22223	C	-3.49599	-2.02967	0.43634
H	4.33473	6.50981	-1.41403	C	-4.88760	-1.93347	-0.21158
H	4.54539	10.21599	-2.64237	C	-6.03771	-2.31120	0.73352
H	4.26800	9.15961	-1.23969	C	-5.12787	-0.53373	-0.79420
H	5.88228	9.23119	-2.00591	N	-2.78300	-3.12322	3.27331
H	4.52234	3.05690	-2.94494	C	-3.09225	-3.29163	4.68907
H	4.56769	3.92548	-0.21482	C	-3.92264	-2.09119	5.16924
H	9.02692	3.08106	-3.64782	O	-3.49250	-0.93822	5.07398
H	6.68242	3.86855	-4.03635	C	-1.81074	-3.40402	5.53394
H	2.05538	2.17423	-6.32825	C	-0.98618	-4.59274	5.02414
H	1.63912	0.18010	1.70166	O	-1.34378	-5.74117	5.26111
H	-1.09291	-0.13997	0.85733	N	0.10804	-4.25936	4.29179
H	-0.21445	-1.37552	-0.02057	C	-6.05085	2.61904	4.49811
H	7.63913	-0.74585	-4.18973	C	-5.42527	3.21117	3.23975
H	3.53584	0.85568	-1.00311	O	-5.38597	4.42571	3.04331
H	3.92232	-0.83444	-0.82593	N	-4.88931	2.32269	2.34399
H	3.58483	-0.99556	-3.40758	C	-4.01354	2.86190	1.29716
H	2.46003	1.70605	-2.95870	C	-4.75239	3.27049	0.02307
N	-5.24380	-2.03019	5.76202	O	-5.89964	2.91966	-0.25254
H	-5.68470	-1.17449	6.07260	C	-2.93912	1.77100	1.05253
C	-6.03655	-3.26032	5.75895	C	-3.00651	0.96944	2.35424
H	-7.06568	-3.00312	6.01583	C	-4.49418	0.94678	2.68081
H	-6.03023	-3.72796	4.77029	N	-3.98656	4.02893	-0.81864
H	-5.67101	-3.98158	6.49788	C	-4.60923	4.79640	-1.89568
H	0.89477	-0.91915	-2.91917	C	-5.28292	3.95725	-2.99071
N	-9.70741	1.59614	-3.92437	O	-6.11963	4.47085	-3.72570
H	-8.97575	2.27988	-4.05648	C	-3.56032	5.70843	-2.54371

N	-4.85743	2.66803	-3.13385	C	-2.13062	5.84985	1.80373
C	-5.41428	1.78433	-4.13946	N	-1.18074	6.41669	2.59453
C	-6.48360	0.80715	-3.60067	N	3.82375	4.00308	-1.09926
O	-6.61286	-0.31689	-4.08364	C	4.58199	4.11698	-2.34717
C	-4.31700	1.03059	-4.91962	C	6.09130	4.16719	-2.03423
C	-3.33171	0.31600	-4.05124	O	6.50800	4.25408	-0.88220
N	-3.42145	-1.01136	-3.66843	C	4.14413	5.37624	-3.13968
C	-2.19005	0.78698	-3.44780	C	4.41672	6.67405	-2.37816
C	-2.36882	-1.30827	-2.87538	S	3.78638	8.10526	-3.33549
N	-1.60317	-0.22959	-2.72501	C	4.17752	9.43243	-2.14219
N	-7.30674	1.31470	-2.64469	N	6.90518	4.14175	-3.12776
C	-8.34181	0.48292	-2.02544	C	8.35413	4.35650	-3.07443
C	-9.57633	0.25411	-2.92107	C	1.41402	1.87770	-5.26825
O	-10.31953	-0.69681	-2.69528	C	2.11286	0.67137	-4.67296
C	-8.71750	1.08309	-0.64350	O	2.20130	-0.39473	-5.29573
C	-9.41980	2.44373	-0.76941	O	6.38891	-1.03817	-0.17177
C	-9.54779	0.10161	0.19198	C	6.46954	-0.50114	-1.28357
C	9.05744	-1.80157	1.97864	N	7.48112	-0.66372	-2.15137
C	9.01992	-2.36302	0.57371	C	7.36011	0.12501	-3.36852
O	9.47656	-1.76773	-0.40511	C	5.87481	0.56254	-3.35579
N	8.44938	-3.60103	0.49069	C	5.45125	0.48652	-1.87194
C	8.01931	-4.16581	-0.77337	C	3.98873	0.13030	-1.48535
C	6.51041	-3.97014	-0.92287	C	3.06763	-0.29164	-2.63051
O	5.77284	-4.01987	0.07821	N	2.60935	0.84064	-3.41980
C	8.31733	-5.67186	-0.84440	C	1.89239	-1.17380	-2.21007
N	6.05037	-3.85697	-2.17068	O	2.06356	-2.15251	-1.46740
C	4.62512	-3.87760	-2.45664	H	-5.31788	-5.69923	-5.59964
C	4.02249	-5.14311	-1.77896	H	-2.14422	-6.92260	-2.42297
O	4.59551	-6.22239	-1.84784	H	-2.01987	-8.54580	-0.48476
C	4.38046	-3.92762	-3.97712	H	-3.49787	-7.83598	0.18665
C	5.19906	-2.91054	-4.76963	H	-2.01045	-6.86877	0.06372
O	6.43577	-2.90672	-4.71345	H	-3.19138	-8.98895	-2.62718
N	4.51625	-2.05410	-5.56280	H	-4.85057	-6.21623	-1.23534
N	2.86054	-4.91456	-1.11971	H	-4.50364	-6.59727	-3.73849
C	2.31403	-5.81677	-0.12609	H	-2.75566	-1.64650	-0.26992
C	2.33976	-5.22452	1.29276	H	-3.44670	-1.38137	1.31236
O	1.56297	-5.64119	2.14979	H	-4.90276	-2.62791	-1.05544
N	3.25245	-4.24088	1.50608	H	-5.93900	-0.58601	-1.51692
C	3.37714	-3.53510	2.76780	H	-5.40379	0.20516	-0.03749
C	2.53536	-2.23953	2.84681	H	-4.24863	-0.15407	-1.32335
O	2.56072	-1.57810	3.87569	H	-6.99834	-2.20323	0.21896
C	4.84800	-3.19886	3.08014	H	-5.96168	-3.33627	1.10066
O	5.38892	-2.21732	2.20957	H	-6.05885	-1.65531	1.61233
C	0.93006	-0.56493	1.71170	H	-1.94253	-3.49662	0.82442
C	0.10705	-0.47204	2.98823	H	-4.36126	-5.00033	0.47202
O	-0.42005	-1.48257	3.50162	H	-2.09787	-3.61443	6.56793
C	-0.05653	-0.45180	0.51334	H	-1.27197	-2.45692	5.50039
S	0.52696	0.60868	-0.86874	H	0.56379	-4.97927	3.73696
N	-0.06522	0.75379	3.49027	H	0.19030	-3.30582	3.95935
C	-0.82126	1.03795	4.70249	H	-3.63644	-4.23054	4.77653
C	0.10876	1.05222	5.90647	H	-1.99802	-2.51597	3.04559
O	0.32108	2.08071	6.56454	H	-5.27270	2.25977	5.18055
N	0.70663	-0.12717	6.15395	H	-1.96086	2.22306	0.87154
C	1.77566	-0.24072	7.11637	H	-3.19466	1.14787	0.19179
C	0.92131	5.46016	6.87754	H	-2.51053	1.54204	3.13270
C	1.38953	5.40323	5.42079	H	-2.54955	-0.01748	2.32796
O	1.62290	6.41705	4.75940	H	-5.03887	0.23182	2.05636
N	1.60164	4.14411	4.94466	H	-4.67634	0.69704	3.72303
C	2.41425	3.86298	3.77553	H	-3.52832	3.75208	1.69574
C	1.59650	3.72075	2.47754	H	-4.02989	6.30326	-3.32931
O	0.46995	3.20960	2.46422	H	-3.12045	6.37491	-1.79682
C	3.20196	2.56229	4.04849	H	-2.75504	5.11149	-2.98513
C	4.11413	2.11703	2.94639	H	-5.42513	5.40610	-1.48965
N	4.80746	2.99063	2.12223	H	-3.10541	4.40339	-0.44755
C	4.46986	0.82046	2.65820	H	-3.77303	1.76270	-5.52266
C	5.57411	2.21640	1.36376	H	-4.80650	0.32609	-5.59472
N	5.40436	0.90092	1.65610	H	-1.75710	1.77592	-3.48346
N	2.21097	4.16083	1.35156	H	-2.21267	-2.28661	-2.44026
C	1.57104	4.03332	0.05007	H	-5.94397	2.44054	-4.83968
C	2.48657	3.76086	-1.14742	H	-4.23869	2.28619	-2.43166
O	1.94223	3.43387	-2.21364	H	-7.76318	1.25004	-0.12860
C	0.73301	5.31098	-0.31449	H	-9.74432	0.52907	1.18095
C	-0.25043	5.70613	0.74276	H	-10.50137	-0.12390	-0.29075
N	-1.60415	5.40512	0.67253	H	-9.01769	-0.84615	0.33161
C	0.02188	6.34018	1.93290	H	-9.58778	2.87115	0.22352

H	-10.39156	2.34222	-1.26456	H	-10.58485	0.92949	-5.84853
H	-8.82387	3.16724	-1.33477	H	5.74588	1.55762	-3.78515
H	-7.94286	-0.52559	-1.87799	H	5.69748	1.44067	-1.38926
H	-6.96737	2.10736	-2.10785	H	5.29407	-0.13419	-3.95979
H	9.64650	-0.88514	1.98600	H	8.03767	0.98974	-3.33905
H	7.95636	-6.09079	-1.78722	H	8.33553	-1.11794	-1.82367
H	7.80416	-6.19510	-0.03185	H	8.02910	-1.58205	2.29068
H	8.55639	-3.63372	-1.56166	H	9.48367	-2.52150	2.68402
H	7.89748	-3.89845	1.28569	H	0.32274	6.36027	7.02642
H	3.30831	-3.81557	-4.15977	H	0.35741	4.56953	7.16575
H	4.68307	-4.91808	-4.33512	H	-6.61490	3.40936	4.99317
H	5.07494	-1.38393	-6.07290	H	-6.71400	1.77996	4.27014
H	3.53212	-1.81689	-5.45008	H	-6.38414	-4.33420	-5.17159
H	4.15998	-2.98408	-2.03081	H	-4.78706	-4.01634	-5.84317
H	6.67400	-3.71870	-2.96293	H	0.34493	1.64858	-5.32869
H	2.89687	-6.74155	-0.14945	H	1.54764	2.78417	-4.67433
H	1.26661	-6.04081	-0.33145	H	2.66457	-0.65731	6.63241
H	2.48021	-3.97701	-1.14260	H	1.99762	0.75314	7.50483
H	5.43114	-4.12931	3.05686	H	8.62319	5.31815	-3.52262
H	4.88500	-2.78164	4.08938	H	8.65057	4.35303	-2.02541
H	5.61742	-2.62903	1.35606	H	9.39258	-5.84422	-0.75523
H	2.99108	-4.18619	3.56168	H	-4.19863	-1.66052	-3.81980
H	3.93513	-4.04727	0.77895	H	-0.60632	0.11499	-1.86955
H	-1.61473	0.29610	4.83223	O	0.03409	-3.71943	-0.37514
H	-1.24467	2.03839	4.61897	H	0.60245	-3.12295	-0.89449
H	0.30427	1.57746	3.00827	H	-0.71039	-3.96079	-0.95855
H	1.49339	-0.89017	7.95245	C	1.70058	-1.88632	1.64733
H	0.55973	-0.88770	5.50125	H	1.00627	-2.72068	1.49048
H	1.80792	5.52942	7.51645	H	2.33942	-1.89869	0.75937
H	2.49737	1.75104	4.26754				
H	3.77206	2.73618	4.96992	Int-N3			
H	4.17594	-0.11950	3.08870	C	-5.23695	-4.89951	-5.19538
H	5.81050	0.10042	1.16404	C	-4.60189	-4.70104	-3.82707
H	6.25712	2.57651	0.60947	O	-4.60064	-3.58996	-3.28515
H	3.11435	4.69381	3.65091	N	-4.07470	-5.81852	-3.27176
H	1.26523	3.36283	5.50455	C	-3.52477	-6.01161	-1.93476
H	0.21236	5.10447	-1.25207	C	-2.94654	-4.75052	-1.29662
H	1.43378	6.13539	-0.49639	O	-2.06894	-4.09732	-1.88775
H	0.93646	6.66957	2.40022	C	-2.37774	-7.04256	-2.03460
H	-1.30645	6.78916	3.52365	O	-2.98096	-8.18854	-2.64635
H	-3.17262	5.78746	2.09128	C	-1.75349	-7.37696	-0.68288
H	0.88557	3.18460	0.10088	N	-3.35572	-4.52175	-0.04676
H	3.19569	4.38727	1.44695	C	-2.86996	-3.45785	0.82324
H	3.07663	5.27634	-3.34917	C	-3.33053	-3.82706	2.24402
H	4.65598	5.39536	-4.10872	O	-4.24283	-4.64205	2.42677
H	5.48966	6.80519	-2.19712	C	-3.37262	-2.05004	0.39334
H	3.91414	6.64764	-1.40580	C	-4.74892	-1.99135	-0.29041
H	3.84854	10.37384	-2.58714	C	-5.90687	-2.44944	0.60796
H	3.64385	9.28088	-1.19989	C	-5.03423	-0.58299	-0.83363
H	5.25298	9.48698	-1.95200	N	-2.68234	-3.18299	3.23435
H	4.36910	3.23665	-2.96413	C	-3.01311	-3.41280	4.63561
H	4.34024	4.12719	-0.23398	C	-3.90297	-2.26885	5.14056
H	8.87724	3.55277	-3.59995	O	-1.09055	-1.09055	5.04237
H	6.47155	4.11662	-4.03876	C	-1.74824	-3.50243	5.50738
H	1.77315	2.03079	-6.28849	C	-0.87450	-4.65266	4.99012
H	1.63516	0.27286	1.69715	O	-1.21177	-5.81578	5.18302
H	-0.99598	-0.01134	0.84416	N	0.23279	-4.26951	4.30612
H	-0.28047	-1.45094	0.13517	C	-6.15761	2.33291	4.52863
H	7.59810	-0.48450	-4.24445	C	-5.57177	2.99727	3.28890
H	3.52237	0.96917	-0.96298	O	-5.60227	4.21652	3.12846
H	4.02173	-0.68689	-0.75865	N	-4.98718	2.16763	2.36462
H	3.61508	-0.95501	-3.31013	C	-4.13148	2.79136	1.35035
H	2.37467	1.70195	-2.92526	C	-4.86645	3.18392	0.06939
N	-5.13007	-2.35457	5.72377	O	-5.99803	2.80049	-0.22852
H	-5.62276	-1.52788	6.03499	C	-2.97510	1.78638	1.10421
C	-5.84485	-3.63135	5.71733	C	-3.02342	0.93055	2.37164
H	-6.88478	-3.44098	5.98835	C	-4.51384	0.80760	2.66314
H	-5.82124	-4.08884	4.72408	N	-4.11152	3.97484	-0.75353
H	-5.42664	-4.33512	6.44495	C	-4.74176	4.75745	-1.81510
H	1.02804	-1.12816	-2.88791	C	-5.36679	3.94231	-2.95547
N	-9.80028	1.16849	-3.90312	O	-6.14768	4.47975	-3.73222
H	-9.11788	1.90424	-4.01618	C	-3.71500	5.73023	-2.40893
C	-10.92189	1.07988	-4.81637	N	-4.96658	2.64079	-3.08783
H	-11.52642	0.22453	-4.51216	C	-5.50942	1.78038	-4.11946
H	-11.53592	1.98626	-4.77528	C	-6.51524	0.73205	-3.59562

O	-6.55405	-0.40067	-4.07848	C	4.40803	4.19851	-2.36066
C	-4.40103	1.10236	-4.95189	C	5.90677	4.34463	-2.03295
C	-3.42066	0.34059	-4.12179	O	6.29598	4.55936	-0.88768
N	-3.53543	-1.00166	-3.78720	C	3.92219	5.41053	-3.19834
C	-2.28029	0.77831	-3.50096	C	4.11862	6.74272	-2.47340
C	-2.51010	-1.36701	-3.00647	S	3.42588	8.11032	-3.47974
N	-1.73758	-0.29393	-2.82395	C	3.74530	9.49210	-2.32777
N	-7.37451	1.17477	-2.64218	N	6.73827	4.26770	-3.10944
C	-8.33327	0.26222	-2.00902	C	8.16985	4.57409	-3.05858
C	-9.54836	-0.08426	-2.89375	C	1.36782	1.82258	-5.21417
O	-10.19236	-1.10218	-2.65836	C	2.05432	0.62610	-4.57868
C	-8.75070	0.84137	-0.62981	O	2.12250	-0.45597	-5.17819
C	-9.57104	2.13348	-0.76321	O	6.49088	-0.79239	-0.12748
C	-9.48763	-0.20069	-0.21989	C	6.51046	-0.31359	-1.26848
C	9.08165	-1.58257	1.96278	N	7.49671	-0.49028	-2.16323
C	9.07801	-2.13823	0.55517	C	7.30524	0.22399	-3.41709
O	9.53788	-1.53218	-0.41527	C	5.80730	0.61384	-3.37013
N	8.53084	-3.38681	0.46072	C	5.43818	0.60530	-1.87074
C	8.09990	-3.94020	-0.80812	C	4.00231	0.22211	-1.41712
C	6.58761	-3.75580	-0.94463	C	3.03522	-0.26082	-2.49701
O	5.86125	-3.79357	-0.06479	N	2.56667	0.83452	-3.34148
C	8.41013	-5.44283	-0.89862	C	1.84575	-1.07784	-1.93523
N	6.11285	-3.66664	-2.18867	O	2.14589	-2.07888	-1.18174
C	4.68549	-3.73639	-2.46052	H	-5.11552	-5.90609	-5.60209
C	4.12766	-5.00378	-1.75315	H	-1.62000	-6.60291	-2.69936
O	4.72779	-6.07075	-1.81055	H	-1.01380	-8.17471	-0.80482
C	4.43143	-3.82977	-3.97669	H	-2.51223	-7.72315	0.02526
C	5.21647	-2.80991	-4.79657	H	-1.23570	-6.51406	-0.25406
O	6.45486	-2.79594	-4.77616	H	-2.28659	-8.83434	-2.82886
N	4.50046	-1.96209	-5.56888	H	-4.30278	-6.44029	-1.28881
N	2.97110	-4.78477	-1.08579	H	-4.13071	-6.68615	-3.78864
C	2.45345	-5.69471	-0.08570	H	-2.62642	-1.63136	-0.28779
C	2.50003	-5.12358	1.34118	H	-3.36701	-1.41352	1.27911
O	1.76638	-5.59027	2.21220	H	-4.71418	-2.66083	-1.15419
N	3.38070	-4.11262	1.55034	H	-5.81392	-0.64471	-1.58954
C	3.51349	-3.41865	2.81864	H	-5.37194	0.11469	-0.06335
C	2.63829	-2.14518	2.93081	H	-4.15296	-0.14020	-1.30983
O	2.66614	-1.48856	3.96398	H	-6.85497	-2.37957	0.06444
C	4.98118	-3.04510	3.10055	H	-5.78656	-3.47808	0.95186
O	5.47417	-2.03991	2.22826	H	-5.98923	-1.81755	1.50042
C	0.97942	-0.51837	1.79513	H	-1.77512	-3.45947	0.80125
C	0.12274	-0.45796	3.05173	H	-4.06018	-5.10853	0.39204
O	-0.36368	-1.49063	3.56369	H	-2.05222	-3.74748	6.52893
C	0.02954	-0.43092	0.56644	H	-1.24086	-2.53770	5.51030
S	0.67817	0.42918	-0.91936	H	0.73104	-4.96050	3.74929
N	-0.11797	0.75718	3.55399	H	0.30060	-3.30506	4.00348
C	-0.88831	0.99014	4.76938	H	-3.51767	-4.37654	4.67859
C	0.04879	1.00056	5.96904	H	-1.90844	-2.54929	3.04277
O	0.27365	2.03023	6.62137	H	-5.35874	1.98494	5.19263
N	0.64829	-0.17937	6.20763	H	-2.02660	2.31362	0.97598
C	1.76222	-0.28406	7.11998	H	-3.16030	1.18001	0.21326
C	0.72290	5.38717	6.91079	H	-2.57703	1.49773	3.18369
C	1.14015	5.36218	5.43710	H	-2.50691	-0.02501	2.31230
O	1.27806	6.39108	4.77095	H	-5.00120	0.08432	2.00239
N	1.42119	4.12092	4.94978	H	-4.70397	0.50822	3.69042
C	2.23668	3.88776	3.77068	H	-3.72281	3.70599	1.77902
C	1.42138	3.72597	2.47076	H	-4.19058	6.33352	-3.18399
O	0.29496	3.21226	2.45806	H	-3.31620	6.38504	-1.62973
C	3.08788	2.62432	4.03413	H	-2.87812	5.17967	-2.85203
C	4.02639	2.23258	2.93359	H	-5.58561	5.32410	-1.40293
N	4.65478	3.14456	2.09816	H	-3.24619	4.36728	-0.36019
C	4.46990	0.96165	2.65391	H	-3.86048	1.88319	-5.49271
C	5.46852	2.41759	1.34077	H	-4.87089	0.43907	-5.68028
N	5.39149	1.09793	1.64654	H	-1.81576	1.75113	-3.48516
N	2.04090	4.15965	1.34442	H	-2.36104	-2.36003	-2.59247
C	1.40324	4.01827	0.04277	H	-6.07463	2.44697	-4.78097
C	2.32364	3.78538	-1.15847	H	-4.41478	2.23651	-2.34436
O	1.78789	3.43318	-2.22061	H	-7.81113	1.09483	-0.12270
C	0.52956	5.27578	-0.31887	H	-9.71658	0.21900	1.20502
C	-0.41986	5.67801	0.76428	H	-10.42008	-0.51421	-0.25496
N	-1.76808	5.34635	0.76838	H	-8.87551	-1.09610	0.36717
C	-0.10059	6.32859	1.93274	H	-9.76679	2.55598	0.22658
C	-2.24162	5.78588	1.92567	H	-10.53450	1.94146	-1.24739
N	-1.26453	6.38188	2.65942	H	-9.04740	2.90075	-1.34284
N	3.64728	4.08516	-1.11539	H	-7.84639	-0.70547	-1.85415

H	-7.09306	1.99195	-2.10757	H	5.22708	-0.13237	-3.91096
H	9.65230	-0.65468	1.98386	H	7.95486	1.10981	-3.46124
H	8.04676	-5.85413	-1.84378	H	8.37212	-0.90977	-1.84613
H	7.90540	-5.97990	-0.08981	H	8.04411	-1.38548	2.25815
H	8.62724	-3.39467	-1.59380	H	9.51130	-2.29726	2.67160
H	7.97107	-3.68989	1.24834	H	0.09328	6.26013	7.08961
H	3.35558	-3.74809	-4.15259	H	0.20804	4.47078	7.20906
H	4.75889	-4.81980	-4.31328	H	-6.75398	3.07777	5.05525
H	5.03794	-1.28074	-6.08697	H	-6.78285	1.47213	4.27535
H	3.52024	-1.72955	-5.40617	H	-6.30300	-4.67212	-5.10801
H	4.19110	-2.85304	-2.04652	H	-4.80513	-4.17603	-5.89165
H	6.72837	-3.55425	-2.99079	H	0.31721	1.56124	-5.37627
H	3.04278	-6.61501	-0.12440	H	1.42371	2.72562	-4.60330
H	1.40408	-5.92714	-0.27070	H	2.63669	-0.66980	6.58674
H	2.57457	-3.84619	-1.12839	H	1.97727	0.70736	7.51823
H	5.58934	-3.95853	3.05348	H	8.39024	5.49998	-3.59926
H	5.03072	-2.63695	4.11314	H	8.44487	4.69473	-2.01067
H	5.69452	-2.43635	1.36494	H	9.48727	-5.60726	-0.81693
H	3.16470	-4.09255	3.61049	H	-4.32623	-1.62515	-3.96894
H	4.01081	-3.85902	0.79526	H	-0.90121	-0.19032	-2.18856
H	-1.66202	0.22411	4.87702	O	0.14185	-3.66071	-0.27803
H	-1.33812	1.98063	4.70836	H	0.80626	-3.04004	-0.66061
H	0.20595	1.60076	3.07308	H	-0.51320	-3.81922	-0.97918
H	1.53206	-0.95612	7.95393	C	1.78195	-1.81698	1.74808
H	0.49451	-0.93279	5.54775	H	1.10327	-2.66805	1.61356
H	1.62898	5.48663	7.51767	H	2.39321	-1.83009	0.84032
H	2.42508	1.77678	4.24659				
H	3.64566	2.82036	4.95874	Reac-N2			
H	4.24177	0.00586	3.08951	C	-5.53408	-4.66007	-4.94154
H	5.84330	0.32181	1.15086	C	-5.00208	-4.58727	-3.51997
H	6.11981	2.81663	0.57794	O	-4.91395	-3.50569	-2.93481
H	2.89734	4.75067	3.64689	N	-4.64038	-5.76918	-2.95959
H	1.15948	3.32285	5.52580	C	-4.27393	-5.99230	-1.56784
H	-0.01400	5.04345	-1.23729	C	-3.41820	-4.86597	-0.97377
H	1.21140	6.10674	-0.53796	O	-2.40287	-4.47368	-1.56816
H	0.82893	6.68074	2.34832	C	-3.45546	-7.29850	-1.49592
H	-1.32974	6.73606	3.60237	O	-4.27048	-8.28088	-2.14735
H	-3.26621	5.70671	2.26548	C	-3.11476	-7.71098	-0.06717
H	0.74604	3.14703	0.08505	N	-3.79977	-4.46566	0.24512
H	3.04054	4.33087	1.44085	C	-3.18316	-3.39689	1.01827
H	2.86441	5.25227	-3.42009	C	-3.69665	-3.55157	2.46345
H	4.45190	5.42402	-4.15770	O	-4.65086	-4.28926	2.73105
H	5.18065	6.93557	-2.28497	C	-3.48558	-1.99848	0.41583
H	3.60705	6.71936	-1.50566	C	-4.89759	-1.79834	-0.16125
H	3.37552	10.40242	-2.80431	C	-6.03045	-1.98796	0.85828
H	3.21310	9.34541	-1.38383	C	-5.01712	-0.42515	-0.83975
H	4.81565	9.60331	-2.13351	N	-3.03023	-2.81214	3.37347
H	4.24793	3.28942	-2.95118	C	-3.30318	-2.90850	4.80284
H	4.15345	4.27393	-0.25607	C	-4.03933	-1.64255	5.26626
H	8.75062	3.75463	-3.49113	O	-3.53943	-0.52207	5.13478
H	6.32324	4.12187	-4.01781	C	-1.99927	-3.08303	5.60705
H	1.80830	2.00299	-6.19828	C	-1.28181	-4.33728	5.09280
H	1.65628	0.34263	1.79440	O	-1.68119	-5.45394	5.40515
H	-0.85459	0.15180	0.82813	N	-0.23881	-4.09963	4.25620
H	-0.29806	-1.43609	0.29397	C	-5.92980	3.13395	4.37561
H	7.52946	-0.42590	-4.26738	C	-5.22177	3.61710	3.11499
H	3.54406	1.06461	-0.89280	O	-5.03734	4.81496	2.89406
H	4.08066	-0.57662	-0.67397	N	-4.78544	2.64963	2.25005
H	3.53732	-0.97623	-3.15455	C	-3.83652	3.04323	1.20318
H	2.34106	1.71909	-2.88673	C	-4.50924	3.41113	-0.12062
N	-5.07371	-2.61413	5.72814	O	-5.66932	3.11622	-0.40480
H	-5.61050	-1.82428	6.06125	C	-2.84765	1.85425	1.06972
C	-5.70225	-3.93514	5.72914	C	-3.07719	1.09241	2.37847
H	-6.73329	-3.82172	6.06837	C	-4.57407	1.24167	2.61574
H	-5.71056	-4.36705	4.72402	N	-3.67422	4.06258	-0.98597
H	-5.19415	-4.62634	6.40975	C	-4.22375	4.80162	-2.12133
H	1.11972	-1.25804	-2.74860	C	-5.01572	3.95235	-3.12400
N	-9.87296	0.80256	-3.87358	O	-5.90987	4.46814	-3.78846
H	-9.26770	1.60086	-3.99770	C	-3.08440	5.51627	-2.85885
C	-10.99399	0.60409	-4.77112	N	-4.62449	2.65609	-3.29161
H	-11.51314	-0.30074	-4.45303	C	-5.25781	1.79461	-4.27474
H	-11.68777	1.45058	-4.72659	C	-6.36364	0.88213	-3.69728
H	-10.65830	0.47733	-5.80680	O	-6.53563	-0.26029	-4.12258
H	5.62573	1.57888	-3.84830	C	-4.22533	0.98492	-5.08232
H	5.67083	1.59200	-1.44883	C	-3.27841	0.17379	-4.25807

N	-3.53081	-1.10020	-3.78682	C	4.45687	5.17200	-3.20656
C	-2.01385	0.47152	-3.80206	C	4.85944	6.45195	-2.47337
C	-2.44306	-1.51277	-3.08346	S	4.33469	7.91876	-3.44021
N	-1.49706	-0.58128	-3.07204	C	4.86553	9.22428	-2.27747
N	-7.17119	1.46877	-2.77429	N	7.11241	3.79404	-3.21674
C	-8.24177	0.72061	-2.11282	C	8.57532	3.81698	-3.17427
C	-9.51254	0.55091	-2.97252	C	1.63909	1.84224	-5.37416
O	-10.30886	-0.34453	-2.70450	C	2.27244	0.62223	-4.73789
C	-8.54441	1.37665	-0.73774	O	2.35198	-0.45454	-5.34213
C	-9.13243	2.78931	-0.87952	O	6.22135	-1.42340	-0.11529
C	-9.44135	0.48711	0.13116	C	6.40914	-0.85695	-1.19892
C	8.96193	-2.11444	2.17539	N	7.45031	-1.07619	-2.01865
C	8.82632	-2.74132	0.80167	C	7.46112	-0.23573	-3.20714
O	9.35840	-2.26890	-0.20693	C	6.01607	0.31723	-3.25759
N	8.10068	-3.89605	0.78567	C	5.51947	0.24247	-1.79695
C	7.71716	-4.55286	-0.44939	C	4.01453	0.03339	-1.47946
C	6.22934	-4.33797	-0.70763	C	3.12702	-0.35712	-2.66567
O	5.41696	-4.38175	0.23430	N	2.73209	0.78892	-3.46907
C	7.97280	-6.06739	-0.37940	C	1.90909	-1.19124	-2.29182
N	5.84955	-4.21608	-1.98240	O	1.98526	-2.12222	-1.50122
C	4.43883	-4.16557	-2.30777	H	-5.57478	-5.67170	-5.35268
C	3.73949	-5.44449	-1.76154	H	-2.53331	-7.12286	-2.06976
O	4.35205	-6.48903	-1.68127	H	-2.59384	-8.67401	-0.07249
C	4.21930	-4.10507	-3.83802	H	-4.02417	-7.82017	0.53131
C	5.13959	-3.13565	-4.58354	H	-2.45873	-6.98416	0.41928
O	6.36862	-3.20092	-4.46225	H	-3.76077	-9.09821	-2.21466
N	4.54915	-2.26641	-5.43394	H	-5.18438	-6.12707	-0.96740
C	1.85516	-6.07895	-0.12656	H	-4.80684	-6.62715	-3.46796
C	1.81704	-5.28148	1.17766	H	-2.75975	-1.82930	-0.38355
O	1.00093	-5.58784	2.04526	H	-3.28192	-1.25040	1.18394
N	2.72633	-4.27335	1.34006	H	-5.02756	-2.54572	-0.94592
C	2.88775	-3.59775	2.62230	H	-5.84119	-0.44690	-1.55053
C	2.20755	-2.22248	2.71406	H	-5.21496	0.38423	-0.13270
O	2.33910	-1.53622	3.73664	H	-4.11362	-0.16767	-1.41014
C	4.36774	-3.44866	3.03039	H	-6.99281	-1.74193	0.39762
O	5.08736	-2.49446	2.26713	H	-6.08963	-3.01079	1.23461
N	1.48035	-1.81770	1.65326	H	-5.90363	-1.33292	1.72785
C	0.81364	-0.52557	1.66496	H	-2.09736	-3.53824	1.03440
C	-0.00758	-0.35235	2.94967	H	-4.61436	-4.87073	0.69585
O	-0.62736	-1.30303	3.45591	H	-2.25905	-3.24944	6.65601
C	-0.15040	-0.38510	0.46460	H	-1.39709	-2.17729	5.52566
S	0.42064	0.87044	-0.74894	H	0.12396	-4.86353	3.69318
N	-0.05436	0.89155	3.42761	H	-0.10782	-3.16337	3.89180
C	-0.76044	1.27344	4.63975	H	-3.90469	-3.80553	4.94082
C	0.18047	1.28648	5.83564	H	-2.21564	-2.26351	3.10650
O	0.37491	2.30521	6.51372	H	-5.21287	2.67952	5.06844
N	0.78185	0.11238	6.10289	H	-1.82376	2.21527	0.94760
C	1.73983	0.03751	7.18212	H	-3.09292	1.23409	0.20376
C	1.15905	5.75408	6.66204	H	-2.57427	1.61767	3.18482
C	1.70621	5.57824	5.24654	H	-2.73138	0.06118	2.39817
O	2.04643	6.53220	4.54402	H	-5.16190	0.59312	1.96051
N	1.85586	4.28273	4.85388	H	-4.84265	1.02812	3.64727
C	2.67082	3.89521	3.71688	H	-3.29595	3.91914	1.55771
C	1.86432	3.76929	2.41471	H	-3.49153	6.09926	-3.68773
O	0.74252	3.24872	2.39378	H	-2.55091	6.18439	-2.17668
C	3.33592	2.54122	4.04141	H	-2.37011	4.78718	-3.25548
C	4.20690	1.98612	2.95701	H	-4.95268	5.53998	-1.76728
N	5.00411	2.77344	2.14037	H	-2.79337	4.42591	-0.60669
C	4.42117	0.65424	2.68736	H	-3.63937	1.69379	-5.67435
C	5.69519	1.91336	1.40396	H	-4.77378	0.33938	-5.77244
N	5.37713	0.62473	1.70263	H	-1.45075	1.38096	-3.96596
N	2.46868	4.21559	1.28707	H	-2.40016	-2.48411	-2.61112
C	1.81360	4.10034	-0.00517	H	-5.77591	2.47440	-4.96114
C	2.69731	3.71783	-1.19439	H	-3.94338	2.25990	-2.65709
O	2.12407	3.40310	-2.24971	H	-7.57055	1.47348	-0.24198
C	1.04724	5.41027	-0.39652	H	-9.56895	0.94162	1.11943
C	0.03225	5.82037	0.62498	H	-10.42523	0.34933	-0.32295
N	-1.32116	5.53721	0.49720	H	-9.00326	-0.50664	0.26831
C	0.26420	6.45360	1.82386	H	-9.25818	3.24147	0.10873
C	-1.89053	5.99756	1.60041	H	-10.11241	2.76161	-1.36813
N	-0.96682	6.55272	2.43039	H	-8.48267	3.45591	-1.45520
N	4.04969	3.85620	-1.15038	H	-7.90175	-0.30693	-1.95001
C	4.80469	3.89131	-2.40545	H	-6.81239	2.28765	-2.29455
C	6.31544	3.79970	-2.11078	H	9.59139	-1.22835	2.10363
O	6.74942	3.74318	-0.96370	H	7.65021	-6.55424	-1.30375

H	7.40317	-6.50511	0.44571	H	7.96707	-1.83287	2.54044
H	8.31450	-4.10409	-1.24585	H	9.39884	-2.82235	2.88615
H	7.49252	-4.07356	1.57539	H	0.59067	6.68427	6.71331
H	3.16556	-3.88870	-4.03424	H	0.54144	4.90849	6.97614
H	4.44060	-5.09306	-4.25919	H	-6.38315	4.00087	4.85597
H	5.17222	-1.64678	-5.93349	H	-6.70144	2.39205	4.15209
H	3.57655	-1.96711	-5.38361	H	-6.53577	-4.22275	-4.94829
H	3.98224	-3.29104	-1.83239	H	-4.90254	-4.03787	-5.58167
H	6.51156	-4.05822	-2.73891	H	0.58082	1.61948	-5.54226
H	2.52020	-6.93858	0.02103	H	1.72388	2.73866	-4.75612
H	0.84229	-6.46958	-0.23009	H	1.30913	0.46553	8.08968
H	4.83626	-4.44092	2.98098	H	1.99758	-1.00803	7.35747
H	4.38334	-3.09689	4.06400	H	8.96226	4.75976	-3.57317
H	5.28858	-2.87834	1.39637	H	8.87829	3.71688	-2.13178
H	2.39832	-4.21558	3.38316	H	9.03643	-6.25876	-0.21872
H	3.49816	-4.19605	0.68434	H	-4.41212	-1.60891	-3.82709
H	-1.58794	0.58172	4.82257	H	-0.40075	0.42274	-1.74071
H	-1.13419	2.29048	4.51989	O	-0.15064	-3.48128	-0.39255
H	0.42170	1.66146	2.94961	H	0.37493	-3.06380	-1.09295
H	2.65663	0.59256	6.94852	H	-0.94794	-3.85778	-0.82102
H	0.74895	-0.63874	5.42331	C	2.26598	-5.33864	-1.41405
H	2.00790	5.83652	7.34882	H	1.94721	-4.30267	-1.38208
H	2.56077	1.80286	4.27802	H	1.73938	-5.80556	-2.25759
H	3.91451	2.69352	4.96162				
H	4.00942	-0.24344	3.11690	TS-1-N2			
H	5.70830	-0.22044	1.23348	C	-5.24479	-4.99620	-4.99432
H	6.42867	2.18927	0.66194	C	-4.62637	-4.80116	-3.61835
H	3.44179	4.65876	3.58243	O	-4.61247	-3.68892	-3.08453
H	1.45296	3.55285	5.43774	N	-4.11824	-5.92267	-3.04783
H	0.55600	5.22947	-1.35508	C	-3.56376	-6.09170	-1.71002
H	1.78358	6.21056	-0.54170	C	-2.97622	-4.81848	-1.10367
H	1.16490	6.77302	2.32536	O	-2.07972	-4.20146	-1.70344
H	-1.13877	6.94586	3.34320	C	-2.42045	-7.12716	-1.79318
H	-2.94412	5.95096	1.84719	O	-3.03653	-8.29472	-2.34834
H	1.06890	3.30986	0.08956	C	-1.76329	-7.40859	-0.44430
H	3.41479	4.56079	1.37683	N	-3.39359	-4.54544	0.13561
H	3.37999	5.16181	-3.39021	C	-2.91789	-3.44353	0.96136
H	4.93882	5.13531	-4.19042	C	-3.38481	-3.74464	2.39737
H	5.94416	6.48981	-2.31990	O	-4.27308	-4.57358	2.62498
H	4.37981	6.48342	-1.48964	C	-3.41755	-2.06129	0.45700
H	4.60949	10.18389	-2.73138	C	-4.81378	-2.02933	-0.18574
H	4.34129	9.13390	-1.32213	C	-5.94831	-2.42284	0.77106
H	5.94560	9.18821	-2.11041	C	-5.09795	-0.65130	-0.80041
H	4.51525	3.02429	-3.01079	N	-2.75978	-3.01739	3.34353
H	4.57596	3.88984	-0.28143	C	-3.03209	-3.18618	4.76565
H	8.98780	2.98429	-3.75126	C	-3.87904	-2.00326	5.25695
H	6.67136	3.88454	-4.11963	O	-3.47916	-0.84050	5.14857
H	2.09461	2.01124	-6.35302	C	-1.72360	-3.26414	5.57472
H	1.58054	0.25889	1.64939	C	-0.90550	-4.45714	5.06364
H	-1.13515	-0.07976	0.81099	O	-1.23313	-5.60213	5.35896
H	-0.27213	-1.34553	-0.03382	N	0.13914	-4.13690	4.26064
H	7.70399	-0.82990	-4.09197	C	-6.12224	2.61162	4.44303
H	3.59720	0.93396	-1.02194	C	-5.50402	3.18284	3.17164
H	3.93472	-0.74950	-0.71895	O	-5.49079	4.39228	2.94211
H	3.68178	-1.03726	-3.32094	N	-4.94471	2.28330	2.30166
H	2.50053	1.65546	-2.98192	C	-4.08108	2.81564	1.24155
N	-5.25243	-1.81218	5.84661	C	-4.83377	3.18309	-0.03700
H	-5.68369	-0.94732	6.14491	O	-5.97524	2.80463	-0.29907
C	-6.04954	-3.03833	5.88724	C	-2.98481	1.74133	1.02103
H	-7.07263	-2.77121	6.15780	C	-3.03271	0.97408	2.34398
H	-6.06553	-3.53037	4.91044	C	-4.51971	0.92484	2.67164
H	-5.67267	-3.74468	6.63483	N	-4.08925	3.94344	-0.89640
H	1.26636	-2.48367	0.92004	C	-4.73806	4.68840	-1.97372
H	0.99056	-1.00899	-2.87378	C	-5.41083	3.82508	-3.04977
N	-9.70644	1.45570	-3.97086	O	-6.26742	4.31378	-3.77889
H	-8.97632	2.13610	-4.12675	C	-3.71275	5.60962	-2.64605
C	-10.85400	1.41445	-4.85443	N	-4.96095	2.54360	-3.18446
H	-11.39461	2.36713	-4.84082	C	-5.50473	1.63976	-4.17878
H	-10.55706	1.19309	-5.88633	C	-6.51863	0.62038	-3.61276
H	-11.51444	0.62275	-4.49843	O	-6.59488	-0.51914	-4.07188
H	5.98829	1.32733	-3.66808	C	-4.39351	0.92847	-4.97728
H	5.84105	1.15316	-1.27761	C	-3.39368	0.22314	-4.11904
H	5.41364	-0.32064	-3.90443	N	-3.48133	-1.10077	-3.72487
H	8.19975	0.57122	-3.10438	C	-2.24750	0.69748	-3.52692
H	8.25536	-1.59261	-1.65928	C	-2.42313	-1.39232	-2.93679

N	-1.65460	-0.31465	-2.80070	C	3.93749	9.44446	-2.32631
N	-7.35595	1.10434	-2.65763	N	6.77523	4.24448	-3.25954
C	-8.34209	0.23724	-2.00726	C	8.22237	4.46592	-3.21591
C	-9.56409	-0.08842	-2.88942	C	1.25662	1.58871	-5.25285
O	-10.25020	-1.07357	-2.63241	C	2.02446	0.44979	-4.61279
C	-8.74571	0.86173	-0.64398	O	2.12346	-0.65245	-5.17075
C	-9.51944	2.17849	-0.81154	O	6.38611	-0.96256	-0.13298
C	-9.52161	-0.13412	0.22604	C	6.45974	-0.42393	-1.24398
C	9.09232	-1.49830	2.03970	N	7.47094	-0.57706	-2.11455
C	9.04345	-2.13560	0.66765	C	7.34217	0.21890	-3.32644
O	9.50677	-1.60146	-0.34328	C	5.85284	0.64332	-3.31012
N	8.46583	-3.37244	0.65569	C	5.43668	0.56220	-1.82460
C	8.08654	-4.03026	-0.57890	C	3.97836	0.21114	-1.42748
C	6.57888	-3.90645	-0.77754	C	3.08614	-0.33932	-2.54092
O	5.80734	-3.98818	0.19570	N	2.56798	0.71708	-3.39902
C	8.44145	-5.52563	-0.55013	C	1.96218	-1.25154	-2.04848
N	6.14498	-3.82094	-2.03779	O	2.18048	-2.12365	-1.19344
C	4.72701	-3.91320	-2.31459	H	-5.18481	-6.02000	-5.37128
C	4.18293	-5.25169	-1.73771	H	-1.67724	-6.71310	-2.49040
O	4.90576	-6.22455	-1.66746	H	-1.04079	-8.22498	-0.54924
C	4.45220	-3.89065	-3.83705	H	-2.50496	-7.70827	0.30194
C	5.26541	-2.85912	-4.62341	H	-1.21919	-6.53487	-0.07334
O	6.50044	-2.83471	-4.55616	H	-2.34901	-8.95447	-2.50466
N	4.57263	-2.03992	-5.44399	H	-4.33849	-6.50364	-1.04926
C	2.45594	-6.00127	0.00883	H	-4.18860	-6.79698	-3.55068
C	2.37706	-5.16094	1.28469	H	-2.69229	-1.69990	-0.27609
O	1.67029	-5.55936	2.20714	H	-3.37773	-1.36859	1.29844
N	3.13715	-4.02337	1.37360	H	-4.80756	-2.74531	-1.01119
C	3.27473	-3.32740	2.65025	H	-5.89780	-0.74601	-1.53123
C	2.47532	-2.01797	2.77216	H	-5.40772	0.09178	-0.06061
O	2.47594	-1.39948	3.84595	H	-4.22658	-0.25093	-1.32765
C	4.74465	-3.06168	3.02588	H	-6.91353	-2.35178	0.25860
O	5.37385	-2.07288	2.22726	H	-5.84062	-3.43989	1.15241
N	1.79183	-1.61686	1.68556	H	-5.98536	-1.75343	1.63917
C	0.94351	-0.43580	1.67342	H	-1.82266	-3.44360	0.95562
C	0.09936	-0.36844	2.95037	H	-4.10958	-5.10803	0.58633
O	-0.43900	-1.38110	3.43010	H	-1.97524	-3.45595	6.62144
C	-0.04568	-0.47981	0.48246	H	-1.19372	-2.31338	5.50394
S	0.46014	0.56580	-0.93512	H	0.59201	-4.86988	3.72221
N	-0.07783	0.85680	3.44769	H	0.21349	-3.19317	3.90024
C	-0.83282	1.14125	4.65841	H	-3.55124	-4.13746	4.87205
C	0.10030	1.19246	5.85805	H	-1.99105	-2.39509	3.10144
O	0.24261	2.21462	6.54433	H	-5.33969	2.28462	5.13661
N	0.77297	0.05403	6.10420	H	-2.01638	2.20824	0.82561
C	1.77949	0.04538	7.13838	H	-3.23018	1.09081	0.17788
C	0.77702	5.71093	6.70998	H	-2.55197	1.58047	3.10625
C	1.25210	5.58810	5.26115	H	-2.55201	-0.00183	2.34621
O	1.46059	6.57210	4.54838	H	-5.04775	0.18301	2.06393
N	1.50074	4.31284	4.85003	H	-4.69665	0.69682	3.71985
C	2.31655	4.00234	3.68955	H	-3.61309	3.72426	1.61892
C	1.50015	3.81872	2.39552	H	-4.20208	6.18760	-3.43221
O	0.37288	3.30862	2.39983	H	-3.27407	6.29192	-1.91287
C	3.11393	2.71677	4.00184	H	-2.90370	5.02054	-3.09113
C	4.03158	2.24677	2.91515	H	-5.55868	5.28947	-1.56429
N	4.72004	3.10218	2.06711	H	-3.21184	4.33857	-0.53804
C	4.40215	0.94523	2.67215	H	-3.86910	1.68499	-5.56729
C	5.50079	2.31255	1.33975	H	-4.86562	0.22383	-5.66475
N	5.34304	1.00505	1.67433	H	-1.81715	1.68723	-3.57225
N	2.11501	4.21661	1.25377	H	-2.26612	-2.36613	-2.49160
C	1.47400	4.03204	-0.04174	H	-6.07383	2.27515	-4.86719
C	2.39251	3.74050	-1.23193	H	-4.31953	2.18407	-2.49076
O	1.85716	3.36301	-2.28579	H	-7.80011	1.09485	-0.13846
C	0.61534	5.28316	-0.45280	H	-9.73925	0.31511	1.20081
C	-0.36953	5.70669	0.59104	H	-10.46266	-0.42567	-0.24588
N	-1.71686	5.37448	0.54656	H	-8.94182	-1.04709	0.39558
C	-0.10010	6.39528	1.75067	H	-9.70755	2.62893	0.16750
C	-2.24199	5.85306	1.66445	H	-10.48564	2.00922	-1.29897
N	-1.29733	6.47256	2.42145	H	-8.96461	2.91362	-1.40330
N	3.72130	4.02869	-1.19684	H	-7.88884	-0.74246	-1.82784
C	4.46451	4.13829	-2.45308	H	-7.05042	1.92473	-2.14247
C	5.97562	4.21523	-2.15613	H	9.63752	-0.55701	1.98050
O	6.40601	4.26485	-1.00693	H	8.11520	-6.01541	-1.47140
C	3.98629	5.37300	-3.25978	H	7.93254	-6.01533	0.28547
C	4.24289	6.68954	-2.52560	H	8.62346	-3.52747	-1.38622
S	3.55881	8.08947	-3.49207	H	7.89773	-3.61926	1.45674

H	3.37863	-3.76293	-4.00059	H	0.24801	4.81644	7.04954
H	4.74113	-4.86204	-4.25569	H	-6.70338	3.40319	4.91576
H	5.12422	-1.37809	-5.97256	H	-6.76780	1.75394	4.23442
H	3.57891	-1.82472	-5.34341	H	-6.29311	-4.69135	-4.93858
H	4.19938	-3.08752	-1.82631	H	-4.74737	-4.32468	-5.69927
H	6.76833	-3.64588	-2.82254	H	0.19768	1.31061	-5.26436
H	3.22299	-6.76954	0.16578	H	1.36901	2.53349	-4.71670
H	1.49400	-6.51310	-0.02467	H	1.34977	0.38808	8.08225
H	5.28720	-4.01587	2.98690	H	2.15763	-0.97094	7.25665
H	4.75372	-2.68829	4.05253	H	8.48148	5.43796	-3.64707
H	5.59924	-2.45913	1.36357	H	8.52937	4.44307	-2.17014
H	2.85295	-3.98125	3.42093	H	9.52045	-5.65024	-0.43184
H	3.88067	-3.88681	0.69480	H	-4.26519	-1.73971	-3.86227
H	-1.60800	0.38371	4.80661	H	-0.64726	0.03956	-1.92046
H	-1.27961	2.13063	4.56438	O	0.14669	-3.77118	-0.18993
H	0.28829	1.68181	2.96678	H	0.79046	-3.22206	-0.67119
H	2.61823	0.70712	6.88986	H	-0.58987	-3.91166	-0.81531
H	0.79078	-0.68199	5.40754	C	2.71993	-5.30429	-1.34122
H	1.65723	5.85446	7.34530	H	2.26929	-4.31779	-1.37453
H	2.41899	1.90432	4.24496	H	2.23444	-5.90295	-2.12356
H	3.68209	2.92422	4.91772				
H	4.10464	0.01795	3.13008	Int-N2			
H	5.76248	0.19387	1.21446	C	-5.17505	-5.15402	-4.99002
H	6.18542	2.65644	0.57955	C	-4.50354	-4.88111	-3.65361
H	3.01122	4.83367	3.53981	O	-4.54284	-3.75320	-3.15108
H	1.19264	3.54910	5.44831	N	-3.89843	-5.95214	-3.08488
H	0.09550	5.03145	-1.37974	C	-3.27100	-6.07118	-1.77270
H	1.30421	6.10903	-0.66974	C	-2.80256	-4.75278	-1.16516
H	0.81199	6.76059	2.19476	O	-1.97435	-4.04722	-1.76992
H	-1.41993	6.87590	3.33801	C	-2.02524	-6.97454	-1.91268
H	-3.27974	5.77958	1.96449	O	-2.53662	-8.19836	-2.45293
H	0.80109	3.17563	0.03824	C	-1.28510	-7.18380	-0.59410
H	3.10508	4.42663	1.34011	N	-3.22765	-4.52595	0.07796
H	2.91783	5.24514	-3.44886	C	-2.79538	-3.41997	0.92308
H	4.47803	5.38723	-4.23937	C	-3.27867	-3.75427	2.34490
H	5.31619	6.84846	-2.36997	O	-4.15333	-4.60594	2.54367
H	3.76120	6.66716	-1.54262	C	-3.30944	-2.04370	0.42155
H	3.57590	10.37007	-2.77904	C	-4.69046	-2.02939	-0.25412
H	3.42537	9.29376	-1.37200	C	-5.83736	-2.47873	0.66232
H	5.01449	9.52968	-2.15738	C	-4.99842	-0.64266	-0.84005
H	4.26335	3.24365	-3.05311	N	-2.67654	-3.03933	3.31354
H	4.24205	4.17576	-0.33782	C	-2.96149	-3.25547	4.72586
H	8.74580	3.67648	-3.76264	C	-3.86630	-2.12900	5.23885
H	6.33115	4.24456	-4.16567	O	-3.54276	-0.94274	5.12566
H	1.57770	1.69735	-6.29141	C	-1.66437	-3.29679	5.55391
H	1.56758	0.46481	1.62155	C	-0.80576	-4.46496	5.05124
H	-1.01750	-0.10835	0.80490	O	-1.13022	-5.61970	5.31277
H	-0.18308	-1.51771	0.17195	N	0.26438	-4.11249	4.30090
H	7.58695	-0.38298	-4.20562	C	-6.17706	2.39039	4.48576
H	3.48515	1.08570	-0.99633	C	-5.59995	3.02769	3.22791
H	4.01562	-0.53184	-0.62521	O	-5.64244	4.24215	3.03631
H	3.67079	-1.01629	-3.17486	N	-5.00983	2.18065	2.32234
H	2.32456	1.60277	-2.95466	C	-4.16114	2.78862	1.29287
N	-5.07090	-2.29239	5.83310	C	-4.90040	3.13896	0.00231
H	-5.57786	-1.47654	6.14985	O	-6.03110	2.74291	-0.28185
C	-5.75134	-3.58736	5.85112	C	-2.98919	1.79417	1.07598
H	-6.78996	-3.42269	6.14326	C	-3.02948	0.97188	2.36564
H	-5.73790	-4.05306	4.86137	C	-4.51956	0.83360	2.65250
H	-5.29887	-4.27490	6.57370	N	-4.15174	3.91196	-0.84388
H	1.86405	-2.17220	0.84369	C	-4.79148	4.67492	-1.91406
H	1.11332	-1.34101	-2.74190	C	-5.42540	3.84016	-3.03464
N	-9.84423	0.78245	-3.89627	O	-6.20867	4.36540	-3.81731
H	-9.20666	1.55319	-4.03390	C	-3.77049	5.63771	-2.53371
C	-10.96178	0.60215	-4.80099	N	-5.03063	2.53482	-3.14458
H	-11.62447	1.47440	-4.78697	C	-5.58244	1.65925	-4.15820
H	-10.62005	0.43596	-5.82921	C	-6.55573	0.59771	-3.60202
H	-11.51753	-0.27442	-4.46574	O	-6.57941	-0.54320	-4.06840
H	5.71749	1.63779	-3.73823	C	-4.48214	0.99373	-5.01065
H	5.68682	1.51508	-1.34226	C	-3.48988	0.23223	-4.19550
H	5.27443	-0.05702	-3.91205	N	-3.61776	-1.10352	-3.83936
H	8.01119	1.09003	-3.29115	C	-2.33126	0.66124	-3.60427
H	8.33358	-1.01446	-1.78647	C	-2.58403	-1.47446	-3.07364
H	8.06583	-1.31108	2.37714	N	-1.79148	-0.41160	-2.92439
H	9.57549	-2.16048	2.76462	N	-7.40536	1.03400	-2.63853
H	0.14097	6.59241	6.80522	C	-8.32777	0.10845	-1.97055

C	-9.52848	-0.31666	-2.84001	C	1.24846	1.55035	-5.19781
O	-10.12965	-1.35157	-2.56891	C	1.96238	0.39305	-4.52152
C	-8.76445	0.72110	-0.61211	O	1.99677	-0.72578	-5.05607
C	-9.63166	1.97669	-0.79010	O	6.48186	-0.78219	-0.11074
C	-9.46199	-0.31619	0.27581	C	6.49308	-0.30025	-1.24945
C	9.11123	-1.38940	2.00961	N	7.47902	-0.46313	-2.14806
C	9.08287	-1.99830	0.62398	C	7.27563	0.25822	-3.39606
O	9.55086	-1.44160	-0.37226	C	5.77250	0.62744	-3.34374
N	8.51288	-3.23868	0.58395	C	5.41236	0.61360	-1.84224
C	8.11445	-3.85987	-0.66322	C	3.98267	0.23037	-1.37518
C	6.60076	-3.74245	-0.82358	C	3.04131	-0.35837	-2.42435
O	5.85411	-3.81469	0.16929	N	2.53869	0.67590	-3.33012
C	8.48258	-5.35240	-0.69028	C	1.87130	-1.16853	-1.80620
N	6.13432	-3.67485	-2.07293	O	2.19782	-2.07469	-0.93542
C	4.71249	-3.80841	-2.31704	H	-5.03134	-6.17014	-5.36489
C	4.21461	-5.14668	-1.70395	H	-1.36180	-6.47917	-2.63676
O	4.95717	-6.10634	-1.64497	H	-0.48428	-7.91779	-0.73486
C	4.40970	-3.83097	-3.83389	H	-1.95705	-7.56338	0.18129
C	5.19182	-2.80931	-4.66150	H	-0.82137	-6.25659	-0.24365
O	6.42894	-2.77759	-4.63468	H	-1.79145	-8.78761	-2.62573
N	4.46643	-2.00699	-5.46986	H	-3.96930	-6.57546	-1.09161
C	2.56894	-5.90812	0.10399	H	-3.91877	-6.83422	-3.57910
C	2.52062	-5.07248	1.38414	H	-2.57153	-1.66290	-0.29075
O	1.88414	-5.51187	2.34170	H	-3.29911	-1.35900	1.27011
N	3.22962	-3.90630	1.44216	H	-4.64899	-2.72639	-1.09512
C	3.37793	-3.18634	2.70065	H	-5.77148	-0.73935	-1.59943
C	2.55406	-1.89148	2.82976	H	-5.35417	0.06976	-0.09125
O	2.48389	-1.33317	3.93688	H	-4.12127	-0.19693	-1.32205
C	4.84938	-2.90121	3.05209	H	-6.78914	-2.43517	0.12231
O	5.45980	-1.92353	2.22522	H	-5.70104	-3.49761	1.02866
N	1.92950	-1.44609	1.72849	H	-5.92377	-1.82702	1.53994
C	1.01041	-0.32269	1.73129	H	-1.69962	-3.40171	0.93548
C	0.13362	-0.33197	2.98703	H	-3.89246	-5.14609	0.53303
O	-0.38010	-1.37841	3.42039	H	-1.92626	-3.50076	6.59598
C	0.04574	-0.43273	0.52761	H	-1.16162	-2.33056	5.49725
S	0.62445	0.34108	-1.02193	H	0.75944	-4.82696	3.77242
N	-0.11042	0.86937	3.51847	H	0.33834	-3.16177	3.95995
C	-0.88444	1.07627	4.73328	H	-3.43724	-4.23201	4.80173
C	0.05931	1.12325	5.92542	H	-1.91071	-2.40390	3.09529
O	0.22648	2.15032	6.59889	H	-5.37405	2.05859	5.15305
N	0.72628	-0.02085	6.16195	H	-2.04779	2.33135	0.93675
C	1.78626	-0.02240	7.14119	H	-3.16391	1.16204	0.20078
C	0.66411	5.62285	6.74279	H	-2.59740	1.56853	3.16434
C	1.07682	5.52930	5.27280	H	-2.49726	0.02347	2.33614
O	1.19802	6.52574	4.55599	H	-4.99292	0.09052	2.00352
N	1.37623	4.27059	4.84442	H	-4.71158	0.55352	3.68487
C	2.19463	4.00234	3.67374	H	-3.76690	3.72060	1.69738
O	1.38159	3.80440	2.37753	H	-4.25296	6.22658	-3.31555
C	0.25008	3.30211	2.38148	H	-3.36582	6.30659	-1.76966
C	3.04521	2.74874	3.97995	H	-2.93678	5.07978	-2.97363
C	3.98077	2.31503	2.89399	H	-5.63224	5.24866	-1.50521
N	4.61618	3.19225	2.02645	H	-3.28667	4.31639	-0.46231
C	4.41909	1.03238	2.66738	H	-3.95315	1.78132	-5.55294
C	5.43091	2.43252	1.30289	H	-4.95673	0.33207	-5.73770
N	5.34630	1.12588	1.66057	H	-1.85385	1.62774	-3.60998
N	2.00601	4.18662	1.23491	H	-2.43790	-2.45973	-2.64019
C	1.36626	3.98959	-0.05972	H	-6.17296	2.31274	-4.81066
C	2.28777	3.72793	-1.25335	H	-4.47119	2.14335	-2.39989
O	1.75844	3.33812	-2.30535	H	-7.83394	1.02591	-0.11629
C	0.48223	5.22627	-0.47128	H	-9.70601	0.13019	1.24543
C	-0.46242	5.67222	0.59774	H	-10.38247	-0.68077	-0.18582
N	-1.80662	5.32690	0.63150	H	-8.81713	-1.18230	0.45446
C	-0.13749	6.37632	1.73272	H	-9.84172	2.42747	0.18415
C	-2.27142	5.80971	1.77499	H	-10.58806	1.73206	-1.26448
N	-1.29296	6.44774	2.47071	H	-9.13732	2.74073	-1.39908
N	3.60585	4.05306	-1.22078	H	-7.80444	-0.83369	-1.78111
C	4.35144	4.16285	-2.47411	H	-7.13450	1.86757	-2.12365
C	5.85293	4.31061	-2.16460	H	9.65458	-0.44561	1.97793
O	6.26052	4.48066	-1.01837	H	8.14270	-5.81575	-1.62014
C	3.84341	5.36580	-3.31101	H	7.99415	-5.87389	0.13829
C	4.04770	6.70383	-2.59933	H	8.62907	-3.32780	-1.46627
S	3.31287	8.05941	-3.59176	H	7.94192	-3.50029	1.37850
C	3.65183	9.45050	-2.45666	H	3.33180	-3.72100	-3.97920
N	6.66641	4.27772	-3.25652	H	4.70683	-4.80866	-4.23176
C	8.09780	4.57938	-3.21501	H	4.99568	-1.34138	-6.01618

H	3.47714	-1.79450	-5.31938	H	-6.24517	-4.96090	-4.87526
H	4.16675	-2.99038	-1.83474	H	-4.79255	-4.44253	-5.72650
H	6.74010	-3.52782	-2.87664	H	0.20211	1.26263	-5.33934
H	3.35733	-6.65953	0.23461	H	1.29536	2.47921	-4.62603
H	1.61916	-6.44243	0.10879	H	1.41538	0.36661	8.09156
H	5.39978	-3.85141	3.02501	H	2.14180	-1.04458	7.27729
H	4.87007	-2.50787	4.07169	H	8.31325	5.52241	-3.72736
H	5.67026	-2.32438	1.36363	H	8.38773	4.66459	-2.16763
H	2.97906	-3.83759	3.48477	H	9.56475	-5.47046	-0.59608
H	3.89287	-3.70120	0.70281	H	-4.42866	-1.70416	-3.99380
H	-1.63083	0.28498	4.84818	H	-0.95069	-0.31999	-2.29948
H	-1.37063	2.04986	4.67591	O	0.19141	-3.73708	-0.08126
H	0.21552	1.72334	3.05959	H	0.91885	-3.15200	-0.39347
H	2.62976	0.60289	6.82349	H	-0.42882	-3.78991	-0.82805
H	0.74269	-0.74198	5.44928	C	2.76843	-5.20782	-1.25477
H	1.56819	5.78650	7.33855	H	2.31760	-4.21874	-1.27260
H	2.38514	1.90797	4.22452	H	2.25573	-5.80990	-2.01751
H	3.60539	2.97919	4.89532				
H	4.17206	0.09847	3.14024				
H	5.79880	0.33060	1.20051	Reac-N23			
H	6.08869	2.79932	0.52964	C	-5.54401	-4.46256	-5.12022
H	2.85580	4.86103	3.52485	C	-5.09390	-4.43403	-3.66934
H	1.13710	3.49409	5.45774	O	-5.03456	-3.37194	-3.04571
H	-0.06416	4.94970	-1.37561	N	-4.76780	-5.63407	-3.12715
H	1.15901	6.04946	-0.73132	C	-4.46647	-5.88640	-1.72664
H	0.79319	6.75451	2.12116	C	-3.54358	-4.82053	-1.11474
H	-1.34706	6.83383	3.40186	O	-2.54337	-4.43152	-1.73255
H	-3.29108	5.73381	2.12990	C	-3.75231	-7.25222	-1.63537
H	0.71505	3.11576	0.01448	O	-4.59393	-8.16324	-2.35423
H	3.00972	4.34141	1.32418	C	-3.53257	-7.71658	-0.19918
H	2.78218	5.19947	-3.51011	N	-3.86912	-4.46185	0.13501
H	4.35074	5.37641	-4.28247	C	-3.21184	-3.42858	0.92444
H	5.11327	6.90706	-2.44376	C	-3.66348	-3.63927	2.38180
H	3.56490	6.68089	-1.61691	O	-4.64381	-4.34219	2.65179
H	3.25802	10.35421	-2.92645	C	-3.54117	-2.00098	0.40145
H	3.14970	9.30308	-1.49653	C	-4.95562	-1.79365	-0.16803
H	4.72625	9.57424	-2.29528	C	-6.08472	-2.02836	0.84627
H	4.18844	3.24966	-3.05711	C	-5.09223	-0.39987	-0.79879
H	4.11766	4.25082	-0.36674	N	-2.92832	-2.98677	3.30770
H	8.67174	3.77428	-3.68248	C	-3.21649	-3.10178	4.73427
H	6.23739	4.16858	-4.16338	C	-3.97049	-1.84988	5.20963
H	1.67640	1.69857	-6.19310	O	-3.47083	-0.72546	5.11319
H	1.55981	0.62611	1.68806	C	-1.92767	-3.26383	5.56032
H	-0.87831	0.09667	0.76328	C	-1.17104	-4.49925	5.05869
H	-0.19480	-1.48618	0.36893	O	-1.58362	-5.62593	5.31065
H	7.50792	-0.38196	-4.25135	N	-0.06770	-4.22876	4.31414
H	3.49700	1.09916	-0.92299	C	-5.89459	2.95986	4.49728
H	4.07144	-0.50577	-0.57105	C	-5.19709	3.47603	3.24262
H	3.57345	-1.09373	-3.03418	O	-5.03548	4.68068	3.04068
H	2.33509	1.58932	-2.92487	N	-4.74370	2.53276	2.36042
N	-5.01845	-2.49689	5.84921	C	-3.81632	2.96652	1.30909
H	-5.56736	-1.71752	6.18712	C	-4.51750	3.39417	0.01871
C	-5.61192	-3.83356	5.87908	O	-5.68145	3.10594	-0.25657
H	-6.63949	-3.74221	6.23529	C	-2.83674	1.78084	1.10547
H	-5.62707	-4.28008	4.88040	C	-3.01118	0.99781	2.40892
H	-5.07369	-4.50230	6.55893	C	-4.50129	1.12265	2.69883
H	2.13090	-1.85636	0.80903	N	-3.70366	4.09090	-0.83125
H	1.20262	-1.49454	-2.62239	C	-4.27965	4.87385	-1.92318
N	-9.89022	0.52209	-3.84880	C	-5.07065	4.05957	-2.95547
H	-9.32029	1.34111	-4.00076	O	-5.96987	4.59575	-3.59662
C	-11.00111	0.24528	-4.73818	C	-3.16231	5.64194	-2.64017
H	-11.72869	1.06397	-4.72482	N	-4.67454	2.77230	-3.17076
H	-10.65916	0.09384	-5.76851	C	-5.31152	1.93969	-4.17578
H	-11.48351	-0.66751	-4.38674	C	-6.41686	1.01210	-3.62194
H	5.57960	1.59044	-3.82099	O	-6.60426	-0.10888	-4.09436
H	5.64590	1.59965	-1.42013	C	-4.28171	1.15049	-5.00652
H	5.19875	-0.12591	-3.88131	C	-3.33676	0.31737	-4.20244
H	7.91181	1.15397	-3.43446	N	-3.58777	-0.97090	-3.77109
H	8.36322	-0.86364	-1.83158	C	-2.07695	0.60677	-3.72767
H	8.07892	-1.21279	2.33452	C	-2.50306	-1.39972	-3.07247
H	9.58622	-2.06524	2.72748	N	-1.56144	-0.46501	-3.02552
H	0.00565	6.48243	6.87703	N	-7.20918	1.56532	-2.66570
H	0.18018	4.70783	7.09460	C	-8.28491	0.80041	-2.03312
H	-6.77313	3.14530	4.99812	C	-9.55035	0.66345	-2.90553
H	-6.80077	1.52218	4.25476	O	-10.35526	-0.23320	-2.66881
				C	-8.59240	1.41542	-0.64054

C	-9.18246	2.83054	-0.74406	C	6.35366	-0.77686	-1.33524
C	-9.48977	0.49894	0.19930	N	7.39150	-0.93708	-2.17234
C	8.99677	-2.14711	1.98406	C	7.35781	-0.06420	-3.33676
C	8.90190	-2.68800	0.57265	C	5.89346	0.43576	-3.35569
O	9.34606	-2.08930	-0.40999	C	5.42322	0.31211	-1.88973
N	8.29889	-3.90969	0.48810	C	3.93046	0.05346	-1.55126
C	7.86146	-4.47078	-0.77540	C	3.02476	-0.29675	-2.73571
C	6.35125	-4.28764	-0.91063	N	2.62493	0.87830	-3.49204
O	5.62012	-4.38574	0.09297	C	1.80627	-1.14227	-2.37940
C	8.17522	-5.97289	-0.85924	O	1.89210	-2.12489	-1.65427
N	5.87656	-4.12646	-2.14658	H	-5.57635	-5.46320	-5.55805
C	4.44674	-4.08415	-2.38115	H	-2.78651	-7.13773	-2.15037
C	3.79907	-5.38448	-1.81890	H	-3.06645	-8.70728	-0.19520
O	4.41990	-6.42741	-1.83922	H	-4.48720	-7.78821	0.33082
C	4.13409	-3.99719	-3.89421	H	-2.87537	-7.03868	0.35093
C	5.00293	-3.01433	-4.68339	H	-4.13795	-9.01258	-2.40999
O	6.23768	-3.04833	-4.61196	H	-5.40177	-5.94615	-1.15277
N	4.36160	-2.16972	-5.52161	H	-4.92788	-6.47741	-3.66109
C	2.06542	-6.13908	-0.07337	H	-2.81617	-1.77086	-0.38373
C	2.09007	-5.38826	1.25666	H	-3.35501	-1.29573	1.21321
O	1.25878	-5.64151	2.12841	H	-5.08130	-2.51302	-0.97945
N	3.06936	-4.45580	1.42993	H	-5.92554	-0.40525	-1.49896
C	3.22055	-3.73593	2.68431	H	-5.28491	0.38598	-0.06404
C	2.41546	-2.42151	2.76620	H	-4.19889	-0.11955	-1.36498
O	2.47533	-1.75590	3.79154	H	-7.05254	-1.80051	0.38749
C	4.69842	-3.44680	3.00729	H	-6.11719	-3.05681	1.21021
O	5.28195	-2.47247	2.15687	H	-5.97643	-1.38166	1.72482
C	0.90006	-0.66564	1.65572	H	-2.12787	-3.57013	0.87535
C	0.10549	-0.49045	2.94218	H	-4.68648	-4.85628	0.58925
O	-0.48769	-1.44948	3.47737	H	-2.20900	-3.44177	6.60209
C	-0.08761	-0.47951	0.46771	H	-1.34295	-2.34554	5.50171
S	0.42856	0.86777	-0.66987	H	0.33968	-4.97203	3.75380
N	0.03050	0.75459	3.41995	H	0.05695	-3.28352	3.97194
C	-0.68906	1.12379	4.63012	H	-3.80837	-4.00749	4.85550
C	0.23684	1.12156	5.83665	H	-2.10763	-2.44400	3.04800
O	0.45712	2.14302	6.50320	H	-5.16600	2.51942	5.18696
N	0.80856	-0.06857	6.09236	H	-1.81803	2.14145	0.94662
C	1.80558	-0.21746	7.12411	H	-3.12094	1.17642	0.24057
C	1.20285	5.51305	6.83230	H	-2.48880	1.52329	3.20206
C	1.74086	5.42079	5.40402	H	-2.64857	-0.02805	2.40404
O	2.06537	6.41355	4.74929	H	-5.10030	0.47254	2.05489
N	1.90149	4.14816	4.94797	H	-4.73192	0.89196	3.73585
C	2.70675	3.81490	3.78887	H	-3.26125	3.82375	1.68758
C	1.88304	3.71058	2.49559	H	-3.59062	6.25570	-3.43539
O	0.76511	3.18329	2.47907	H	-2.63045	6.28618	-1.93424
C	3.40114	2.46407	4.06596	H	-2.44152	4.94471	-3.08008
C	4.25451	1.94016	2.95237	H	-5.01572	5.58195	-1.52489
N	5.02904	2.74815	2.13538	H	-2.81660	4.44100	-0.45423
C	4.47125	0.61623	2.64798	H	-3.69512	1.87332	-5.58079
C	5.70799	1.90873	1.36448	H	-4.83245	0.52375	-5.71185
N	5.40457	0.61226	1.64109	H	-1.51641	1.52292	-3.86029
N	2.47265	4.18676	1.37162	H	-2.45860	-2.38478	-2.62933
C	1.80468	4.10442	0.08396	H	-5.83096	2.63813	-4.84219
C	2.67915	3.75945	-1.12436	H	-3.98864	2.35784	-2.55329
O	2.09766	3.46466	-2.18074	H	-7.62018	1.49903	-0.13913
C	1.02905	5.42228	-0.25942	H	-9.62620	0.92663	1.19833
C	0.02491	5.79600	0.78691	H	-10.46984	0.36757	-0.26486
N	-1.32800	5.50802	0.66656	H	-9.04601	-0.49530	0.31339
C	0.26732	6.39118	2.00342	H	-9.30874	3.25628	0.25583
C	-1.88698	5.92752	1.79113	H	-10.16258	2.81436	-1.23292
N	-0.95685	6.46182	2.62761	H	-8.53397	3.51236	-1.30320
N	4.03070	3.90951	-1.08975	H	-7.95083	-0.23340	-1.90025
C	4.77825	3.97785	-2.34809	H	-6.83701	2.35647	-2.15077
C	6.29261	3.90202	-2.06062	H	9.61269	-1.24859	1.98543
O	6.73011	3.84939	-0.91465	H	7.81632	-6.38772	-1.80486
C	4.41374	5.27042	-3.12243	H	7.67242	-6.50779	-0.04785
C	4.80343	6.54022	-2.36499	H	8.38624	-3.92861	-1.56485
S	4.26218	8.01957	-3.30320	H	7.76021	-4.21126	1.29037
C	4.77761	9.30806	-2.11483	H	3.06981	-3.78055	-4.01950
N	7.08839	3.91203	-3.16806	H	4.32976	-4.97824	-4.34381
C	8.55141	3.98752	-3.12654	H	4.95125	-1.54149	-6.05025
C	1.51341	1.99780	-5.34810	H	3.38731	-1.88629	-5.43810
C	2.14411	0.75367	-4.75778	H	4.01130	-3.22271	-1.86423
O	2.20359	-0.30633	-5.39304	H	6.48209	-3.92544	-2.94048
O	6.19492	-1.38308	-0.26858	H	2.76933	-6.97850	-0.02286

H	1.05950	-6.55356	-0.13430	H	2.12566	0.77438	7.44420
H	5.25300	-4.39454	2.97800	H	8.90292	4.95533	-3.49756
H	4.73910	-3.04279	4.02141	H	8.85995	3.86731	-2.08787
H	5.48283	-2.87767	1.29510	H	9.25272	-6.13393	-0.77679
H	2.81462	-4.36678	3.48521	H	-4.46573	-1.48469	-3.83346
H	3.81930	-4.37914	0.74858	H	-0.43375	0.49909	-1.65787
H	-1.52048	0.43201	4.79515	O	-0.21778	-3.67628	-0.47527
H	-1.05673	2.14314	4.51552	H	0.33222	-3.15432	-1.08039
H	0.47840	1.53535	2.93537	H	-1.00331	-3.95700	-0.98552
H	1.40875	-0.75322	7.99413	C	1.56406	-2.04496	1.58482
H	0.64195	-0.83872	5.45626	H	0.81054	-2.83289	1.46094
H	2.05654	5.54984	7.51711	H	2.17314	-2.11484	0.67856
H	2.63970	1.71192	4.30370	C	2.36937	-5.29071	-1.32424
H	3.99779	2.60328	4.97633	H	2.08496	-4.25671	-1.16600
H	4.08388	-0.29297	3.07229	H	1.74855	-5.65433	-2.15437
H	5.73204	-0.22036	1.14823				
H	6.42300	2.20543	0.61239	TS-1-N23			
H	3.45979	4.59842	3.66806	C	-5.54401	-4.46256	-5.12022
H	1.48649	3.39072	5.48781	C	-5.09390	-4.43403	-3.66934
H	0.52685	5.26928	-1.21720	O	-5.03456	-3.37194	-3.04571
H	1.76075	6.22959	-0.38851	N	-4.76780	-5.63407	-3.12715
H	1.17122	6.70108	2.50545	C	-4.46647	-5.88640	-1.72664
H	-1.11921	6.82270	3.55541	C	-3.54358	-4.82053	-1.11474
H	-2.93735	5.86424	2.04808	O	-2.54337	-4.43152	-1.73255
H	1.06547	3.30702	0.16422	C	-3.75231	-7.25222	-1.63537
H	3.41612	4.53909	1.46017	O	-4.59393	-8.16324	-2.35423
H	3.33649	5.25141	-3.30333	C	-3.53257	-7.71658	-0.19918
H	4.89420	5.25833	-4.10765	N	-3.86912	-4.46185	0.13501
H	5.88776	6.58700	-2.21122	C	-3.21184	-3.42858	0.92444
H	4.32433	6.54767	-1.38053	C	-3.66348	-3.63927	2.38180
H	4.51104	10.27338	-2.55018	O	-4.64381	-4.34219	2.65179
H	4.25383	9.19323	-1.16186	C	-3.54117	-2.00098	0.40145
H	5.85791	9.28090	-1.94759	C	-4.95562	-1.79365	-0.16803
H	4.49259	3.12080	-2.96893	C	-6.08472	-2.02836	0.84627
H	4.56320	3.93741	-0.22452	C	-5.09223	-0.39987	-0.79879
H	8.99103	3.18773	-3.72900	N	-2.92832	-2.98677	3.30770
H	6.64401	4.00613	-4.06909	C	-3.21649	-3.10178	4.73427
H	1.94620	2.18413	-6.33402	C	-3.97049	-1.84988	5.20963
H	1.68139	0.10278	1.63267	O	-3.47083	-0.72546	5.11319
H	-1.08540	-0.23565	0.83035	C	-1.92767	-3.26383	5.56032
H	-0.17260	-1.40443	-0.09949	C	-1.17104	-4.49925	5.05869
H	7.61164	-0.62318	-4.24124	O	-1.58362	-5.62593	5.31065
H	3.50406	0.91888	-1.03838	N	-0.06770	-4.22876	4.31414
H	3.88881	-0.76901	-0.83091	C	-5.89459	2.95986	4.49728
H	3.57262	-0.95230	-3.41987	C	-5.19709	3.47603	3.24262
H	2.41743	1.73322	-2.97484	O	-5.03548	4.68068	3.04068
N	-5.19062	-2.03761	5.76864	N	-4.74370	2.53276	2.36042
H	-5.62895	-1.18122	6.08089	C	-3.81632	2.96652	1.30909
C	-5.98692	-3.26535	5.76306	C	-4.51750	3.39417	0.01871
H	-7.01818	-3.00382	6.00701	O	-5.68145	3.10594	-0.25657
H	-5.97089	-3.73762	4.77682	C	-2.83674	1.78084	1.10547
H	-5.63181	-3.98411	6.50962	C	-3.01118	0.99781	2.40892
H	0.87223	-0.91314	-2.91775	C	-4.50129	1.12265	2.69883
N	-9.72830	1.59617	-3.88046	N	-3.70366	4.09090	-0.83125
H	-8.99482	2.27896	-4.00720	C	-4.27965	4.87385	-1.92318
C	-10.86887	1.58886	-4.77377	C	-5.07065	4.05957	-2.95547
H	-11.53362	0.78646	-4.45122	O	-5.96987	4.59575	-3.59662
H	-11.40818	2.54151	-4.73099	C	-3.16231	5.64194	-2.64017
H	-10.56375	1.40355	-5.81033	N	-4.67454	2.77230	-3.17076
H	5.82298	1.45213	-3.74520	C	-5.31152	1.93969	-4.17578
H	5.72927	1.21820	-1.35234	C	-6.41686	1.01210	-3.62194
H	5.30463	-0.21052	-4.00701	O	-6.60426	-0.10888	-4.09436
H	8.06678	0.76702	-3.21956	C	-4.28171	1.15049	-5.00652
H	8.21822	-1.43274	-1.83369	C	-3.33676	0.31737	-4.20244
H	7.98481	-1.90117	2.32919	N	-3.58777	-0.97090	-3.77109
H	9.42061	-2.88917	2.66730	C	-2.07695	0.60677	-3.72767
H	0.63887	6.44068	6.94359	C	-2.50306	-1.39972	-3.07247
H	0.58440	4.65214	7.09820	N	-1.56144	-0.46501	-3.02552
H	-6.37303	3.80881	4.98531	N	-7.20918	1.56532	-2.66570
H	-6.64389	2.19821	4.26450	C	-8.28491	0.80041	-2.03312
H	-6.53612	-4.00726	-5.17488	C	-9.55035	0.66345	-2.90553
H	-4.86514	-3.83719	-5.70679	O	-10.35526	-0.23320	-2.66881
H	0.44778	1.79484	-5.49340	C	-8.59240	1.41542	-0.64054
H	1.62759	2.87744	-4.71088	C	-9.18246	2.83054	-0.74406
H	2.66159	-0.77272	6.72987	C	-9.48977	0.49894	0.19930

C	8.99677	-2.14711	1.98406	C	7.35781	-0.06420	-3.33676
C	8.90190	-2.68800	0.57265	C	5.89346	0.43576	-3.35569
O	9.34606	-2.08930	-0.40999	C	5.42322	0.31211	-1.88973
N	8.29889	-3.90969	0.48810	C	3.93046	0.05346	-1.55126
C	7.86146	-4.47078	-0.77540	C	3.02476	-0.29675	-2.73571
C	6.35125	-4.28764	-0.91063	N	2.62493	0.87830	-3.49204
O	5.62012	-4.38574	0.09297	C	1.80627	-1.14227	-2.37940
C	8.17522	-5.97289	-0.85924	O	1.89210	-2.12489	-1.65427
N	5.87656	-4.12646	-2.14658	H	-5.57635	-5.46320	-5.55805
C	4.44674	-4.08415	-2.38115	H	-2.78651	-7.13773	-2.15037
C	3.79907	-5.38448	-1.81890	H	-3.06645	-8.70728	-0.19520
O	4.41990	-6.42741	-1.83922	H	-4.48720	-7.78821	0.33082
C	4.13409	-3.99719	-3.89421	H	-2.87537	-7.03868	0.35093
C	5.00293	-3.01433	-4.68339	H	-4.13795	-9.01258	-2.40999
O	6.23768	-3.04833	-4.61196	H	-5.40177	-5.94615	-1.15277
N	4.36160	-2.16972	-5.52161	H	-4.92788	-6.47741	-3.66109
C	2.06542	-6.13908	-0.07337	H	-2.81617	-1.77086	-0.38373
C	2.09007	-5.38826	1.25666	H	-3.35501	-1.29573	1.21321
O	1.25878	-5.64151	2.12841	H	-5.08130	-2.51302	-0.97945
N	3.06936	-4.45580	1.42993	H	-5.92554	-0.40525	-1.49896
C	3.22055	-3.73593	2.68431	H	-5.28491	0.38598	-0.06404
C	2.41546	-2.42151	2.76620	H	-4.19889	-0.11955	-1.36498
O	2.47533	-1.75590	3.79154	H	-7.05254	-1.80051	0.38749
C	4.69842	-3.44680	3.00729	H	-6.11719	-3.05681	1.21021
O	5.28195	-2.47247	2.15687	H	-5.97643	-1.38166	1.72482
C	0.90006	-0.66564	1.65572	H	-2.12787	-3.57013	0.87535
C	0.10549	-0.49045	2.94218	H	-4.68648	-4.85628	0.58925
O	-0.48769	-1.44948	3.47737	H	-2.20900	-3.44177	6.60209
C	-0.08761	-0.47951	0.46771	H	-1.34295	-2.34554	5.50171
S	0.42856	0.86777	-0.66987	H	0.33968	-4.97203	3.75380
N	0.03050	0.75459	3.41995	H	0.05695	-3.28352	3.97194
C	-0.68906	1.12379	4.63012	H	-3.80837	-4.00749	4.85550
C	0.23684	1.12156	5.83665	H	-2.10763	-2.44400	3.04800
O	0.45712	2.14302	6.50320	H	-5.16600	2.51942	5.18696
N	0.80856	-0.06857	6.09236	H	-1.81803	2.14145	0.94662
C	1.80558	-0.21746	7.12411	H	-3.12094	1.17642	0.24057
C	1.20285	5.51305	6.83230	H	-2.48880	1.52329	3.20206
C	1.74086	5.42079	5.40402	H	-2.64857	-0.02805	2.40404
O	2.06537	6.41355	4.74929	H	-5.10030	0.47254	2.05489
N	1.90149	4.14816	4.94797	H	-4.73192	0.89196	3.73585
C	2.70675	3.81490	3.78887	H	-3.26125	3.82375	1.68758
C	1.88304	3.71058	2.49559	H	-3.59062	6.25570	-3.43539
O	0.76511	3.18329	2.47907	H	-2.63045	6.28618	-1.93424
C	3.40114	2.46407	4.06596	H	-2.44152	4.94471	-3.08008
C	4.25451	1.94016	2.95237	H	-5.01572	5.58195	-1.52489
N	5.02904	2.74815	2.13538	H	-2.81660	4.44100	-0.45423
C	4.47125	0.61623	2.64798	H	-3.69512	1.87332	-5.58079
C	5.70799	1.90873	1.36448	H	-4.83245	0.52375	-5.71185
N	5.40457	0.61226	1.64109	H	-1.51641	1.52292	-3.86029
N	2.47265	4.18676	1.37162	H	-2.45860	-2.38478	-2.62933
C	1.80468	4.10442	0.08396	H	-5.83096	2.63813	-4.84219
C	2.67915	3.75945	-1.12436	H	-3.98864	2.35784	-2.55329
O	2.09766	3.46466	-2.18074	H	-7.62018	1.49903	-0.13913
C	1.02905	5.42228	-0.25942	H	-9.62620	0.92663	1.19833
C	0.02491	5.79600	0.78691	H	-10.46984	0.36757	-0.26486
N	-1.32800	5.50802	0.66656	H	-9.04601	-0.49530	0.31339
C	0.26732	6.39118	2.00342	H	-9.30874	3.25628	0.25583
C	-1.88698	5.92752	1.79113	H	-10.16258	2.81436	-1.23292
N	-0.95685	6.46182	2.62761	H	-8.53397	3.51236	-1.30320
N	4.03070	3.90951	-1.08975	H	-7.95083	-0.23340	-1.90025
C	4.77825	3.97785	-2.34809	H	-6.83701	2.35647	-2.15077
C	6.29261	3.90202	-2.06062	H	9.61269	-1.24859	1.98543
O	6.73011	3.84939	-0.91465	H	7.81632	-6.38772	-1.80486
C	4.41374	5.27042	-3.12243	H	7.67242	-6.50779	-0.04785
C	4.80343	6.54022	-2.36499	H	8.38624	-3.92861	-1.56485
S	4.26218	8.01957	-3.30320	H	7.76021	-4.21126	1.29037
C	4.77761	9.30806	-2.11483	H	3.06981	-3.78055	-4.01950
N	7.08839	3.91203	-3.16806	H	4.32976	-4.97824	-4.34381
C	8.55141	3.98752	-3.12654	H	4.95125	-1.54149	-6.05025
C	1.51341	1.99780	-5.34810	H	3.38731	-1.88629	-5.43810
C	2.14411	0.75367	-4.75778	H	4.01130	-3.22271	-1.86423
O	2.20359	-0.30633	-5.39304	H	6.48209	-3.92544	-2.94048
O	6.19492	-1.38308	-0.26858	H	2.76933	-6.97850	-0.02286
C	6.35366	-0.77686	-1.33524	H	1.05950	-6.55356	-0.13430
N	7.39150	-0.93708	-2.17234	H	5.25300	-4.39454	2.97800

H	4.73910	-3.04279	4.02141	H	8.85995	3.86731	-2.08787
H	5.48283	-2.87767	1.29510	H	9.25272	-6.13393	-0.77679
H	2.81462	-4.36678	3.48521	H	-4.46573	-1.48469	-3.83346
H	3.81930	-4.37914	0.74858	H	-0.43375	0.49909	-1.65787
H	-1.52048	0.43201	4.79515	O	-0.21778	-3.67628	-0.47527
H	-1.05673	2.14314	4.51552	H	0.33222	-3.15432	-1.08039
H	0.47840	1.53535	2.93537	H	-1.00331	-3.95700	-0.98552
H	1.40875	-0.75322	7.99413	C	1.56406	-2.04496	1.58482
H	0.64195	-0.83872	5.45626	H	0.81054	-2.83289	1.46094
H	2.05654	5.54984	7.51711	H	2.17314	-2.11484	0.67856
H	2.63970	1.71192	4.30370	C	2.36937	-5.29071	-1.32424
H	3.99779	2.60328	4.97633	H	2.08496	-4.25671	-1.16600
H	4.08388	-0.29297	3.07229	H	1.74855	-5.65433	-2.15437
H	5.73204	-0.22036	1.14823				
H	6.42300	2.20543	0.61239	Int-N23			
H	3.45979	4.59842	3.66806	C	-5.54401	-4.46256	-5.12022
H	1.48649	3.39072	5.48781	C	-5.09390	-4.43403	-3.66934
H	0.52685	5.26928	-1.21720	O	-5.03456	-3.37194	-3.04571
H	1.76075	6.22959	-0.38851	N	-4.76780	-5.63407	-3.12715
H	1.17122	6.70108	2.50545	C	-4.46647	-5.88640	-1.72664
H	-1.11921	6.82270	3.55541	C	-3.54358	-4.82053	-1.11474
H	-2.93735	5.86424	2.04808	O	-2.54337	-4.43152	-1.73255
H	1.06547	3.30702	0.16422	C	-3.75231	-7.25222	-1.63537
H	3.41612	4.53909	1.46017	O	-4.59393	-8.16324	-2.35423
H	3.33649	5.25141	-3.30333	C	-3.53257	-7.71658	-0.19918
H	4.89420	5.25833	-4.10765	N	-3.86912	-4.46185	0.13501
H	5.88776	6.58700	-2.21122	C	-3.21184	-3.42858	0.92444
H	4.32433	6.54767	-1.38053	C	-3.66348	-3.63927	2.38180
H	4.51104	10.27338	-2.55018	O	-4.64381	-4.34219	2.65179
H	4.25383	9.19323	-1.16186	C	-3.54117	-2.00098	0.40145
H	5.85791	9.28090	-1.94759	C	-4.95562	-1.79365	-0.16803
H	4.49259	3.12080	-2.96893	C	-6.08472	-2.02836	0.84627
H	4.56320	3.93741	-0.22452	C	-5.09223	-0.39987	-0.79879
H	8.99103	3.18773	-3.72900	N	-2.92832	-2.98677	3.30770
H	6.64401	4.00613	-4.06909	C	-3.21649	-3.10178	4.73427
H	1.94620	2.18413	-6.33402	C	-3.97049	-1.84988	5.20963
H	1.68139	0.10278	1.63267	O	-3.47083	-0.72546	5.11319
H	-1.08540	-0.23565	0.83035	C	-1.92767	-3.26383	5.56032
H	-0.17260	-1.40443	-0.09949	C	-1.17104	-4.49925	5.05869
H	7.61164	-0.62318	-4.24124	O	-1.58362	-5.62593	5.31065
H	3.50406	0.91888	-1.03838	N	-0.06770	-4.22876	4.31414
H	3.88881	-0.76901	-0.83091	C	-5.89459	2.95986	4.49728
H	3.57262	-0.95230	-3.41987	C	-5.19709	3.47603	3.24262
H	2.41743	1.73322	-2.97484	O	-5.03548	4.68068	3.04068
N	-5.19062	-2.03761	5.76864	N	-4.74370	2.53276	2.36042
H	-5.62895	-1.18122	6.08089	C	-3.81632	2.96652	1.30909
C	-5.98692	-3.26535	5.76306	C	-4.51750	3.39417	0.01871
H	-7.01818	-3.00382	6.00701	O	-5.68145	3.10594	-0.25657
H	-5.97089	-3.73762	4.77682	C	-2.83674	1.78084	1.10547
H	-5.63181	-3.98411	6.50962	C	-3.01118	0.99781	2.40892
H	0.87223	-0.91314	-2.91775	C	-4.50129	1.12265	2.69883
N	-9.72830	1.59617	-3.88046	N	-3.70366	4.09090	-0.83125
H	-8.99482	2.27896	-4.00720	C	-4.27965	4.87385	-1.92318
C	-10.86887	1.58886	-4.77377	C	-5.07065	4.05957	-2.95547
H	-11.53362	0.78646	-4.45122	O	-5.96987	4.59575	-3.59662
H	-11.40818	2.54151	-4.73099	C	-3.16231	5.64199	-2.64017
H	-10.56375	1.40355	-5.81033	N	-4.67454	2.77230	-3.17076
H	5.82298	1.45213	-3.74520	C	-5.31152	1.93969	-4.17578
H	5.72927	1.21820	-1.35234	C	-6.41686	1.01210	-3.62194
H	5.30463	-0.21052	-4.00701	O	-6.60426	-0.10888	-4.09436
H	8.06678	0.76702	-3.21956	C	-4.28171	1.15049	-5.00652
H	8.21822	-1.43274	-1.83369	C	-3.33676	0.31737	-4.20244
H	7.98481	-1.90117	2.32919	N	-3.58777	-0.97090	-3.77109
H	9.42061	-2.88917	2.66730	C	-2.07695	0.60677	-3.72767
H	0.63887	6.44068	6.94359	C	-2.50306	-1.39972	-3.07247
H	0.58440	4.65214	7.09820	N	-1.56144	-0.46501	-3.02552
H	-6.37303	3.80881	4.98531	N	-7.20918	1.56532	-2.66570
H	-6.64389	2.19821	4.26450	C	-8.28491	0.80041	-2.03312
H	-6.53612	-4.00726	-5.17488	C	-9.55035	0.66345	-2.90553
H	-4.86514	-3.83719	-5.70679	O	-10.35526	-0.23320	-2.66881
H	0.44778	1.79484	-5.49340	C	-8.59240	1.41542	-0.64054
H	1.62759	2.87744	-4.71088	C	-9.18246	2.83054	-0.74406
H	2.66159	-0.77272	6.72987	C	-9.48977	0.49894	0.19930
H	2.12566	0.77438	7.44420	C	8.99677	-2.14711	1.98406
H	8.90292	4.95533	-3.49756	C	8.90190	-2.68800	0.57265

O	9.34606	-2.08930	-0.40999	C	5.42322	0.31211	-1.88973
N	8.29889	-3.90969	0.48810	C	3.93046	0.05346	-1.55126
C	7.86146	-4.47078	-0.77540	C	3.02476	-0.29675	-2.73571
C	6.35125	-4.28764	-0.91063	N	2.62493	0.87830	-3.49204
O	5.62012	-4.38574	0.09297	C	1.80627	-1.14227	-2.37940
C	8.17522	-5.97289	-0.85924	O	1.89210	-2.12489	-1.65427
N	5.87656	-4.12646	-2.14658	H	-5.57635	-5.46320	-5.55805
C	4.44674	-4.08415	-2.38115	H	-2.78651	-7.13773	-2.15037
C	3.79907	-5.38448	-1.81890	H	-3.06645	-8.70728	-0.19520
O	4.41990	-6.42741	-1.83922	H	-4.48720	-7.78821	0.33082
C	4.13409	-3.99719	-3.89421	H	-2.87537	-7.03868	0.35093
C	5.00293	-3.01433	-4.68339	H	-4.13795	-9.01258	-2.40999
O	6.23768	-3.04833	-4.61196	H	-5.40177	-5.94615	-1.15277
N	4.36160	-2.16972	-5.52161	H	-4.92788	-6.47741	-3.66109
C	2.06542	-6.13908	-0.07337	H	-2.81617	-1.77086	-0.38373
C	2.09007	-5.38826	1.25666	H	-3.35501	-1.29573	1.21321
O	1.25878	-5.64151	2.12841	H	-5.08130	-2.51302	-0.97945
N	3.06936	-4.45580	1.42993	H	-5.92554	-0.40525	-1.49896
C	3.22055	-3.73593	2.68431	H	-5.28491	0.38598	-0.06404
C	2.41546	-2.42151	2.76620	H	-4.19889	-0.11955	-1.36498
O	2.47533	-1.75590	3.79154	H	-7.05254	-1.80051	0.38749
C	4.69842	-3.44680	3.00729	H	-6.11719	-3.05681	1.21021
O	5.28195	-2.47247	2.15687	H	-5.97643	-1.38166	1.72482
C	0.90006	-0.66564	1.65572	H	-2.12787	-3.57013	0.87535
C	0.10549	-0.49045	2.94218	H	-4.68648	-4.85628	0.58925
O	-0.48769	-1.44948	3.47737	H	-2.20900	-3.44177	6.60209
C	-0.08761	-0.47951	0.46771	H	-1.34295	-2.34554	5.50171
S	0.42856	0.86777	-0.66987	H	0.33968	-4.97203	3.75380
N	0.03050	0.75459	3.41995	H	0.05695	-3.28352	3.97194
C	-0.68906	1.12379	4.63012	H	-3.80837	-4.00749	4.85550
C	0.23684	1.12156	5.83665	H	-2.10763	-2.44400	3.04800
O	0.45712	2.14302	6.50320	H	-5.16600	2.51942	5.18696
N	0.80856	-0.06857	6.09236	H	-1.81803	2.14145	0.94662
C	1.80558	-0.21746	7.12411	H	-3.12094	1.17642	0.24057
C	1.20285	5.51305	6.83230	H	-2.48880	1.52329	3.20206
C	1.74086	5.42079	5.40402	H	-2.64857	-0.02805	2.40404
O	2.06537	6.41355	4.74929	H	-5.10030	0.47254	2.05489
N	1.90149	4.14816	4.94797	H	-4.73192	0.89196	3.73585
C	2.70675	3.81490	3.78887	H	-3.26125	3.82375	1.68758
C	1.88304	3.71058	2.49559	H	-3.59062	6.25570	-3.43539
O	0.76511	3.18329	2.47907	H	-2.63045	6.28618	-1.93424
C	3.40114	2.46407	4.06596	H	-2.44152	4.94471	-3.08008
C	4.25451	1.94016	2.95237	H	-5.01572	5.58195	-1.52489
N	5.02904	2.74815	2.13538	H	-2.81660	4.44100	-0.45423
C	4.47125	0.61623	2.64798	H	-3.69512	1.87332	-5.58079
C	5.70799	1.90873	1.36448	H	-4.83245	0.52375	-5.71185
N	5.40457	0.61226	1.64109	H	-1.51641	1.52292	-3.86029
N	2.47265	4.18676	1.37162	H	-2.45860	-2.38478	-2.62933
C	1.80468	4.10442	0.08396	H	-5.83096	2.63813	-4.84219
C	2.67915	3.75945	-1.12436	H	-3.98864	2.35784	-2.55329
O	2.09766	3.46466	-2.18074	H	-7.62018	1.49903	-0.13913
C	1.02905	5.42228	-0.25942	H	-9.62620	0.92663	1.19833
C	0.02491	5.79600	0.78691	H	-10.46984	0.36757	-0.26486
N	-1.32800	5.50802	0.66656	H	-9.04601	-0.49530	0.31339
C	0.26732	6.39118	2.00342	H	-9.30874	3.25628	0.25583
C	-1.88698	5.92752	1.79113	H	-10.16258	2.81436	-1.23292
N	-0.95685	6.46182	2.62761	H	-8.53397	3.51236	-1.30320
N	4.03070	3.90951	-1.08975	H	-7.95083	-0.23340	-1.90025
C	4.77825	3.97785	-2.34809	H	-6.83701	2.35647	-2.15077
C	6.29261	3.90202	-2.06062	H	9.61269	-1.24859	1.98543
O	6.73011	3.84939	-0.91465	H	7.81632	-6.38772	-1.80486
C	4.41374	5.27042	-3.12243	H	7.67242	-6.50779	-0.04785
C	4.80343	6.54022	-2.36499	H	8.38624	-3.92861	-1.56485
S	4.26218	8.01957	-3.30320	H	7.76021	-4.21126	1.29037
C	4.77761	9.30806	-2.11483	H	3.06981	-3.78055	-4.01950
N	7.08839	3.91203	-3.16806	H	4.32976	-4.97824	-4.34381
C	8.55141	3.98752	-3.12654	H	4.95125	-1.54149	-6.05025
C	1.51341	1.99780	-5.34810	H	3.38731	-1.88629	-5.43810
C	2.14411	0.75367	-4.75778	H	4.01130	-3.22271	-1.86423
O	2.20359	-0.30633	-5.39304	H	6.48209	-3.92544	-2.94048
O	6.19492	-1.38308	-0.26858	H	2.76933	-6.97850	-0.02286
C	6.35366	-0.77686	-1.33524	H	1.05950	-6.55356	-0.13430
N	7.39150	-0.93708	-2.17234	H	5.25300	-4.39454	2.97800
C	7.35781	-0.06420	-3.33676	H	4.73910	-3.04279	4.02141
C	5.89346	0.43576	-3.35569	H	5.48283	-2.87767	1.29510

H	2.81462	-4.36678	3.48521	H	-4.46573	-1.48469	-3.83346
H	3.81930	-4.37914	0.74858	H	-0.43375	0.49909	-1.65787
H	-1.52048	0.43201	4.79515	O	-0.21778	-3.67628	-0.47527
H	-1.05673	2.14314	4.51552	H	0.33222	-3.15432	-1.08039
H	0.47840	1.53535	2.93537	H	-1.00331	-3.95700	-0.98552
H	1.40875	-0.75322	7.99413	C	1.56406	-2.04496	1.58482
H	0.64195	-0.83872	5.45626	H	0.81054	-2.83289	1.46094
H	2.05654	5.54984	7.51711	H	2.17314	-2.11484	0.67856
H	2.63970	1.71192	4.30370	C	2.36937	-5.29071	-1.32424
H	3.99779	2.60328	4.97633	H	2.08496	-4.25671	-1.16600
H	4.08388	-0.29297	3.07229	H	1.74855	-5.65433	-2.15437
H	5.73204	-0.22036	1.14823				
H	6.42300	2.20543	0.61239				
H	3.45979	4.59842	3.66806				
H	1.48649	3.39072	5.48781				
H	0.52685	5.26928	-1.21720				
H	1.76075	6.22959	-0.38851				
H	1.17122	6.70108	2.50545				
H	-1.11921	6.82270	3.55541				
H	-2.93735	5.86424	2.04808				
H	1.06547	3.30702	0.16422				
H	3.41612	4.53909	1.46017				
H	3.33649	5.25141	-3.30333				
H	4.89420	5.25833	-4.10765				
H	5.88776	6.58700	-2.21122				
H	4.32433	6.54767	-1.38053				
H	4.51104	10.27338	-2.55018				
H	4.25383	9.19323	-1.16186				
H	5.85791	9.28090	-1.94759				
H	4.49259	3.12080	-2.96893				
H	4.56320	3.93741	-0.22452				
H	8.99103	3.18773	-3.72900				
H	6.64401	4.00613	-4.06909				
H	1.94620	2.18413	-6.33402				
H	1.68139	0.10278	1.63267				
H	-1.08540	-0.23565	0.83035				
H	-0.17260	-1.40443	-0.09949				
H	7.61164	-0.62318	-4.24124				
H	3.50406	0.91888	-1.03838				
H	3.88881	-0.76901	-0.83091				
H	3.57262	-0.95230	-3.41987				
H	2.41743	1.73322	-2.97484				
N	-5.19062	-2.03761	5.76864				
H	-5.62895	-1.18122	6.08089				
C	-5.98692	-3.26535	5.76306				
H	-7.01818	-3.00382	6.00701				
H	-5.97089	-3.73762	4.77682				
H	-5.63181	-3.98411	6.50962				
H	0.87223	-0.91314	-2.91775				
N	-9.72830	1.59617	-3.88046				
H	-8.99482	2.27896	-4.00720				
C	-10.86887	1.58886	-4.77377				
H	-11.53362	0.78646	-4.45122				
H	-11.40818	2.54151	-4.73099				
H	-10.56375	1.40355	-5.81033				
H	5.82298	1.45213	-3.74520				
H	5.72927	1.21820	-1.35234				
H	5.30463	-0.21052	-4.00701				
H	8.06678	0.76702	-3.21956				
H	8.21822	-1.43274	-1.83369				
H	7.98481	-1.90117	2.32919				
H	9.42061	-2.88917	2.66730				
H	0.63887	6.44068	6.94359				
H	0.58440	4.65214	7.09820				
H	-6.37303	3.80881	4.98531				
H	-6.64389	2.19821	4.26450				
H	-6.53612	-4.00726	-5.17488				
H	-4.86514	-3.83719	-5.70679				
H	0.44778	1.79484	-5.49340				
H	1.62759	2.87744	-4.71088				
H	2.66159	-0.77272	6.72987				
H	2.12566	0.77438	7.44420				
H	8.90292	4.95533	-3.49756				
H	8.85995	3.86731	-2.08787				
H	9.25272	-6.13393	-0.77679				