

Supporting information

QM/MM studies of the type II isopentenyl diphosphate-dimethylallyl diphosphate isomerase demonstrate a novel role for flavin coenzyme

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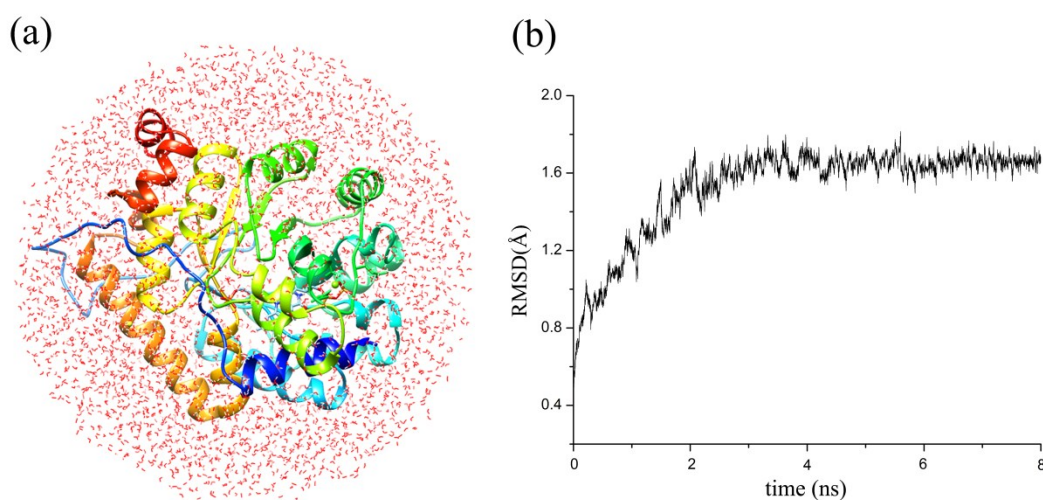


Figure S1 (a)The constructed solvation model. (b) RMSD for the model in 8-ns MD simulation.

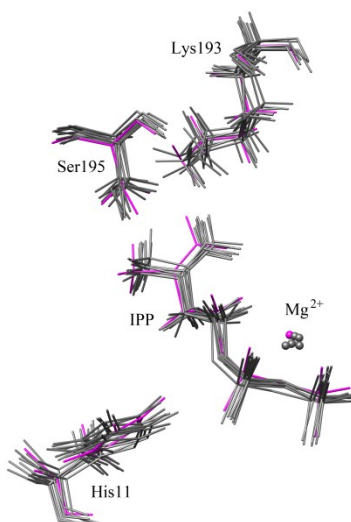


Figure S2 A total of 11 optimized structures, B3LYP/6-31G(d,p) for QM region and CHARMM22 force field for MM region. They were selected after MD calculation, at interval of 200ps from 4ns to 6ns. The RMSDs of 11 snapshots were calculated relative to the average one, 0.422(4.0 ns), 0.437(4.2 ns), 0.505(4.4 ns), 0.478(4.6 ns), 0.399(4.8 ns), 0.407(5.0 ns), 0.425(5.2 ns).

ns), 0.405(5.4 ns), 0.355(5.6 ns), 0.453(5.8 ns), 0.392(6.0 ns). The RMS deviation at 5.6 ns corresponds to the smallest value, it means this structure (shown in purple) is the most representative configuration and chosen as the reactant structure.

Cartesian coordinates of QM regions of all computed species:

React _A				-5.349	1.344	-0.388	H
-13.375	-1.114	-10.321	N	-3.660	5.817	2.872	C
-14.001	-1.115	-9.531	H	-4.667	6.425	3.244	O
-11.973	-0.837	-10.039	C				
-11.687	0.046	-10.602	H	-4.521	6.556	-1.738	N
-11.739	-0.582	-8.517	C	-4.549	7.571	-1.723	H
-12.240	-1.393	-7.975	H	-4.761	5.946	-3.036	C
-10.666	-0.654	-8.296	H	-4.221	5.008	-3.091	H
-12.336	1.031	-6.691	N	-6.250	5.643	-3.342	C
-12.235	0.760	-8.044	C	-6.348	5.302	-4.381	H
-12.652	2.316	-6.597	C	-6.493	4.797	-2.690	H
-12.812	2.852	-5.670	H	-7.074	6.756	-3.057	O
-12.775	2.890	-7.811	N	-7.956	6.502	-3.405	H
-12.795	3.931	-7.963	H	-4.190	6.803	-4.149	C
-12.504	1.916	-8.743	C	-4.898	7.445	-4.922	O
-12.511	2.118	-9.801	H				
-11.014	-1.940	-10.495	C	-6.944	0.339	-1.129	N
-9.940	-1.657	-11.022	O	-7.645	0.231	0.037	C
				-7.194	0.645	1.116	O
-3.330	4.888	5.167	N	-8.910	-0.364	0.011	N
-4.310	4.787	5.363	H	-9.327	-0.581	0.922	H
-2.913	4.853	3.776	C	-9.570	-0.742	-1.139	C
-1.882	5.170	3.730	H	-10.771	-1.135	-1.116	O
-2.985	3.423	3.178	C	-8.793	-0.632	-2.304	C
-2.322	3.382	2.284	H	-9.455	-0.981	-3.563	N
-2.552	2.724	3.928	H	-8.492	-1.260	-4.643	C
-4.373	2.884	2.818	C	-8.918	-2.009	-5.735	C
-4.992	2.853	3.739	H	-9.953	-2.341	-5.771	H
-4.883	3.537	2.085	H	-8.046	-2.346	-6.772	C
-4.320	1.462	2.252	C	-8.531	-3.139	-7.958	C
-3.743	0.862	2.964	H	-9.601	-3.347	-7.877	H
-5.331	1.053	2.202	H	-8.007	-4.099	-8.048	H
-3.636	1.261	0.901	C	-8.376	-2.603	-8.902	H
-2.632	1.687	0.852	H	-6.705	-1.916	-6.674	C
-3.541	0.194	0.695	H	-5.702	-2.253	-7.753	C
-4.417	1.807	-0.281	N	-4.722	-1.819	-7.536	H
-4.541	2.828	-0.221	H	-6.023	-1.876	-8.731	H
-3.903	1.629	-1.166	H	-5.576	-3.339	-7.859	H

-6.301	-1.162	-5.572	C	-8.181	3.014	-0.038	H
-5.277	-0.814	-5.553	H	-12.654	3.324	-0.644	O
-7.176	-0.796	-4.534	C	-13.938	3.334	-1.616	P
-6.750	-0.042	-3.429	N	-14.238	4.761	-2.075	O
-7.497	-0.103	-2.266	C	-13.768	2.321	-2.751	O
-5.512	0.792	-3.502	C	-15.100	2.806	-0.656	O
-5.575	1.296	-4.467	H	-15.661	3.679	0.778	P
-5.633	1.559	-2.739	H	-15.194	2.847	1.937	O
-4.152	0.075	-3.279	C	-14.925	5.054	0.615	O
-3.976	-0.520	-4.212	H	-17.154	3.786	0.507	O
-4.145	-0.504	-2.468	O	-14.863	5.874	-0.897	Mg
-4.830	-1.175	-2.271	H	-11.657	0.412	-4.181	O
-3.032	1.225	-3.468	C	-12.122	1.150	-3.749	H
-2.138	0.560	-3.544	H	-11.896	0.495	-5.158	H
-2.948	1.950	-2.722	O				
-2.240	2.621	-2.753	H	TS1 _A			
-3.071	1.791	-4.966	C	-13.387	-1.122	-10.336	N
-3.678	2.719	-4.807	H	-14.004	-1.132	-9.540	H
-3.440	1.219	-5.728	O	-11.985	-0.833	-10.069	C
-2.833	0.764	-6.352	H	-11.711	0.049	-10.639	H
-1.640	2.373	-5.244	C	-11.747	-0.567	-8.551	C
-1.678	3.007	-6.163	H	-12.241	-1.376	-8.000	H
-1.365	3.075	-4.429	H	-10.673	-0.628	-8.333	H
-0.605	1.366	-5.342	O	-12.382	1.044	-6.738	N
-0.324	0.595	-6.692	P	-12.252	0.774	-8.088	C
0.449	-0.736	-6.800	O	-12.685	2.332	-6.653	C
0.616	1.311	-7.599	O	-12.859	2.872	-5.732	H
-1.620	0.155	-7.277	O	-12.777	2.909	-7.870	N
-10.203	-0.262	-3.836	H	-12.790	3.950	-8.017	H
-9.990	-1.847	-3.394	H	-12.496	1.931	-8.795	C
				-12.484	2.128	-9.854	H
-11.404	3.853	-1.133	C	-11.020	-1.930	-10.525	C
-11.564	4.482	-2.014	H	-9.955	-1.642	-11.066	O
-11.000	4.487	-0.339	H				
-10.492	2.663	-1.440	C	-3.315	4.957	5.191	N
-10.398	2.083	-0.513	H	-4.298	4.860	5.371	H
-11.010	2.036	-2.171	H	-2.875	4.926	3.807	C
-9.126	3.025	-1.972	C	-1.855	5.278	3.774	H
-8.821	2.834	-3.261	C	-2.892	3.490	3.228	C
-9.553	2.426	-3.955	H	-2.201	3.451	2.356	H
-7.855	3.102	-3.678	H	-2.469	2.815	4.006	H
-8.156	3.594	-0.966	C	-4.252	2.903	2.839	C
-7.130	3.580	-1.343	H	-4.896	2.863	3.742	H
-8.408	4.629	-0.710	H	-4.764	3.527	2.081	H

-4.129	1.476	2.299	C	-4.960	-2.466	-7.175	H
-3.536	0.913	3.028	H	-6.267	-2.486	-8.365	H
-5.120	1.024	2.240	H	-6.074	-3.841	-7.255	H
-3.417	1.282	0.962	C	-6.356	-1.281	-5.319	C
-2.428	1.743	0.920	H	-5.278	-1.192	-5.284	H
-3.275	0.217	0.778	H	-7.152	-0.619	-4.379	C
-4.199	1.781	-0.239	N	-6.640	0.154	-3.303	N
-4.359	2.797	-0.193	H	-7.346	0.125	-2.111	C
-3.664	1.613	-1.114	H	-5.356	0.899	-3.432	C
-5.119	1.284	-0.365	H	-5.433	1.410	-4.394	H
-3.638	5.854	2.880	C	-5.384	1.670	-2.663	H
-4.658	6.448	3.236	O	-4.027	0.117	-3.287	C
				-3.901	-0.429	-4.257	H
-4.480	6.548	-1.742	N	-4.021	-0.503	-2.507	O
-4.518	7.562	-1.727	H	-4.726	-1.157	-2.320	H
-4.713	5.931	-3.036	C	-2.872	1.235	-3.450	C
-4.160	5.000	-3.090	H	-2.005	0.542	-3.569	H
-6.198	5.603	-3.333	C	-2.749	1.924	-2.677	O
-6.292	5.238	-4.364	H	-2.055	2.610	-2.722	H
-6.418	4.766	-2.661	H	-2.921	1.868	-4.921	C
-7.041	6.706	-3.068	O	-3.483	2.816	-4.718	H
-7.905	6.466	-3.468	H	-3.330	1.346	-5.697	O
-4.159	6.791	-4.155	C	-2.761	0.846	-6.323	H
-4.881	7.418	-4.926	O	-1.472	2.394	-5.207	C
				-1.497	3.047	-6.113	H
-6.725	0.399	-0.953	N	-1.156	3.066	-4.381	H
-7.453	0.275	0.199	C	-0.484	1.345	-5.338	O
-7.001	0.605	1.305	O	-0.263	0.585	-6.704	P
-8.746	-0.258	0.127	N	0.321	-0.769	-6.997	O
-9.166	-0.534	1.022	H	0.665	1.299	-7.626	O
-9.483	-0.415	-1.036	C	-1.582	0.178	-7.256	O
-10.704	-0.714	-0.997	O	-9.268	1.329	-3.682	H
-8.722	-0.159	-2.198	C	-10.325	-0.206	-3.525	H
-9.302	-0.058	-3.497	N				
-8.541	-0.773	-4.480	C	-11.500	3.876	-1.176	C
-9.114	-1.558	-5.472	C	-11.673	4.490	-2.066	H
-10.194	-1.670	-5.500	H	-11.013	4.502	-0.425	H
-8.313	-2.215	-6.412	C	-10.676	2.614	-1.488	C
-8.945	-3.073	-7.480	C	-10.486	2.120	-0.529	H
-10.028	-3.136	-7.344	H	-11.310	1.965	-2.093	H
-8.544	-4.095	-7.464	H	-9.397	2.871	-2.214	C
-8.760	-2.681	-8.488	H	-9.335	2.666	-3.592	C
-6.913	-2.062	-6.337	C	-10.283	2.709	-4.135	H
-6.005	-2.747	-7.332	C	-8.471	3.049	-4.138	H

-8.257	3.395	-1.406	C	-4.813	2.869	3.776	H
-7.294	3.161	-1.863	H	-4.689	3.539	2.118	H
-8.345	4.490	-1.350	H	-3.985	1.511	2.334	C
-8.276	3.019	-0.380	H	-3.362	0.971	3.056	H
-12.732	3.412	-0.616	O	-4.956	1.018	2.288	H
-14.024	3.371	-1.584	P	-3.276	1.352	0.991	C
-14.319	4.790	-2.069	O	-2.300	1.840	0.950	H
-13.853	2.343	-2.702	O	-3.106	0.294	0.793	H
-15.164	2.844	-0.611	O	-4.073	1.849	-0.202	N
-15.699	3.729	0.825	P	-4.216	2.871	-0.171	H
-15.217	2.901	1.980	O	-3.566	1.652	-1.089	H
-14.949	5.095	0.642	O	-5.002	1.379	-0.295	H
-17.191	3.842	0.559	O	-3.623	5.893	2.906	C
-14.897	5.911	-0.874	Mg	-4.662	6.461	3.247	O
-11.988	0.534	-4.092	O				
-12.594	1.219	-3.757	H	-4.500	6.532	-1.699	N
-12.117	0.533	-5.078	H	-4.548	7.546	-1.697	H
				-4.763	5.896	-2.979	C
Int1 _A				-4.227	4.956	-3.024	H
-13.395	-1.119	-10.357	N	-6.263	5.588	-3.235	C
-14.006	-1.130	-9.556	H	-6.370	5.149	-4.236	H
-11.992	-0.820	-10.103	C	-6.518	4.815	-2.496	H
-11.730	0.065	-10.673	H	-7.066	6.739	-3.063	O
-11.740	-0.558	-8.587	C	-7.931	6.502	-3.461	H
-12.221	-1.370	-8.032	H	-4.203	6.735	-4.116	C
-10.664	-0.613	-8.379	H	-4.921	7.336	-4.913	O
-12.376	1.039	-6.762	N				
-12.248	0.778	-8.113	C	-6.727	0.589	-0.929	N
-12.681	2.326	-6.669	C	-7.387	0.413	0.257	C
-12.851	2.862	-5.745	H	-6.861	0.640	1.345	O
-12.774	2.912	-7.882	N	-8.685	-0.136	0.241	N
-12.791	3.953	-8.022	H	-9.013	-0.559	1.123	H
-12.493	1.940	-8.813	C	-9.478	-0.201	-0.857	C
-12.482	2.144	-9.870	H	-10.592	-0.727	-0.834	O
-11.027	-1.910	-10.573	C	-8.901	0.479	-2.108	C
-9.988	-1.617	-11.161	O	-9.446	-0.195	-3.257	N
				-8.665	-0.710	-4.269	C
-3.301	5.015	5.223	N	-9.221	-1.513	-5.278	C
-4.285	4.916	5.394	H	-10.288	-1.706	-5.246	H
-2.847	4.993	3.846	C	-8.438	-2.109	-6.265	C
-1.836	5.371	3.820	H	-9.078	-2.997	-7.304	C
-2.825	3.554	3.278	C	-10.152	-3.098	-7.130	H
-2.119	3.524	2.418	H	-8.638	-4.003	-7.296	H
-2.401	2.897	4.071	H	-8.939	-2.608	-8.320	H
-4.163	2.930	2.877	C				

-7.043	-1.891	-6.269	C	-9.476	3.668	-3.547	H
-6.148	-2.519	-7.312	C	-8.324	2.426	-4.014	H
-5.110	-2.193	-7.190	H	-8.368	2.988	-1.237	C
-6.455	-2.254	-8.331	H	-7.338	2.973	-1.598	H
-6.159	-3.616	-7.256	H	-8.708	4.026	-1.296	H
-6.495	-1.076	-5.277	C	-8.371	2.720	-0.177	H
-5.429	-0.892	-5.313	H	-12.664	3.332	-0.744	O
-7.282	-0.472	-4.294	C	-14.006	3.340	-1.638	P
-6.709	0.290	-3.224	N	-14.308	4.767	-2.089	O
-7.381	0.395	-2.063	C	-13.895	2.313	-2.765	O
-5.370	0.939	-3.383	C	-15.125	2.819	-0.631	O
-5.447	1.415	-4.362	H	-15.664	3.699	0.801	P
-5.345	1.736	-2.640	H	-15.181	2.867	1.954	O
-4.083	0.096	-3.234	C	-14.918	5.067	0.622	O
-3.988	-0.481	-4.191	H	-17.159	3.810	0.544	O
-4.101	-0.502	-2.440	O	-14.880	5.888	-0.891	Mg
-4.785	-1.185	-2.278	H	-12.085	0.495	-4.109	O
-2.882	1.164	-3.436	C	-12.626	1.252	-3.816	H
-2.046	0.437	-3.578	H	-12.158	0.494	-5.102	H
-2.711	1.853	-2.673	O				
-2.006	2.525	-2.754	H	TS2 _A			
-2.952	1.791	-4.909	C	-13.409	-1.075	-10.366	N
-3.534	2.726	-4.704	H	-14.018	-1.092	-9.563	H
-3.355	1.252	-5.676	O	-12.011	-0.752	-10.117	C
-2.779	0.782	-6.320	H	-11.766	0.139	-10.687	H
-1.518	2.351	-5.209	C	-11.756	-0.493	-8.602	C
-1.565	2.996	-6.121	H	-12.223	-1.317	-8.052	H
-1.213	3.041	-4.394	H	-10.679	-0.536	-8.401	H
-0.506	1.326	-5.336	O	-12.425	1.049	-6.745	N
-0.271	0.573	-6.706	P	-12.276	0.827	-8.102	C
0.360	-0.803	-6.849	O	-12.738	2.331	-6.624	C
0.659	1.294	-7.619	O	-12.932	2.839	-5.689	H
-1.584	0.160	-7.267	O	-12.816	2.949	-7.822	N
-10.062	2.100	-4.134	H	-12.853	3.991	-7.944	H
-10.440	-0.044	-3.459	H	-12.514	2.005	-8.775	C
				-12.482	2.241	-9.825	H
				-11.032	-1.829	-10.591	C
-11.404	3.561	-1.407	C	-9.999	-1.525	-11.182	O
-11.554	4.006	-2.396	H				
-10.858	4.281	-0.795	H				
-10.721	2.195	-1.463	C	-3.309	5.021	5.225	N
-10.700	1.847	-0.425	H	-4.294	4.922	5.394	H
-11.391	1.537	-2.017	H	-2.849	4.992	3.849	C
-9.308	2.102	-2.077	C	-1.836	5.365	3.826	H
-9.294	2.592	-3.535	C	-2.829	3.551	3.290	C
				-2.124	3.509	2.429	H

-2.410	2.898	4.088	H	-9.324	-3.831	-6.718	H
-4.170	2.931	2.895	C	-9.512	-2.597	-7.954	H
-4.826	2.895	3.791	H	-7.522	-1.706	-6.090	C
-4.685	3.525	2.117	H	-6.740	-2.438	-7.157	C
-4.000	1.496	2.394	C	-5.673	-2.207	-7.095	H
-3.371	0.980	3.128	H	-7.079	-2.168	-8.165	H
-4.971	1.002	2.371	H	-6.853	-3.526	-7.069	H
-3.310	1.290	1.048	C	-6.846	-0.917	-5.155	C
-2.345	1.795	0.964	H	-5.768	-0.853	-5.230	H
-3.123	0.227	0.898	H	-7.518	-0.251	-4.125	C
-4.146	1.714	-0.145	N	-6.850	0.382	-3.043	N
-4.337	2.724	-0.124	H	-7.427	0.189	-1.796	C
-3.641	1.533	-1.034	H	-5.508	1.004	-3.227	C
-5.058	1.185	-0.221	H	-5.595	1.558	-4.165	H
-3.616	5.890	2.899	C	-5.409	1.745	-2.434	H
-4.652	6.469	3.231	O	-4.242	0.108	-3.211	C
				-4.243	-0.425	-4.196	H
-4.348	6.569	-1.752	N	-4.220	-0.531	-2.449	O
-4.352	7.584	-1.752	H	-4.904	-1.214	-2.276	H
-4.588	5.933	-3.034	C	-3.010	1.138	-3.430	C
-4.036	5.001	-3.075	H	-2.199	0.388	-3.593	H
-6.073	5.604	-3.292	C	-2.802	1.818	-2.666	O
-6.161	5.101	-4.261	H	-2.055	2.441	-2.743	H
-6.318	4.880	-2.506	H	-3.091	1.766	-4.899	C
-6.927	6.734	-3.205	O	-3.686	2.690	-4.686	H
-7.522	6.664	-3.982	H	-3.486	1.221	-5.666	O
-4.055	6.766	-4.183	C	-2.902	0.768	-6.315	H
-4.793	7.339	-4.981	O	-1.667	2.352	-5.207	C
				-1.727	2.990	-6.124	H
-6.692	0.312	-0.678	N	-1.375	3.054	-4.400	H
-7.315	0.081	0.516	C	-0.632	1.348	-5.328	O
-6.767	0.323	1.602	O	-0.376	0.594	-6.695	P
-8.613	-0.450	0.520	N	0.428	-0.681	-6.783	O
-8.985	-0.707	1.443	H	0.583	1.298	-7.592	O
-9.448	-0.470	-0.583	C	-1.684	0.193	-7.280	O
-10.678	-0.753	-0.500	O	-9.934	4.611	-3.391	H
-8.798	-0.101	-1.769	C	-10.544	-0.087	-2.884	H
-9.571	0.228	-2.927	N				
-8.916	-0.339	-4.086	C	-11.607	3.214	-2.144	C
-9.603	-1.126	-5.007	C	-11.904	2.790	-3.106	H
-10.678	-1.231	-4.906	H	-11.563	4.302	-2.229	H
-8.923	-1.839	-5.996	C	-10.274	2.632	-1.678	C
-9.667	-2.801	-6.888	C	-10.376	2.029	-0.772	H
-10.742	-2.778	-6.693	H	-9.891	1.663	-2.556	H

-9.136	3.430	-1.761	C	-2.991	3.429	3.210	C
-9.009	4.426	-2.846	C	-2.320	3.383	2.323	H
-8.606	5.375	-2.479	H	-2.563	2.735	3.969	H
-8.280	4.055	-3.579	H	-4.373	2.882	2.839	C
-7.972	3.270	-0.852	C	-5.002	2.852	3.753	H
-7.075	2.975	-1.409	H	-4.880	3.529	2.097	H
-7.756	4.252	-0.414	H	-4.304	1.458	2.280	C
-8.157	2.551	-0.056	H	-3.725	0.866	2.997	H
-12.591	2.895	-1.138	O	-5.311	1.041	2.226	H
-14.101	3.088	-1.729	P	-3.611	1.256	0.933	C
-14.292	4.543	-2.159	O	-2.610	1.692	0.886	H
-14.216	2.019	-2.815	O	-3.502	0.189	0.736	H
-15.097	2.687	-0.571	O	-4.391	1.787	-0.255	N
-15.629	3.688	0.789	P	-4.522	2.807	-0.204	H
-15.151	2.934	1.996	O	-3.877	1.603	-1.139	H
-14.856	5.020	0.508	O	-5.322	1.321	-0.357	H
-17.121	3.793	0.520	O	-3.673	5.819	2.887	C
-14.865	5.763	-1.046	Mg	-4.677	6.431	3.255	O
-12.148	0.558	-4.025	O				
-12.941	1.070	-3.769	H	-4.492	6.535	-1.740	N
-12.171	0.539	-5.014	H	-4.526	7.550	-1.724	H
				-4.719	5.923	-3.040	C
Prod _A				-4.164	4.994	-3.097	H
-13.361	-1.130	-10.295	N	-6.201	5.598	-3.353	C
-13.991	-1.136	-9.507	H	-6.299	5.293	-4.402	H
-11.960	-0.856	-10.004	C	-6.425	4.725	-2.731	H
-11.669	0.025	-10.567	H	-7.042	6.690	-3.025	O
-11.736	-0.598	-8.480	C	-7.898	6.481	-3.457	H
-12.242	-1.406	-7.940	H	-4.166	6.791	-4.152	C
-10.665	-0.671	-8.252	H	-4.887	7.426	-4.918	O
-12.355	1.025	-6.665	N				
-12.235	0.746	-8.015	C	-6.939	0.339	-1.091	N
-12.674	2.311	-6.585	C	-7.646	0.257	0.075	C
-12.854	2.849	-5.663	H	-7.186	0.669	1.151	O
-12.780	2.877	-7.804	N	-8.920	-0.319	0.053	N
-12.808	3.916	-7.970	H	-9.347	-0.508	0.965	H
-12.495	1.897	-8.726	C	-9.585	-0.692	-1.094	C
-12.492	2.093	-9.786	H	-10.781	-1.095	-1.071	O
-10.998	-1.960	-10.451	C	-8.813	-0.583	-2.264	C
-9.902	-1.680	-10.931	O	-9.481	-0.932	-3.520	N
				-8.525	-1.240	-4.597	C
-3.342	4.904	5.191	N	-8.962	-2.001	-5.676	C
-4.321	4.816	5.390	H	-10.001	-2.320	-5.705	H
-2.925	4.862	3.799	C	-8.095	-2.373	-6.705	C
-1.895	5.181	3.750	H				

-8.589	-3.191	-7.870	C	-10.134	4.157	0.012	H
-9.660	-3.392	-7.780	H	-10.223	-0.203	-3.794	H
-8.069	-4.155	-7.939	H	-9.037	3.491	-1.634	C
-8.434	-2.677	-8.827	H	-8.922	3.042	-3.071	C
-6.749	-1.957	-6.618	C	-8.481	3.820	-3.702	H
-5.751	-2.332	-7.688	C	-8.260	2.175	-3.148	H
-4.771	-1.889	-7.490	H	-7.736	3.617	-0.861	C
-6.076	-1.990	-8.677	H	-6.926	3.069	-1.350	H
-5.624	-3.420	-7.755	H	-7.440	4.669	-0.783	H
-6.334	-1.189	-5.530	C	-7.839	3.213	0.148	H
-5.305	-0.855	-5.516	H	-12.528	3.279	-0.939	O
-7.200	-0.798	-4.495	C	-13.951	3.285	-1.702	P
-6.758	-0.043	-3.396	N	-14.307	4.712	-2.126	O
-7.502	-0.092	-2.228	C	-13.868	2.265	-2.844	O
-5.507	0.772	-3.478	C	-15.022	2.745	-0.651	O
-5.571	1.276	-4.443	H	-15.612	3.642	0.761	P
-5.609	1.541	-2.715	H	-15.144	2.829	1.932	O
-4.155	0.041	-3.262	C	-14.886	5.021	0.581	O
-3.986	-0.553	-4.197	H	-17.105	3.731	0.482	O
-4.151	-0.539	-2.453	O	-14.879	5.838	-0.934	Mg
-4.832	-1.218	-2.262	H	-11.661	0.488	-4.113	O
-3.025	1.184	-3.452	C	-12.140	1.223	-3.689	H
-2.137	0.513	-3.537	H	-11.915	0.539	-5.085	H
-2.932	1.905	-2.704	O				
-2.220	2.574	-2.738	H	React _B			
-3.070	1.756	-4.948	C	-14.346	-1.136	-10.074	N
-3.681	2.680	-4.784	H	-14.945	-1.213	-9.267	H
-3.439	1.184	-5.710	O	-12.964	-0.740	-9.807	C
-2.832	0.741	-6.344	H	-12.785	0.213	-10.293	H
-1.642	2.345	-5.229	C	-12.675	-0.617	-8.277	C
-1.687	2.985	-6.144	H	-13.062	-1.523	-7.799	H
-1.366	3.044	-4.412	H	-11.589	-0.601	-8.110	H
-0.604	1.343	-5.336	O	-13.566	0.605	-6.276	N
-0.325	0.583	-6.694	P	-13.286	0.597	-7.630	C
0.469	-0.656	-7.002	O	-13.965	1.839	-5.990	C
0.617	1.304	-7.595	O	-14.272	2.184	-5.008	H
-1.620	0.149	-7.282	O	-13.971	2.624	-7.092	N
-9.882	2.761	-3.512	H	-14.082	3.664	-7.097	H
-10.030	-1.787	-3.338	H	-13.531	1.851	-8.143	C
				-13.430	2.254	-9.138	H
				-11.936	-1.711	-10.383	C
				-11.047	-1.324	-11.143	O
				-4.056	5.504	5.158	N
				-5.054	5.442	5.220	H
-11.503	4.021	-1.673	C	-3.511	5.704	3.826	C
-11.496	3.685	-2.715	H	-2.584	6.256	3.907	H
-11.795	5.076	-1.665	H	-3.221	4.351	3.127	C
-10.179	3.842	-1.027	C	-2.449	3.841	3.746	H
				-2.758	4.533	2.132	H

-4.416	3.397	2.990	C	-5.357	1.052	-4.287	H
-5.172	3.811	2.295	H	-5.369	1.166	-2.557	H
-4.899	3.278	3.982	H	-3.932	-0.284	-3.253	C
-4.016	1.992	2.525	C	-3.780	-0.798	-4.235	H
-4.882	1.329	2.671	H	-3.887	-0.929	-2.479	O
-3.224	1.643	3.201	H	-4.516	-1.679	-2.367	H
-3.536	1.844	1.067	C	-2.864	0.907	-3.402	C
-3.074	0.856	0.946	H	-1.936	0.301	-3.506	H
-2.733	2.550	0.833	H	-2.840	1.583	-2.609	O
-4.598	1.970	0.035	N	-3.353	1.421	-1.798	H
-4.755	2.957	-0.165	H	-2.938	1.520	-4.891	C
-5.465	1.638	0.463	H	-3.465	2.488	-4.690	H
-4.437	6.549	2.963	C	-3.376	1.005	-5.659	O
-5.639	6.638	3.220	O	-2.809	0.519	-6.289	H
				-1.480	1.989	-5.210	C
-5.487	7.041	-1.134	N	-1.510	2.671	-6.093	H
-6.406	7.130	-0.733	H	-1.122	2.607	-4.359	H
-5.379	6.306	-2.390	C	-0.537	0.908	-5.412	O
-4.744	5.450	-2.181	H	-0.350	0.163	-6.790	P
-6.750	5.742	-2.850	C	0.331	-1.151	-6.582	O
-6.614	5.158	-3.769	H	0.533	0.939	-7.710	O
-7.060	5.051	-2.055	H	-1.657	-0.257	-7.359	O
-7.680	6.793	-3.006	O				
-8.545	6.425	-3.282	H	-11.542	2.469	-1.701	C
-4.723	7.019	-3.578	C	-11.663	3.427	-1.188	H
-5.218	8.016	-4.106	O	-11.418	1.681	-0.950	H
				-10.400	2.484	-2.699	C
-6.768	-0.157	-1.061	N	-10.397	1.531	-3.248	H
-7.468	-0.214	0.127	C	-10.604	3.254	-3.455	H
-6.994	0.231	1.178	O	-9.017	2.717	-2.151	C
-8.693	-0.817	0.026	N	-7.958	2.711	-3.216	C
-9.230	-0.897	0.903	H	-7.977	1.769	-3.770	H
-9.321	-1.249	-1.157	C	-6.954	2.854	-2.813	H
-10.467	-1.738	-1.091	O	-8.150	3.495	-3.956	H
-8.564	-1.061	-2.346	C	-8.751	2.907	-0.851	C
-9.143	-1.322	-3.615	N	-9.529	2.889	-0.092	H
-8.244	-1.521	-4.682	C	-7.733	3.054	-0.500	H
-8.649	-2.146	-5.863	C	-12.730	2.189	-2.471	O
-9.670	-2.513	-5.918	H	-14.176	2.690	-1.925	P
-7.786	-2.315	-6.954	C	-14.033	4.175	-1.546	O
-8.300	-2.953	-8.222	C	-15.166	2.285	-2.981	O
-9.327	-3.308	-8.094	H	-14.323	1.826	-0.575	O
-7.683	-3.805	-8.536	H	-15.722	2.010	0.414	P
-8.301	-2.242	-9.058	H	-15.476	1.074	1.574	O
-6.465	-1.847	-6.856	C	-15.662	3.516	0.808	O
-5.494	-1.959	-8.007	C	-16.882	1.605	-0.489	O
-4.533	-1.501	-7.759	H	-14.771	4.686	-0.067	Mg
-5.865	-1.451	-8.907	H	-13.258	-0.434	-3.683	O
-5.314	-3.006	-8.289	H	-13.338	-0.242	-4.650	H
-6.054	-1.222	-5.668	C	-12.874	0.381	-3.318	H
-5.055	-0.805	-5.642	H				
-6.921	-1.047	-4.588	C	TS1 _B			
-6.517	-0.373	-3.395	N	-14.366	-1.151	-10.073	N
-7.289	-0.536	-2.281	C	-14.968	-1.231	-9.270	H
-5.836	0.245	-1.002	H	-12.984	-0.761	-9.795	C
-9.862	-2.045	-3.571	H	-12.799	0.195	-10.274	H
-5.289	0.456	-3.382	C				

-12.710	-0.649	-8.262	C	-8.485	6.439	-3.341	H
-13.129	-1.545	-7.792	H	-4.683	7.056	-3.603	C
-11.627	-0.668	-8.078	H	-5.192	8.050	-4.123	O
-13.576	0.603	-6.267	N				
-13.295	0.582	-7.621	C	-7.150	0.244	-1.116	N
-13.958	1.844	-5.990	C	-7.830	-0.055	0.049	C
-14.264	2.198	-5.011	H	-7.517	0.460	1.127	O
-13.950	2.621	-7.097	N	-8.931	-0.900	-0.047	N
-14.059	3.662	-7.109	H	-9.434	-1.069	0.836	H
-13.521	1.836	-8.143	C	-9.513	-1.312	-1.242	C
-13.410	2.231	-9.140	H	-10.591	-1.944	-1.240	O
-11.955	-1.729	-10.372	C	-8.766	-0.974	-2.420	C
-11.067	-1.338	-11.130	O	-9.273	-1.329	-3.679	N
				-8.319	-1.496	-4.710	C
-4.079	5.448	5.129	N	-8.634	-2.223	-5.855	C
-5.076	5.373	5.194	H	-9.618	-2.682	-5.910	H
-3.537	5.647	3.795	C	-7.724	-2.385	-6.910	C
-2.591	6.168	3.876	H	-8.133	-3.144	-8.150	C
-3.290	4.294	3.077	C	-9.101	-3.633	-8.007	H
-2.586	3.722	3.720	H	-7.399	-3.912	-8.424	H
-2.764	4.479	2.114	H	-8.227	-2.478	-9.019	H
-4.531	3.419	2.838	C	-6.459	-1.791	-6.799	C
-5.203	3.894	2.097	H	-5.441	-1.873	-7.912	C
-5.094	3.316	3.788	H	-4.527	-1.330	-7.654	H
-4.193	1.999	2.364	C	-5.818	-1.439	-8.847	H
-5.124	1.413	2.345	H	-5.168	-2.915	-8.137	H
-3.541	1.565	3.138	H	-6.145	-1.059	-5.641	C
-3.501	1.872	0.989	C	-5.192	-0.550	-5.626	H
-3.097	0.858	0.878	H	-7.045	-0.904	-4.584	C
-2.619	2.520	0.927	H	-6.725	-0.170	-3.405	N
-4.343	2.117	-0.198	N	-7.544	-0.328	-2.297	C
-4.675	3.081	-0.178	H	-7.726	1.645	-1.202	H
-5.179	1.531	-0.142	H	-9.932	-2.110	-3.629	H
-4.442	6.529	2.944	C	-5.453	0.600	-3.321	C
-5.641	6.642	3.202	O	-5.475	1.271	-4.178	H
				-5.511	1.208	-2.421	H
-5.453	7.052	-1.158	N	-4.115	-0.189	-3.236	C
-6.375	7.133	-0.760	H	-4.006	-0.721	-4.212	H
-5.329	6.331	-2.419	C	-4.066	-0.831	-2.463	O
-4.686	5.479	-2.216	H	-4.802	-1.437	-2.223	H
-6.688	5.764	-2.901	C	-3.000	0.955	-3.445	C
-6.548	5.233	-3.851	H	-2.102	0.307	-3.557	H
-6.961	5.022	-2.138	H	-2.918	1.659	-2.682	O
-7.645	6.796	-2.983	O	-3.431	1.607	-1.847	H

-3.075	1.537	-4.948	C	-12.825	0.265	-10.302	H
-3.618	2.499	-4.764	H	-12.689	-0.608	-8.302	C
-3.499	1.004	-5.712	O	-13.082	-1.518	-7.837	H
-2.910	0.531	-6.333	H	-11.603	-0.603	-8.135	H
-1.624	2.032	-5.274	C	-13.582	0.587	-6.287	N
-1.666	2.689	-6.175	H	-13.296	0.600	-7.639	C
-1.284	2.681	-4.440	H	-13.978	1.819	-5.986	C
-0.653	0.971	-5.442	O	-14.293	2.154	-5.004	H
-0.422	0.206	-6.800	P	-13.975	2.620	-7.077	N
0.383	-1.021	-6.406	O	-14.081	3.661	-7.072	H
0.497	0.965	-7.700	O	-13.533	1.862	-8.136	C
-1.712	-0.208	-7.410	O	-13.419	2.283	-9.122	H
				-11.938	-1.638	-10.430	C
-11.458	2.423	-1.756	C	-11.062	-1.227	-11.191	O
-11.528	3.410	-1.288	H				
-11.288	1.675	-0.973	H	-4.069	5.552	5.191	N
-10.397	2.372	-2.849	C	-5.065	5.456	5.231	H
-10.420	1.379	-3.334	H	-3.497	5.790	3.877	C
-10.706	3.059	-3.649	H	-2.606	6.394	3.992	H
-8.980	2.698	-2.522	C	-3.101	4.463	3.184	C
-8.119	2.916	-3.710	C	-2.379	3.956	3.864	H
-8.244	2.079	-4.405	H	-2.547	4.685	2.244	H
-7.061	3.005	-3.470	H	-4.246	3.483	2.892	C
-8.447	3.811	-4.256	H	-4.905	3.883	2.097	H
-8.409	2.703	-1.231	C	-4.859	3.351	3.807	H
-9.078	2.645	-0.371	H	-3.756	2.089	2.479	C
-7.570	3.391	-1.084	H	-4.637	1.438	2.396	H
-12.684	2.125	-2.442	O	-3.142	1.713	3.310	H
-14.128	2.661	-1.896	P	-2.941	1.996	1.170	C
-13.953	4.141	-1.510	O	-2.454	1.014	1.119	H
-15.115	2.284	-2.965	O	-2.105	2.706	1.167	H
-14.295	1.792	-0.556	O	-3.695	2.162	-0.088	N
-15.706	2.006	0.419	P	-4.064	3.111	-0.134	H
-15.486	1.069	1.583	O	-4.515	1.554	-0.068	H
-15.622	3.510	0.809	O	-4.435	6.587	2.983	C
-16.859	1.618	-0.500	O	-5.638	6.671	3.236	O
-14.710	4.680	-0.047	Mg				
-13.286	-0.482	-3.707	O	-5.476	6.947	-1.114	N
-13.371	-0.255	-4.668	H	-6.390	7.006	-0.697	H
-12.868	0.304	-3.321	H	-5.360	6.196	-2.362	C
				-4.696	5.364	-2.148	H
Int1 _B				-6.724	5.580	-2.799	C
-14.359	-1.118	-10.089	N	-6.596	4.994	-3.719	H
-14.952	-1.200	-9.279	H	-6.997	4.879	-1.994	H
-12.981	-0.699	-9.832	C				

-7.667	6.620	-2.934	O	-2.718	1.569	-1.689	H
-8.526	6.270	-3.250	H	-2.570	1.613	-4.795	C
-4.734	6.923	-3.563	C	-3.036	2.598	-4.536	H
-5.263	7.899	-4.098	O	-3.074	1.149	-5.552	O
				-2.564	0.653	-6.223	H
-6.404	0.410	-0.832	N	-1.112	2.018	-5.179	C
-7.070	0.124	0.327	C	-1.150	2.721	-6.045	H
-6.656	0.398	1.450	O	-0.681	2.597	-4.333	H
-8.272	-0.619	0.227	N	-0.244	0.893	-5.451	O
-8.733	-0.916	1.102	H	-0.186	0.164	-6.846	P
-8.978	-0.799	-0.916	C	0.468	-1.144	-6.552	O
-9.965	-1.527	-0.972	O	0.693	0.909	-7.790	O
-8.485	0.016	-2.116	C	-1.545	-0.151	-7.358	O
-8.892	-0.690	-3.316	N				
-8.002	-0.955	-4.346	C	-11.553	2.527	-2.010	C
-8.387	-1.761	-5.430	C	-11.149	3.439	-2.462	H
-9.393	-2.174	-5.421	H	-11.706	2.713	-0.943	H
-7.517	-2.059	-6.478	C	-10.687	1.297	-2.270	C
-7.968	-2.966	-7.600	C	-11.063	0.494	-1.630	H
-8.989	-3.322	-7.433	H	-10.854	0.978	-3.302	H
-7.315	-3.845	-7.693	H	-9.171	1.505	-2.067	C
-7.946	-2.456	-8.571	H	-8.610	2.334	-3.237	C
-6.231	-1.479	-6.484	C	-8.735	1.811	-4.185	H
-5.257	-1.721	-7.613	C	-7.550	2.567	-3.111	H
-4.319	-1.184	-7.447	H	-9.142	3.287	-3.317	H
-5.650	-1.384	-8.580	H	-8.922	2.272	-0.752	C
-5.023	-2.790	-7.719	H	-9.363	1.784	0.122	H
-5.860	-0.655	-5.418	C	-9.394	3.256	-0.831	H
-4.887	-0.186	-5.466	H	-12.816	2.244	-2.641	O
-6.703	-0.426	-4.322	C	-14.218	2.748	-1.991	P
-6.245	0.218	-3.131	N	-14.041	4.229	-1.610	O
-6.978	0.185	-2.000	C	-15.249	2.333	-3.002	O
-7.859	2.438	-0.563	H	-14.309	1.884	-0.637	O
-9.571	-1.431	-3.143	H	-15.700	2.056	0.382	P
-4.891	0.847	-3.103	C	-15.430	1.126	1.538	O
-4.918	1.532	-3.948	H	-15.642	3.562	0.769	O
-4.843	1.438	-2.193	H	-16.875	1.646	-0.500	O
-3.656	-0.088	-3.112	C	-14.757	4.726	-0.114	Mg
-3.650	-0.595	-4.109	H	-13.292	-0.437	-3.679	O
-3.648	-0.758	-2.366	O	-13.360	-0.313	-4.656	H
-4.438	-1.274	-2.093	H	-13.019	0.445	-3.369	H
-2.442	0.942	-3.335	C				
-1.627	0.214	-3.544	H	TS _{2B}			
-2.236	1.587	-2.544	O	-14.344	-1.134	-10.096	N
				-14.932	-1.220	-9.282	H

-12.966	-0.712	-9.852	C	-6.889	4.964	-1.911	H
-12.813	0.248	-10.334	H	-7.607	6.647	-2.913	O
-12.657	-0.600	-8.328	C	-8.456	6.283	-3.235	H
-13.016	-1.519	-7.852	H	-4.684	6.992	-3.544	C
-11.570	-0.557	-8.176	H	-5.206	7.989	-4.046	O
-13.576	0.566	-6.312	N				
-13.292	0.591	-7.664	C	-6.429	-0.043	-0.753	N
-13.991	1.789	-6.003	C	-6.978	-0.403	0.442	C
-14.317	2.110	-5.019	H	-6.370	-0.317	1.516	O
-14.004	2.596	-7.090	N	-8.296	-0.915	0.448	N
-14.111	3.637	-7.079	H	-8.743	-1.053	1.365	H
-13.549	1.851	-8.154	C	-9.108	-1.019	-0.661	C
-13.445	2.279	-9.138	H	-10.295	-1.410	-0.598	O
-11.924	-1.656	-10.442	C	-8.478	-0.623	-1.870	C
-11.035	-1.248	-11.190	O	-9.292	-0.621	-3.040	N
				-8.494	-0.817	-4.248	C
-4.075	5.523	5.194	N	-9.067	-1.427	-5.363	C
-5.072	5.446	5.241	H	-10.113	-1.718	-5.308	H
-3.509	5.750	3.876	C	-8.322	-1.693	-6.517	C
-2.596	6.321	3.986	H	-8.966	-2.375	-7.701	C
-3.163	4.419	3.162	C	-10.003	-2.648	-7.484	H
-2.462	3.877	3.836	H	-8.432	-3.293	-7.981	H
-2.599	4.637	2.227	H	-8.973	-1.735	-8.593	H
-4.337	3.481	2.847	C	-6.970	-1.282	-6.552	C
-4.975	3.908	2.051	H	-6.116	-1.492	-7.783	C
-4.960	3.359	3.757	H	-5.135	-1.024	-7.670	H
-3.883	2.075	2.429	C	-6.584	-1.061	-8.676	H
-4.766	1.425	2.367	H	-5.963	-2.560	-7.990	H
-3.260	1.694	3.250	H	-6.406	-0.663	-5.434	C
-3.089	1.958	1.107	C	-5.375	-0.334	-5.498	H
-2.557	1.000	1.095	H	-7.132	-0.453	-4.246	C
-2.292	2.709	1.050	H	-6.527	0.055	-3.085	N
-3.877	2.019	-0.141	N	-7.138	-0.201	-1.873	C
-4.367	2.912	-0.181	H	-7.635	2.010	-0.271	H
-4.609	1.308	-0.104	H	-9.981	-1.383	-2.963	H
-4.427	6.589	3.003	C	-5.188	0.705	-3.129	C
-5.631	6.682	3.251	O	-5.253	1.395	-3.969	H
				-5.104	1.296	-2.220	H
-5.418	7.022	-1.095	N	-3.931	-0.202	-3.204	C
-6.339	7.104	-0.697	H	-3.992	-0.714	-4.197	H
-5.289	6.268	-2.334	C	-3.847	-0.868	-2.459	O
-4.610	5.448	-2.118	H	-4.594	-1.412	-2.123	H
-6.641	5.632	-2.748	C	-2.754	0.859	-3.478	C
-6.509	5.015	-3.645	H	-1.915	0.154	-3.672	H

-2.562	1.544	-2.715	O	-14.947	-1.214	-9.263	H
-2.983	1.498	-1.830	H	-12.961	-0.744	-9.790	C
-2.927	1.459	-4.959	C	-12.778	0.210	-10.274	H
-3.477	2.409	-4.736	H	-12.680	-0.625	-8.258	C
-3.381	0.916	-5.697	O	-13.074	-1.531	-7.786	H
-2.818	0.455	-6.349	H	-11.593	-0.618	-8.088	H
-1.507	1.985	-5.355	C	-13.530	0.619	-6.248	N
-1.599	2.623	-6.264	H	-13.287	0.592	-7.611	C
-1.149	2.660	-4.547	H	-13.952	1.849	-5.976	C
-0.519	0.942	-5.535	O	-14.254	2.201	-4.994	H
-0.330	0.153	-6.883	P	-14.005	2.611	-7.092	N
0.478	-1.109	-6.925	O	-14.125	3.651	-7.106	H
0.578	0.900	-7.801	O	-13.571	1.831	-8.139	C
-1.639	-0.240	-7.467	O	-13.500	2.218	-9.143	H
				-11.931	-1.714	-10.363	C
-11.475	2.555	-2.805	C	-11.025	-1.323	-11.101	O
-11.171	2.632	-3.855	H				
-11.512	3.563	-2.375	H	-4.080	5.429	5.109	N
-10.527	1.676	-1.973	C	-5.078	5.374	5.177	H
-11.053	1.225	-1.127	H	-3.541	5.640	3.776	C
-10.045	0.521	-2.794	H	-2.605	6.177	3.863	H
-9.265	2.197	-1.690	C	-3.261	4.298	3.049	C
-8.529	2.919	-2.778	C	-2.552	3.737	3.696	H
-8.796	2.562	-3.774	H	-2.727	4.501	2.094	H
-7.447	2.835	-2.660	H	-4.474	3.393	2.784	C
-8.783	3.988	-2.750	H	-5.135	3.841	2.016	H
-8.695	2.278	-0.314	C	-5.062	3.288	3.719	H
-9.261	1.697	0.414	H	-4.083	1.975	2.344	C
-8.754	3.334	-0.006	H	-4.992	1.357	2.317	H
-12.790	2.007	-2.785	O	-3.433	1.577	3.138	H
-14.133	2.615	-2.055	P	-3.358	1.841	0.984	C
-13.891	4.092	-1.678	O	-2.860	0.865	0.936	H
-15.220	2.256	-3.028	O	-2.537	2.562	0.898	H
-14.231	1.753	-0.708	O	-4.200	1.944	-0.223	N
-15.636	1.986	0.315	P	-4.642	2.862	-0.245	H
-15.392	1.063	1.481	O	-4.968	1.274	-0.152	H
-15.520	3.492	0.677	O	-4.455	6.516	2.931	C
-16.817	1.598	-0.565	O	-5.653	6.629	3.199	O
-14.613	4.650	-0.192	Mg				
-13.185	-0.596	-3.770	O	-5.468	6.992	-1.151	N
-13.309	-0.418	-4.733	H	-6.387	7.058	-0.746	H
-12.917	0.276	-3.428	H	-5.342	6.254	-2.403	C
				-4.677	5.422	-2.195	H
Prod _B				-6.696	5.642	-2.854	C
-14.344	-1.137	-10.066	N				

-6.562	5.078	-3.785	H	-2.025	0.225	-3.644	H
-6.952	4.922	-2.066	H	-2.841	1.562	-2.748	O
-7.659	6.670	-2.961	O	-3.313	1.491	-1.889	H
-8.515	6.310	-3.273	H	-3.054	1.442	-5.008	C
-4.721	6.986	-3.597	C	-3.620	2.388	-4.813	H
-5.237	7.985	-4.103	O	-3.474	0.893	-5.762	O
				-2.879	0.438	-6.389	H
-6.818	-0.134	-1.061	N	-1.623	1.974	-5.358	C
-7.490	-0.326	0.109	C	-1.691	2.618	-6.266	H
-7.038	0.040	1.201	O	-1.292	2.643	-4.536	H
-8.742	-0.970	0.061	N	-0.625	0.936	-5.520	O
-9.245	-1.057	0.955	H	-0.391	0.155	-6.865	P
-9.388	-1.353	-1.099	C	0.368	-1.084	-7.275	O
-10.530	-1.878	-1.086	O	0.516	0.919	-7.771	O
-8.639	-1.102	-2.272	C	-1.680	-0.274	-7.469	O
-9.288	-1.437	-3.543	N				
-8.342	-1.468	-4.683	C	-11.544	3.170	-2.560	C
-8.772	-2.074	-5.860	C	-11.120	3.028	-3.559	H
-9.770	-2.505	-5.888	H	-11.960	4.181	-2.490	H
-7.947	-2.148	-6.981	C	-10.520	2.962	-1.496	C
-8.445	-2.785	-8.255	C	-10.906	2.957	-0.477	H
-9.450	-3.195	-8.119	H	-10.087	-0.813	-3.734	H
-7.790	-3.599	-8.592	H	-9.198	2.901	-1.721	C
-8.498	-2.059	-9.076	H	-8.609	2.900	-3.121	C
-6.653	-1.586	-6.885	C	-9.118	2.181	-3.773	H
-5.704	-1.615	-8.060	C	-7.551	2.633	-3.111	H
-4.775	-1.085	-7.837	H	-8.696	3.872	-3.617	H
-6.145	-1.142	-8.946	H	-8.227	2.879	-0.565	C
-5.454	-2.646	-8.344	H	-8.716	2.556	0.358	H
-6.239	-0.983	-5.698	C	-7.793	3.875	-0.386	H
-5.261	-0.523	-5.681	H	-12.643	2.228	-2.455	O
-7.062	-0.908	-4.552	C	-14.122	2.689	-1.940	P
-6.627	-0.319	-3.367	N	-14.040	4.182	-1.570	O
-7.371	-0.509	-2.211	C	-15.106	2.255	-2.998	O
-7.390	2.204	-0.753	H	-14.274	1.820	-0.599	O
-9.717	-2.386	-3.466	H	-15.702	1.992	0.364	P
-5.363	0.477	-3.315	C	-15.466	1.058	1.527	O
-5.435	1.169	-4.151	H	-15.662	3.497	0.760	O
-5.410	1.056	-2.397	H	-16.839	1.574	-0.563	O
-4.023	-0.302	-3.297	C	-14.768	4.690	-0.080	Mg
-3.965	-0.817	-4.288	H	-13.056	-0.369	-3.656	O
-3.933	-0.958	-2.541	O	-13.201	-0.153	-4.612	H
-4.660	-1.554	-2.255	H	-12.759	0.469	-3.254	H
-2.930	0.859	-3.512	C				