

Exploring the substrate specificity and catalytic mechanism of imidazolonepropionase (HutI) from *Bacillus subtilis*

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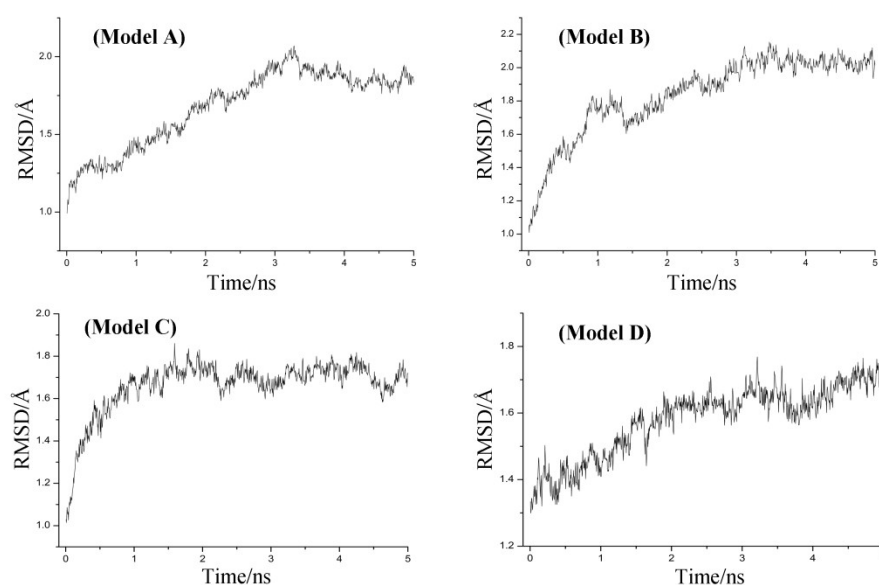


Fig. S1 The root-mean-squared deviations (RMSDs) of Models A and B for activation of water molecule, and Models C and D for cleavage of substrate.

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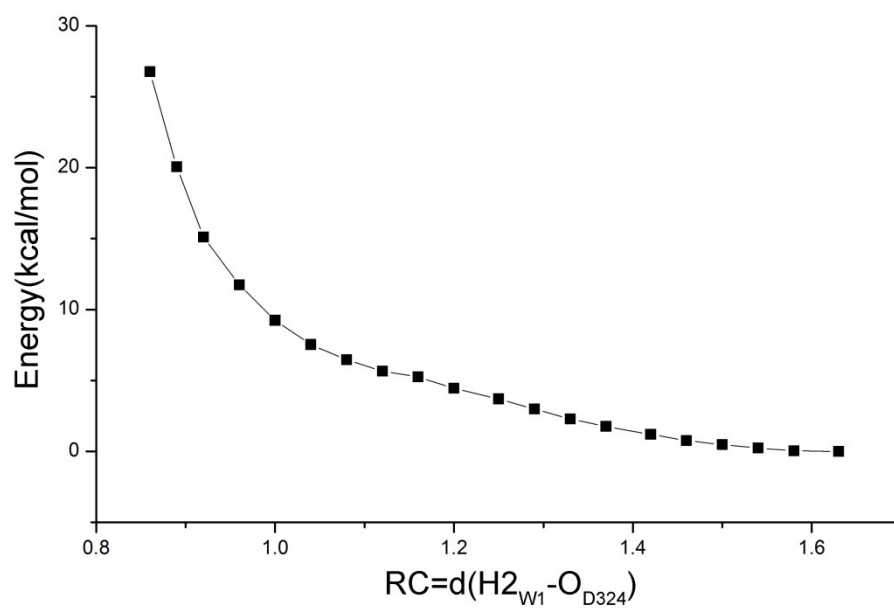


Fig. S2 Scanned energy profile along the reaction coordinate defined as: $RC = d(H2_{W1}-O_{D324})$ for the activation of water molecule by D324 in Model A.

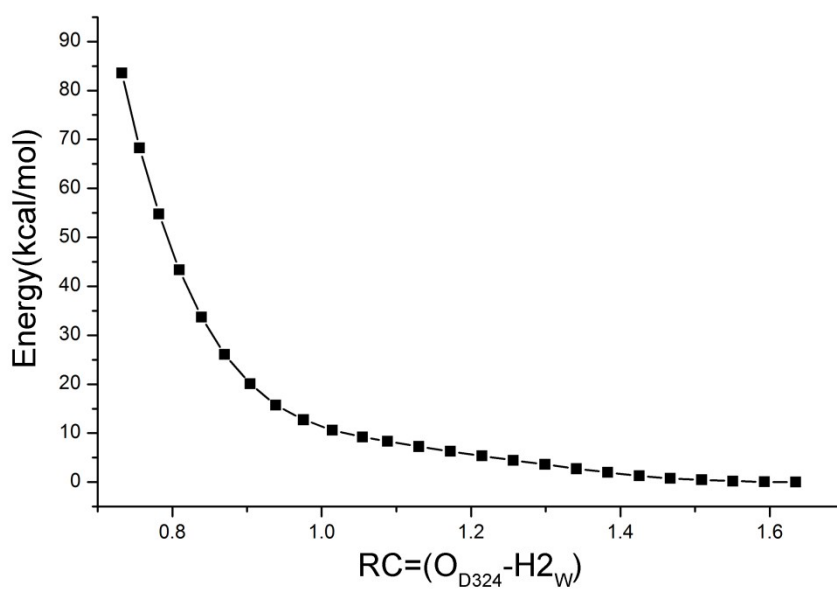


Fig. S3 Scanned energy profile along the reaction coordinate defined as $RC = d(H1_W-N_{H272})$ for the activation of water molecule by H272 in Model B.

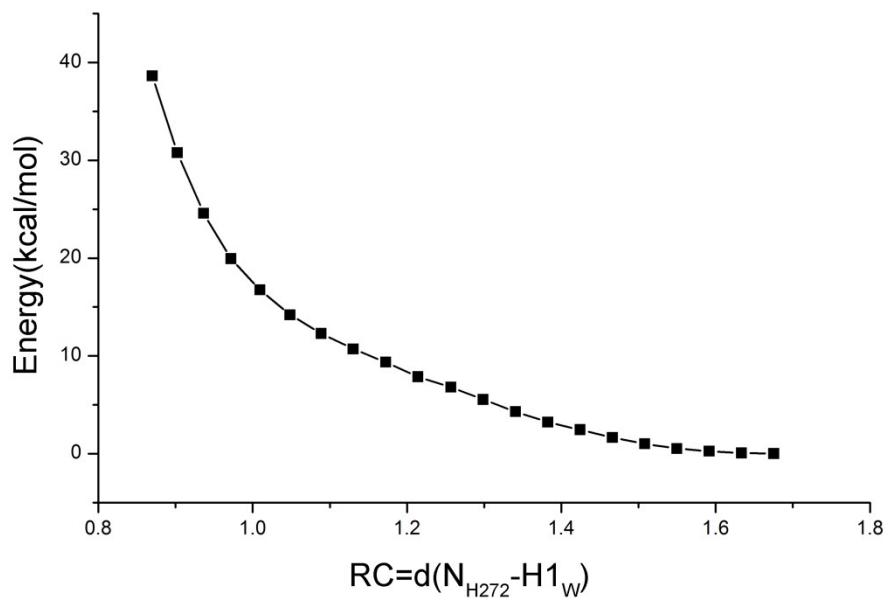


Fig. S4 Scanned energy profile along the reaction coordinate defined as $RC=d(H2_W-O_{D324})$ for the activation of water molecule by D324 in Model B.

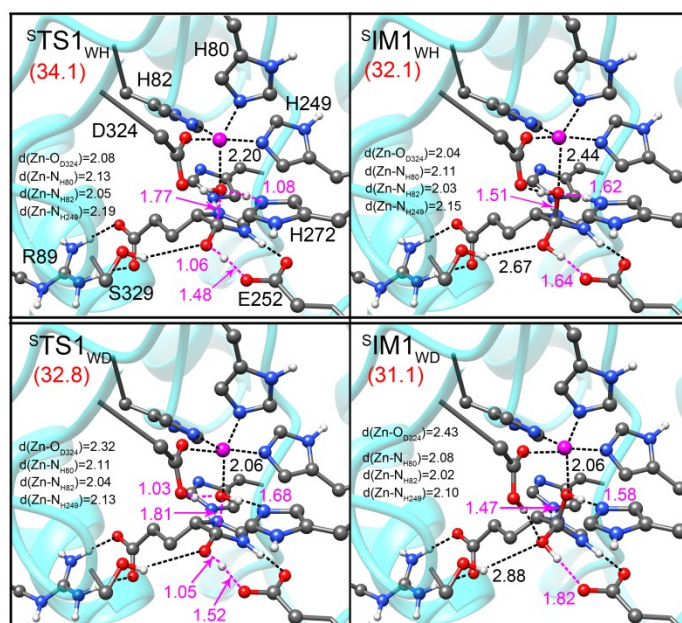


Fig. S5 Optimized structures of transition states and intermediates for Model B with H272 as the proton acceptor ($^{S}TS1_{WH}$, $^{S}IM1_{WH}$) and D324 as the proton acceptor ($^{S}TS1_{WD}$, $^{S}IM1_{WD}$) respectively. Key distances are shown in angstrom. Relative energies (kcal/mol) are given in parentheses.

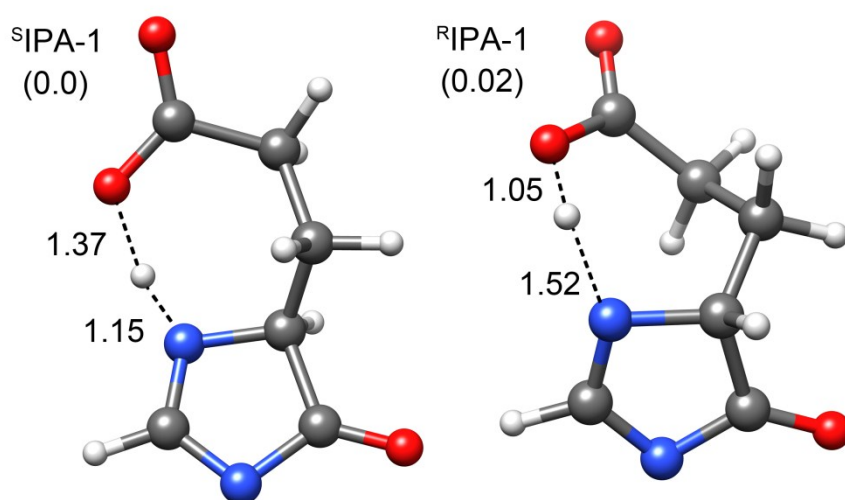


Fig. S6 Optimized structures of $^S\text{IPA-1}$ and $^R\text{IPA-1}$, the relative energies (kcal/mol) are shown in parentheses.

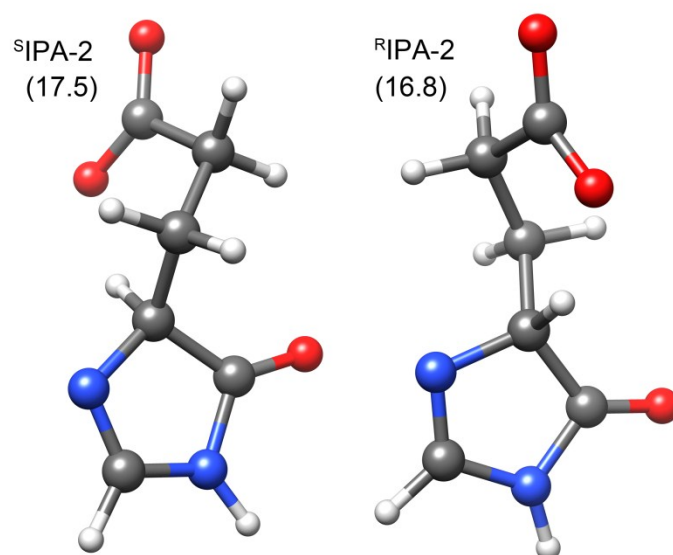


Fig. S7 Optimized structures of $^S\text{IPA-2}$ and $^R\text{IPA-2}$, the relative energies (kcal/mol) to $^S\text{IPA-1}$ are shown in parentheses.

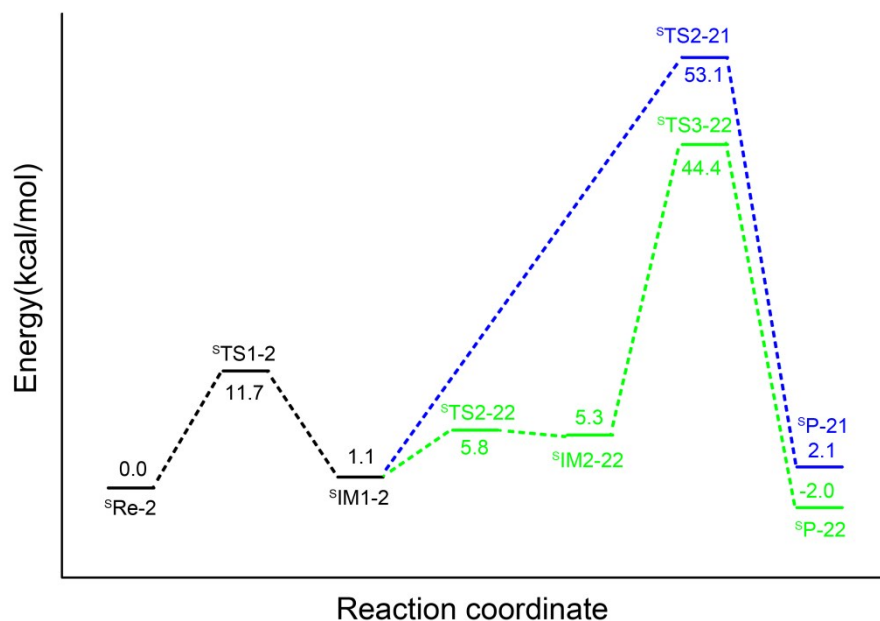


Fig. S8 Calculated energy profiles for the catalytic mechanism of $^5\text{IPA-2}$. The nucleophilic attack step of the mechanism is shown in black color and the cleavage of $\text{C}_1\text{-N}_1$ bond step without the assistance of water molecule are shown in green and blue color.

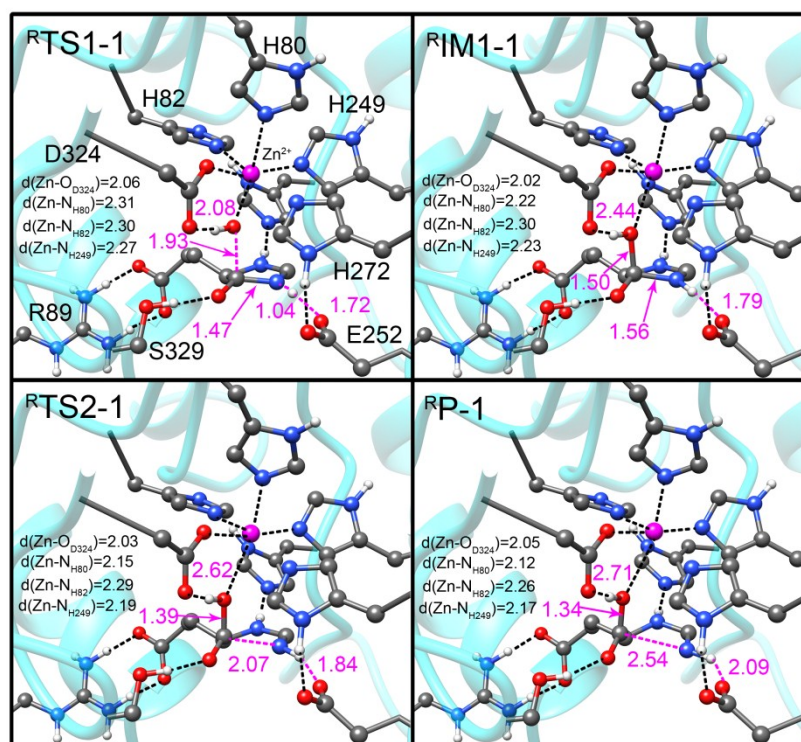


Fig. S9 The optimized structures of all the stationary points involved in the catalytic mechanism of Model $^{\text{RC}}$.

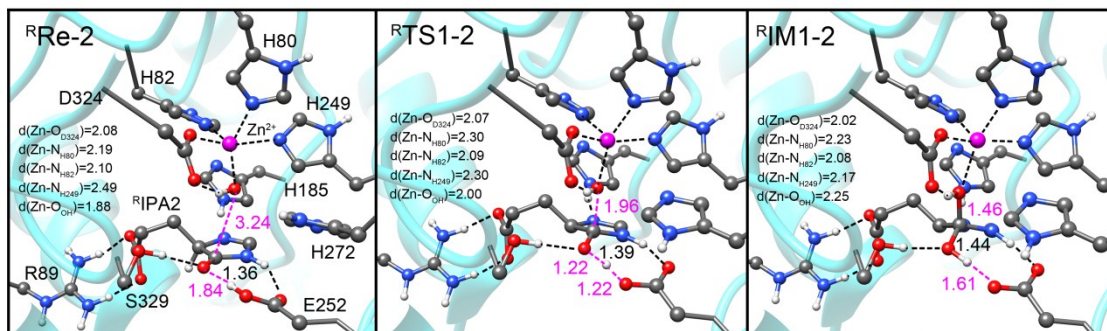


Fig. S10 Optimized structures of reactant, transition state and intermediate for the nucleophilic attack step in Model R^D . Key distances are shown in angstrom.

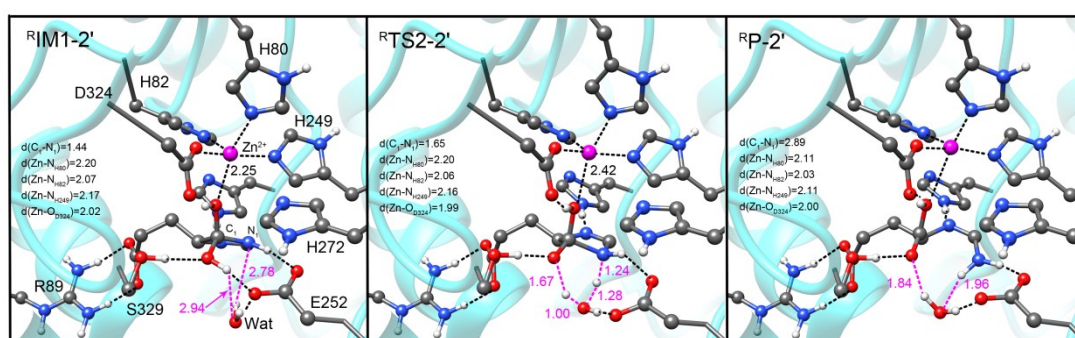


Fig. S11 Optimized structures of intermediate and transition state for the water-assisted C1-N1 cleavage step in Model R^D . Key distances are shown in angstrom.

Cartesian coordinates of QM regions of Re_W , TS, Re_{OH} from Model A; SRe_W , from Model B; $SRe-1$, $STs1-1$, $SiM1-1$, $STs2-1$ and $SP-1$ from Model C; $RRe-1$, $RTs1-1$, $RiM1-1$, $RTs2-1$ and $RP-1$ from Model R^C ; $SRe-2$, $STs1-2$, $SiM1-2$, $SiM1-2'$, $STs2-2'$ and $SP-2'$ from Model D; $RRe-2$, $RTs1-2$, $RiM1-2$, $RiM1-2'$, $RTs2-2'$ and $RP-2'$ from Model R^D .

Re_W :				H	-8.685	-5.033	-3.969
C	-3.051	1.331	-0.254	N	-9.403	-3.030	-2.409
H	-2.713	1.864	0.639	H	-10.058	-3.830	-2.292
H	-2.539	1.773	-1.111	C	-8.285	-3.059	-3.223
N	-5.249	2.288	0.476	C	-9.553	-1.786	-1.908
H	-4.870	2.818	1.295	H	-10.360	-1.491	-1.256
C	-4.529	1.475	-0.376	N	-8.582	-0.995	-2.359
C	-6.544	2.264	0.109	C	-7.789	-1.776	-3.184
H	-7.327	2.756	0.667	H	-6.953	-1.343	-3.712
N	-6.701	1.480	-0.954	C	-14.983	-3.708	-12.037
C	-5.450	0.983	-1.263	H	-15.877	-3.641	-12.657
H	-5.310	0.338	-2.113	H	-15.217	-4.395	-11.224
C	-7.881	-4.293	-3.976	N	-14.732	-2.365	-11.513
H	-7.656	-4.035	-5.013	H	-15.191	-1.608	-12.020

C	-14.286	-2.046	-10.288
N	-14.302	-0.753	-9.917
H	-13.822	-0.512	-9.040
H	-14.368	-0.043	-10.646
N	-13.821	-2.962	-9.430
H	-13.430	-2.637	-8.546
H	-13.913	-3.967	-9.589
C	-15.792	-3.298	-0.352
H	-15.092	-3.757	0.358
H	-16.427	-4.113	-0.711
N	-14.313	-3.546	-2.322
H	-14.351	-4.566	-2.264
C	-15.036	-2.698	-1.502
C	-13.680	-2.799	-3.259
H	-13.047	-3.227	-4.024
N	-13.941	-1.512	-3.095
C	-14.788	-1.438	-2.000
H	-15.182	-0.495	-1.648
C	-11.461	4.028	1.655
H	-12.414	3.704	2.083
H	-11.671	4.688	0.806
N	-10.279	1.721	1.776
H	-10.344	1.474	2.792
C	-10.676	2.872	1.115
C	-9.644	0.934	0.885
H	-9.219	-0.019	1.161
N	-9.624	1.478	-0.330
C	-10.271	2.694	-0.186
H	-10.438	3.362	-1.015
C	-12.403	7.905	-1.219
H	-11.418	8.040	-0.765
H	-13.107	7.769	-0.388
C	-12.362	6.595	-2.019
O	-13.131	6.440	-2.994
O	-11.510	5.726	-1.612
H	-11.389	4.694	-2.560
C	-8.512	8.048	-0.777
H	-8.460	6.960	-0.687
H	-9.250	8.374	-0.036
N	-9.180	9.629	-2.682
H	-9.046	10.500	-2.191
C	-8.923	8.360	-2.185
C	-9.585	9.510	-3.978
H	-9.846	10.365	-4.586

N	-9.606	8.244	-4.351
C	-9.201	7.527	-3.243
H	-9.181	6.447	-3.251
C	-5.177	2.468	-4.909
H	-4.757	3.232	-4.247
H	-5.188	2.896	-5.911
C	-6.614	2.218	-4.421
O	-6.899	1.180	-3.755
O	-7.446	3.153	-4.671
C	-10.301	3.184	-8.598
H	-10.075	4.254	-8.549
H	-11.394	3.083	-8.660
O	-9.773	2.502	-7.472
H	-9.829	3.149	-6.721
Zn	-8.368	1.027	-2.066
O	-9.425	2.140	-3.339
H	-8.708	2.584	-3.906
O	-9.926	4.355	-5.550
H	-10.513	4.212	-4.756
H	-9.018	4.227	-5.225
O	-11.216	3.905	-3.259
H	-12.054	3.384	-3.333
H	-10.146	2.838	-3.144
O	-10.680	0.731	-5.358
H	-10.466	1.187	-6.194
H	-10.238	1.239	-4.641
O	-13.355	0.305	-5.166
H	-12.383	0.468	-5.110
H	-13.570	-0.364	-4.457
O	-12.826	-0.799	-7.618
H	-13.089	-0.472	-6.722
H	-11.855	-0.847	-7.639

TS:

C	-3.062	1.330	-0.259
H	-2.727	1.864	0.635
H	-2.549	1.774	-1.115
N	-5.260	2.287	0.470
H	-4.881	2.813	1.289
C	-4.541	1.474	-0.384
C	-6.556	2.266	0.098
H	-7.338	2.759	0.656
N	-6.713	1.486	-0.968
C	-5.462	0.988	-1.275

H	-5.322	0.346	-2.127	C	-10.283	2.671	-0.184
C	-7.882	-4.289	-3.977	H	-10.457	3.323	-1.025
H	-7.657	-4.035	-5.014	C	-12.378	7.878	-1.248
H	-8.687	-5.028	-3.967	H	-11.383	8.001	-0.815
N	-9.400	-3.020	-2.410	H	-13.063	7.725	-0.404
H	-10.055	-3.819	-2.290	C	-12.367	6.594	-2.075
C	-8.283	-3.052	-3.226	O	-13.149	6.429	-3.019
C	-9.548	-1.773	-1.915	O	-11.481	5.712	-1.700
H	-10.354	-1.474	-1.262	H	-11.393	4.865	-2.418
N	-8.579	-0.984	-2.371	C	-8.498	8.045	-0.785
C	-7.787	-1.769	-3.193	H	-8.437	6.958	-0.697
H	-6.953	-1.337	-3.725	H	-9.236	8.366	-0.041
C	-14.982	-3.707	-12.036	N	-9.175	9.631	-2.681
H	-15.876	-3.639	-12.655	H	-9.032	10.500	-2.190
H	-15.217	-4.394	-11.223	C	-8.911	8.361	-2.192
N	-14.730	-2.363	-11.510	C	-9.582	9.517	-3.977
H	-15.189	-1.607	-12.017	H	-9.845	10.374	-4.581
C	-14.284	-2.046	-10.286	N	-9.601	8.252	-4.356
N	-14.300	-0.753	-9.914	C	-9.188	7.531	-3.253
H	-13.819	-0.513	-9.037	H	-9.158	6.451	-3.272
H	-14.365	-0.043	-10.643	C	-5.166	2.476	-4.923
N	-13.820	-2.962	-9.427	H	-4.742	3.239	-4.263
H	-13.428	-2.636	-8.544	H	-5.165	2.900	-5.928
H	-13.911	-3.966	-9.587	C	-6.613	2.248	-4.448
C	-15.793	-3.299	-0.352	O	-6.909	1.214	-3.777
H	-15.092	-3.758	0.358	O	-7.423	3.191	-4.718
H	-16.428	-4.113	-0.711	C	-10.300	3.186	-8.595
N	-14.312	-3.545	-2.322	H	-10.075	4.258	-8.549
H	-14.348	-4.565	-2.264	H	-11.394	3.086	-8.658
C	-15.037	-2.698	-1.502	O	-9.772	2.507	-7.470
C	-13.680	-2.796	-3.258	H	-9.832	3.153	-6.718
H	-13.045	-3.223	-4.022	Zn	-8.384	1.056	-2.114
N	-13.942	-1.510	-3.094	O	-9.474	2.158	-3.328
C	-14.789	-1.438	-1.999	H	-8.770	2.574	-3.899
H	-15.185	-0.496	-1.646	O	-9.928	4.354	-5.544
C	-11.463	4.013	1.662	H	-10.511	4.189	-4.745
H	-12.415	3.691	2.096	H	-9.018	4.202	-5.230
H	-11.680	4.670	0.814	O	-11.181	3.881	-3.249
N	-10.274	1.713	1.785	H	-12.016	3.358	-3.335
H	-10.335	1.472	2.802	H	-10.279	2.965	-3.166
C	-10.680	2.857	1.119	O	-10.678	0.736	-5.335
C	-9.640	0.923	0.894	H	-10.461	1.191	-6.169
H	-9.210	-0.026	1.172	H	-10.250	1.255	-4.608
N	-9.631	1.460	-0.324	O	-13.345	0.310	-5.166

H	-12.371	0.471	-5.112
H	-13.562	-0.358	-4.459
O	-12.826	-0.799	-7.616
H	-13.087	-0.469	-6.720
H	-11.855	-0.844	-7.638

Re_{OH}:

C	-3.080	1.335	-0.275
H	-2.750	1.869	0.620
H	-2.564	1.779	-1.129
N	-5.281	2.285	0.451
H	-4.903	2.808	1.273
C	-4.559	1.477	-0.406
C	-6.575	2.269	0.072
H	-7.359	2.761	0.627
N	-6.728	1.499	-1.000
C	-5.477	1.000	-1.305
H	-5.335	0.366	-2.162
C	-7.880	-4.292	-3.988
H	-7.654	-4.044	-5.026
H	-8.688	-5.029	-3.974
N	-9.382	-3.013	-2.415
H	-10.038	-3.809	-2.287
C	-8.273	-3.051	-3.243
C	-9.520	-1.763	-1.922
H	-10.318	-1.458	-1.262
N	-8.553	-0.979	-2.391
C	-7.774	-1.768	-3.219
H	-6.943	-1.341	-3.761
C	-14.981	-3.705	-12.033
H	-15.875	-3.636	-12.652
H	-15.216	-4.393	-11.220
N	-14.727	-2.362	-11.507
H	-15.185	-1.605	-12.014
C	-14.280	-2.045	-10.283
N	-14.295	-0.752	-9.911
H	-13.811	-0.513	-9.035
H	-14.361	-0.042	-10.640
N	-13.817	-2.962	-9.424
H	-13.422	-2.636	-8.542
H	-13.908	-3.966	-9.584
C	-15.794	-3.301	-0.352
H	-15.093	-3.760	0.357
H	-16.429	-4.114	-0.712

N	-14.309	-3.543	-2.320
H	-14.342	-4.563	-2.262
C	-15.038	-2.699	-1.502
C	-13.677	-2.792	-3.255
H	-13.039	-3.216	-4.017
N	-13.945	-1.507	-3.091
C	-14.793	-1.438	-1.998
H	-15.192	-0.497	-1.645
C	-11.464	3.986	1.676
H	-12.412	3.664	2.120
H	-11.692	4.637	0.826
N	-10.270	1.692	1.810
H	-10.326	1.462	2.830
C	-10.680	2.829	1.137
C	-9.638	0.896	0.922
H	-9.205	-0.050	1.207
N	-9.633	1.421	-0.300
C	-10.287	2.631	-0.166
H	-10.456	3.273	-1.013
C	-12.394	7.920	-1.230
H	-11.398	8.042	-0.798
H	-13.078	7.778	-0.384
C	-12.387	6.634	-2.039
O	-13.141	6.433	-2.990
O	-11.493	5.757	-1.628
H	-11.459	4.951	-2.286
C	-8.479	8.037	-0.796
H	-8.404	6.949	-0.717
H	-9.219	8.344	-0.048
N	-9.178	9.634	-2.673
H	-9.027	10.499	-2.177
C	-8.898	8.361	-2.199
C	-9.586	9.531	-3.970
H	-9.855	10.392	-4.565
N	-9.596	8.270	-4.362
C	-9.171	7.540	-3.269
H	-9.118	6.461	-3.308
C	-5.144	2.503	-4.963
H	-4.717	3.268	-4.306
H	-5.125	2.917	-5.971
C	-6.602	2.300	-4.502
O	-6.911	1.272	-3.826
O	-7.390	3.253	-4.793
C	-10.290	3.187	-8.608

H	-10.063	4.257	-8.561
H	-11.384	3.088	-8.671
O	-9.762	2.501	-7.489
H	-9.794	3.148	-6.739
Zn	-8.395	1.072	-2.167
O	-9.531	2.135	-3.305
H	-8.846	2.547	-3.876
O	-9.872	4.340	-5.546
H	-10.497	4.152	-4.805
H	-8.981	4.114	-5.205
O	-11.307	3.844	-3.259
H	-12.143	3.323	-3.358
H	-10.550	3.111	-3.156
O	-10.681	0.746	-5.266
H	-10.441	1.192	-6.097
H	-10.255	1.263	-4.519
O	-13.326	0.299	-5.178
H	-12.352	0.471	-5.110
H	-13.545	-0.368	-4.470
O	-12.819	-0.798	-7.620
H	-13.074	-0.470	-6.721
H	-11.846	-0.840	-7.646

^sRe_w:

C	3.269	1.235	0.082
H	2.933	1.713	-0.841
H	2.759	1.722	0.915
N	5.502	2.048	-0.736
H	5.137	2.534	-1.586
C	4.749	1.365	0.199
C	6.797	2.012	-0.359
H	7.596	2.423	-0.958
N	6.920	1.338	0.782
C	5.650	0.933	1.135
H	5.488	0.380	2.043
C	8.065	-4.285	4.155
H	7.887	-3.990	5.190
H	8.874	-5.020	4.151
N	9.611	-3.050	2.588
H	10.331	-3.800	2.527
C	8.466	-3.077	3.360
C	9.757	-1.821	2.064
H	10.584	-1.532	1.433
N	8.756	-1.032	2.448

C	7.947	-1.807	3.265
H	7.080	-1.381	3.744
C	14.630	-3.976	12.543
H	15.454	-4.077	13.254
H	14.794	-4.748	11.795
N	14.710	-2.659	11.915
H	14.630	-1.833	12.528
C	14.295	-2.400	10.656
N	14.020	-1.123	10.348
H	14.019	-0.860	9.351
H	14.397	-0.408	10.989
N	14.113	-3.341	9.734
H	13.853	-3.035	8.779
H	14.352	-4.323	9.883
C	15.714	-3.822	0.187
H	14.954	-4.353	-0.394
H	16.350	-4.601	0.621
N	14.214	-3.686	2.169
C	15.037	-3.031	1.273
C	13.717	-2.747	2.953
H	13.023	-2.920	3.765
N	14.175	-1.511	2.620
H	13.830	-0.624	2.993
C	15.025	-1.679	1.545
H	15.544	-0.847	1.096
C	11.973	3.409	-1.784
H	12.825	2.967	-2.302
H	12.349	4.012	-0.952
N	10.560	1.246	-1.836
H	10.630	0.950	-2.838
C	11.084	2.359	-1.203
C	9.842	0.563	-0.919
H	9.326	-0.352	-1.158
N	9.878	1.146	0.276
C	10.662	2.266	0.100
H	10.890	2.934	0.916
C	12.422	8.302	3.412
H	13.004	8.811	4.189
H	11.400	8.683	3.476
C	12.442	6.832	3.764
O	13.326	6.051	3.428
O	11.413	6.489	4.538
H	11.488	5.535	4.818
C	8.997	8.209	0.532

H	9.643	8.107	-0.340
H	9.361	9.064	1.118
N	8.601	6.900	2.665
H	8.143	7.657	3.188
C	9.070	6.976	1.363
C	8.802	5.635	3.106
H	8.471	5.270	4.068
N	9.394	4.902	2.178
C	9.564	5.727	1.090
H	10.012	5.376	0.172
C	5.390	2.373	4.857
H	4.963	3.088	4.145
H	5.352	2.844	5.840
C	6.843	2.144	4.420
O	7.113	1.156	3.667
O	7.689	3.013	4.790
C	10.365	3.073	9.451
H	10.037	4.122	9.431
H	11.439	3.046	9.664
O	10.054	2.398	8.244
H	10.452	2.889	7.512
N	12.836	3.353	3.529
C	12.036	3.021	4.579
O	11.485	3.822	5.355
C	12.018	1.502	4.605
N	12.866	1.096	3.469
C	13.286	2.178	2.930
C	12.545	0.952	5.931
C	12.542	-0.569	5.970
C	13.381	-1.132	7.112
O	13.311	-2.373	7.305
O	14.100	-0.315	7.769
H	11.526	-0.973	6.054
H	12.960	-0.978	5.046
H	13.569	1.307	6.083
H	11.934	1.350	6.748
H	10.994	1.162	4.421
H	13.950	2.227	2.076
H	13.127	4.322	3.337
Zn	8.510	0.952	2.047
O	9.525	2.390	3.027
H	9.570	3.284	2.576
H	7.930	-8.222	22.726
O	-23.149	-11.158	-15.491

H	-23.002	-10.259	-15.226
^s TS1 _{WH} :			
C	3.322	1.226	0.071
H	3.010	1.697	-0.865
H	2.801	1.734	0.885
N	5.559	2.048	-0.711
H	5.192	2.523	-1.567
C	4.805	1.352	0.213
C	6.849	2.039	-0.316
H	7.646	2.463	-0.909
N	6.974	1.374	0.831
C	5.706	0.942	1.164
H	5.542	0.376	2.063
C	8.092	-4.229	4.167
H	7.906	-3.948	5.206
H	8.904	-4.960	4.161
N	9.658	-2.970	2.641
H	10.366	-3.729	2.551
C	8.505	-3.005	3.401
C	9.832	-1.728	2.161
H	10.674	-1.436	1.552
N	8.841	-0.932	2.561
C	8.010	-1.722	3.344
H	7.141	-1.301	3.827
C	14.621	-3.928	12.504
H	15.452	-4.016	13.210
H	14.785	-4.705	11.761
N	14.687	-2.616	11.865
H	14.613	-1.786	12.475
C	14.282	-2.362	10.601
N	14.032	-1.084	10.280
H	14.003	-0.819	9.284
H	14.412	-0.368	10.920
N	14.085	-3.307	9.685
H	13.834	-2.992	8.731
H	14.318	-4.289	9.837
C	15.745	-3.845	0.168
H	14.979	-4.365	-0.415
H	16.377	-4.634	0.587
N	14.291	-3.724	2.189
C	15.082	-3.062	1.268
C	13.802	-2.783	2.977
H	13.132	-2.957	3.810

N	14.233	-1.544	2.624
H	13.855	-0.655	2.974
C	15.056	-1.709	1.529
H	15.550	-0.873	1.060
C	11.997	3.398	-1.789
H	12.821	2.919	-2.319
H	12.412	4.001	-0.974
N	10.553	1.250	-1.740
H	10.618	0.911	-2.730
C	11.091	2.388	-1.166
C	9.843	0.613	-0.783
H	9.319	-0.310	-0.968
N	9.896	1.256	0.382
C	10.679	2.364	0.143
H	10.949	3.045	0.934
C	12.407	7.973	3.267
H	12.993	8.291	4.138
H	11.433	8.469	3.368
C	12.163	6.452	3.376
O	12.474	5.688	2.426
O	11.610	6.074	4.469
H	11.345	4.633	4.692
C	8.960	8.139	0.596
H	9.622	7.983	-0.255
H	9.352	8.992	1.167
N	8.480	6.957	2.788
H	8.045	7.763	3.264
C	8.960	6.938	1.480
C	8.624	5.745	3.334
H	8.284	5.433	4.310
N	9.193	4.950	2.434
C	9.415	5.667	1.278
H	9.883	5.228	0.413
C	5.450	2.492	4.886
H	5.024	3.216	4.183
H	5.395	2.940	5.879
C	6.919	2.298	4.469
O	7.206	1.363	3.651
O	7.756	3.133	4.913
C	10.256	3.207	9.532
H	9.914	4.251	9.541
H	11.329	3.191	9.749
O	9.965	2.574	8.298
H	10.464	3.046	7.618

N	12.250	3.122	3.005
C	11.379	2.744	4.023
O	11.150	3.632	4.993
C	11.758	1.271	4.330
N	12.745	0.930	3.280
C	12.976	2.015	2.632
C	12.342	0.982	5.718
C	12.482	-0.533	5.875
C	13.316	-1.027	7.050
O	13.291	-2.271	7.258
O	13.996	-0.180	7.707
H	11.496	-1.011	5.938
H	12.957	-0.951	4.983
H	13.320	1.463	5.822
H	11.687	1.383	6.500
H	10.872	0.645	4.198
H	13.707	2.095	1.835
H	12.404	4.129	2.728
Zn	8.618	1.060	2.155
O	9.795	2.561	3.257
H	9.474	3.930	2.669
H	7.930	-8.222	22.726
O	-23.149	-11.158	-15.491
H	-23.002	-10.259	-15.226

^sIM1_{WH}

C	3.300	1.220	0.072
H	2.978	1.691	-0.860
H	2.785	1.723	0.893
N	5.531	2.048	-0.720
H	5.164	2.535	-1.570
C	4.783	1.339	0.198
C	6.827	2.013	-0.344
H	7.622	2.436	-0.941
N	6.958	1.315	0.783
C	5.690	0.893	1.124
H	5.529	0.304	2.009
C	8.085	-4.270	4.158
H	7.913	-3.991	5.199
H	8.892	-5.007	4.139
N	9.663	-3.006	2.651
H	10.381	-3.759	2.575
C	8.497	-3.048	3.390
C	9.831	-1.769	2.159

H	10.681	-1.474	1.563	H	11.288	4.543	4.759
N	8.822	-0.982	2.532	C	8.968	8.151	0.587
C	7.986	-1.773	3.308	H	9.627	7.989	-0.265
H	7.104	-1.360	3.774	H	9.362	9.007	1.151
C	14.635	-3.925	12.506	N	8.499	6.988	2.791
H	15.465	-4.010	13.214	H	8.062	7.796	3.261
H	14.805	-4.700	11.762	C	8.975	6.959	1.482
N	14.698	-2.612	11.866	C	8.657	5.787	3.354
H	14.623	-1.783	12.477	H	8.335	5.489	4.340
C	14.281	-2.360	10.605	N	9.223	4.989	2.456
N	14.022	-1.083	10.286	C	9.441	5.691	1.291
H	13.979	-0.819	9.289	H	9.915	5.242	0.434
H	14.406	-0.367	10.922	C	5.487	2.488	4.853
N	14.080	-3.307	9.692	H	5.061	3.212	4.150
H	13.813	-2.993	8.741	H	5.430	2.936	5.846
H	14.316	-4.288	9.844	C	6.957	2.297	4.440
C	15.743	-3.820	0.170	O	7.239	1.400	3.577
H	14.979	-4.343	-0.413	O	7.802	3.098	4.927
H	16.371	-4.609	0.598	C	10.260	3.199	9.487
N	14.271	-3.677	2.176	H	9.934	4.249	9.506
C	15.077	-3.027	1.261	H	11.336	3.167	9.682
C	13.787	-2.728	2.960	O	9.932	2.575	8.257
H	13.112	-2.895	3.789	H	10.467	2.995	7.570
N	14.234	-1.495	2.608	N	12.143	3.110	2.965
H	13.880	-0.598	2.973	C	11.247	2.695	4.006
C	15.065	-1.672	1.522	O	11.171	3.574	5.065
H	15.573	-0.842	1.055	C	11.735	1.238	4.326
C	11.993	3.376	-1.778	N	12.835	0.986	3.365
H	12.808	2.886	-2.311	C	13.008	2.081	2.713
H	12.419	3.975	-0.966	C	12.209	0.935	5.750
N	10.527	1.245	-1.719	C	12.470	-0.568	5.863
H	10.596	0.901	-2.708	C	13.277	-1.046	7.063
C	11.078	2.379	-1.148	O	13.249	-2.288	7.286
C	9.814	0.616	-0.762	O	13.955	-0.195	7.716
H	9.278	-0.301	-0.945	H	11.531	-1.134	5.836
N	9.878	1.261	0.404	H	13.047	-0.894	4.992
C	10.672	2.362	0.163	H	13.127	1.492	5.961
H	10.974	3.024	0.959	H	11.458	1.244	6.486
C	12.416	8.013	3.304	H	10.907	0.559	4.094
H	13.044	8.315	4.152	H	13.789	2.211	1.970
H	11.461	8.535	3.447	H	12.350	4.130	2.795
C	12.141	6.494	3.430	Zn	8.579	0.985	2.095
O	12.522	5.709	2.520	O	9.869	2.594	3.408
O	11.508	6.147	4.483	H	9.521	4.006	2.698

H	7.930	-8.222	22.726
O	-23.149	-11.158	-15.491
H	-23.002	-10.259	-15.226

^sTS1_{WD}:

C	3.334	1.206	0.064
H	3.026	1.676	-0.874
H	2.816	1.723	0.875
N	5.569	2.047	-0.699
H	5.200	2.537	-1.547
C	4.819	1.320	0.203
C	6.861	2.021	-0.315
H	7.656	2.465	-0.895
N	6.992	1.313	0.807
C	5.723	0.870	1.132
H	5.557	0.271	2.009
C	8.101	-4.255	4.145
H	7.920	-3.948	5.177
H	8.903	-4.998	4.157
N	9.711	-3.041	2.627
H	10.423	-3.802	2.581
C	8.532	-3.060	3.345
C	9.892	-1.818	2.105
H	10.753	-1.540	1.517
N	8.879	-1.017	2.438
C	8.026	-1.786	3.218
H	7.135	-1.362	3.652
C	14.632	-3.901	12.501
H	15.461	-3.976	13.210
H	14.808	-4.680	11.762
N	14.686	-2.592	11.853
H	14.607	-1.759	12.460
C	14.278	-2.349	10.588
N	14.031	-1.074	10.255
H	13.965	-0.817	9.258
H	14.408	-0.352	10.888
N	14.078	-3.304	9.682
H	13.811	-2.999	8.729
H	14.308	-4.285	9.844
C	15.750	-3.890	0.182
H	14.986	-4.409	-0.405
H	16.389	-4.678	0.590
N	14.354	-3.811	2.246
C	15.087	-3.126	1.295

C	13.844	-2.882	3.036
H	13.206	-3.074	3.889
N	14.209	-1.629	2.656
H	13.789	-0.754	2.992
C	15.008	-1.772	1.541
H	15.453	-0.921	1.049
C	12.020	3.472	-1.826
H	12.883	3.044	-2.337
H	12.373	4.078	-0.986
N	10.637	1.282	-1.891
H	10.706	0.981	-2.893
C	11.133	2.412	-1.263
C	9.917	0.595	-0.982
H	9.420	-0.332	-1.219
N	9.930	1.194	0.207
C	10.691	2.331	0.032
H	10.892	3.010	0.844
C	12.426	7.830	3.293
H	12.989	8.169	4.171
H	11.430	8.282	3.379
C	12.233	6.299	3.398
O	12.578	5.547	2.453
O	11.681	5.899	4.485
H	11.227	4.458	4.654
C	8.968	8.168	0.552
H	9.622	8.038	-0.310
H	9.353	9.015	1.136
N	8.560	6.943	2.725
H	8.149	7.737	3.232
C	8.978	6.944	1.403
C	8.679	5.680	3.198
H	8.383	5.392	4.196
N	9.165	4.873	2.271
C	9.356	5.652	1.150
H	9.754	5.243	0.234
C	5.446	2.393	4.832
H	5.060	3.109	4.099
H	5.429	2.884	5.806
C	6.862	2.057	4.392
O	7.132	1.122	3.635
O	7.785	2.894	4.828
C	10.205	3.250	9.486
H	9.860	4.294	9.507
H	11.281	3.240	9.688

O	9.898	2.625	8.250	C	8.519	-3.056	3.347
H	10.511	2.984	7.593	C	9.874	-1.828	2.087
N	12.180	3.003	3.003	H	10.735	-1.555	1.495
C	11.252	2.616	3.957	N	8.864	-1.022	2.421
O	10.920	3.488	4.900	C	8.015	-1.783	3.214
C	11.594	1.142	4.267	H	7.128	-1.355	3.654
N	12.601	0.791	3.236	C	14.633	-3.875	12.476
C	12.884	1.886	2.623	H	15.468	-3.936	13.180
C	12.159	0.878	5.669	H	14.813	-4.655	11.739
C	12.356	-0.625	5.852	N	14.667	-2.567	11.823
C	13.212	-1.063	7.036	H	14.590	-1.735	12.431
O	13.228	-2.303	7.268	C	14.244	-2.329	10.561
O	13.865	-0.182	7.674	N	13.984	-1.055	10.231
H	11.392	-1.142	5.927	H	13.886	-0.797	9.236
H	12.845	-1.042	4.967	H	14.370	-0.333	10.859
H	13.112	1.401	5.796	N	14.043	-3.285	9.657
H	11.469	1.263	6.428	H	13.751	-2.981	8.709
H	10.708	0.517	4.132	H	14.279	-4.264	9.818
H	13.644	1.971	1.853	C	15.749	-3.861	0.179
H	12.366	4.017	2.736	H	14.986	-4.382	-0.407
Zn	8.725	0.959	1.950	H	16.384	-4.649	0.595
O	9.674	2.382	3.104	N	14.338	-3.758	2.231
H	9.527	3.290	2.692	C	15.083	-3.085	1.282
H	7.930	-8.222	22.726	C	13.824	-2.819	3.007
O	-23.149	-11.158	-15.491	H	13.179	-3.001	3.857
H	-23.002	-10.259	-15.226	N	14.196	-1.571	2.620
^s IM1 _{WD} :				H	13.773	-0.688	2.948
C	3.352	1.210	0.089	C	15.006	-1.728	1.516
H	3.058	1.684	-0.852	H	15.458	-0.883	1.020
H	2.825	1.727	0.895	C	12.043	3.451	-1.847
N	5.590	2.040	-0.663	H	12.901	3.032	-2.371
H	5.220	2.521	-1.517	H	12.400	4.044	-1.000
C	4.838	1.325	0.248	N	10.633	1.279	-1.947
C	6.880	2.025	-0.277	H	10.696	0.992	-2.954
H	7.675	2.463	-0.863	C	11.160	2.382	-1.297
N	7.012	1.336	0.857	C	9.910	0.584	-1.049
C	5.743	0.895	1.188	H	9.391	-0.326	-1.305
H	5.582	0.294	2.066	N	9.950	1.152	0.155
C	8.093	-4.251	4.150	C	10.737	2.276	0.001
H	7.911	-3.942	5.182	H	10.981	2.918	0.831
H	8.898	-4.990	4.163	C	12.367	7.851	3.336
N	9.694	-3.045	2.621	H	12.926	8.191	4.217
H	10.409	-3.803	2.577	H	11.380	8.327	3.405
				C	12.138	6.318	3.457

O	12.481	5.564	2.508
O	11.570	5.929	4.533
H	10.938	4.231	4.727
C	8.966	8.103	0.577
H	9.622	7.961	-0.282
H	9.366	8.941	1.163
N	8.517	6.897	2.752
H	8.125	7.705	3.251
C	8.946	6.879	1.432
C	8.618	5.644	3.245
H	8.319	5.380	4.248
N	9.098	4.818	2.329
C	9.309	5.579	1.198
H	9.717	5.152	0.294
C	5.495	2.472	4.920
H	5.143	3.186	4.168
H	5.391	2.948	5.896
C	6.959	2.182	4.603
O	7.333	1.337	3.801
O	7.784	2.984	5.281
C	10.224	3.244	9.511
H	9.879	4.288	9.530
H	11.296	3.234	9.726
O	9.938	2.629	8.265
H	10.608	2.944	7.643
N	12.126	3.022	3.090
C	10.998	2.492	3.792
O	10.584	3.301	4.861
C	11.478	1.049	4.146
N	12.633	0.820	3.242
C	12.939	1.983	2.767
C	11.926	0.815	5.598
C	12.281	-0.662	5.781
C	13.100	-1.056	7.008
O	13.123	-2.294	7.265
O	13.738	-0.162	7.641
H	11.380	-1.286	5.763
H	12.888	-0.985	4.931
H	12.801	1.437	5.814
H	11.135	1.105	6.299
H	10.677	0.340	3.912
H	13.806	2.156	2.135
H	12.266	4.047	2.839
Zn	8.775	0.927	1.886

O	9.831	2.379	2.905
H	9.539	3.338	2.651
H	7.930	-8.222	22.726
O	-23.149	-11.158	-15.491
H	-23.002	-10.259	-15.226

^sRe-1:

C	3.307	1.060	-0.029
H	3.013	1.481	-0.994
H	2.792	1.636	0.742
N	5.536	1.991	-0.719
H	5.182	2.568	-1.509
C	4.792	1.176	0.120
C	6.817	1.995	-0.286
H	7.608	2.541	-0.774
N	6.947	1.227	0.785
C	5.693	0.714	1.048
H	5.530	0.099	1.917
C	8.261	-4.307	4.143
H	8.126	-4.048	5.196
H	9.050	-5.060	4.077
N	9.722	-3.042	2.506
H	10.453	-3.757	2.438
C	8.626	-3.087	3.354
C	9.777	-1.806	1.948
H	10.540	-1.481	1.257
N	8.776	-1.059	2.382
C	8.060	-1.837	3.266
H	7.212	-1.421	3.790
C	13.779	-3.532	12.763
H	14.387	-4.425	12.941
H	12.921	-3.838	12.156
N	14.529	-2.489	12.066
H	14.723	-1.619	12.584
C	14.442	-2.288	10.733
N	14.738	-1.090	10.251
H	14.719	-0.888	9.222
H	14.944	-0.311	10.890
N	14.042	-3.259	9.896
H	13.930	-2.983	8.904
H	14.286	-4.229	10.098
C	15.589	-3.372	0.306
H	14.902	-4.011	-0.263
H	16.234	-4.046	0.882

N	13.757	-2.897	1.973
H	13.355	-3.832	2.034
C	14.808	-2.445	1.196
C	13.234	-1.831	2.632
H	12.396	-1.925	3.307
N	13.877	-0.717	2.338
C	14.861	-1.090	1.448
H	15.557	-0.367	1.050
C	11.850	3.620	-1.711
H	12.796	3.239	-2.101
H	12.074	4.239	-0.836
N	10.436	1.471	-1.989
H	10.482	1.305	-3.014
C	10.990	2.491	-1.230
C	9.790	0.641	-1.139
H	9.253	-0.230	-1.487
N	9.905	1.036	0.122
C	10.665	2.184	0.071
H	10.860	2.731	0.980
C	12.070	8.748	3.442
H	12.867	9.178	4.062
H	11.155	9.307	3.652
C	11.860	7.322	3.936
O	10.821	7.023	4.532
O	12.873	6.522	3.721
H	12.691	5.498	3.936
C	9.055	8.173	0.453
H	9.705	8.319	-0.414
H	9.365	8.867	1.244
N	9.124	6.368	2.249
H	9.260	6.956	3.063
C	9.135	6.754	0.919
C	9.108	5.005	2.284
H	9.101	4.435	3.201
N	9.082	4.494	1.068
C	9.114	5.571	0.219
H	9.101	5.440	-0.854
C	5.244	2.381	4.729
H	4.781	3.053	3.997
H	5.201	2.881	5.698
C	6.720	2.207	4.294
O	7.021	1.172	3.605
O	7.486	3.145	4.612
C	10.694	3.340	9.148

H	10.364	4.385	9.064
H	11.786	3.343	9.275
O	10.295	2.540	8.055
H	10.631	2.990	7.242
N	12.635	3.998	4.044
C	11.995	3.322	5.073
O	11.384	3.860	5.989
C	12.192	1.820	4.874
N	13.061	1.818	3.694
C	13.188	3.064	3.277
C	12.782	1.137	6.106
C	12.932	-0.375	5.957
C	13.667	-1.016	7.126
O	13.478	-2.239	7.365
O	14.475	-0.278	7.780
H	11.961	-0.869	5.836
H	13.523	-0.609	5.062
H	13.760	1.573	6.329
H	12.126	1.365	6.953
H	11.212	1.426	4.544
H	13.724	3.299	2.365
H	13.334	0.982	3.156
O	9.877	1.987	3.111
H	9.331	2.411	3.794
Zn	8.579	1.041	2.156

^RRe-1

C	3.324	1.055	-0.027
H	3.039	1.472	-0.996
H	2.803	1.636	0.737
N	5.555	1.984	-0.709
H	5.202	2.556	-1.504
C	4.810	1.174	0.134
C	6.833	2.002	-0.266
H	7.624	2.547	-0.757
N	6.962	1.247	0.815
C	5.709	0.729	1.073
H	5.545	0.116	1.944
C	8.260	-4.284	4.188
H	8.106	-4.017	5.236
H	9.057	-5.029	4.141
N	9.693	-3.033	2.513
H	10.420	-3.750	2.431
C	8.622	-3.067	3.392

C	9.738	-1.799	1.947	O	12.669	6.426	3.589
H	10.482	-1.479	1.233	H	12.481	5.429	3.870
N	8.754	-1.045	2.404	C	9.035	8.161	0.471
C	8.060	-1.814	3.312	H	9.691	8.288	-0.394
H	7.226	-1.393	3.856	H	9.348	8.864	1.253
C	13.871	-3.516	12.644	N	9.010	6.389	2.296
H	14.535	-4.369	12.813	H	9.078	7.002	3.099
H	13.024	-3.874	12.052	C	9.098	6.750	0.962
N	14.542	-2.430	11.928	C	9.000	5.026	2.357
H	14.719	-1.558	12.454	H	8.914	4.476	3.284
C	14.395	-2.233	10.600	N	9.049	4.492	1.152
N	14.640	-1.024	10.101	C	9.122	5.554	0.284
H	14.503	-0.806	9.096	H	9.167	5.404	-0.786
H	14.902	-0.253	10.730	C	5.283	2.427	4.733
N	13.994	-3.216	9.781	H	4.819	3.100	4.002
H	13.849	-2.942	8.791	H	5.233	2.923	5.704
H	14.241	-4.181	9.997	C	6.764	2.269	4.302
C	15.621	-3.358	0.288	O	7.081	1.229	3.628
H	14.930	-3.996	-0.275	O	7.516	3.221	4.607
H	16.266	-4.032	0.865	C	10.691	3.420	9.320
N	13.717	-2.834	1.856	H	10.343	4.460	9.230
H	13.279	-3.754	1.887	H	11.777	3.441	9.485
C	14.845	-2.421	1.172	O	10.347	2.621	8.208
C	13.221	-1.766	2.530	H	10.818	3.021	7.442
H	12.331	-1.830	3.136	N	12.561	3.914	4.114
N	13.954	-0.685	2.336	C	12.322	3.316	5.339
C	14.968	-1.084	1.493	O	11.744	3.854	6.277
H	15.729	-0.390	1.168	C	12.890	1.886	5.312
C	11.830	3.640	-1.720	N	13.308	1.801	3.908
H	12.787	3.270	-2.093	C	13.050	2.959	3.328
H	12.032	4.259	-0.840	C	11.880	0.821	5.743
N	10.439	1.478	-2.028	C	12.447	-0.600	5.806
H	10.487	1.320	-3.053	C	13.316	-0.980	7.007
C	10.973	2.502	-1.258	O	13.367	-2.210	7.297
C	9.799	0.634	-1.185	O	13.981	-0.077	7.607
H	9.277	-0.242	-1.545	H	11.622	-1.317	5.759
N	9.901	1.020	0.078	H	13.070	-0.805	4.928
C	10.643	2.180	0.039	H	11.502	1.106	6.729
H	10.826	2.717	0.958	H	11.049	0.857	5.027
C	12.004	8.715	3.419	H	13.771	1.848	5.964
H	12.794	9.121	4.065	H	13.251	3.115	2.274
H	11.100	9.296	3.620	H	13.562	0.948	3.389
C	11.740	7.293	3.905	O	10.054	1.895	3.057
O	10.742	7.055	4.589	H	9.627	2.416	3.752

Zn	8.615	1.064	2.200
^s TS1-1			
C	3.314	1.048	-0.024
H	3.019	1.474	-0.986
H	2.807	1.628	0.751
N	5.535	1.988	-0.712
H	5.176	2.568	-1.498
C	4.801	1.158	0.120
C	6.816	2.000	-0.283
H	7.596	2.561	-0.771
N	6.960	1.220	0.779
C	5.710	0.692	1.039
H	5.552	0.065	1.900
C	8.297	-4.210	4.129
H	8.153	-3.980	5.186
H	9.101	-4.946	4.055
N	9.815	-2.902	2.605
H	10.517	-3.656	2.543
C	8.671	-2.964	3.379
C	9.932	-1.651	2.105
H	10.749	-1.325	1.479
N	8.918	-0.897	2.508
C	8.130	-1.701	3.310
H	7.257	-1.289	3.796
C	13.807	-3.500	12.740
H	14.427	-4.387	12.913
H	12.951	-3.814	12.136
N	14.543	-2.447	12.041
H	14.725	-1.573	12.559
C	14.450	-2.256	10.708
N	14.739	-1.059	10.213
H	14.673	-0.845	9.193
H	14.953	-0.277	10.847
N	14.051	-3.236	9.882
H	13.950	-2.964	8.886
H	14.290	-4.204	10.097
C	15.781	-3.559	0.247
H	15.127	-4.227	-0.328
H	16.514	-4.194	0.757
N	14.209	-3.435	2.180
H	14.162	-4.444	2.313
C	14.973	-2.781	1.235
C	13.520	-2.496	2.881

H	12.845	-2.754	3.684
N	13.797	-1.275	2.450
C	14.707	-1.446	1.429
H	15.130	-0.601	0.904
C	11.894	3.680	-1.720
H	12.799	3.247	-2.150
H	12.190	4.321	-0.883
N	10.477	1.513	-1.802
H	10.517	1.262	-2.812
C	11.026	2.606	-1.146
C	9.826	0.773	-0.877
H	9.288	-0.127	-1.132
N	9.930	1.300	0.339
C	10.689	2.437	0.175
H	10.874	3.095	1.007
C	12.138	8.557	3.408
H	13.024	8.788	4.015
H	11.354	9.261	3.707
C	11.637	7.135	3.788
O	10.558	7.111	4.450
O	12.330	6.142	3.430
H	11.997	4.546	3.600
C	9.065	8.145	0.409
H	9.708	8.235	-0.470
H	9.413	8.847	1.175
N	9.007	6.449	2.283
H	9.286	7.035	3.078
C	9.077	6.744	0.936
C	8.923	5.101	2.400
H	8.892	4.612	3.359
N	8.890	4.503	1.222
C	8.996	5.523	0.304
H	8.997	5.324	-0.759
C	5.199	2.380	4.742
H	4.715	3.055	4.026
H	5.162	2.865	5.718
C	6.666	2.251	4.289
O	7.007	1.250	3.570
O	7.409	3.203	4.620
C	10.601	3.217	8.982
H	10.268	4.261	8.890
H	11.701	3.221	9.011
O	10.101	2.376	7.969
H	10.315	2.750	7.076

N	11.986	3.476	3.645	H	7.273	-1.262	3.804
C	11.132	2.700	4.560	C	13.814	-3.493	12.732
O	10.668	3.261	5.558	H	14.435	-4.378	12.904
C	11.760	1.282	4.544	H	12.957	-3.807	12.128
N	12.687	1.386	3.405	N	14.547	-2.438	12.032
C	12.790	2.652	3.018	H	14.728	-1.563	12.550
C	12.476	0.929	5.852	C	14.450	-2.246	10.698
C	12.950	-0.523	5.823	N	14.738	-1.049	10.202
C	13.655	-1.008	7.080	H	14.658	-0.830	9.183
O	13.555	-2.233	7.369	H	14.954	-0.269	10.837
O	14.352	-0.171	7.734	N	14.050	-3.227	9.873
H	12.108	-1.193	5.619	H	13.947	-2.953	8.878
H	13.666	-0.662	5.002	H	14.288	-4.194	10.090
H	13.318	1.605	6.027	C	15.803	-3.566	0.233
H	11.765	1.082	6.672	H	15.152	-4.236	-0.341
H	10.975	0.558	4.326	H	16.541	-4.199	0.740
H	13.492	2.969	2.256	N	14.245	-3.458	2.180
H	13.169	0.577	2.998	H	14.214	-4.468	2.313
O	9.717	2.312	3.390	C	14.995	-2.797	1.228
H	8.994	2.689	3.942	C	13.556	-2.524	2.889
Zn	8.615	1.184	2.194	H	12.893	-2.787	3.700
^s IM1-1				N	13.818	-1.302	2.455
C	3.316	1.043	-0.027	C	14.719	-1.464	1.425
H	3.025	1.466	-0.991	H	15.129	-0.614	0.898
H	2.808	1.626	0.744	C	11.902	3.679	-1.728
N	5.535	1.985	-0.712	H	12.787	3.224	-2.176
H	5.174	2.567	-1.497	H	12.230	4.320	-0.904
C	4.804	1.151	0.118	N	10.473	1.517	-1.735
C	6.817	1.993	-0.291	H	10.510	1.234	-2.738
H	7.595	2.551	-0.788	C	11.027	2.631	-1.120
N	6.968	1.205	0.765	C	9.821	0.813	-0.784
C	5.717	0.678	1.028	H	9.277	-0.092	-1.002
H	5.563	0.042	1.883	N	9.929	1.386	0.413
C	8.306	-4.189	4.128	C	10.694	2.514	0.206
H	8.159	-3.965	5.185	H	10.901	3.199	1.011
H	9.112	-4.923	4.054	C	12.148	8.583	3.421
N	9.838	-2.874	2.626	H	13.043	8.803	4.019
H	10.535	-3.632	2.564	H	11.376	9.297	3.728
C	8.684	-2.939	3.387	C	11.632	7.166	3.806
C	9.969	-1.619	2.142	O	10.547	7.165	4.467
H	10.799	-1.293	1.534	O	12.303	6.163	3.450
N	8.953	-0.863	2.540	H	11.906	4.479	3.605
C	8.150	-1.672	3.325	C	9.047	8.125	0.424
				H	9.694	8.195	-0.453

H	9.397	8.840	1.178
N	9.011	6.496	2.349
H	9.315	7.104	3.121
C	9.048	6.738	0.991
C	8.941	5.156	2.523
H	8.951	4.716	3.505
N	8.885	4.506	1.372
C	8.961	5.492	0.409
H	8.940	5.251	-0.646
C	5.219	2.389	4.732
H	4.733	3.069	4.022
H	5.183	2.867	5.711
C	6.683	2.273	4.278
O	7.035	1.292	3.536
O	7.428	3.219	4.628
C	10.603	3.203	8.963
H	10.278	4.250	8.869
H	11.703	3.205	8.990
O	10.095	2.361	7.960
H	10.325	2.710	7.046
N	11.878	3.424	3.608
C	10.928	2.588	4.492
O	10.592	3.161	5.570
C	11.688	1.209	4.503
N	12.657	1.361	3.403
C	12.755	2.642	3.049
C	12.379	0.896	5.831
C	12.937	-0.527	5.809
C	13.638	-0.996	7.073
O	13.553	-2.223	7.366
O	14.322	-0.150	7.730
H	12.138	-1.239	5.579
H	13.678	-0.622	5.004
H	13.175	1.622	6.024
H	11.645	1.010	6.634
H	10.976	0.418	4.256
H	13.513	2.985	2.353
H	13.198	0.580	3.024
O	9.713	2.342	3.579
H	8.963	2.747	4.099
Zn	8.625	1.202	2.195

^sTS2-1:

C	3.304	1.041	-0.022
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H	2.999	1.472	-0.978
H	2.808	1.618	0.762
N	5.518	1.983	-0.725
H	5.154	2.573	-1.502
C	4.792	1.141	0.101
C	6.807	1.970	-0.325
H	7.584	2.524	-0.827
N	6.964	1.162	0.716
C	5.713	0.643	0.989
H	5.563	-0.006	1.836
C	8.297	-4.203	4.139
H	8.143	-3.964	5.193
H	9.100	-4.941	4.079
N	9.843	-2.906	2.634
H	10.541	-3.667	2.584
C	8.681	-2.964	3.383
C	9.975	-1.661	2.130
H	10.814	-1.340	1.530
N	8.951	-0.903	2.505
C	8.143	-1.702	3.294
H	7.259	-1.289	3.758
C	13.834	-3.510	12.708
H	14.470	-4.385	12.875
H	12.981	-3.837	12.106
N	14.546	-2.440	12.009
H	14.724	-1.568	12.533
C	14.440	-2.242	10.677
N	14.715	-1.040	10.186
H	14.629	-0.817	9.168
H	14.939	-0.263	10.822
N	14.043	-3.222	9.849
H	13.941	-2.945	8.854
H	14.287	-4.188	10.063
C	15.822	-3.591	0.227
H	15.181	-4.265	-0.353
H	16.569	-4.218	0.729
N	14.278	-3.528	2.183
H	14.281	-4.540	2.313
C	15.002	-2.843	1.228
C	13.563	-2.616	2.894
H	12.912	-2.900	3.709
N	13.784	-1.387	2.460
C	14.685	-1.520	1.426
H	15.066	-0.657	0.897

C	11.908	3.677	-1.724	N	12.507	1.297	3.338
H	12.798	3.229	-2.168	C	12.772	2.599	3.071
H	12.228	4.317	-0.895	C	12.324	0.856	5.786
N	10.467	1.524	-1.761	C	12.954	-0.537	5.758
H	10.506	1.252	-2.766	C	13.636	-0.990	7.039
C	11.033	2.622	-1.127	O	13.559	-2.217	7.337
C	9.808	0.811	-0.823	O	14.295	-0.134	7.707
H	9.254	-0.084	-1.056	H	12.197	-1.283	5.498
N	9.922	1.365	0.384	H	13.717	-0.586	4.969
C	10.701	2.487	0.198	H	13.084	1.624	5.959
H	10.927	3.149	1.017	H	11.605	0.929	6.607
C	12.152	8.674	3.444	H	10.913	0.293	4.251
H	13.031	8.962	4.035	H	13.603	2.832	2.405
H	11.336	9.350	3.722	H	13.074	0.518	3.008
C	11.736	7.234	3.860	O	9.650	2.301	3.569
O	10.618	7.166	4.470	H	8.838	2.738	4.012
O	12.505	6.287	3.575	Zn	8.616	1.132	2.113
H	12.158	4.493	3.591				
C	9.067	8.111	0.420	^s P-1:			
H	9.707	8.187	-0.462	C	3.285	1.044	-0.020
H	9.420	8.827	1.171	H	2.969	1.481	-0.970
N	9.131	6.489	2.349	H	2.798	1.614	0.773
H	9.468	7.094	3.115	N	5.497	1.990	-0.735
C	9.084	6.726	0.991	H	5.131	2.588	-1.507
C	9.061	5.151	2.533	C	4.773	1.143	0.087
H	9.141	4.721	3.516	C	6.790	1.957	-0.355
N	8.931	4.495	1.391	H	7.568	2.504	-0.864
C	8.956	5.476	0.421	N	6.950	1.131	0.672
H	8.876	5.230	-0.630	C	5.698	0.620	0.955
C	5.221	2.378	4.675	H	5.552	-0.038	1.795
H	4.726	3.048	3.962	C	8.280	-4.230	4.166
H	5.202	2.871	5.647	H	8.116	-3.968	5.213
C	6.673	2.245	4.199	H	9.078	-4.975	4.125
O	7.020	1.250	3.480	N	9.840	-2.968	2.642
O	7.427	3.202	4.511	H	10.538	-3.730	2.607
C	10.618	3.243	9.111	C	8.678	-3.009	3.390
H	10.255	4.277	9.004	C	9.973	-1.737	2.106
H	11.716	3.281	9.158	H	10.815	-1.428	1.505
O	10.159	2.371	8.109	N	8.946	-0.972	2.463
H	10.388	2.703	7.205	C	8.137	-1.751	3.272
N	11.999	3.461	3.624	H	7.254	-1.329	3.727
C	10.710	2.406	4.536	C	13.866	-3.535	12.676
O	10.388	2.945	5.604	H	14.523	-4.395	12.841
C	11.590	1.127	4.465	H	13.021	-3.882	12.073

N	14.551	-2.447	11.979	C	9.436	5.201	2.532
H	14.728	-1.580	12.511	H	9.686	4.775	3.490
C	14.425	-2.234	10.650	N	9.166	4.540	1.417
N	14.677	-1.022	10.172	C	9.036	5.516	0.455
H	14.589	-0.788	9.155	H	8.827	5.263	-0.576
H	14.911	-0.255	10.815	C	5.250	2.374	4.620
N	14.032	-3.209	9.814	H	4.732	3.065	3.947
H	13.923	-2.922	8.823	H	5.297	2.858	5.596
H	14.289	-4.175	10.017	C	6.666	2.218	4.058
C	15.803	-3.573	0.237	O	7.015	1.160	3.444
H	15.172	-4.253	-0.348	O	7.408	3.234	4.200
H	16.545	-4.196	0.751	C	10.655	3.286	9.264
N	14.251	-3.522	2.182	H	10.264	4.306	9.134
H	14.273	-4.532	2.318	H	11.749	3.351	9.336
C	14.965	-2.828	1.225	O	10.243	2.379	8.268
C	13.510	-2.619	2.880	H	10.436	2.695	7.368
H	12.862	-2.914	3.694	N	12.201	3.704	4.256
N	13.702	-1.388	2.439	C	10.253	2.000	4.624
C	14.614	-1.511	1.412	O	9.799	2.368	5.690
H	14.980	-0.643	0.879	C	11.460	1.078	4.466
C	11.920	3.635	-1.724	N	12.355	1.558	3.423
H	12.809	3.191	-2.176	C	12.780	2.876	3.482
H	12.243	4.262	-0.888	C	12.142	0.792	5.819
N	10.445	1.509	-1.812	C	12.988	-0.480	5.715
H	10.489	1.259	-2.824	C	13.635	-0.946	7.009
C	11.043	2.571	-1.146	O	13.543	-2.173	7.305
C	9.776	0.780	-0.898	O	14.276	-0.094	7.700
H	9.202	-0.095	-1.160	H	12.373	-1.302	5.336
N	9.912	1.289	0.327	H	13.794	-0.330	4.986
C	10.721	2.396	0.176	H	12.754	1.649	6.110
H	10.969	3.020	1.017	H	11.376	0.666	6.590
C	12.183	8.921	3.618	H	11.036	0.134	4.093
H	13.060	9.325	4.141	H	13.598	3.094	2.785
H	11.326	9.563	3.848	H	12.962	0.854	3.015
C	11.913	7.493	4.162	O	9.572	2.254	3.479
O	10.710	7.293	4.556	H	8.696	2.794	3.785
O	12.861	6.683	4.175	Zn	8.593	1.014	2.003
H	12.526	4.677	4.202				
C	9.113	8.148	0.419	^R TS1-1:			
H	9.739	8.239	-0.472	C	3.288	1.088	-0.011
H	9.452	8.884	1.157	H	2.964	1.520	-0.961
N	9.449	6.540	2.340	H	2.794	1.651	0.782
H	9.775	7.160	3.109	N	5.487	1.982	-0.815
C	9.202	6.771	1.004	H	5.107	2.551	-1.596

C	4.778	1.214	0.094	H	10.523	1.272	-2.756
C	6.779	2.021	-0.417	C	11.110	2.688	-1.183
H	7.542	2.527	-0.988	C	9.831	0.938	-0.780
N	6.958	1.318	0.690	H	9.240	0.056	-0.965
C	5.715	0.811	1.015	N	9.974	1.540	0.395
H	5.580	0.235	1.915	C	10.782	2.624	0.146
C	8.337	-4.004	4.076	H	11.028	3.327	0.925
H	8.191	-3.772	5.131	C	11.971	8.824	3.437
H	9.177	-4.699	4.008	H	12.894	8.862	4.028
N	9.710	-2.678	2.427	H	11.332	9.656	3.751
H	10.413	-3.413	2.295	C	11.214	7.522	3.749
C	8.646	-2.747	3.311	O	10.047	7.693	4.255
C	9.780	-1.409	1.944	O	11.757	6.428	3.479
H	10.532	-1.077	1.244	H	11.704	4.714	3.574
N	8.821	-0.656	2.453	C	8.935	7.629	0.685
C	8.111	-1.476	3.309	H	9.623	7.641	-0.164
H	7.282	-1.080	3.879	H	9.314	8.300	1.463
C	13.873	-3.502	12.657	N	8.742	6.050	2.642
H	14.534	-4.357	12.828	H	9.065	6.726	3.369
H	13.025	-3.860	12.066	C	8.806	6.241	1.273
N	14.548	-2.421	11.934	C	8.672	4.727	2.880
H	14.727	-1.547	12.457	H	8.652	4.310	3.875
C	14.378	-2.221	10.608	N	8.647	4.023	1.755
N	14.594	-1.007	10.108	C	8.732	4.969	0.742
H	14.449	-0.793	9.102	H	8.736	4.680	-0.300
H	14.864	-0.237	10.734	C	5.238	2.487	4.865
N	13.978	-3.209	9.795	H	4.807	3.168	4.122
H	13.796	-2.934	8.811	H	5.137	2.947	5.848
H	14.236	-4.172	10.008	C	6.733	2.325	4.520
C	15.668	-3.339	0.221	O	7.012	1.628	3.485
H	14.979	-3.980	-0.341	O	7.557	2.925	5.245
H	16.298	-4.008	0.818	C	10.644	3.244	9.106
N	13.739	-2.746	1.738	H	10.318	4.290	9.007
H	13.276	-3.654	1.772	H	11.742	3.249	9.183
C	14.892	-2.375	1.073	O	10.189	2.412	8.067
C	13.250	-1.653	2.372	H	10.416	2.833	7.199
H	12.349	-1.685	2.963	N	11.920	3.703	3.722
N	14.010	-0.592	2.171	C	11.326	2.920	4.821
C	15.036	-1.034	1.364	O	10.798	3.512	5.766
H	15.822	-0.367	1.043	C	12.324	1.744	4.959
C	11.995	3.698	-1.830	N	12.972	1.763	3.627
H	12.830	3.209	-2.335	C	12.758	2.937	3.059
H	12.398	4.322	-1.026	C	11.784	0.408	5.442
N	10.504	1.585	-1.762	C	12.854	-0.708	5.545

C	13.422	-1.027	6.929
O	13.312	-2.224	7.324
O	14.026	-0.109	7.565
H	12.443	-1.640	5.154
H	13.719	-0.465	4.918
H	11.327	0.594	6.420
H	10.981	0.107	4.767
H	13.077	2.104	5.679
H	13.243	3.228	2.135
H	13.471	0.990	3.161
O	9.926	2.056	3.820
H	9.240	2.266	4.485
Zn	8.652	1.631	2.236

^RIM1-1:

C	3.268	1.094	-0.015
H	2.937	1.525	-0.963
H	2.775	1.652	0.781
N	5.460	1.986	-0.835
H	5.077	2.555	-1.616
C	4.755	1.226	0.082
C	6.753	2.027	-0.448
H	7.514	2.525	-1.028
N	6.935	1.330	0.664
C	5.695	0.826	1.001
H	5.566	0.253	1.904
C	8.340	-3.964	4.068
H	8.191	-3.739	5.124
H	9.186	-4.651	4.000
N	9.716	-2.623	2.436
H	10.417	-3.360	2.302
C	8.645	-2.699	3.312
C	9.797	-1.351	1.968
H	10.558	-1.016	1.279
N	8.835	-0.596	2.477
C	8.115	-1.425	3.320
H	7.284	-1.034	3.890
C	13.871	-3.504	12.664
H	14.528	-4.362	12.838
H	13.022	-3.859	12.072
N	14.551	-2.426	11.943
H	14.729	-1.551	12.466
C	14.380	-2.225	10.617
N	14.597	-1.012	10.117

H	14.446	-0.796	9.110
H	14.866	-0.241	10.744
N	13.977	-3.213	9.806
H	13.795	-2.938	8.820
H	14.237	-4.175	10.018
C	15.680	-3.353	0.212
H	14.992	-3.995	-0.351
H	16.313	-4.021	0.807
N	13.758	-2.770	1.741
H	13.300	-3.678	1.772
C	14.904	-2.393	1.067
C	13.271	-1.676	2.379
H	12.378	-1.714	2.981
N	14.024	-0.613	2.171
C	15.044	-1.051	1.357
H	15.825	-0.381	1.030
C	12.001	3.696	-1.827
H	12.834	3.204	-2.332
H	12.406	4.320	-1.024
N	10.501	1.589	-1.755
H	10.526	1.270	-2.748
C	11.112	2.692	-1.178
C	9.815	0.954	-0.777
H	9.220	0.074	-0.961
N	9.953	1.564	0.397
C	10.776	2.639	0.149
H	11.035	3.336	0.930
C	11.963	8.835	3.431
H	12.883	8.861	4.027
H	11.329	9.670	3.745
C	11.192	7.537	3.724
O	10.012	7.720	4.209
O	11.720	6.440	3.457
H	11.633	4.653	3.566
C	8.937	7.576	0.690
H	9.626	7.575	-0.158
H	9.327	8.243	1.466
N	8.748	6.026	2.666
H	9.087	6.721	3.382
C	8.797	6.191	1.294
C	8.673	4.713	2.932
H	8.673	4.324	3.938
N	8.635	3.981	1.821
C	8.712	4.910	0.785

H	8.706	4.602	-0.250	C	5.674	0.826	0.973
C	5.254	2.481	4.853	H	5.553	0.249	1.875
H	4.825	3.162	4.109	C	8.337	-3.951	4.063
H	5.153	2.942	5.836	H	8.186	-3.722	5.118
C	6.748	2.317	4.515	H	9.187	-4.634	3.998
O	7.038	1.639	3.469	N	9.714	-2.609	2.432
O	7.572	2.896	5.255	H	10.416	-3.347	2.306
C	10.646	3.235	9.096	C	8.637	-2.687	3.300
H	10.326	4.285	8.998	C	9.790	-1.341	1.954
H	11.745	3.241	9.174	H	10.555	-1.005	1.271
O	10.190	2.408	8.060	N	8.819	-0.589	2.450
H	10.427	2.829	7.171	C	8.098	-1.417	3.296
N	11.812	3.641	3.691	H	7.263	-1.028	3.860
C	11.112	2.790	4.797	C	13.873	-3.512	12.671
O	10.733	3.468	5.808	H	14.532	-4.369	12.844
C	12.240	1.709	4.989	H	13.026	-3.868	12.078
N	12.946	1.744	3.686	N	14.552	-2.431	11.953
C	12.731	2.922	3.109	H	14.729	-1.558	12.476
C	11.766	0.341	5.452	C	14.383	-2.229	10.627
C	12.880	-0.731	5.554	N	14.598	-1.015	10.130
C	13.433	-1.049	6.943	H	14.454	-0.797	9.121
O	13.316	-2.247	7.336	H	14.864	-0.245	10.758
O	14.031	-0.134	7.586	N	13.983	-3.217	9.813
H	12.515	-1.674	5.146	H	13.811	-2.942	8.825
H	13.744	-0.442	4.945	H	14.246	-4.178	10.025
H	11.286	0.493	6.426	C	15.700	-3.377	0.197
H	10.988	-0.007	4.767	H	15.022	-4.026	-0.369
H	12.926	2.130	5.736	H	16.340	-4.038	0.792
H	13.293	3.235	2.234	N	13.769	-2.829	1.722
H	13.493	0.998	3.245	H	13.326	-3.743	1.745
O	9.968	2.149	4.064	C	14.911	-2.431	1.053
H	9.200	2.381	4.644	C	13.265	-1.745	2.364
Zn	8.560	1.657	2.134	H	12.372	-1.796	2.966
^R TS2-1:				N	14.004	-0.672	2.163
C	3.243	1.099	-0.016	C	15.032	-1.090	1.350
H	2.902	1.533	-0.958	H	15.804	-0.405	1.030
H	2.756	1.651	0.788	C	12.007	3.694	-1.826
N	5.426	1.996	-0.854	H	12.839	3.203	-2.331
H	5.039	2.569	-1.632	H	12.410	4.313	-1.020
C	4.728	1.235	0.067	N	10.495	1.597	-1.781
C	6.722	2.031	-0.484	H	10.529	1.283	-2.776
H	7.481	2.527	-1.069	C	11.112	2.688	-1.188
N	6.911	1.327	0.621	C	9.795	0.959	-0.819
				H	9.194	0.086	-1.017

N	9.929	1.557	0.363	H	13.812	-0.414	4.954
C	10.767	2.626	0.137	H	11.355	0.441	6.457
H	11.041	3.298	0.934	H	11.028	-0.076	4.809
C	11.918	8.929	3.418	H	12.900	2.166	5.688
H	12.831	8.954	4.026	H	13.405	2.992	2.115
H	11.279	9.765	3.720	H	13.375	0.899	3.251
C	11.158	7.622	3.686	O	9.949	2.117	4.157
O	9.969	7.780	4.172	H	9.117	2.428	4.623
O	11.688	6.541	3.394	Zn	8.507	1.635	2.021
H	11.926	4.720	3.220				
C	8.942	7.562	0.690	¹⁸ P-1:			
H	9.630	7.566	-0.159	C	3.218	1.111	-0.011
H	9.331	8.225	1.469	H	2.855	1.552	-0.942
N	8.780	6.012	2.663	H	2.745	1.652	0.808
H	9.123	6.719	3.376	N	5.386	2.017	-0.880
C	8.806	6.175	1.291	H	4.993	2.594	-1.651
C	8.704	4.701	2.929	C	4.702	1.248	0.044
H	8.711	4.320	3.936	C	6.689	2.042	-0.534
N	8.641	3.964	1.821	H	7.441	2.539	-1.126
C	8.709	4.894	0.783	N	6.892	1.325	0.561
H	8.689	4.586	-0.252	C	5.660	0.825	0.929
C	5.271	2.479	4.837	H	5.550	0.240	1.827
H	4.838	3.164	4.099	C	8.309	-3.899	4.084
H	5.182	2.938	5.821	H	8.129	-3.651	5.131
C	6.758	2.309	4.479	H	9.170	-4.570	4.050
O	7.040	1.640	3.428	N	9.695	-2.585	2.442
O	7.598	2.881	5.215	H	10.386	-3.338	2.331
C	10.642	3.249	9.216	C	8.610	-2.648	3.301
H	10.304	4.290	9.100	C	9.777	-1.328	1.940
H	11.739	3.263	9.296	H	10.554	-1.002	1.266
O	10.198	2.393	8.194	N	8.798	-0.568	2.411
H	10.447	2.794	7.322	C	8.068	-1.380	3.265
N	11.994	3.743	3.515	H	7.227	-0.982	3.813
C	10.990	2.613	4.929	C	13.862	-3.546	12.699
O	10.705	3.348	5.881	H	14.517	-4.405	12.873
C	12.224	1.689	4.965	H	13.017	-3.898	12.101
N	12.857	1.681	3.649	N	14.548	-2.464	11.991
C	12.783	2.873	3.008	H	14.726	-1.594	12.517
C	11.813	0.303	5.471	C	14.385	-2.251	10.666
C	12.954	-0.738	5.552	N	14.599	-1.034	10.182
C	13.484	-1.061	6.945	H	14.481	-0.812	9.167
O	13.360	-2.259	7.334	H	14.853	-0.267	10.818
O	14.062	-0.144	7.605	N	13.991	-3.234	9.842
H	12.613	-1.683	5.127	H	13.831	-2.956	8.854

H	14.262	-4.196	10.045	C	6.754	2.319	4.420
C	15.754	-3.441	0.180	O	7.021	1.660	3.364
H	15.110	-4.115	-0.396	O	7.610	2.872	5.156
H	16.420	-4.077	0.773	C	10.674	3.302	9.392
N	13.824	-3.047	1.731	H	10.307	4.332	9.267
H	13.467	-3.994	1.740	H	11.767	3.347	9.509
C	14.917	-2.554	1.047	O	10.294	2.432	8.353
C	13.248	-2.013	2.396	H	10.589	2.814	7.497
H	12.371	-2.143	3.010	N	12.295	3.792	3.420
N	13.898	-0.884	2.194	C	10.881	2.428	5.023
C	14.941	-1.211	1.358	O	10.663	3.218	5.931
H	15.654	-0.466	1.032	C	12.174	1.626	4.918
C	12.022	3.691	-1.844	N	12.647	1.546	3.547
H	12.857	3.208	-2.351	C	12.814	2.747	2.904
H	12.418	4.304	-1.029	C	11.900	0.246	5.543
N	10.495	1.605	-1.838	C	13.129	-0.694	5.575
H	10.533	1.301	-2.835	C	13.595	-1.077	6.973
C	11.122	2.679	-1.224	O	13.412	-2.273	7.340
C	9.779	0.963	-0.891	O	14.169	-0.186	7.672
H	9.168	0.100	-1.107	H	12.904	-1.623	5.049
N	9.911	1.544	0.300	H	13.977	-0.229	5.064
C	10.766	2.605	0.096	H	11.530	0.419	6.561
H	11.046	3.260	0.905	H	11.086	-0.230	4.986
C	11.860	8.990	3.411	H	12.892	2.176	5.541
H	12.763	9.043	4.032	H	13.387	2.679	1.969
H	11.197	9.817	3.689	H	13.167	0.738	3.211
C	11.127	7.665	3.677	O	9.886	2.028	4.212
O	9.926	7.806	4.152	H	9.027	2.397	4.617
O	11.665	6.590	3.393	Zn	8.483	1.622	1.932
H	12.414	4.685	2.949				
C	8.943	7.551	0.688	^s Re-2:			
H	9.634	7.569	-0.159	C	3.351	1.083	-0.043
H	9.325	8.207	1.476	H	3.011	1.565	-0.964
N	8.831	5.985	2.648	H	2.823	1.566	0.785
H	9.163	6.704	3.365	N	5.559	2.032	-0.798
C	8.820	6.157	1.278	H	5.206	2.535	-1.632
C	8.770	4.674	2.908	C	4.830	1.259	0.090
H	8.808	4.292	3.912	C	6.843	2.073	-0.368
N	8.675	3.942	1.797	H	7.634	2.577	-0.901
C	8.713	4.879	0.763	N	6.985	1.377	0.749
H	8.670	4.576	-0.273	C	5.738	0.863	1.040
C	5.277	2.498	4.803	H	5.595	0.271	1.926
H	4.830	3.178	4.069	C	8.375	-4.340	3.982
H	5.205	2.960	5.787	H	8.183	-4.111	5.031

H	9.206	-5.049	3.949	H	12.979	8.646	4.373
N	9.790	-3.032	2.356	H	11.376	8.493	3.670
H	10.441	-3.811	2.156	C	12.460	6.660	3.951
C	8.724	-3.088	3.235	O	13.352	5.900	3.595
C	9.874	-1.778	1.859	O	11.464	6.301	4.763
H	10.624	-1.454	1.154	H	11.534	5.325	4.994
N	8.914	-1.015	2.366	C	9.087	8.427	0.384
C	8.196	-1.817	3.234	H	9.691	8.753	-0.464
H	7.374	-1.403	3.800	H	9.260	9.133	1.210
C	15.040	-4.124	12.651	N	9.230	6.217	1.728
H	15.869	-4.484	13.264	H	8.427	6.319	2.334
H	14.917	-4.865	11.865	C	9.638	7.087	0.733
N	15.423	-2.840	12.059	C	10.107	5.167	1.762
H	15.761	-2.123	12.686	H	9.959	4.268	2.367
C	15.028	-2.393	10.845	N	11.074	5.331	0.875
N	15.192	-1.095	10.561	C	10.785	6.515	0.239
H	14.930	-0.762	9.620	H	11.431	6.925	-0.525
H	15.429	-0.434	11.318	C	5.357	2.286	4.670
N	14.471	-3.195	9.943	H	4.884	3.041	4.033
H	14.225	-2.834	8.995	H	5.348	2.700	5.679
H	14.489	-4.212	10.035	C	6.820	2.164	4.200
C	15.656	-3.728	0.102	O	7.172	1.111	3.563
H	14.968	-4.242	-0.574	O	7.544	3.157	4.449
H	16.285	-4.511	0.545	C	10.716	3.101	8.660
N	13.944	-3.717	1.923	H	10.401	4.153	8.669
C	14.852	-3.013	1.155	H	11.812	3.076	8.748
C	13.372	-2.817	2.708	O	10.261	2.408	7.519
H	12.614	-3.028	3.451	H	10.576	2.900	6.734
N	13.848	-1.568	2.484	N	12.816	3.192	3.505
H	13.503	-0.690	2.909	C	12.059	2.868	4.585
C	14.801	-1.678	1.496	O	11.519	3.677	5.361
H	15.362	-0.822	1.155	C	12.114	1.348	4.678
C	11.891	3.519	-1.843	N	12.892	0.943	3.495
H	12.818	3.145	-2.284	C	13.239	2.021	2.898
H	12.122	4.113	-0.954	C	12.776	0.882	5.986
N	10.542	1.318	-2.104	C	12.928	-0.634	6.060
H	10.622	1.097	-3.115	C	13.694	-1.139	7.283
C	11.028	2.393	-1.372	O	13.669	-2.385	7.476
C	9.887	0.503	-1.239	O	14.324	-0.294	8.004
H	9.426	-0.409	-1.587	H	11.951	-1.128	6.060
N	9.921	0.970	0.002	H	13.462	-1.013	5.182
C	10.639	2.145	-0.077	H	13.760	1.353	6.071
H	10.818	2.733	0.808	H	12.159	1.235	6.816
C	12.404	8.130	3.595	H	11.093	0.966	4.575

H	13.831	2.065	1.992
H	13.046	4.157	3.251
Zn	8.658	1.055	2.100
O	9.828	2.328	2.850
H	9.263	2.671	3.567

^RRe-2:

C	3.371	1.072	-0.044
H	3.041	1.554	-0.969
H	2.840	1.560	0.779
N	5.586	2.018	-0.782
H	5.235	2.518	-1.617
C	4.851	1.242	0.100
C	6.867	2.062	-0.342
H	7.661	2.569	-0.868
N	7.003	1.367	0.777
C	5.754	0.849	1.057
H	5.606	0.253	1.941
C	8.383	-4.358	3.997
H	8.187	-4.124	5.045
H	9.209	-5.072	3.970
N	9.817	-3.049	2.385
H	10.473	-3.824	2.188
C	8.741	-3.109	3.251
C	9.900	-1.794	1.888
H	10.653	-1.466	1.189
N	8.929	-1.037	2.383
C	8.206	-1.841	3.243
H	7.373	-1.434	3.797
C	15.028	-3.849	12.558
H	15.914	-4.090	13.151
H	14.966	-4.610	11.783
N	15.215	-2.538	11.938
H	15.441	-1.744	12.535
C	14.927	-2.195	10.666
N	15.056	-0.901	10.340
H	14.902	-0.582	9.372
H	15.345	-0.256	11.083
N	14.492	-3.063	9.749
H	14.343	-2.741	8.780
H	14.494	-4.073	9.900
C	15.689	-3.779	0.080
H	14.978	-4.268	-0.591
H	16.326	-4.579	0.481

N	14.008	-3.787	1.937
C	14.930	-3.090	1.179
C	13.526	-2.908	2.804
H	12.789	-3.125	3.567
N	14.067	-1.679	2.633
H	13.892	-0.810	3.163
C	14.970	-1.779	1.603
H	15.559	-0.930	1.292
C	11.902	3.499	-1.833
H	12.830	3.130	-2.277
H	12.134	4.092	-0.944
N	10.560	1.295	-2.097
H	10.633	1.082	-3.109
C	11.046	2.367	-1.361
C	9.913	0.473	-1.232
H	9.453	-0.438	-1.584
N	9.952	0.932	0.011
C	10.666	2.109	-0.064
H	10.851	2.691	0.824
C	12.388	8.021	3.589
H	12.924	8.552	4.385
H	11.345	8.346	3.647
C	12.482	6.547	3.929
O	13.324	5.781	3.485
O	11.568	6.181	4.839
H	11.686	5.219	5.066
C	9.084	8.391	0.409
H	9.692	8.712	-0.438
H	9.260	9.097	1.235
N	9.211	6.186	1.767
H	8.412	6.298	2.376
C	9.620	7.045	0.762
C	10.075	5.123	1.796
H	9.930	4.227	2.407
N	11.034	5.272	0.898
C	10.754	6.455	0.259
H	11.397	6.854	-0.514
C	5.350	2.238	4.694
H	4.893	3.020	4.077
H	5.343	2.628	5.713
C	6.817	2.116	4.231
O	7.177	1.064	3.597
O	7.539	3.107	4.487
C	10.723	3.078	8.720

H	10.392	4.125	8.673	C	9.949	-1.771	1.878
H	11.815	3.078	8.849	H	10.727	-1.440	1.208
O	10.325	2.328	7.595	N	8.973	-1.013	2.367
H	10.776	2.720	6.820	C	8.229	-1.828	3.201
N	13.007	3.030	3.570	H	7.391	-1.424	3.750
C	12.491	2.689	4.782	C	15.127	-3.978	12.627
O	11.855	3.449	5.529	H	15.979	-4.251	13.255
C	12.975	1.251	5.017	H	15.088	-4.732	11.842
N	13.648	0.888	3.764	N	15.398	-2.669	12.031
C	13.616	1.923	3.011	H	15.679	-1.918	12.649
C	11.947	0.176	5.435	C	14.981	-2.266	10.810
C	12.108	-0.356	6.870	N	15.099	-0.966	10.505
C	13.480	-0.896	7.281	H	14.796	-0.636	9.574
O	14.314	-0.049	7.767	H	15.342	-0.307	11.258
O	13.691	-2.135	7.191	N	14.453	-3.103	9.922
H	11.402	-1.181	6.988	H	14.178	-2.750	8.977
H	11.824	0.438	7.566	H	14.488	-4.116	10.038
H	12.043	-0.651	4.727	C	15.740	-3.822	0.097
H	10.934	0.567	5.306	H	15.059	-4.348	-0.577
H	13.745	1.322	5.800	H	16.394	-4.592	0.525
H	14.017	1.972	2.007	N	14.046	-3.872	1.936
H	12.975	3.977	3.190	C	14.928	-3.141	1.164
Zn	8.677	1.033	2.151	C	13.461	-2.989	2.732
O	9.895	2.260	2.890	H	12.714	-3.221	3.480
H	9.368	2.594	3.636	N	13.906	-1.728	2.514
^s TS1-2:				H	13.501	-0.853	2.904
C	3.376	1.070	-0.056	C	14.849	-1.810	1.515
H	3.047	1.546	-0.984	H	15.383	-0.938	1.169
H	2.846	1.566	0.764	C	11.928	3.557	-1.819
N	5.582	2.042	-0.775	H	12.848	3.168	-2.262
H	5.227	2.547	-1.606	H	12.197	4.176	-0.958
C	4.856	1.236	0.086	N	10.608	1.331	-1.979
C	6.862	2.089	-0.335	H	10.698	1.066	-2.979
H	7.646	2.636	-0.834	C	11.063	2.454	-1.299
N	7.007	1.363	0.763	C	9.936	0.566	-1.084
C	5.764	0.825	1.031	H	9.487	-0.369	-1.384
H	5.620	0.206	1.899	N	9.933	1.113	0.127
C	8.403	-4.361	3.930	C	10.639	2.291	-0.003
H	8.233	-4.147	4.985	H	10.731	2.969	0.834
H	9.227	-5.076	3.874	C	12.428	7.747	3.220
N	9.848	-3.031	2.354	H	13.033	8.068	4.078
H	10.499	-3.811	2.156	H	11.449	8.223	3.341
C	8.756	-3.100	3.199	C	12.228	6.228	3.344
				O	12.733	5.456	2.501

O	11.538	5.867	4.372	H	9.228	2.663	3.705
H	11.378	4.538	4.653				
C	8.881	8.411	0.388	^s IM1-2:			
H	9.536	8.504	-0.480	C	3.371	1.067	-0.060
H	9.163	9.184	1.115	H	3.041	1.542	-0.988
N	8.757	6.753	2.301	H	2.843	1.565	0.760
H	8.395	7.412	2.992	N	5.570	2.054	-0.774
C	9.045	7.058	0.982	H	5.212	2.563	-1.603
C	8.952	5.410	2.461	C	4.851	1.232	0.078
H	8.758	4.890	3.388	C	6.852	2.095	-0.345
N	9.357	4.848	1.339	H	7.630	2.652	-0.843
C	9.420	5.864	0.420	N	7.008	1.350	0.739
H	9.717	5.690	-0.605	C	5.767	0.806	1.008
C	5.396	2.305	4.677	H	5.628	0.167	1.862
H	4.943	3.069	4.036	C	8.413	-4.353	3.913
H	5.372	2.712	5.688	H	8.247	-4.135	4.969
C	6.863	2.176	4.229	H	9.235	-5.070	3.858
O	7.208	1.158	3.540	N	9.882	-3.027	2.355
O	7.606	3.139	4.546	H	10.536	-3.810	2.167
C	10.695	3.030	8.538	C	8.774	-3.095	3.179
H	10.451	4.100	8.565	C	10.002	-1.770	1.885
H	11.789	2.931	8.570	H	10.801	-1.445	1.237
O	10.137	2.376	7.419	N	9.019	-1.006	2.355
H	10.390	2.864	6.614	C	8.252	-1.820	3.173
N	12.472	2.923	3.116	H	7.408	-1.415	3.710
C	11.602	2.594	4.118	C	15.133	-3.937	12.610
O	11.223	3.485	4.991	H	15.990	-4.192	13.238
C	11.880	1.117	4.435	H	15.102	-4.695	11.829
N	12.728	0.694	3.300	N	15.381	-2.628	12.005
C	13.025	1.760	2.645	H	15.650	-1.865	12.615
C	12.611	0.878	5.771	C	14.961	-2.240	10.779
C	12.888	-0.614	5.959	N	15.074	-0.942	10.461
C	13.592	-1.030	7.250	H	14.741	-0.615	9.539
O	13.605	-2.271	7.482	H	15.319	-0.283	11.212
O	14.143	-0.136	7.973	N	14.435	-3.087	9.898
H	11.954	-1.185	5.910	H	14.144	-2.738	8.954
H	13.512	-0.989	5.140	H	14.472	-4.099	10.024
H	13.543	1.449	5.792	C	15.728	-3.791	0.086
H	11.968	1.240	6.578	H	15.041	-4.311	-0.586
H	10.948	0.553	4.428	H	16.372	-4.567	0.518
H	13.682	1.783	1.782	N	14.027	-3.788	1.924
H	12.584	3.910	2.757	C	14.929	-3.086	1.148
Zn	8.715	1.059	2.096	C	13.473	-2.881	2.719
O	9.872	2.262	3.084	H	12.729	-3.091	3.476

N	13.953	-1.636	2.494
H	13.591	-0.732	2.894
C	14.887	-1.752	1.494
H	15.444	-0.896	1.143
C	11.937	3.566	-1.832
H	12.836	3.147	-2.289
H	12.238	4.189	-0.984
N	10.588	1.347	-1.904
H	10.678	1.044	-2.894
C	11.056	2.495	-1.277
C	9.918	0.626	-0.975
H	9.461	-0.319	-1.226
N	9.927	1.232	0.213
C	10.639	2.398	0.025
H	10.779	3.101	0.830
C	12.437	7.731	3.208
H	13.066	8.013	4.062
H	11.484	8.254	3.349
C	12.150	6.213	3.319
O	12.590	5.436	2.434
O	11.470	5.874	4.344
H	11.262	4.268	4.709
C	8.897	8.337	0.399
H	9.553	8.390	-0.472
H	9.207	9.116	1.107
N	8.737	6.778	2.381
H	8.423	7.486	3.045
C	9.009	6.996	1.041
C	8.875	5.443	2.616
H	8.700	4.997	3.582
N	9.224	4.794	1.522
C	9.313	5.754	0.541
H	9.586	5.506	-0.476
C	5.456	2.309	4.647
H	5.019	3.071	3.991
H	5.424	2.725	5.654
C	6.925	2.163	4.220
O	7.264	1.184	3.475
O	7.704	3.077	4.603
C	10.682	3.010	8.534
H	10.489	4.090	8.574
H	11.771	2.861	8.536
O	10.064	2.396	7.427
H	10.397	2.817	6.607

N	12.137	2.866	2.939
C	11.223	2.416	3.955
O	11.115	3.308	5.012
C	11.809	0.997	4.321
N	12.862	0.758	3.310
C	12.999	1.865	2.656
C	12.398	0.812	5.729
C	12.855	-0.639	5.905
C	13.516	-1.026	7.227
O	13.547	-2.265	7.476
O	14.037	-0.117	7.954
H	12.010	-1.323	5.762
H	13.583	-0.891	5.126
H	13.238	1.499	5.868
H	11.641	1.053	6.479
H	11.003	0.267	4.185
H	13.760	2.011	1.894
H	12.281	3.884	2.702
Zn	8.730	1.039	2.047
O	9.893	2.245	3.369
H	9.194	2.643	3.970

^sIM1-2':

C	3.354	1.070	-0.051
H	3.017	1.549	-0.974
H	2.828	1.558	0.775
N	5.551	2.074	-0.758
H	5.193	2.587	-1.584
C	4.833	1.239	0.081
C	6.836	2.097	-0.338
H	7.617	2.652	-0.832
N	6.991	1.332	0.733
C	5.748	0.790	0.999
H	5.610	0.143	1.847
C	8.405	-4.443	3.887
H	8.269	-4.226	4.946
H	9.212	-5.174	3.810
N	9.879	-3.118	2.332
H	10.549	-3.891	2.165
C	8.766	-3.188	3.149
C	9.987	-1.865	1.847
H	10.784	-1.537	1.198
N	8.991	-1.108	2.303
C	8.230	-1.921	3.125

H	7.379	-1.517	3.654	H	9.269	9.131	1.084
C	15.136	-3.925	12.606	N	9.325	6.795	2.328
H	15.999	-4.155	13.236	H	9.419	7.497	3.061
H	15.122	-4.690	11.831	C	9.168	7.009	0.970
N	15.355	-2.615	11.990	C	9.481	5.456	2.522
H	15.620	-1.843	12.591	H	9.676	5.037	3.497
C	14.918	-2.245	10.765	N	9.425	4.795	1.381
N	15.019	-0.947	10.436	C	9.240	5.754	0.412
H	14.647	-0.628	9.528	H	9.159	5.492	-0.634
H	15.259	-0.283	11.183	C	5.444	2.228	4.628
N	14.393	-3.102	9.896	H	5.000	3.001	3.991
H	14.086	-2.763	8.953	H	5.449	2.639	5.637
H	14.439	-4.113	10.028	C	6.892	2.056	4.153
C	15.746	-3.784	0.076	O	7.218	1.034	3.461
H	15.059	-4.306	-0.595	O	7.676	3.003	4.442
H	16.389	-4.560	0.512	C	10.621	2.861	8.438
N	14.034	-3.759	1.906	H	10.534	3.956	8.471
C	14.948	-3.072	1.132	H	11.689	2.606	8.368
C	13.484	-2.845	2.693	O	9.864	2.295	7.397
H	12.733	-3.044	3.446	H	10.165	2.659	6.537
N	13.981	-1.606	2.467	N	12.015	2.866	2.959
H	13.637	-0.696	2.859	C	11.081	2.288	3.918
C	14.920	-1.735	1.474	O	10.886	3.132	5.009
H	15.485	-0.885	1.124	C	11.750	0.888	4.213
C	11.906	3.519	-1.825	N	12.889	0.801	3.279
H	12.814	3.114	-2.278	C	12.993	1.950	2.706
H	12.193	4.130	-0.965	C	12.242	0.678	5.657
N	10.561	1.299	-1.953	C	12.791	-0.737	5.844
H	10.650	1.021	-2.951	C	13.412	-1.081	7.201
C	11.032	2.429	-1.296	O	13.480	-2.315	7.468
C	9.896	0.550	-1.043	O	13.871	-0.144	7.934
H	9.441	-0.387	-1.323	H	12.009	-1.480	5.653
N	9.912	1.118	0.163	H	13.578	-0.926	5.104
C	10.625	2.288	0.006	H	13.019	1.416	5.877
H	10.763	2.971	0.828	H	11.413	0.845	6.350
C	12.928	7.972	3.507	H	11.016	0.112	3.970
H	13.877	8.121	4.036	H	13.798	2.199	2.022
H	12.211	8.685	3.923	H	12.208	3.874	2.951
C	12.448	6.554	3.843	Zn	8.683	0.920	2.000
O	13.160	5.586	3.402	O	9.794	2.117	3.326
O	11.446	6.450	4.588	H	9.056	2.583	3.869
H	11.791	3.524	5.252	O	13.288	3.928	5.379
C	8.969	8.361	0.365	H	13.545	4.363	6.205
H	9.597	8.464	-0.523	H	13.334	4.609	4.639

^sTS2-2':

C	3.371	1.063	-0.054
H	3.038	1.543	-0.979
H	2.848	1.558	0.770
N	5.567	2.061	-0.763
H	5.208	2.575	-1.589
C	4.852	1.227	0.079
C	6.853	2.089	-0.345
H	7.631	2.645	-0.843
N	7.014	1.326	0.726
C	5.772	0.782	0.995
H	5.638	0.130	1.841
C	8.416	-4.408	3.905
H	8.262	-4.189	4.961
H	9.228	-5.135	3.842
N	9.887	-3.098	2.337
H	10.540	-3.882	2.157
C	8.784	-3.154	3.169
C	10.010	-1.843	1.858
H	10.804	-1.526	1.201
N	9.034	-1.073	2.333
C	8.269	-1.878	3.161
H	7.432	-1.463	3.702
C	15.160	-4.011	12.625
H	16.006	-4.280	13.263
H	15.126	-4.774	11.848
N	15.440	-2.710	12.018
H	15.734	-1.958	12.629
C	14.993	-2.306	10.806
N	15.106	-1.008	10.494
H	14.715	-0.683	9.597
H	15.348	-0.344	11.242
N	14.439	-3.145	9.936
H	14.144	-2.805	8.991
H	14.476	-4.158	10.058
C	15.729	-3.806	0.080
H	15.051	-4.334	-0.595
H	16.376	-4.574	0.520
N	14.034	-3.833	1.918
C	14.913	-3.111	1.133
C	13.448	-2.941	2.701
H	12.713	-3.166	3.463
N	13.886	-1.681	2.459

H	13.494	-0.806	2.849
C	14.827	-1.775	1.461
H	15.364	-0.907	1.108
C	11.925	3.565	-1.816
H	12.836	3.167	-2.268
H	12.208	4.191	-0.964
N	10.597	1.334	-1.920
H	10.686	1.047	-2.915
C	11.064	2.472	-1.273
C	9.932	0.592	-1.004
H	9.478	-0.349	-1.275
N	9.942	1.172	0.196
C	10.653	2.342	0.030
H	10.751	3.053	0.835
C	12.598	7.948	3.087
H	13.135	8.387	3.933
H	11.590	8.381	3.117
C	12.456	6.460	3.404
O	12.589	5.579	2.529
O	12.162	6.271	4.643
H	12.246	3.743	5.805
C	8.945	8.323	0.415
H	9.585	8.408	-0.465
H	9.243	9.100	1.129
N	9.168	6.769	2.410
H	9.139	7.470	3.145
C	9.121	6.978	1.042
C	9.338	5.434	2.620
H	9.439	5.007	3.607
N	9.391	4.772	1.481
C	9.264	5.725	0.498
H	9.274	5.462	-0.551
C	5.477	2.249	4.606
H	5.010	3.027	3.992
H	5.494	2.646	5.622
C	6.924	2.122	4.106
O	7.289	1.075	3.465
O	7.661	3.118	4.320
C	10.642	2.875	8.608
H	10.448	3.958	8.602
H	11.734	2.731	8.592
O	9.990	2.192	7.573
H	10.253	2.557	6.685
N	12.281	2.971	3.442

C	11.057	2.317	4.240	N	9.010	-1.220	2.230
O	10.762	3.038	5.278	C	8.227	-2.008	3.060
C	11.671	0.881	4.408	H	7.364	-1.595	3.559
N	12.642	0.725	3.303	C	15.146	-3.928	12.597
C	12.922	1.877	2.832	H	16.006	-4.164	13.229
C	12.354	0.656	5.768	H	15.125	-4.696	11.825
C	12.827	-0.786	5.924	N	15.376	-2.624	11.976
C	13.461	-1.159	7.268	H	15.635	-1.847	12.576
O	13.552	-2.400	7.492	C	14.944	-2.252	10.749
O	13.883	-0.235	8.032	N	15.053	-0.958	10.420
H	11.991	-1.478	5.765	H	14.660	-0.632	9.524
H	13.574	-1.034	5.160	H	15.300	-0.293	11.162
H	13.199	1.343	5.890	N	14.408	-3.106	9.881
H	11.627	0.891	6.551	H	14.111	-2.765	8.937
H	10.879	0.136	4.283	H	14.447	-4.117	10.014
H	13.633	2.044	2.027	C	15.695	-3.756	0.100
H	12.107	3.822	2.869	H	15.029	-4.291	-0.583
Zn	8.726	0.957	2.029	H	16.322	-4.522	0.572
O	9.944	2.247	3.300	N	13.983	-3.719	1.926
H	9.171	2.701	3.771	C	14.861	-3.024	1.117
O	13.100	4.137	5.472	C	13.366	-2.793	2.647
H	12.732	5.086	5.151	H	12.631	-2.993	3.416
H	12.899	3.497	4.371	N	13.778	-1.539	2.343
^{sp-2} :				H	13.350	-0.640	2.688
C	3.396	1.041	-0.055	C	14.743	-1.673	1.373
H	3.086	1.519	-0.989	H	15.278	-0.818	0.988
H	2.863	1.548	0.756	C	11.949	3.532	-1.833
N	5.604	2.056	-0.697	H	12.872	3.162	-2.284
H	5.252	2.577	-1.523	H	12.210	4.138	-0.960
C	4.878	1.192	0.105	N	10.597	1.325	-2.048
C	6.885	2.064	-0.269	H	10.678	1.084	-3.057
H	7.672	2.635	-0.737	C	11.099	2.408	-1.335
N	7.035	1.261	0.778	C	9.932	0.535	-1.179
C	5.786	0.710	1.014	H	9.459	-0.377	-1.507
H	5.635	0.027	1.832	N	9.975	1.034	0.057
C	8.380	-4.495	3.911	C	10.714	2.196	-0.037
H	8.244	-4.241	4.962	H	10.867	2.834	0.818
H	9.173	-5.245	3.859	C	12.728	8.032	3.267
N	9.895	-3.226	2.345	H	13.294	8.560	4.044
H	10.573	-4.002	2.220	H	11.709	8.423	3.319
C	8.764	-3.271	3.136	C	12.761	6.566	3.719
C	10.018	-1.991	1.825	O	13.715	5.846	3.367
H	10.838	-1.680	1.196	O	11.820	6.265	4.538
				H	11.845	3.767	6.102

C	8.989	8.296	0.397	H	12.367	5.089	5.528
H	9.618	8.433	-0.486	H	12.831	3.280	4.452
H	9.285	9.044	1.142				
N	9.466	6.671	2.291	^R TS1-2			
H	9.562	7.339	3.055	C	3.418	1.046	-0.057
C	9.200	6.925	0.957	H	3.104	1.523	-0.990
C	9.650	5.330	2.433	H	2.888	1.554	0.756
H	9.941	4.885	3.375	N	5.626	2.025	-0.750
N	9.504	4.700	1.281	H	5.270	2.527	-1.581
C	9.236	5.685	0.360	C	4.902	1.201	0.097
H	9.086	5.453	-0.686	C	6.904	2.078	-0.301
C	5.395	2.211	4.571	H	7.682	2.641	-0.791
H	4.944	2.976	3.930	N	7.054	1.343	0.790
H	5.455	2.650	5.568	C	5.813	0.789	1.042
C	6.793	1.958	4.041	H	5.671	0.152	1.897
O	7.184	0.899	3.542	C	8.390	-4.380	3.982
O	7.552	3.035	4.128	H	8.201	-4.139	5.030
C	10.636	2.860	8.581	H	9.210	-5.100	3.957
H	10.534	3.953	8.594	N	9.864	-3.089	2.397
H	11.706	2.623	8.511	H	10.522	-3.869	2.219
O	9.882	2.258	7.552	C	8.763	-3.138	3.231
H	10.155	2.596	6.678	C	9.976	-1.838	1.904
N	13.239	3.101	3.537	H	10.763	-1.523	1.236
C	10.544	1.964	4.145	N	8.999	-1.068	2.368
O	10.438	2.857	5.008	C	8.241	-1.865	3.206
C	11.573	0.816	4.260	H	7.398	-1.451	3.739
N	12.552	0.838	3.162	C	14.870	-3.851	12.491
C	13.236	1.922	2.914	H	15.784	-4.112	13.034
C	12.195	0.669	5.668	H	14.728	-4.621	11.737
C	12.843	-0.709	5.818	N	15.049	-2.554	11.840
C	13.419	-1.071	7.193	H	15.285	-1.738	12.429
O	13.498	-2.310	7.436	C	14.787	-2.226	10.562
O	13.822	-0.138	7.957	N	14.933	-0.931	10.220
H	12.120	-1.493	5.564	H	14.752	-0.613	9.254
H	13.668	-0.812	5.102	H	15.197	-0.274	10.952
H	12.934	1.453	5.858	N	14.366	-3.091	9.634
H	11.408	0.782	6.419	H	14.221	-2.763	8.666
H	10.971	-0.089	4.090	H	14.382	-4.102	9.783
H	13.905	1.873	2.052	C	15.684	-3.778	0.099
H	13.721	3.927	3.184	H	14.959	-4.251	-0.570
Zn	8.836	0.773	1.833	H	16.312	-4.591	0.484
O	9.749	1.975	3.114	N	14.036	-3.787	1.986
H	8.464	2.810	3.752	C	14.948	-3.089	1.216
O	12.643	4.312	6.099	C	13.575	-2.912	2.868

H	12.855	-3.130	3.647
N	14.121	-1.685	2.701
H	13.908	-0.808	3.213
C	15.002	-1.782	1.651
H	15.587	-0.933	1.331
C	11.939	3.551	-1.806
H	12.851	3.157	-2.261
H	12.223	4.179	-0.955
N	10.601	1.329	-1.911
H	10.675	1.053	-2.910
C	11.085	2.455	-1.257
C	9.956	0.575	-0.988
H	9.493	-0.361	-1.263
N	9.998	1.132	0.219
C	10.707	2.302	0.055
H	10.854	2.978	0.883
C	12.386	7.700	3.178
H	12.942	8.022	4.066
H	11.395	8.162	3.253
C	12.183	6.180	3.267
O	12.534	5.426	2.345
O	11.612	5.805	4.375
H	11.488	4.613	4.621
C	8.896	8.279	0.444
H	9.555	8.345	-0.423
H	9.201	9.049	1.164
N	8.715	6.674	2.397
H	8.366	7.365	3.063
C	9.008	6.926	1.066
C	8.867	5.331	2.604
H	8.656	4.842	3.546
N	9.251	4.717	1.502
C	9.344	5.701	0.546
H	9.640	5.480	-0.470
C	5.428	2.233	4.696
H	4.998	3.041	4.094
H	5.402	2.592	5.725
C	6.908	2.118	4.266
O	7.272	1.129	3.543
O	7.649	3.060	4.639
C	10.659	3.085	8.585
H	10.352	4.139	8.556
H	11.753	3.061	8.680
O	10.206	2.354	7.466

H	10.528	2.801	6.657
N	12.579	2.875	3.138
C	11.806	2.539	4.238
O	11.361	3.469	5.029
C	12.492	1.245	4.772
N	13.413	0.859	3.688
C	13.406	1.828	2.842
C	11.665	0.047	5.267
C	11.944	-0.413	6.711
C	13.335	-0.903	7.133
O	14.123	-0.044	7.664
O	13.588	-2.136	7.035
H	11.278	-1.258	6.903
H	11.657	0.403	7.382
H	11.823	-0.783	4.572
H	10.608	0.308	5.188
H	13.115	1.618	5.601
H	14.009	1.849	1.942
H	12.519	3.796	2.666
Z	8.837	1.007	2.196
O	10.142	1.932	3.403
H	9.509	2.402	3.980

^RIM1-2

C	3.393	1.049	-0.063
H	3.065	1.526	-0.991
H	2.872	1.552	0.758
N	5.587	2.044	-0.771
H	5.225	2.557	-1.594
C	4.877	1.204	0.069
C	6.872	2.080	-0.348
H	7.645	2.650	-0.841
N	7.039	1.317	0.721
C	5.801	0.762	0.985
H	5.670	0.101	1.824
C	8.428	-4.335	3.954
H	8.243	-4.091	5.002
H	9.248	-5.055	3.930
N	9.919	-3.044	2.385
H	10.582	-3.824	2.218
C	8.803	-3.096	3.199
C	10.038	-1.796	1.889
H	10.841	-1.484	1.240

N	9.047	-1.026	2.331	C	8.907	8.191	0.461
C	8.276	-1.825	3.158	H	9.567	8.229	-0.408
H	7.422	-1.415	3.678	H	9.239	8.959	1.171
C	14.880	-3.846	12.487	N	8.707	6.653	2.456
H	15.795	-4.098	13.032	H	8.423	7.381	3.112
H	14.746	-4.619	11.734	C	8.973	6.846	1.111
N	15.048	-2.549	11.834	C	8.814	5.320	2.713
H	15.276	-1.730	12.424	H	8.637	4.888	3.687
C	14.787	-2.225	10.555	N	9.135	4.643	1.627
N	14.931	-0.933	10.206	C	9.241	5.587	0.628
H	14.730	-0.620	9.241	H	9.503	5.313	-0.385
H	15.191	-0.269	10.932	C	5.503	2.233	4.685
N	14.369	-3.095	9.629	H	5.090	3.056	4.091
H	14.230	-2.774	8.658	H	5.469	2.573	5.720
H	14.384	-4.105	9.784	C	6.982	2.103	4.270
C	15.641	-3.704	0.104	O	7.319	1.195	3.437
H	14.905	-4.162	-0.564	O	7.770	2.952	4.759
H	16.246	-4.531	0.496	C	10.658	3.064	8.606
N	14.035	-3.668	2.025	H	10.368	4.123	8.571
C	14.928	-2.986	1.220	H	11.752	3.027	8.694
C	13.596	-2.774	2.901	O	10.188	2.330	7.499
H	12.906	-2.980	3.710	H	10.507	2.773	6.684
N	14.136	-1.549	2.696	N	12.208	2.787	3.031
H	13.931	-0.664	3.209	C	11.398	2.365	4.147
C	14.991	-1.669	1.627	O	11.171	3.361	5.092
H	15.571	-0.828	1.279	C	12.297	1.202	4.755
C	11.971	3.560	-1.837	N	13.350	0.960	3.745
H	12.856	3.136	-2.314	C	13.253	1.926	2.896
H	12.294	4.185	-0.998	C	11.621	-0.099	5.217
N	10.596	1.355	-1.870	C	11.911	-0.504	6.678
H	10.672	1.046	-2.859	C	13.314	-0.951	7.114
C	11.100	2.496	-1.256	O	14.071	-0.078	7.661
C	9.935	0.649	-0.924	O	13.599	-2.179	7.011
H	9.454	-0.288	-1.159	H	11.270	-1.362	6.903
N	9.982	1.257	0.262	H	11.600	0.326	7.319
C	10.714	2.407	0.056	H	11.898	-0.910	4.536
H	10.898	3.103	0.858	H	10.537	0.014	5.123
C	12.440	7.682	3.141	H	12.788	1.670	5.618
H	13.060	7.945	4.007	H	13.944	2.058	2.069
H	11.491	8.215	3.279	H	12.231	3.781	2.699
C	12.119	6.169	3.237	Z	8.789	1.017	2.062
O	12.475	5.387	2.321	O	10.091	1.929	3.658
O	11.486	5.847	4.298	H	9.388	2.384	4.195
H	11.289	4.303	4.716				

^RIM1-2'

C	3.391	1.045	-0.070
H	3.060	1.525	-1.007
H	2.865	1.557	0.756
N	5.585	2.053	-0.765
H	5.221	2.572	-1.589
C	4.874	1.200	0.060
C	6.870	2.081	-0.343
H	7.648	2.663	-0.833
N	7.036	1.300	0.711
C	5.802	0.741	0.970
H	5.668	0.059	1.804
C	8.428	-4.359	3.938
H	8.254	-4.118	4.998
H	9.252	-5.089	3.904
N	9.933	-3.055	2.388
H	10.605	-3.835	2.228
C	8.807	-3.117	3.185
C	10.046	-1.808	1.891
H	10.865	-1.488	1.249
N	9.043	-1.047	2.319
C	8.267	-1.848	3.134
H	7.395	-1.443	3.646
C	14.850	-3.858	12.486
H	15.772	-4.137	13.027
H	14.691	-4.630	11.723
N	15.030	-2.562	11.842
H	15.262	-1.749	12.445
C	14.783	-2.225	10.562
N	14.933	-0.931	10.225
H	14.696	-0.601	9.267
H	15.165	-0.260	10.965
N	14.379	-3.090	9.625
H	14.226	-2.761	8.650
H	14.379	-4.106	9.778
C	15.660	-3.720	0.106
H	14.919	-4.189	-0.565
H	16.275	-4.552	0.500
N	14.068	-3.698	2.043
C	14.941	-3.011	1.226
C	13.625	-2.812	2.920
H	12.942	-3.025	3.746
N	14.145	-1.580	2.707

H	13.923	-0.686	3.211
C	14.990	-1.688	1.632
H	15.561	-0.833	1.274
C	11.951	3.582	-1.823
H	12.859	3.167	-2.290
H	12.255	4.218	-0.973
N	10.597	1.360	-1.879
H	10.679	1.059	-2.876
C	11.088	2.502	-1.258
C	9.938	0.642	-0.942
H	9.461	-0.305	-1.191
N	9.971	1.243	0.246
C	10.689	2.400	0.054
H	10.859	3.102	0.864
C	12.469	7.644	3.072
H	13.057	7.924	3.965
H	11.490	8.153	3.178
C	12.174	6.131	3.154
O	12.331	5.385	2.171
O	11.738	5.762	4.305
H	11.288	4.259	4.707
C	8.907	8.189	0.473
H	9.575	8.219	-0.402
H	9.244	8.966	1.186
N	8.719	6.660	2.483
H	8.457	7.397	3.146
C	8.966	6.846	1.133
C	8.812	5.327	2.743
H	8.632	4.895	3.727
N	9.109	4.645	1.655
C	9.211	5.577	0.652
H	9.462	5.294	-0.371
C	5.513	2.224	4.698
H	5.098	3.071	4.120
H	5.488	2.551	5.748
C	6.988	2.091	4.269
O	7.314	1.203	3.421
O	7.789	2.923	4.759
C	10.661	3.018	8.578
H	10.409	4.098	8.558
H	11.764	2.939	8.638
O	10.137	2.318	7.480
H	10.460	2.743	6.650
N	12.185	2.771	3.026

C	11.358	2.331	4.122	H	10.847	-1.566	1.198
O	11.127	3.319	5.076	N	9.043	-1.107	2.276
C	12.266	1.163	4.712	C	8.268	-1.902	3.104
N	13.294	0.920	3.685	H	7.415	-1.490	3.620
C	13.204	1.890	2.843	C	14.792	-3.917	12.536
C	11.593	-0.134	5.190	H	15.693	-4.245	13.063
C	11.848	-0.511	6.662	H	14.600	-4.659	11.765
C	13.243	-0.939	7.148	N	15.035	-2.616	11.917
O	13.950	-0.065	7.742	H	15.247	-1.812	12.534
O	13.558	-2.152	7.026	C	14.761	-2.250	10.651
H	11.206	-1.382	6.878	N	14.899	-0.947	10.343
H	11.503	0.329	7.286	H	14.658	-0.605	9.399
H	11.896	-0.962	4.526	H	15.106	-0.295	11.097
H	10.502	-0.034	5.063	N	14.346	-3.095	9.703
H	12.783	1.635	5.567	H	14.186	-2.741	8.743
H	13.882	2.016	1.992	H	14.386	-4.108	9.823
H	12.131	3.725	2.603	C	15.815	-3.845	0.072
Z	8.770	0.981	2.032	H	15.172	-4.400	-0.614
O	10.063	1.918	3.624	H	16.465	-4.590	0.546
H	9.343	2.370	4.166	N	14.063	-3.833	1.872
O	14.174	4.529	5.190	C	14.958	-3.137	1.083
H	14.198	3.690	4.704	C	13.454	-2.913	2.605
H	13.298	4.930	4.997	H	12.703	-3.116	3.358
^R TS2-2'				N	13.887	-1.662	2.318
C	3.382	1.045	-0.060	H	13.588	-0.760	2.733
H	3.046	1.530	-0.981	C	14.858	-1.790	1.358
H	2.869	1.543	0.769	H	15.398	-0.931	0.990
N	5.576	2.036	-0.775	C	11.934	3.588	-1.816
H	5.213	2.558	-1.594	H	12.836	3.177	-2.274
C	4.865	1.192	0.060	H	12.233	4.223	-0.976
C	6.866	2.051	-0.368	N	10.610	1.356	-1.870
H	7.640	2.614	-0.865	H	10.697	1.054	-2.861
N	7.034	1.269	0.688	C	11.075	2.508	-1.247
C	5.793	0.726	0.959	C	9.955	0.628	-0.938
H	5.664	0.053	1.789	H	9.503	-0.321	-1.184
C	8.420	-4.407	3.912	N	9.968	1.233	0.251
H	8.256	-4.160	4.961	C	10.671	2.403	0.060
H	9.232	-5.137	3.874	H	10.782	3.122	0.858
N	9.914	-3.122	2.339	C	12.261	8.056	3.057
H	10.573	-3.907	2.178	H	12.616	8.610	3.931
C	8.796	-3.171	3.150	H	11.213	8.349	2.905
C	10.036	-1.878	1.839	C	12.289	6.573	3.432
				O	12.384	5.684	2.560
				O	12.179	6.393	4.702

H	12.499	3.816	5.769	O	13.284	4.288	5.361
C	8.910	8.224	0.458	H	13.063	3.628	4.287
H	9.565	8.259	-0.414	H	12.821	5.223	5.099
H	9.236	9.007	1.154				
N	8.775	6.711	2.483	^R P-2'			
H	8.456	7.438	3.130				
C	9.011	6.892	1.130	C	3.321	1.062	-0.054
C	8.942	5.388	2.760	H	2.960	1.550	-0.963
H	8.791	4.959	3.740	H	2.819	1.542	0.792
N	9.276	4.708	1.678	N	5.508	2.052	-0.810
C	9.325	5.638	0.664	H	5.143	2.587	-1.621
H	9.583	5.360	-0.349	C	4.801	1.215	0.034
C	5.562	2.182	4.688	C	6.807	2.034	-0.438
H	5.140	3.044	4.160	H	7.583	2.580	-0.949
H	5.564	2.466	5.741	N	6.978	1.236	0.605
C	7.029	2.076	4.220	C	5.735	0.719	0.905
O	7.361	1.146	3.404	H	5.610	0.044	1.733
O	7.810	2.959	4.646	C	8.394	-4.418	3.924
C	10.551	2.925	8.674	H	8.221	-4.151	4.968
H	10.315	3.999	8.624	H	9.205	-5.149	3.903
H	11.646	2.829	8.697	N	9.886	-3.154	2.331
O	9.968	2.176	7.640	H	10.558	-3.932	2.193
H	10.371	2.461	6.777	C	8.765	-3.197	3.139
N	12.398	3.025	3.427	C	9.990	-1.925	1.791
C	11.392	2.200	4.441	H	10.804	-1.615	1.153
O	11.126	2.916	5.485	N	8.980	-1.160	2.198
C	12.384	0.979	4.585	C	8.217	-1.940	3.051
N	13.044	0.853	3.273	H	7.359	-1.525	3.560
C	13.023	1.998	2.706	C	14.845	-3.964	12.569
C	11.842	-0.352	5.113	H	15.730	-4.297	13.120
C	11.882	-0.486	6.650	H	14.673	-4.707	11.795
C	13.230	-0.900	7.261	N	15.115	-2.667	11.955
O	13.918	-0.013	7.868	H	15.326	-1.864	12.569
O	13.542	-2.123	7.169	C	14.821	-2.293	10.695
H	11.206	-1.302	6.915	N	14.968	-0.993	10.392
H	11.507	0.425	7.123	H	14.708	-0.645	9.454
H	12.440	-1.165	4.689	H	15.167	-0.347	11.157
H	10.816	-0.494	4.760	N	14.382	-3.131	9.753
H	13.146	1.342	5.290	H	14.223	-2.776	8.793
H	13.456	2.189	1.728	H	14.409	-4.145	9.871
H	12.038	3.844	2.905	C	15.811	-3.841	0.076
Z	8.754	0.910	2.007	H	15.187	-4.417	-0.611
O	10.214	1.877	3.681	H	16.461	-4.568	0.576
H	9.479	2.374	4.130	N	14.046	-3.814	1.862

C	14.924	-3.122	1.053	H	11.674	2.837	8.845
C	13.387	-2.882	2.536	O	9.986	2.246	7.764
H	12.636	-3.077	3.291	H	10.321	2.605	6.923
N	13.773	-1.629	2.197	N	13.073	3.153	2.891
H	13.375	-0.713	2.530	C	11.182	1.839	4.636
C	14.764	-1.768	1.261	O	11.162	2.720	5.495
H	15.283	-0.909	0.861	C	12.415	0.947	4.417
C	11.939	3.611	-1.794	N	12.752	0.812	3.005
H	12.856	3.206	-2.227	C	13.017	1.927	2.378
H	12.211	4.245	-0.943	C	12.180	-0.453	5.025
N	10.607	1.385	-1.913	C	12.053	-0.496	6.563
H	10.711	1.096	-2.906	C	13.322	-0.941	7.301
C	11.067	2.523	-1.257	O	13.971	-0.069	7.964
C	9.926	0.644	-1.013	O	13.610	-2.170	7.229
H	9.474	-0.295	-1.292	H	11.319	-1.265	6.807
N	9.915	1.228	0.187	H	11.688	0.449	6.971
C	10.631	2.399	0.038	H	13.020	-1.083	4.720
H	10.751	3.096	0.855	H	11.284	-0.876	4.558
C	12.439	7.933	2.891	H	13.217	1.435	4.991
H	12.903	8.295	3.815	H	13.192	1.857	1.303
H	11.415	8.331	2.892	H	13.035	4.029	2.340
C	12.345	6.398	3.008	Z	8.646	0.812	1.826
O	12.668	5.680	2.027	O	10.102	1.594	3.898
O	11.919	6.016	4.146	H	9.321	2.171	4.233
H	12.649	3.748	5.830	O	13.400	4.311	5.576
C	8.925	8.174	0.461	H	13.145	3.335	3.891
H	9.578	8.212	-0.413	H	12.934	5.047	5.096
H	9.263	8.945	1.165				
N	8.855	6.665	2.486				
H	8.633	7.403	3.153				
C	9.010	6.833	1.121				
C	8.988	5.339	2.761				
H	8.917	4.933	3.758				
N	9.212	4.639	1.665				
C	9.233	5.564	0.642				
H	9.411	5.270	-0.383				
C	5.576	2.194	4.594				
H	5.171	2.995	3.964				
H	5.559	2.577	5.614				
C	7.044	2.005	4.164				
O	7.328	1.108	3.300				
O	7.891	2.793	4.663				
C	10.584	2.952	8.828				
H	10.353	4.027	8.811				