Supporting Information:

Quantum mechanics/molecular mechanics studies on the sulfoxidation of dimethyl sulfide by Compound I and Compound 0 of Cytochrome P450: which is the better oxidant?

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Table S1: Relative energies (ΔE) of Cpd I of $P450_{cam}$ (values in kcal mol^{-1} relative to the quartet spin state).

	inner region MM ΔE	inner region QM ΔE	outer region MM ΔE	Total Energy ΔE	ΔE + ZPE
Doublet	0.34	–0.01	0.39	0.03	0.02
Quartet	0.00	0.00	0.00	0.00	0.00

Optimized geometries of Cpd I of $P450_{cam}$ All distances are in Å. The average value of the four Fe–N distances is given as well as the displacement of the iron from the plane through the four nitrogen atoms (*Δ*).

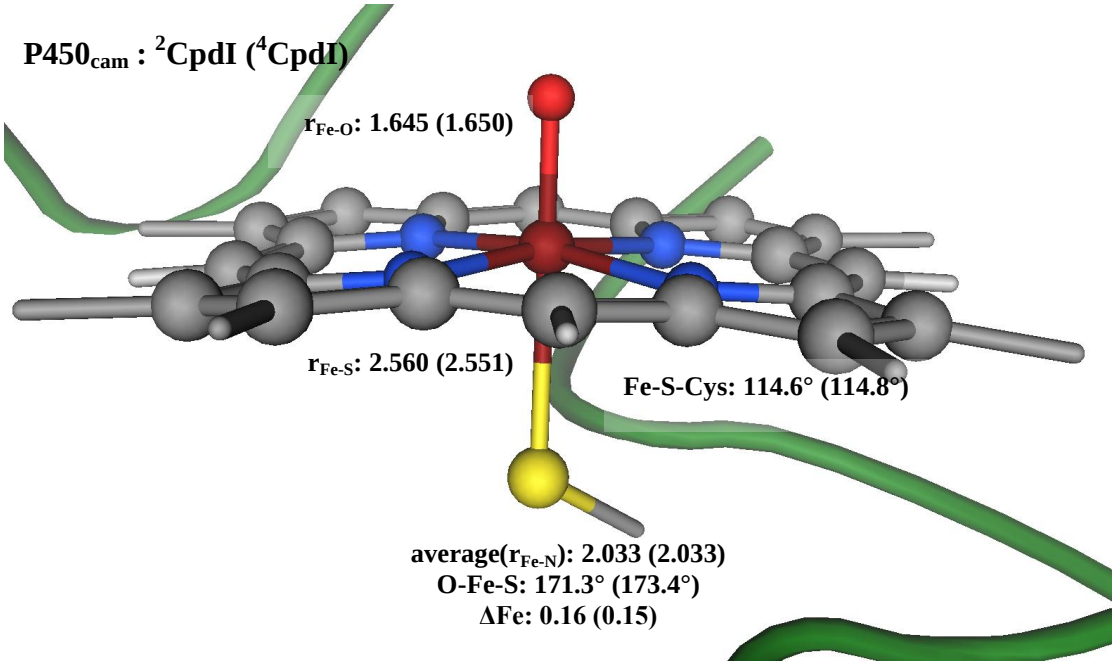

Table S2: Energies of Cpd 0 of $P450_{cam}$ species in Hartrees.

	inner region MM ΔE	inner region QM ΔE	outer region MM ΔE	Total Energy ΔE	ΔE + ZPE
Doublet	0.27	–1363.3631	–0.0214	–1363.6551	–1357.2017

Optimized geometries of Cpd 0 of $P450_{cam}$ All distances are in Å. The average value of the four Fe–N distances is given as well as the displacement of the iron from the plane through the four nitrogen atoms (*Δ*).

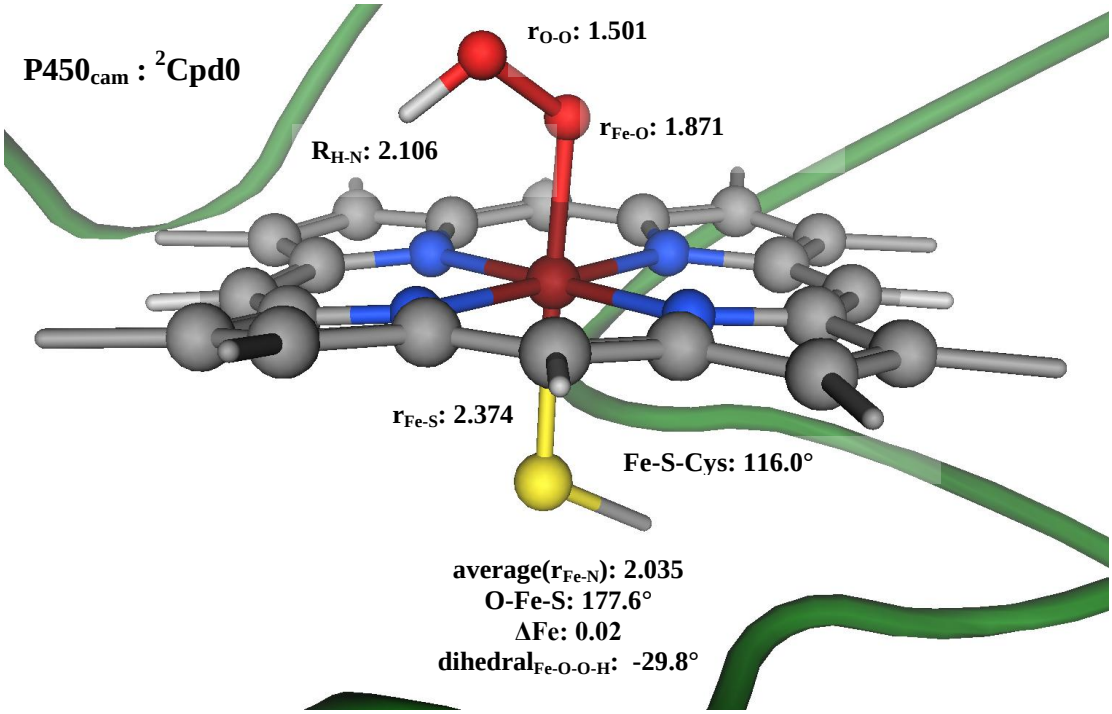

Table S3: Energies of Cpd I of $P450_{BM3}$ species in kcal mol^{-1} relative to the doublet state.

	inner region MM ΔE	inner region QM	outer region MM	Total Energy LANL2DZ	ΔE+ ZPE G03
Doublet	0.00	0.00	0.00	0.00	0.00
Quartet	–1.44	0.12	–1.27	0.29	0.28

Optimized geometries of Cpd I of $P450_{BM3}$. All distances are in Å. The average value of the four Fe–N distances is given as well as the displacement of the iron from the plane through the four nitrogen atoms (*Δ*).

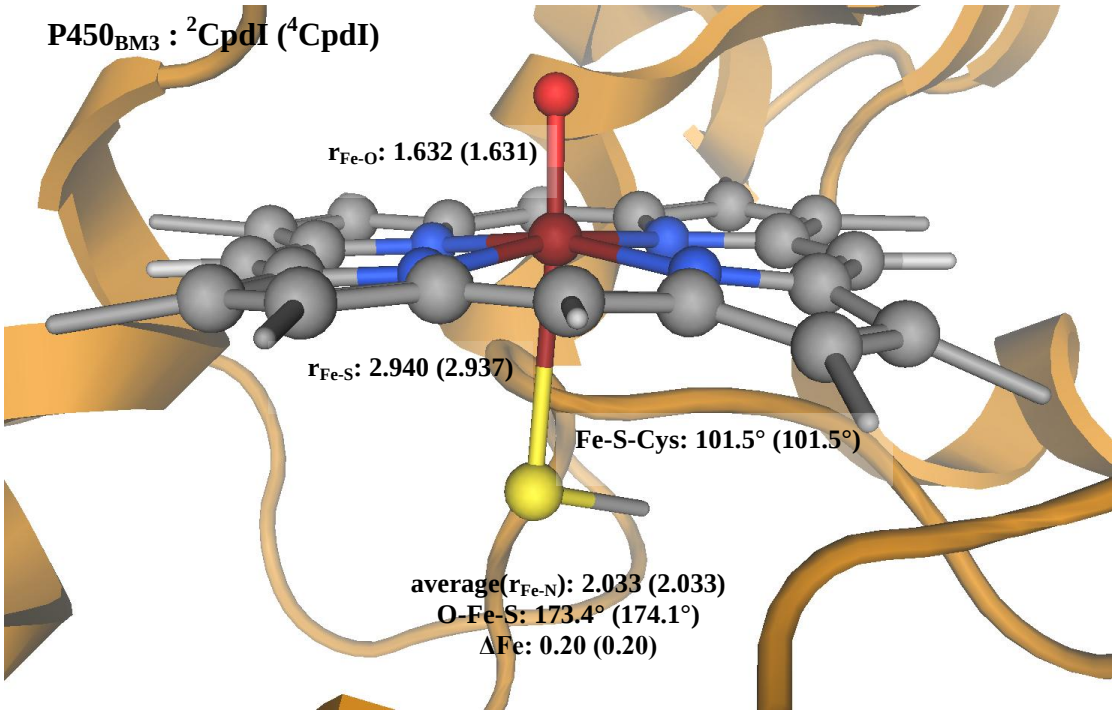

Table S4: Energies of Cpd 0 of $P450_{BM3}$ species in Hartrees.

	inner region MM E	inner region QM	outer region MM	Total Energy LANL2DZ
Doublet	0.621	–1363.363	–25.426	–1389.410

Optimized geometries of Cpd 0 of $P450_{BM3}$. All distances in Å. The average value of the four Fe–N distances is given as well as the displacement of the iron from the plane through the four nitrogen atoms (Δ).

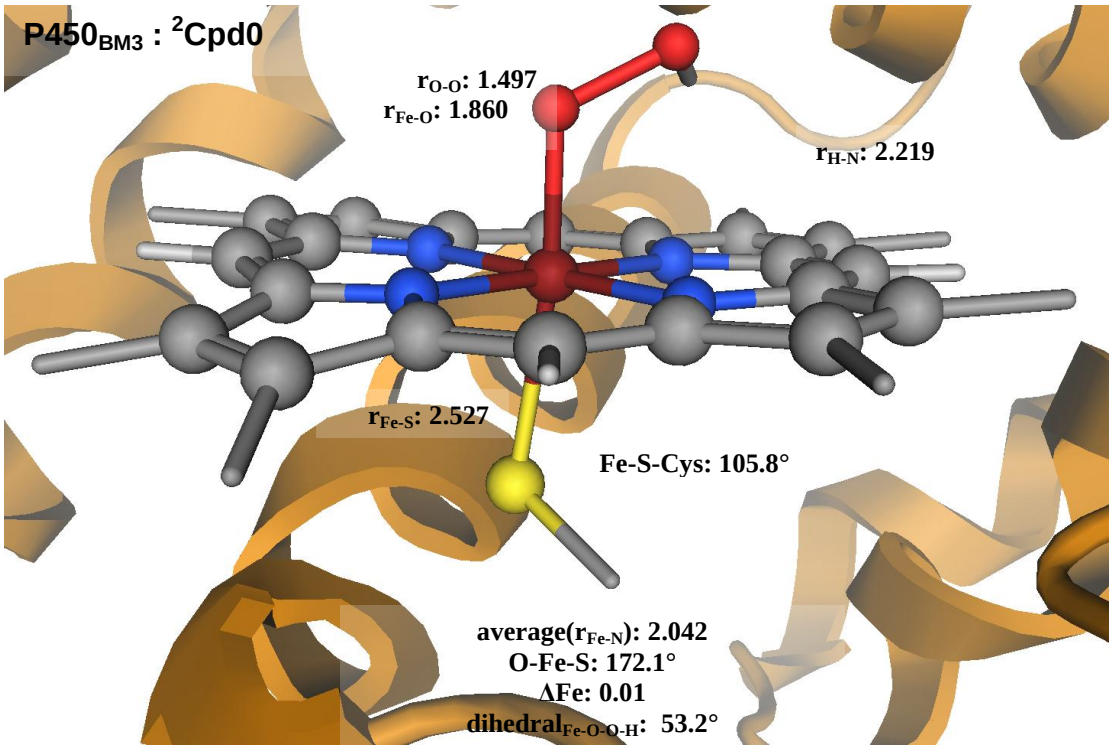

Table S5: Energies of transition state species of Cpd I of $P450_{cam}$ in Hartrees

	S–O Distance	inner region MM E	inner region QM	outer region MM	Total Energy LANL2DZ
$^{2}\mathbf{TS}_{I}$	2.108	0.310	–1287.4482	0.237	–1287.521
$^{4}\mathbf{TS}_{I}$	2.000	0.488	–1287.459	0.414	–1287.533

Table S6: Energies of transition state species of Cpd 0 of $P450_{cam}$ in Hartrees

	S–O Distance	inner region MM E	inner region QM	outer region MM	Total Energy LANL2DZ
$^{2}\mathbf{TS}_{0}$	1.736	2.607	–1363.254	2.322	–1363.538

Optimized geometries of the transition state species of the reaction between (a) doublet and (b) quartet Cpd I and DMS, both for $P450_{cam}$. All distances are in Å.

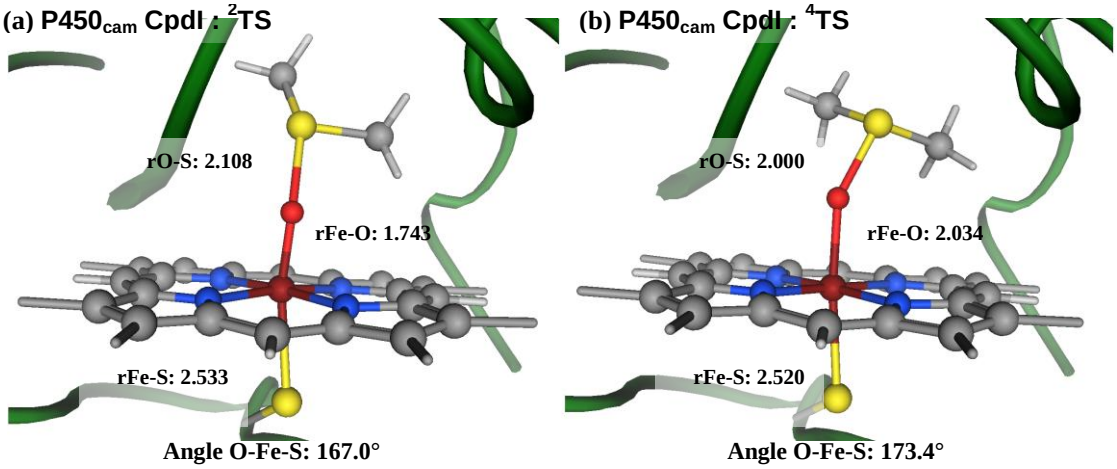

Table S7: Energies of transition state species of Cpd I of $P450_{BM3}$ in Hartrees

	S–O Distance	inner region MM E	inner region QM	outer region MM	Total Energy LANL2DZ
$^{2}\mathbf{TS}_{I}$	1.9349	1.426	–1287.427	–23.739	–1312.591
$^{4}\mathbf{TS}_{I}$	2.0488	1.109	–1287.434	–24.087	–1312.629

Table S8: Energies of transition state species of Cpd 0 of $P450_{BM3}$ in Hartrees

	S–O Distance	inner region MM E	inner region QM	outer region MM	Total Energy LANL2DZ
$^{2}\mathbf{TS}_{0}$	1.7980	2.371	–1363.258	–23.670	–1389.298

Optimized geometries of the transition state species of the reaction between (a) Cpd I and DMS and (b) Cpd 0 and DMS, both for $P450_{BM3}$. All distances are in Å. The average value of the four Fe–N distances is given as well as the displacement of the iron from the plane through the four nitrogen atoms (Δ).

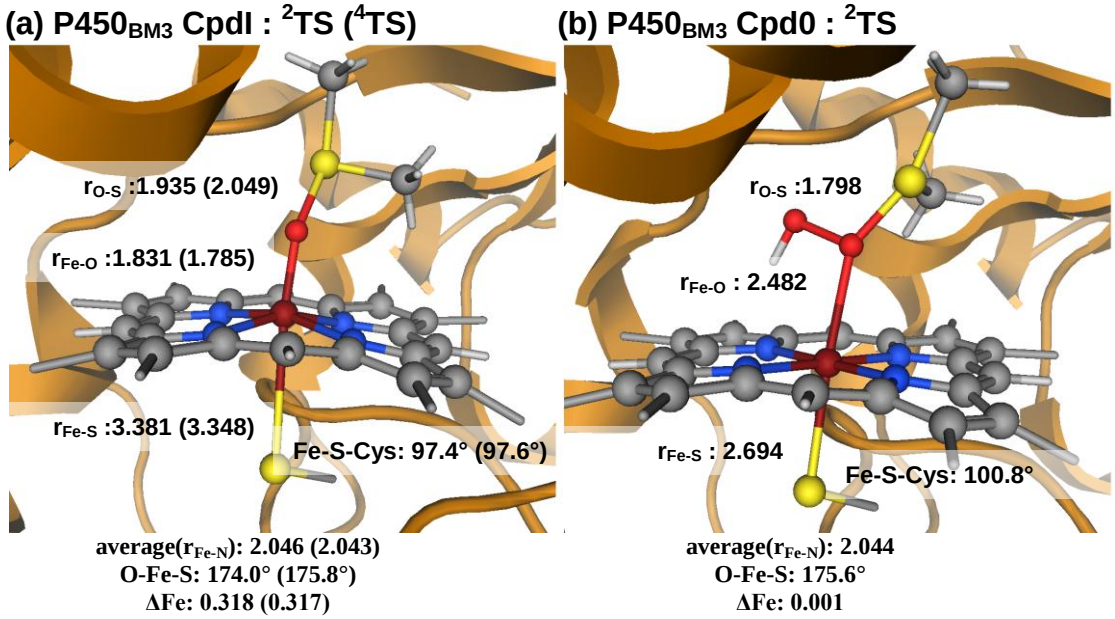

Table S9. Group spin densities (ρ) and Fe–S distances (r_{FeS}) of ^{4,2}CpdI structures optimized from different MD snapshots.

SNAPSHOTS	ρ_{Fe}	ρ_{Cys}	ρ_{Por}	ρ_{O}	ρ_{DMS}	r_{FeS}
Sn_3 doublet	1.21	–0.87	–0.20	0.86	0.00	3.481
Sn_2 doublet	1.20	–0.74	–0.36	0.90	0.00	2.945
Sn_3 quartet	1.14	0.88	0.12	0.86	0.00	3.506
Sn_2 quartet	1.08	0.71	0.30	0.90	0.00	2.944

Cartesian Coordinates of optimized structures:

$P450_{cam}$ ^{2}Cpd I; active site only

H	-1.597561	-0.501504	-3.424378
H	-1.202463	0.431063	-2.98
H	-2.332184	-0.248269	-4.198975
S	-2.438409	-1.462382	-2.159298
C	2.815911	-1.333775	5.292366
H	2.593284	-2.159606	5.97215
H	3.226433	-0.491578	5.857437
H	3.5553	-1.655805	4.553343
S	1.247937	-0.749388	4.426992
C	0.774975	-2.39225	3.634306
H	0.538789	-3.130678	4.407664
H	-0.099042	-2.194944	3.013424
H	1.594615	-2.7651	3.010356
Fe	-1.873836	-0.788323	0.244459
C	1.404453	-0.50551	-0.842616
H	2.437566	-0.40127	-1.141735
C	-2.303772	2.595241	-0.173761
H	-2.42604	3.670358	-0.256054
C	-5.252673	-1.168071	0.727694
H	-6.316877	-1.289418	0.890018
C	-1.448398	-4.202966	0.557958
H	-1.293886	-5.268817	0.673092
N	-0.695904	0.729338	-0.402584
C	0.645224	0.664743	-0.772728
C	1.14559	2.004196	-1.074854
C	0.105666	2.878912	-0.856521
C	-1.042161	2.079999	-0.448938
H	0.124571	4.372031	-0.996807
H	-0.570667	4.689148	-1.798883
H	1.133614	4.750776	-1.24139
H	-0.18893	4.833768	-0.048811
H	2.557267	2.364384	-1.4423
H	3.048179	1.525001	-1.984161
H	2.554751	3.192784	-2.179364
C	3.345511	2.77195	-0.177481
H	3.094559	3.807277	0.131996
H	3.101705	2.098764	0.668758
C	4.814426	2.7277	-0.393502
O	5.321651	3.323946	-1.374011
O	5.523489	1.95526	0.299382
N	-3.457781	0.469356	0.305413
C	-3.432942	1.848245	0.157832
C	-4.769549	2.404234	0.341221
C	-5.61122	1.337613	0.587883
C	-4.781032	0.134239	0.557685
H	-5.103131	3.867916	0.28641
H	-4.975582	4.236397	-0.754171
H	-4.423051	4.434551	0.9515
H	-6.139873	4.060239	0.620032
H	-7.062711	1.353024	0.870131
H	-7.444524	0.691596	1.638927
C	-7.916451	2.105485	0.17804
H	-8.971559	2.086023	0.411758
H	-7.580315	2.729168	-0.64058
N	-3.097721	-2.375005	0.602864
C	-4.476038	-2.325981	0.777379
C	-4.986946	-3.654892	1.101498
C	-3.898868	-4.502317	1.158972

C	-2.727798	-3.703034	0.801923
H	-6.416855	-3.977128	1.436262
H	-6.514779	-5.011052	1.819065
H	-7.053813	-3.852563	0.536415
H	-6.76215	-3.30399	2.249575
H	-3.938278	-5.950944	1.464349
H	-4.785811	-6.530463	1.131436
C	-3.03026	-6.546463	2.233737
H	-3.135474	-7.592356	2.496041
H	-2.222432	-5.991858	2.689284
N	-0.345025	-2.094391	-0.137793
C	-0.358859	-3.470701	0.101663
C	0.944116	-4.043543	-0.2081
C	1.759212	-3.011225	-0.61927
C	0.958153	-1.78929	-0.554321
H	1.305409	-5.49523	-0.074792
H	2.352979	-5.688871	-0.38057
H	0.635951	-6.100986	-0.71913
H	1.190819	-5.805563	0.985203
H	3.172257	-3.146997	-1.124356
H	3.720119	-2.180126	-1.096773
H	3.746784	-3.816171	-0.443466
C	3.168375	-3.702269	-2.563049
H	2.562796	-4.626939	-2.620441
H	2.73338	-2.962466	-3.267059
C	4.542269	-4.012259	-3.040591
O	4.842909	-5.183662	-3.385323
O	5.337608	-3.072736	-3.284025
O	-1.494924	-0.599986	1.834042

$P450_{cam}$ ^{4}Cpd I; active site only

H	-1.617221	-0.471029	-3.452513
H	-1.221554	0.464658	-3.015408
H	-2.355072	-0.222994	-4.225716
S	-2.4521	-1.425866	-2.178893
C	2.805971	-1.264034	5.260871
H	2.581874	-2.100617	5.926802
H	3.206014	-0.426855	5.84084
H	3.554396	-1.571546	4.524617
S	1.243373	-0.677253	4.389184
C	0.782812	-2.313938	3.577517
H	0.520986	-3.055213	4.339903
H	-0.07136	-2.109674	2.931888
H	1.617939	-2.688515	2.975157
Fe	-1.887399	-0.742042	0.213007
C	1.388071	-0.458692	-0.876134
H	2.420774	-0.355339	-1.176782
C	-2.324624	2.640436	-0.225842
H	-2.448701	3.71481	-0.31509
C	-5.266913	-1.120264	0.705148
H	-6.33069	-1.242281	0.869829
C	-1.458859	-4.150958	0.552254
H	-1.302808	-5.215855	0.673834
N	-0.713506	0.775348	-0.443893
C	0.627575	0.711103	-0.813998
C	1.125146	2.04929	-1.125969
C	0.08402	2.923554	-0.911721
C	-1.062482	2.125269	-0.499049
H	0.100611	4.415826	-1.061326
H	-0.596575	4.727551	-1.863815
H	1.108803	4.794549	-1.309468
H	-0.211774	4.882591	-0.115293
H	2.535382	2.409716	-1.498598
H	3.026635	1.566986	-2.034964
H	2.529725	3.232238	-2.242226
C	3.325715	2.828255	-0.238896
H	3.073445	3.865356	0.063421
H	3.085283	2.160826	0.612817
C	4.794167	2.785212	-0.458509
O	5.297643	3.375336	-1.444648
O	5.506374	2.018456	0.237442
N	-3.475766	0.516439	0.268013
C	-3.45205	1.894584	0.113426
C	-4.788777	2.450527	0.297313
C	-5.628818	1.384676	0.552232
C	-4.797622	0.181697	0.526124
H	-5.122922	3.91393	0.239024
H	-4.99803	4.279326	-0.802982
H	-4.441349	4.482654	0.900737
H	-6.159023	4.106744	0.574432
H	-7.080128	1.40027	0.835233
H	-7.460959	0.742271	1.607448
C	-7.93478	2.148663	0.139816
H	-8.989823	2.129304	0.373802
H	-7.599372	2.768803	-0.681806
N	-3.109225	-2.324704	0.588696
C	-4.488239	-2.276274	0.762391
C	-4.997144	-3.603598	1.096055
C	-3.908286	-4.449653	1.157148
C	-2.738498	-3.651115	0.795243

H	-6.426673	-3.926002	1.432053
H	-6.523462	-4.95819	1.819756
H	-7.063772	-3.806381	0.531603
H	-6.772727	-3.249355	2.24213
H	-3.945551	-5.896566	1.470519
H	-4.791868	-6.479293	1.14009
C	-3.03717	-6.486066	2.24404
H	-3.140977	-7.530509	2.512564
H	-2.230694	-5.92733	2.696935
N	-0.359178	-2.044197	-0.156193
C	-0.37207	-3.420164	0.087778
C	0.929746	-3.993769	-0.224199
C	1.74343	-2.963081	-0.64192
C	0.942542	-1.740969	-0.580158
H	1.29269	-5.444312	-0.083348
H	2.338921	-5.639418	-0.392675
H	0.620878	-6.054441	-0.721103
H	1.182829	-5.748333	0.978989
H	3.156203	-3.101222	-1.147254
H	3.703948	-2.134153	-1.123611
H	3.731317	-3.767397	-0.463917
C	3.151957	-3.661766	-2.583703
H	2.547513	-4.587358	-2.637003
H	2.715626	-2.925089	-3.290167
C	4.526041	-3.971702	-3.060757
O	4.828623	-5.144357	-3.399422
O	5.31966	-3.032043	-3.309301
O	-1.523233	-0.515383	1.803149

$P450_{cam}$ ^{2}Cpd 0; active site only

H	0.362364	3.644207	-1.54865
H	-0.52983	3.316789	-0.97304
H	0.104961	4.53651	-2.13674
S	0.872684	2.370208	-2.71883
C	-1.34264	-3.0381	5.102514
H	-0.7103	-3.88934	5.373125
H	-2.31835	-3.14978	5.585954
H	-0.87109	-2.11712	5.458049
S	-1.63584	-3.00334	3.236111
C	0.113981	-3.4267	2.675159
H	0.34173	-4.47552	2.894404
H	0.18443	-3.25877	1.600652
H	0.850962	-2.7792	3.158278
Fe	0.428332	0.129113	-2.07398
C	1.168374	0.903787	1.173074
H	1.405393	1.181801	2.191911
C	-2.92577	0.573923	-1.45806
H	-3.9858	0.694074	-1.25381
C	-0.26716	-0.34634	-5.43562
H	-0.48323	-0.48977	-6.48723
C	3.73224	-0.6724	-2.67358
H	4.783483	-0.88055	-2.84024
N	-0.66108	0.648077	-0.46366
C	-0.17433	0.969069	0.795925
C	-1.28914	1.31631	1.682038
C	-2.44553	1.139269	0.954646
C	-2.04243	0.74265	-0.39243
H	-3.85851	1.209715	1.453179
H	-4.49883	1.765596	0.740904
H	-3.90692	1.710897	2.438103
H	-4.25807	0.182363	1.568412
H	-1.18599	1.752504	3.115924
H	-0.18907	2.19794	3.321114
H	-1.90423	2.575472	3.30927
C	-1.45417	0.567984	4.062177
H	-2.48751	0.179982	3.942848
H	-0.75166	-0.26108	3.844827
C	-1.28582	0.960055	5.485205
O	-2.01659	1.852127	5.982287
O	-0.33092	0.495227	6.155939
N	-1.2635	0.120588	-3.22405
C	-2.56044	0.317346	-2.77734
C	-3.49984	0.246066	-3.89673
C	-2.7482	0.007174	-5.03052
C	-1.34946	-0.07917	-4.59598
H	-4.99261	0.356388	-3.76453
H	-5.26125	1.386641	-3.4445
H	-5.34854	-0.36364	-3.00259
H	-5.50383	0.121043	-4.71619
H	-3.2161	-0.22884	-6.41439
H	-2.74519	-1.02233	-6.98172
C	-4.15965	0.515253	-6.9897
H	-4.4783	0.303053	-8.00059

H	-4.61204	1.349217	-6.46826
N	1.52373	-0.43431	-3.72846
C	1.054719	-0.55852	-5.03328
C	2.120452	-1.05942	-5.90035
C	3.228651	-1.27502	-5.0982
C	2.863356	-0.8193	-3.75419
H	1.953155	-1.39573	-7.35687
H	2.858872	-1.87492	-7.77259
H	1.727582	-0.47331	-7.93173
H	1.120513	-2.12386	-7.46301
H	4.505835	-1.90147	-5.52007
H	4.843346	-1.76843	-6.53699
C	5.194303	-2.73272	-4.73859
H	6.085953	-3.22126	-5.11454
H	4.849745	-3.00146	-3.75043
N	2.11994	0.138997	-0.97216
C	3.389459	-0.21032	-1.40278
C	4.34855	-0.02913	-0.31376
C	3.632921	0.41012	0.778227
C	2.231592	0.501128	0.361195
H	5.819539	-0.32666	-0.38435
H	6.341857	-0.0236	0.545036
H	6.275884	0.221479	-1.23381
H	5.956224	-1.41889	-0.51879
H	4.185349	0.721102	2.137909
H	3.396326	0.6306	2.913159
H	4.942299	-0.05056	2.405502
C	4.80171	2.131608	2.162081
H	5.578663	2.218135	1.382348
H	4.029556	2.905168	1.970875
C	5.414667	2.441651	3.480062
O	6.655574	2.614892	3.582799
O	4.673915	2.656726	4.470097
O	0.130164	-1.62935	-1.50742
O	0.684583	-2.72363	-2.3731
H	0.650994	-2.2946	-3.27188

$P450_{BM3}$ ^{2}Cpd I; QM region only

C	-4.02493	-7.15409	1.826837
H	-3.43646	-6.6251	1.05249
H	-5.00904	-7.38094	1.373698
S	-4.24675	-6.07044	3.265592
Fe	-1.79491	-4.45091	3.165002
N	-1.30453	-5.29951	1.396806
C	-0.46074	-6.39565	1.176147
C	-0.19359	-6.51971	-0.25918
C	0.574288	-7.60537	-0.95168
H	0.63555	-8.49771	-0.31046
H	0.013279	-7.9318	-1.85704
C	1.985833	-7.11947	-1.31127
H	1.94299	-6.21081	-1.94485
H	2.53371	-6.85915	-0.38527
C	2.751591	-8.15862	-2.05354
O	2.48143	-8.39137	-3.25711
O	3.765215	-8.69064	-1.53679
C	-0.83777	-5.47575	-0.88514
C	-0.82843	-5.13183	-2.34965
H	-0.27984	-5.88463	-2.94628
H	-0.36125	-4.13968	-2.49737
H	-1.87002	-5.08698	-2.73044
C	-1.53588	-4.72903	0.145831
C	-2.35528	-3.63367	-0.11192
H	-2.44952	-3.32525	-1.148
C	-3.07431	-2.92143	0.836738
N	-3.04222	-3.17346	2.209652
C	-3.92137	-1.76973	0.552392
C	-4.16462	-1.19063	-0.80906
H	-3.20314	-1.03002	-1.33772
H	-4.68785	-0.22088	-0.74369
H	-4.78516	-1.89745	-1.39632
C	-4.38614	-1.30991	1.764685
C	-5.17674	-0.09426	2.040313
H	-4.85876	0.542633	2.861053
C	-6.28391	0.198948	1.362772
H	-6.8481	1.093499	1.597015
H	-6.65634	-0.46597	0.593197
C	-3.82886	-2.18044	2.790615
C	-4.0572	-2.01697	4.150955
H	-4.72604	-1.21623	4.429204
C	-3.4864	-2.77131	5.169126
N	-2.58845	-3.82013	4.951859
C	-3.70242	-2.56973	6.603888
C	-4.69746	-1.64761	7.257279
H	-5.39723	-1.19965	6.533299
H	-4.17401	-0.81741	7.771408
H	-5.3018	-2.21928	7.99376
C	-2.90258	-3.48513	7.254362
C	-2.83692	-3.76234	8.707177
H	-2.75786	-4.79042	9.023432
C	-2.82046	-2.80383	9.632894
H	-2.7574	-3.06314	10.68267

H	-2.82691	-1.75649	9.366379
C	-2.23526	-4.2736	6.222515
C	-1.43556	-5.38414	6.466494
H	-1.25072	-5.64957	7.501365
C	-0.90274	-6.23116	5.495821
N	-0.89254	-5.99752	4.125254
C	-0.33196	-7.53822	5.792273
C	-0.38306	-8.20302	7.140536
H	0.008447	-9.23891	7.108624
H	-1.43935	-8.25191	7.481005
H	0.20734	-7.61728	7.873568
C	0.077166	-8.08639	4.592881
C	-0.23785	-7.09373	3.554883
C	0.029937	-7.22547	2.188251
H	0.667591	-8.05091	1.894218
C	0.432508	-9.53563	4.365097
H	-0.32815	-10.1729	4.86654
H	0.36172	-9.80338	3.287509
C	1.83573	-9.89388	4.901931
H	2.624926	-9.40367	4.307346
H	1.970014	-9.58243	5.952431
C	2.074254	-11.3617	4.861599
O	1.632622	-12.0751	5.799141
O	2.340205	-11.9075	3.760017
O	-0.53138	-3.43061	3.003175
C	2.315338	-3.03965	0.8549
H	1.249303	-3.03673	1.091324
H	2.812768	-3.75611	1.516736
H	2.481547	-3.32422	-0.18929
S	2.987691	-1.30522	1.197492
C	4.806912	-1.74333	1.461067
H	5.293827	-0.91362	1.979874
H	5.32543	-1.91873	0.514212
H	4.888943	-2.63961	2.085077

$P450_{BM3}$ ^{4}Cpd I; QM region only

C	-4.0247	-7.15154	1.822237
H	-3.43564	-6.62278	1.048257
H	-5.00838	-7.37909	1.36847
S	-4.24834	-6.06764	3.260643
Fe	-1.79821	-4.45182	3.159349
N	-1.30398	-5.29595	1.395476
C	-0.46055	-6.39422	1.175304
C	-0.19535	-6.51923	-0.26039
C	0.575462	-7.60331	-0.95215
H	0.636017	-8.49635	-0.31186
H	0.017491	-7.92996	-1.85926
C	1.987282	-7.11496	-1.30728
H	1.94454	-6.20634	-1.94104
H	2.531911	-6.85362	-0.37955
C	2.757204	-8.15278	-2.04693
O	2.494006	-8.38313	-3.2526
O	3.769237	-8.68408	-1.52624
C	-0.84042	-5.4763	-0.88694
C	-0.83534	-5.13576	-2.35222
H	-0.28586	-5.88825	-2.94841
H	-0.37119	-4.14269	-2.5033
H	-1.878	-5.09447	-2.73055
C	-1.53767	-4.72839	0.143685
C	-2.35796	-3.63385	-0.11455
H	-2.4532	-3.32577	-1.15065
C	-3.07778	-2.92354	0.834801
N	-3.04398	-3.17639	2.208074
C	-3.9248	-1.7719	0.552096
C	-4.16825	-1.19179	-0.80886
H	-3.20682	-1.02968	-1.33715
H	-4.69257	-0.22273	-0.74248
H	-4.78801	-1.89857	-1.39698
C	-4.3881	-1.31179	1.764959
C	-5.17711	-0.09505	2.041005
H	-4.8569	0.54251	2.86044
C	-6.28587	0.197921	1.366037
H	-6.84929	1.092751	1.60111
H	-6.66033	-0.46753	0.597966
C	-3.8314	-2.1825	2.790652
C	-4.05838	-2.01698	4.150392
H	-4.72669	-1.21584	4.428642
C	-3.48549	-2.76982	5.169154
N	-2.58919	-3.81831	4.951266
C	-3.69985	-2.56683	6.604007
C	-4.6947	-1.64457	7.257352
H	-5.39763	-1.20065	6.533959
H	-4.1712	-0.81156	7.766913
H	-5.29558	-2.21476	7.997771
C	-2.89905	-3.48177	7.254063
C	-2.83121	-3.75741	8.707127
H	-2.7493	-4.78498	9.024374
C	-2.81586	-2.79797	9.631905
H	-2.75074	-3.05616	10.68183

H	-2.82535	-1.75089	9.364411
C	-2.2339	-4.2716	6.221387
C	-1.43468	-5.38245	6.464679
H	-1.24841	-5.64738	7.499428
C	-0.90122	-6.22954	5.493969
N	-0.8911	-5.99774	4.123231
C	-0.32909	-7.53571	5.791561
C	-0.37888	-8.19889	7.140774
H	0.011965	-9.23507	7.109606
H	-1.43489	-8.24726	7.48219
H	0.212272	-7.61254	7.872686
C	0.078724	-8.08542	4.592127
C	-0.23696	-7.09318	3.553652
C	0.029999	-7.22469	2.186206
H	0.666273	-8.051	1.891833
C	0.434103	-9.53493	4.365897
H	-0.32783	-10.171	4.866938
H	0.364053	-9.8033	3.288423
C	1.836287	-9.89462	4.904175
H	2.626558	-9.41011	4.306441
H	1.972207	-9.57817	5.952943
C	2.069954	-11.3635	4.870898
O	1.626062	-12.071	5.811813
O	2.334188	-11.9154	3.772027
O	-0.52775	-3.4378	3.021466
C	2.31666	-3.04481	0.859004
H	1.248919	-3.04327	1.08797
H	2.810472	-3.76106	1.523573
H	2.489907	-3.3281	-0.18425
S	2.985085	-1.30986	1.207974
C	4.806874	-1.74296	1.464158
H	5.288434	-0.92168	2.001033
H	5.3274	-1.89562	0.514471
H	4.893538	-2.65172	2.069309

$P450_{BM3}$ ^{2}Cpd 0; QM region only

H	-4.55053	-5.96681	2.147245
S	-4.04864	-6.08906	3.432599
C	2.542075	-3.14898	0.794573
H	1.470119	-3.1411	1.004897
H	3.011274	-3.97341	1.340863
H	2.733945	-3.25038	-0.27943
S	3.206199	-1.50424	1.44028
C	5.063255	-1.8579	1.371095
H	5.580938	-1.13641	2.013022
H	5.467675	-1.77333	0.357653
H	5.267728	-2.86404	1.755005
Fe	-2.0155	-4.60785	3.179168
N	-1.34395	-5.31926	1.404114
C	-0.48878	-6.40146	1.206229
C	-0.18101	-6.51913	-0.22683
H	0.459697	-7.27982	-0.65605
C	-0.82529	-5.47963	-0.86362
H	-0.82888	-5.23601	-1.91884
C	-1.56281	-4.74782	0.158442
C	-2.40293	-3.66792	-0.11455
H	-2.48934	-3.36341	-1.15298
C	-3.1429	-2.95681	0.825484
N	-3.10001	-3.19179	2.198269
C	-4.02032	-1.8253	0.538576
H	-4.22282	-1.43801	-0.45213
C	-4.50528	-1.3811	1.753018
H	-5.18348	-0.55946	1.947496
C	-3.92129	-2.2345	2.784885
C	-4.16628	-2.09054	4.151399
H	-4.85268	-1.29922	4.42302
C	-3.59576	-2.84131	5.181019
N	-2.68877	-3.87897	4.987787
C	-3.80693	-2.62326	6.621678
H	-4.46824	-1.87542	7.041438
C	-2.98971	-3.52138	7.280087
H	-2.86828	-3.6657	8.346598
C	-2.32126	-4.31965	6.25014
C	-1.48839	-5.41056	6.502777
H	-1.29313	-5.66142	7.540582
C	-0.93135	-6.25209	5.538897
N	-0.95257	-6.04199	4.17077
C	-0.28817	-7.53234	5.83996
H	-0.17934	-7.94533	6.835352
C	0.107322	-8.08026	4.635398
C	-0.26945	-7.10456	3.593791
C	-0.0016	-7.23113	2.224537
H	0.652367	-8.04581	1.931436
H	0.613528	-9.0191	4.449006
O	-0.48967	-3.54715	3.248603
O	-0.29903	-2.58166	2.119801

H	-1.16692	-2.09727	2.132537

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$P450_{cam}$ $^{2}TS_{I}$; active site only

H	-1.30499	-0.92148	-3.00009
H	-0.88352	-0.0519	-2.46374
H	-2.0202	-0.57217	-3.75378
S	-2.21199	-1.95848	-1.84118
C	1.522788	-0.95045	4.828214
H	1.702086	-1.49783	5.76083
H	1.334944	0.104226	5.044628
H	2.380494	-1.05668	4.158421
S	-0.06985	-1.65092	3.99071
C	0.602215	-3.39822	3.75284
H	0.623302	-3.92469	4.712552
H	-0.0616	-3.90843	3.057681
H	1.608954	-3.35613	3.327187
Fe	-1.59655	-1.59896	0.589582
C	1.68589	-1.24097	-0.35081
H	2.724521	-1.13191	-0.63088
C	-1.98182	1.869636	0.515846
H	-2.07967	2.951254	0.501514
C	-5.03449	-1.88471	0.999728
H	-6.1076	-1.98799	1.106264
C	-1.29879	-4.97435	0.628217
H	-1.1788	-6.0514	0.627791
N	-0.39653	-0.01048	0.208133
C	0.946804	-0.06799	-0.17891
C	1.463901	1.281872	-0.39158
C	0.4362	2.153633	-0.11337
C	-0.72374	1.345551	0.238133
H	0.470675	3.652524	-0.15493
H	-0.22288	4.034308	-0.93314
H	1.482008	4.032959	-0.37496
H	0.161269	4.051981	0.822969
H	2.875865	1.646974	-0.74491
H	3.352956	0.838598	-1.34083
H	2.88196	2.522266	-1.42693
C	3.664321	1.957191	0.542781
H	3.413912	2.966612	0.92975
H	3.42285	1.219719	1.334066
C	5.131655	1.928881	0.316221
O	5.640719	2.630021	-0.59039
O	5.845336	1.10305	0.940102
N	-3.18065	-0.26504	0.780659
C	-3.13378	1.121367	0.746983
C	-4.46992	1.688023	0.929627
C	-5.33843	0.62415	1.060463
C	-4.52247	-0.58861	0.957037
H	-4.77858	3.155094	0.980616
H	-4.61934	3.597204	-0.02542
H	-4.10555	3.648124	1.703335
H	-5.81966	3.338744	1.305518
H	-6.80163	0.641582	1.302964
H	-7.22197	-0.0849	1.992724
C	-7.62581	1.469459	0.659648

H	-8.68729	1.45029	0.863833
H	-7.25601	2.160976	-0.08674
N	-2.91117	-3.12579	0.851563
C	-4.28943	-3.06364	0.97755
C	-4.83672	-4.40978	1.15453
C	-3.76866	-5.28325	1.158863
C	-2.5708	-4.47484	0.913468
H	-6.28073	-4.7332	1.418266
H	-6.40974	-5.79538	1.706528
H	-6.88913	-4.51724	0.516114
H	-6.6348	-4.12581	2.276969
H	-3.84224	-6.75474	1.329555
H	-4.69124	-7.29083	0.927408
C	-2.96193	-7.43197	2.063045
H	-3.08951	-8.4937	2.235605
H	-2.15842	-6.92809	2.581491
N	-0.10337	-2.84813	0.161409
C	-0.175	-4.23652	0.258407
C	1.11497	-4.8176	-0.08898
C	1.968937	-3.77327	-0.37868
C	1.207126	-2.53985	-0.20132
H	1.433532	-6.28519	-0.09263
H	2.480795	-6.47739	-0.40174
H	0.758892	-6.81251	-0.79826
H	1.296362	-6.68845	0.932518
H	3.383265	-3.89632	-0.87231
H	3.949753	-2.95024	-0.73848
H	3.923703	-4.64314	-0.24971
C	3.393736	-4.30554	-2.35863
H	2.773717	-5.20841	-2.51722
H	2.984288	-3.4922	-2.9935
C	4.770423	-4.59155	-2.8392
O	5.062576	-5.73083	-3.28364
O	5.587539	-3.6482	-2.96744
O	-1.34251	-1.70372	2.31106

$P450_{cam}$ $^{4}TS_{I}$; active site only

H	-1.35061	-0.8739	-3.07191
H	-0.94723	0.009095	-2.54103
H	-2.05326	-0.54032	-3.84572
S	-2.26103	-1.90697	-1.91633
C	1.047439	-0.63409	4.111774
H	1.869196	-0.89781	4.785169
H	0.52274	0.253393	4.46851
H	1.388499	-0.48287	3.086485
S	-0.21676	-2.02723	4.086317
C	0.890258	-3.431	3.480269
H	1.567785	-3.70593	4.294983
H	0.2515	-4.27927	3.230897
H	1.436526	-3.1061	2.59512
Fe	-1.64315	-1.50228	0.493498
C	1.686698	-1.19945	-0.39314
H	2.719764	-1.09624	-0.69464
C	-1.99633	1.921943	0.409191
H	-2.10178	3.001648	0.375137
C	-5.02727	-1.84019	0.985894
H	-6.09822	-1.95426	1.101209
C	-1.2735	-4.94082	0.645239
H	-1.15494	-6.01826	0.653377
N	-0.40911	0.043104	0.085874
C	0.941363	-0.02521	-0.27029
C	1.460827	1.325823	-0.47051
C	0.427894	2.200978	-0.20661
C	-0.73784	1.396365	0.123269
H	0.466177	3.701133	-0.24402
H	-0.22781	4.08171	-1.02035
H	1.478717	4.081195	-0.47038
H	0.162554	4.106229	0.734618
H	2.880567	1.694103	-0.79197
H	3.381651	0.877711	-1.35853
H	2.89546	2.553668	-1.49395
C	3.641501	2.041013	0.507379
H	3.379874	3.058215	0.864012
H	3.388557	1.324957	1.314298
C	5.112751	2.015196	0.314718
O	5.632274	2.678567	-0.61406
O	5.812548	1.195762	0.962119
N	-3.18287	-0.21486	0.751251
C	-3.13558	1.173996	0.679446
C	-4.47177	1.736787	0.863529
C	-5.33543	0.671877	1.018221
C	-4.52454	-0.54521	0.935454
H	-4.78228	3.206931	0.894001
H	-4.63682	3.637576	-0.12008
H	-4.10177	3.720307	1.60065
H	-5.8184	3.39658	1.231014
H	-6.79401	0.692693	1.269827
H	-7.20352	-0.02521	1.971162
C	-7.62218	1.517088	0.62958
H	-8.68247	1.493671	0.840467

H	-7.26204	2.204106	-0.12546
N	-2.89211	-3.08144	0.799978
C	-4.27002	-3.01379	0.948332
C	-4.81614	-4.3538	1.139738
C	-3.74788	-5.22841	1.144238
C	-2.54896	-4.43114	0.884829
H	-6.26057	-4.67192	1.410942
H	-6.38672	-5.73073	1.707973
H	-6.87023	-4.46128	0.508364
H	-6.61536	-4.05808	2.266356
H	-3.82689	-6.69545	1.31957
H	-4.66155	-7.22935	0.890747
C	-2.97164	-7.36356	2.088137
H	-3.10096	-8.42519	2.260002
H	-2.18905	-6.85355	2.632904
N	-0.08108	-2.81227	0.205617
C	-0.14396	-4.19566	0.305545
C	1.155177	-4.77379	-0.01968
C	2.003392	-3.7264	-0.31966
C	1.219881	-2.4971	-0.17481
H	1.475831	-6.24063	-0.02486
H	2.527806	-6.43119	-0.31708
H	0.812276	-6.76023	-0.74586
H	1.319393	-6.65196	0.994797
H	3.412565	-3.84833	-0.83461
H	3.982562	-2.90171	-0.71119
H	3.969528	-4.59471	-0.22285
C	3.392658	-4.25955	-2.32024
H	2.783014	-5.17243	-2.46155
H	2.955262	-3.45366	-2.94629
C	4.76019	-4.52529	-2.83659
O	5.058129	-5.66116	-3.28588
O	5.558212	-3.56938	-2.98958
O	-1.2266	-1.39049	2.481705

$P450_{cam}$ $^2TS_0$; active site only

H	-1.07055	-1.05915	-3.18557
H	-0.70157	-0.08371	-2.80096
H	-1.73105	-0.88608	-4.04628
S	-2.06033	-1.8969	-1.93667
C	1.883972	-0.6038	2.973319
H	2.045646	0.060024	3.828475
H	1.370152	-0.08936	2.162058
H	2.848094	-0.97233	2.612642
S	0.850498	-2.12237	3.47057
C	2.624731	-2.6833	4.810746
H	2.651856	-1.96294	5.634452
H	2.391779	-3.70707	5.122163
H	3.526735	-2.64556	4.186754
Fe	-1.28617	-1.62333	0.364255
C	1.980287	-1.51866	-0.65702
H	2.990571	-1.50065	-1.04442
C	-1.4714	1.817515	0.255597
H	-1.51774	2.901804	0.215257
C	-4.69947	-1.74158	1.017401
H	-5.77014	-1.79708	1.169508
C	-1.08684	-4.99836	0.866615
H	-1.00773	-6.07356	0.988262
N	0.010559	-0.14807	-0.07842
C	1.320329	-0.29316	-0.53489
C	1.89305	1.02595	-0.81286
C	0.9277	1.956295	-0.48643
C	-0.24914	1.217488	-0.04927
H	1.034775	3.451808	-0.54501
H	0.158496	3.88189	-1.06885
H	1.948151	3.765833	-1.0844
H	1.071684	3.861788	0.48475
H	3.274609	1.316722	-1.32644
H	3.732585	0.41008	-1.77509
H	3.213885	2.042867	-2.16636
C	4.172525	1.859096	-0.19657
H	3.809899	2.836753	0.18081
H	4.200319	1.1482	0.653791
C	5.56453	2.05926	-0.66837
O	5.805464	2.902585	-1.56722
O	6.462514	1.257808	-0.3115
N	-2.78162	-0.23035	0.663162
C	-2.65887	1.145459	0.531329
C	-3.96397	1.792172	0.66019
C	-4.89094	0.783675	0.843507
C	-4.14167	-0.47474	0.844571
H	-4.18303	3.278877	0.645434
H	-3.96807	3.676377	-0.37057
H	-3.50351	3.759443	1.374778
H	-5.21873	3.539605	0.930551
H	-6.34129	0.896966	1.12248
H	-6.7646	0.238354	1.872022
C	-7.14058	1.743776	0.473699
H	-8.19321	1.791826	0.718014

H	-6.76497	2.380087	-0.31744
N	-2.61442	-3.07133	0.92253
C	-3.98496	-2.93753	1.118892
C	-4.55704	-4.21229	1.547789
C	-3.50921	-5.1075	1.651819
C	-2.30873	-4.40315	1.185214
H	-5.99813	-4.42213	1.923626
H	-6.16477	-5.42838	2.350861
H	-6.64237	-4.28568	1.02991
H	-6.27592	-3.68503	2.707429
H	-3.58549	-6.48562	2.189164
H	-4.49371	-7.05505	2.053093
C	-2.62213	-7.00438	2.946937
H	-2.73961	-7.98944	3.383205
H	-1.74192	-6.43171	3.206703
N	0.154849	-2.99195	0.10655
C	0.026569	-4.35399	0.32402
C	1.261143	-5.03182	-0.06481
C	2.14126	-4.05378	-0.47445
C	1.443998	-2.77331	-0.35047
H	1.534977	-6.50186	0.076509
H	2.493658	-6.78271	-0.40246
H	0.71929	-7.09325	-0.38623
H	1.613555	-6.74051	1.157035
H	3.591218	-4.24587	-0.79939
H	4.153807	-3.30687	-0.62292
H	4.030851	-4.98571	-0.08831
C	3.759715	-4.70131	-2.2568
H	3.245143	-5.66361	-2.41458
H	3.332079	-3.95607	-2.95875
C	5.190836	-4.8623	-2.60881
O	5.655933	-5.9942	-2.89427
O	5.906871	-3.84197	-2.74881
O	-0.52992	-1.79669	2.469531
O	-1.74438	-1.54968	3.386735
H	-2.47527	-1.63505	2.71447

$P450_{BM3}$ $^{2}TS_{I}$; QM region only

H	-3.34664	-7.20705	2.934243
S	-4.09685	-6.27463	3.633063
Fe	-1.4758	-4.22529	3.034687
N	-1.20869	-5.17571	1.238351
C	-0.5035	-6.35601	0.993175
C	-0.25048	-6.48661	-0.4436
H	0.267517	-7.31772	-0.90461
C	-0.77455	-5.36147	-1.04805
H	-0.77823	-5.10674	-2.0998
C	-1.39297	-4.56572	-0.00068
C	-2.08706	-3.37829	-0.2222
H	-2.16258	-3.03557	-1.2486
C	-2.74361	-2.63699	0.75387
N	-2.70744	-2.90914	2.11978
C	-3.59353	-1.48067	0.496153
H	-3.78793	-1.06488	-0.4837
C	-4.08499	-1.06986	1.716811
H	-4.76065	-0.25168	1.929107
C	-3.52547	-1.96257	2.721315
C	-3.80362	-1.86726	4.083985
H	-4.50044	-1.09476	4.376236
C	-3.23928	-2.65041	5.08276
N	-2.2954	-3.65956	4.844732
C	-3.47726	-2.50839	6.522652
H	-4.17311	-1.80773	6.965087
C	-2.63971	-3.40638	7.153118
H	-2.53003	-3.59521	8.212939
C	-1.93154	-4.13473	6.103264
C	-1.09594	-5.22636	6.328106
H	-0.86617	-5.47883	7.357202
C	-0.63644	-6.09561	5.341462
N	-0.73245	-5.89047	3.965629
C	-0.10502	-7.42418	5.618297
H	0.037921	-7.83288	6.610052
C	0.118927	-8.03479	4.400544
C	-0.2288	-7.05321	3.365717
C	-0.07965	-7.24282	1.990593
H	0.420266	-8.15073	1.672603
H	0.495826	-9.02994	4.203628
O	0.057315	-3.2674	2.746779
C	2.301759	-4.27087	1.452422
H	1.556712	-4.97951	1.104779
H	2.652113	-4.55724	2.445813
H	3.129306	-4.20534	0.740448
S	1.437425	-2.60668	1.562473
C	3.094735	-1.59195	1.804132
H	2.822999	-0.54125	1.921536
H	3.709757	-1.74241	0.909089
H	3.620921	-1.9549	2.692252

$P450_{BM3}$ $^{4}TS_{I}$; QM region only

H	-3.37622	-7.22523	2.964712
S	-4.10839	-6.23391	3.598593
Fe	-1.48515	-4.23189	3.032853
N	-1.21129	-5.17923	1.241125
C	-0.49809	-6.35537	0.995221
C	-0.24561	-6.48351	-0.44154
H	0.278054	-7.31099	-0.90254
C	-0.77588	-5.36191	-1.04565
H	-0.78134	-5.10691	-2.0972
C	-1.39955	-4.57125	0.001509
C	-2.10501	-3.39166	-0.22173
H	-2.18623	-3.05214	-1.24873
C	-2.76547	-2.6546	0.753946
N	-2.72475	-2.92528	2.119722
C	-3.62179	-1.50373	0.495777
H	-3.82093	-1.09155	-0.48461
C	-4.10706	-1.08866	1.717394
H	-4.78354	-0.27143	1.930538
C	-3.54177	-1.97804	2.722021
C	-3.81304	-1.879	4.085227
H	-4.50803	-1.10536	4.378672
C	-3.24325	-2.65826	5.08341
N	-2.2985	-3.66636	4.844636
C	-3.47625	-2.51051	6.523374
H	-4.17329	-1.81082	6.965316
C	-2.63159	-3.40147	7.15423
H	-2.5165	-3.58528	8.214282
C	-1.92603	-4.13216	6.104519
C	-1.0887	-5.22174	6.328575
H	-0.85247	-5.47188	7.356769
C	-0.63553	-6.09332	5.341906
N	-0.73841	-5.89058	3.965439
C	-0.10595	-7.42207	5.619353
H	0.037045	-7.83029	6.611192
C	0.11895	-8.03209	4.401781
C	-0.22829	-7.05136	3.367308
C	-0.07135	-7.23883	1.993155
H	0.438406	-8.14208	1.677873
H	0.496424	-9.02694	4.20489
O	-0.00898	-3.26361	2.766812
C	2.293198	-4.25375	1.45803
H	1.520181	-4.93909	1.122492
H	2.650392	-4.55459	2.445059
H	3.112532	-4.22012	0.734368
S	1.49728	-2.55841	1.570378
C	3.161365	-1.59527	1.804951
H	2.915539	-0.53577	1.90132
H	3.790387	-1.76928	0.923684
H	3.674081	-1.94776	2.70546

$P450_{BM3}$ $^{2}TS_{0}$; QM region only

H	-3.79497	-7.13936	2.027499
S	-3.95866	-6.01979	3.445842
C	1.829869	-3.29638	0.428339
H	0.756732	-3.41758	0.276345
H	2.369662	-4.16654	0.045315
H	2.192936	-2.37941	-0.0424
S	2.057746	-3.1896	2.301195
C	4.094391	-2.50018	2.108244
H	4.356069	-2.14681	3.109224
H	4.080058	-1.68454	1.378336
H	4.734299	-3.33199	1.789582
Fe	-1.75908	-4.49522	3.140597
N	-1.1227	-5.27864	1.387031
C	-0.29243	-6.384	1.189605
C	-0.05325	-6.5609	-0.24941
H	0.751605	-7.63824	-0.91238
C	-0.7147	-5.54117	-0.89855
H	-0.68283	-5.20982	-2.36526
C	-1.39918	-4.75932	0.125375
C	-2.23617	-3.67668	-0.15789
H	-2.36967	-3.42882	-1.20633
C	-2.94531	-2.91515	0.769279
N	-2.84697	-3.07787	2.151793
C	-3.87668	-1.83641	0.461201
H	-4.16661	-1.30144	-0.91062
C	-4.35692	-1.35924	1.668439
H	-5.22612	-0.18596	1.904779
C	-3.71894	-2.14265	2.717964
C	-3.97744	-1.99533	4.081226
H	-4.7102	-1.24132	4.341595
C	-3.38731	-2.72251	5.118236
N	-2.40631	-3.69659	4.930453
C	-3.66426	-2.55898	6.555564
H	-4.77928	-1.75938	7.179739
C	-2.8173	-3.42469	7.221134
H	-2.75295	-3.71418	8.67322
C	-2.06616	-4.15383	6.195402
C	-1.21545	-5.23137	6.453825
H	-1.02637	-5.47339	7.495073
C	-0.66079	-6.09657	5.507149
N	-0.6688	-5.91487	4.130876
C	-0.05658	-7.38689	5.840537
H	-0.04466	-7.99194	7.218339
C	0.330527	-7.97373	4.649288
C	-0.02058	-7.01625	3.58498
C	0.218642	-7.18756	2.215527
H	0.856248	-8.01775	1.930453
H	0.687397	-9.42499	4.442334
O	0.304932	-3.18788	2.701752
O	-0.24129	-1.80596	2.348811
H	-1.22393	-2.00051	2.372199