Supporting Information for

Spectroscopic and Computational Investigation of Fe(III) Cysteine Dioxygenase: Implications for the Nature of the Putative Superoxo-Fe(III) Intermediate

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Table S1. Experimentally derived[a] and computationally predicted[b] EPR parameters for various species mentioned in this work, where D is given in wavenumbers

Species	g_1	g_2	g_3	D	E/D
S1, Azide-bound Fe(III)CDO	***2.001***	***2.011***	***2.017***	***| 2.985 |***	***0.305***
(N_3^-/2H_2O)-Fe(III)CDO	2.001	2.010	2.017	1.403	0.109
(N_3^-/OH^-)-Fe(III)CDO	2.009	2.011	2.017	-2.988	0.320
(N_3^-/OH^-/H_2O)-Fe(III)CDO	2.008	2.012	2.016	1.365	0.321
(N_3^-/2OH^-)-Fe(III)CDO	2.009	2.011	2.012	1.447	0.107
S2, Cys-bound Fe(III)CDO	***2.030***	***2.030***	***2.030***	***| 0.726 |***	***0.317***
(Cys/OH^-)-Fe(III)CDO	2.011	2.016	2.028	0.868	0.207
(Cys/H_2O)-Fe(III)CDO	2.025	2.039	2.048	-1.963	0.100
Cys-Fe(III)CDO	2.021	2.051	2.067	-4.142	0.171
S3, (Cys/N_3^-)-Fe(III)CDO	***1.888***	***2.550***	***2.435***	***N/A***	***N/A***
(Cys/N_3^-)-Fe(III)CDO	2.027	2.156	2.193	N/A	N/A

a Obtained from fits of experimental spectra using EasySpin
b EPR parameters were computed as described in the Experimental Section

Table S2. Relevant active site bond lengths (in Å) as derived from QM/MM optimized models of azide-bound Fe(III)CDO

Species	Fe-His_{86}	Fe-His_{88}	Fe-His_{140}	Fe-N_{Az}	Fe-O_{H2O}	Fe-O_{OH}
(N_3^-/2H_2O)-Fe(III)CDO	2.108	2.072	2.111	1.938	2.203, 2.364	N/A
(N_3^-/OH^-)-Fe(III)CDO	2.127	2.039	2.152	2.026	3.313	1.896
(N_3^-/OH^-/H_2O)-Fe(III)CDO	2.105	2.236	2.200	2.011	2.326	1.876
(N_3^-/2OH^-)-Fe(III)CDO	2.179	2.316	2.288	2.116	N/A	1.900, 1.949

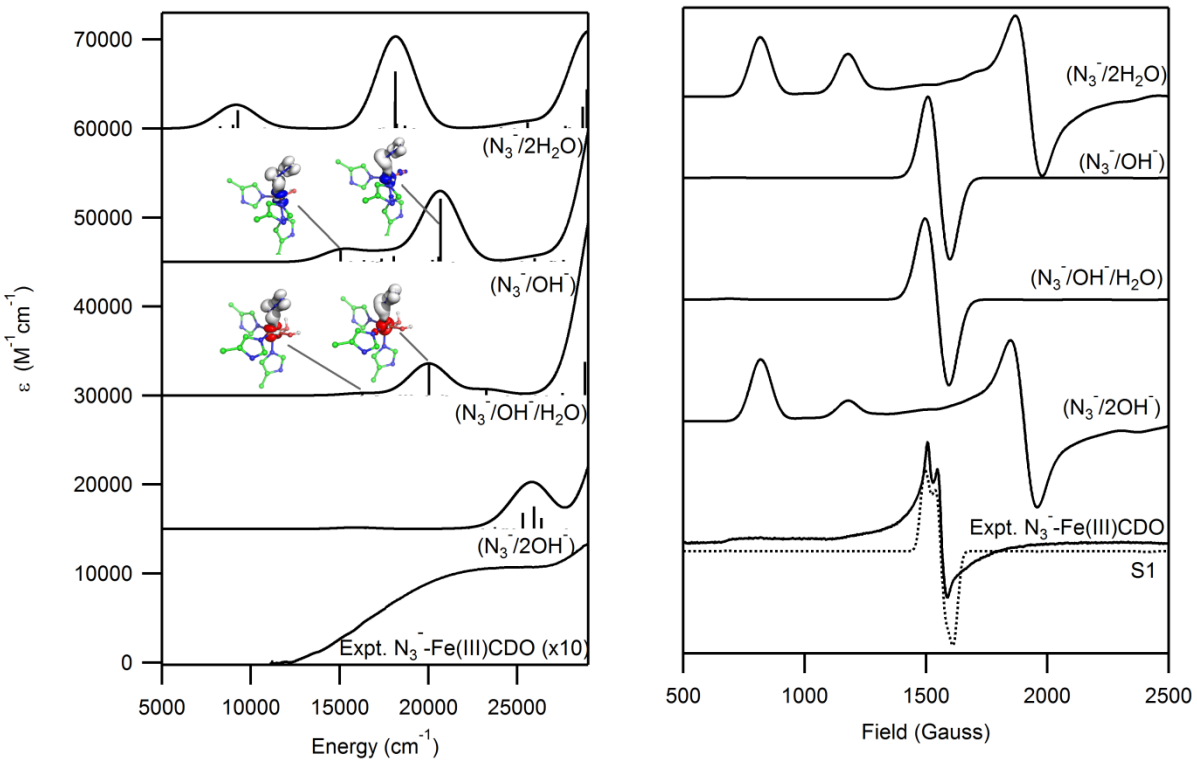

Figure S1. Comparison of the INDO/S-CI predicted Abs spectra (left) and DFT-computed EPR spectra (right) with their experimentally derived counterparts. EDDMs are shown next to relevant INDO/S-CI-computed transitions, where loss and gain of electron density are denoted by white and colored lobes, respectively. Also shown is the simulated EPR spectrum (S1, dotted line) for the N_3^--Fe(III)CDO species, which has been slightly offset for clarity (see **Table S1** for all EPR parameters used).

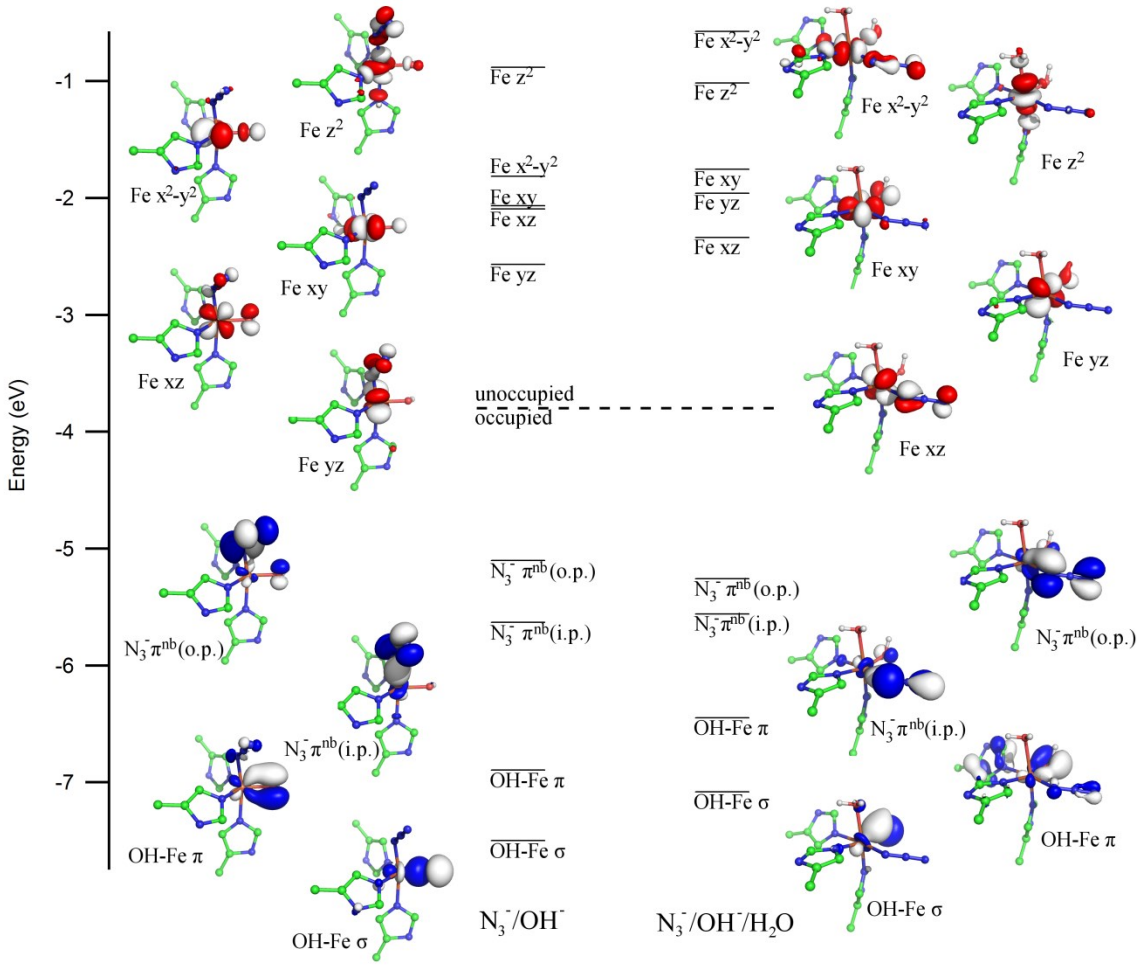

Figure S2. DFT-computed energies of relevant spin-down MOs for the active sites of (from left to right) the (N_3^-/OH^-)-Fe(III)CDO and (N_3^-/OH^-/H_2O)-Fe(III)CDO models. Boundary surface plots of key MOs for the each model are also shown. Note that the orientations of the molecular axes differ between these models, and orbitals lacking significant Fe, azide, hydroxide, or water character are omitted for clarity. The orbital energies for each species were adjusted such that α-LUMO (a ligand-based orbital with essentially identical compositions for both species) lies at 0 eV.

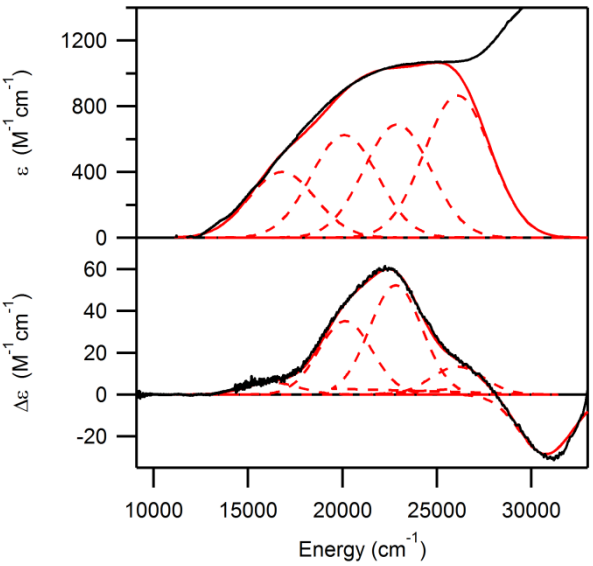

Figure S3. RT Abs (top) and 4.5 K MCD (bottom) spectra of Fe(III)CDO in presence of azide. Individual bands obtained from an interative Gaussian deconvolution (red, dotted lines) and the resultant fit (solid red line) are also shown. For band positions, see **Table 1**.

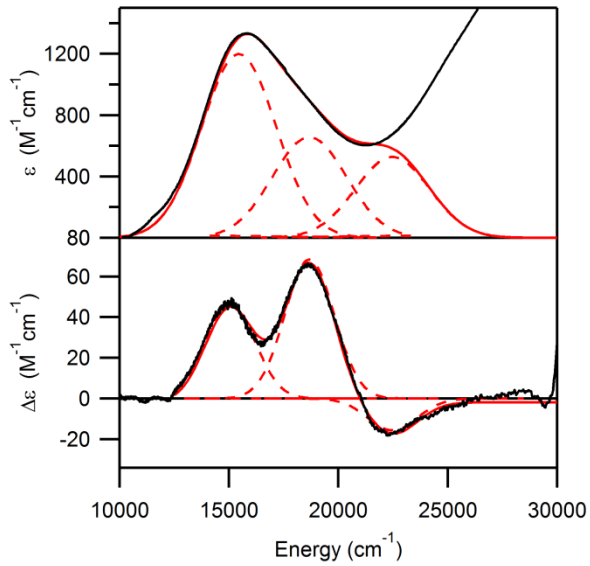

Figure S4. RT Abs (top) and 4.5 K MCD (bottom) spectra of Fe(III)CDO in the presence of Cys. Individual bands obtained from an iterative Gaussian deconvolution (red, dotted lines) and the resultant fit (solid red line) are also shown. For band positions, see **Table 1**.

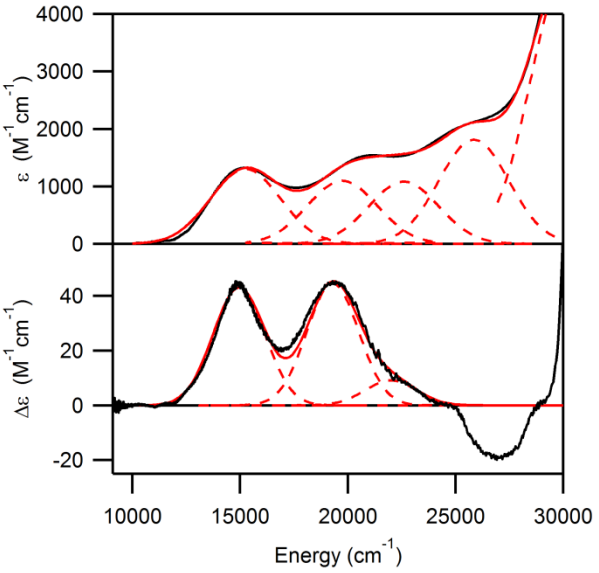

Figure S5. RT Abs (top) and 4.5 K MCD spectra (bottom) of Cys-Fe(III)CDO in the presence of azide. Individual bands obtained from an iterative Gaussian deconvolution (red, dotted lines) and the resultant fit (solid red line) are also shown. For band positions, see **Table 1**.

(N_3^-/$2H_2O$)-Fe(III)CDO, QM/MM-optimized active site (single-point energy: -2376.30058434 Eh)

C	-5.359482	-1.441177	0.410355
C	-4.156311	-0.563431	0.438782
C	-2.981857	-0.623627	-0.274872
N	-3.945633	0.452377	1.375381
C	-2.684769	0.931808	1.242340
N	-2.072525	0.302109	0.236800
H	-5.412186	-2.146927	1.252441
H	-5.340042	-2.027161	-0.513062
H	-6.286057	-0.858139	0.388123
H	-2.730667	-1.242996	-1.117203
H	-4.586853	0.723114	2.113815
H	-2.253403	1.686096	1.875824
C	0.901200	-5.151657	-2.005814
C	1.022812	-3.965714	-1.102203
C	0.865143	-2.623062	-1.337463
N	0.983368	-4.082657	0.289474
C	0.780670	-2.864944	0.847000
N	0.703506	-1.945100	-0.124344
H	-0.153564	-5.291611	-2.284897
H	1.262054	-6.059600	-1.513200
H	1.489151	-5.033188	-2.916534
H	0.811874	-2.096176	-2.271042
H	0.908569	-4.960541	0.806442
H	0.642151	-2.746735	1.910233
C	-0.477448	-0.825928	5.672684
C	-0.160416	-0.306320	4.312988
C	-0.538269	-0.670105	3.037216
N	0.733521	0.741974	4.119980
C	0.901535	0.963989	2.797180
N	0.127914	0.128937	2.103638
H	-1.519791	-1.141083	5.828247
H	-0.256500	-0.050064	6.413147
H	0.157318	-1.680496	5.927246
H	-1.213486	-1.455643	2.741089
H	1.328323	1.211044	4.803604
H	1.542130	1.738403	2.412521
N	-0.527939	0.990219	-2.664917
N	-0.116959	0.137756	-1.929459
N	-0.924133	1.794464	-3.370636
Fe	0.000000	0.000000	0.000000
O	0.000000	2.363693	-0.000015
H	-0.611359	2.852020	-0.560928
H	0.895737	2.640778	-0.235641
O	2.086136	0.702591	0.076279
H	2.527451	0.298965	0.837845
H	2.559250	0.323792	-0.712067

(N_3^-/OH^-)-Fe(III)CDO, QM/MM-optimized active site (single-point energy: -2299.55660646 Eh)

C	-4.315308	-3.398224	0.877900
C	-2.929443	-2.990051	0.512772
C	-2.198563	-1.886932	0.881668
N	-2.119629	-3.656906	-0.410950
C	-0.967606	-2.951370	-0.583664
N	-0.987167	-1.874329	0.194687
H	-5.076416	-3.129486	0.130585
H	-4.590851	-2.904953	1.814468
H	-4.379883	-4.475037	1.067505
H	-2.431808	-1.119568	1.597733
H	-2.383240	-4.477936	-0.942886
H	-0.161575	-3.238480	-1.235016
C	-2.969269	4.132156	1.996918
C	-2.128387	3.448975	0.969131
C	-1.089249	2.571671	1.124619
N	-2.539368	3.275223	-0.357391
C	-1.791962	2.302612	-0.938004
N	-0.894440	1.853851	-0.053909
H	-3.586868	3.383194	2.514221
H	-3.620453	4.883667	1.541260
H	-2.361084	4.647888	2.740479
H	-0.508484	2.351500	1.999420
H	-3.395920	3.646591	-0.768555
H	-1.987350	1.945374	-1.935944
C	-2.100769	-0.822556	-5.390091
C	-1.270752	-0.691498	-4.149246
C	-1.550491	-0.556976	-2.805206
N	0.117493	-0.563736	-4.220169
C	0.619568	-0.325760	-2.984573
N	-0.368210	-0.329178	-2.094147
H	-3.012146	-1.434769	-5.322296
H	-1.481491	-1.251022	-6.186279
H	-2.410645	0.166351	-5.745911
H	-2.510071	-0.566849	-2.318573
H	0.713379	-0.502884	-5.046112
H	1.666870	-0.182800	-2.782425
N	0.528900	-0.872971	2.650040
N	0.000000	-0.000046	2.026230
N	1.035919	-1.706696	3.252502
Fe	0.000000	0.000000	0.000000
O	1.869705	0.224075	-0.220062
H	2.065033	1.120087	-0.533400

(N_3^-/OH^-/H_2O)-Fe(III)CDO, QM/MM-optimized active site (single-point energy: -2375.99768973 Eh)

C	-1.385651	-5.510132	-0.073303
C	-0.619797	-4.239349	-0.183853
C	-0.827408	-3.005508	0.385880
N	0.456635	-4.053528	-1.055618
C	0.847656	-2.750748	-1.000900
N	0.087814	-2.099045	-0.129990
H	-2.107071	-5.663300	-0.889481
H	-1.946686	-5.509903	0.865479
H	-0.718506	-6.377914	-0.033340
H	-1.550140	-2.701675	1.123154
H	0.813629	-4.739182	-1.709885
H	1.649872	-2.318405	-1.572433
C	-5.294968	0.566971	2.250397
C	-4.156036	0.720383	1.284683
C	-2.790619	0.716812	1.451920
N	-4.334579	0.598160	-0.095840
C	-3.116043	0.503708	-0.698074
N	-2.149368	0.575790	0.218430
H	-5.372849	-0.480164	2.601349
H	-6.242584	0.851715	1.779755
H	-5.173813	1.212921	3.121216
H	-2.211761	0.757050	2.356354
H	-5.220779	0.410202	-0.566864
H	-3.024490	0.336761	-1.757477
C	-1.495407	-0.891464	-5.629822
C	-0.905258	-0.465866	-4.327576
C	-1.109467	-0.829987	-3.012161
N	0.033524	0.559280	-4.258804
C	0.337097	0.803085	-2.959259
N	-0.332000	-0.032349	-2.174042
H	-1.730286	-1.962296	-5.719986
H	-0.798325	-0.642502	-6.437805
H	-2.419235	-0.342500	-5.843353
H	-1.774841	-1.582855	-2.623642
H	0.345398	1.188553	-4.997940
H	1.047791	1.549255	-2.651566
N	0.966293	-0.328568	2.636398
N	0.000000	0.000015	2.011093
N	1.868546	-0.655396	3.260773
Fe	0.000000	0.000000	0.000000
O	1.862656	0.085022	-0.207855
H	2.255783	0.962662	-0.250824
O	0.156693	2.281677	-0.425583
H	-0.564087	2.440262	-1.051086
H	-0.150620	2.714417	0.401443

(N_3^-/2OH^-)-Fe(III)CDO, QM/MM-optimized active site (single-point energy: -2375.55295256 Eh)

C	-1.209106	-5.641525	-0.337997
C	-0.491562	-4.341873	-0.311127
C	-0.852554	-3.116180	0.195374
N	0.703308	-4.110992	-0.996796
C	1.011780	-2.785385	-0.891464
N	0.089325	-2.170425	-0.170074
H	-1.783386	-5.794922	-1.263550
H	-1.914886	-5.689850	0.495789
H	-0.521881	-6.485260	-0.209793
H	-1.709427	-2.842773	0.787613
H	1.185089	-4.774902	-1.589325
H	1.873962	-2.312256	-1.327972
C	-5.777893	0.090469	1.271622
C	-4.475327	0.187592	0.531097
C	-3.162888	0.158798	0.942261
N	-4.407211	0.044006	-0.856766
C	-3.095200	-0.067551	-1.223328
N	-2.311295	0.010254	-0.150970
H	-5.904526	-0.926056	1.672348
H	-6.621658	0.313675	0.606888
H	-5.838684	0.803818	2.095749
H	-2.759232	0.222992	1.936279
H	-5.202850	-0.135178	-1.469040
H	-2.810272	-0.236206	-2.245544
C	-0.954865	-0.968811	-5.850998
C	-0.531036	-0.508072	-4.482178
C	-0.583420	-1.018677	-3.201172
N	0.018005	0.769730	-4.315247
C	0.249527	0.986359	-2.988373
N	-0.084991	-0.085175	-2.284805
H	-1.106461	-2.043625	-6.029297
H	-0.200592	-0.635162	-6.575760
H	-1.888016	-0.473328	-6.142212
H	-0.965775	-1.973526	-2.878906
H	0.120895	1.487625	-5.034180
H	0.655853	1.897644	-2.582291
N	0.453094	-0.318619	2.908936
N	-0.372513	-0.292984	2.062195
N	1.236771	-0.352890	3.762695
Fe	0.000000	0.000000	0.000000
O	1.892944	-0.081039	0.137543
O	0.000031	1.948990	-0.000015
H	2.200943	-0.583023	0.899429
H	-0.849472	2.281189	-0.314346

(OH^-/Cys)-Fe(III)CDO, QM/MM-optimized active site (single-point energy: -2855.97322593 Eh)

C	-0.980774	0.472046	5.835953
C	-0.308365	0.322632	4.511322
C	-0.737732	0.620193	3.237900
N	0.952087	-0.250702	4.328491
C	1.224350	-0.281158	2.988846
N	0.222046	0.251053	2.302200
H	-1.485229	-0.489059	6.236908
H	-1.760239	1.235992	5.751831
H	-0.281342	0.835068	6.596207
H	-1.634415	1.128311	2.934296
H	1.515427	-0.696060	5.041122
H	2.133759	-0.667221	2.561707
C	-5.914215	0.933900	0.250595
C	-4.543442	0.340485	0.128326
C	-3.301758	0.862213	-0.178391
N	-4.264694	-0.944138	0.587387
C	-2.913040	-1.137482	0.587479
N	-2.294861	-0.054993	0.130676
H	-6.120178	1.357803	1.312042
H	-6.682205	0.185028	0.030014
H	-6.048874	1.740753	-0.473770
H	-3.076920	1.787476	-0.683182
H	-4.947250	-1.600067	0.973862
H	-2.478683	-2.063004	0.925613
C	-0.095398	-5.490402	1.844604
C	0.040543	-4.208664	1.104935
C	-0.143906	-2.892456	1.454819
N	0.427994	-4.162094	-0.232864
C	0.447083	-2.871475	-0.646957
N	0.123871	-2.075806	0.365463
H	-0.089081	-5.389771	2.991745
H	0.734879	-6.152161	1.569138
H	-1.015900	-6.019043	1.558960
H	-0.482758	-2.485611	2.392395
H	0.605743	-4.931168	-0.875977
H	0.669266	-2.554504	-1.649292
O	-0.167694	-0.365800	-1.836044
Fe	0.000000	0.000000	0.000000
H	0.598404	-0.095795	-2.352814
N	-0.000015	2.222534	0.000000
C	1.332733	2.821548	0.322617
C	1.423538	4.328537	0.039000
O	0.779968	4.793839	-1.000900
C	2.419693	2.096710	-0.488312
S	2.423676	0.288666	-0.140335
O	2.190704	5.040039	0.764206
H	-0.706345	2.622391	0.621643
H	-0.267731	2.458145	-0.961441
H	1.506638	2.659042	1.387283
H	3.397705	2.509689	-0.235641
H	2.248383	2.251556	-1.558273

(H_2O/Cys)-Fe(III)CDO QM/MM-optimized active site (single-point energy: -2865.40635266 Eh)

C	-1.609695	0.187744	5.478317
C	-0.746400	0.128600	4.268204
C	-1.018173	0.472382	2.966766
N	0.516830	-0.463181	4.220032
C	0.949554	-0.468842	2.928925
N	0.039566	0.105225	2.144363
H	-2.133560	-0.757431	5.683655
H	-2.371140	0.959595	5.337189
H	-1.044098	0.476761	6.368423
H	-1.869614	0.991272	2.570694
H	0.985107	-0.933655	4.985031
H	1.889908	-0.880585	2.606735
C	-5.822571	0.912216	-0.757919
C	-4.444946	0.315536	-0.752609
C	-3.173096	0.838791	-0.890472
N	-4.223511	-0.997574	-0.346054
C	-2.886047	-1.213608	-0.208679
N	-2.206680	-0.111633	-0.529175
H	-6.130829	1.229492	0.208710
H	-6.555603	0.182465	-1.117340
H	-5.870605	1.764450	-1.440231
H	-2.893723	1.798203	-1.296036
H	-4.949127	-1.667206	-0.076996
H	-2.506302	-2.165939	0.125870
C	-0.184662	-5.585159	1.259125
C	0.012222	-4.264145	0.604950
C	-0.251587	-2.971390	0.989792
N	0.563141	-4.140625	-0.669098
C	0.605331	-2.833038	-1.017639
N	0.132004	-2.092010	-0.018600
H	-0.333420	-5.552292	2.348511
H	0.692856	-6.214203	1.067978
H	-1.042175	-6.113708	0.820923
H	-0.719467	-2.622116	1.894562
H	0.844193	-4.880005	-1.312866
H	0.964417	-2.481369	-1.966873
O	0.217026	-0.177582	-2.201645
H	1.100891	0.078903	-2.494781
H	-0.425629	0.302261	-2.768768
Fe	0.000000	0.000000	0.000000
N	0.000000	2.204727	-0.000015
C	1.294327	2.776093	0.492767
C	1.434952	4.291016	0.253632
O	0.913498	4.771347	-0.849152
C	2.480347	2.086090	-0.203308
S	2.400116	0.256104	-0.106674
O	2.122467	4.970230	1.068924
H	-0.769272	2.577652	0.568588
H	-0.166000	2.514526	-0.963013
H	1.337296	2.589676	1.566895
H	3.416183	2.425552	0.245438
H	2.510773	2.361313	-1.264984

Cys-Fe(III)CDO, QM/MM-optimized active site (single-point energy: -2779.9046462 Eh)

C	-2.839554	-0.300064	4.787033
C	-1.655579	-0.198196	3.887436
C	-1.561707	0.290741	2.608124
N	-0.400574	-0.757675	4.141357
C	0.379227	-0.619949	3.033554
N	-0.297821	0.026642	2.086060
H	-3.348373	-1.339859	4.769196
H	-3.587250	0.432739	4.468628
H	-2.588470	-0.050140	5.821289
H	-2.284332	0.849243	2.043350
H	-0.143112	-1.296280	4.960098
H	1.384903	-0.993790	2.948898
C	-5.112534	0.477844	-2.484695
C	-3.754227	-0.042480	-2.144379
C	-2.547028	0.568878	-1.883606
N	-3.553528	-1.369446	-1.772919
C	-2.298996	-1.518784	-1.275100
N	-1.649551	-0.350891	-1.326721
H	-5.725388	0.751328	-1.538040
H	-5.682434	-0.261490	-3.055054
H	-5.036346	1.367020	-3.115082
H	-2.234665	1.567352	-2.140839
H	-4.276123	-2.093277	-1.744736
H	-1.953156	-2.466858	-0.893600
C	0.307388	-5.647232	0.975037
C	0.500092	-4.273376	0.432358
C	-0.071548	-3.058121	0.727509
N	1.381897	-3.996033	-0.611557
C	1.314682	-2.676926	-0.920197
N	0.448044	-2.075012	-0.109634
H	-0.185562	-5.706512	2.017349
H	1.279343	-6.150055	1.042160
H	-0.302246	-6.249008	0.287323
H	-0.841843	-2.838318	1.447281
H	1.958389	-4.648560	-1.143509
H	1.902145	-2.216309	-1.695404
Fe	0.000000	0.000000	0.000000
N	0.000031	2.198593	0.000031
C	1.189300	2.678452	0.783127
C	1.313339	4.214035	0.897461
O	1.094238	4.919724	-0.188187
C	2.460297	2.106277	0.134705
S	2.328918	0.289948	-0.065796
O	1.702637	4.680862	2.003510
H	-0.866119	2.587448	0.389786
H	0.089905	2.539886	-0.965134
H	1.082474	2.290710	1.796646
H	3.337830	2.329300	0.744202
H	2.619812	2.521057	-0.866165

(N_3^-/Cys)-Fe(III)CDO S=1/2, QM/MM-optimized active site (single-point energy: -2944.32513165 Eh)

C	-1.446884	-0.035248	5.480759
C	-0.651917	-0.053314	4.219391
C	-0.972153	0.336136	2.939056
N	0.620285	-0.614487	4.109665
C	1.011627	-0.560303	2.804581
N	0.070114	0.023361	2.071228
H	-1.834976	-1.022018	5.773468
H	-2.232742	0.720123	5.396423
H	-0.831055	0.261017	6.335739
H	-1.843597	0.859451	2.593231
H	1.119095	-1.112656	4.835205
H	1.950211	-0.929810	2.433289
C	-5.763916	0.871613	-0.478241
C	-4.373032	0.293503	-0.452850
C	-3.099060	0.830246	-0.508698
N	-4.157120	-1.032700	-0.082779
C	-2.824341	-1.237045	0.120071
N	-2.147003	-0.120789	-0.121384
H	-6.120346	1.166641	0.519730
H	-6.471313	0.139832	-0.884552
H	-5.809891	1.745850	-1.131729
H	-2.801758	1.788712	-0.901535
H	-4.884293	-1.719910	0.128600
H	-2.443405	-2.196976	0.422180
C	-0.093704	-5.559021	1.060822
C	0.092697	-4.194580	0.494293
C	-0.205917	-2.928558	0.943985
N	0.673645	-3.989609	-0.751266
C	0.696732	-2.660660	-1.025345
N	0.178253	-1.986588	-0.005203
N	-0.109314	-0.089096	-1.924622
N	0.736023	-0.068893	-2.765945
N	1.490800	-0.113937	-3.631027
Fe	0.000000	0.000000	0.000000
N	0.000015	2.068909	-0.000031
C	1.300034	2.662094	0.461472
C	1.400055	4.192337	0.317520
O	0.814270	4.753647	-0.705231
C	2.412292	1.963806	-0.327576
S	2.255646	0.149597	-0.056442
O	2.113998	4.824707	1.159714
H	-0.178497	-5.602676	2.156677
H	0.759933	-6.185135	0.773087
H	-0.982452	-6.043610	0.635269
H	-0.692093	-2.643829	1.861450
H	0.967484	-4.675156	-1.443649
H	1.114853	-2.267548	-1.932724
H	-0.758270	2.458008	0.565384
H	-0.177719	2.343246	-0.973114
H	1.399582	2.421844	1.521210
H	3.394104	2.298019	0.009415
H	2.315887	2.173279	-1.398392

(N_3^-/Cys)-Fe(III)CDO S=5/2, QM/MM-optimized active site (single-point energy: -2944.29705305 Eh)

C	-1.569717	0.217148	-5.412155
C	-0.736221	0.174118	-4.177292
C	-1.024734	-0.271637	-2.907944
N	0.519241	0.772720	-4.063507
C	0.922104	0.683258	-2.756256
N	0.007858	0.047958	-2.034409
H	-2.111603	1.227005	-5.575790
H	-2.340881	-0.557632	-5.350128
H	-0.980438	-0.009064	-6.307129
H	-1.877762	-0.831757	-2.571396
H	0.984055	1.332031	-4.764800
H	1.861176	1.044281	-2.376480
C	-5.693802	-0.967834	0.671524
C	-4.308853	-0.379898	0.624420
C	-3.026627	-0.904007	0.613297
N	-4.121780	0.958389	0.292084
C	-2.792618	1.177322	0.043167
N	-2.093430	0.065400	0.225769
H	-6.099655	-1.255722	-0.381516
H	-6.394287	-0.250885	1.116898
H	-5.717728	-1.858398	1.303467
H	-2.706909	-1.874100	0.958298
H	-4.863007	1.638321	0.112305
H	-2.427856	2.146027	-0.244919
C	-0.198700	5.604614	-0.787384
C	0.031174	4.219421	-0.287766
C	-0.267395	2.970917	-0.784195
N	0.670425	3.963837	0.921005
C	0.720016	2.614349	1.121307
N	0.166687	1.984879	0.094315
N	0.000000	-0.000031	2.016113
N	0.823257	0.005936	2.864532
N	1.569077	0.033142	3.755905
Fe	0.000000	0.000000	0.000000
N	0.061447	-2.105469	-0.032135
C	1.368484	-2.660751	-0.504669
C	1.490753	-4.181473	-0.372192
O	0.961624	-4.764160	0.674469
C	2.487747	-1.946320	0.276550
S	2.389374	-0.139496	-0.050507
O	2.167664	-4.835281	-1.241821
H	-0.321960	5.699800	-1.930649
H	0.655731	6.232117	-0.501053
H	-1.083450	6.060608	-0.318146
H	-0.782425	2.722000	-1.696930
H	0.971573	4.617859	1.639496
H	1.187134	2.171692	1.981049
H	-0.692245	-2.535233	-0.570724
H	-0.084229	-2.353790	0.949341
H	1.459610	-2.405487	-1.562271
H	3.461000	-2.337341	-0.025940
H	2.354874	-2.130737	1.349411