

Supporting Information

Computational insights into the binding modes, keto-enol tautomerization and stereo-electronically controlled decarboxylation of oxaloacetate in the active site of Macrophomate synthase

Xinyi Li,[†] Fa-Guang Zhang,[‡] Jun-An Ma^{‡,*} and Yongjun Liu^{†,*}

[†] School of Chemistry and Chemical Engineering, Shandong University, Jinan, Shandong 250100, China.

[‡] Department of Chemistry, Tianjin Key Laboratory of Molecular Optoelectronic Sciences, Frontiers Science Center for Synthetic Biology (Ministry of Education), Tianjin University, Tianjin 300072, China.

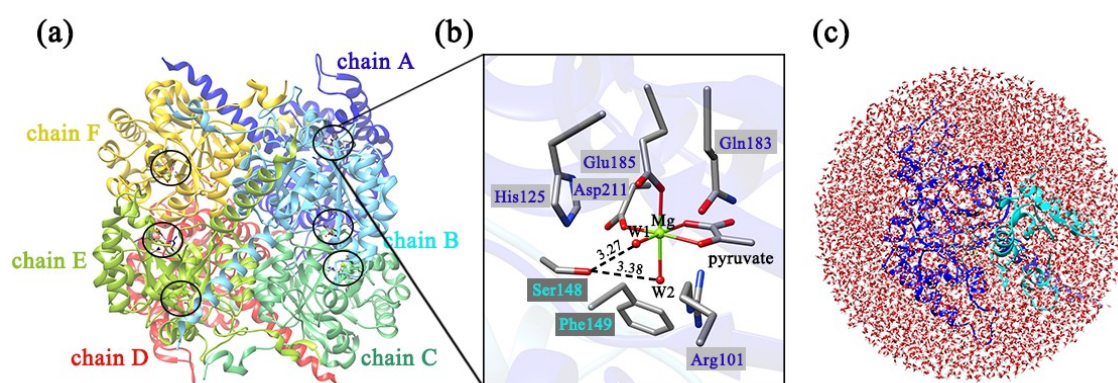


Figure S1. (a) Hexameric crystal structure of MPS (PDB code: 1IZC). (b) Active site of MPS, in which pocket residues His125, Asp211, Glu185, Gln183 and Arg101 are from chain A, while Ser148 and Phe149 are from chain B. (c) Solvated model of pretreatment in this work.

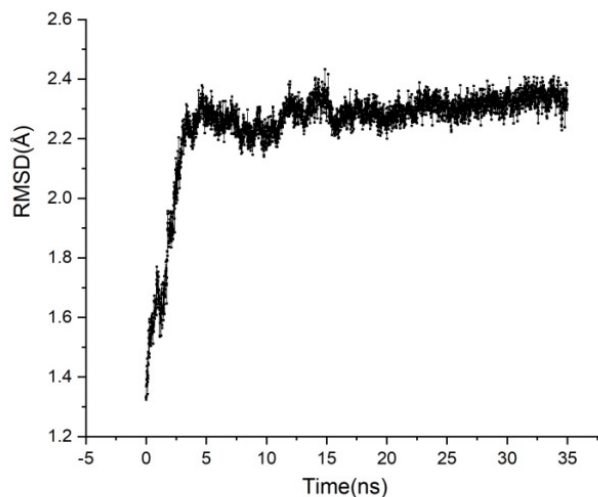


Figure S2. RMSD for the backbone atoms of enzyme-oxaloacetate complex in 35-ns MD simulation.

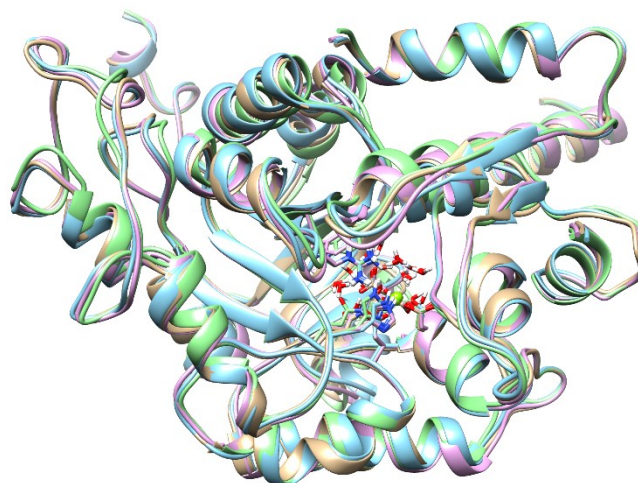


Figure S3. Overlay of four QM/MM-optimized structures which were first derived from snapshots of MD trajectory at 15 (plum), 20 (blue), 25 (tan), 30 (light green) ns and then optimized at B3LYP/B2 level. The structure (shown in blue) at 20 ns is considered to be representative, which was chosen for the QM/MM calculation.

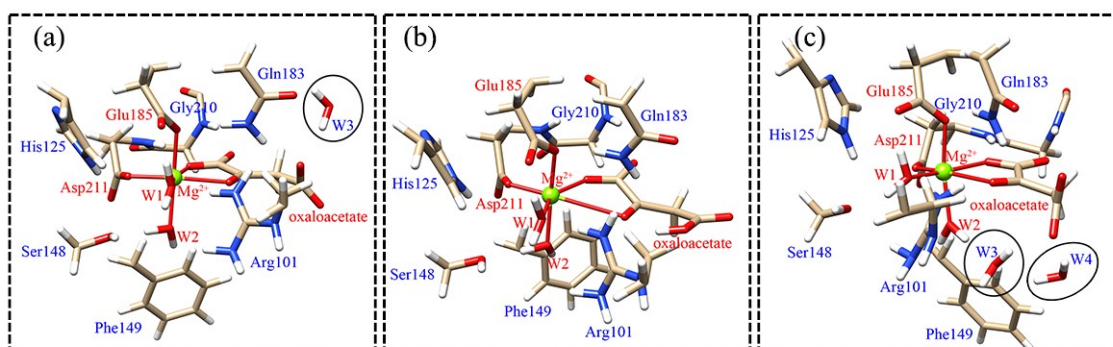


Figure S4. QM regions used for exploring different reactions in this work. (a) QM region for the decarboxylation of the doubly deprotonated oxaloacetate. An additional water

molecule was included in the QM region when the hydration-assisted decarboxylation of OAA was investigated. (b) QM region for the proton migration-assisted decarboxylation of the singly protonated oxaloacetate. (c) QM regions selected for the keto-enol tautomerization of oxaloacetate with the assistance of one or two water molecules.

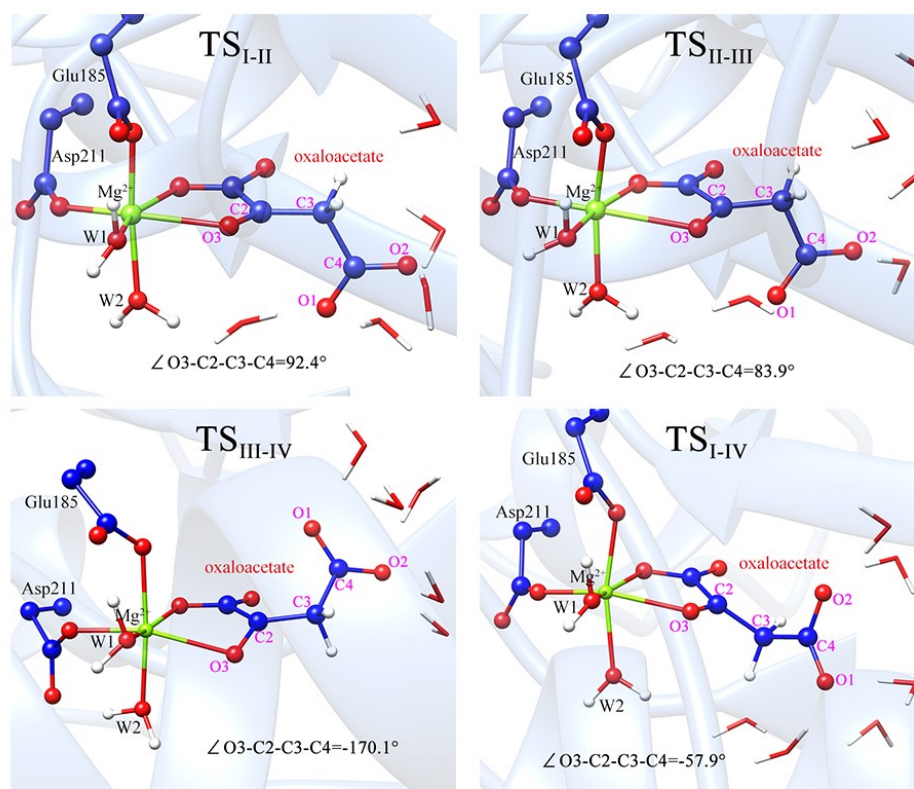


Figure S5. Optimized transition states involved in isomerization of four binding conformations of oxaloacetate from K-I to K-II, K-III and K-IV.

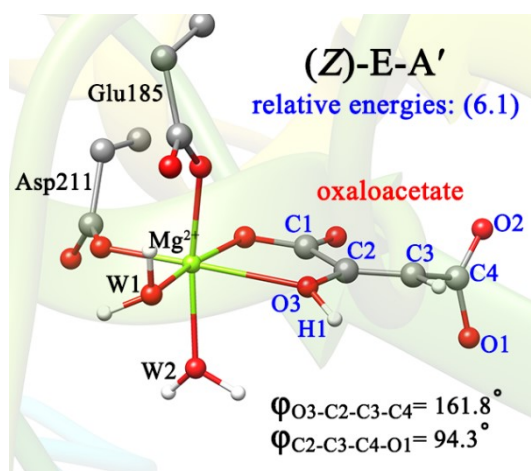


Figure S6. A QM/MM-optimized enolate structure of oxaloacetate binding to the magnesium ion in MPS, which was considered to be dynamically unstable via MD

simulations and easily isomerized into (Z)-E-A. The data in brackets is the QM/MM relative energy when K-I was set to zero in kcal/mol. All distances are present in angstrom.

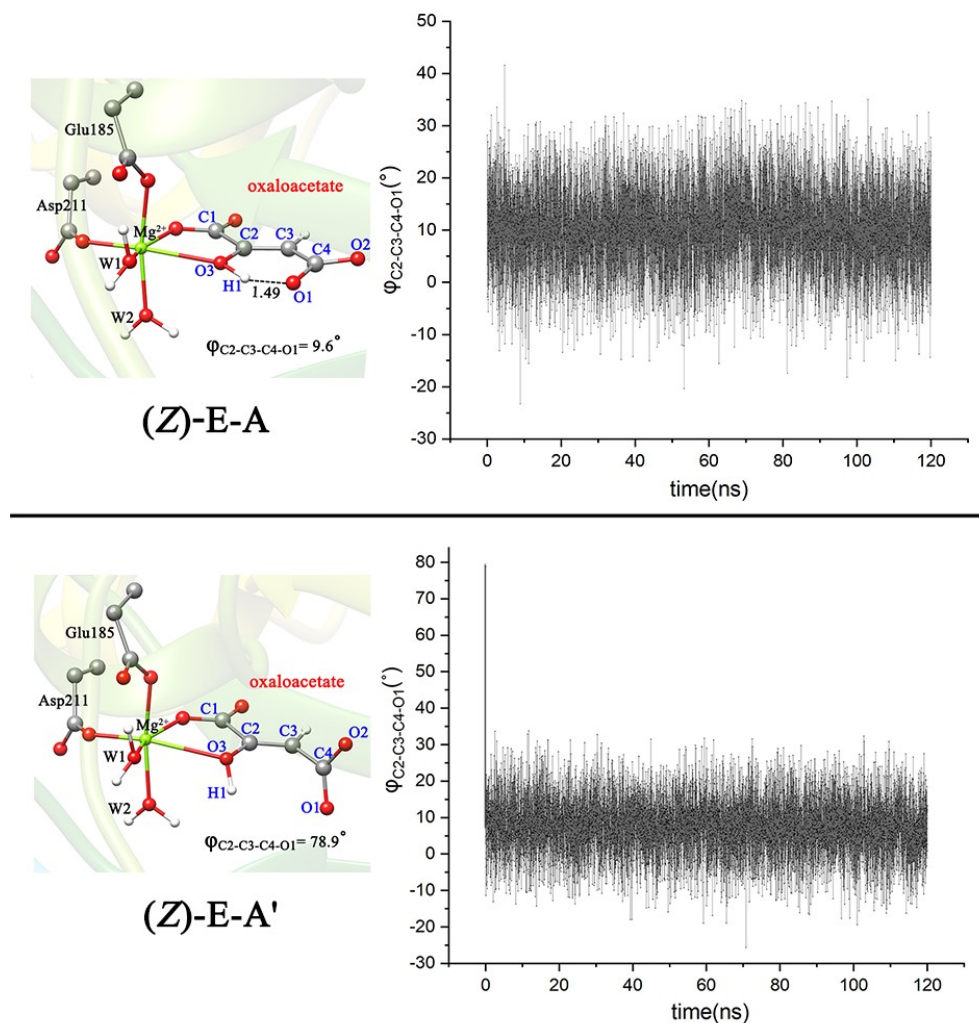


Figure S7. Time evolution of the dihedral of C2-C3-C4-O1 during 120-ns MD simulations of (Z)-E-A (upper panel) and (Z)-E-A' (lower panel). The dihedrals of $\phi_{O3-C2-C3-C4}$ of (Z)-E-A and (Z)-E-A' all fluctuate around 0 degree and those of $\phi_{C2-C3-C4-O1}$ all fluctuate around 10 degrees. This indicates that (Z)-E-A' is unstable in MD simulations and can be easily converted into (Z)-E-A, that is, the carboxylate group tends to be parallel to the plane of C=C bond.

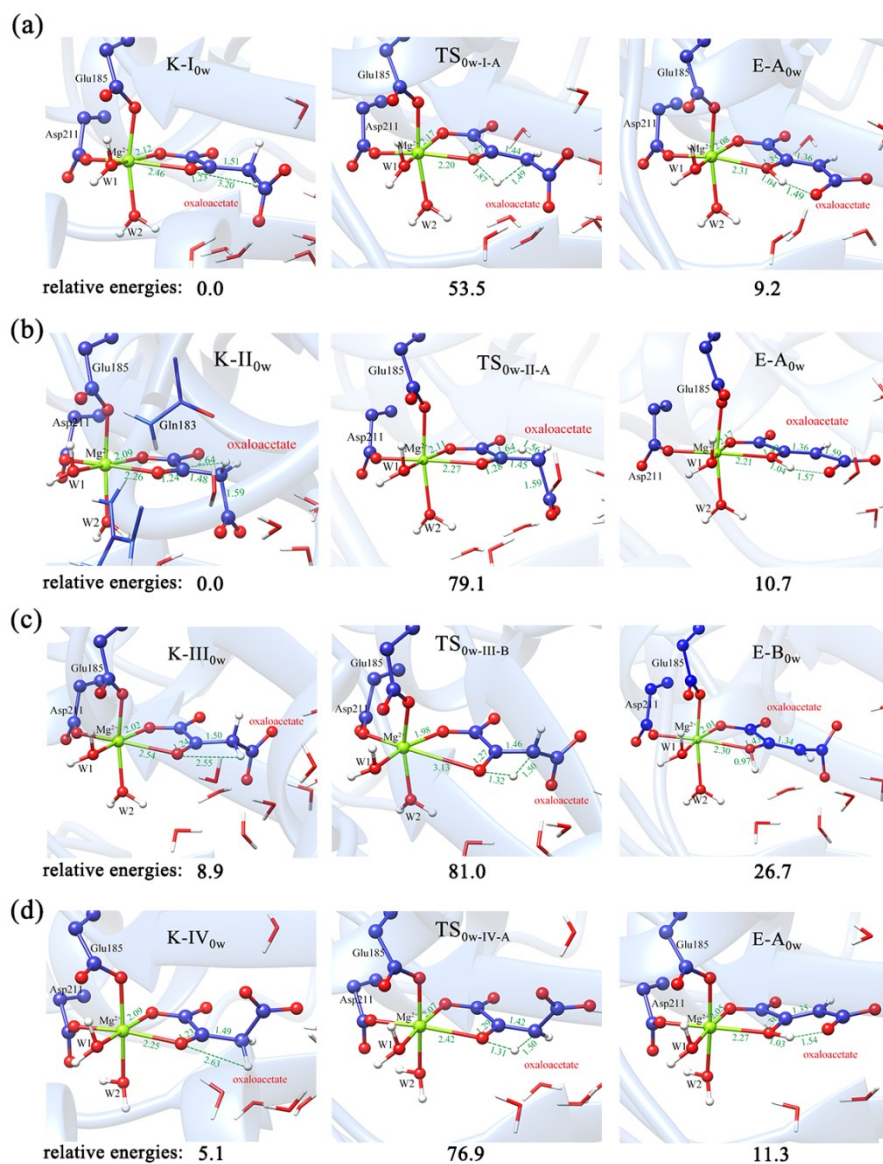


Figure S8. Optimized structures of keto-enol tautomerization without the assistance of water molecule. All distances are given in angstrom and relative energies are in kcal/mol.

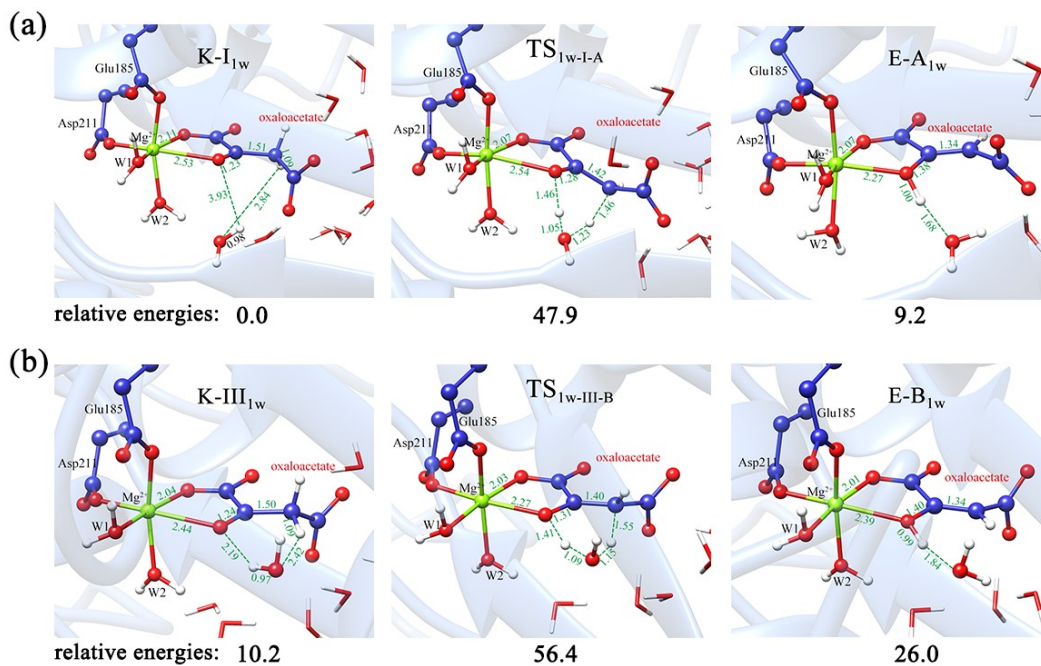


Figure S9. Optimized structures of keto-enol tautomerization of K-I to E-A and K-III to E-B with the assistance of one water molecule. All distances are given in angstrom and relative energies are in kcal/mol.

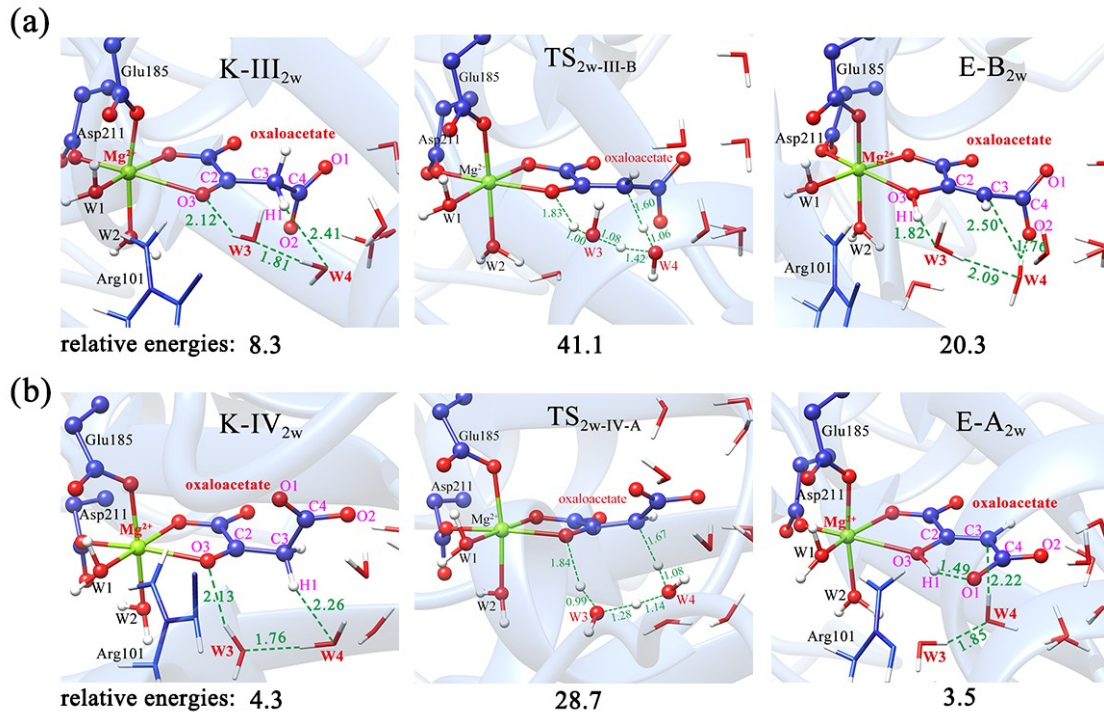


Figure S10. Optimized structures of keto-enol tautomerization of K-III to E-B and K-IV to E-A with the assistance of two water molecules. All distances are given in angstrom and relative energies are in kcal/mol.

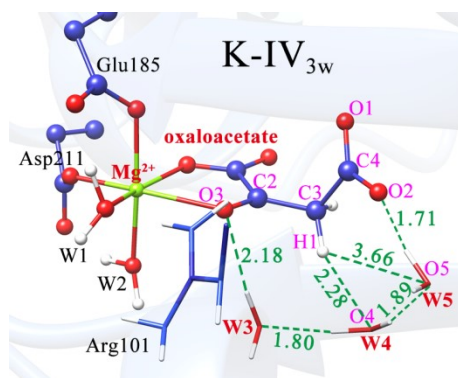


Figure S11. Optimized structures of K-IV in which the QM region contains three mediate water molecules (W3, W4 and W5). All distances are given in angstrom.

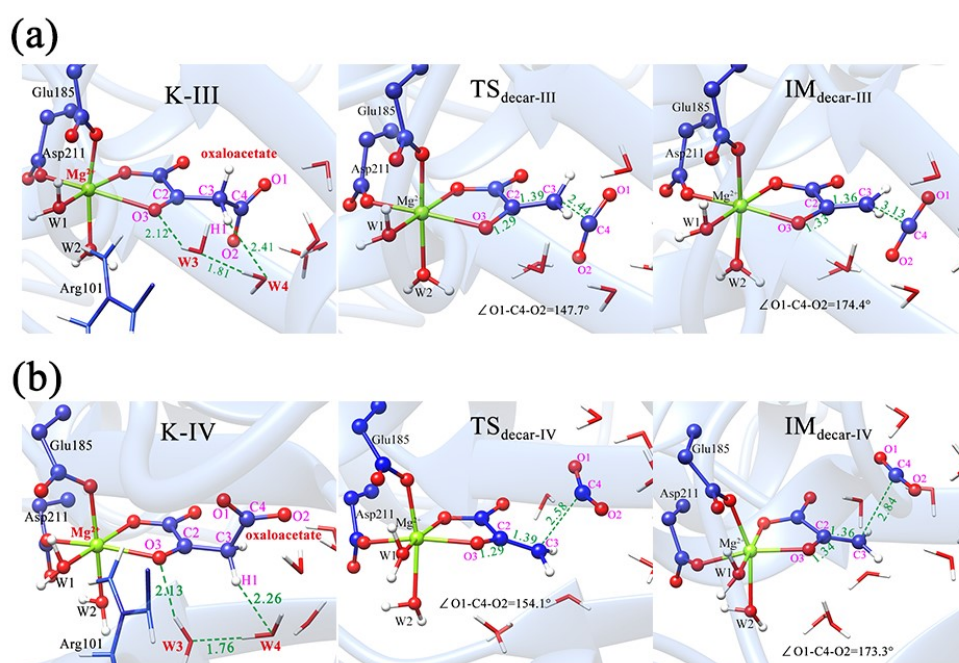


Figure S12. Optimized structures of transition states and intermediates for decarboxylation starting from K-III (a) and K-IV (b). All distances are given in angstrom.

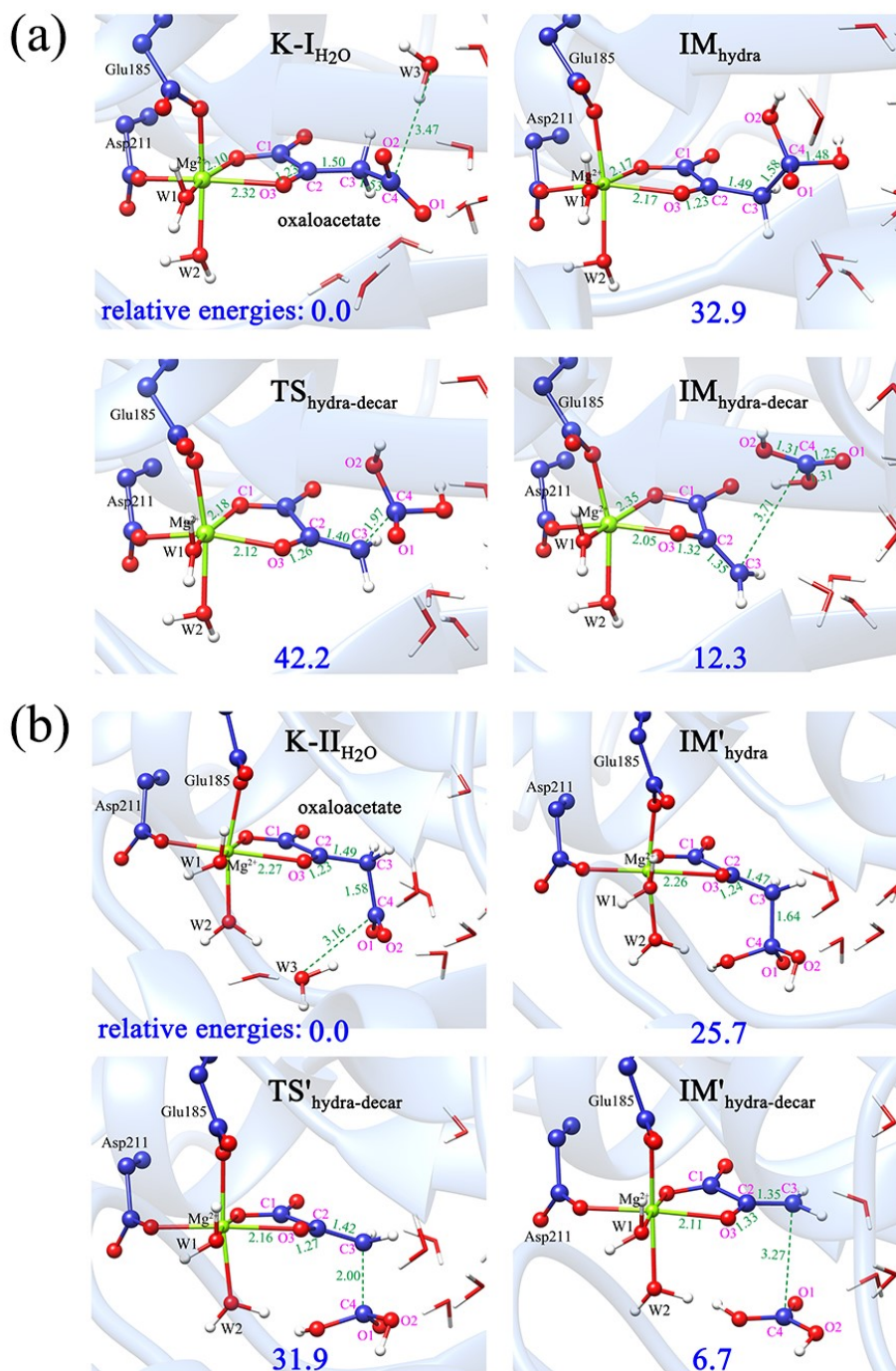


Figure S13. Optimized structures involved in hydration-assisted decarboxylation of oxaloacetate starting from K-I-H₂O (a) and K-II-H₂O (b). All distances are given in angstrom and relative energies are in kcal/mol.

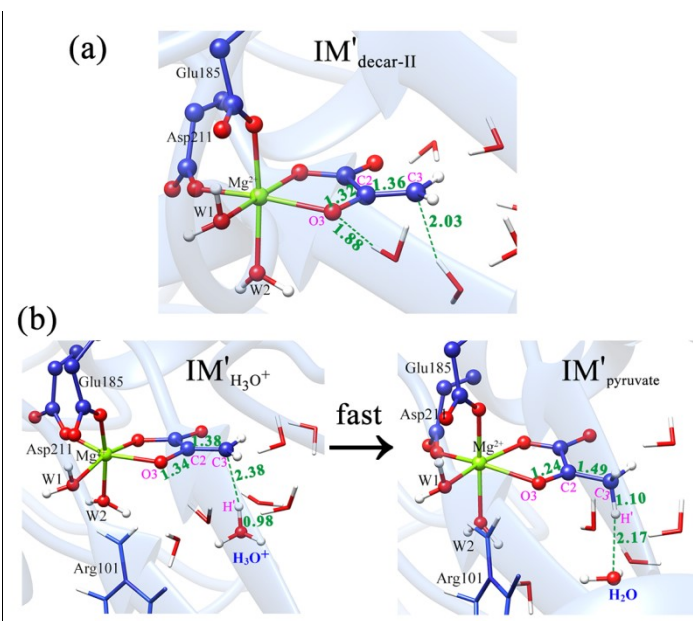


Figure S14. (a) Optimized intermediate structure generated by the decarboxylation of K-II, in which the carbon dioxide has escaped from the active site. (b) Schematic representation of the protonation process of the enolpyruvate intermediate. $IM1'_{H_3O^+}$ represents the model where a hydrated proton comes from bulk solvent to approach the enolpyruvate, and our optimization indicated that this proton immediately transfers to the enolpyruvate to generate the more stable pyruvate (IM'_{pyruvate}). All distances are given in angstrom.

Cartesian coordinates of QM regions of key transition states and intermediates

K-I				H	8.378	5.905	2.537
C	9.718	5.478	0.176	C	6.987	7.522	2.692
H	9.640	6.563	0.333	H	6.306	7.231	1.912
H	9.728	5.304	-0.909	C	2.428	4.184	7.210
O	8.639	4.799	0.809	H	3.363	4.735	7.341
H	7.829	5.098	0.325	H	2.080	3.870	8.201
C	12.520	0.653	2.336	C	2.599	2.923	6.397
H	13.384	1.253	2.643	O	1.631	2.163	6.186
H	11.744	0.833	3.083	N	3.826	2.627	5.938
C	12.882	-0.824	2.268	H	3.923	1.780	5.392
C	14.099	-1.264	1.728	H	4.650	3.220	6.001
H	14.821	-0.533	1.378	C	6.860	5.435	7.816
C	14.379	-2.626	1.615	H	7.803	4.912	7.655
H	15.318	-2.943	1.171	H	6.138	4.679	8.136
C	13.454	-3.578	2.049	C	6.350	6.091	6.532
H	13.662	-4.639	1.932	H	5.423	6.655	6.692
C	11.973	-1.792	2.724	H	7.071	6.813	6.129
H	11.024	-1.456	3.139	C	6.065	5.087	5.408
C	12.253	-3.155	2.619	O	6.513	3.886	5.520
H	11.530	-3.892	2.966	O	5.382	5.479	4.425
C	0.155	2.774	0.447	C	10.064	0.559	10.316
H	0.710	3.342	-0.307	O	11.161	0.714	10.871
H	-0.466	3.496	0.986	N	9.932	0.187	9.033
C	1.116	2.136	1.440	H	9.018	0.117	8.590
H	1.560	2.915	2.065	C	11.100	-0.026	8.191
H	0.604	1.455	2.128	H	10.769	-0.565	7.298
N	2.227	1.457	0.749	H	11.848	-0.620	8.719
H	2.100	1.199	-0.244	C	11.783	1.290	7.798
C	3.495	1.750	1.054	O	12.969	1.505	8.025
N	3.815	2.133	2.280	N	10.938	2.220	7.259
H	4.742	2.524	2.496	H	10.003	1.934	6.979
H	3.218	1.792	3.042	C	11.369	3.551	6.825
N	4.443	1.625	0.075	H	12.314	3.464	6.280
H	5.137	2.411	0.083	C	10.311	4.194	5.927
H	3.996	1.530	-0.844	H	9.313	4.134	6.369
C	5.982	9.692	3.728	H	10.532	5.258	5.783
H	5.503	9.935	2.776	C	10.267	3.592	4.508
H	6.482	10.586	4.108	O	11.317	3.166	3.997
N	8.089	8.493	4.394	O	9.134	3.628	3.911
C	6.984	8.583	3.566	Mg	7.464	2.683	4.096
C	8.726	7.389	4.037	C	7.564	0.472	6.154
H	9.639	7.022	4.478	O	5.766	0.879	4.615
N	8.097	6.769	3.004	O	7.895	-0.259	7.114

C	6.213	0.122	5.468	C	1.335	2.337	1.428
O	8.154	1.480	5.691	H	1.762	3.198	1.951
C	5.524	-1.132	5.948	H	0.926	1.683	2.206
H	6.263	-1.937	5.869	N	2.418	1.666	0.704
H	5.319	-1.006	7.017	H	2.209	1.266	-0.226
C	4.252	-1.508	5.190	C	3.707	1.991	0.837
O	4.390	-2.042	4.048	N	4.167	2.642	1.896
O	3.137	-1.285	5.743	H	5.126	3.005	1.946
O	6.138	3.622	2.738	H	3.565	2.831	2.684
H	5.754	4.416	3.238	N	4.573	1.611	-0.149
H	6.229	3.834	1.780	H	5.252	2.393	-0.340
O	7.826	1.214	2.658	H	4.053	1.342	-0.997
H	8.637	1.098	2.128	C	6.038	9.698	3.785
H	7.263	0.426	2.483	H	5.610	9.840	2.791
O	6.302	-1.037	2.186	H	6.473	10.641	4.124
H	5.965	-1.118	1.262	N	8.155	8.730	4.698
H	5.520	-1.164	2.763	C	7.106	8.639	3.798
O	6.926	-3.232	3.715	C	8.866	7.629	4.550
H	7.046	-2.626	2.961	H	9.762	7.379	5.094
H	6.006	-3.008	3.960	N	8.349	6.831	3.578
K-II				H	8.674	5.886	3.382
C	9.489	5.441	0.320	C	7.222	7.466	3.086
H	9.342	6.478	0.649	H	6.628	7.045	2.292
H	9.557	5.450	-0.774	C	2.467	4.026	6.956
O	8.389	4.620	0.728	H	3.340	4.651	7.172
H	7.669	4.838	0.083	H	2.117	3.582	7.890
C	12.588	0.676	2.343	C	2.871	2.881	6.042
H	13.399	1.352	2.632	O	2.493	1.716	6.265
H	11.828	0.764	3.124	N	3.671	3.162	4.985
C	13.087	-0.758	2.226	H	4.200	2.364	4.638
C	14.246	-1.072	1.503	H	4.157	4.066	4.906
H	14.830	-0.274	1.060	C	6.877	5.558	7.982
C	14.642	-2.397	1.328	H	7.822	5.038	7.833
H	15.531	-2.614	0.745	H	6.150	4.804	8.297
C	13.888	-3.437	1.874	C	6.371	6.204	6.691
H	14.178	-4.470	1.700	H	5.414	6.722	6.823
C	12.367	-1.809	2.813	H	7.074	6.956	6.312
H	11.485	-1.585	3.406	C	6.172	5.177	5.579
C	12.758	-3.138	2.636	O	6.827	4.095	5.621
H	12.171	-3.936	3.084	O	5.333	5.458	4.653
C	0.267	2.861	0.470	C	10.035	0.626	10.383
H	0.747	3.450	-0.318	O	11.126	0.765	10.953
H	-0.379	3.552	1.022	N	9.913	0.265	9.095
				H	9.003	0.209	8.643

C	11.082	0.032	8.259	C	14.224	-1.086	1.474
H	10.745	-0.500	7.364	H	14.771	-0.293	0.978
H	11.817	-0.575	8.790	C	14.626	-2.409	1.308
C	11.788	1.337	7.872	H	15.485	-2.630	0.682
O	12.970	1.545	8.135	C	13.916	-3.445	1.917
N	10.969	2.276	7.304	H	14.208	-4.479	1.749
H	10.056	1.988	6.957	C	12.432	-1.812	2.904
C	11.443	3.594	6.879	H	11.588	-1.583	3.550
H	12.397	3.485	6.355	C	12.827	-3.141	2.734
C	10.424	4.284	5.969	H	12.276	-3.934	3.234
H	9.418	4.277	6.398	C	0.277	2.747	0.531
H	10.699	5.337	5.825	H	0.752	3.384	-0.224
C	10.361	3.692	4.551	H	-0.358	3.403	1.134
O	11.357	3.136	4.066	C	1.354	2.142	1.434
O	9.249	3.863	3.916	H	1.742	2.939	2.074
Mg	7.614	2.807	4.208	H	0.969	1.371	2.108
C	7.643	0.661	6.199	N	2.464	1.606	0.648
O	5.944	1.356	4.670	H	2.262	1.216	-0.289
O	7.884	-0.092	7.164	C	3.740	1.967	0.785
C	6.240	0.533	5.545	N	4.190	2.633	1.840
O	8.365	1.578	5.717	H	5.144	3.013	1.882
C	5.332	-0.549	6.001	H	3.571	2.861	2.601
H	5.682	-0.953	6.949	N	4.621	1.600	-0.193
H	4.313	-0.162	6.077	H	5.289	2.392	-0.382
C	5.333	-1.703	4.908	H	4.121	1.307	-1.043
O	6.108	-2.654	5.098	C	6.040	9.689	3.786
O	4.542	-1.508	3.941	H	5.611	9.844	2.793
O	6.532	3.916	2.779	H	6.482	10.626	4.132
H	6.082	4.646	3.286	N	8.150	8.693	4.687
H	7.155	4.282	2.110	C	7.101	8.623	3.784
O	7.930	1.436	2.649	C	8.856	7.592	4.522
H	8.760	1.224	2.184	H	9.751	7.328	5.060
H	7.329	0.677	2.478	N	8.335	6.814	3.535
				H	8.659	5.876	3.313
K-III				C	7.212	7.462	3.052
C	9.493	5.420	0.333	H	6.615	7.055	2.252
H	9.343	6.459	0.656	C	2.406	4.006	6.886
H	9.560	5.424	-0.761	H	3.278	4.619	7.137
O	8.393	4.599	0.744	H	2.050	3.516	7.794
H	7.671	4.814	0.099	C	2.810	2.915	5.913
C	12.597	0.664	2.372	O	2.371	1.754	6.025
H	13.406	1.346	2.657	N	3.671	3.237	4.920
H	11.841	0.748	3.157	H	4.188	2.453	4.539
C	13.105	-0.767	2.255	H	4.172	4.136	4.888

C	6.882	5.486	7.988	H	6.121	4.585	3.290
H	7.828	4.958	7.864	H	7.197	4.211	2.125
H	6.144	4.743	8.299	O	7.863	1.288	2.675
C	6.407	6.126	6.683	H	8.684	1.079	2.190
H	5.463	6.670	6.800	H	7.299	0.487	2.605
H	7.130	6.859	6.305	O	3.057	0.210	3.801
C	6.188	5.104	5.571	H	2.755	0.684	4.610
O	6.776	3.984	5.623	H	4.020	0.349	3.799
O	5.388	5.432	4.625				
C	10.082	0.596	10.422	K-IV			
O	11.196	0.784	10.932	C	9.509	5.470	0.320
N	9.912	0.158	9.165	H	9.363	6.508	0.643
H	8.987	0.072	8.747	H	9.571	5.469	-0.775
C	11.055	-0.065	8.292	O	8.418	4.646	0.745
H	10.691	-0.592	7.406	H	7.672	4.899	0.139
H	11.810	-0.674	8.794	C	12.438	0.641	2.345
C	11.752	1.244	7.893	H	13.263	1.278	2.685
O	12.945	1.443	8.104	H	11.645	0.734	3.092
N	10.919	2.197	7.364	C	12.887	-0.810	2.236
H	9.993	1.918	7.049	C	14.129	-1.154	1.685
C	11.399	3.506	6.920	H	14.804	-0.370	1.358
H	12.350	3.383	6.392	C	14.497	-2.491	1.538
C	10.381	4.190	6.003	H	15.455	-2.734	1.088
H	9.371	4.162	6.420	C	13.637	-3.511	1.950
H	10.638	5.249	5.869	H	13.915	-4.552	1.808
C	10.348	3.609	4.579	C	12.043	-1.843	2.670
O	11.365	3.089	4.098	H	11.077	-1.588	3.102
O	9.239	3.754	3.931	C	12.413	-3.181	2.532
Mg	7.611	2.703	4.213	H	11.741	-3.968	2.868
C	7.571	0.581	6.266	C	0.255	2.862	0.587
O	5.825	1.018	4.677	H	0.787	3.427	-0.186
O	7.847	-0.100	7.264	H	-0.395	3.579	1.102
C	6.165	0.330	5.647	C	1.260	2.315	1.603
O	8.257	1.485	5.703	H	1.694	3.156	2.149
C	5.247	-0.648	6.327	H	0.790	1.682	2.365
H	4.844	-0.141	7.212	N	2.356	1.601	0.929
H	4.409	-0.880	5.668	H	2.144	1.205	0.003
C	5.901	-1.977	6.787	C	3.631	2.018	1.001
O	5.835	-2.287	7.994	N	4.112	2.674	2.043
O	6.405	-2.694	5.867	H	5.083	3.014	2.046
O	2.989	-2.471	4.536	H	3.618	2.745	2.930
H	3.810	-2.813	4.125	N	4.457	1.715	-0.044
H	2.936	-1.549	4.199	H	5.124	2.508	-0.238
O	6.558	3.846	2.781	H	3.901	1.452	-0.875

C	6.042	9.826	3.771	C	10.130	3.814	4.757
H	5.637	10.008	2.773	O	10.948	3.115	4.105
H	6.466	10.755	4.158	O	8.939	4.064	4.369
N	8.151	8.816	4.672	Mg	7.476	2.689	4.364
C	7.104	8.764	3.765	C	7.598	0.486	6.275
C	8.834	7.699	4.511	O	6.193	0.824	4.374
H	9.717	7.413	5.057	O	7.852	-0.290	7.222
N	8.304	6.936	3.516	C	6.479	0.045	5.289
H	8.564	5.972	3.334	O	8.124	1.605	6.021
C	7.196	7.604	3.033	C	5.805	-1.264	5.533
H	6.578	7.195	2.251	H	5.656	-1.816	4.598
C	2.221	4.098	6.549	H	6.412	-1.878	6.195
H	3.182	4.604	6.673	C	4.394	-1.124	6.173
H	1.942	3.667	7.519	O	3.893	-2.167	6.669
C	2.302	2.920	5.587	O	3.829	-0.001	6.104
O	1.306	2.253	5.290	O	6.585	3.704	2.766
N	3.542	2.613	5.092	H	6.116	4.477	3.229
H	3.704	1.611	4.978	H	7.234	4.066	2.123
H	4.363	3.098	5.451	O	8.817	1.559	3.175
C	6.781	5.489	7.795	H	9.677	2.017	3.321
H	7.724	4.967	7.632	H	8.904	1.070	2.333
H	6.068	4.734	8.133	O	6.146	-1.118	2.182
C	6.239	6.105	6.506	H	5.928	-1.069	1.223
H	5.290	6.634	6.666	H	5.876	-0.276	2.576
H	6.924	6.850	6.086	O	4.849	-3.321	3.114
C	5.980	5.077	5.399	H	3.964	-3.124	3.478
O	6.276	3.843	5.603	H	5.195	-2.494	2.715
O	5.477	5.494	4.320				
C	10.012	0.677	10.360	TS_{I-II}			
O	11.113	0.852	10.903	C	9.737	5.417	0.167
N	9.871	0.284	9.085	H	9.660	6.503	0.321
H	8.951	0.173	8.659	H	9.743	5.241	-0.918
C	11.026	0.042	8.238	O	8.658	4.743	0.804
H	10.678	-0.492	7.349	H	7.847	5.035	0.318
H	11.766	-0.570	8.758	C	12.647	0.603	2.277
C	11.747	1.330	7.833	H	13.526	1.194	2.555
O	12.957	1.468	7.977	H	11.895	0.797	3.045
N	10.934	2.331	7.366	C	12.987	-0.879	2.216
H	9.958	2.130	7.158	C	14.206	-1.341	1.701
C	11.481	3.622	6.955	H	14.947	-0.625	1.360
H	12.429	3.451	6.438	C	14.465	-2.709	1.602
C	10.523	4.444	6.092	H	15.407	-3.045	1.178
H	9.596	4.687	6.619	C	13.518	-3.643	2.026
H	10.998	5.401	5.837	H	13.713	-4.707	1.924

C	12.053	-1.829	2.660	C	6.254	5.081	5.469
H	11.095	-1.481	3.042	O	6.959	4.030	5.438
C	12.311	-3.197	2.568	O	5.325	5.335	4.627
H	11.563	-3.913	2.901	C	10.089	0.528	10.226
C	0.221	2.707	0.460	O	11.185	0.701	10.777
H	0.766	3.280	-0.297	N	9.957	0.153	8.944
H	-0.387	3.427	1.019	H	9.043	0.080	8.500
C	1.198	2.050	1.428	C	11.130	-0.050	8.104
H	1.658	2.818	2.056	H	10.800	-0.567	7.198
H	0.692	1.366	2.118	H	11.871	-0.660	8.624
N	2.292	1.370	0.713	C	11.819	1.274	7.752
H	2.151	1.131	-0.284	O	12.997	1.494	8.018
C	3.569	1.637	1.010	N	10.983	2.208	7.205
N	3.902	1.999	2.240	H	10.073	1.910	6.861
H	4.840	2.352	2.455	C	11.437	3.534	6.782
H	3.318	1.640	3.004	H	12.404	3.437	6.279
N	4.514	1.503	0.032	C	10.426	4.170	5.827
H	5.215	2.280	0.055	H	9.405	4.134	6.218
H	4.077	1.417	-0.891	H	10.670	5.228	5.670
C	5.961	9.615	3.741	C	10.454	3.533	4.422
H	5.456	9.845	2.800	O	11.530	3.091	3.982
H	6.474	10.514	4.094	O	9.360	3.548	3.756
N	8.083	8.423	4.369	Mg	7.638	2.702	4.012
C	6.959	8.504	3.567	C	7.597	0.505	6.044
C	8.718	7.322	4.001	O	5.877	1.194	4.538
H	9.639	6.957	4.427	O	7.833	-0.234	7.026
N	8.069	6.692	2.986	C	6.180	0.383	5.415
H	8.360	5.840	2.502	O	8.320	1.405	5.541
C	6.946	7.437	2.697	C	5.221	-0.626	5.973
H	6.257	7.148	1.923	H	5.489	-0.816	7.015
C	2.414	4.052	7.222	H	4.205	-0.221	5.939
H	3.282	4.691	7.410	C	5.203	-2.032	5.291
H	2.073	3.640	8.174	O	5.986	-2.285	4.345
C	2.804	2.886	6.340	O	4.350	-2.815	5.786
O	2.288	1.759	6.490	O	6.195	3.620	2.733
N	3.733	3.114	5.401	H	5.782	4.368	3.252
H	4.116	2.312	4.914	H	6.213	3.831	1.768
H	4.175	4.020	5.219	O	7.923	1.363	2.445
C	6.958	5.429	7.883	H	8.768	1.143	2.005
H	7.909	4.914	7.747	H	7.339	0.580	2.315
H	6.228	4.669	8.174				
C	6.487	6.097	6.588	TS_{II-III}			
H	5.549	6.648	6.720	C	9.493	5.420	0.343
H	7.222	6.823	6.218	H	9.344	6.461	0.659

H	9.553	5.415	-0.752	H	3.279	4.584	7.162
O	8.397	4.602	0.769	H	2.065	3.486	7.849
H	7.670	4.815	0.130	C	2.814	2.854	5.972
C	12.634	0.682	2.368	O	2.410	1.687	6.118
H	13.443	1.365	2.653	N	3.646	3.169	4.949
H	11.876	0.765	3.151	H	4.145	2.370	4.569
C	13.142	-0.748	2.248	H	4.156	4.062	4.904
C	14.282	-1.061	1.495	C	6.900	5.450	8.015
H	14.849	-0.263	1.031	H	7.851	4.933	7.885
C	14.677	-2.384	1.313	H	6.173	4.698	8.330
H	15.550	-2.600	0.706	C	6.409	6.088	6.716
C	13.942	-3.426	1.881	H	5.466	6.631	6.842
H	14.230	-4.459	1.701	H	7.126	6.821	6.328
C	12.443	-1.800	2.858	C	6.178	5.065	5.608
H	11.579	-1.577	3.478	O	6.768	3.944	5.661
C	12.833	-3.128	2.673	O	5.375	5.395	4.668
H	12.260	-3.928	3.137	C	10.106	0.550	10.341
C	0.271	2.803	0.489	O	11.206	0.741	10.876
H	0.748	3.415	-0.284	N	9.968	0.141	9.069
H	-0.366	3.479	1.070	H	9.052	0.052	8.634
C	1.344	2.234	1.416	C	11.133	-0.065	8.220
H	1.751	3.062	2.003	H	10.796	-0.590	7.322
H	0.940	1.518	2.140	H	11.882	-0.668	8.736
N	2.439	1.630	0.658	C	11.819	1.256	7.845
H	2.236	1.244	-0.281	O	13.006	1.466	8.069
C	3.724	1.950	0.811	N	10.976	2.202	7.324
N	4.174	2.599	1.877	H	10.055	1.914	7.003
H	5.132	2.963	1.931	C	11.435	3.526	6.903
H	3.552	2.833	2.635	H	12.383	3.426	6.366
N	4.609	1.567	-0.156	C	10.402	4.213	6.009
H	5.286	2.352	-0.339	H	9.398	4.189	6.443
H	4.114	1.280	-1.011	H	10.660	5.271	5.874
C	6.034	9.661	3.800	C	10.342	3.634	4.586
H	5.598	9.813	2.810	O	11.350	3.114	4.086
H	6.480	10.599	4.139	O	9.219	3.779	3.966
N	8.143	8.659	4.696	Mg	7.604	2.694	4.236
C	7.093	8.593	3.795	C	7.579	0.485	6.223
C	8.846	7.557	4.526	O	5.770	0.984	4.707
H	9.742	7.290	5.063	O	7.917	-0.293	7.138
N	8.323	6.782	3.538	C	6.129	0.326	5.690
H	8.644	5.844	3.313	O	8.249	1.427	5.710
C	7.200	7.434	3.060	C	5.229	-0.638	6.415
H	6.602	7.031	2.259	H	5.556	-0.800	7.439
C	2.410	3.962	6.928	H	4.198	-0.269	6.403

C	5.255	-2.008	5.672	H	3.971	1.529	-0.941
O	4.824	-2.980	6.330	C	6.049	9.853	3.769
O	5.731	-2.029	4.511	H	5.649	10.046	2.772
O	6.535	3.829	2.815	H	6.471	10.778	4.169
H	6.093	4.566	3.322	N	8.157	8.829	4.662
H	7.166	4.192	2.153	C	7.111	8.791	3.754
O	7.951	1.385	2.662	C	8.837	7.713	4.489
H	8.795	1.179	2.220	H	9.720	7.417	5.033
H	7.381	0.593	2.519	N	8.307	6.964	3.484
				H	8.561	6.003	3.287
TS_{III-IV}				C	7.200	7.639	3.008
C	9.555	5.527	0.276	H	6.581	7.240	2.224
H	9.410	6.563	0.611	C	2.246	4.058	6.567
H	9.620	5.539	-0.819	H	3.209	4.561	6.682
O	8.461	4.702	0.689	H	1.965	3.653	7.548
H	7.717	4.958	0.083	C	2.328	2.856	5.638
C	12.469	0.683	2.294	O	1.330	2.200	5.311
H	13.314	1.300	2.621	N	3.572	2.508	5.202
H	11.685	0.805	3.046	H	3.671	1.533	4.954
C	12.875	-0.782	2.205	H	4.419	2.963	5.548
C	14.101	-1.174	1.652	C	6.748	5.473	7.711
H	14.795	-0.418	1.300	H	7.692	4.953	7.543
C	14.432	-2.525	1.536	H	6.039	4.717	8.055
H	15.379	-2.806	1.086	C	6.199	6.082	6.421
C	13.547	-3.510	1.980	H	5.240	6.594	6.584
H	13.795	-4.561	1.864	H	6.871	6.840	6.006
C	12.005	-1.781	2.670	C	5.957	5.057	5.301
H	11.052	-1.487	3.105	O	6.235	3.819	5.499
C	12.337	-3.132	2.562	O	5.490	5.490	4.212
H	11.647	-3.892	2.923	C	9.919	0.598	10.096
C	0.273	2.882	0.578	O	11.079	0.747	10.509
H	0.777	3.468	-0.198	N	9.628	0.246	8.832
H	-0.373	3.579	1.122	H	8.665	0.132	8.517
C	1.314	2.330	1.555	C	10.691	-0.008	7.874
H	1.736	3.170	2.114	H	10.227	-0.401	6.965
H	0.875	1.664	2.306	H	11.401	-0.742	8.261
N	2.412	1.667	0.841	C	11.516	1.240	7.544
H	2.201	1.288	-0.095	O	12.740	1.226	7.550
C	3.688	2.064	0.935	N	10.782	2.371	7.279
N	4.163	2.700	1.996	H	9.776	2.285	7.158
H	5.140	3.022	2.020	C	11.450	3.619	6.933
H	3.642	2.779	2.860	H	12.391	3.369	6.437
N	4.523	1.784	-0.108	C	10.607	4.556	6.065
H	5.175	2.592	-0.291	H	9.704	4.900	6.577

H	11.198	5.448	5.817	C	0.187	2.766	0.471
C	10.176	3.939	4.740	H	0.741	3.333	-0.285
O	11.002	3.297	4.036	H	-0.435	3.490	1.007
O	8.955	4.117	4.423	C	1.151	2.136	1.469
Mg	7.573	2.684	4.285	H	1.598	2.922	2.084
C	7.164	0.534	6.183	H	0.640	1.463	2.166
O	6.533	0.626	3.920	N	2.259	1.448	0.782
O	7.310	-0.340	7.056	H	2.127	1.181	-0.207
C	6.157	0.223	5.028	C	3.530	1.745	1.075
O	7.841	1.590	6.010	N	3.866	2.131	2.297
C	5.096	-0.838	5.136	H	4.794	2.528	2.502
H	4.274	-0.601	4.454	H	3.279	1.799	3.069
H	5.569	-1.738	4.711	N	4.467	1.618	0.085
C	4.525	-1.110	6.532	H	5.164	2.403	0.088
O	4.135	-2.279	6.822	H	4.007	1.527	-0.828
O	4.330	-0.065	7.194	C	5.987	9.694	3.725
O	6.659	3.699	2.702	H	5.509	9.940	2.774
H	6.174	4.470	3.152	H	6.488	10.586	4.108
H	7.287	4.064	2.041	N	8.090	8.487	4.392
O	9.011	1.693	3.148	C	6.987	8.584	3.561
H	9.849	2.203	3.260	C	8.725	7.383	4.033
H	9.086	1.175	2.323	H	9.635	7.010	4.476
				N	8.098	6.768	2.995
TS_{I-IV}				H	8.378	5.906	2.526
C	9.738	5.443	0.177	C	6.990	7.525	2.682
H	9.661	6.529	0.330	H	6.309	7.239	1.901
H	9.750	5.265	-0.907	C	2.471	4.118	7.221
O	8.656	4.769	0.810	H	3.402	4.679	7.342
H	7.848	5.069	0.323	H	2.124	3.833	8.221
C	12.570	0.619	2.329	C	2.666	2.823	6.463
H	13.449	1.201	2.626	O	1.708	2.054	6.251
H	11.804	0.820	3.082	N	3.912	2.508	6.067
C	12.898	-0.867	2.273	H	4.025	1.607	5.620
C	14.088	-1.344	1.706	H	4.725	3.120	6.098
H	14.817	-0.637	1.324	C	6.842	5.455	7.817
C	14.333	-2.715	1.608	H	7.784	4.935	7.645
H	15.252	-3.062	1.145	H	6.125	4.695	8.140
C	13.398	-3.637	2.080	C	6.318	6.115	6.540
H	13.577	-4.704	1.975	H	5.382	6.664	6.707
C	11.980	-1.806	2.771	H	7.027	6.851	6.141
H	11.055	-1.443	3.217	C	6.050	5.113	5.412
C	12.224	-3.177	2.678	O	6.510	3.918	5.532
H	11.497	-3.891	3.060				
O	5.379	5.497	4.418	C	10.061	0.627	10.404

O	11.174	0.762	10.931	H	11.819	0.849	3.072
N	9.891	0.259	9.124	C	12.931	-0.826	2.259
H	8.962	0.204	8.707	C	14.143	-1.286	1.724
C	11.036	0.013	8.259	H	14.876	-0.567	1.372
H	10.673	-0.520	7.375	C	14.403	-2.652	1.615
H	11.778	-0.600	8.773	H	15.338	-2.985	1.173
C	11.750	1.306	7.845	C	13.464	-3.589	2.050
O	12.947	1.484	8.050	H	13.657	-4.653	1.937
N	10.927	2.257	7.310	C	12.008	-1.780	2.715
H	9.972	2.009	7.057	H	11.060	-1.424	3.117
C	11.406	3.564	6.858	C	12.268	-3.148	2.616
H	12.358	3.436	6.335	H	11.533	-3.872	2.962
C	10.388	4.230	5.931	C	0.099	2.890	0.279
H	9.385	4.235	6.366	H	0.662	3.429	-0.490
H	10.667	5.276	5.756	H	-0.529	3.630	0.784
C	10.323	3.590	4.530	C	1.033	2.288	1.312
O	11.362	3.139	4.017	H	1.442	3.090	1.932
O	9.183	3.622	3.945	H	0.507	1.619	1.999
Mg	7.502	2.712	4.158	N	2.171	1.602	0.685
C	7.535	0.620	6.340	H	2.090	1.300	-0.302
O	6.115	0.992	4.455	C	3.425	1.845	1.067
O	7.740	-0.133	7.319	N	3.691	2.294	2.286
C	6.379	0.223	5.378	H	4.626	2.654	2.530
O	8.180	1.628	5.956	H	2.976	2.186	3.007
C	6.013	-1.227	5.321	N	4.433	1.601	0.168
H	6.637	-1.679	4.546	H	5.147	2.367	0.168
H	6.304	-1.678	6.274	H	4.043	1.479	-0.772
C	4.525	-1.546	5.127	C	5.989	9.692	3.728
O	4.218	-2.365	4.208	H	5.504	9.933	2.778
O	3.713	-0.957	5.891	H	6.487	10.589	4.105
O	6.188	3.631	2.748	N	8.103	8.500	4.387
H	5.789	4.423	3.238	C	6.995	8.588	3.562
H	6.291	3.843	1.792	C	8.740	7.397	4.029
O	7.985	1.227	2.680	H	9.652	7.029	4.471
H	8.787	1.125	2.131	N	8.111	6.776	2.997
H	7.416	0.460	2.475	H	8.388	5.909	2.533
				C	6.998	7.526	2.687
E-A				H	6.314	7.231	1.912
C	9.727	5.460	0.178	C	2.555	4.141	7.378
O	8.654	4.786	0.825	H	3.463	4.745	7.460
H	9.648	6.546	0.325				
C	12.587	0.655	2.318				
H	9.730	5.276	-0.905				
H	13.460	1.247	2.612				

H	2.217	3.888	8.388	H	11.797	-0.671	8.623
C	2.785	2.834	6.658	C	11.748	1.262	7.751
O	1.916	1.942	6.669	O	12.941	1.454	7.965
N	3.938	2.669	5.994	N	10.910	2.215	7.242
H	4.057	1.801	5.494	H	9.968	1.946	6.967
H	4.727	3.309	5.977	C	11.366	3.539	6.818
C	6.875	5.434	7.826	H	12.314	3.436	6.281
H	7.813	4.898	7.682	C	10.329	4.201	5.910
H	6.137	4.687	8.134	H	9.327	4.172	6.347
C	6.398	6.097	6.533	H	10.581	5.257	5.755
H	5.471	6.667	6.675	C	10.277	3.580	4.499
H	7.132	6.815	6.148	O	11.327	3.152	3.987
C	6.129	5.096	5.402	O	9.140	3.603	3.913
O	6.583	3.899	5.512	Mg	7.481	2.619	4.081
O	5.443	5.487	4.419	C	7.457	0.431	6.195
C	10.069	0.535	10.273	O	5.843	0.866	4.471
O	11.182	0.677	10.800	O	7.806	-0.304	7.151
N	9.901	0.164	8.994	C	6.113	0.121	5.549
H	8.976	0.100	8.568	O	8.083	1.414	5.711
C	11.049	-0.051	8.126	C	5.236	-0.808	6.029
H	10.688	-0.559	7.227	H	6.384	-2.261	4.798
H	5.478	-1.341	6.941	C	12.611	0.692	2.347
C	3.914	-0.981	5.390	H	13.425	1.370	2.625
O	3.731	-0.364	4.280	H	11.857	0.790	3.132
O	3.026	-1.709	5.930	C	13.107	-0.743	2.243
O	6.123	3.590	2.753	C	14.207	-1.084	1.444
H	5.792	4.410	3.254	H	14.748	-0.304	0.923
H	6.220	3.797	1.793	C	14.597	-2.413	1.293
O	7.925	1.225	2.623	H	15.442	-2.650	0.655
H	8.740	1.122	2.098	C	13.892	-3.433	1.933
H	7.386	0.412	2.458	H	14.171	-4.472	1.773
O	6.416	-0.943	2.196	C	12.441	-1.773	2.925
H	5.997	-1.137	1.331	H	11.618	-1.525	3.591
H	4.967	0.439	4.093	C	12.822	-3.107	2.768
O	6.822	-2.855	4.161	H	12.278	-3.889	3.293
H	6.507	-1.779	2.684	C	0.287	2.701	0.590
H	6.491	-3.750	4.377	H	0.784	3.334	-0.153
				H	-0.352	3.364	1.183
E-B				C	1.339	2.078	1.514
C	9.495	5.437	0.306	H	1.724	2.863	2.169
H	9.349	6.478	0.624	H	0.920	1.311	2.174
H	9.562	5.435	-0.788	N	2.459	1.525	0.754
O	8.394	4.622	0.724	H	2.258	1.126	-0.177
H	7.669	4.843	0.084	C	3.721	1.957	0.851

N	4.165	2.668	1.876	H	9.998	1.901	6.956
H	5.115	3.062	1.899	C	11.401	3.495	6.878
H	3.591	2.820	2.692	H	12.352	3.375	6.349
N	4.586	1.613	-0.147	C	10.387	4.198	5.971
H	5.249	2.408	-0.342	H	9.376	4.169	6.387
H	4.072	1.316	-0.988	H	10.650	5.258	5.852
C	6.049	9.698	3.777	C	10.350	3.642	4.537
H	5.614	9.847	2.786	O	11.363	3.112	4.055
H	6.489	10.639	4.116	O	9.248	3.817	3.887
N	8.158	8.706	4.681	Mg	7.620	2.748	4.193
C	7.114	8.635	3.775	C	7.729	0.456	6.053
C	8.864	7.604	4.519	O	5.873	1.199	4.653
H	9.756	7.339	5.063	O	8.189	-0.389	6.842
N	8.349	6.826	3.529	C	6.296	0.276	5.612
H	8.669	5.883	3.319	O	8.317	1.503	5.617
C	7.228	7.475	3.042	C	5.464	-0.646	6.108
H	6.632	7.066	2.244	H	4.422	-0.601	5.817
C	2.343	3.972	6.924	H	4.441	-2.716	5.140
H	3.204	4.557	7.261	C	5.838	-1.913	6.833
H	1.925	3.445	7.784	O	5.907	-1.998	8.066
C	2.816	2.926	5.932	O	5.944	-2.921	6.027
O	2.421	1.745	5.996	O	3.555	-2.699	4.686
N	3.703	3.310	4.982	H	3.755	-3.119	3.837
H	4.356	2.584	4.707	H	3.387	-0.725	4.022
H	4.133	4.243	4.981	O	6.536	3.888	2.774
C	6.908	5.503	7.982	H	6.112	4.629	3.293
H	7.861	4.994	7.837	H	7.171	4.249	2.113
H	6.189	4.734	8.278	O	7.907	1.372	2.611
C	6.415	6.169	6.698	H	8.737	1.160	2.144
H	5.457	6.686	6.829	H	7.358	0.560	2.544
H	7.118	6.930	6.338	O	3.402	0.232	3.835
C	6.221	5.169	5.562	H	2.939	0.662	4.589
O	6.837	4.066	5.594	H	5.101	0.803	4.172
O	5.412	5.498	4.622				
C	10.063	0.577	10.301				
O	11.179	0.789	10.799	K-IV_{1W}			
N	9.897	0.105	9.057	C	9.510	5.474	0.318
H	8.980	-0.029	8.636	H	9.363	6.513	0.641
C	11.048	-0.099	8.187	H	9.574	5.474	-0.777
H	10.680	-0.601	7.289	O	8.418	4.651	0.741
H	11.801	-0.715	8.682	H	7.675	4.898	0.131
C	11.744	1.221	7.820	C	12.439	0.645	2.351
O	12.937	1.415	8.039	H	13.265	1.281	2.688
N	10.914	2.182	7.304				

H	11.648	0.739	3.099	H	8.578	5.986	3.340
C	12.886	-0.807	2.241	C	7.204	7.614	3.033
C	14.127	-1.151	1.689	H	6.589	7.203	2.250
H	14.802	-0.369	1.360	C	2.218	4.108	6.553
C	14.494	-2.489	1.541	H	3.178	4.613	6.685
H	15.451	-2.733	1.089	H	1.933	3.670	7.518
C	13.634	-3.508	1.953	C	2.303	2.938	5.583
H	13.910	-4.550	1.811	O	1.309	2.267	5.284
C	12.041	-1.839	2.676	N	3.542	2.642	5.079
H	11.077	-1.584	3.110	H	3.709	1.642	4.959
C	12.410	-3.178	2.537	H	4.362	3.129	5.439
H	11.738	-3.964	2.874	C	6.779	5.507	7.799
C	0.265	2.874	0.585	H	7.721	4.985	7.631
H	0.790	3.439	-0.193	H	6.065	4.751	8.132
H	-0.383	3.589	1.102	C	6.236	6.135	6.516
C	1.280	2.335	1.596	H	5.286	6.661	6.680
H	1.717	3.183	2.131	H	6.920	6.883	6.101
H	0.819	1.709	2.367	C	5.978	5.113	5.403
N	2.373	1.619	0.919	O	6.286	3.880	5.600
H	2.159	1.221	-0.006	O	5.465	5.530	4.329
C	3.651	2.023	0.995	C	10.005	0.674	10.353
N	4.133	2.682	2.035	O	11.107	0.842	10.895
H	5.104	3.023	2.038	N	9.860	0.286	9.076
H	3.634	2.767	2.917	H	8.939	0.181	8.652
N	4.479	1.705	-0.045	C	11.014	0.044	8.228
H	5.147	2.498	-0.243	H	10.663	-0.482	7.335
H	3.925	1.442	-0.876	H	11.751	-0.576	8.743
C	6.041	9.833	3.769	C	11.742	1.331	7.832
H	5.635	10.010	2.771	O	12.952	1.464	7.980
H	6.462	10.764	4.153	N	10.934	2.337	7.367
N	8.151	8.829	4.674	H	9.958	2.141	7.155
C	7.106	8.774	3.764	C	11.487	3.627	6.961
C	8.837	7.714	4.515	H	12.436	3.454	6.445
H	9.720	7.430	5.063	C	10.532	4.454	6.099
N	8.313	6.950	3.519	H	9.602	4.691	6.623

H	11.006	5.414	5.853	C	12.881	-0.794	2.250
C	10.148	3.834	4.758	C	14.111	-1.151	1.681
O	10.962	3.126	4.113	H	14.785	-0.375	1.334
O	8.964	4.100	4.358	C	14.469	-2.492	1.539
Mg	7.490	2.743	4.361	H	15.417	-2.746	1.075
C	7.601	0.536	6.262	C	13.609	-3.503	1.974
O	6.206	0.934	4.364	H	13.878	-4.547	1.837
O	7.829	-0.260	7.199	C	12.038	-1.819	2.707
C	6.488	0.132	5.259	H	11.083	-1.553	3.158
O	8.146	1.651	6.028	C	12.397	-3.161	2.575
C	5.810	-1.186	5.433	H	11.727	-3.940	2.931
H	5.621	-1.596	4.438	C	0.289	2.890	0.576
H	6.440	-1.873	5.993	H	0.802	3.452	-0.212
C	4.428	-1.084	6.144	H	-0.356	3.605	1.097
O	3.972	-2.136	6.660	C	1.321	2.367	1.579
O	3.838	0.027	6.090	H	1.764	3.225	2.092
O	6.595	3.752	2.764	H	0.876	1.751	2.369
H	6.117	4.519	3.223	N	2.406	1.645	0.896
H	7.241	4.115	2.118	H	2.196	1.246	-0.033
O	8.826	1.584	3.184	C	3.692	1.999	0.999
H	9.690	2.035	3.332	N	4.172	2.660	2.039
H	8.911	1.100	2.339	H	5.138	3.018	2.044
O	5.991	-1.158	2.230	H	3.648	2.791	2.902
H	5.819	-1.143	1.261	N	4.544	1.619	-0.010
H	5.810	-0.264	2.551	H	5.199	2.417	-0.230
				H	4.005	1.333	-0.843
TS_{1W-IV-A}				C	6.043	9.849	3.769
C	9.514	5.484	0.321	H	5.637	10.022	2.770
H	9.365	6.522	0.644	H	6.460	10.783	4.152
H	9.576	5.484	-0.774	N	8.157	8.859	4.679
O	8.426	4.657	0.747	C	7.114	8.795	3.769
H	7.679	4.904	0.139	C	8.848	7.746	4.527
C	12.442	0.660	2.355	H	9.731	7.468	5.079
H	13.270	1.293	2.694	N	8.328	6.974	3.535
H	11.649	0.761	3.102	H	8.594	6.007	3.369

C	7.217	7.631	3.044	C	10.151	3.841	4.749
H	6.603	7.213	2.264	O	10.963	3.129	4.104
C	2.192	4.099	6.559	O	8.976	4.130	4.337
H	3.157	4.590	6.708	Mg	7.476	2.790	4.391
H	1.889	3.656	7.516	C	7.802	0.509	6.154
C	2.274	2.938	5.576	O	6.138	1.107	4.534
O	1.277	2.277	5.265	O	8.207	-0.347	6.969
N	3.515	2.638	5.080	C	6.518	0.192	5.359
H	3.678	1.634	4.954	O	8.283	1.664	5.952
H	4.330	3.128	5.444	C	5.849	-1.042	5.527
C	6.787	5.547	7.804	H	5.521	-1.113	4.004
H	7.731	5.035	7.621	H	6.432	-1.784	6.060
H	6.080	4.782	8.130	C	4.383	-1.093	5.904
C	6.230	6.189	6.534	O	3.962	-2.139	6.477
H	5.276	6.705	6.708	O	3.658	-0.088	5.642
H	6.906	6.948	6.123	O	6.589	3.796	2.780
C	5.979	5.170	5.419	H	6.109	4.563	3.238
O	6.304	3.945	5.617	H	7.243	4.156	2.143
O	5.460	5.580	4.344	O	8.791	1.626	3.127
C	10.040	0.655	10.331	H	9.654	2.062	3.317
O	11.118	0.836	10.916	H	8.908	1.175	2.269
N	9.950	0.262	9.052	O	5.080	-0.544	3.111
H	9.053	0.138	8.588	H	5.492	-0.689	2.219
C	11.133	0.045	8.236	H	5.395	0.374	3.539
H	10.814	-0.494	7.340				
H	11.874	-0.548	8.777	E-A_{1W}			
C	11.827	1.353	7.849	C	9.502	5.485	0.335
O	13.026	1.533	8.044	H	9.357	6.521	0.668
N	11.000	2.323	7.347	H	9.562	5.494	-0.760
H	10.046	2.084	7.080	O	8.410	4.659	0.755
C	11.512	3.632	6.948	H	7.664	4.919	0.153
H	12.463	3.497	6.425	C	12.394	0.632	2.328
C	10.526	4.440	6.102	H	13.226	1.259	2.670
H	9.591	4.638	6.635	H	11.603	0.734	3.076
H	10.965	5.421	5.870	C	12.826	-0.825	2.223

C	14.053	-1.189	1.654	H	6.580	7.185	2.265
H	14.727	-0.418	1.296	C	2.179	4.056	6.635
C	14.410	-2.532	1.528	H	3.158	4.520	6.775
H	15.357	-2.792	1.066	H	1.858	3.651	7.602
C	13.550	-3.536	1.977	C	2.221	2.868	5.683
H	13.819	-4.583	1.854	O	1.201	2.249	5.364
C	11.982	-1.842	2.693	N	3.450	2.497	5.221
H	11.030	-1.570	3.145	H	3.530	1.522	4.932
C	12.339	-3.186	2.575	H	4.304	2.940	5.556
H	11.670	-3.962	2.942	C	6.783	5.486	7.803
C	0.242	2.894	0.589	H	7.728	4.972	7.631
H	0.770	3.458	-0.187	H	6.076	4.729	8.148
H	-0.410	3.609	1.102	C	6.222	6.096	6.519
C	1.252	2.357	1.605	H	5.270	6.617	6.689
H	1.690	3.208	2.133	H	6.896	6.844	6.090
H	0.789	1.736	2.380	C	5.959	5.063	5.416
N	2.344	1.636	0.930	O	6.261	3.829	5.617
H	2.132	1.240	0.005	O	5.456	5.481	4.337
C	3.622	2.034	1.014	C	10.075	0.646	10.427
N	4.092	2.696	2.059	O	11.140	0.818	11.037
H	5.068	3.020	2.079	N	10.005	0.266	9.144
H	3.574	2.774	2.928	H	9.114	0.150	8.667
N	4.452	1.730	-0.024	C	11.193	0.050	8.335
H	5.122	2.521	-0.215	H	10.885	-0.518	7.453
H	3.902	1.465	-0.858	H	11.944	-0.515	8.891
C	6.039	9.819	3.782	C	11.862	1.360	7.916
H	5.631	9.997	2.785	O	13.052	1.577	8.130
H	6.463	10.749	4.166	N	11.021	2.297	7.373
N	8.148	8.812	4.685	H	10.081	2.026	7.088
C	7.102	8.757	3.777	C	11.503	3.615	6.958
C	8.832	7.696	4.526	H	12.453	3.497	6.428
H	9.716	7.412	5.073	C	10.492	4.393	6.114
N	8.304	6.930	3.533	H	9.555	4.566	6.652
H	8.567	5.966	3.355	H	10.902	5.384	5.878
C	7.195	7.595	3.048	C	10.118	3.785	4.762

O	10.932	3.075	4.117	H	14.830	-0.513	1.447
O	8.941	4.069	4.353	C	14.397	-2.611	1.649
Mg	7.467	2.701	4.366	H	15.347	-2.916	1.221
C	7.801	0.475	6.263	C	13.470	-3.574	2.050
O	6.129	0.865	4.585	H	13.687	-4.631	1.926
O	8.292	-0.316	7.097	C	11.958	-1.808	2.708
C	6.469	0.103	5.657	H	10.992	-1.477	3.089
O	8.274	1.600	5.913	C	12.252	-3.167	2.596
C	5.668	-0.837	6.203	H	11.527	-3.915	2.914
H	6.761	-0.624	2.415	C	0.140	2.812	0.453
H	6.045	-1.401	7.046	H	0.699	3.371	-0.305
C	4.281	-1.054	5.760	H	-0.485	3.540	0.979
O	3.540	-1.853	6.422	C	1.095	2.187	1.459
O	3.870	-0.384	4.748	H	1.539	2.974	2.075
O	6.569	3.709	2.779	H	0.579	1.517	2.155
H	6.098	4.481	3.245	N	2.204	1.496	0.781
H	7.215	4.069	2.134	H	2.092	1.240	-0.213
O	8.780	1.564	3.117	C	3.471	1.751	1.120
H	9.643	1.989	3.336	N	3.776	2.118	2.354
H	8.897	1.177	2.228	H	4.718	2.461	2.589
O	5.819	-0.785	2.283	H	3.152	1.800	3.103
H	5.722	-0.922	1.315	N	4.440	1.598	0.160
H	5.267	0.478	4.242	H	5.132	2.386	0.155
				H	4.012	1.477	-0.765
TS_{2W-1A}				C	5.987	9.727	3.732
C	9.699	5.455	0.205	H	5.519	9.965	2.774
H	9.615	6.537	0.372	H	6.474	10.625	4.121
H	9.697	5.288	-0.881	N	8.097	8.551	4.428
O	8.641	4.758	0.852	C	6.999	8.625	3.590
H	7.818	5.057	0.390	C	8.728	7.434	4.107
C	12.491	0.645	2.350	H	9.629	7.067	4.571
H	13.338	1.253	2.685	N	8.107	6.794	3.082
H	11.689	0.801	3.077	H	8.360	5.894	2.678
C	12.872	-0.828	2.286	C	7.003	7.542	2.742
C	14.105	-1.252	1.772	H	6.322	7.230	1.970

C	2.436	4.149	7.185	O	8.811	3.958	4.356
H	3.381	4.690	7.283	Mg	7.355	2.573	4.233
H	2.101	3.880	8.194	C	7.381	0.473	6.234
C	2.578	2.843	6.435	O	6.112	0.810	4.196
O	1.578	2.119	6.237	O	7.623	-0.264	7.225
N	3.803	2.473	6.039	C	6.201	0.099	5.310
H	3.889	1.577	5.574	O	8.028	1.508	5.898
H	4.644	3.057	6.062	C	5.369	-0.890	5.756
C	6.788	5.418	7.787	H	6.829	-2.394	4.545
H	7.720	4.878	7.616	H	5.550	-1.219	6.775
H	6.063	4.671	8.123	C	4.146	-1.457	5.128
C	6.263	6.060	6.502	O	4.234	-2.123	4.020
H	5.340	6.631	6.671	O	3.035	-1.339	5.712
H	6.978	6.772	6.076	O	6.145	3.523	2.748
C	5.952	5.041	5.396	H	5.775	4.337	3.234
O	6.258	3.807	5.580	H	6.253	3.742	1.794
O	5.390	5.462	4.350	O	8.747	1.638	2.951
C	10.030	0.596	10.199	H	9.578	2.148	3.093
O	11.172	0.736	10.663	H	8.900	1.036	2.199
N	9.785	0.228	8.933	O	6.807	-0.726	2.334
H	8.835	0.161	8.556	H	6.244	-0.807	1.524
C	10.873	-0.013	8.002	H	6.435	-0.019	3.002
H	10.439	-0.476	7.111	O	6.547	-2.721	3.671
H	11.617	-0.685	8.437	H	6.757	-1.736	2.925
C	11.625	1.266	7.620	H	5.414	-2.489	3.790
O	12.845	1.352	7.716				
N	10.827	2.311	7.234	TS_{decar-I}			
H	9.847	2.132	7.013	C	9.751	5.330	0.304
C	11.409	3.592	6.837	H	9.624	6.394	0.543
H	12.349	3.397	6.312	H	9.765	5.235	-0.791
C	10.470	4.445	5.980	O	8.706	4.554	0.881
H	9.564	4.732	6.521	H	7.881	4.875	0.434
H	10.987	5.374	5.706	C	12.514	0.541	2.440
C	10.030	3.795	4.663	H	13.393	1.132	2.721
O	10.868	3.166	3.958	H	11.749	0.746	3.195
				C	12.845	-0.945	2.397
				C	13.981	-1.434	1.733
				H	14.673	-0.735	1.272

C	14.213	-2.806	1.636	H	6.050	4.825	8.165
H	15.087	-3.164	1.099	C	6.289	6.244	6.571
C	13.317	-3.717	2.201	H	5.380	6.836	6.734
H	13.484	-4.786	2.093	H	7.033	6.941	6.166
C	11.976	-1.871	2.993	C	5.968	5.237	5.463
H	11.104	-1.506	3.532	O	6.440	4.049	5.570
C	12.204	-3.244	2.896	O	5.230	5.601	4.509
H	11.506	-3.940	3.356	C	10.012	0.619	10.315
C	0.127	2.851	0.335	O	11.127	0.737	10.847
H	0.715	3.365	-0.432	N	9.837	0.288	9.028
H	-0.502	3.612	0.809	H	8.912	0.256	8.589
C	1.029	2.260	1.406	C	10.981	0.059	8.158
H	1.454	3.073	2.002	H	10.617	-0.459	7.266
H	0.464	1.640	2.109	H	11.726	-0.557	8.665
N	2.150	1.506	0.824	C	11.687	1.362	7.771
H	2.078	1.229	-0.171	O	12.884	1.545	7.985
C	3.412	1.759	1.201	N	10.859	2.321	7.258
N	3.687	2.173	2.426	H	9.913	2.065	6.967
H	4.620	2.534	2.680	C	11.332	3.644	6.854
H	2.961	2.127	3.138	H	12.270	3.541	6.300
N	4.408	1.546	0.283	C	10.287	4.366	6.001
H	5.097	2.335	0.276	H	9.304	4.362	6.477
H	3.995	1.436	-0.649	H	10.572	5.417	5.867
C	5.979	9.741	3.702	C	10.130	3.813	4.572
H	5.525	9.899	2.721	O	11.103	3.292	3.998
H	6.430	10.677	4.041	O	8.974	3.997	4.040
N	8.131	8.741	4.510	Mg	7.378	2.764	4.182
C	7.036	8.671	3.666	C	7.555	0.629	6.158
C	8.812	7.624	4.323	O	6.123	1.107	4.293
H	9.725	7.353	4.827	O	7.766	-0.084	7.171
N	8.229	6.842	3.376	C	6.461	0.210	5.154
H	8.508	5.887	3.154	O	8.187	1.683	5.828
C	7.094	7.498	2.948	C	5.996	-1.089	5.213
H	6.438	7.075	2.208	H	5.691	-1.548	4.283
C	2.690	4.081	7.297	H	6.347	-1.742	6.000
H	3.583	4.712	7.320	C	3.369	-1.685	4.430
H	2.377	3.892	8.329	O	3.633	-2.485	3.599
C	2.956	2.719	6.688	O	2.721	-0.995	5.140
O	2.123	1.792	6.828	O	5.984	3.726	2.806
N	4.092	2.541	6.004	H	5.599	4.515	3.298
H	4.294	1.632	5.606	H	6.026	3.907	1.838
H	4.851	3.223	5.911	O	8.195	2.058	2.296
C	6.790	5.567	7.849	H	8.678	2.866	2.038
H	7.718	5.022	7.680	H	8.735	1.303	1.995

IM_{decar-I}				H	8.362	5.929	2.641
C	9.766	5.404	0.240	C	6.974	7.559	2.718
H	9.703	6.489	0.404	H	6.293	7.238	1.950
H	9.756	5.240	-0.847	C	2.618	4.083	7.363
O	8.700	4.729	0.890	H	3.501	4.717	7.476
H	7.886	5.000	0.394	H	2.249	3.827	8.360
C	12.559	0.593	2.417	C	2.941	2.777	6.670
H	13.427	1.202	2.692	O	2.151	1.802	6.748
H	11.794	0.784	3.175	N	4.071	2.711	5.968
C	12.920	-0.887	2.372	H	4.331	1.876	5.449
C	14.080	-1.347	1.732	H	4.783	3.439	5.931
H	14.771	-0.630	1.299	C	6.831	5.597	7.879
C	14.340	-2.713	1.623	H	7.758	5.047	7.722
H	15.234	-3.047	1.104	H	6.079	4.860	8.175
C	13.449	-3.648	2.155	C	6.358	6.290	6.600
H	13.638	-4.712	2.036	H	5.448	6.882	6.754
C	12.054	-1.837	2.936	H	7.109	6.989	6.212
H	11.160	-1.496	3.452	C	6.051	5.290	5.481
C	12.311	-3.205	2.829	O	6.542	4.110	5.579
H	11.614	-3.918	3.263	O	5.296	5.649	4.538
C	0.189	2.958	0.181	C	10.050	0.490	10.044
H	0.722	3.464	-0.631	O	11.178	0.636	10.540
H	-0.428	3.720	0.670	N	9.846	0.124	8.768
C	1.163	2.428	1.215	H	8.913	0.055	8.355
H	1.597	3.272	1.759	C	10.980	-0.060	7.874
H	0.643	1.826	1.970	H	10.600	-0.513	6.955
N	2.273	1.675	0.618	H	11.729	-0.713	8.328
H	2.218	1.388	-0.377	C	11.681	1.269	7.567
C	3.515	1.805	1.097	O	12.883	1.439	7.748
N	3.722	2.216	2.336	N	10.831	2.257	7.154
H	4.666	2.426	2.674	H	9.886	2.002	6.864
H	2.959	2.192	3.016	C	11.296	3.590	6.786
N	4.581	1.486	0.289	H	12.237	3.501	6.235
H	5.259	2.280	0.271	C	10.255	4.308	5.927
H	4.274	1.271	-0.663	H	9.261	4.287	6.384
C	5.953	9.751	3.698	H	10.527	5.362	5.800
H	5.468	9.969	2.743	C	10.152	3.741	4.502
H	6.444	10.657	4.061	O	11.164	3.269	3.952
N	8.073	8.591	4.385	O	9.006	3.846	3.935
C	6.966	8.649	3.558	Mg	7.308	2.761	4.172
C	8.713	7.478	4.065	C	7.446	0.489	5.968
H	9.623	7.124	4.523	O	5.884	1.301	4.327
N	8.088	6.822	3.052	O	7.702	-0.316	6.896
				C	6.150	0.318	5.138

O	8.142	1.507	5.646	H	5.074	3.017	1.979
C	5.362	-0.783	5.335	H	3.537	2.768	2.743
H	4.461	-0.911	4.728	N	4.529	1.629	-0.131
H	5.674	-1.583	5.995	H	5.204	2.419	-0.314
C	1.932	-2.085	4.619	H	4.001	1.377	-0.979
O	2.519	-3.086	4.502	C	6.028	9.701	3.769
O	1.315	-1.097	4.720	H	5.592	9.846	2.778
O	6.047	3.780	2.786	H	6.468	10.642	4.106
H	5.658	4.563	3.272	N	8.152	8.725	4.658
H	6.063	3.945	1.815	C	7.094	8.639	3.769
O	8.229	1.997	2.276	C	8.854	7.619	4.505
H	8.853	2.746	2.395	H	9.752	7.364	5.042
H	8.772	1.233	2.003	N	8.324	6.824	3.539
				H	8.630	5.870	3.348
TS_{decar-II}				C	7.197	7.465	3.057
C	9.491	5.463	0.292	H	6.591	7.045	2.272
H	9.347	6.505	0.607	C	2.456	4.026	6.957
H	9.555	5.458	-0.803	H	3.323	4.648	7.200
O	8.393	4.650	0.719	H	2.085	3.572	7.879
H	7.664	4.876	0.086	C	2.878	2.888	6.043
C	12.651	0.732	2.297	O	2.436	1.735	6.203
H	13.461	1.416	2.576	N	3.765	3.163	5.058
H	11.896	0.824	3.082	H	4.344	2.375	4.757
C	13.157	-0.700	2.191	H	4.220	4.081	4.980
C	14.289	-1.022	1.429	C	6.902	5.546	7.982
H	14.845	-0.230	0.943	H	7.849	5.026	7.841
C	14.691	-2.346	1.271	H	6.175	4.789	8.287
H	15.558	-2.569	0.658	C	6.408	6.200	6.691
C	13.971	-3.380	1.872	H	5.464	6.742	6.825
H	14.265	-4.414	1.712	H	7.125	6.936	6.308
C	12.471	-1.743	2.830	C	6.172	5.178	5.583
H	11.613	-1.512	3.455	O	6.774	4.067	5.626
C	12.869	-3.072	2.670	O	5.342	5.493	4.658
H	12.309	-3.865	3.162	C	9.992	0.519	10.210
C	0.247	2.835	0.486	O	11.077	0.678	10.789
H	0.746	3.424	-0.292	N	9.885	0.163	8.921
H	-0.399	3.530	1.032	H	8.983	0.090	8.452
C	1.292	2.285	1.456	C	11.070	-0.028	8.096
H	1.715	3.128	2.009	H	10.752	-0.539	7.182
H	0.855	1.618	2.208	H	11.809	-0.636	8.621
N	2.385	1.618	0.744	C	11.756	1.300	7.755
H	2.182	1.226	-0.189	O	12.937	1.514	8.014
C	3.668	1.979	0.870	N	10.919	2.244	7.226
N	4.121	2.628	1.930	H	10.002	1.956	6.886

C	11.375	3.575	6.827	H	11.674	-1.532	3.524
H	12.325	3.486	6.291	C	12.928	-3.081	2.713
C	10.339	4.269	5.941	H	12.386	-3.879	3.215
H	9.338	4.243	6.381	C	0.251	2.846	0.492
H	10.603	5.326	5.809	H	0.746	3.440	-0.285
C	10.260	3.696	4.514	H	-0.395	3.537	1.044
O	11.262	3.166	4.006	C	1.303	2.296	1.455
O	9.136	3.857	3.906	H	1.716	3.135	2.020
Mg	7.500	2.737	4.189	H	0.872	1.613	2.198
C	7.610	0.488	6.003	N	2.404	1.651	0.739
O	5.883	1.198	4.475	H	2.210	1.252	-0.193
O	7.921	-0.293	6.931	C	3.681	2.030	0.872
C	6.234	0.290	5.307	N	4.116	2.703	1.924
O	8.271	1.500	5.621	H	5.070	3.088	1.984
C	5.474	-0.827	5.695	H	3.553	2.787	2.760
H	5.830	-1.352	6.575	N	4.560	1.667	-0.110
H	4.398	-0.785	5.562	H	5.241	2.450	-0.297
C	5.666	-2.414	4.147	H	4.058	1.383	-0.962
O	6.553	-3.152	4.475	C	6.013	9.754	3.766
O	4.776	-2.189	3.365	H	5.580	9.893	2.773
O	6.445	3.920	2.779	H	6.445	10.700	4.103
H	6.029	4.661	3.304	N	8.139	8.795	4.669
H	7.093	4.269	2.128	C	7.085	8.699	3.776
O	7.973	1.578	2.511	C	8.840	7.686	4.532
H	8.847	1.400	2.125	H	9.734	7.434	5.078
H	7.421	0.796	2.288	N	8.315	6.881	3.570
				H	8.607	5.915	3.415
				C	7.190	7.517	3.078
IM_{decar-II}				H	6.586	7.088	2.296
C	9.483	5.436	0.302	C	2.438	3.979	6.930
H	9.350	6.484	0.604	H	3.306	4.580	7.219
H	9.543	5.418	-0.793	H	2.033	3.505	7.827
O	8.387	4.637	0.749	H	2.033	3.505	7.827
H	7.657	4.837	0.111	C	2.879	2.859	5.998
C	12.660	0.719	2.335	O	2.417	1.707	6.112
H	13.459	1.414	2.616	N	3.805	3.150	5.055
H	11.899	0.797	3.117	H	4.432	2.380	4.776
C	13.185	-0.707	2.230	H	4.229	4.082	5.001
C	14.304	-1.019	1.444	C	6.858	5.594	8.000
H	14.842	-0.223	0.945	H	7.797	5.062	7.850
C	14.713	-2.340	1.275	H	6.123	4.844	8.302
H	15.568	-2.555	0.642	C	6.366	6.261	6.716
C	14.014	-3.380	1.890	H	5.432	6.818	6.855
H	14.312	-4.411	1.720	H	7.093	6.985	6.327
C	12.523	-1.756	2.884	C	6.109	5.239	5.613

O	6.667	4.108	5.685	H	9.596	6.376	0.527
O	5.307	5.568	4.670	H	9.768	5.238	-0.823
C	9.983	0.553	10.260	O	8.689	4.527	0.822
O	11.072	0.686	10.839	H	7.870	4.860	0.373
N	9.863	0.205	8.971	C	12.527	0.553	2.429
H	8.957	0.165	8.495	H	13.415	1.136	2.699
C	11.033	-0.003	8.132	H	11.770	0.772	3.188
H	10.694	-0.512	7.226	C	12.840	-0.937	2.400
H	11.773	-0.617	8.649	C	13.962	-1.449	1.731
C	11.728	1.314	7.774	H	14.658	-0.766	1.251
O	12.914	1.518	8.026	C	14.178	-2.825	1.655
N	10.898	2.264	7.245	H	15.042	-3.202	1.115
H	9.975	1.986	6.908	C	13.279	-3.717	2.244
C	11.370	3.590	6.848	H	13.433	-4.790	2.152
H	12.316	3.491	6.307	C	11.968	-1.843	3.022
C	10.336	4.318	5.987	H	11.110	-1.458	3.569
H	9.351	4.338	6.463	C	12.179	-3.221	2.945
H	10.637	5.363	5.840	H	11.480	-3.902	3.426
C	10.154	3.752	4.571	C	0.137	2.693	0.594
O	11.081	3.132	4.011	H	0.738	3.253	-0.130
O	9.022	4.005	4.024	H	-0.504	3.425	1.095
Mg	7.385	2.771	4.274	C	1.042	2.043	1.639
C	7.573	0.590	6.103	H	1.438	2.828	2.288
O	5.907	1.202	4.423	H	0.499	1.350	2.292
O	7.936	-0.189	7.020	N	2.185	1.373	1.001
C	6.211	0.371	5.431	H	2.061	1.040	0.032
O	8.239	1.599	5.702	C	3.444	1.760	1.242
C	5.436	-0.622	5.931	N	3.787	2.335	2.383
H	5.806	-1.212	6.759	H	4.734	2.706	2.531
H	4.425	-0.807	5.589	H	3.191	2.292	3.197
C	5.520	-2.987	3.467	N	4.381	1.531	0.275
O	6.515	-3.440	3.884	H	5.060	2.321	0.194
O	4.513	-2.600	3.020	H	3.925	1.315	-0.623
O	6.412	3.968	2.810	C	5.975	9.745	3.734
H	6.001	4.718	3.324	H	5.530	9.912	2.750
H	7.098	4.298	2.189				
O	8.266	1.876	2.581				
H	9.228	1.988	2.589				
H	8.071	0.962	2.301				
hydration decarboxylation:							
R							
C	9.741	5.319	0.272				

H	6.421	10.679	4.086	N	10.918	2.272	7.212
N	8.127	8.753	4.546	H	9.996	1.997	6.882
C	7.035	8.680	3.698	C	11.371	3.611	6.832
C	8.819	7.645	4.352	H	12.309	3.533	6.275
H	9.735	7.378	4.854	C	10.314	4.337	5.999
N	8.245	6.864	3.398	H	9.330	4.299	6.475
H	8.539	5.914	3.174	H	10.570	5.398	5.898
C	7.104	7.512	2.973	C	10.167	3.828	4.556
H	6.455	7.092	2.224	O	11.128	3.287	3.984
C	2.488	4.087	7.001	O	9.023	4.063	4.013
H	3.418	4.655	6.927	Mg	7.451	2.869	4.031
H	2.279	3.898	8.060	C	7.659	0.565	5.870
C	2.567	2.719	6.350	O	6.009	1.066	4.215
O	1.660	1.888	6.535	O	7.932	-0.193	6.823
N	3.637	2.422	5.580	C	6.357	0.259	5.071
H	3.723	1.439	5.302	O	8.276	1.593	5.474
H	4.461	3.017	5.529	C	5.634	-1.007	5.437
C	6.798	5.482	7.786	H	6.334	-1.829	5.247
H	7.738	4.958	7.617	H	5.502	-0.989	6.527
H	6.078	4.730	8.120	C	4.273	-1.293	4.794
C	6.263	6.127	6.508	O	4.126	-2.417	4.229
H	5.351	6.711	6.682	O	3.371	-0.420	4.936
H	6.987	6.829	6.076	O	6.101	3.830	2.697
C	5.924	5.120	5.404	H	5.645	4.575	3.208
O	6.379	3.920	5.477	H	6.070	3.981	1.721
O	5.198	5.522	4.452	O	8.157	2.075	2.197
C	9.992	0.538	10.185	H	8.546	2.880	1.796
O	11.080	0.694	10.757	H	8.734	1.332	1.932
N	9.880	0.178	8.895	O	2.291	-0.662	7.571
H	8.973	0.124	8.439	H	2.558	-0.710	6.637
C	11.059	-0.011	8.064	H	2.164	0.293	7.682
H	10.738	-0.519	7.149				
H	11.797	-0.625	8.583				
C	11.751	1.315	7.725	IM-hydration			
O	12.937	1.515	7.972	C	9.767	5.380	0.233
				H	9.603	6.426	0.521

H	9.805	5.333	-0.864	N	8.145	8.822	4.578
O	8.728	4.554	0.746	C	7.039	8.649	3.766
H	7.890	4.884	0.329	C	8.880	7.733	4.437
C	12.605	0.592	2.326	H	9.815	7.538	4.935
H	13.480	1.177	2.630	N	8.320	6.867	3.554
H	11.831	0.781	3.075	H	8.666	5.921	3.381
C	12.941	-0.892	2.260	C	7.141	7.437	3.117
C	14.140	-1.354	1.699	H	6.502	6.943	2.406
H	14.868	-0.639	1.331	C	2.404	4.078	7.174
C	14.396	-2.722	1.592	H	3.300	4.700	7.269
H	15.322	-3.058	1.135	H	2.096	3.754	8.170
C	13.463	-3.655	2.050	C	2.722	2.825	6.385
H	13.654	-4.719	1.940	O	2.212	1.722	6.705
C	12.024	-1.840	2.742	N	3.571	2.949	5.358
H	11.091	-1.496	3.182	H	3.909	2.099	4.926
C	12.281	-3.208	2.641	H	4.039	3.830	5.116
H	11.550	-3.923	3.012	C	6.870	5.563	7.833
C	0.349	2.642	0.569	H	7.816	5.052	7.656
H	0.879	3.221	-0.196	H	6.158	4.798	8.156
H	-0.242	3.360	1.148	C	6.332	6.218	6.557
C	1.354	1.979	1.513	H	5.400	6.766	6.728
H	1.868	2.739	2.109	H	7.053	6.936	6.148
H	0.859	1.321	2.234	C	6.053	5.177	5.468
N	2.397	1.262	0.748	O	6.831	4.181	5.382
H	2.227	1.098	-0.259	O	5.043	5.358	4.711
C	3.693	1.397	1.038	C	9.997	0.552	10.131
N	4.100	1.589	2.290	O	11.079	0.684	10.721
H	5.095	1.732	2.430	N	9.899	0.218	8.834
H	3.710	0.974	3.031	H	9.002	0.193	8.354
N	4.612	1.315	0.018	C	11.088	0.034	8.015
H	5.250	2.142	0.040	H	10.775	-0.462	7.092
H	4.136	1.262	-0.890	H	11.816	-0.587	8.540
C	5.947	9.683	3.757	C	11.793	1.359	7.698
H	5.486	9.788	2.771	O	12.973	1.552	7.979
H	6.378	10.642	4.053	N	10.978	2.321	7.166

H	10.065	2.054	6.801	O	8.736	4.564	0.745
C	11.458	3.651	6.789	H	7.895	4.890	0.331
H	12.417	3.554	6.271	C	12.602	0.594	2.326
C	10.450	4.378	5.898	H	13.476	1.179	2.632
H	9.438	4.351	6.311	H	11.827	0.782	3.074
H	10.720	5.437	5.801	C	12.940	-0.890	2.261
C	10.391	3.851	4.456	C	14.141	-1.350	1.700
O	11.362	3.247	3.969	H	14.867	-0.633	1.332
O	9.306	4.120	3.813	C	14.399	-2.717	1.592
Mg	7.650	3.029	3.920	H	15.326	-3.051	1.135
C	7.853	0.674	5.739	C	13.468	-3.652	2.049
O	6.388	1.267	3.967	H	13.660	-4.716	1.939
O	8.067	-0.141	6.664	C	12.025	-1.839	2.742
C	6.685	0.373	4.761	H	11.091	-1.498	3.181
O	8.465	1.745	5.470	C	12.284	-3.207	2.640
C	5.989	-0.940	4.817	H	11.555	-3.924	3.011
H	6.076	-1.431	3.845	C	0.355	2.655	0.560
H	6.473	-1.556	5.573	H	0.879	3.236	-0.207
C	4.453	-0.774	5.139	H	-0.238	3.370	1.141
O	3.684	-0.488	4.113	C	1.369	2.000	1.501
O	4.442	0.139	6.229	H	1.876	2.767	2.095
O	6.205	3.911	2.650	H	0.878	1.339	2.222
H	5.603	4.495	3.167	N	2.414	1.291	0.735
H	6.000	3.944	1.686	H	2.249	1.128	-0.274
O	8.266	2.182	2.064	C	3.710	1.399	1.038
H	8.615	2.991	1.629	N	4.107	1.585	2.293
H	8.869	1.456	1.809	H	5.107	1.623	2.492
O	4.036	-2.076	5.707	H	3.600	1.090	3.030
H	3.527	0.467	6.362	N	4.640	1.299	0.032
H	4.402	-2.067	6.603	H	5.278	2.127	0.055
				H	4.174	1.245	-0.880
				C	5.949	9.680	3.755
TS-decarboxylation				H	5.488	9.785	2.770
C	9.772	5.388	0.229	H	6.381	10.639	4.051
H	9.613	6.435	0.515	N	8.147	8.817	4.574
H	9.811	5.339	-0.869				

C	7.038	8.644	3.765	C	11.447	3.650	6.789
C	8.877	7.724	4.435	H	12.404	3.554	6.267
H	9.813	7.527	4.932	C	10.434	4.375	5.902
N	8.313	6.857	3.557	H	9.423	4.343	6.319
H	8.651	5.906	3.388	H	10.700	5.435	5.805
C	7.135	7.429	3.120	C	10.368	3.848	4.460
H	6.494	6.933	2.412	O	11.344	3.259	3.964
C	2.409	4.075	7.163	O	9.276	4.107	3.828
H	3.297	4.705	7.272	Mg	7.621	2.990	3.937
H	2.093	3.744	8.154	C	7.822	0.668	5.772
C	2.760	2.829	6.378	O	6.452	1.226	3.905
O	2.264	1.714	6.693	O	8.009	-0.130	6.721
N	3.634	2.963	5.376	C	6.765	0.306	4.701
H	4.027	2.122	4.975	O	8.418	1.762	5.546
H	4.082	3.859	5.133	C	6.202	-0.981	4.681
C	6.869	5.567	7.833	H	6.062	-1.393	3.686
H	7.813	5.052	7.656	H	6.662	-1.675	5.378
H	6.155	4.804	8.155	C	4.314	-0.796	5.198
C	6.334	6.226	6.558	O	3.598	-0.535	4.174
H	5.406	6.781	6.732	O	4.400	0.103	6.250
H	7.058	6.938	6.146	O	6.201	3.913	2.658
C	6.039	5.184	5.476	H	5.599	4.503	3.162
O	6.803	4.180	5.389	H	6.000	3.936	1.692
O	5.020	5.369	4.728	O	8.283	2.197	2.060
C	9.997	0.550	10.131	H	8.657	3.007	1.651
O	11.080	0.679	10.720	H	8.871	1.460	1.803
N	9.894	0.219	8.833	O	4.072	-2.102	5.730
H	8.996	0.201	8.349	H	3.518	0.532	6.387
C	11.083	0.034	8.015	H	4.519	-2.101	6.588
H	10.771	-0.464	7.093				
H	11.813	-0.585	8.541				
C	11.786	1.359	7.694	IM-decarboxylation			
O	12.969	1.551	7.968	C	9.688	5.450	0.259
N	10.969	2.320	7.167	H	9.536	6.496	0.553
H	10.046	2.058	6.817	H	9.722	5.410	-0.838
				O	8.645	4.629	0.775

H	7.800	4.965	0.373	C	8.831	7.631	4.366
C	12.486	0.639	2.321	H	9.760	7.389	4.855
H	13.335	1.248	2.652	N	8.230	6.806	3.470
H	11.691	0.798	3.055	H	8.520	5.849	3.265
C	12.871	-0.831	2.249	C	7.073	7.432	3.054
C	14.086	-1.249	1.687	H	6.417	6.975	2.336
H	14.787	-0.507	1.318	C	2.538	4.191	6.988
C	14.395	-2.606	1.579	H	3.391	4.876	7.024
H	15.332	-2.906	1.120	H	2.287	3.883	8.006
C	13.500	-3.573	2.042	C	2.932	2.924	6.261
H	13.731	-4.630	1.933	O	2.484	1.823	6.682
C	11.992	-1.813	2.732	N	3.789	3.018	5.242
H	11.046	-1.505	3.172	H	4.309	2.197	4.927
C	12.302	-3.171	2.634	H	4.206	3.932	4.999
H	11.601	-3.913	3.010	C	6.834	5.579	7.862
C	0.481	2.891	0.211	H	7.767	5.038	7.703
H	0.909	3.404	-0.657	H	6.086	4.836	8.153
H	-0.078	3.649	0.770	C	6.354	6.276	6.584
C	1.612	2.400	1.108	H	5.460	6.886	6.749
H	2.106	3.289	1.520	H	7.125	6.946	6.186
H	1.233	1.822	1.964	C	6.008	5.259	5.496
N	2.622	1.612	0.399	O	6.706	4.210	5.406
H	2.492	1.379	-0.606	O	4.997	5.502	4.750
C	3.785	1.306	0.972	C	9.951	0.402	9.906
N	4.036	1.631	2.227	O	11.081	0.554	10.386
H	4.948	1.439	2.736	N	9.736	0.053	8.622
H	3.422	2.280	2.694	H	8.794	-0.009	8.246
N	4.717	0.561	0.289	C	10.862	-0.108	7.713
H	5.669	0.850	0.496	H	10.478	-0.522	6.777
H	4.530	0.399	-0.713	H	11.602	-0.791	8.138
C	5.965	9.703	3.753	C	11.591	1.217	7.452
H	5.513	9.855	2.770	O	12.803	1.334	7.591
H	6.422	10.639	4.082	N	10.762	2.249	7.113
N	8.141	8.745	4.535	H	9.801	2.035	6.850
C	7.022	8.633	3.729	C	11.269	3.571	6.752

H	12.213	3.449	6.213	H	5.195	6.915	4.440
C	10.263	4.317	5.878	C	8.764	3.623	9.030
H	9.255	4.311	6.303	H	9.230	4.362	9.692
H	10.556	5.368	5.769	H	7.692	3.647	9.246
C	10.190	3.761	4.444	C	9.327	2.232	9.290
O	11.199	3.230	3.945	C	10.707	1.993	9.383
O	9.079	3.935	3.826	H	11.402	2.824	9.297
Mg	7.347	2.953	3.894	C	11.194	0.698	9.565
C	7.406	0.421	5.552	H	12.267	0.533	9.615
O	6.024	1.386	3.883	C	10.315	-0.383	9.659
O	7.401	-0.480	6.468	H	10.702	-1.393	9.775
C	6.551	0.248	4.305	C	8.456	1.139	9.415
O	8.075	1.486	5.576	H	7.382	1.315	9.367
C	6.498	-0.947	3.672	C	8.940	-0.158	9.598
H	6.073	-1.023	2.672	H	8.243	-0.989	9.690
H	6.996	-1.815	4.085	C	-0.813	3.132	0.612
C	4.163	-1.152	6.552	H	-0.067	3.839	0.233
O	3.026	-1.679	6.543	H	-1.767	3.665	0.615
O	4.355	0.142	6.520	C	-0.476	2.745	2.045
O	6.081	4.067	2.627	H	-0.658	3.619	2.678
H	5.535	4.701	3.137	H	-1.117	1.942	2.431
H	5.773	4.014	1.682	N	0.942	2.384	2.161
O	7.989	2.151	1.941	H	1.436	2.044	1.315
H	8.368	2.971	1.558	C	1.764	2.944	3.044
H	8.639	1.452	1.728	N	1.312	3.503	4.164
O	5.251	-1.874	6.587	H	1.919	4.118	4.733
H	3.499	0.703	6.579	H	0.321	3.612	4.311
H	6.109	-1.283	6.518	N	3.109	2.888	2.808
				H	3.552	3.816	3.008
				H	3.283	2.579	1.840
				C	0.777	11.090	5.880
				H	0.921	11.209	4.804
				H	0.734	12.079	6.344
				N	2.282	10.561	7.814
				C	1.890	10.301	6.512
proton-assisted decarboxylation:							
R							
C	6.665	7.775	5.350				
H	6.180	8.756	5.407				
H	7.292	7.760	4.450				
O	5.674	6.740	5.293				

C	3.206	9.665	8.109	H	5.959	6.242	11.963
H	3.731	9.586	9.047	C	4.323	6.697	10.612
N	3.452	8.844	7.053	H	3.255	6.488	10.493
H	4.054	8.026	7.085	H	4.425	7.790	10.601
C	2.619	9.240	6.025	C	5.055	6.218	9.354
H	2.611	8.742	5.071	O	6.247	5.884	9.410
C	-2.666	4.540	7.281	O	4.349	6.246	8.273
H	-2.085	5.309	7.797	Mg	3.355	4.807	7.462
H	-3.407	4.140	7.978	C	2.895	2.239	9.099
C	-1.813	3.373	6.840	O	2.329	2.312	6.765
O	-2.317	2.283	6.517	O	2.775	1.531	10.117
N	-0.474	3.551	6.804	C	2.332	1.626	7.786
H	0.074	2.737	6.574	O	3.360	3.401	8.970
H	0.036	4.340	7.205	C	1.761	0.227	7.828
C	0.199	6.934	10.065	H	2.571	-0.462	8.101
H	1.161	6.622	10.470	H	1.052	0.156	8.662
H	-0.424	6.038	10.002	C	1.085	-0.303	6.570
C	0.332	7.526	8.662	O	0.642	-1.436	6.511
H	-0.624	7.892	8.269	O	0.977	0.508	5.513
H	1.008	8.389	8.647	H	1.531	1.321	5.674
C	0.869	6.536	7.630	O	2.705	5.428	5.544
O	1.450	5.450	8.020	H	1.915	6.055	5.690
O	0.712	6.805	6.407	H	3.191	5.630	4.705
C	2.674	2.609	14.107	O	5.020	4.203	6.334
O	3.259	2.976	15.132	H	5.384	5.070	6.045
N	3.318	2.292	12.966	H	5.799	3.637	6.512
H	2.802	2.037	12.131				
C	4.766	2.412	12.880	TS			
H	5.089	1.926	11.955	C	6.674	7.831	5.334
H	5.241	1.921	13.731	H	6.213	8.825	5.367
C	5.242	3.871	12.900	H	7.300	7.779	4.434
O	6.142	4.253	13.636	O	5.657	6.820	5.308
N	4.548	4.709	12.066	H	5.184	6.977	4.447
H	3.881	4.310	11.417	C	8.883	3.873	9.176
C	4.873	6.125	11.917	H	9.421	4.651	9.731

H	7.835	3.972	9.469	H	4.092	7.991	6.790
C	9.394	2.492	9.560	C	2.617	9.249	5.865
C	10.633	1.976	9.147	H	2.584	8.806	4.886
H	11.316	2.601	8.576	C	-2.545	4.528	7.261
C	10.984	0.655	9.428	H	-1.927	5.309	7.711
H	11.932	0.265	9.073	H	-3.274	4.195	8.007
C	10.107	-0.176	10.125	C	-1.746	3.294	6.888
H	10.351	-1.224	10.273	O	-2.320	2.236	6.574
C	8.569	1.676	10.354	N	-0.397	3.376	6.928
H	7.657	2.099	10.770	H	0.113	2.510	6.796
C	8.915	0.349	10.627	H	0.119	4.169	7.318
H	8.249	-0.275	11.218	C	0.172	6.956	10.017
C	-0.796	3.022	0.717	H	1.148	6.655	10.396
H	-0.024	3.726	0.389	H	-0.438	6.051	9.963
H	-1.739	3.576	0.710	C	0.265	7.550	8.611
C	-0.518	2.555	2.144	H	-0.707	7.888	8.232
H	-0.733	3.380	2.827	H	0.918	8.431	8.581
H	-1.170	1.727	2.448	C	0.816	6.568	7.576
N	0.899	2.188	2.310	O	1.382	5.480	7.968
H	1.391	1.854	1.464	O	0.692	6.857	6.353
C	1.713	2.896	3.104	C	2.794	2.558	13.880
N	1.266	3.510	4.189	O	3.482	2.877	14.856
H	1.859	4.160	4.724	N	3.310	2.248	12.671
H	0.332	3.353	4.535	H	2.695	2.034	11.893
N	3.035	2.954	2.775	C	4.737	2.285	12.424
H	3.450	3.897	2.967	H	4.942	1.723	11.509
H	3.167	2.652	1.797	H	5.275	1.813	13.249
C	0.780	11.102	5.862	C	5.339	3.687	12.277
H	0.903	11.262	4.789	O	6.543	3.855	12.417
H	0.752	12.073	6.363	N	4.448	4.682	11.986
N	2.323	10.458	7.738	H	3.476	4.429	11.853
C	1.901	10.279	6.431	C	4.840	6.079	11.885
C	3.250	9.544	7.958	H	5.932	6.101	11.914
H	3.792	9.405	8.880	C	4.324	6.763	10.621
N	3.469	8.789	6.848	H	3.239	6.683	10.522

H	4.567	7.834	10.648	H	11.388	2.736	8.867
C	4.982	6.219	9.349	C	11.101	0.686	9.451
O	6.187	5.921	9.358	H	12.142	0.425	9.287
O	4.213	6.150	8.322	C	10.196	-0.291	9.872
Mg	3.254	4.796	7.374	H	10.525	-1.317	10.009
C	2.804	1.866	8.671	C	8.444	1.374	9.876
O	3.798	0.998	6.674	H	7.412	1.655	10.078
O	2.581	1.528	9.851	C	8.868	0.063	10.113
C	3.000	0.706	7.681	H	8.160	-0.678	10.481
O	2.882	3.027	8.183	C	-0.777	3.061	0.688
C	2.340	-0.499	7.806	H	0.002	3.752	0.352
H	2.764	-1.367	7.312	H	-1.716	3.622	0.673
H	1.807	-0.680	8.732	C	-0.508	2.616	2.124
C	0.778	-0.501	6.344	H	-0.705	3.461	2.789
O	0.471	-1.665	6.330	H	-1.187	1.812	2.435
O	0.615	0.592	5.883	N	0.897	2.211	2.305
H	3.814	0.258	6.011	H	1.390	1.878	1.458
O	2.664	5.478	5.498	C	1.721	2.905	3.107
H	1.867	6.106	5.647	N	1.277	3.515	4.195
H	3.140	5.661	4.648	H	1.872	4.162	4.741
O	4.982	4.238	6.296	H	0.322	3.412	4.500
H	5.379	5.102	6.053	N	3.043	2.940	2.788
H	5.722	3.662	6.562	H	3.471	3.876	2.985
				H	3.183	2.631	1.814
IM				C	0.785	11.101	5.872
C	6.660	7.816	5.334	H	0.925	11.244	4.798
H	6.193	8.807	5.378	H	0.749	12.079	6.358
H	7.288	7.779	4.435	N	2.302	10.508	7.783
O	5.653	6.798	5.297	C	1.899	10.291	6.476
H	5.178	6.960	4.439	C	3.221	9.597	8.044
C	8.797	3.740	9.078	H	3.750	9.484	8.977
H	9.300	4.497	9.691	N	3.453	8.807	6.961
H	7.735	3.803	9.331	H	4.059	7.993	6.947
C	9.329	2.351	9.394	C	2.618	9.241	5.952
C	10.675	1.993	9.214	H	2.596	8.768	4.986

C	-2.533	4.496	7.252	O	4.251	6.134	8.317
H	-1.950	5.282	7.737	Mg	3.288	4.749	7.404
H	-3.269	4.126	7.973	C	2.877	1.865	8.787
C	-1.684	3.294	6.881	O	3.830	0.995	6.747
O	-2.207	2.225	6.509	O	2.639	1.591	9.983
N	-0.344	3.411	6.997	C	3.094	0.684	7.843
H	0.204	2.567	6.892	O	2.928	3.022	8.261
H	0.144	4.216	7.405	C	2.588	-0.532	8.111
C	0.178	6.961	10.021	H	2.790	-1.388	7.475
H	1.152	6.662	10.406	H	2.011	-0.684	9.014
H	-0.430	6.054	9.966	C	0.550	-0.631	5.794
C	0.278	7.552	8.614	O	0.483	-1.787	5.982
H	-0.694	7.886	8.229	O	0.578	0.508	5.543
H	0.927	8.435	8.588	H	3.784	0.254	6.101
C	0.837	6.568	7.588	O	2.667	5.444	5.519
O	1.407	5.486	7.989	H	1.880	6.085	5.674
O	0.712	6.848	6.362	H	3.160	5.642	4.684
C	2.739	2.602	13.962	O	4.981	4.219	6.273
O	3.389	2.942	14.958	H	5.380	5.082	6.034
N	3.304	2.275	12.782	H	5.726	3.618	6.468
H	2.728	2.052	11.975				
C	4.743	2.329	12.605	R' _{pyrone}			
H	4.985	1.814	11.671	C	6.581	7.870	5.194
H	5.250	1.824	13.429	H	6.038	8.818	5.295
C	5.315	3.751	12.555	H	7.181	7.919	4.276
O	6.442	3.994	12.959	O	5.673	6.773	5.156
N	4.473	4.692	12.021	H	5.122	6.917	4.342
H	3.547	4.404	11.729	C	9.144	3.906	8.707
C	4.844	6.093	11.905	H	9.311	4.787	9.335
H	5.934	6.140	11.949	H	8.103	3.620	8.874
C	4.325	6.736	10.621	C	10.119	2.812	9.098
H	3.243	6.628	10.512	C	11.237	3.130	9.878
H	4.537	7.813	10.627	H	11.393	4.155	10.194
C	5.004	6.191	9.359	C	12.164	2.155	10.237
O	6.206	5.886	9.384	H	13.027	2.442	10.829

C	11.978	0.828	9.844	C	-1.940	3.690	6.120
H	12.707	0.065	10.103	O	-2.348	2.571	5.766
C	9.925	1.466	8.743	N	-0.748	4.191	5.739
H	9.059	1.185	8.148	H	-0.111	3.591	5.237
C	10.843	0.483	9.112	H	-0.389	5.085	6.081
H	10.686	-0.546	8.800	C	0.156	7.025	10.176
C	-0.394	3.264	0.648	H	1.145	6.743	10.535
H	0.339	3.917	0.163	H	-0.437	6.108	10.123
H	-1.326	3.838	0.709	C	0.214	7.642	8.776
C	0.041	2.955	2.077	H	-0.772	7.945	8.408
H	-0.106	3.852	2.691	H	0.846	8.538	8.759
H	-0.597	2.185	2.526	C	0.793	6.663	7.755
N	1.468	2.594	2.183	O	1.666	5.837	8.158
H	2.050	2.471	1.331	O	0.375	6.732	6.554
C	2.061	2.508	3.374	C	2.520	2.706	14.277
N	1.374	2.136	4.455	O	3.083	3.072	15.314
H	1.774	2.307	5.381	N	3.183	2.394	13.140
H	0.519	1.568	4.389	H	2.680	2.262	12.260
N	3.378	2.832	3.494	C	4.625	2.562	13.045
H	3.753	2.740	4.437	H	4.944	2.001	12.167
H	3.577	3.781	3.106	H	5.108	2.162	13.940
C	0.745	11.043	5.869	C	5.100	4.015	12.963
H	0.874	11.098	4.786	O	5.908	4.458	13.779
H	0.729	12.056	6.280	N	4.526	4.773	11.984
N	2.276	10.623	7.804	H	3.987	4.328	11.241
C	1.852	10.272	6.533	C	4.874	6.185	11.779
C	3.178	9.724	8.152	H	5.960	6.296	11.858
H	3.710	9.698	9.089	C	4.393	6.694	10.419
N	3.385	8.817	7.162	H	3.338	6.465	10.241
H	3.953	7.974	7.261	H	4.485	7.787	10.376
C	2.544	9.154	6.120	C	5.195	6.182	9.205
H	2.513	8.583	5.209	O	6.368	5.781	9.338
C	-2.823	4.621	6.934	O	4.575	6.259	8.082
H	-2.234	5.325	7.528	Mg	3.268	4.906	7.372
H	-3.439	4.014	7.600	C	2.826	2.646	9.340

O	2.668	1.911	10.339	H	2.901	5.568	4.575
O	3.398	3.771	9.257	O	4.882	4.304	6.164
C	2.302	2.121	7.978	H	5.381	5.128	5.995
O	2.393	2.887	7.013	H	5.479	3.536	6.123
C	1.767	0.736	7.831				
H	1.998	0.152	8.724	R''_{pyrone}			
O	-0.227	-0.323	7.027	C	6.734	7.880	5.184
C	0.220	0.724	7.623	H	6.322	8.897	5.211
O	-0.427	1.688	8.028	H	7.387	7.815	4.305
H	2.222	0.273	6.953	O	5.680	6.915	5.106
C	4.542	-1.120	7.965	H	5.291	7.049	4.198
O	4.637	-0.298	6.897	C	9.117	3.763	8.845
C	5.188	0.998	6.958	H	9.413	4.596	9.494
O	5.087	1.638	5.927	H	8.061	3.581	9.062
C	5.768	1.377	8.207	C	9.949	2.528	9.153
H	6.249	2.344	8.241	C	11.328	2.475	8.906
C	3.817	-2.375	7.639	H	11.827	3.328	8.463
H	2.789	-2.137	7.347	C	12.064	1.332	9.202
H	3.808	-3.054	8.487	H	13.129	1.327	8.999
H	4.294	-2.880	6.795	C	11.437	0.202	9.729
C	5.669	0.545	9.295	H	12.013	-0.700	9.918
O	6.155	0.783	10.519	C	9.339	1.405	9.727
C	6.993	1.941	10.732	H	8.283	1.444	9.978
H	7.915	1.831	10.162	C	10.071	0.248	10.005
H	6.470	2.864	10.463	H	9.569	-0.615	10.438
H	7.223	1.942	11.796	C	-0.687	3.089	0.656
C	5.013	-0.734	9.175	H	0.040	3.811	0.270
C	4.915	-1.653	10.352	H	-1.646	3.613	0.721
O	5.568	-2.691	10.346	C	-0.284	2.630	2.055
C	3.943	-1.300	11.445	H	-0.434	3.450	2.762
H	3.760	-0.226	11.501	H	-0.920	1.812	2.413
H	2.986	-1.778	11.193	N	1.139	2.255	2.110
H	4.261	-1.713	12.405	H	1.583	2.026	1.209
O	2.548	5.522	5.493	C	1.984	2.939	2.910
H	1.723	6.053	5.603	N	1.547	3.399	4.085

H	2.183	3.899	4.704	N	2.931	2.598	13.570
H	0.805	2.836	4.520	H	2.382	2.452	12.726
N	3.237	3.140	2.491	C	4.382	2.578	13.430
H	3.681	4.048	2.769	H	4.624	2.005	12.532
H	3.368	2.883	1.506	H	4.844	2.105	14.294
C	0.784	10.968	5.891	C	4.985	3.984	13.329
H	0.794	11.160	4.815	O	5.762	4.421	14.174
H	0.843	11.924	6.418	N	4.519	4.739	12.286
N	2.462	10.104	7.562	H	3.947	4.298	11.567
C	1.936	10.089	6.282	C	4.970	6.113	12.037
C	3.426	9.198	7.570	H	6.057	6.160	12.154
H	4.057	8.953	8.411	C	4.577	6.591	10.637
N	3.561	8.608	6.352	H	3.508	6.454	10.444
H	4.266	7.920	6.082	H	4.783	7.665	10.542
C	2.615	9.168	5.520	C	5.386	5.926	9.506
H	2.511	8.874	4.489	O	6.611	5.760	9.625
C	-2.832	4.709	7.505	O	4.732	5.615	8.445
H	-2.359	5.524	8.062	Mg	3.158	4.514	8.045
H	-3.522	4.185	8.169	C	2.356	2.446	9.961
C	-1.795	3.716	7.033	O	3.062	3.485	9.882
O	-2.054	2.497	6.956	O	2.146	1.739	10.978
N	-0.595	4.202	6.687	C	1.626	2.059	8.644
H	0.124	3.525	6.462	O	1.832	2.771	7.662
H	-0.321	5.185	6.728	C	0.661	0.923	8.627
C	0.073	7.026	10.429	H	0.077	0.952	9.554
H	1.006	6.675	10.870	H	-0.019	1.032	7.782
H	-0.573	6.151	10.312	C	1.280	-0.520	8.628
C	0.308	7.648	9.050	O	2.356	-0.722	9.221
H	-0.621	7.984	8.575	O	0.547	-1.375	8.051
H	0.968	8.524	9.094	C	2.800	-2.653	6.172
C	0.970	6.642	8.117	C	3.736	-2.485	7.159
O	1.696	5.744	8.640	C	4.448	-1.215	7.180
O	0.747	6.728	6.864	C	4.225	-0.263	6.218
C	2.338	2.835	14.754	C	3.320	-0.490	5.151
O	2.965	2.982	15.810	O	2.607	-1.717	5.215

O	3.060	0.212	4.191	H	11.680	3.205	9.091
H	4.731	0.688	6.227	C	11.805	1.087	9.425
C	1.873	-3.799	5.932	H	12.889	1.095	9.470
H	0.869	-3.516	6.264	C	11.106	-0.113	9.567
H	2.169	-4.694	6.474	H	11.646	-1.047	9.704
H	1.820	-3.994	4.857	C	9.034	1.099	9.304
O	5.304	-1.049	8.188	H	7.948	1.107	9.281
C	6.113	0.147	8.251	C	9.712	-0.101	9.523
H	6.775	0.211	7.385	H	9.151	-1.024	9.657
H	5.489	1.042	8.308	C	-0.724	3.077	0.696
H	6.705	0.038	9.157	H	-0.006	3.815	0.323
C	3.970	-3.536	8.189	H	-1.689	3.590	0.774
O	3.070	-4.304	8.538	C	-0.315	2.588	2.083
C	5.335	-3.713	8.806	H	-0.517	3.373	2.815
H	6.149	-3.443	8.138	H	-0.901	1.722	2.406
H	5.418	-3.086	9.699	N	1.124	2.285	2.146
H	5.433	-4.756	9.111	H	1.587	2.076	1.248
O	2.801	5.192	6.066	C	1.936	2.983	2.965
H	2.061	5.863	6.185	N	1.478	3.426	4.137
H	3.531	5.616	5.586	H	2.075	3.957	4.773
O	4.686	3.198	7.446	H	0.672	2.931	4.532
H	5.419	3.792	7.692	N	3.200	3.193	2.570
H	4.830	3.003	6.486	H	3.636	4.107	2.841
				H	3.345	2.938	1.588
TS''_{pyrone}				C	0.789	10.955	5.923
C	6.748	7.830	5.235	H	0.791	11.157	4.849
H	6.345	8.851	5.266	H	0.859	11.906	6.457
H	7.402	7.764	4.356	N	2.486	10.069	7.567
O	5.685	6.876	5.148	C	1.940	10.065	6.294
H	5.302	7.016	4.239	C	3.444	9.156	7.551
C	8.956	3.590	8.850	H	4.093	8.904	8.376
H	9.256	4.377	9.550	N	3.555	8.573	6.328
H	7.884	3.441	9.005	H	4.258	7.888	6.046
C	9.723	2.305	9.124	C	2.601	9.147	5.514
C	11.123	2.282	9.208	H	2.482	8.864	4.482

C	-2.841	4.654	7.526	O	4.654	5.582	8.462
H	-2.388	5.466	8.102	Mg	3.069	4.398	8.106
H	-3.560	4.135	8.163	C	2.457	2.388	10.089
C	-1.788	3.645	7.123	O	3.150	3.442	9.973
O	-2.074	2.434	7.004	O	2.455	1.622	11.092
N	-0.549	4.104	6.908	C	1.567	2.049	8.881
H	0.221	3.435	6.897	O	1.803	2.713	7.816
H	-0.301	5.091	6.951	C	0.611	1.043	9.046
C	0.026	7.017	10.490	H	0.324	0.832	10.066
H	0.935	6.635	10.953	H	-0.180	0.965	8.303
H	-0.639	6.161	10.336	C	1.390	-0.919	9.248
C	0.320	7.653	9.130	O	2.584	-0.897	9.180
H	-0.581	8.030	8.635	O	0.372	-1.537	9.407
H	1.012	8.502	9.206	C	2.814	-3.265	5.706
C	0.967	6.631	8.204	C	3.602	-2.838	6.745
O	1.678	5.725	8.731	C	4.216	-1.529	6.605
O	0.735	6.709	6.951	C	3.982	-0.761	5.485
C	2.254	2.922	14.845	C	3.358	-1.332	4.338
O	2.815	3.191	15.916	O	2.731	-2.577	4.549
N	2.919	2.633	13.713	O	3.285	-0.878	3.210
H	2.433	2.374	12.856	H	4.413	0.220	5.360
C	4.373	2.634	13.678	C	1.952	-4.477	5.640
H	4.689	1.945	12.896	H	0.910	-4.174	5.793
H	4.771	2.294	14.633	H	2.210	-5.213	6.397
C	4.986	4.021	13.451	H	2.024	-4.907	4.638
O	5.789	4.495	14.254	O	4.965	-1.144	7.628
N	4.511	4.715	12.374	C	5.514	0.183	7.657
H	3.938	4.240	11.677	H	6.127	0.385	6.779
C	4.926	6.093	12.071	H	4.719	0.926	7.734
H	6.013	6.171	12.167	H	6.143	0.205	8.543
C	4.494	6.525	10.665	C	3.830	-3.678	7.958
H	3.430	6.345	10.489	O	2.950	-4.416	8.408
H	4.656	7.606	10.550	C	5.184	-3.673	8.621
C	5.309	5.878	9.526	H	5.991	-3.386	7.953
O	6.537	5.718	9.641	H	5.164	-2.965	9.455

H	5.369	-4.670	9.024	H	1.585	2.073	1.265
O	2.710	5.147	6.130	C	1.939	2.996	2.973
H	1.978	5.827	6.287	N	1.490	3.439	4.147
H	3.455	5.599	5.703	H	2.084	3.990	4.772
O	4.706	3.244	7.431	H	0.701	2.932	4.559
H	5.343	3.968	7.592	N	3.196	3.213	2.562
H	4.831	2.960	6.493	H	3.633	4.127	2.832
				H	3.330	2.962	1.577
IM''_{pyrone}				C	0.791	10.986	5.898
C	6.756	7.836	5.223	H	0.794	11.185	4.823
H	6.357	8.859	5.255	H	0.856	11.938	6.430
H	7.415	7.771	4.348	N	2.485	10.106	7.547
O	5.690	6.888	5.126	C	1.945	10.101	6.273
H	5.311	7.035	4.217	C	3.442	9.192	7.538
C	8.914	3.557	8.827	H	4.083	8.935	8.368
H	9.197	4.330	9.549	N	3.561	8.610	6.316
H	7.838	3.407	8.951	H	4.258	7.916	6.044
C	9.674	2.267	9.094	C	2.611	9.182	5.497
C	11.050	2.261	9.362	H	2.493	8.895	4.466
H	11.590	3.200	9.402	C	-2.843	4.686	7.487
C	11.732	1.062	9.564	H	-2.402	5.493	8.080
H	12.801	1.082	9.750	H	-3.560	4.149	8.111
C	11.056	-0.159	9.513	C	-1.775	3.696	7.071
H	11.599	-1.092	9.642	O	-2.062	2.485	6.926
C	9.002	1.036	9.070	N	-0.542	4.172	6.879
H	7.935	1.026	8.871	H	0.273	3.545	6.913
C	9.681	-0.165	9.278	H	-0.328	5.166	6.942
H	9.135	-1.107	9.230	C	0.025	7.052	10.431
C	-0.722	3.076	0.709	H	0.939	6.666	10.881
H	-0.002	3.813	0.337	H	-0.636	6.195	10.261
H	-1.686	3.589	0.786	C	0.311	7.721	9.084
C	-0.313	2.587	2.099	H	-0.599	8.073	8.587
H	-0.516	3.372	2.831	H	0.974	8.590	9.182
H	-0.899	1.720	2.420	C	1.006	6.734	8.152
N	1.125	2.284	2.163	O	1.790	5.890	8.674

O	0.742	6.783	6.903	C	3.919	-0.747	5.437
C	2.197	2.966	14.786	C	3.297	-1.333	4.295
O	2.750	3.249	15.859	O	2.658	-2.573	4.523
N	2.873	2.669	13.662	O	3.238	-0.898	3.161
H	2.399	2.424	12.794	H	4.341	0.236	5.303
C	4.327	2.665	13.662	C	1.868	-4.452	5.648
H	4.662	1.947	12.916	H	0.831	-4.144	5.821
H	4.690	2.355	14.640	H	2.139	-5.187	6.401
C	4.961	4.040	13.419	H	1.915	-4.888	4.648
O	5.773	4.503	14.220	O	4.877	-1.092	7.596
N	4.495	4.738	12.341	C	5.357	0.264	7.632
H	3.930	4.267	11.631	H	6.003	0.484	6.781
C	4.926	6.114	12.046	H	4.524	0.968	7.656
H	6.013	6.180	12.155	H	5.932	0.330	8.551
C	4.517	6.554	10.637	C	3.756	-3.634	7.939
H	3.455	6.378	10.441	O	2.850	-4.321	8.424
H	4.680	7.636	10.530	C	5.121	-3.661	8.576
C	5.348	5.915	9.504	H	5.918	-3.403	7.884
O	6.565	5.699	9.661	H	5.139	-2.941	9.400
O	4.725	5.690	8.407	H	5.291	-4.657	8.990
Mg	3.126	4.506	8.023	O	2.748	5.255	6.038
C	2.473	2.471	9.949	H	2.003	5.915	6.211
O	3.208	3.506	9.884	H	3.463	5.716	5.573
O	2.464	1.673	10.934	O	4.788	3.350	7.371
C	1.566	2.239	8.732	H	5.424	4.080	7.500
O	1.849	2.954	7.678	H	4.890	3.036	6.442
C	0.531	1.359	8.847				
H	0.341	0.875	9.794				
H	-0.244	1.320	8.087				
C	1.530	-1.326	9.463				
O	2.659	-1.077	9.315				
O	0.413	-1.644	9.627				
C	2.739	-3.245	5.687				
C	3.536	-2.810	6.716				
C	4.149	-1.501	6.565				