Supporting information

Catalytic mechanisms of the PrhA (V150L/A232S) double mutant involved in the fungal meroterpenoid biosynthetic pathway: A QM/MM study

Jie Bai, Lijuan Yan and Yongjun Liu*

Key Lab of Colloid and Interface Chemistry, Ministry of Education, School of Chemistry and Chemical Engineering, Shandong University, Jinan, Shandong 250100, China

Table S1 Spin densities of key atoms in ^{1}Re, ^{3}Re, ^{5}Re and ^{7}Re at the B3LYP/6-31G(d, p)/ LANL2DZ basis set.

	Fe	**O**
^{1}Re	-0.69	0.57
^{3}Re	2.71	-0.57
^{5}Re	3.01	0.74
^{7}Re	4.06	1.23

Table S2 Spin densities of key atoms of species involved in desaturation process at the B3LYP/6-31G(d, p)/ LANL2DZ basis set.

	Fe	**O**	C2	C1
^{3}Re	2.71	-0.57	0	0
^{3}TS1	1.02	0.55	0.39	0
^{3}IM1	0.94	0.06	0.74	0
^{3}TS2	0.89	0.12	0.73	0
^{3}IM2	0.97	0.06	0.72	0
^{3}TS3	1.44	-0.05	0.46	0
^{3}IM3	1.93	0	0	0

	Fe	**O**	C2	C1
^{5}Re	3.01	0.74	0	0
^{5}TS1	2.93	0.45	0.27	0
^{5}IM1	2.75	0.10	0.74	0
^{5}TS2	2.80	0.12	0.74	0
^{5}IM2	2.74	0.12	0.72	0
^{5}TS3	3.24	-0.08	0.50	0
^{5}IM3	3.67	0.07	0	0

Table S3 Spin densities of key atoms of involved species in ring rearrangement process at the B3LYP/6-31G(d, p)/ LANL2DZ basis set.

	Fe	**O**	C5	C2	C10	C9
^{3}IM3'	1.33	0.70	0	0	0	0
^{3}TS4	2.62	-0.20	-0.35	0.01	0	0
^{3}IM4	2.72	0.09	-0.86	-0.01	0.02	-0.01
^{3}TS5	2.72	0.10	-0.53	-0.40	0.01	0
^{3}IM5	2.72	0.09	-0.03	-0.70	-0.09	-0.01
^{3}TS6	2.72	0.09	0.02	-0.36	-0.51	0.01
^{3}IM6	2.72	0.09	0.02	-0.16	-0.73	0.02
^{3}TS7	1.94	0	0	0	-0.02	0
^{3}IM7	1.92	0	0	0	0	0

	Fe	**O**	C5	C2	C10	C9
^{5}IM3'	3.06	0.70	0	0	0	0
^{5}TS4	3.96	0.11	-0.33	0	0	0
^{5}IM4	4.07	0.39	-0.86	-0.01	0.02	0
^{5}TS5	4.23	0.29	-0.45	-0.38	0	0
^{5}IM5	4.23	0.30	-0.03	-0.61	-0.09	0
^{5}TS6	4.23	0.29	0	-0.18	-0.64	-0.01
^{5}IM6	4.23	0.29	0	-0.14	-0.68	-0.01
^{5}TS7	3.65	-0.01	0	0.01	0.07	-0.01
^{5}IM7	3.66	0.04	0	0	0	0

Table S4 Spin densities of key atoms in involved species in hydroxylation process at the B3LYP/6-31G(d, p)/ LANL2DZ basis set.

	Fe	**O**	C13	C9
^{5}IM7'	3.06	0.67	0	0
^{5}TS8	3.85	0.09	-0.18	-0.16
^{5}IM8	4.09	0.33	-0.47	-0.61
^{5}TS9	4.09	0.34	-0.41	-0.65
^{5}IM9	4.08	0.37	-0.47	-0.61
^{5}TS10	4.16	0.22	-0.38	-0.42
^{5}P	3.65	0.03	0	0

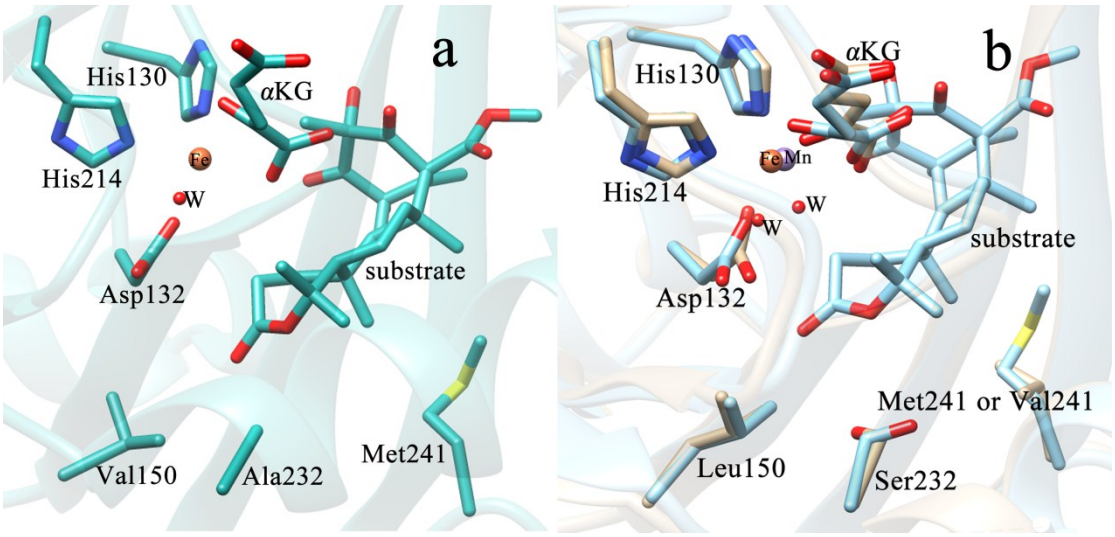

Figure S1 a) Active site of PrhA-Fe/αKG/substrate (PDB code: 5ybo). B) Comparison of active sites of AusE-Mn/*α*KG (PDB code: 5ybl) and PrhA (V150L/A232S)-Fe/*α*KG/substrate. Key residues, *α*-ketoglutarate and substrate are shown as stick models. Mn(II) and Fe(II) are shown as spheres. The active site structures of AusE and PrhA(V150L/A232S) are highly similar, except for the Met241 and Ser232 near the A/B-ring of substrate. Val241 and Met241 residues are derived from AusE and PrhA(V150L/A232S), respectively.

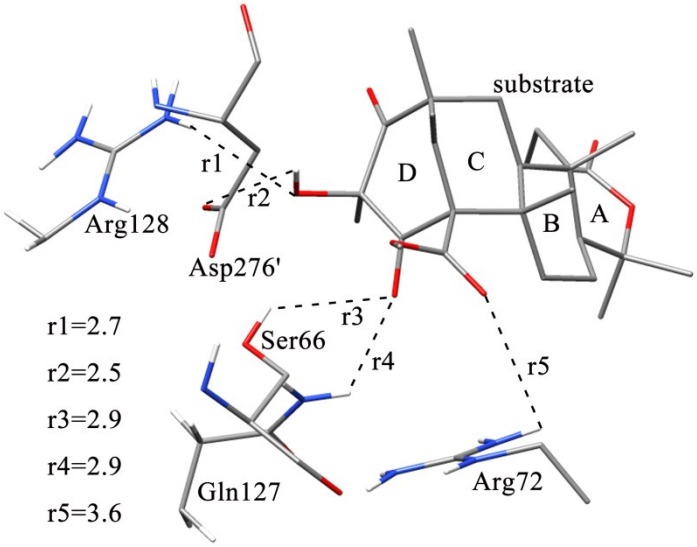

Figure S2 Several residues that form hydrogen bonds with the substrate. Possible hydrogen bonds are shown by black dashed lines. All distances are shown in angstroms.

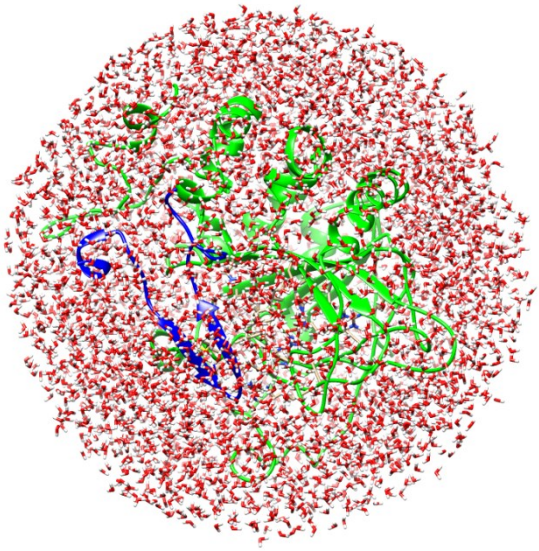

Figure S3 Constructed solvation model for the MD simulations.

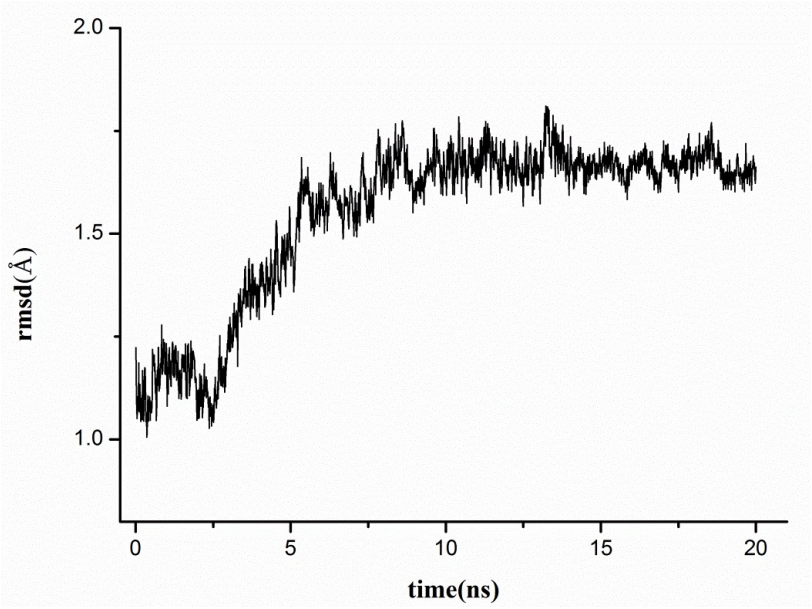

Figure S4 Calculated RMSD for backbone atoms of PrhA(V150L/A232S) double mutant in MD-I.

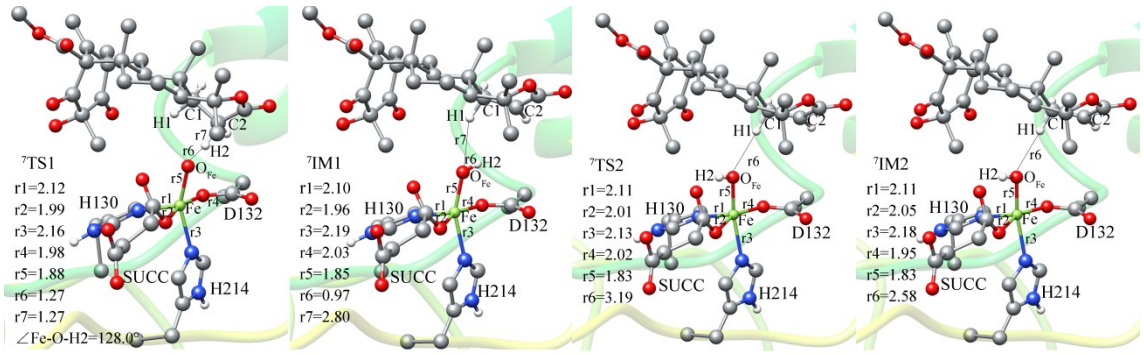

Figure S5 Optimized structures of transition states and intermediates involved in the desaturation process in septet. All distances are shown in angstroms.

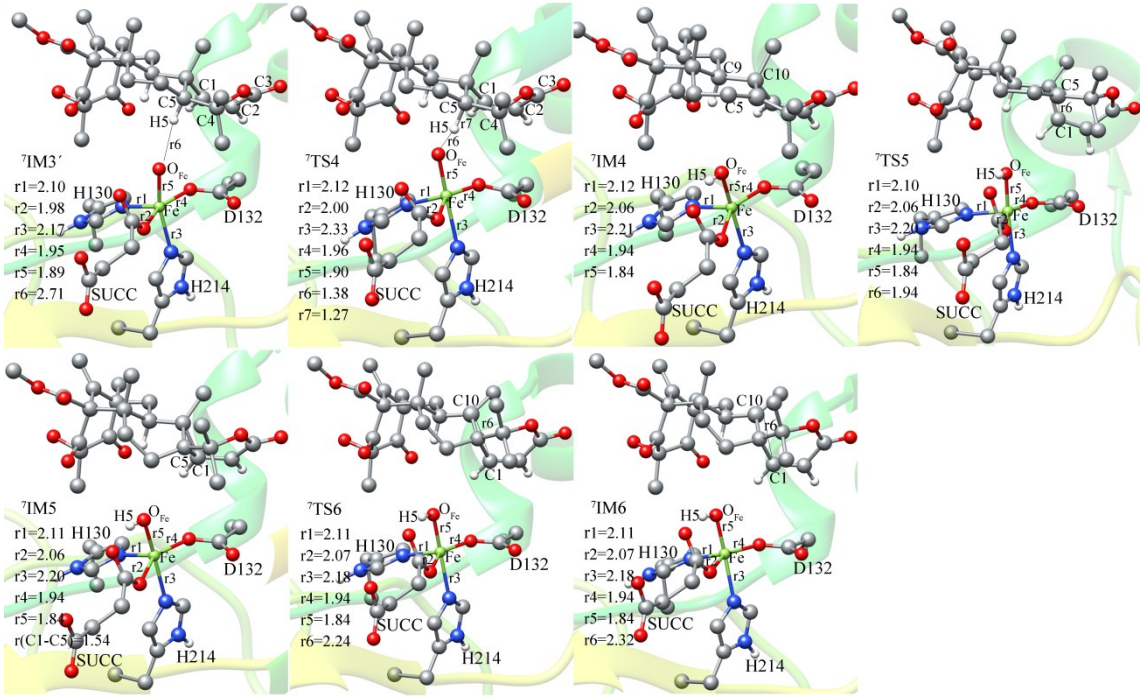

Figure S6 Optimized structures of transition states and intermediates involved in ring rearrangement at septet spin state. All distances are shown in angstroms.

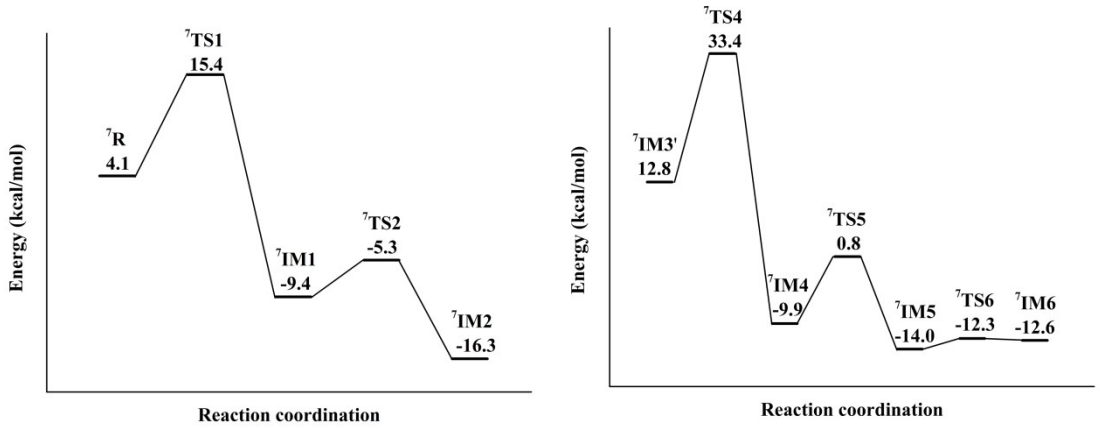

Figure S7 Energy profiles of desaturation (left) and ring rearrangement (right) processes at septet. All energies are given in kcal/mol relative to ^{5}Re.

Absolute QM/MM single-point energies (E, a.u.) at the B3LYP/6-311++G(2d, 2p) / LANL2TZf level, as well as cartesian coordinates of QM regions:

^{3}Re

E=-3040.565573 (a.u.)

C	10.045	-4.659	7.169
H	9.126	-5.128	7.532
H	10.597	-4.303	8.047

N	10.495	-2.430	5.959
H	11.457	-2.267	6.267
C	9.690	-3.527	6.248
C	9.841	-1.654	5.060
H	10.222	-0.717	4.681
N	8.660	-2.174	4.766
C	8.555	-3.335	5.502
H	7.673	-3.954	5.439
C	4.498	-4.881	3.182
H	4.427	-5.562	2.330
H	3.489	-4.496	3.367
C	5.336	-3.659	2.747
O	6.232	-3.230	3.587
O	5.095	-3.144	1.651
C	11.699	-3.946	0.404
H	12.069	-2.998	0.008
H	11.687	-4.664	-0.423
N	9.448	-4.794	1.264
H	9.596	-5.788	1.115
C	10.337	-3.762	0.988
C	8.356	-4.271	1.849
H	7.519	-4.868	2.166
N	8.475	-2.955	1.953
C	9.706	-2.627	1.418
H	10.042	-1.603	1.397
FE	7.300	-1.685	3.070
OE	6.120	-0.622	3.649
C2	8.052	0.995	2.519
O5	8.388	-0.234	2.330
O	7.102	1.363	3.239
C	8.815	2.059	1.725
H13	8.561	1.898	0.670
H23	8.419	3.036	2.009
C4	10.347	2.096	1.865
H14	10.810	1.235	1.379
H24	10.613	2.072	2.928
C5	10.900	3.409	1.270
O3	10.408	4.481	1.738
O4	11.794	3.347	0.383
C7	3.675	1.312	2.237
H9	3.169	1.404	1.269
H10	4.193	0.353	2.312
H11	4.460	2.073	2.286
C24	1.971	2.885	3.114

H33	1.285	3.171	3.914
H34	1.400	2.802	2.185
H35	2.701	3.684	2.985
C6	2.666	1.538	3.375
C5	1.475	-0.694	3.441
O3	1.516	0.632	3.185
O4	0.441	-1.283	3.185
C4	2.662	-1.339	4.093
H7	2.511	-2.418	4.022
H8	3.586	-1.090	3.568
C9	3.395	1.414	4.785
H15	4.336	0.887	4.580
C10	2.705	0.575	5.928
C23	2.782	-0.953	5.580
H31	1.999	-1.488	6.126
H32	3.740	-1.365	5.914
C11	3.799	2.824	5.264
H16	2.909	3.443	5.416
H17	4.379	3.311	4.471
C18	1.214	0.951	6.158
H21	0.997	2.004	5.968
H22	0.551	0.379	5.508
H23	0.902	0.734	7.183
C12	4.648	2.852	6.535
H18	4.897	3.885	6.773
H19	5.598	2.339	6.336
C14	3.600	0.721	7.242
H20	4.561	0.316	6.905
C13	3.936	2.175	7.728
C19	2.673	2.956	8.162
H24	2.914	3.981	8.445
H25	1.944	3.021	7.359
H26	2.176	2.483	9.013
C	3.132	-0.195	8.384
H	2.966	-1.212	8.025
H1	2.190	0.152	8.823
C15	4.910	2.134	9.037
C16	4.326	1.154	10.074
C17	4.181	-0.270	9.537
C20	5.482	-0.817	8.914
O	5.599	-2.003	8.668
C3	3.714	-1.303	10.578
H4	3.730	-2.298	10.132
H5	4.372	-1.310	11.453

H6	2.697	-1.098	10.910
C1	3.846	1.468	11.281
H2	3.445	0.696	11.925
H3	3.820	2.468	11.683
C25	5.147	3.595	9.544
O5	5.177	4.591	8.836
O6	5.352	3.680	10.859
C8	5.365	5.004	11.434
H12	4.354	5.420	11.431
H13	5.714	4.869	12.456
H14	6.023	5.666	10.876
C2	6.672	0.120	8.603
O2	7.753	-0.251	9.458
H30	7.597	-0.029	10.402
C21	6.362	1.629	8.772
O1	7.290	2.414	8.787
C22	7.207	-0.155	7.192
H27	8.105	0.443	7.046
H28	6.506	0.075	6.388
H29	7.454	-1.215	7.133

^{5}Re

E=-3040.585826 (a.u.)

C	10.025	-4.713	7.200
H	9.115	-5.192	7.573
H	10.583	-4.357	8.073
N	10.447	-2.485	5.981
H	11.408	-2.310	6.286
C	9.650	-3.582	6.288
C	9.784	-1.714	5.087
H	10.158	-0.779	4.699
N	8.601	-2.243	4.814
C	8.503	-3.402	5.556
H	7.626	-4.027	5.504
C	4.427	-4.977	3.150
H	4.387	-5.670	2.304
H	3.406	-4.618	3.315
C	5.237	-3.736	2.715
O	6.254	-3.414	3.455
O	4.877	-3.117	1.711
C	11.709	-3.934	0.418
H	12.077	-2.981	0.033
H	11.700	-4.643	-0.417
N	9.470	-4.808	1.268
H	9.626	-5.798	1.103

C	10.346	-3.762	1.004
C	8.380	-4.308	1.878
H	7.555	-4.915	2.203
N	8.489	-2.992	2.007
C	9.708	-2.641	1.462
H	10.029	-1.612	1.449
FE	7.269	-1.777	3.175
O	6.114	-0.896	3.924
C	8.027	0.957	2.518
O	8.175	-0.338	2.301
O	7.307	1.441	3.387
C	8.814	1.866	1.564
H	8.752	1.461	0.549
H	8.309	2.836	1.585
C	10.299	2.104	1.932
H	10.919	1.256	1.627
H	10.384	2.219	3.018
C	10.821	3.409	1.289
O	10.285	4.480	1.709
O	11.728	3.343	0.414
C	3.755	1.258	2.259
H	3.288	1.405	1.278
H	4.205	0.264	2.319
H	4.584	1.967	2.351
C	2.058	2.867	3.089
H	1.365	3.172	3.877
H	1.496	2.778	2.154
H	2.800	3.655	2.957
C	2.731	1.512	3.375
C	1.498	-0.700	3.454
O	1.569	0.622	3.180
O	0.457	-1.270	3.191
C	2.665	-1.362	4.126
H	2.488	-2.437	4.072
H	3.598	-1.149	3.600
C	3.445	1.396	4.792
H	4.382	0.857	4.601
C	2.738	0.577	5.938
C	2.795	-0.956	5.607
H	2.007	-1.474	6.163
H	3.749	-1.375	5.941
C	3.857	2.808	5.257
H	2.972	3.436	5.395
H	4.448	3.281	4.463

C	1.251	0.972	6.156
H	1.044	2.024	5.949
H	0.584	0.396	5.513
H	0.932	0.775	7.184
C	4.698	2.845	6.533
H	4.950	3.879	6.763
H	5.647	2.327	6.344
C	3.633	0.726	7.253
H	4.591	0.313	6.919
C	3.975	2.183	7.728
C	2.714	2.973	8.148
H	2.958	3.997	8.428
H	1.992	3.039	7.338
H	2.206	2.506	8.996
C	3.159	-0.180	8.401
H	2.993	-1.200	8.048
H	2.218	0.171	8.836
C	4.943	2.149	9.042
C	4.349	1.179	10.082
C	4.206	-0.250	9.557
C	5.508	-0.801	8.941
O	5.627	-1.991	8.708
C	3.737	-1.275	10.604
H	3.760	-2.273	10.168
H	4.389	-1.269	11.484
H	2.717	-1.071	10.928
C	3.854	1.506	11.280
H	3.444	0.741	11.927
H	3.824	2.510	11.671
C	5.179	3.612	9.542
O	5.206	4.605	8.830
O	5.385	3.700	10.856
C	5.384	5.025	11.430
H	4.367	5.426	11.434
H	5.742	4.896	12.450
H	6.028	5.696	10.866
C	6.700	0.130	8.623
O	7.780	-0.241	9.480
H	7.623	-0.020	10.424
C	6.395	1.640	8.782
O	7.325	2.423	8.787
C	7.233	-0.155	7.214
H	8.138	0.433	7.069
H	6.538	0.079	6.408

H	7.469	-1.219	7.162

^{3}IM3'

E=-3039.601263 (a.u.)

C	13.195	-4.295	1.267
H	12.640	-4.755	2.089
H	14.114	-3.894	1.705
N	12.828	-2.143	-0.093
H	13.805	-1.951	-0.330
C	12.352	-3.210	0.663
C	11.779	-1.411	-0.519
H	11.848	-0.541	-1.149
N	10.653	-1.938	-0.050
C	10.991	-3.054	0.691
H	10.238	-3.655	1.173
C	6.289	-4.516	0.653
H	5.828	-5.101	-0.148
H	5.480	-4.150	1.294
C	6.955	-3.271	0.017
O	8.209	-3.065	0.279
O	6.285	-2.520	-0.705
C	11.075	-3.582	-5.334
H	11.149	-2.619	-5.846
H	10.641	-4.293	-6.044
N	9.643	-4.490	-3.424
H	9.659	-5.478	-3.678
C	10.230	-3.436	-4.108
C	9.044	-4.000	-2.321
H	8.520	-4.620	-1.616
N	9.196	-2.685	-2.254
C	9.929	-2.324	-3.369
H	10.187	-1.294	-3.549
FE	8.858	-1.464	-0.575
O	8.383	-0.502	0.623
C	9.280	1.248	-1.781
O	9.271	-0.041	-1.850
O	9.364	1.933	-0.742
C	9.237	1.977	-3.124
H	8.695	1.394	-3.873
H	8.701	2.915	-2.953
C	10.664	2.325	-3.621
H	11.074	1.513	-4.225
H	11.320	2.458	-2.755
C	10.706	3.647	-4.396
O	10.439	4.692	-3.712

O	11.013	3.632	-5.616
C	4.619	1.067	0.590
H	3.669	0.990	0.051
H	5.116	0.094	0.591
H	5.263	1.766	0.044
C	3.643	2.956	1.899
H	3.440	3.397	2.879
H	2.688	2.791	1.393
H	4.219	3.677	1.315
C	4.382	1.612	2.006
C	3.378	-0.547	2.852
O	3.340	0.789	2.662
O	2.317	-1.117	3.068
C	4.673	-1.246	2.861
H	4.651	-2.267	2.497
C	5.740	1.669	2.823
H	6.507	1.324	2.115
C	5.863	0.669	4.034
C	5.771	-0.728	3.422
H	6.672	-1.336	3.414
C	6.153	3.085	3.253
H	5.448	3.488	3.987
H	6.094	3.765	2.397
C	4.772	0.875	5.136
H	4.338	1.876	5.105
H	3.950	0.166	5.052
H	5.189	0.733	6.133
C	7.588	3.146	3.796
H	7.836	4.178	4.044
H	8.278	2.843	3.001
C	7.323	0.797	4.627
H	7.962	0.516	3.774
C	7.788	2.241	5.035
C	7.005	2.825	6.234
H	7.386	3.812	6.493
H	5.949	2.939	5.999
H	7.083	2.204	7.127
C	7.573	-0.238	5.735
H	7.250	-1.234	5.426
H	7.015	0.003	6.644
C	9.349	2.155	5.497
C	9.482	1.079	6.598
C	9.075	-0.313	6.121
C	9.832	-0.694	4.840

O	9.634	-1.749	4.269
C	9.276	-1.435	7.155
H	8.977	-2.387	6.713
H	10.323	-1.512	7.463
H	8.657	-1.263	8.039
C	9.813	1.301	7.874
H	9.867	0.481	8.580
H	10.008	2.282	8.279
C	9.882	3.549	5.914
O	9.428	4.623	5.558
O	10.983	3.452	6.660
C	11.445	4.656	7.312
H	10.842	4.825	8.206
H	12.487	4.464	7.565
H	11.351	5.513	6.645
C	10.860	0.313	4.306
O	11.966	0.305	5.232
H	11.719	0.746	6.061
C	10.281	1.751	4.305
O	10.612	2.556	3.458
C	11.414	-0.110	2.963
H	12.222	0.567	2.680
H	10.642	-0.090	2.191
H	11.800	-1.128	3.039

^{5}IM3'

E=-3039.619204 (a.u.)

C	13.277	-4.437	1.304
H	12.714	-4.913	2.110
H	14.203	-4.068	1.755
N	12.973	-2.254	-0.001
H	13.955	-2.083	-0.234
C	12.460	-3.319	0.728
C	11.945	-1.485	-0.417
H	12.059	-0.609	-1.033
N	10.797	-1.974	0.028
C	11.101	-3.115	0.745
H	10.331	-3.703	1.219
C	6.193	-4.601	0.617
H	5.760	-5.242	-0.156
H	5.370	-4.285	1.268
C	6.713	-3.314	-0.074
O	7.957	-2.998	0.142
O	5.930	-2.662	-0.767
C	11.114	-3.572	-5.316

H	11.200	-2.611	-5.830
H	10.667	-4.278	-6.023
N	9.680	-4.463	-3.403
H	9.688	-5.450	-3.661
C	10.275	-3.414	-4.087
C	9.073	-3.971	-2.308
H	8.534	-4.581	-1.605
N	9.231	-2.655	-2.246
C	9.975	-2.297	-3.354
H	10.234	-1.268	-3.539
FE	8.828	-1.433	-0.603
O	8.424	-0.495	0.667
C	9.066	1.280	-1.809
O	8.957	-0.011	-1.911
O	9.258	1.914	-0.757
C	9.011	2.046	-3.126
H	8.382	1.533	-3.857
H	8.575	3.024	-2.903
C	10.436	2.276	-3.692
H	10.726	1.458	-4.352
H	11.152	2.304	-2.864
C	10.584	3.622	-4.415
O	10.355	4.661	-3.709
O	10.948	3.624	-5.619
C	4.599	1.085	0.596
H	3.648	1.017	0.057
H	5.089	0.109	0.588
H	5.246	1.786	0.055
C	3.623	2.962	1.922
H	3.426	3.397	2.906
H	2.666	2.797	1.421
H	4.194	3.687	1.338
C	4.367	1.618	2.017
C	3.374	-0.550	2.848
O	3.330	0.787	2.670
O	2.316	-1.125	3.067
C	4.672	-1.244	2.841
H	4.654	-2.259	2.459
C	5.726	1.674	2.830
H	6.493	1.341	2.116
C	5.859	0.661	4.031
C	5.771	-0.729	3.404
H	6.674	-1.332	3.382
C	6.133	3.087	3.275

H	5.430	3.475	4.019
H	6.061	3.779	2.430
C	4.771	0.852	5.138
H	4.330	1.851	5.116
H	3.954	0.138	5.053
H	5.193	0.707	6.132
C	7.570	3.150	3.810
H	7.815	4.180	4.066
H	8.258	2.857	3.009
C	7.321	0.791	4.620
H	7.959	0.519	3.764
C	7.781	2.234	5.038
C	7.003	2.805	6.246
H	7.383	3.790	6.512
H	5.945	2.918	6.018
H	7.086	2.176	7.133
C	7.577	-0.251	5.721
H	7.261	-1.247	5.403
H	7.016	-0.022	6.630
C	9.344	2.149	5.491
C	9.481	1.071	6.590
C	9.079	-0.321	6.110
C	9.840	-0.697	4.830
O	9.645	-1.750	4.255
C	9.281	-1.444	7.142
H	8.986	-2.396	6.698
H	10.328	-1.518	7.453
H	8.660	-1.275	8.026
C	9.811	1.293	7.867
H	9.866	0.472	8.572
H	10.003	2.274	8.273
C	9.879	3.542	5.909
O	9.424	4.616	5.557
O	10.983	3.444	6.651
C	11.447	4.647	7.304
H	10.845	4.817	8.198
H	12.489	4.453	7.556
H	11.354	5.504	6.637
C	10.866	0.315	4.301
O	11.967	0.321	5.233
H	11.711	0.760	6.061
C	10.271	1.747	4.293
O	10.581	2.548	3.434
C	11.432	-0.106	2.963

H	12.229	0.584	2.678
H	10.664	-0.109	2.188
H	11.838	-1.116	3.046

^{3}IM7'

E=-3066.07782 (a.u.)

C	5.657	-13.052	-0.152
H	4.666	-13.122	-0.607
H	5.758	-13.922	0.504
N	6.630	-11.509	1.659
H	7.320	-12.158	2.055
C	5.750	-11.765	0.614
C	6.489	-10.227	2.046
H	7.057	-9.743	2.822
N	5.540	-9.653	1.317
C	5.064	-10.594	0.426
H	4.283	-10.358	-0.275
C	2.524	-7.143	-1.932
H	2.913	-6.509	-2.734
H	1.558	-6.729	-1.625
C	3.464	-7.014	-0.713
O	4.006	-8.101	-0.258
O	3.663	-5.898	-0.207
C	10.255	-7.823	-0.854
H	10.752	-7.375	0.010
H	10.641	-7.322	-1.747
N	7.875	-7.811	-1.772
H	8.090	-7.991	-2.754
C	8.772	-7.669	-0.724
C	6.627	-7.721	-1.281
H	5.745	-7.819	-1.887
N	6.658	-7.511	0.027
C	7.993	-7.469	0.383
H	8.286	-7.309	1.407
FE	5.060	-7.800	1.326
O	3.791	-7.867	2.315
C	6.161	-6.682	3.847
O	6.317	-7.100	2.634
O	5.242	-7.003	4.628
C	7.256	-5.746	4.351
H	7.524	-5.016	3.583
H	6.847	-5.214	5.214
C	8.511	-6.529	4.812
H	9.237	-6.607	4.002
H	8.223	-7.547	5.093

C	9.169	-5.927	6.059
O	8.417	-5.802	7.082
O	10.394	-5.643	6.016
C	1.015	-4.020	4.780
H	0.607	-3.011	4.886
H	1.856	-3.972	4.082
H	1.374	-4.341	5.760
C	-1.227	-5.005	5.290
H	-2.083	-5.565	4.908
H	-1.561	-3.993	5.539
H	-0.896	-5.471	6.213
C	-0.100	-4.949	4.269
C	-0.229	-4.317	1.877
O	-0.736	-4.249	3.134
O	-0.860	-3.783	0.979
C	0.989	-5.107	1.684
H	1.555	-4.960	0.770
C	0.421	-6.356	3.785
C	-0.660	-7.371	3.331
C	1.272	-6.092	2.548
H	2.097	-6.771	2.352
C	1.312	-7.067	4.834
H	2.035	-6.373	5.267
H	1.915	-7.802	4.291
C	-1.448	-7.077	2.065
H	-2.344	-7.691	1.999
H	-1.800	-6.047	2.057
H	-0.873	-7.236	1.147
C	0.558	-7.771	5.961
H	0.075	-7.048	6.620
H	1.287	-8.278	6.591
C	-0.852	-8.550	3.969
C	-0.513	-8.780	5.454
C	-1.866	-8.523	6.184
H	-1.738	-8.510	7.265
H	-2.262	-7.556	5.871
H	-2.608	-9.286	5.940
C	-1.611	-9.658	3.262
H	-1.630	-9.488	2.187
H	-2.650	-9.743	3.602
C	-0.079	-10.318	5.779
C	-0.994	-11.277	4.996
C	-0.925	-11.029	3.496
C	0.530	-10.905	3.018

O	0.803	-10.497	1.906
C	-1.590	-12.104	2.617
H	-1.438	-11.846	1.567
H	-1.147	-13.088	2.802
H	-2.665	-12.158	2.800
C	-1.880	-12.137	5.511
H	-2.496	-12.747	4.860
H	-2.049	-12.261	6.570
C	-0.073	-10.545	7.310
O	0.058	-9.672	8.152
O	-0.155	-11.837	7.613
C	-0.382	-12.190	8.995
H	-1.447	-12.095	9.212
H	-0.058	-13.225	9.085
H	0.184	-11.537	9.657
C	1.615	-11.337	4.011
O	1.438	-12.740	4.298
H	0.647	-12.873	4.846
C	1.398	-10.582	5.345
O	2.336	-10.274	6.054
C	3.009	-11.181	3.442
H	3.742	-11.520	4.177
H	3.222	-10.142	3.179
H	3.097	-11.791	2.542

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E=-3066.096551 (a.u.)

C	5.653	-13.169	-0.256
H	4.673	-13.228	-0.737
H	5.742	-14.060	0.372
N	6.607	-11.709	1.612
H	7.300	-12.366	1.986
C	5.730	-11.912	0.557
C	6.476	-10.440	2.045
H	7.063	-10.008	2.839
N	5.537	-9.819	1.349
C	5.060	-10.721	0.420
H	4.277	-10.454	-0.272
C	2.523	-7.062	-2.019
H	2.912	-6.485	-2.862
H	1.540	-6.647	-1.771
C	3.420	-6.772	-0.791
O	3.961	-7.796	-0.201
O	3.554	-5.599	-0.428
C	10.255	-7.862	-0.838

H	10.759	-7.416	0.023
H	10.628	-7.351	-1.731
N	7.865	-7.861	-1.731
H	8.075	-8.025	-2.717
C	8.772	-7.717	-0.691
C	6.621	-7.775	-1.230
H	5.730	-7.856	-1.827
N	6.667	-7.567	0.078
C	8.003	-7.524	0.425
H	8.308	-7.355	1.445
FE	5.082	-7.770	1.388
O	3.825	-7.931	2.412
C	6.124	-6.473	3.840
O	6.211	-6.752	2.572
O	5.263	-6.906	4.625
C	7.231	-5.576	4.375
H	7.509	-4.816	3.641
H	6.835	-5.084	5.267
C	8.470	-6.407	4.793
H	9.190	-6.465	3.976
H	8.161	-7.430	5.033
C	9.147	-5.874	6.062
O	8.400	-5.763	7.090
O	10.380	-5.627	6.026
C	1.021	-4.026	4.783
H	0.613	-3.016	4.879
H	1.868	-3.983	4.093
H	1.368	-4.341	5.771
C	-1.220	-5.015	5.287
H	-2.075	-5.575	4.902
H	-1.554	-4.004	5.538
H	-0.891	-5.483	6.211
C	-0.091	-4.957	4.268
C	-0.221	-4.322	1.878
O	-0.727	-4.256	3.135
O	-0.853	-3.789	0.981
C	1.002	-5.107	1.683
H	1.566	-4.950	0.769
C	0.435	-6.361	3.782
C	-0.643	-7.378	3.326
C	1.288	-6.091	2.547
H	2.118	-6.767	2.355
C	1.325	-7.072	4.831
H	2.049	-6.379	5.264

H	1.927	-7.809	4.289
C	-1.429	-7.086	2.059
H	-2.324	-7.702	1.990
H	-1.785	-6.056	2.051
H	-0.852	-7.242	1.142
C	0.571	-7.775	5.959
H	0.086	-7.051	6.616
H	1.299	-8.281	6.591
C	-0.836	-8.556	3.965
C	-0.500	-8.785	5.451
C	-1.854	-8.528	6.179
H	-1.727	-8.513	7.260
H	-2.250	-7.562	5.864
H	-2.595	-9.292	5.935
C	-1.592	-9.665	3.257
H	-1.606	-9.497	2.182
H	-2.633	-9.750	3.593
C	-0.066	-10.323	5.779
C	-0.982	-11.281	4.996
C	-0.909	-11.037	3.496
C	0.548	-10.916	3.022
O	0.827	-10.505	1.912
C	-1.573	-12.113	2.618
H	-1.419	-11.857	1.567
H	-1.131	-13.096	2.805
H	-2.649	-12.165	2.799
C	-1.874	-12.135	5.511
H	-2.489	-12.745	4.860
H	-2.045	-12.256	6.570
C	-0.063	-10.548	7.310
O	0.069	-9.675	8.152
O	-0.149	-11.840	7.614
C	-0.381	-12.191	8.995
H	-1.447	-12.096	9.208
H	-0.058	-13.227	9.087
H	0.183	-11.538	9.658
C	1.628	-11.354	4.018
O	1.440	-12.754	4.313
H	0.647	-12.878	4.860
C	1.412	-10.587	5.347
O	2.350	-10.269	6.050
C	3.025	-11.211	3.455
H	3.754	-11.544	4.198
H	3.245	-10.178	3.180

H	3.116	-11.832	2.562