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Supplementary Data

A computational study of ligand binding affinities in iron(III) porphine and protoporphyrin IX complexes

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Table S1. Calculated energies and uncorrected zero point energies (ZPE) (Hartrees), and entropies S (cal mol^{-1} K^{-1}) of iron(III) porphine complexes and free ligands, computed *in vacuo*, and in water and *n*-octanol solvents for **method 1**.

All structures were geometry optimized *in vacuo* at the B3LYP/LanL2DZ level. Single point calculations were then run at the B3LYP/LanL2DZ level, using the SMD solvent method.

core porphine						
species	S	ZPE	vacuum	water	octanol	Fe spin
m=2	133.500	0.274721	-1111.497726	-1111.578237	-1111.578627	2.02
m=4	133.305	0.277911	-1111.501063	-1111.596130	-1111.593599	2.85
m=6	137.783	0.272882	-1111.490774	-1111.578344	-1111.575342	3.71

H_2O						
species	S	ZPE	vacuum	water	octanol	Fe spin
m=2	146.985	0.299347	-1187.937503	-1188.016880	-1188.020278	1.98
m=4	149.410	0.302085	-1187.943417	-1188.039901	-1188.042716	3.01
m=6	149.372	0.299866	-1187.940921	-1188.030719	-1188.031038	4.08
H_2O	46.507	0.020764	-76.414316	-76.432623	-76.429402	

OH^-						
species	S	ZPE	vacuum	water	octanol	Fe spin
m=2	138.726	0.290869	-1187.540503	-1187.573665	-1187.576910	1.00
m=4	144.072	0.289047	-1187.545651	-1187.580507	-1187.583411	2.59
m=6	147.026	0.287489	-1187.550704	-1187.582056	-1187.585346	4.02
OH^-	41.320	0.007607	-75.751486	-75.921763	-75.896403	

Cl^-						
species	S	ZPE	vacuum	water	octanol	Fe spin
m=2	140.923	0.278794	-1126.692067	-1126.719473	-1126.727411	1.25
m=4	142.628	0.278788	-1126.707627	-1126.737442	-1126.745051	2.61
m=6	144.419	0.277111	-1126.705000	-1126.731697	-1126.739701	3.97
Cl^-	36.586	0.000000	-14.998633	-15.107025	-15.100075	

OMe^-						
species	S	ZPE	vacuum	water	octanol	Fe spin
m=2	147.123	0.319196	-1226.834059	-1226.861267	-1226.866054	0.99
m=4	152.378	0.318142	-1226.840354	-1226.867096	-1226.872034	2.54
m=6	156.782	0.316739	-1226.846091	-1226.869630	-1226.875341	3.99
OMe^-	55.068	0.034812	-115.070523	-115.209187	-115.190012	

OAc^-						
species	S	ZPE	vacuum	water	octanol	Fe spin
m=2	158.921	0.328540	-1340.179289	-1340.212391	-1340.216051	1.12
m=4	163.309	0.328045	-1340.190966	-1340.227928	-1340.230298	2.71
m=6	165.739	0.326458	-1340.189981	-1340.224129	-1340.226967	4.06
OAc^-	69.450	0.047875	-228.486772	-228.608525	-228.592448	

Pyridine						
species	S	ZPE	vacuum	water	octanol	Fe spin
m=2	155.124	0.371190	-1359.779990	-1359.849316	-1359.856671	1.17
m=4	160.282	0.369859	-1359.792109	-1359.860488	-1359.868020	2.79
m=6	163.439	0.367785	-1359.780544	-1359.850908	-1359.857292	4.08
pyridine	68.617	0.089264	-248.239421	-248.248805	-248.247215	

$MeNH_2$						
species	S	ZPE	vacuum	water	octanol	Fe spin
m=2	149.932	0.346872	-1207.393797	-1207.462373	-1207.466912	1.19
m=4	151.385	0.346175	-1207.396825	-1207.470191	-1207.475917	2.78
m=6	154.100	0.344135	-1207.383967	-1207.459806	-1207.464742	4.07
$MeNH_2$	58.009	0.063841	-95.843063	-95.849469	-95.849167	

***N*-bound oxazole**						
species	S	ZPE	vacuum	water	octanol	Fe spin
m=2	154.341	0.339141	-1357.550607	-1357.624286	-1357.628265	1.19
m=4	158.974	0.338380	-1357.565114	-1357.636894	-1357.641149	2.81
m=6	162.116	0.336172	-1357.552360	-1357.626179	-1357.629717	4.08
oxazole	64.742	0.058059	-246.018609	-246.028694	-246.025605	

***O*-bound oxazole**						
species	S	ZPE	vacuum	water	octanol	Fe spin
m=2	164.692	0.333354	-1357.523183	-1357.611610	-1357.603772	2.05
m=4	161.351	0.337006	-1357.538170	-1357.623400	-1357.619503	2.85
m=6	166.194	0.333239	-1357.521724	-1357.609237	-1357.605917	4.07
oxazole	64.742	0.058059	-246.018609	-246.028694	-246.025605	

$(imidazolide)^-$						
species	S	ZPE	vacuum	water	octanol	Fe spin
m=2	152.471	0.338615	-1337.290662	-1337.323993	-1337.330384	1.03
m=4	158.551	0.337571	-1337.289362	-1337.327362	-1337.333179	2.67
m=6	161.114	0.335903	-1337.289244	-1337.322534	-1337.328866	4.06
$C_3H_3N_2^-$	64.498	0.057365	-225.592791	-225.698833	-225.687621	

imidazole						
species	S	ZPE	vacuum	water	octanol	Fe spin
m=2	154.606	0.352851	-1337.721659	-1337.797805	-1337.804641	1.15
m=4	158.919	0.352269	-1337.733349	-1337.806904	-1337.814254	2.80
m=6	162.069	0.350232	-1337.722509	-1337.798204	-1337.804885	4.08
$C_3H_4N_2$	65.001	0.071612	-226.173778	-226.190831	-226.190597	

1,3,5-triazine						
species	S	ZPE	vacuum	water	octanol	Fe spin
m=2	157.106	0.345194	-1391.811946	-1391.896694	-1391.899878	1.23
m=4	161.210	0.344738	-1391.827050	-1391.912226	-1391.915604	2.80
m=6	163.984	0.342445	-1391.813116	-1391.899294	-1391.901502	4.07
$C_3H_3N_3$	68.256	0.064811	-280.289773	-280.307768	-280.305865	

Me_3NO						
species	S	ZPE	vacuum	water	octanol	Fe spin
m=2	166.034	0.406465	-1361.146128	-1361.226005	-1361.230812	1.09
m=4	168.596	0.406078	-1361.164161	-1361.243650	-1361.248154	2.77
m=6	171.063	0.404278	-1361.156513	-1361.239491	-1361.242819	4.06
Me_3NO	75.586	0.125472	-249.588399	-249.621972	-249.619468	

Me_3N						
species	S	ZPE	vacuum	water	octanol	Fe spin
m=2	157.853	0.403177	-1285.973040	-1286.044101	-1286.050448	1.29
m=4	160.496	0.402511	-1285.989980	-1286.058580	-1286.065619	2.76
m=6	164.368	0.400403	-1285.979818	-1286.051341	-1286.057951	4.07
Me_3N	71.913	0.120330	-174.442307	-174.447869	-174.448749	

MeS^-						
species	S	ZPE	vacuum	water	octanol	Fe spin
m=2	152.237	0.316711	-1161.739587	-1161.760257	-1161.769299	1.35
m=4	155.786	0.316245	-1161.739697	-1161.763192	-1161.771920	2.43
m=6	158.164	0.314621	-1161.738846	-1161.760507	-1161.769465	3.90
MeS^-	58.381	0.035892	-50.020370	-50.119887	-50.113982	

***N*-bound (2-hydroxypyridine)$^-$**						
species	S	ZPE	vacuum	water	octanol	Fe spin
m=2	158.436	0.360651	-1434.583442	-1434.614865	-1434.621015	1.04
m=4	163.166	0.359867	-1434.587344	-1434.622174	-1434.627373	2.69
m=6	166.446	0.358196	-1434.587525	-1434.620946	-1434.625941	4.06
$C_5H_4NO^-$	73.417	0.079315	-322.895934	-323.006804	-322.993013	

***O*-bound (2-hydroxypyridine)$^-$**						
species	S	ZPE	vacuum	water	octanol	Fe spin
m=2	164.234	0.360424	-1434.583967	-1434.613140	-1434.620256	1.00
m=4	169.849	0.359721	-1434.597658	-1434.629587	-1434.635324	2.68
m=6	171.928	0.358233	-1434.599138	-1434.630373	-1434.635765	4.04
$C_5H_4NO^-$	73.417	0.079315	-322.895934	-323.006804	-322.993013	

MeOH						
species	S	ZPE	vacuum	water	octanol	Fe spin
m=2	155.611	0.328709	-1227.230884	-1227.303548	-1227.307948	1.95
m=4	156.267	0.331533	-1227.250508	-1227.327994	-1227.331760	2.85
m=6	157.756	0.329314	-1227.236304	-1227.316510	-1227.320071	4.08
MeOH	56.963	0.050934	-115.708436	-115.720004	-115.718522	

PhO^-						
species	S	ZPE	vacuum	water	octanol	Fe spin
m=2	165.827	0.372091	-1418.552879	-1418.582098	-1418.589224	1.20
m=4	170.199	0.371699	-1418.563257	-1418.591398	-1418.599343	2.60
m=6	171.161	0.370228	-1418.567309	-1418.592183	-1418.600623	4.01
PhO^-	73.659	0.091046	-306.855544	-306.960892	-306.950736	

AcOH						
species	S	ZPE	vacuum	water	octanol	Fe spin
m=2	165.427	0.337994	-1340.570464	-1340.647857	-1340.649812	1.99
m=4	169.612	0.340645	-1340.589138	-1340.669443	-1340.670636	2.84
m=6	169.278	0.338416	-1340.575113	-1340.658506	-1340.657857	4.08
AcOH	69.476	0.061286	-229.053218	-229.067968	-229.065932	

Me_3P						
species	S	ZPE	vacuum	water	octanol	Fe spin
m=2	169.453	0.394902	-1237.755244	-1237.825376	-1237.831608	1.40
m=4	176.851	0.393774	-1237.762384	-1237.829339	-1237.836798	2.63
m=6	178.761	0.391703	-1237.749669	-1237.819212	-1237.826445	3.98
Me_3P	79.352	0.113707	-126.221562	-126.220711	-126.224483	

Quinoline						
species	S	ZPE	vacuum	water	octanol	Fe spin
m=2	167.847	0.417393	-1513.390328	-1513.457206	-1513.466435	1.15
m=4	171.697	0.416892	-1513.405801	-1513.473218	-1513.482151	2.79
m=6	174.325	0.415066	-1513.396315	-1513.465048	-1513.473430	4.08
C_9H_7N	81.322	0.136646	-401.860324	-401.870696	-401.873357	

Thiophene						
species	S	ZPE	vacuum	water	octanol	Fe spin
m=2	169.377	0.342701	-1276.381507	-1276.452203	-1276.459157	2.04
m=4	168.780	0.345681	-1276.393847	-1276.465626	-1276.471999	2.75
m=6	173.126	0.342239	-1276.378506	-1276.447814	-1276.454543	3.93
C_4H_4S	68.106	0.066912	-164.878827	-164.881560	-164.885253	

Aniline						
species	S	ZPE	vacuum	water	octanol	Fe spin
m=2	167.978	0.399356	-1399.091221	-1399.170293	-1399.176393	1.27
m=4	170.057	0.398896	-1399.105390	-1399.182871	-1399.189320	2.76
m=6	173.692	0.396881	-1399.091951	-1399.170680	-1399.177070	4.06
$PhNH_2$	75.988	0.117693	-287.564867	-287.574427	-287.577283	

Me_3PO						
species	S	ZPE	vacuum	water	octanol	Fe spin
m=2	175.508	0.398308	-1312.973163	-1313.053894	-1313.057874	1.12
m=4	181.919	0.397831	-1312.993482	-1313.071578	-1313.076389	2.80
m=6	186.327	0.396162	-1312.986842	-1313.067056	-1313.071232	4.08
Me_3PO	85.133	0.117775	-201.421231	-201.448129	-201.446088	

***O*-bound DMSO**						
species	S	ZPE	vacuum	water	octanol	Fe spin
m=2	169.031	0.359432	-1276.592174	-1276.671436	-1276.675478	1.12
m=4	174.449	0.359124	-1276.608210	-1276.687098	-1276.691022	2.79
m=6	176.193	0.357247	-1276.598292	-1276.678984	-1276.682237	4.06
DMSO	75.872	0.079009	-165.040337	-165.066131	-165.062249	

***S*-bound DMSO**						
species	S	ZPE	vacuum	water	octanol	Fe spin
m=2	dissociated	-	-	-	-	-
m=4	174.135	0.358445	-1276.558501	-1276.652149	-1276.651044	2.72
m=6	dissociated	-	-	-	-	-
DMSO	75.872	0.079009	-165.040337	-165.066131	-165.062249	

F^-						
species	S	ZPE	vacuum	water	octanol	Fe spin
m=2	137.868	0.279696	-1211.587038	-1211.618280	-1211.624239	1.03
m=4	139.246	0.279569	-1211.603578	-1211.636386	-1211.642139	2.70
m=6	140.652	0.278103	-1211.603783	-1211.633059	-1211.639296	4.06
F^-	34.767	0.000000	-99.827418	-99.974492	-99.962766	

$Me_2PO_2^-$						
species	S	ZPE	vacuum	water	octanol	Fe spin
m=2	170.868	0.362280	-1348.471441	-1348.517144	-1348.518900	1.05
m=4	176.692	0.361831	-1348.486251	-1348.533952	-1348.535361	2.70
m=6	181.191	0.360256	-1348.487591	-1348.532739	-1348.534830	4.06
$Me_2PO_2^-$	80.030	0.081688	-236.775963	-236.901865	-236.885498	

$Me3SiO^-$						
species	S	ZPE	vacuum	water	octanol	Fe spin
2	178.638	0.394571	-1310.619990	-1310.644858	-1310.652248	1.02
4	184.298	0.394119	-1310.637101	-1310.658412	-1310.667921	2.61
6	185.508	0.392847	-1310.644386	-1310.664539	-1310.673650	4.03
$Me3SiO^-$	86.592	0.113166	-198.901565	-199.012895	-199.000427	

***N*-bound morpholine**						
species	S	ZPE	vacuum	water	octanol	Fe spin
2	160.695	0.417125	-1399.287677	-1399.372632	-1399.375800	1.22
4	166.442	0.415706	-1399.299313	-1399.382812	-1399.386585	2.92
6	167.376	0.414179	-1399.288445	-1399.373905	-1399.377049	4.08
C_4H_9NO	73.602	0.135221	-287.751029	-287.767282	-287.765069	

***O*-bound morpholine**						
species	S	ZPE	vacuum	water	octanol	Fe spin
2	167.387	0.412655	-1399.273962	-1399.348595	-1399.353043	1.85
4	168.175	0.415053	-1399.295109	-1399.372173	-1399.376207	2.83
6	171.837	0.413047	-1399.282914	-1399.362462	-1399.364292	4.08
C_4H_9NO	73.602	0.135221	-287.751029	-287.767282	-287.765069	

4-methylpyridine						
species	S	ZPE	vacuum	water	octanol	Fe spin
2	168.843	0.397800	-1399.096945	-1399.164282	-1399.172765	1.16
4	171.592	0.397386	-1399.108310	-1399.174766	-1399.183413	2.79
6	174.862	0.395335	-1399.097232	-1399.165683	-1399.173145	4.08
C_6H_7N	78.866	0.116965	-287.552748	-287.562023	-287.563496	

4-dimethylaminopyridine						
species	S	ZPE	vacuum	water	octanol	Fe spin
2	177.262	0.444241	-1493.747214	-1493.814248	-1493.822997	1.12
4	181.508	0.443434	-1493.756087	-1493.821951	-1493.830871	2.78
6	184.628	0.441536	-1493.746901	-1493.815268	-1493.822980	4.08
$C_7H_{10}N_2$	90.531	0.162716	-382.190374	-382.204534	-382.205583	

***n*-butylamine**						
species	S	ZPE	vacuum	water	octanol	Fe spin
2	172.231	0.432570	-1325.310674	-1325.386528	-1325.394340	1.19
4	175.815	0.431682	-1325.322674	-1325.394170	-1325.403140	2.77
6	178.798	0.429645	-1325.310331	-1325.384078	-1325.392429	4.08
$BuNH_2$	81.105	0.150109	-213.766607	-213.772308	-213.775404	

Table S2. Calculated energies of iron(III) porphine complexes and free ligands (kcal mol^{-1}), computed *in vacuo*, and in water and *n*-octanol solvents for **method 2**.

Single point calculations were run at the method 1 geometries, using OPBE/6-311+G(d,p) and the SMD solvent method.

core porphine				
species	vacuum	water	octanol	Fe spin
m=2	-2251.966908	-2252.050934	-2252.050631	2.37
m=4	-2251.994435	-2252.085276	-2252.083308	2.93
m=6	-2251.971189	-2252.075531	-2252.069847	4.22

H_2O				
species	vacuum	water	octanol	Fe spin
m=4	-2328.425950	-2328.506820	-2328.510195	2.97
m=6	-2328.414624	-2328.501272	-2328.502000	4.25
H_2O	-76.418443	-76.431164	-76.429483	

OH^-				
species	vacuum	water	octanol	Fe spin
m=4	-2328.013098	-2328.041374	-2328.045859	2.68
m=6	-2328.020563	-2328.046446	-2328.050945	4.14
OH^-	-75.776668	-75.927803	-75.907977	

Cl^-				
species	vacuum	water	octanol	Fe spin
m=4	-2712.427774	-2712.454781	-2712.462595	2.85
m=6	-2712.431533	-2712.455114	-2712.463381	4.13
Cl^-	-460.255231	-460.359360	-460.352750	

OMe^-				
species	vacuum	water	octanol	Fe spin
m=4	-2367.303515	-2367.324452	-2367.330720	2.57
m=6	-2367.312583	-2367.331594	-2367.338251	4.07
OMe^-	-115.080589	-115.206846	-115.190707	

OAc^-				
species	vacuum	water	octanol	Fe spin
m=4	-2480.652008	-2480.681973	-2480.685997	2.78
m=6	-2480.656675	-2480.684206	-2480.688548	4.19
OAc^-	-228.482029	-228.593865	-228.580287	

Pyridine				
species	vacuum	water	octanol	Fe spin
m=4	-2480.652008	-2480.681973	-2480.685997	2.75
m=6	-2480.656675	-2480.684206	-2480.688548	4.13
pyridine	-248.237797	-248.245287	-248.246086	

$MeNH_2$				
species	vacuum	water	octanol	Fe spin
m=4	-2347.871728	-2347.943362	-2347.949295	2.84
m=6	-2347.862673	-2347.937095	-2347.942184	4.25
$MeNH_2$	-95.846535	-95.851638	-95.851491	

***N*-bound oxazole**				
species	vacuum	water	octanol	Fe spin
m=4	-2498.048120	-2498.116374	-2498.121186	2.76
m=6	-2498.039597	-2498.110186	-2498.114214	4.17
oxazole	-246.029193	-246.036612	-246.034008	

***O*-bound oxazole**				
species	vacuum	water	octanol	Fe spin
m=4	-2498.020043	-2498.101651	-2498.098444	2.87
m=6	-2498.006998	-2498.093123	-2498.089749	4.13
oxazole	-246.029193	-246.036612	-246.034008	

(imidazolide)$^-$				
species	vacuum	water	octanol	Fe spin
m=2	-2477.776777	-2477.804455	-2477.811445	1.02
m=4	-2477.778370	-2477.810697	-2477.817046	2.63
m=6	-2477.783433	-2477.811517	-2477.818398	4.15
$C_3H_3N_2^-$	-225.612824	-225.713967	-225.703142	

imidazole				
species	vacuum	water	octanol	Fe spin
m=4	-2478.216501	-2478.287788	-2478.295402	2.75
m=6	-2478.209793	-2478.283480	-2478.290364	4.15
$C_3H_4N_2$	-226.187758	-226.202258	-226.202371	

1,3,5-triazine				
species	vacuum	water	octanol	Fe spin
m=4	-2532.322387	-2532.401939	-2532.406094	2.79
m=6	-2532.312419	-2532.393216	-2532.396237	4.19
$C_3H_3N_3$	-280.311880	-280.326253	-280.324879	

Me_3NO				
species	vacuum	water	octanol	Fe spin
m=4	-2501.608063	-2501.683787	-2501.689218	2.84
m=6	-2501.605347	-2501.684825	-2501.689004	4.14
Me_3NO	-249.568803	-249.595239	-249.593883	

Me_3N				
species	vacuum	water	octanol	Fe spin
m=4	-2426.451113	-2426.518058	-2426.525297	2.81
m=6	-2426.445154	-2426.514986	-2426.521801	4.11
Me_3N	-174.442057	-174.446241	-174.447314	

MeS^-				
species	vacuum	water	octanol	Fe spin
m=2	-2690.291464	-2690.309572	-2690.318914	1.17
m=4	-2690.289743	-2690.310237	-2690.319305	2.66
m=6	-2690.295517	-2690.314465	-2690.323741	4.06
MeS^-	-438.097221	-438.193396	-438.187622	

***N*-bound (2-hydroxypyridine)$^-$**				
species	vacuum	water	octanol	Fe spin
m=4	-2575.051213	-2575.079689	-2575.086256	2.63
m=6	-2575.057020	-2575.084049	-2575.090506	4.06
$C_5H_4NO^-$	-322.895364	-322.997606	-322.985564	

***O*-bound (2-hydroxypyridine)$^-$**				
species	vacuum	water	octanol	Fe spin
m=4	-2575.063383	-2575.089010	-2575.096061	2.67
m=6	-2575.069170	-2575.094334	-2575.100911	4.14
$C_5H_4NO^-$	-322.895364	-322.997606	-322.985564	

MeOH				
species	vacuum	water	octanol	Fe spin
m=4	-2367.712924	-2367.787662	-2367.791875	2.92
m=6	-2367.702033	-2367.780163	-2367.783948	4.24
MeOH	-115.704072	-115.711706	-115.711308	

PhO^-				
species	vacuum	water	octanol	Fe spin
m=4	-2559.019320	-2559.042418	-2559.051421	2.60
m=6	-2559.026394	-2559.047400	-2559.056588	4.13
PhO^-	-306.846513	-306.944364	-306.935860	

AcOH				
species	vacuum	water	octanol	Fe spin
m=4	-2481.059737	-2481.134082	-2481.136622	2.90
m=6	-2481.049599	-2481.127467	-2481.128124	4.21
AcOH	-229.051030	-229.061432	-229.060610	

Me_3P				
species	vacuum	water	octanol	Fe spin
m=4	-2713.081993	-2713.147227	-2713.154885	2.91
m=6	-2713.073959	-2713.141791	-2713.149224	4.16
Me_3P	-461.054864	-461.053988	-461.057750	

Quinoline				
species	vacuum	water	octanol	Fe spin
m=4	-2653.865596	-2653.931036	-2653.940208	2.75
m=6	-2653.859713	-2653.926554	-2653.935135	4.04
C_9H_7N	-401.851207	-401.859746	-401.862635	

Thiophene				
species	vacuum	water	octanol	Fe spin
m=4	-2804.964793	-2805.034700	-2805.041280	2.98
m=6	-2804.952262	-2805.021639	-2805.028217	4.07
C_4H_4S	-552.965884	-552.968202	-552.971941	

Aniline				
species	vacuum	water	octanol	Fe spin
m=4	-2539.571519	-2539.646915	-2539.653612	2.77
m=6	-2539.562237	-2539.639224	-2539.645798	4.20
$PhNH_2$	-287.556108	-287.565117	-287.568029	

Me_3PO				
species	vacuum	water	octanol	Fe spin
m=4	-2788.319849	-2788.391679	-2788.397788	2.87
m=6	-2788.316787	-2788.391073	-2788.396296	4.20
Me_3PO	-536.287294	-536.306562	-536.306604	

***O*-bound DMSO**				
species	vacuum	water	octanol	Fe spin
m=4	-2805.165242	-2805.239362	-2805.244269	2.83
m=6	-2805.159309	-2805.235787	-2805.239839	4.20
DMSO	-553.131881	-553.152778	-553.150276	

***S*-bound DMSO**				
species	vacuum	water	octanol	Fe spin
m=4	-2805.137751	-2805.223859	-2805.224543	2.89
DMSO	-553.131881	-553.152778	-553.150276	

F^-				
species	vacuum	water	octanol	Fe spin
m=4	-2352.046277	-2352.074343	-2352.080615	2.82
m=6	-2352.051824	-2352.076614	-2352.083361	4.23
F^-	-99.825486	-99.965673	-99.954523	

$Me_2PO_2^-$				
species	vacuum	water	octanol	Fe spin
m=4	-2823.818966	-2823.855769	-2823.859974	2.74
m=6	-2823.825573	-2823.860322	-2823.864936	4.18
$Me_2PO_2^-$	-571.650454	-571.763166	-571.750533	

Me3SiO$^-$				
species	vacuum	water	octanol	Fe spin
m=4	-2736.669971	-2736.686892	-2736.697363	2.64
m=6	-2736.680230	-2736.696499	-2736.706463	4.13
Me3SiO$^-$	-484.471825	-484.574106	-484.563680	

***N*-bound morpholine**				
species	vacuum	water	octanol	Fe spin
m=4	-2539.759287	-2539.837301	-2539.842103	2.79
m=6	-2539.752257	-2539.832395	-2539.836580	4.14
C_4H_9NO	-287.741296	-287.753559	-287.752523	

***O*-bound morpholine**				
species	vacuum	water	octanol	Fe spin
m=4	-2539.749482	-2539.824084	-2539.828462	2.86
m=6	-2539.740682	-2539.818371	-2539.820450	4.20
C_4H_9NO	-287.741296	-287.753559	-287.752523	

4-methylpyridine				
species	vacuum	water	octanol	Fe spin
m=4	-2539.574824	-2539.639707	-2539.648517	2.74
m=6	-2539.567729	-2539.634680	-2539.642308	4.13
C_6H_7N	-287.549759	-287.557359	-287.559020	

4-dimethylaminopyridine				
species	vacuum	water	octanol	Fe spin
m=4	-2634.217364	-2634.282001	-2634.291036	2.74
m=6	-2634.212297	-2634.279674	-2634.287490	4.17
$C_7H_{10}N_2$	-382.182550	-382.195048	-382.196259	

***n*-butylamine**				
species	vacuum	water	octanol	Fe spin
m=4	-2465.795350	-2465.865282	-2465.874447	2.75
m=6	-2465.786874	-2465.859364	-2465.867856	4.18
$BuNH_2$	-213.767782	-213.772397	-213.775631	

Table S3. Calculated energies of iron(III) porphine complexes and free ligands (kcal mol^{-1}), computed *in vacuo*, and in water and *n*-octanol solvents for **method 3**.

Single point calculations were run at the method 1 geometries, using B3LYP/6-311+G(d,p) and the SMD solvent method.

core porphine				
species	vacuum	water	octanol	Fe spin
m=4	-2252.171509	-2252.266096	-2252.263531	2.96

H_2O				
species	vacuum	water	octanol	Fe spin
m=4	-2328.654417	-2328.737281	-2328.740358	2.97
H_2O	-76.457365	-76.470876	-76.469064	

OH^-				
species	vacuum	water	octanol	Fe spin
m=6	-2328.253782	-2328.281205	-2328.285276	4.15
OH^-	-75.826120	-75.977213	-75.957477	

Cl^-				
species	vacuum	water	octanol	Fe spin
m=4	-2712.659260	-2712.687543	-2712.695243	2.83
m=6	-2712.660400	-2712.684928	-2712.693123	4.13
Cl^-	-460.303727	-460.407712	-460.401115	

OMe^-				
species	vacuum	water	octanol	Fe spin
m=6	-2367.564242	-2367.584322	-2367.590638	4.07
OMe^-	-115.144191	-115.272208	-115.255796	

OAc^-				
species	vacuum	water	octanol	Fe spin
m=4	-2480.961242	-2480.993842	-2480.997336	2.79
m=6	-2480.962533	-2480.992860	-2480.996576	4.18
OAc^-	-228.599114	-228.713171	-228.699278	

Pyridine				
species	vacuum	water	octanol	Fe spin
m=4	-2500.563889	-2500.631666	-2500.639297	2.81
pyridine	-248.349415	-248.357399	-248.358130	

$MeNH_2$				
species	vacuum	water	octanol	Fe spin
m=4	-2348.107153	-2348.180046	-2348.185843	2.84
$MeNH_2$	-95.892159	-95.897352	-95.897191	

***N*-bound oxazole**				
species	vacuum	water	octanol	Fe spin
m=4	-2498.346544	-2498.416573	-2498.421152	2.80
oxazole	-246.136899	-246.145150	-246.142415	

***O*-bound oxazole**				
species	vacuum	water	octanol	Fe spin
m=4	-2498.319500	-2498.403595	-2498.399469	2.91
oxazole	-246.136899	-246.145150	-246.142415	

(imidazolide)$^-$				
species	vacuum	water	octanol	Fe spin
m=2	-2478.063769	-2478.094176	-2478.100867	1.02
m=4	-2478.067126	-2478.101748	-2478.107923	2.67
m=6	-2478.068952	-2478.099150	-2478.105797	4.11
$C_3H_3N_2^-$	-225.711420	-225.812648	-225.801798	

imidazole				
species	vacuum	water	octanol	Fe spin
m=4	-2478.501331	-2478.573740	-2478.581253	2.78
$C_3H_4N_2$	-226.280668	-226.295781	-226.295813	

1,3,5-triazine				
species	vacuum	water	octanol	Fe spin
m=4	-2532.636449	-2532.718561	-2532.722370	2.83
$C_3H_3N_3$	-280.435205	-280.450794	-280.449238	

Me_3NO				
species	vacuum	water	octanol	Fe spin
m=4	-2501.930679	-2502.008298	-2502.013263	2.86
m=6	-2501.925404	-2502.006721	-2502.010395	4.15
Me_3NO	-249.697632	-249.726123	-249.724489	

Me_3N				
species	vacuum	water	octanol	Fe spin
m=4	-2426.734436	-2426.802668	-2426.809760	2.83
Me_3N	-174.526750	-174.531025	-174.532080	

MeS^-				
species	vacuum	water	octanol	Fe spin
m=4	-2690.541706	-2690.563437	-2690.572310	2.60
m=6	-2690.545159	-2690.564589	-2690.573796	4.03
MeS^-	-438.166977	-438.262749	-438.257011	

***N*-bound (2-hydroxypyridine)$^-$**				
species	vacuum	water	octanol	Fe spin
m=4	-2575.395677	-2575.427004	-2575.433028	2.72
m=6	-2575.397816	-2575.427795	-2575.433557	4.11
$C_5H_4NO^-$	-323.045876	-323.150388	-323.137860	

***O*-bound (2-hydroxypyridine)$^-$**				
species	vacuum	water	octanol	Fe spin
m=6	-2575.410916	-2575.437599	-2575.443777	4.12
$C_5H_4NO^-$	-323.045876	-323.150388	-323.137860	

MeOH				
species	vacuum	water	octanol	Fe spin
m=4	-2367.964793	-2368.041282	-2368.045165	2.92
MeOH	-115.763717	-115.772179	-115.771639	

PhO^-				
species	vacuum	water	octanol	Fe spin
m=6	-2559.361754	-2559.383557	-2559.392474	4.10
PhO^-	-306.991574	-307.090798	-307.081961	

AcOH				
species	vacuum	water	octanol	Fe spin
m=4	-2481.361560	-2481.438355	-2481.440425	2.92
AcOH	-229.161199	-229.173005	-229.171947	

Me_3P				
species	vacuum	water	octanol	Fe spin
m=4	-2713.374476	-2713.440911	-2713.448423	2.87
Me_3P	-461.162547	-461.161142	-461.164980	

Quinoline				
species	vacuum	water	octanol	Fe spin
m=4	-2654.236719	-2654.303241	-2654.312323	2.80
C_9H_7N	-402.028743	-402.037576	-402.040430	

Thiophene				
species	vacuum	water	octanol	Fe spin
m=4	-2805.254610	-2805.325448	-2805.331946	3.02
C_4H_4S	-553.069396	-553.071400	-553.075189	

Aniline				
species	vacuum	water	octanol	Fe spin
m=4	-2539.891234	-2539.967635	-2539.974231	2.80
$PhNH_2$	-287.685056	-287.693211	-287.696275	

Me_3PO				
species	vacuum	water	octanol	Fe spin
m=4	-2788.660688	-2788.734511	-2788.740325	2.87
m=6	-2788.655177	-2788.731479	-2788.736350	4.19
Me_3PO	-536.431920	-536.454437	-536.453906	

***O*-bound DMSO**				
species	vacuum	water	octanol	Fe spin
m=4	-2805.474340	-2805.550544	-2805.555071	2.84
DMSO	-553.247838	-553.271945	-553.268842	

***S*-bound DMSO**				
species	vacuum	water	octanol	Fe spin
m=4	-2805.437190	-2805.528441	-2805.528134	2.92
DMSO	-553.247838	-553.271945	-553.268842	

F^-				
species	vacuum	water	octanol	Fe spin
m=4	-2352.295951	-2352.326302	-2352.332315	2.81
m=6	-2352.299102	-2352.325821	-2352.332346	4.24
F^-	-99.888693	-100.028972	-100.017816	

$Me_2PO_2^-$				
species	vacuum	water	octanol	Fe spin
m=4	-2824.186138	-2824.226506	-2824.229956	2.75
m=6	-2824.188959	-2824.227469	-2824.231258	4.16
$Me_2PO_2^-$	-571.824910	-571.940780	-571.927577	

$Me3SiO^-$				
species	vacuum	water	octanol	Fe spin
m=4	-2737.031874	-2737.049310	-2737.059618	2.65
m=6	-2737.040267	-2737.056853	-2737.066629	4.12
$Me3SiO^-$	-484.643982	-484.748119	-484.737382	

***N*-bound morpholine**				
species	vacuum	water	octanol	Fe spin
m=4	-2540.089871	-2540.170162	-2540.174878	2.83
m=6	-2540.079807	-2540.162540	-2540.166319	4.14
C_4H_9NO	-287.879579	-287.892455	-287.891554	

***O*-bound morpholine**				
species	vacuum	water	octanol	Fe spin
m=4	-2540.083167	-2540.159365	-2540.163513	2.89
C_4H_9NO	-287.879579	-287.892455	-287.891554	

4-methylpyridine				
species	vacuum	water	octanol	Fe spin
m=4	-2539.895936	-2539.961899	-2539.970633	2.80
C_6H_7N	-287.678658	-287.686632	-287.688245	

4-dimethylaminopyridine				
species	vacuum	water	octanol	Fe spin
m=4	-2634.584570	-2634.649669	-2634.658744	2.80
$C_7H_{10}N_2$	-382.357824	-382.370146	-382.371403	

***n*-butylamine**				
species	vacuum	water	octanol	Fe spin
m=4	-2466.085003	-2466.156146	-2466.165174	2.78
m=6	-2466.073971	-2466.147738	-2466.156079	4.15
$BuNH_2$	-213.868223	-213.872811	-213.876043	

Table S4. Calculated ground state geometries (method 3, water) of porphine complexes.

1. Core porphine (m=4)

Fe	0	-0.005676	-0.106761	-0.052516
N	0	1.687048	0.114016	-1.050286
N	0	-0.988504	0.774378	-1.524597
N	0	0.977565	-0.987252	1.420394
N	0	-1.698376	-0.328443	0.945143
C	0	2.981554	-0.285767	-0.654897
C	0	3.945775	0.057792	-1.666384
C	0	3.260670	0.670634	-2.692955
C	0	1.871903	0.707111	-2.317503
C	0	-0.462678	1.283748	-2.731127
C	0	-1.511150	1.849110	-3.538605
C	0	-2.690659	1.695849	-2.842889
C	0	-2.373140	1.035329	-1.604370
C	0	-2.992646	0.072639	0.550467
C	0	-3.956981	-0.271642	1.561622
C	0	-3.272111	-0.886250	2.587294
C	0	-1.883365	-0.922771	2.211787
C	0	0.451542	-1.497497	2.626317
C	0	2.362330	-1.246584	1.500868
C	0	2.680023	-1.906575	2.739794
C	0	1.500289	-2.061568	3.434612
C	0	-0.883238	-1.470278	3.000782
C	0	-3.313243	0.709748	-0.638613
C	0	0.871783	1.254504	-3.106563
C	0	3.302411	-0.921169	0.535036
H	0	-1.158563	-1.898371	3.958597
H	0	-4.351047	0.965997	-0.822412
H	0	1.146932	1.681374	-4.064976
H	0	4.340348	-1.176571	0.719257
H	0	5.005656	-0.145175	-1.596042
H	0	3.654662	1.063349	-3.620354
H	0	-1.359987	2.302237	-4.508822
H	0	-3.685940	1.999989	-3.136890
H	0	-5.016769	-0.068065	1.491620
H	0	3.675576	-2.209332	3.034311
H	0	-3.666231	-1.280053	3.514189
H	0	1.348871	-2.515042	4.404640

2. H_2O complex (m=4)

Fe	0	0.019308	0.005963	0.034449
N	0	-0.583591	1.936743	-0.028792
N	0	-1.875627	-0.582155	-0.157996
N	0	1.910064	0.595079	-0.192884
N	0	0.620739	-1.924466	-0.049957
C	0	0.232172	3.073725	-0.033127
C	0	-0.585897	4.268822	-0.065998
C	0	-1.897144	3.861873	-0.116060
C	0	-1.896912	2.413349	-0.104657
C	0	-3.021226	0.233139	-0.193959
C	0	-4.207915	-0.586760	-0.212416
C	0	-3.800254	-1.900697	-0.157502
C	0	-2.358422	-1.902611	-0.115319
C	0	-0.195003	-3.061453	-0.043458
C	0	0.622192	-4.256341	-0.098286
C	0	1.932203	-3.849097	-0.172503
C	0	1.932266	-2.400644	-0.154212
C	0	3.054682	-0.219981	-0.255520
C	0	2.393676	1.915340	-0.153551
C	0	3.834382	1.913695	-0.224439
C	0	4.240807	0.600053	-0.293702
C	0	3.071436	-1.610171	-0.245591
C	0	-1.584599	-3.056115	-0.049559
C	0	-3.037713	1.623265	-0.177095
C	0	1.621370	3.068482	-0.066916
H	0	4.033621	-2.106878	-0.312610
H	0	-2.098532	-4.011510	-0.036859
H	0	-4.001018	2.120240	-0.222586
H	0	2.135500	4.023830	-0.059909
H	0	-0.194929	5.277078	-0.072977
H	0	-2.788186	4.472409	-0.168881
H	0	-5.217005	-0.199925	-0.253544
H	0	-4.412823	-2.791913	-0.147847
H	0	0.231114	-5.264571	-0.102272
H	0	4.447064	2.804884	-0.222747
H	0	2.821987	-4.459334	-0.245951
H	0	5.248860	0.213465	-0.356749
O	0	0.040551	0.000891	2.168630
H	0	0.308447	-0.769307	2.703278
H	0	-0.216607	0.768528	2.712159

3. OH^- complex (m=6)

Fe	0	0.000102	0.000163	0.404327
N	0	1.359101	-1.528860	-0.088088
N	0	1.527147	1.359553	-0.082290
N	0	-1.533750	-1.358197	-0.081222
N	0	-1.366703	1.526492	-0.085612
C	0	1.077278	-2.891020	-0.126646
C	0	2.320279	-3.645727	-0.187359
C	0	3.348977	-2.730666	-0.189048
C	0	2.744812	-1.407916	-0.128846
C	0	2.889475	1.078700	-0.123050
C	0	3.643042	2.322473	-0.177479
C	0	2.727341	3.350703	-0.173403
C	0	1.405197	2.745239	-0.116813
C	0	-1.082437	2.889952	-0.125813
C	0	-2.323996	3.644842	-0.198797
C	0	-3.354302	2.731011	-0.209369
C	0	-2.753273	1.407717	-0.141978
C	0	-2.897797	-1.078485	-0.140135
C	0	-1.410241	-2.745880	-0.126603
C	0	-2.731046	-3.350363	-0.201343
C	0	-3.648104	-2.322558	-0.210540
C	0	-3.463792	0.201737	-0.154076
C	0	0.198279	3.454195	-0.124492
C	0	3.454570	-0.201758	-0.133377
C	0	-0.203748	-3.455201	-0.131454
H	0	-4.547706	0.264538	-0.202281
H	0	0.261180	4.538766	-0.156124
H	0	4.539077	-0.264739	-0.165738
H	0	-0.267345	-4.539603	-0.167146
H	0	2.385336	-4.725189	-0.229485
H	0	4.413410	-2.921330	-0.232301
H	0	4.722456	2.388447	-0.219098
H	0	2.917356	4.415454	-0.211200
H	0	-2.387595	4.724261	-0.244732
H	0	-2.920164	-4.414856	-0.250480
H	0	-4.417857	2.923543	-0.265187
H	0	-4.726735	-2.389943	-0.268460
O	0	0.015130	0.002461	2.221860
H	0	-0.599906	-0.078303	2.972427

4. Cl^- complex (m=4)

Fe	0	-0.038799	-0.171973	-0.109946
N	0	1.488733	-1.251087	0.647183
N	0	1.138557	0.333321	-1.668659
N	0	-1.290185	-1.124580	1.153906
N	0	-1.640382	0.459698	-1.161976
C	0	1.476164	-2.019871	1.813381
C	0	2.815212	-2.469386	2.133800
C	0	3.649942	-1.970764	1.161897
C	0	2.825304	-1.213667	0.242974
C	0	2.521353	0.161721	-1.766779
C	0	3.029768	0.837631	-2.942560
C	0	1.954548	1.428178	-3.563163
C	0	0.783633	1.115622	-2.770136
C	0	-1.628309	1.225422	-2.330202
C	0	-2.971071	1.652478	-2.665431
C	0	-3.806651	1.148828	-1.696849
C	0	-2.978660	0.412076	-0.764513
C	0	-2.674599	-0.962673	1.245665
C	0	-0.935794	-1.910164	2.253234
C	0	-2.110325	-2.244590	3.031847
C	0	-3.186355	-1.658857	2.408081
C	0	-3.468420	-0.245178	0.358230
C	0	-0.502676	1.539851	-3.082910
C	0	3.315405	-0.554330	-0.878392
C	0	0.351631	-2.327634	2.570477
H	0	-4.535291	-0.196784	0.552792
H	0	-0.636789	2.150681	-3.970212
H	0	4.382225	-0.603032	-1.073158
H	0	0.486610	-2.933202	3.461248
H	0	3.067211	-3.081353	2.989570
H	0	4.720369	-2.093795	1.064972
H	0	4.070085	0.851271	-3.239045
H	0	1.940794	2.020754	-4.468155
H	0	-3.224444	2.256058	-3.526733
H	0	-2.097926	-2.845418	3.931400
H	0	-4.879242	1.258807	-1.608539
H	0	-4.228799	-1.685357	2.696100
Cl	0	0.285258	1.780371	1.176620

5. OMe^- complex (m=6)

Fe	0	0.081066	0.207433	0.098338
N	0	1.531879	-1.050079	0.960364
N	0	1.206395	0.112669	-1.678613
N	0	-1.267213	-0.553350	1.522532
N	0	-1.592339	0.600834	-1.120292
C	0	1.480123	-1.603882	2.235574
C	0	2.783686	-2.152003	2.582570
C	0	3.615436	-1.928512	1.508178
C	0	2.828387	-1.241496	0.493910
C	0	2.548787	-0.246980	-1.776269
C	0	3.045576	0.083091	-3.103696
C	0	1.995543	0.634447	-3.804513
C	0	0.845448	0.647598	-2.912841
C	0	-1.564611	1.067723	-2.431841
C	0	-2.899894	1.492134	-2.826364
C	0	-3.729445	1.273139	-1.748864
C	0	-2.910345	0.711908	-0.684519
C	0	-2.629173	-0.277134	1.587779
C	0	-0.928083	-1.176297	2.719355
C	0	-2.108983	-1.285909	3.563898
C	0	-3.158388	-0.731121	2.865955
C	0	-3.386788	0.320113	0.572541
C	0	-0.433548	1.103248	-3.256903
C	0	3.302604	-0.858508	-0.766930
C	0	0.345773	-1.650965	3.055252
H	0	-4.445223	0.470519	0.768883
H	0	-0.565752	1.495492	-4.261923
H	0	4.343167	-1.078086	-0.991626
H	0	0.459029	-2.116846	4.030696
H	0	3.017220	-2.644183	3.517773
H	0	4.656528	-2.203931	1.400275
H	0	4.056541	-0.095812	-3.446315
H	0	1.988439	0.990323	-4.826649
H	0	-3.158629	1.891877	-3.798330
H	0	-2.124021	-1.733902	4.549004
H	0	-4.792878	1.460668	-1.675636
H	0	-4.192240	-0.640864	3.173164
O	0	0.505340	1.845112	0.738224
C	0	0.781595	3.224405	0.486504
H	0	-0.153040	3.805792	0.489092
H	0	1.276559	3.353566	-0.488648
H	0	1.440863	3.616949	1.273946

6. OAc^- complex (m=6)

Fe	0	0.104068	-0.099482	0.049165
N	0	1.524279	-1.221299	1.108740
N	0	1.309736	-0.349830	-1.634229
N	0	-1.292412	-0.704841	1.492007
N	0	-1.504890	0.166163	-1.251234
C	0	1.422514	-1.638618	2.435166
C	0	2.711999	-2.126659	2.894051
C	0	3.590107	-2.006352	1.839512
C	0	2.846058	-1.443874	0.725342
C	0	2.662585	-0.690254	-1.638286
C	0	3.217102	-0.468846	-2.963048
C	0	2.195180	0.001706	-3.757081
C	0	1.005129	0.073057	-2.927439
C	0	-1.417596	0.517191	-2.597772
C	0	-2.729184	0.904487	-3.087016
C	0	-3.608446	0.782499	-2.034284
C	0	-2.843376	0.319164	-0.889078
C	0	-2.659935	-0.434318	1.474589
C	0	-1.003048	-1.193823	2.765228
C	0	-2.216124	-1.222962	3.564690
C	0	-3.238066	-0.754297	2.768709
C	0	-3.376579	0.050962	0.375221
C	0	-0.254977	0.481236	-3.371575
C	0	3.376472	-1.187166	-0.543691
C	0	0.255639	-1.615317	3.205850
H	0	-4.441871	0.216851	0.510606
H	0	-0.339064	0.792550	-4.408950
H	0	4.429034	-1.409579	-0.696471
H	0	0.328967	-1.974480	4.228777
H	0	2.907661	-2.512293	3.886083
H	0	4.637907	-2.275070	1.808128
H	0	4.247395	-0.652422	-3.238329
H	0	2.233952	0.277105	-4.802743
H	0	-2.938597	1.225390	-4.098907
H	0	-2.270174	-1.562762	4.590721
H	0	-4.671830	0.982768	-2.024675
H	0	-4.283796	-0.639139	3.022221
O	0	0.500999	1.651296	0.607387
C	0	0.649776	2.879308	0.045876
C	0	0.985971	3.957470	1.063121
O	0	0.522264	3.092675	-1.178113
H	0	1.914968	3.695623	1.583459
H	0	0.192208	4.011809	1.817672
H	0	1.095658	4.923949	0.565302

7. Pyridine complex (m=4)

Fe	0	-0.049318	-0.384191	-0.232408
N	0	1.475981	-1.354036	0.632044
N	0	1.166749	0.121441	-1.742364
N	0	-1.312076	-1.253566	1.057586
N	0	-1.621305	0.222011	-1.316760
C	0	1.449122	-2.051135	1.849859
C	0	2.775045	-2.508518	2.195807
C	0	3.619124	-2.107785	1.185435
C	0	2.818011	-1.389384	0.221499
C	0	2.548453	-0.103365	-1.848211
C	0	3.068453	0.520235	-3.043105
C	0	2.010804	1.136797	-3.671710
C	0	0.834045	0.883635	-2.872901
C	0	-1.587776	0.971061	-2.503163
C	0	-2.928199	1.315346	-2.917509
C	0	-3.791185	0.767585	-1.996029
C	0	-2.984015	0.096234	-1.003651
C	0	-2.714483	-1.190028	1.065911
C	0	-0.972723	-1.963923	2.219474
C	0	-2.164116	-2.330953	2.949419
C	0	-3.240477	-1.860423	2.232509
C	0	-3.500743	-0.564360	0.105127
C	0	-0.444191	1.305356	-3.218397
C	0	3.324261	-0.810443	-0.936652
C	0	0.314562	-2.315144	2.607603
H	0	-4.578466	-0.593355	0.227463
H	0	-0.561306	1.891364	-4.124080
H	0	4.384642	-0.916544	-1.140681
H	0	0.436020	-2.867351	3.533723
H	0	3.015762	-3.073445	3.086121
H	0	4.682786	-2.280190	1.092105
H	0	4.103886	0.482987	-3.353429
H	0	2.015181	1.698818	-4.595756
H	0	-3.168123	1.886409	-3.804115
H	0	-2.167784	-2.887338	3.876872
H	0	-4.871987	0.806558	-1.983389
H	0	-4.293002	-1.956402	2.462269
N	0	0.186166	1.450416	0.876987
C	0	1.421389	1.993477	1.053135
C	0	1.612043	3.184117	1.768357
C	0	0.492347	3.835351	2.319522
C	0	-0.783532	3.270007	2.134826
C	0	-0.898935	2.076662	1.408093
H	0	2.257219	1.462223	0.613655
H	0	2.612822	3.585758	1.887236
H	0	0.610946	4.759128	2.878275
H	0	-1.672490	3.739397	2.542789
H	0	-1.862892	1.609947	1.243937

8. $MeNH_2$ complex (m=4)

Fe	0	0.036948	-0.048617	0.015958
N	0	-0.992104	0.472528	-1.616855
N	0	-1.679358	-0.230161	1.024703
N	0	1.693375	-0.216339	-1.102569
N	0	1.005418	-0.919918	1.541115
C	0	-0.479979	0.759735	-2.893061
C	0	-1.540169	1.192010	-3.773361
C	0	-2.708534	1.165104	-3.046142
C	0	-2.371445	0.720243	-1.714245
C	0	-2.969240	0.109272	0.583719
C	0	-3.929103	-0.082177	1.645552
C	0	-3.235414	-0.540457	2.742557
C	0	-1.846451	-0.637072	2.358867
C	0	0.487799	-1.239252	2.808079
C	0	1.529485	-1.768976	3.656656
C	0	2.688852	-1.785340	2.914931
C	0	2.366709	-1.262402	1.607742
C	0	2.964933	-0.650355	-0.690709
C	0	1.855392	0.159515	-2.447044
C	0	3.225638	-0.033803	-2.860380
C	0	3.910036	-0.535857	-1.776822
C	0	3.285910	-1.131242	0.573346
C	0	-0.837836	-1.093439	3.199511
C	0	-3.296606	0.559379	-0.689727
C	0	0.848538	0.630834	-3.281232
H	0	4.310469	-1.436667	0.758689
H	0	-1.106367	-1.379248	4.211225
H	0	-4.337054	0.783636	-0.900743
H	0	1.109215	0.886082	-4.303124
H	0	-1.402379	1.466735	-4.810321
H	0	-3.708346	1.414168	-3.374928
H	0	-4.990535	0.104072	1.553754
H	0	-3.621381	-0.800902	3.718747
H	0	1.382942	-2.092767	4.678133
H	0	3.602940	0.178296	-3.851537
H	0	3.671213	-2.124316	3.214640
H	0	4.953854	-0.811753	-1.712898
N	0	0.543557	1.968677	0.684888
H	0	0.911707	1.829701	1.630716
C	0	-0.548259	2.996441	0.673504
H	0	1.317831	2.243936	0.073180
H	0	-1.363823	2.660614	1.317971
H	0	-0.930153	3.102888	-0.344374
H	0	-0.188203	3.970734	1.026677

9. *N*-bound oxazole complex (m=4)

Fe	0	-0.064540	-0.342797	-0.096173
N	0	0.489316	-1.074163	1.683402
N	0	1.784939	-0.682139	-0.788748
N	0	-1.972159	-0.362375	0.511775
N	0	-0.686391	-0.022279	-1.972115
C	0	-0.310251	-1.229659	2.826773
C	0	0.492410	-1.663777	3.946633
C	0	1.788110	-1.774808	3.497924
C	0	1.787358	-1.409718	2.100154
C	0	2.913001	-1.083478	-0.052413
C	0	4.077095	-1.130327	-0.904843
C	0	3.670470	-0.766369	-2.169379
C	0	2.254499	-0.493936	-2.100229
C	0	0.107004	0.094260	-3.124555
C	0	-0.707278	0.458341	-4.260950
C	0	-2.003063	0.569009	-3.812431
C	0	-1.990820	0.273587	-2.398389
C	0	-3.112190	-0.034829	-0.241521
C	0	-2.453838	-0.623795	1.805694
C	0	-3.885900	-0.447216	1.852734
C	0	-4.292477	-0.083331	0.588378
C	0	-3.124708	0.276582	-1.595773
C	0	1.478584	-0.117093	-3.189949
C	0	2.922147	-1.409359	1.298617
C	0	-1.681135	-1.014587	2.892556
H	0	-4.077259	0.515846	-2.057007
H	0	1.968573	-0.001672	-4.151185
H	0	3.865892	-1.700221	1.748200
H	0	-2.180076	-1.181071	3.841603
H	0	0.106593	-1.860493	4.937673
H	0	2.665886	-2.079924	4.051208
H	0	5.066929	-1.416329	-0.575791
H	0	4.264617	-0.698295	-3.070595
H	0	-0.330224	0.601675	-5.264450
H	0	-4.493196	-0.595673	2.735329
H	0	-2.889764	0.820144	-4.378462
H	0	-5.295606	0.122485	0.240239
C	0	-0.002416	3.836134	1.088923
C	0	-0.632428	2.630930	0.942715
O	0	1.317460	3.684522	0.621481
N	0	0.291884	1.717428	0.382217
C	0	1.422232	2.380974	0.211281
H	0	-0.279243	4.808170	1.458590
H	0	-1.642074	2.347552	1.184883
H	0	2.360446	2.038200	-0.189102

10. *O*-bound oxazole complex (m=4)

Fe	0	-0.080415	-0.410094	-0.103123
N	0	0.513535	-1.107031	1.666920
N	0	1.760353	-0.694926	-0.811546
N	0	-1.967461	-0.405937	0.535447
N	0	-0.720791	0.005357	-1.943291
C	0	-0.265946	-1.251625	2.829075
C	0	0.549797	-1.707511	3.927676
C	0	1.832437	-1.854286	3.449274
C	0	1.812766	-1.481732	2.055885
C	0	2.900817	-1.121350	-0.106413
C	0	4.056254	-1.117375	-0.969948
C	0	3.637106	-0.685328	-2.208184
C	0	2.220868	-0.429225	-2.114010
C	0	0.063603	0.178011	-3.098206
C	0	-0.765695	0.552067	-4.217344
C	0	-2.064277	0.604185	-3.762710
C	0	-2.038276	0.270409	-2.359624
C	0	-3.125903	-0.087609	-0.196730
C	0	-2.422732	-0.641888	1.845394
C	0	-3.852090	-0.464486	1.920001
C	0	-4.287207	-0.127245	0.657994
C	0	-3.165168	0.229229	-1.548570
C	0	1.437320	-0.006629	-3.179392
C	0	2.931498	-1.489424	1.232614
C	0	-1.631737	-1.020158	2.921963
H	0	-4.128208	0.451365	-1.996046
H	0	1.921128	0.161972	-4.135682
H	0	3.879143	-1.803737	1.657055
H	0	-2.112329	-1.170078	3.882973
H	0	0.181901	-1.895649	4.927093
H	0	2.713267	-2.184130	3.983119
H	0	5.051631	-1.408603	-0.663263
H	0	4.224408	-0.557156	-3.107201
H	0	-0.397676	0.739292	-5.216899
H	0	-4.439015	-0.591784	2.819403
H	0	-2.960215	0.842900	-4.319489
H	0	-5.297553	0.074538	0.329098
C	0	0.075319	3.931952	0.697858
C	0	-0.558424	2.833312	0.194338
N	0	1.322047	3.550402	1.263361
O	0	0.287638	1.715697	0.434522
C	0	1.425590	2.265601	1.100857
H	0	-0.247590	4.960359	0.706780
H	0	-1.490429	2.641741	-0.308189
H	0	2.209116	1.582733	1.382081

11. Imidazolide complex (m=4)

Fe	0	0.005200	0.000029	-0.282680
N	0	0.001425	2.002242	-0.576166
N	0	-1.995647	-0.005247	-0.571361
N	0	2.009336	0.005338	-0.554884
N	0	0.012059	-2.002155	-0.576256
C	0	1.109983	2.851219	-0.579868
C	0	0.682647	4.236157	-0.601956
C	0	-0.691537	4.232490	-0.607799
C	0	-1.111614	2.845328	-0.589350
C	0	-2.845141	1.104611	-0.596372
C	0	-4.227474	0.676773	-0.637106
C	0	-4.223828	-0.699114	-0.636779
C	0	-2.839247	-1.119603	-0.595898
C	0	-1.096517	-2.851110	-0.588955
C	0	-0.669127	-4.236031	-0.607621
C	0	0.705061	-4.232436	-0.602487
C	0	1.125085	-2.845260	-0.580504
C	0	2.858821	-1.104553	-0.576118
C	0	2.852922	1.119726	-0.575551
C	0	4.237584	0.699342	-0.609628
C	0	4.241234	-0.676812	-0.610011
C	0	2.453905	-2.435682	-0.575820
C	0	-2.427435	-2.448536	-0.593097
C	0	-2.440382	2.435712	-0.593880
C	0	2.440949	2.448687	-0.574832
H	0	3.222983	-3.201728	-0.581991
H	0	-3.192537	-3.218464	-0.602546
H	0	-3.209543	3.201579	-0.603704
H	0	3.205962	3.218796	-0.580560
H	0	1.354056	5.084346	-0.610156
H	0	-1.367439	5.077020	-0.621363
H	0	-5.076106	1.347200	-0.662203
H	0	-5.068900	-1.374033	-0.661561
H	0	-1.340570	-5.084115	-0.620889
H	0	5.082760	1.374270	-0.632476
H	0	1.380932	-5.077070	-0.611059
H	0	5.089974	-1.347241	-0.633230
C	0	0.598530	-0.000285	3.881922
C	0	1.090814	-0.000126	2.581262
N	0	-0.805617	-0.000361	3.857131
N	0	-0.011201	-0.000111	1.716403
C	0	-1.124962	-0.000264	2.552858
H	0	1.140098	-0.000346	4.816671
H	0	2.106294	-0.000030	2.216941
H	0	-2.137278	-0.000292	2.179272

12. Imidazole complex (m=4)

Fe	0	-0.142684	-0.277207	-0.126557
N	0	-0.642258	-1.105112	1.630961
N	0	1.542219	-1.369086	-0.134146
N	0	-1.997826	0.469706	-0.274914
N	0	0.164190	0.165003	-2.058949
C	0	-1.809724	-0.879784	2.374687
C	0	-1.727542	-1.546650	3.654490
C	0	-0.508947	-2.182459	3.702013
C	0	0.162962	-1.908322	2.451782
C	0	2.055435	-2.152820	0.912155
C	0	3.340794	-2.699332	0.544664
C	0	3.619579	-2.260235	-0.730501
C	0	2.506745	-1.441995	-1.152354
C	0	1.314807	-0.094193	-2.818007
C	0	1.201894	0.512048	-4.125453
C	0	-0.016858	1.147552	-4.173017
C	0	-0.658036	0.934031	-2.895261
C	0	-2.544139	1.187767	-1.350468
C	0	-2.995069	0.477608	0.713181
C	0	-4.152703	1.207692	0.251532
C	0	-3.874158	1.646350	-1.023345
C	0	-1.918200	1.420023	-2.569377
C	0	2.412701	-0.836202	-2.399988
C	0	1.423263	-2.394572	2.126377
C	0	-2.907161	-0.137480	1.956330
H	0	-2.452814	1.996743	-3.317048
H	0	3.234368	-0.969486	-3.096154
H	0	1.933818	-3.017865	2.853280
H	0	-3.752549	-0.050180	2.630961
H	0	-2.506007	-1.530379	4.405139
H	0	-0.097969	-2.787179	4.499008
H	0	3.936549	-3.343695	1.176974
H	0	4.486724	-2.477148	-1.339560
H	0	1.956009	0.447773	-4.898090
H	0	-5.057184	1.350367	0.827202
H	0	-0.452365	1.703936	-4.991869
H	0	-4.507259	2.216403	-1.689724
C	0	1.014312	3.579215	1.454034
C	0	0.094247	2.683417	0.944297
N	0	2.233491	2.897316	1.485787
N	0	0.743800	1.472858	0.669607
C	0	2.034563	1.630800	1.006252
H	0	0.906795	4.599916	1.781994
H	0	-0.957662	2.822420	0.762075
H	0	2.806587	0.884985	0.918276
H	0	3.116506	3.273841	1.808504

13. Triazene complex (m=4)

Fe	0	-0.140002	-0.393238	-0.204104
N	0	0.764905	-1.609267	1.099887
N	0	1.446032	-0.548095	-1.411783
N	0	-1.836723	-0.549272	0.842210
N	0	-1.155600	0.511891	-1.669466
C	0	0.259863	-2.056594	2.332707
C	0	1.253896	-2.838735	3.028462
C	0	2.370324	-2.885991	2.224539
C	0	2.070912	-2.125535	1.034614
C	0	2.664834	-1.200222	-1.155463
C	0	3.583717	-0.995556	-2.249824
C	0	2.938037	-0.214895	-3.181811
C	0	1.616232	0.056585	-2.668925
C	0	-0.644054	0.977483	-2.892804
C	0	-1.672325	1.663456	-3.638475
C	0	-2.822936	1.614705	-2.884383
C	0	-2.505048	0.906140	-1.667525
C	0	-3.098958	-0.019140	0.522570
C	0	-2.000412	-1.135665	2.108843
C	0	-3.356430	-0.960276	2.571855
C	0	-4.036313	-0.275690	1.590001
C	0	-3.416038	0.662797	-0.646342
C	0	0.652634	0.786537	-3.353742
C	0	2.962705	-1.936114	-0.014556
C	0	-1.020780	-1.820579	2.817037
H	0	-4.433019	1.019431	-0.771455
H	0	0.917110	1.200478	-4.321201
H	0	3.943794	-2.393560	0.058230
H	0	-1.282218	-2.225988	3.788925
H	0	1.105843	-3.296928	3.996871
H	0	3.309676	-3.388566	2.410884
H	0	4.585429	-1.400974	-2.293406
H	0	3.310739	0.138231	-4.133689
H	0	-1.528489	2.109800	-4.613033
H	0	-3.733332	-1.325202	3.517608
H	0	-3.798710	2.014982	-3.123825
H	0	-5.074444	0.027430	1.580486
N	0	0.518511	1.456398	0.755937
C	0	1.803356	1.627832	1.176809
N	0	2.250837	2.752540	1.773335
C	0	1.331555	3.740087	1.941267
N	0	0.031088	3.656952	1.553445
C	0	-0.334197	2.498754	0.965062
H	0	2.505082	0.817185	1.024633
H	0	1.658253	4.657710	2.417509
H	0	-1.362227	2.392878	0.641534

14. Me_3NO complex (m=6)

Fe	0	0.156933	-0.000003	-0.219241
N	0	2.215518	-0.001252	-0.401457
N	0	0.188576	2.040031	-0.631639
N	0	0.186084	-2.040107	-0.631803
N	0	-1.836852	0.001188	-0.822920
C	0	3.051331	-1.119368	-0.348321
C	0	4.434164	-0.691551	-0.249814
C	0	4.435000	0.686339	-0.249757
C	0	3.052694	1.115841	-0.348324
C	0	1.307783	2.875270	-0.552919
C	0	0.894044	4.260565	-0.683086
C	0	-0.472978	4.264040	-0.851579
C	0	-0.911676	2.880527	-0.823208
C	0	-2.659482	1.122740	-1.016587
C	0	-4.014604	0.692082	-1.294097
C	0	-4.015430	-0.687044	-1.294158
C	0	-2.660811	-1.119355	-1.016762
C	0	-0.915137	-2.879277	-0.823600
C	0	1.304297	-2.876680	-0.553090
C	0	0.888944	-4.261461	-0.683568
C	0	-0.478089	-4.263310	-0.852024
C	0	-2.235835	-2.451264	-0.990314
C	0	-2.232896	2.454128	-0.989930
C	0	2.630173	2.447466	-0.406445
C	0	2.627193	-2.450472	-0.406499
H	0	-2.989281	-3.215805	-1.157191
H	0	-2.985404	3.219617	-1.156695
H	0	3.398208	3.214379	-0.363121
H	0	3.394294	-3.218322	-0.363192
H	0	5.284489	-1.358317	-0.198657
H	0	5.286137	1.352064	-0.198547
H	0	1.565180	5.108871	-0.665034
H	0	-1.124405	5.115591	-0.996118
H	0	-4.845450	1.357450	-1.487732
H	0	1.559068	-5.110569	-0.665633
H	0	-4.847076	-1.351393	-1.487858
H	0	-1.130516	-5.114072	-0.996694
O	0	0.154901	0.000000	1.743948
N	0	-0.842125	0.000143	2.797420
C	0	-0.048069	-0.000159	4.092144
C	0	-1.690550	1.254065	2.689252
C	0	-1.691162	-1.253330	2.688987
H	0	-0.737480	0.000398	4.942039
H	0	0.580025	-0.891636	4.098188
H	0	0.581113	0.890550	4.097857
H	0	-2.390201	1.288157	3.529820
H	0	-1.018959	2.113418	2.709189
H	0	-2.229808	1.224855	1.742507
H	0	-2.390552	-1.287470	3.529773
H	0	-2.230727	-1.223467	1.742435
H	0	-1.019962	-2.112998	2.708335

15. Me_3N complex (m=4)

Fe	0	0.000948	0.007880	-0.197704
N	0	0.414682	1.955888	-0.442462
N	0	-1.948979	0.424525	-0.420190
N	0	1.947266	-0.407021	-0.452476
N	0	-0.417177	-1.942077	-0.430139
C	0	1.681200	2.559208	-0.491022
C	0	1.552838	3.997034	-0.549509
C	0	0.207371	4.284183	-0.538354
C	0	-0.495806	3.023831	-0.472889
C	0	-2.552692	1.691791	-0.446705
C	0	-3.990753	1.563730	-0.497652
C	0	-4.277203	0.217927	-0.513743
C	0	-3.016753	-0.486242	-0.468692
C	0	-1.685090	-2.544344	-0.481970
C	0	-1.556976	-3.980869	-0.562640
C	0	-0.211191	-4.268083	-0.573774
C	0	0.493429	-3.009283	-0.499968
C	0	2.549295	-1.674184	-0.514733
C	0	3.015222	0.503458	-0.492908
C	0	4.274706	-0.200334	-0.566185
C	0	3.986508	-1.545765	-0.582219
C	0	1.877893	-2.890616	-0.525386
C	0	-2.900709	-1.870739	-0.485909
C	0	-1.880379	2.908037	-0.456559
C	0	2.897946	1.888224	-0.496250
H	0	2.467607	-3.799551	-0.584667
H	0	-3.810929	-2.459586	-0.532819
H	0	-2.470357	3.818326	-0.483796
H	0	3.807594	2.478487	-0.535912
H	0	2.385454	4.685314	-0.602464
H	0	-0.272496	5.252558	-0.580408
H	0	-4.679877	2.396662	-0.531026
H	0	-5.245688	-0.261137	-0.561863
H	0	-2.389885	-4.668644	-0.617285
H	0	5.243192	0.278838	-0.613303
H	0	0.267449	-5.235753	-0.639224
H	0	4.674174	-2.378271	-0.644069
N	0	0.013484	-0.022463	2.082241
C	0	0.310778	1.347566	2.623429
C	0	-1.330040	-0.473555	2.581841
C	0	1.063199	-0.984916	2.561792
H	0	0.314710	1.324509	3.723893
H	0	1.289334	1.682612	2.272565
H	0	-0.450478	2.054611	2.286519
H	0	-1.319772	-0.542450	3.680153
H	0	-2.098214	0.239910	2.277877
H	0	-1.568821	-1.455190	2.167335
H	0	1.043347	-1.047359	3.660356
H	0	0.873341	-1.976970	2.146819
H	0	2.050852	-0.646572	2.243039

16. MeS$^-$ complex (m=6)

Fe	0	-0.067973	0.104957	0.009760
N	0	-1.150520	0.374867	-1.760961
N	0	-1.819828	-0.659578	0.851974
N	0	1.678248	0.111628	-1.138491
N	0	1.010027	-0.935070	1.470095
C	0	-0.631394	0.834756	-2.969168
C	0	-1.722183	1.143594	-3.881896
C	0	-2.896306	0.860514	-3.220497
C	0	-2.536179	0.378697	-1.895120
C	0	-3.113891	-0.512420	0.359444
C	0	-4.069989	-0.954571	1.362829
C	0	-3.345719	-1.371364	2.457855
C	0	-1.938778	-1.191635	2.134549
C	0	0.488423	-1.436094	2.661354
C	0	1.576552	-1.872943	3.522386
C	0	2.751752	-1.642928	2.840899
C	0	2.395373	-1.058437	1.557122
C	0	2.972324	-0.155824	-0.694196
C	0	1.795904	0.602811	-2.438112
C	0	3.200288	0.658996	-2.810887
C	0	3.925229	0.188654	-1.737237
C	0	3.304522	-0.689089	0.557633
C	0	-0.872756	-1.537902	2.973564
C	0	-3.446142	-0.024607	-0.910483
C	0	0.729241	0.952628	-3.275808
H	0	4.359752	-0.845940	0.765295
H	0	-1.125679	-1.948253	3.947750
H	0	-4.502826	0.036887	-1.156907
H	0	0.981577	1.324346	-4.265532
H	0	-1.596568	1.518277	-4.889348
H	0	-3.909940	0.961801	-3.585911
H	0	-5.144840	-0.946936	1.236895
H	0	-3.718094	-1.769051	3.392893
H	0	1.449292	-2.304354	4.506712
H	0	3.571297	1.001221	-3.768212
H	0	3.763067	-1.851046	3.165353
H	0	4.998511	0.076285	-1.654725
S	0	-0.107884	2.310471	0.910466
C	0	1.695480	2.708164	1.331201
H	0	2.291791	2.730694	0.415685
H	0	2.093083	1.954944	2.015984
H	0	1.709295	3.690907	1.810274

17. *N*-bound 2-hydroxypyridyl complex (m=6)

Fe	0	-0.025150	-0.235482	-0.061095
N	0	-1.528783	-0.058575	-1.537485
N	0	-1.574081	-0.876983	1.227667
N	0	1.314416	-0.510049	-1.629219
N	0	1.269128	-1.329971	1.145497
C	0	-1.314013	0.281212	-2.874882
C	0	-2.583638	0.579600	-3.514779
C	0	-3.567487	0.402930	-2.566961
C	0	-2.908401	0.003079	-1.335431
C	0	-2.947427	-0.702548	1.050270
C	0	-3.646899	-1.030544	2.280756
C	0	-2.693746	-1.406716	3.201368
C	0	-1.402799	-1.320779	2.540686
C	0	1.052588	-1.703095	2.469803
C	0	2.298868	-2.164061	3.058873
C	0	3.263365	-2.079637	2.079755
C	0	2.619516	-1.557741	0.886937
C	0	2.658489	-0.853307	-1.495435
C	0	1.141378	-0.100279	-2.949090
C	0	2.408984	-0.177584	-3.656182
C	0	3.342777	-0.647622	-2.760026
C	0	3.261286	-1.341286	-0.334223
C	0	-0.183428	-1.679478	3.123842
C	0	-3.564880	-0.286944	-0.134432
C	0	-0.074397	0.286457	-3.522117
H	0	4.323653	-1.563520	-0.382543
H	0	-0.204341	-2.003125	4.160849
H	0	-4.647922	-0.199738	-0.126330
H	0	-0.060965	0.579165	-4.568399
H	0	-2.698028	0.869913	-4.550966
H	0	-4.636707	0.523396	-2.682941
H	0	-4.720131	-0.982516	2.411382
H	0	-2.841904	-1.725320	4.224889
H	0	2.408584	-2.508438	4.078825
H	0	2.552481	0.087549	-4.695435
H	0	4.311609	-2.338649	2.149972
H	0	4.395039	-0.835660	-2.928007
N	0	0.045175	1.697364	0.513567
C	0	1.338901	2.243978	0.695280
C	0	1.416282	3.636469	1.110508
C	0	0.271900	4.380713	1.314961
C	0	-1.017031	3.786735	1.119305
C	0	-1.077111	2.461131	0.724199
O	0	2.357769	1.503998	0.490491
H	0	2.411465	4.047802	1.247533
H	0	0.344814	5.421159	1.625445
H	0	-1.929847	4.352033	1.273926
H	0	-2.030892	1.969318	0.563806

18. *O*-bound 2-hydroxypyridyl complex (m=6)

Fe	0	0.189416	-0.395219	-0.126778
N	0	-0.841367	0.046103	-1.890996
N	0	-1.609406	-1.150945	0.623463
N	0	1.936891	-0.478367	-1.293398
N	0	1.168222	-1.676376	1.223133
C	0	-0.284001	0.554555	-3.063254
C	0	-1.342866	1.010556	-3.948901
C	0	-2.538157	0.767549	-3.309711
C	0	-2.222798	0.164553	-2.025394
C	0	-2.883848	-0.865815	0.138747
C	0	-3.881910	-1.326964	1.089401
C	0	-3.204976	-1.891838	2.147237
C	0	-1.785426	-1.785574	1.852135
C	0	0.607093	-2.237635	2.368117
C	0	1.656434	-2.806919	3.198170
C	0	2.850279	-2.591343	2.546044
C	0	2.542562	-1.886303	1.312079
C	0	3.204349	-0.854923	-0.854592
C	0	2.108685	0.102607	-2.547921
C	0	3.519272	0.096249	-2.900612
C	0	4.195013	-0.495658	-1.856568
C	0	3.486666	-1.497950	0.355426
C	0	-0.759566	-2.275792	2.666621
C	0	-3.168319	-0.251897	-1.084172
C	0	1.081809	0.594087	-3.361737
H	0	4.527707	-1.731353	0.562299
H	0	-1.050525	-2.748488	3.600880
H	0	-4.215180	-0.091779	-1.327702
H	0	1.368559	1.021748	-4.318722
H	0	-1.183549	1.448567	-4.925597
H	0	-3.539714	0.970681	-3.665795
H	0	-4.951438	-1.229845	0.955787
H	0	-3.616736	-2.343947	3.040109
H	0	1.491759	-3.307239	4.143560
H	0	3.925669	0.485904	-3.824847
H	0	3.844804	-2.882113	2.858558
H	0	5.257636	-0.680345	-1.767044
N	0	-1.535410	2.540472	0.742784
C	0	-0.224566	2.384147	1.069551
C	0	0.506389	3.383796	1.769129
C	0	-0.149190	4.566928	2.131693
C	0	-1.510884	4.735198	1.795046
C	0	-2.152370	3.693225	1.102696
O	0	0.403563	1.242972	0.718572
H	0	1.550202	3.203016	2.002542
H	0	0.388255	5.346068	2.667080
H	0	-2.054668	5.637300	2.058056
H	0	-3.200107	3.775241	0.821089

19. Methanol complex (m=4)

Fe	0	0.027169	-0.041520	-0.045049
N	0	1.725036	0.061587	-1.099071
N	0	-1.007403	0.461915	-1.682068
N	0	1.031671	-0.936087	1.436984
N	0	-1.689690	-0.442076	0.890511
C	0	3.022591	-0.281300	-0.678959
C	0	3.980326	0.019894	-1.715451
C	0	3.278711	0.542243	-2.779128
C	0	1.885249	0.558846	-2.404771
C	0	-0.487688	0.911618	-2.906755
C	0	-1.559263	1.293430	-3.796817
C	0	-2.740751	1.081629	-3.124307
C	0	-2.400633	0.574885	-1.815337
C	0	-2.997194	-0.218500	0.423452
C	0	-3.958846	-0.565313	1.441856
C	0	-3.250714	-1.008197	2.536712
C	0	-1.850597	-0.942824	2.194410
C	0	0.515080	-1.365659	2.669887
C	0	2.417442	-1.142176	1.532609
C	0	2.753399	-1.710319	2.817571
C	0	1.579110	-1.844369	3.521407
C	0	-0.824942	-1.357146	3.034765
C	0	-3.334743	0.259749	-0.836540
C	0	0.858584	0.973388	-3.244001
C	0	3.351709	-0.839524	0.550125
H	0	-1.088596	-1.723172	4.021553
H	0	-4.386333	0.387285	-1.071257
H	0	1.121528	1.337662	-4.231674
H	0	4.395532	-1.056813	0.751020
H	0	5.044575	-0.155878	-1.636738
H	0	3.660338	0.873116	-3.735468
H	0	-1.417563	1.665696	-4.802318
H	0	-3.750643	1.248328	-3.473664
H	0	-5.031118	-0.486140	1.324766
H	0	3.756062	-1.968897	3.129786
H	0	-3.634052	-1.361312	3.484370
H	0	1.436464	-2.235180	4.519686
O	0	0.277300	1.926870	0.674568
C	0	-0.727298	2.883531	1.185581
H	0	-1.650138	2.316725	1.302458
H	0	-0.869248	3.693722	0.463260
H	0	-0.401577	3.275254	2.154231
H	0	1.164083	2.323050	0.569321

20. Phenoxide complex (m=6)

Fe	0	0.163659	-0.376469	-0.144722
N	0	-1.141105	-0.098458	-1.768163
N	0	-1.482208	-1.162140	0.898846
N	0	1.728734	-0.448939	-1.542751
N	0	1.387222	-1.516259	1.125275
C	0	-0.779857	0.347873	-3.037891
C	0	-1.975930	0.683012	-3.795148
C	0	-3.056681	0.429410	-2.980071
C	0	-2.532898	-0.061633	-1.714720
C	0	-2.826656	-0.977439	0.584173
C	0	-3.653775	-1.431890	1.691548
C	0	-2.802322	-1.894282	2.670171
C	0	-1.445768	-1.730018	2.170743
C	0	1.020899	-2.031279	2.365637
C	0	2.205589	-2.500343	3.068465
C	0	3.283464	-2.270870	2.242643
C	0	2.768748	-1.657351	1.027646
C	0	3.062937	-0.737596	-1.269360
C	0	1.687204	0.050347	-2.841530
C	0	3.032878	0.084619	-3.394418
C	0	3.881162	-0.402584	-2.425196
C	0	3.546316	-1.286774	-0.075901
C	0	-0.287987	-2.116549	2.855403
C	0	-3.313050	-0.455838	-0.620815
C	0	0.528411	0.432903	-3.527864
H	0	4.617266	-1.458767	-0.007583
H	0	-0.418867	-2.545602	3.845308
H	0	-4.391642	-0.372765	-0.725341
H	0	0.653803	0.804460	-4.541447
H	0	-1.978555	1.052537	-4.812327
H	0	-4.107718	0.552281	-3.207012
H	0	-4.735574	-1.403504	1.706056
H	0	-3.058055	-2.314326	3.634205
H	0	2.201583	-2.949344	4.053146
H	0	3.282545	0.427472	-4.390067
H	0	4.325781	-2.497140	2.426096
H	0	4.954228	-0.532331	-2.480096
C	0	-1.447388	2.919100	0.881103
C	0	-0.082978	2.538740	0.960966
C	0	0.871993	3.450892	1.477068
C	0	0.463161	4.724004	1.905471
C	0	-0.893041	5.105064	1.826791
C	0	-1.841337	4.195787	1.313109
O	0	0.325880	1.309107	0.549779
H	0	1.911686	3.139777	1.529973
H	0	1.200611	5.419424	2.300627
H	0	-1.204724	6.091996	2.159685
H	0	-2.888874	4.482641	1.249483
H	0	-2.169574	2.210868	0.484148

21. AcOH complex (m=4)

Fe	0	-0.062800	-0.291440	-0.103755
N	0	1.530132	-1.491477	-0.073049
N	0	0.589401	0.503080	-1.824709
N	0	-0.866705	-1.338119	1.391810
N	0	-1.810637	0.656638	-0.357863
C	0	1.845594	-2.457229	0.895231
C	0	3.147468	-3.024634	0.633900
C	0	3.636568	-2.412645	-0.497211
C	0	2.639153	-1.463049	-0.932249
C	0	1.817157	0.261163	-2.464666
C	0	1.948588	1.100154	-3.631896
C	0	0.808172	1.866240	-3.714421
C	0	-0.033909	1.496369	-2.601690
C	0	-2.126175	1.630227	-1.322952
C	0	-3.459545	2.139321	-1.106088
C	0	-3.972686	1.479064	-0.012933
C	0	-2.955583	0.566580	0.452343
C	0	-2.127410	-1.158008	1.980992
C	0	-0.239781	-2.323781	2.169760
C	0	-1.112489	-2.751998	3.237530
C	0	-2.280202	-2.033966	3.119053
C	0	-3.106617	-0.272919	1.547708
C	0	-1.290091	2.043226	-2.356239
C	0	2.779291	-0.649591	-2.049664
C	0	1.029691	-2.842191	1.950853
H	0	-4.044465	-0.240611	2.092241
H	0	-1.657619	2.803613	-3.037181
H	0	3.689116	-0.735549	-2.634427
H	0	1.396202	-3.604446	2.630347
H	0	3.613583	-3.792582	1.236070
H	0	4.580036	-2.583098	-0.997676
H	0	2.801319	1.095018	-4.297082
H	0	0.549485	2.605798	-4.459891
H	0	-3.935420	2.892773	-1.718824
H	0	-0.860102	-3.506259	3.970337
H	0	-4.948600	1.590961	0.439527
H	0	-3.166301	-2.087307	3.736819
O	0	0.795292	1.190631	1.145163
C	0	0.945723	2.435506	1.260652
C	0	1.681796	3.082858	2.395569
O	0	0.453136	3.322063	0.362018
H	0	2.520652	3.670431	2.004682
H	0	2.046523	2.322937	3.086894
H	0	1.017211	3.780830	2.917667
H	0	-0.038165	2.931495	-0.401200

22. Me_3P complex (m=4)

Fe	0	0.003022	-0.007256	-0.448736
N	0	1.415271	-1.413654	-0.600621
N	0	1.409630	1.404209	-0.609953
N	0	-1.402964	-1.420255	-0.604200
N	0	-1.409540	1.398052	-0.613344
c	0	1.235527	-2.806073	-0.621134
c	0	2.513894	-3.478284	-0.656578
c	0	3.484795	-2.503007	-0.657806
c	0	2.806867	-1.227796	-0.623509
c	0	2.802255	1.224425	-0.630174
c	0	3.473971	2.502571	-0.675018
c	0	2.498257	3.473330	-0.685681
c	0	1.223120	2.795753	-0.646396
c	0	-1.229334	2.790518	-0.649681
c	0	-2.507607	3.461982	-0.694143
c	0	-3.478804	2.486644	-0.687509
c	0	-2.801379	1.211779	-0.639631
c	0	-2.795324	-1.240519	-0.633052
c	0	-1.216742	-2.811911	-0.623360
c	0	-2.491807	-3.489984	-0.662009
c	0	-3.467130	-2.518991	-0.668779
c	0	-3.452902	-0.016070	-0.639400
c	0	-0.004489	3.447403	-0.656894
c	0	3.459283	-0.000519	-0.626631
c	0	0.011012	-3.463650	-0.621947
H	0	-4.537733	-0.018922	-0.667714
H	0	-0.006895	4.532022	-0.691852
H	0	4.544229	0.001617	-0.649721
H	0	0.013768	-4.548616	-0.643225
H	0	2.642022	-4.551842	-0.686207
H	0	4.558893	-2.626165	-0.688591
H	0	4.547479	2.630880	-0.705432
H	0	2.621365	4.547104	-0.726519
H	0	-2.635834	4.535126	-0.735692
H	0	-2.614820	-4.564164	-0.690837
H	0	-4.552769	2.609830	-0.722667
H	0	-4.540501	-2.647292	-0.703679
P	0	-0.009384	0.026600	2.201613
c	0	1.377842	-0.957501	3.012525
c	0	0.151067	1.743297	2.959390
c	0	-1.576558	-0.667679	2.983631
H	0	1.307592	-0.893687	4.104491
H	0	1.311638	-2.006182	2.708093
H	0	2.346472	-0.563027	2.691237
H	0	0.131115	1.683591	4.053684
H	0	1.092815	2.199689	2.640824
H	0	-0.674852	2.374357	2.618026
H	0	-1.518306	-0.613016	4.076765
H	0	-2.442883	-0.094243	2.640899
H	0	-1.708725	-1.710963	2.682012

23. Quinoline complex (m=4)

Fe	0	-0.519846	0.000190	-0.670802
N	0	-1.898533	1.402218	-0.295439
N	0	-1.898554	-1.401965	-0.296287
N	0	0.619292	1.399308	-1.523202
N	0	0.619307	-1.398620	-1.523837
C	0	-1.677996	2.785873	-0.247199
C	0	-2.871473	3.466750	0.201299
C	0	-3.838304	2.505774	0.394364
C	0	-3.231590	1.226267	0.104584
C	0	-3.231583	-1.226118	0.103867
C	0	-3.838345	-2.505738	0.393130
C	0	-2.871580	-3.466675	0.199569
C	0	-1.678048	-2.785646	-0.248555
C	0	0.522362	-2.783271	-1.322099
C	0	1.599224	-3.464032	-2.004189
C	0	2.331676	-2.504013	-2.665420
C	0	1.736057	-1.224527	-2.355892
C	0	1.736104	1.225514	-2.355221
C	0	0.522298	2.783889	-1.321003
C	0	1.599186	3.464909	-2.002800
C	0	2.331778	2.505120	-2.664199
C	0	2.242687	0.000601	-2.777135
C	0	-0.520570	-3.432074	-0.669745
C	0	-3.869404	0.000022	0.265029
C	0	-0.520570	3.432447	-0.668316
H	0	3.106873	0.000787	-3.433125
H	0	-0.474045	-4.512166	-0.577265
H	0	-4.909582	-0.000089	0.573754
H	0	-0.474042	4.512510	-0.575484
H	0	-2.958667	4.538142	0.320790
H	0	-4.864249	2.641274	0.708957
H	0	-4.864287	-2.641304	0.707708
H	0	-2.958810	-4.538123	0.318530
H	0	1.748216	-4.535255	-1.999994
H	0	1.748104	4.536141	-1.998263
H	0	3.198003	-2.640379	-3.298477
H	0	3.198237	2.641685	-3.297031
N	0	0.274632	-0.000577	1.408621
C	0	-0.699616	-0.000969	2.337091
C	0	-0.456347	-0.001220	3.732511
C	0	0.854797	-0.001222	4.185026
C	0	1.922521	-0.000889	3.242001
C	0	1.605587	-0.000455	1.832628
H	0	-1.720216	-0.001135	1.979238
H	0	-1.298021	-0.001377	4.416115
H	0	1.079140	-0.001438	5.248755
C	0	2.675805	0.000092	0.894795
C	0	3.995314	0.000055	1.330210
C	0	4.311561	-0.000510	2.720749
C	0	3.289551	-0.000937	3.658003
H	0	2.456266	0.000564	-0.161343
H	0	4.800453	0.000489	0.600446
H	0	5.350214	-0.000607	3.037865
H	0	3.512897	-0.001321	4.722188

24. Thiophene complex (m=4)

Fe	0	0.082541	-0.429225	-0.337700
N	0	-1.563547	-0.053466	-1.391176
N	0	-1.038756	-0.875211	1.242203
N	0	1.170853	-0.258909	-1.997898
N	0	1.701086	-1.036504	0.648176
C	0	-1.649964	0.318316	-2.745545
C	0	-3.021798	0.570729	-3.111366
C	0	-3.789137	0.351562	-1.988968
C	0	-2.892027	-0.035083	-0.928151
C	0	-2.434194	-0.753040	1.364933
C	0	-2.855897	-1.109955	2.697370
C	0	-1.724878	-1.450682	3.403844
C	0	-0.603463	-1.304527	2.508482
C	0	1.783577	-1.443226	1.992547
C	0	3.150265	-1.738104	2.345887
C	0	3.917373	-1.518443	1.223422
C	0	3.025219	-1.089109	0.174996
C	0	2.562803	-0.410066	-2.129281
C	0	0.732257	0.140798	-3.272843
C	0	1.846297	0.226657	-4.185518
C	0	2.977175	-0.113630	-3.479044
C	0	3.433956	-0.790961	-1.118004
C	0	0.712033	-1.564990	2.866540
C	0	-3.303288	-0.355499	0.358350
C	0	-0.581203	0.417483	-3.626291
H	0	4.489921	-0.871352	-1.353596
H	0	0.911972	-1.894541	3.880711
H	0	-4.362985	-0.305581	0.585665
H	0	-0.785335	0.716229	-4.649086
H	0	-3.347859	0.866524	-4.099236
H	0	-4.862573	0.432913	-1.884589
H	0	-3.882581	-1.103485	3.037299
H	0	-1.649136	-1.776312	4.432387
H	0	3.471561	-2.076897	3.321472
H	0	1.765188	0.508868	-5.226362
H	0	4.985407	-1.642207	1.106448
H	0	3.998511	-0.163153	-3.831179
S	0	0.488869	2.235064	0.296939
C	0	1.004844	2.357522	2.032887
C	0	-1.106426	2.993499	0.714813
C	0	-1.158895	3.322127	2.041497
C	0	0.038109	2.961596	2.788773
H	0	1.987171	2.008389	2.315327
H	0	-1.831520	3.158341	-0.068576
H	0	-2.010829	3.818354	2.493384
H	0	0.157904	3.165196	3.847277

25. $PhNH_2$ complex (m=4)

Fe	0	0.583079	0.000001	-0.405183
N	0	-0.648998	1.408760	-1.095674
N	0	-0.649187	-1.408549	-1.095755
N	0	1.959826	1.410525	-0.031754
N	0	1.959640	-1.410728	-0.031844
C	0	-0.469709	2.800741	-1.049804
C	0	-1.638303	3.474568	-1.566118
C	0	-2.539166	2.500936	-1.932242
C	0	-1.928712	1.225108	-1.642281
C	0	-1.928881	-1.224693	-1.642342
C	0	-2.539512	-2.500423	-1.932367
C	0	-1.638777	-3.474197	-1.566305
C	0	-0.470087	-2.800556	-1.049966
C	0	1.802911	-2.804271	-0.131112
C	0	3.004894	-3.476775	0.301731
C	0	3.907941	-2.502769	0.663526
C	0	3.265554	-1.226507	0.455513
C	0	3.265714	1.226101	0.455596
C	0	1.803281	2.804096	-0.130929
C	0	3.005349	3.476414	0.301967
C	0	3.908266	2.502265	0.663699
C	0	3.874324	-0.000251	0.695442
C	0	0.666241	-3.457449	-0.592758
C	0	-2.534294	0.000255	-1.891417
C	0	0.666701	3.457454	-0.592543
H	0	4.892168	-0.000330	1.071422
H	0	0.675299	-4.542182	-0.619221
H	0	-3.531738	0.000335	-2.318265
H	0	0.675903	4.542187	-0.618936
H	0	-1.742593	4.548315	-1.643610
H	0	-3.522499	2.625643	-2.364877
H	0	-3.522866	-2.624973	-2.364999
H	0	-1.743212	-4.547925	-1.643854
H	0	3.136351	-4.550223	0.314667
H	0	3.136946	4.549844	0.314976
H	0	4.918093	-2.628280	1.029027
H	0	4.918433	2.627620	1.029213
N	0	-0.118061	0.000001	1.706439
H	0	0.344551	-0.836443	2.070632
C	0	-1.549758	-0.000004	1.963256
H	0	0.344548	0.836443	2.070641
C	0	-2.236777	1.222954	2.085381
C	0	-3.619969	1.218000	2.335974
C	0	-4.316451	-0.000016	2.462181
C	0	-3.619943	-1.218026	2.336062
C	0	-2.236751	-1.222968	2.085469
H	0	-1.702331	2.166638	1.994208
H	0	-4.149117	2.161196	2.440714
H	0	-5.383685	-0.000020	2.664229
H	0	-4.149070	-2.161226	2.440871
H	0	-1.702282	-2.166647	1.994366

26. Me_3PO complex (m=4)

Fe	0	0.290289	0.000313	-0.479842
N	0	1.723912	1.410079	-0.440941
N	0	-1.041503	1.413797	-1.030056
N	0	1.721494	-1.411938	-0.441867
N	0	-1.043953	-1.410539	-1.030878
C	0	3.085146	1.223555	-0.177591
C	0	3.754379	2.501697	-0.060989
C	0	2.801334	3.474547	-0.247888
C	0	1.543644	2.797313	-0.482694
C	0	-0.853958	2.802265	-1.004109
C	0	-2.088121	3.481060	-1.331396
C	0	-3.034717	2.509967	-1.566813
C	0	-2.386765	1.230315	-1.380263
C	0	-2.388907	-1.224524	-1.380942
C	0	-3.039064	-2.502943	-1.568255
C	0	-2.094123	-3.475812	-1.333498
C	0	-0.858783	-2.799346	-1.005838
C	0	1.538852	-2.798835	-0.484532
C	0	3.083050	-1.227916	-0.178416
C	0	3.750100	-2.507277	-0.062681
C	0	2.795390	-3.478372	-0.250209
C	0	0.338459	-3.452732	-0.735069
C	0	-3.022689	0.003493	-1.538108
C	0	0.344383	3.453427	-0.732854
C	0	3.725990	-0.002772	-0.049231
H	0	0.341964	-4.537933	-0.749259
H	0	-4.069855	0.004485	-1.823668
H	0	0.349743	4.538630	-0.746325
H	0	4.791967	-0.003753	0.153823
H	0	4.811686	2.624903	0.130680
H	0	2.927438	4.548776	-0.240447
H	0	-2.200430	4.555309	-1.390064
H	0	-4.069230	2.637866	-1.856003
H	0	-4.073804	-2.628886	-1.857490
H	0	4.807199	-2.632416	0.128881
H	0	-2.208279	-4.549828	-1.392854
H	0	2.919661	-4.552820	-0.243486
O	0	-0.069058	0.000017	1.457849
P	0	-1.204736	-0.000049	2.642301
C	0	-0.328767	-0.154425	4.271666
C	0	-2.186541	1.579480	2.638015
C	0	-2.377092	-1.431632	2.455157
H	0	-1.044241	-0.159425	5.100296
H	0	0.247312	-1.084013	4.279007
H	0	0.359491	0.687690	4.386555
H	0	-2.918298	1.576195	3.452561
H	0	-1.503966	2.424222	2.767175
H	0	-2.705480	1.685235	1.681592
H	0	-3.108770	-1.434726	3.269773
H	0	-2.897966	-1.355267	1.496989
H	0	-1.807008	-2.364765	2.476249

27. *O*-bound DMSO complex (m=4)

Fe	0	0.055079	-0.388597	-0.159726
N	0	-0.933126	-0.658144	-1.883285
N	0	-1.110382	-1.776038	0.695298
N	0	1.461524	0.653045	-1.152207
N	0	1.288741	-0.473393	1.425608
C	0	-0.694295	-0.010879	-3.102815
C	0	-1.717655	-0.357852	-4.064359
C	0	-2.585806	-1.220126	-3.436971
C	0	-2.102343	-1.401809	-2.086097
C	0	-2.257387	-2.373006	0.157447
C	0	-2.901942	-3.206212	1.148366
C	0	-2.154553	-3.117273	2.299216
C	0	-1.044697	-2.233480	2.017926
C	0	1.045429	-1.115532	2.649161
C	0	2.121500	-0.851073	3.577049
C	0	3.033470	-0.053765	2.923842
C	0	2.518499	0.181324	1.594000
C	0	2.669199	1.161447	-0.648758
C	0	1.391569	1.117592	-2.474657
C	0	2.550916	1.922668	-2.785036
C	0	3.341964	1.946099	-1.658663
C	0	3.165667	0.947987	0.632027
C	0	-0.050846	-1.920340	2.937326
C	0	-2.726493	-2.204273	-1.139253
C	0	0.378264	0.827718	-3.381493
H	0	4.119321	1.395998	0.891789
H	0	-0.117071	-2.356974	3.928663
H	0	-3.629939	-2.730536	-1.429416
H	0	0.447682	1.253256	-4.377482
H	0	-1.751461	0.006185	-5.082299
H	0	-3.468574	-1.696642	-3.841206
H	0	-3.801480	-3.780992	0.974477
H	0	-2.323030	-3.607094	3.248720
H	0	2.172724	-1.241938	4.584305
H	0	2.736473	2.386745	-3.744336
H	0	3.972288	0.334476	3.295179
H	0	4.296809	2.435036	-1.519889
S	0	-0.485696	2.652301	1.090620
O	0	-1.082658	1.171819	0.441310
C	0	-1.232522	3.870515	-0.142294
C	0	-1.678578	2.855410	2.538366
H	0	-1.103033	4.884420	0.244463
H	0	-0.681378	3.733393	-1.073453
H	0	-2.283985	3.607270	-0.270056
H	0	-1.563236	3.861899	2.948211
H	0	-2.686646	2.674625	2.161213
H	0	-1.396697	2.099120	3.271797

28. *S*-bound DMSO complex (m=4)

Fe	0	0.323781	-0.404115	-0.122973
N	0	-0.581628	-0.749928	-1.860280
N	0	-1.075243	-1.459854	0.808113
N	0	1.817787	0.492587	-1.084711
N	0	1.318210	-0.209382	1.585464
C	0	-0.181151	-0.315109	-3.138400
C	0	-1.127360	-0.748908	-4.136105
C	0	-2.110634	-1.459568	-3.483770
C	0	-1.777518	-1.460006	-2.081299
C	0	-2.214408	-2.066082	0.248817
C	0	-3.020027	-2.672566	1.280617
C	0	-2.390794	-2.431412	2.480520
C	0	-1.191481	-1.685696	2.190421
C	0	0.894022	-0.604173	2.867011
C	0	1.872586	-0.231926	3.857928
C	0	2.907999	0.388016	3.195208
C	0	2.564735	0.409207	1.794306
C	0	3.005416	1.014351	-0.535852
C	0	1.908691	0.767122	-2.462904
C	0	3.139165	1.458174	-2.757656
C	0	3.818509	1.606349	-1.568472
C	0	3.359011	0.977299	0.806987
C	0	-0.282769	-1.279350	3.156445
C	0	-2.543700	-2.076069	-1.099872
C	0	0.971157	0.406419	-3.422230
H	0	4.307297	1.415439	1.100238
H	0	-0.498489	-1.512342	4.193570
H	0	-3.449194	-2.590891	-1.403482
H	0	1.165777	0.675532	-4.455193
H	0	-1.039008	-0.544731	-5.194567
H	0	-2.979435	-1.944885	-3.907345
H	0	-3.944672	-3.204665	1.103107
H	0	-2.702805	-2.726908	3.472801
H	0	1.775467	-0.425939	4.917320
H	0	3.443515	1.773128	-3.746594
H	0	3.819948	0.796365	3.609106
H	0	4.782680	2.066851	-1.400842
S	0	-1.076700	1.876513	0.509580
O	0	-1.751687	1.751963	2.041081
C	0	-2.505873	2.355274	-0.643294
C	0	-0.061649	3.478570	0.528848
H	0	-2.116233	2.530691	-1.647984
H	0	-3.195122	1.510129	-0.625056
H	0	-2.973609	3.244548	-0.216183
H	0	0.343099	3.661989	-0.468362
H	0	-0.730430	4.275096	0.860916
H	0	0.733120	3.312474	1.257120

29. Fluoride complex (m=6)

Fe	0	0.085599	0.610323	0.213506
N	0	1.629706	-0.426907	1.172230
N	0	1.262950	0.565106	-1.515962
N	0	-1.210676	-0.195404	1.645181
N	0	-1.577435	0.796593	-1.043016
C	0	1.603073	-0.917440	2.476796
C	0	2.945103	-1.301825	2.880862
C	0	3.778883	-1.045502	1.815251
C	0	2.955589	-0.501529	0.748355
C	0	2.639737	0.352732	-1.566761
C	0	3.136936	0.690838	-2.889842
C	0	2.055834	1.103243	-3.636539
C	0	0.886128	1.021776	-2.777969
C	0	-1.560035	1.221056	-2.370705
C	0	-2.915630	1.508371	-2.808740
C	0	-3.749420	1.252002	-1.743147
C	0	-2.912535	0.805272	-0.642219
C	0	-2.596700	-0.049114	1.672853
C	0	-0.843070	-0.718015	2.884112
C	0	-2.026380	-0.896848	3.708601
C	0	-3.107451	-0.484168	2.962008
C	0	-3.383740	0.424378	0.618188
C	0	-0.418745	1.335959	-3.170828
C	0	3.425406	-0.130564	-0.515528
C	0	0.460413	-1.042139	3.273491
H	0	-4.455369	0.486059	0.787025
H	0	-0.560091	1.683542	-4.190586
H	0	4.489929	-0.243087	-0.702156
H	0	0.594647	-1.440609	4.275440
H	0	3.203341	-1.713846	3.847562
H	0	4.846453	-1.208770	1.747645
H	0	4.171858	0.616012	-3.196917
H	0	2.041421	1.428686	-4.668436
H	0	-3.183081	1.854472	-3.798509
H	0	-2.021207	-1.288405	4.717357
H	0	-4.826220	1.349236	-1.698652
H	0	-4.151577	-0.475182	3.246046
F	0	0.324644	2.320358	0.811928

30. $Me_2PO_2^-$ complex (m=6)

Fe	0	-0.226780	-0.224756	-0.162114
P	0	1.818079	2.390600	0.536514
O	0	3.214788	1.686960	0.185926
O	0	0.438340	1.424891	0.330813
C	0	1.673518	2.921079	2.319180
C	0	1.435090	3.869512	-0.534163
H	0	0.686504	3.355360	2.502245
H	0	1.802170	2.035435	2.947983
H	0	2.458065	3.647289	2.555691
H	0	0.454618	4.277751	-0.272780
H	0	2.210558	4.631830	-0.406265
H	0	1.424079	3.539469	-1.576882
N	0	-1.629517	-0.650369	1.340841
N	0	1.066098	-1.549730	0.815547
N	0	-1.857823	0.258435	-1.392527
N	0	0.837961	-0.641593	-1.915815
C	0	-2.946428	-0.196346	1.389927
C	0	-3.500622	-0.447663	2.710083
C	0	-2.515484	-1.059256	3.453789
C	0	-1.349065	-1.187419	2.595949
C	0	0.975393	-1.955815	2.146149
C	0	2.213563	-2.606860	2.542840
C	0	3.048281	-2.591127	1.448026
C	0	2.329407	-1.933637	0.370060
C	0	2.133011	-1.151839	-1.981308
C	0	2.649094	-1.002094	-3.331241
C	0	1.660353	-0.404756	-4.080374
C	0	0.529298	-0.180093	-3.194638
C	0	-1.795185	0.588408	-2.745141
C	0	-3.143063	0.586389	-0.964273
C	0	-3.900167	1.142794	-2.073467
C	0	-3.068903	1.143682	-3.171937
C	0	-0.686033	0.397106	-3.576701
C	0	2.827561	-1.739402	-0.920822
C	0	-0.138964	-1.780553	2.972981
C	0	-3.643013	0.388754	0.327211
H	0	-0.784134	0.706598	-4.613801
H	0	3.841198	-2.076426	-1.117544
H	0	-0.065427	-2.154276	3.990778
H	0	-4.669036	0.693950	0.514384
H	0	-4.508210	-0.195620	3.014183
H	0	-2.567129	-1.400762	4.479432
H	0	2.407041	-3.017063	3.525404
H	0	4.054054	-2.981861	1.368072
H	0	3.634838	-1.313121	-3.650952
H	0	-4.928104	1.475853	-2.013015
H	0	1.684149	-0.139531	-5.129289
H	0	-3.290193	1.477470	-4.177350

31. Me_3SiO^- complex (m=6)

Fe	0	-0.012602	0.004865	-0.355986
N	0	-1.537197	1.380964	-0.831938
N	0	-1.393139	-1.510467	-0.848909
N	0	1.354261	1.525309	-0.870561
N	0	1.498163	-1.366345	-0.887477
C	0	-1.404767	2.766114	-0.873761
C	0	-2.722772	3.381829	-0.921277
C	0	-3.646733	2.360838	-0.913322
C	0	-2.902508	1.111079	-0.860993
C	0	-2.778576	-1.377275	-0.875925
C	0	-3.394935	-2.694160	-0.943254
C	0	-2.374102	-3.618077	-0.961928
C	0	-1.123809	-2.875012	-0.906314
C	0	1.364436	-2.751063	-0.939994
C	0	2.680573	-3.365978	-1.030271
C	0	3.604519	-2.344884	-1.037637
C	0	2.862230	-1.095872	-0.952008
C	0	2.738441	1.392549	-0.938049
C	0	1.083428	2.890320	-0.906624
C	0	2.331774	3.634106	-0.989264
C	0	3.352739	2.710165	-1.008759
C	0	3.437661	0.180099	-0.961670
C	0	0.151862	-3.450550	-0.934560
C	0	-3.478161	-0.164867	-0.867364
C	0	-0.192578	3.465744	-0.894137
H	0	4.521783	0.234335	-1.016700
H	0	0.205244	-4.535106	-0.981293
H	0	-4.563392	-0.218766	-0.892988
H	0	-0.247205	4.550720	-0.927771
H	0	-2.904809	4.447857	-0.963847
H	0	-4.725872	2.435539	-0.948630
H	0	-4.461328	-2.875351	-0.979959
H	0	-2.449327	-4.696357	-1.016779
H	0	2.861302	-4.431457	-1.089218
H	0	2.405556	4.712903	-1.035504
H	0	4.682260	-2.419075	-1.103531
H	0	4.417670	2.891990	-1.073825
O	0	0.014132	-0.004653	1.442353
Si	0	0.070533	-0.026442	3.147198
C	0	1.847042	-0.414691	3.676621
C	0	-1.117527	-1.367141	3.761359
C	0	-0.456255	1.677593	3.783165
H	0	2.539802	0.349409	3.300402
H	0	2.168412	-1.384443	3.274799
H	0	1.941506	-0.450755	4.771023
H	0	-0.826076	-2.351605	3.372656
H	0	-2.141657	-1.163974	3.422224
H	0	-1.126751	-1.423287	4.858959
H	0	-1.471531	1.922708	3.445192
H	0	0.218845	2.457495	3.407381
H	0	-0.443792	1.716727	4.881452

32. $BuNH_2$ complex (m=4)

Fe	0	-0.521343	0.000056	-0.428024
N	0	0.587439	-1.408984	-1.313572
N	0	0.587170	1.409574	-1.313128
N	0	-1.834619	-1.411202	0.130813
N	0	-1.834981	1.410781	0.131126
C	0	0.422010	-2.801223	-1.231349
C	0	1.490503	-3.475600	-1.931268
C	0	2.311807	-2.502298	-2.453337
C	0	1.754868	-1.225317	-2.072159
C	0	1.754703	1.226405	-2.071673
C	0	2.311423	2.503630	-2.452343
C	0	1.489948	3.476587	-1.929897
C	0	0.421461	2.801748	-1.230411
C	0	-1.686194	2.803595	0.023158
C	0	-2.810535	3.476884	0.630495
C	0	-3.657898	2.502897	1.107664
C	0	-3.056798	1.226031	0.799505
C	0	-3.056395	-1.226935	0.799391
C	0	-1.685410	-2.803950	0.022606
C	0	-2.809415	-3.477687	0.630080
C	0	-3.657057	-2.504036	1.107438
C	0	-3.626834	-0.000561	1.120124
C	0	-0.627007	3.457291	-0.595433
C	0	2.307170	0.000651	-2.423319
C	0	-0.626176	-3.457209	-0.596365
H	0	-4.580587	-0.000739	1.637608
H	0	-0.634227	4.542267	-0.609387
H	0	3.214170	0.000825	-3.018932
H	0	-0.633114	-4.542183	-0.610613
H	0	1.585225	-4.549572	-2.017202
H	0	3.206811	-2.628065	-3.047426
H	0	3.206441	2.629790	-3.046328
H	0	1.584514	4.550608	-2.015376
H	0	-2.933150	4.550674	0.671791
H	0	-2.931661	-4.551523	0.671275
H	0	-4.605044	2.628343	1.614599
H	0	-4.604103	-2.629861	1.614468
N	0	0.491656	-0.000302	1.496935
H	0	0.126015	0.829182	1.975920
C	0	1.997961	0.000313	1.511270
H	0	0.126725	-0.830524	1.975184
H	0	2.331238	0.884852	0.957678
C	0	2.592123	-0.000462	2.933456
H	0	2.331974	-0.883143	0.956405
C	0	4.138800	0.000141	2.916760
C	0	4.744107	-0.000622	4.335461
H	0	2.234774	0.883908	3.484431
H	0	2.235447	-0.885881	3.483184
H	0	4.497054	-0.881945	2.364548
H	0	4.496363	0.883269	2.365774
H	0	5.839980	-0.000136	4.295216
H	0	4.429845	0.886378	4.901369
H	0	4.430577	-0.888689	4.900098

33. Me_2NPy complex (m=4)

Fe	0	-1.076242	0.000026	0.000021
N	0	-1.310030	-1.412720	1.407660
N	0	-1.310115	-1.412655	-1.407664
N	0	-1.310008	1.412678	1.407709
N	0	-1.310079	1.412750	-1.407594
C	0	-1.280194	-1.226428	2.796990
C	0	-1.348353	-2.500817	3.475829
C	0	-1.433764	-3.472663	2.505625
C	0	-1.404695	-2.800097	1.226348
C	0	-1.404793	-2.800053	-1.226410
C	0	-1.433963	-3.472546	-2.505721
C	0	-1.348606	-2.500656	-3.475882
C	0	-1.280380	-1.226299	-2.796978
C	0	-1.280328	1.226449	-2.796939
C	0	-1.348518	2.500849	-3.475769
C	0	-1.433817	3.472694	-2.505566
C	0	-1.404691	2.800127	-1.226282
C	0	-1.404631	2.800068	1.226466
C	0	-1.280181	1.226322	2.797047
C	0	-1.348337	2.500684	3.475933
C	0	-1.433710	3.472574	2.505776
C	0	-1.452388	3.453807	0.000106
C	0	-1.239453	0.000094	-3.449843
C	0	-1.452499	-3.453768	-0.000046
C	0	-1.239249	-0.000064	3.449899
H	0	-1.532139	4.535978	0.000136
H	0	-1.220639	0.000101	-4.534837
H	0	-1.532284	-4.535939	-0.000054
H	0	-1.220373	-0.000089	4.534892
H	0	-1.346640	-2.623873	4.550386
H	0	-1.513232	-4.543718	2.633766
H	0	-1.513453	-4.543594	-2.633915
H	0	-1.346969	-2.623659	-4.550445
H	0	-1.346882	2.623895	-4.550328
H	0	-1.346642	2.623690	4.550497
H	0	-1.513260	4.543752	-2.633697
H	0	-1.513168	4.543623	2.633970
C	0	6.012144	1.273216	-0.000146
N	0	5.265642	-0.000053	-0.000058
C	0	3.135410	1.214901	-0.000031
C	0	1.747464	1.167757	-0.000016
N	0	1.037644	-0.000032	-0.000029
C	0	1.747419	-1.167851	-0.000072
C	0	3.135365	-1.215032	-0.000095
C	0	3.895902	-0.000078	-0.000045
C	0	6.012261	-1.273247	-0.000143
H	0	5.784088	1.871560	0.892304
H	0	7.083213	1.063367	-0.000071
H	0	5.784174	1.871403	-0.892726
H	0	3.619770	2.183121	-0.000043
H	0	1.171644	2.086141	0.000000
H	0	1.171566	-2.086212	-0.000104
H	0	3.619678	-2.183272	-0.000172
H	0	5.784480	-1.871411	-0.892790
H	0	7.083313	-1.063302	0.000089
H	0	5.784169	-1.871684	0.892237

34. *N*-bound morpholine complex (m=4)

Fe	0	0.000038	0.103682	-0.592455
N	0	1.402656	-1.299391	-0.902347
N	0	1.405258	1.548121	-0.613944
N	0	-1.402628	-1.299326	-0.902442
N	0	-1.405119	1.548190	-0.614009
C	0	1.224507	-2.676817	-1.078138
C	0	2.508800	-3.333030	-1.190012
C	0	3.474067	-2.359623	-1.084042
C	0	2.791998	-1.097382	-0.906859
C	0	2.794798	1.351788	-0.660976
C	0	3.476087	2.624973	-0.594686
C	0	2.510207	3.600709	-0.514608
C	0	1.225964	2.935121	-0.528489
C	0	-1.225769	2.935180	-0.528553
C	0	-2.509984	3.600821	-0.514685
C	0	-3.475902	2.625133	-0.594913
C	0	-2.794666	1.351915	-0.661121
C	0	-2.791961	-1.097256	-0.907021
C	0	-1.224534	-2.676763	-1.078213
C	0	-2.508849	-3.332910	-1.190203
C	0	-3.474079	-2.359472	-1.084182
C	0	-3.440481	0.126468	-0.784938
C	0	0.000112	3.589330	-0.474492
C	0	3.440567	0.126312	-0.784741
C	0	-0.000026	-3.330337	-1.148934
H	0	-4.525143	0.128468	-0.816054
H	0	0.000137	4.672184	-0.409044
H	0	4.525231	0.128261	-0.815792
H	0	-0.000046	-4.406391	-1.286087
H	0	2.641447	-4.396105	-1.338042
H	0	4.548622	-2.472514	-1.130346
H	0	4.550479	2.745626	-0.620952
H	0	2.642840	4.672727	-0.460982
H	0	-2.642573	4.672843	-0.461032
H	0	-2.641538	-4.395974	-1.338279
H	0	-4.550285	2.745836	-0.621270
H	0	-4.548639	-2.472318	-1.130502
C	0	-1.239085	-0.547625	2.258698
C	0	-1.207172	-0.458711	3.795166
N	0	-0.000071	0.054509	1.646436
C	0	1.238833	-0.547731	2.258835
C	0	1.206773	-0.458837	3.795301
O	0	-0.000262	-1.090095	4.321859
H	0	-2.117780	-0.030574	1.860779
H	0	-1.281884	-1.596950	1.951210
H	0	-2.047253	-1.004089	4.233612
H	0	-1.254924	0.593961	4.125371
H	0	-0.000043	1.066078	1.829618
H	0	1.281590	-1.597063	1.951367
H	0	2.117616	-0.030752	1.861009
H	0	1.254599	0.593828	4.125515
H	0	2.046757	-1.004301	4.233828

35. *O*-bound morpholine complex (m=4)

Fe	0	-0.000077	0.140153	-0.530043
N	0	-1.410376	1.560915	-0.548243
N	0	-1.409923	-1.221011	-0.935018
N	0	1.408806	1.562340	-0.548229
N	0	1.411131	-1.219582	-0.935029
C	0	-1.226642	2.931681	-0.305748
C	0	-2.500210	3.612508	-0.284241
C	0	-3.469954	2.667535	-0.530344
C	0	-2.798363	1.398300	-0.685551
C	0	-2.797918	-1.028388	-1.021089
C	0	-3.468356	-2.292728	-1.217425
C	0	-2.497163	-3.267581	-1.241319
C	0	-1.224093	-2.604969	-1.077783
C	0	1.226690	-2.603752	-1.077746
C	0	2.500430	-3.265088	-1.241157
C	0	3.470641	-2.289251	-1.217355
C	0	2.798951	-1.025584	-1.021051
C	0	2.796946	1.401119	-0.685549
C	0	1.223684	2.932918	-0.305774
C	0	2.496566	3.615044	-0.284343
C	0	3.467265	2.671033	-0.530346
C	0	3.451677	0.196878	-0.914818
C	0	0.001622	-3.258341	-1.114394
C	0	-3.451890	0.193405	-0.914841
C	0	-0.001800	3.571360	-0.160391
H	0	4.532689	0.210485	-1.006778
H	0	0.002168	-4.337047	-1.231916
H	0	-4.532913	0.205924	-1.006793
H	0	-0.002331	4.640651	0.023806
H	0	-2.625183	4.674136	-0.119805
H	0	-4.539982	2.807802	-0.601949
H	0	-4.538424	-2.409292	-1.323004
H	0	-2.620802	-4.333813	-1.374002
H	0	2.625170	-4.331205	-1.373742
H	0	2.620452	4.676808	-0.119955
H	0	4.540828	-2.404740	-1.322919
H	0	4.537153	2.812383	-0.601918
C	0	1.225582	-1.226287	3.417910
C	0	1.240525	-0.102232	2.377776
N	0	0.000552	-1.108427	4.220375
C	0	-1.224585	-1.226685	3.418130
C	0	-1.240097	-0.102624	2.378017
O	0	0.000148	-0.167982	1.551971
H	0	2.103799	-1.113915	4.064759
H	0	1.308319	-2.198720	2.893839
H	0	2.070704	-0.203386	1.677924
H	0	1.262546	0.880667	2.864036
H	0	-1.307078	-2.199139	2.894054
H	0	-2.102713	-1.114649	4.065156
H	0	-1.262337	0.880265	2.864280
H	0	-2.070393	-0.204045	1.678341
H	0	0.000726	-1.648565	5.081531

36. 4-Methylpyridine complex (m=4)

Fe	0	-0.000019	-0.004951	-0.683113
N	0	1.411322	-1.412953	-0.892435
N	0	1.411454	1.400149	-0.910274
N	0	-1.411451	-1.412861	-0.892395
N	0	-1.411396	1.400240	-0.910239
C	0	1.225739	-2.803273	-0.854030
C	0	2.499829	-3.481714	-0.916175
C	0	3.471925	-2.511902	-1.006755
C	0	2.800077	-1.232924	-0.986886
C	0	2.800188	1.218817	-1.002420
C	0	3.472137	2.497378	-1.038675
C	0	2.500100	3.468357	-0.960727
C	0	1.225950	2.790875	-0.889941
C	0	-1.225803	2.790953	-0.889903
C	0	-2.499909	3.468519	-0.960633
C	0	-3.472013	2.497603	-1.038558
C	0	-2.800148	1.219000	-1.002329
C	0	-2.800197	-1.232742	-0.986799
C	0	-1.225958	-2.803193	-0.853995
C	0	-2.500093	-3.481552	-0.916106
C	0	-3.472130	-2.511675	-1.006643
C	0	-3.454280	-0.007156	-1.041580
C	0	0.000096	3.444508	-0.853790
C	0	3.454238	-0.007382	-1.041691
C	0	-0.000130	-3.456320	-0.809387
H	0	-4.536493	-0.007634	-1.120007
H	0	0.000131	4.529544	-0.842122
H	0	4.536448	-0.007930	-1.120160
H	0	-0.000165	-4.541111	-0.783699
H	0	2.623319	-4.556157	-0.906884
H	0	4.543034	-2.640885	-1.083658
H	0	4.543265	2.625269	-1.117109
H	0	2.623684	4.542820	-0.965262
H	0	-2.623426	4.542990	-0.965156
H	0	-2.623652	-4.555986	-0.906817
H	0	-4.543136	2.625568	-1.116955
H	0	-4.543250	-2.640587	-1.083507
N	0	0.000028	0.008849	1.463916
C	0	1.170659	0.011483	2.158506
C	0	1.205353	0.017775	3.557190
C	0	0.000089	0.024012	4.296761
C	0	-1.205206	0.017791	3.557243
C	0	-1.170571	0.011500	2.158558
H	0	2.084771	0.005983	1.576668
H	0	2.165520	0.016560	4.064236
C	0	0.000127	0.058684	5.807360
H	0	-2.165353	0.016587	4.064329
H	0	-2.084709	0.006012	1.576760
H	0	-0.888151	-0.429700	6.221834
H	0	0.888700	-0.429206	6.221779
H	0	-0.000159	1.098072	6.165068

Table S5. Calculated method 1 energies and zero point energies (ZPE) (Hartrees), and entropies S (cal mol^{-1} K^{-1}) of iron(III) ferriprotoporphyrin complexes and free ligands, computed *in vacuo*, and in water and *n*-octanol solvents.

All structures were geometry optimized *in vacuo* at the B3LYP/LanL2DZ level. Single point calculations were then run at the B3LYP/LanL2DZ level, using the SMD solvent method. Energies of the free ligands are given in Table S1.

[Fe(PPIXH$_2$)]$^+$							
species	S	ZPE	vacuum	water	octanol	spin, vacuum	spin, water
m=2	236.246	0.599468	-1957.874127	-1957.960229	-1957.963466	2.02	2.11
m=4	238.606	0.600771	-1957.876860	-1957.977817	-1957.978168	2.78	2.92
m=6	241.177	0.597280	-1957.866719	-1957.958368	-1957.958963	3.70	4.02

[Fe(PPIXH)]							
species	S	ZPE	vacuum	water	octanol	spin, vacuum	spin, water
m=2	235.068	0.584072	-1957.418501	-1957.495800	-1957.492623	-0.01	-0.02
m=4	236.444	0.584315	-1957.438689	-1957.529324	-1957.522952	2.01	2.98
m=6	239.94	0.581968	-1957.429688	-1957.513094	-1957.505937	3.70	4.19

[Fe(PPIX)]$^-$							
species	S	ZPE	vacuum	water	octanol	spin, vacuum	spin, water
m=2	248.882	0.570553	-1956.878586	-1957.023736	-1957.002332	0.00	-0.01
m=4	249.484	0.570669	-1956.896741	-1957.059406	-1957.034895	2.09	2.98
m=6	253.684	0.568365	-1956.863893	-1957.042823	-1957.017183	3.70	4.19

[Fe(H$_2$O)(PPIXH$_2$)]$^+$							
species	S	ZPE	vacuum	water	octanol	spin, vacuum	spin, water
m=2	252.427	0.622776	-2034.307777	-2034.396009	-2034.401761	2.06	2.05
m=4	252.011	0.625153	-2034.326831	-2034.421676	-2034.426293	2.83	2.88
m=6	253.96	0.623069	-2034.311824	-2034.411331	-2034.413984	4.06	4.14

[Fe(H$_2$O)(PPIXH)]							
species	S	ZPE	vacuum	water	octanol	spin, vacuum	spin, water
m=2	249.806	0.607203	-2033.866910	-2033.949115	-2033.948535	2.07	2.04
m=4	248.854	0.611133	-2033.884317	-2033.972648	-2033.973066	2.82	2.88
m=6	253.041	0.606687	-2033.868734	-2033.963909	-2033.960988	3.97	4.15

[Fe(H_2O)(PPIX)]$^-$							
species	S	ZPE	vacuum	water	octanol	spin, vacuum	spin, water
m=2	263.04	0.593713	-2033.325556	-2033.477088	-2033.457429	2.07	2.03
m=4	264.929	0.593762	-2033.325194	-2033.501413	-2033.480049	2.10	2.93
m=6	268.52	0.591553	-2033.322115	-2033.489858	-2033.468288	3.78	4.16

[Fe(OH)(PPIXH_2)]							
species	S	ZPE	vacuum	water	octanol	spin, vacuum	spin, water
m=2	245.41	0.613599	-2033.900080	-2033.953237	-2033.957022	1.00	1.02
m=4	248.747	0.612136	-2033.905882	-2033.960573	-2033.954219	2.59	2.71
m=6	252.319	0.610280	-2033.910345	-2033.961671	-2033.965360	4.02	4.06

[Fe(OH)(PPIXH)]$^-$							
species	S	ZPE	vacuum	water	octanol	spin, vacuum	spin, water
m=2	243.294	0.599223	-2033.386855	-2033.504528	-2033.498288	1.00	1.02
m=4	246.48	0.597882	-2033.393943	-2033.512306	-2033.505802	2.60	2.71
m=6	249.48	0.596147	-2033.398109	-2033.513289	-2033.507303	4.02	4.06

[Fe(OH)(PPIX)]$^{2-}$							
species	S	ZPE	vacuum	water	octanol	spin, vacuum	spin, water
m=2	254.584	0.585016	-2032.742072	-2033.018828	-2032.992956	1.00	1.01
m=4	257.13	0.583694	-2032.749474	-2033.026902	-2033.000729	2.61	2.71
m=6	262.47	0.582183	-2032.753671	-2033.028138	-2033.002326	4.02	4.06

[Fe(OAc)(PPIXH_2)]							
species	S	ZPE	vacuum	water	octanol	spin, vacuum	spin, water
m=2	265.402	0.651236	-2186.539044	-2186.592372	-2186.596541	1.12	1.10
m=4	268.901	0.650898	-2186.551663	-2186.608656	-2186.611679	2.72	2.80
m=6	273.19	0.649198	-2186.550360	-2186.605075	-2186.608173	4.06	4.10

[Fe(OAc)(PPIXH)]$^-$							
species	S	ZPE	vacuum	water	octanol	spin, vacuum	spin, water
m=2	263.863	0.636992	-2186.026410	-2186.143394	-2186.137787	1.06	1.06
m=4	266.902	0.636568	-2186.040462	-2186.160373	-2186.153791	2.73	2.80
m=6	270.928	0.634884	-2186.038952	-2186.156135	-2186.149745	4.06	4.10

[Fe(OAc)(PPIX)]$^{2-}$							
species	S	ZPE	vacuum	water	octanol	spin, vacuum	spin, water
m=2	273.048	0.622725	-2185.382599	-2185.658833	-2185.633514	1.11	1.09
m=4	276.923	0.622324	-2185.398287	-2185.675413	-2185.649484	2.75	2.80
m=6	279.989	0.620702	-2185.396523	-2185.672018	-2185.645421	4.06	4.10

[Fe(MeNH$_2$)(PPIXH$_2$)]$^{+}$

species	S	ZPE	vacuum	water	octanol	spin, vacuum	spin, water
m=2	255.391	0.669431	-2053.752729	-2053.840823	-2053.847368	1.14	1.14
m=4	258.378	0.668790	-2053.766715	-2053.850829	-2053.858259	2.76	2.79
m=6	260.558	0.666889	-2053.753964	-2053.840920	-2053.847820	4.06	4.11

[Fe(MeNH$_2$)(PPIXH)]							
species	S	ZPE	vacuum	water	octanol	spin, vacuum	spin, water
m=2	253.522	0.655432	-2053.309929	-2053.392098	-2053.394239	1.16	1.15
m=4	255.21	0.654726	-2053.324055	-2053.401802	-2053.405132	2.76	2.79
m=6	258.053	0.652653	-2053.311010	-2053.391921	-2053.394558	4.06	4.11

[Fe(MeNH$_2$)(PPIX)]$^{-}$							
species	S	ZPE	vacuum	water	octanol	spin, vacuum	spin, water
m=2	268.863	0.636876	-2052.756228	-2052.910165	-2052.893487	2.05	1.31
m=4	270.165	0.637136	-2052.756801	-2052.930065	-2052.914563	2.15	2.83
m=6	277.09	0.634634	-2052.755890	-2052.919845	-2052.903362	3.80	4.13

[Fe(Cl)(PPIXH$_2$)]							
species	S	ZPE	vacuum	water	octanol	spin, vacuum	spin, water
m=2	246.063	0.601666	-1973.053269	-1973.100276	-1973.108789	1.24	1.20
m=4	248.321	0.601620	-1973.069158	-1973.118582	-1973.126851	2.62	2.72
m=6	250.599	0.599833	-1973.066154	-1973.112018	-1973.120735	3.97	4.00

[Fe(Cl)(PPIXH)]$^{-}$							
species	S	ZPE	vacuum	water	octanol	spin, vacuum	spin, water
m=2	244.689	0.587173	-1972.541722	-1972.651601	-1972.650433	1.23	1.19
m=4	246.119	0.587228	-1972.557836	-1972.670058	-1972.668556	2.63	2.72
m=6	248.174	0.585433	-1972.554824	-1972.663389	-1972.662342	3.97	4.00

[Fe(Cl)(PPIX)]$^{2-}$							
species	S	ZPE	vacuum	water	octanol	spin, vacuum	spin, water
m=2	253.696	0.573024	-1971.897188	-1972.165465	-1972.144651	1.24	1.20
m=4	254.768	0.573095	-1971.914447	-1972.184424	-1972.163186	2.64	2.72
m=6	258.408	0.571346	-1971.911612	-1972.178378	-1972.157382	3.97	4.01

Table S6. Calculated energies of iron(III) ferriprotoporphyrin complexes and free ligands (kcal mol^{-1}), computed *in vacuo*, and in water and *n*-octanol solvents for **method 2**.

Single point calculations were run at the method 1 geometries, using OPBE/6-311+G(d,p) and the SMD solvent method. Energies of the free ligands are given in Table S2.

$[Fe(PPIXH_2)]^+$					
species	vacuum	water	octanol	Fe spin, vacuum	Fe spin, water
m=4	-3098.313821	-3098.404576	-3098.407279	2.79	2.95
m=6	-3098.290442	-3098.390472	-3098.691162	4.12	4.32

[Fe(PPIXH)]					
species	vacuum	water	octanol	Fe spin, vacuum	Fe spin, water
m=4	-3097.869204	-3097.946087	-3097.943268	2.64	2.99
m=6	-3097.854026	-3097.935407	-3097.930859	4.08	4.32

$[Fe(PPIX)]^-$					
species	vacuum	water	octanol	Fe spin, vacuum	Fe spin, water
m=4	-3097.333663	-3097.480989	-3097.462183	2.40	3.00
m=6	-3097.322202	-3097.470277	-3097.450878	3.97	4.32

$[Fe(H_2O)(PPIXH_2)]^+$					
species	vacuum	water	octanol	Fe spin, vacuum	Fe spin, water
m=4	-3174.741488	-3174.826026	-3174.833150	2.82	2.88
m=6	-3174.729911	-3174.819622	-3174.824676	4.13	4.22

$[Fe(H_2O)(PPIXH)]$					
species	vacuum	water	octanol	Fe spin, vacuum	Fe spin, water
m=4	-3174.293415	-3174.363926	-3174.367846	2.75	2.88
m=6	-3174.285554	-3174.361620	-3174.362182	4.09	4.23

[Fe(H_2O)(PPIX)]$^-$					
species	vacuum	water	octanol	Fe spin, vacuum	Fe spin, water
m=4	-3173.755031	-3173.904527	-3173.889217	2.50	2.97
m=6	-3173.747807	-3173.895547	-3173.879793	3.98	4.24

[Fe(OH)(PPIXH_2)]					
species	vacuum	water	octanol	Fe spin, vacuum	Fe spin, water
m=4	-3174.316519	-3174.358863	-3174.365520	2.63	2.70
m=6	-3174.324282	-3174.364061	-3174.370848	4.09	4.12

[Fe(OH)(PPIXH)]$^-$					
species	vacuum	water	octanol	Fe spin, vacuum	Fe spin, water
m=4	-3173.795154	-3173.896573	-3173.894241	2.62	2.70
m=6	-3173.802756	-3173.901698	-3173.899651	4.09	4.12

[Fe(OH)(PPIX)]$^{2-}$					
species	vacuum	water	octanol	Fe spin, vacuum	Fe spin, water
m=4	-3173.162740	-3173.415173	-3173.394507	2.74	2.70
m=6	-3173.172114	-3173.420677	-3173.400093	4.01	4.13

[Fe(OAc)(PPIXH_2)]					
species	vacuum	water	octanol	Fe spin, vacuum	Fe spin, water
m=4	-3326.955811	-3327.000192	-3327.006630	2.67	2.73
m=6	-3326.960584	-3327.002881	-3327.009315	4.09	4.12

[Fe(OAc)(PPIXH)]$^-$					
species	vacuum	water	octanol	Fe spin, vacuum	Fe spin, water
m=4	-3326.435484	-3326.538091	-3326.535685	2.69	2.74
m=6	-3326.439812	-3326.540021	-3326.537726	4.08	4.12

[Fe(OAc)(PPIX)]$^{2-}$					
species	vacuum	water	octanol	Fe spin, vacuum	Fe spin, water
m=4	-3325.807156	-3326.057615	-3326.037272	2.88	2.77
m=6	-3325.814368	-3326.060431	-3326.039312	3.99	4.13

[Fe(MeNH$_2$)(PPIXH$_2$)]$^{+}$					
species	vacuum	water	octanol	Fe spin, vacuum	Fe spin, water
m=4	-3194.185501	-3194.261504	-3194.271003	2.72	2.78
m=6	-3194.176989	-3194.256035	-3194.264986	4.13	4.19

[Fe(MeNH$_2$)(PPIXH)]					
species	vacuum	water	octanol	Fe spin, vacuum	Fe spin, water
m=4	-3193.736380	-3193.799261	-3193.805617	2.65	2.78
m=6	-3193.728899	-3193.793700	-3193.799351	4.05	4.19

[Fe(MeNH$_2$)(PPIX)]$^{-}$					
species	vacuum	water	octanol	Fe spin, vacuum	Fe spin, water
m=4	-3193.191775	-3193.336136	-3193.325450	2.38	2.84
m=6	-3193.188431	-3193.330676	-3193.319110	4.03	4.03

[Fe(Cl)(PPIXH$_2$)]					
species	vacuum	water	octanol	Fe spin, vacuum	Fe spin, water
m=4	-3558.732052	-3558.773194	-3558.783417	2.81	2.83
m=6	-3558.735937	-3558.773204	-3558.783960	4.10	4.09

[Fe(Cl)(PPIXH)]$^{-}$					
species	vacuum	water	octanol	Fe spin, vacuum	Fe spin, water
m=4	-3558.211254	-3558.310603	-3558.311869	2.82	2.84
m=6	-3558.214866	-3558.310256	-3558.312051	4.10	4.09

[Fe(Cl)(PPIX)]$^{2-}$					
species	vacuum	water	octanol	Fe spin, vacuum	Fe spin, water
m=4	-3557.581018	-3557.828746	-3557.811661	2.98	2.85
m=6	-3557.588112	-3557.828893	-3557.812094	4.02	4.09

Table S7. Calculated energies of iron(III) ferriprotoporphyrin complexes and free ligands (kcal mol^{-1}), computed *in vacuo*, and in water and *n*-octanol solvents for **method 3**.

Single point calculations were run at the method 1 geometries, using B3LYP/6-311+G(d,p) and the SMD solvent method. Energies of the free ligands are given in Table S3.

$[Fe(PPIXH_2)]^+$					
species	vacuum	water	octanol	Fe spin, vacuum	Fe spin, water
m=4	-3098.903922	-3099.000673	-3099.002392	2.85	3.00

[Fe(PPIXH)]					
species	vacuum	water	octanol	Fe spin, vacuum	Fe spin, water
m=4	-3098.451755	-3098.548643	-3098.544210	2.57	3.04

$[Fe(PPIX)]^-$					
species	vacuum	water	octanol	Fe spin, vacuum	Fe spin, water
m=4	-3097.918706	-3098.084706	-3098.063672	2.09	3.05

$[Fe(H_2O)(PPIXH_2)]^+$					
species	vacuum	water	octanol	Fe spin, vacuum	Fe spin, water
m=4	-3175.383254	-3175.471885	-3175.478325	2.87	2.93
H_2O	-76.457365	-76.470876	-76.469064		

$[Fe(H_2O)(PPIXH)]$					
species	vacuum	water	octanol	Fe spin, vacuum	Fe spin, water
m=4	-3174.938284	-3175.017006	-3175.019854	2.87	2.93
m=6	-3174.918842	-3175.010553	-3175.009662	4.10	4.30

$[Fe(H_2O)(PPIX)]^-$					
species	vacuum	water	octanol	Fe spin, vacuum	Fe spin, water
m=4	-3174.381589	-3174.556240	-3174.539032	2.20	3.02

[Fe(OH)(PPIXH$_2$)]					
species	vacuum	water	octanol	Fe spin, vacuum	Fe spin, water
m=6	-3174.972291	-3175.014633	-3175.020790	4.14	4.19
OH^-	-75.826120	-75.977213	-75.957477		

[Fe(OH)(PPIXH)]$^-$					
species	vacuum	water	octanol	Fe spin, vacuum	Fe spin, water
m=6	-3174.456303	-3174.559489	-3174.556553	4.14	4.19

[Fe(OH)(PPIX)]$^{2-}$					
species	vacuum	water	octanol	Fe spin, vacuum	Fe spin, water
m=6	-3173.821643	-3174.080505	-3174.058769	4.15	4.20

[Fe(OAc)(PPIXH$_2$)]					
species	vacuum	water	octanol	Fe spin, vacuum	Fe spin, water
m=4	-3327.680164	-3327.727836	-3327.733640	2.74	2.79
m=6	-3327.681359	-3327.727229	-3327.732874	4.14	4.18
OAc^-	-228.599114	-228.713171	-228.699278		

[Fe(OAc)(PPIXH)]$^-$					
species	vacuum	water	octanol	Fe spin, vacuum	Fe spin, water
m=4	-3327.165029	-3327.272641	-3327.269346	2.75	2.80
m=6	-3327.165870	-3327.271273	-3327.267945	4.14	4.17

[Fe(OAc)(PPIX)]$^{2-}$					
species	vacuum	water	octanol	Fe spin, vacuum	Fe spin, water
m=4	-3326.532734	-3326.793730	-3326.772150	2.78	2.81
m=6	-3326.533355	-3326.793449	-3326.770955	4.14	4.18

$[Fe(MeNH_2)(PPIXH_2)]^+$					
species	vacuum	water	octanol	Fe spin, vacuum	Fe spin, water
m=4	-3194.834587	-3194.913970	-3194.922968	2.78	2.83
$MeNH_2$	-95.892159	-95.897352	-95.897191		

$[Fe(MeNH_2)(PPIXH)]$					
species	vacuum	water	octanol	Fe spin, vacuum	Fe spin, water
m=4	-3194.389145	-3194.458877	-3194.464379	2.77	2.82

$[Fe(MeNH_2)(PPIX)]^-$					
species	vacuum	water	octanol	Fe spin, vacuum	Fe spin, water
m=4	-3193.823555	-3193.995395	-3193.983409	2.23	2.88
m=6	-3193.819484	-3193.986689	-3193.973628	3.84	4.23

$[Fe(Cl)(PPIXH_2)]$					
species	vacuum	water	octanol	Fe spin, vacuum	Fe spin, water
m=4	-3559.378679	-3559.421848	-3559.431807	2.82	2.87
m=6	-3559.379609	-3559.418486	-3559.429026	4.13	4.15
Cl^-	-460.303727	-460.407712	-460.401115		

$[Fe(Cl)(PPIXH)]^-$					
species	vacuum	water	octanol	Fe spin, vacuum	Fe spin, water
m=4	-3558.863335	-3558.966412	-3558.967125	2.83	2.87
m=6	-3558.864024	-3558.962871	-3558.964080	4.13	4.14

$[Fe(Cl)(PPIX)]^{2-}$					
species	vacuum	water	octanol	Fe spin, vacuum	Fe spin, water
m=4	-3558.229256	-3558.486423	-3558.468508	2.83	2.87
m=6	-3558.229960	-3558.483405	-3558.465823	4.14	4.15

Table S8. Calculated ground state geometries (method 3, water) of iron(III) ferriprotoporphyrin complexes.

1. $[Fe(PPIXH_2)]^+$ (m=4)

Fe	0	1.097743	-0.046021	-0.210451
N	0	-0.442065	-1.271201	-0.334773
N	0	2.317861	-1.598015	-0.117245
N	0	-0.117655	1.500650	-0.390772
N	0	2.625370	1.186081	0.022737
C	0	-1.794179	-0.933469	-0.528025
C	0	-2.638197	-2.110325	-0.450544
C	0	-1.797389	-3.194956	-0.249031
C	0	-0.445413	-2.674820	-0.207032
C	0	1.981811	-2.969160	-0.115939
C	0	3.163828	-3.796717	-0.092754
C	0	4.260021	-2.930871	-0.063655
C	0	3.723011	-1.580524	-0.061789
C	0	3.990350	0.848137	0.139484
C	0	4.803266	2.022631	0.345830
C	0	3.932427	3.116187	0.363501
C	0	2.598819	2.588013	0.133804
C	0	0.204663	2.865469	-0.285700
C	0	-1.496023	1.486643	-0.689084
C	0	-2.017424	2.837213	-0.804012
C	0	-0.958589	3.693310	-0.529590
C	0	1.462762	3.371309	-0.001302
C	0	4.499530	-0.440541	0.063992
C	0	0.685557	-3.467286	-0.116697
C	0	-2.274248	0.343578	-0.771681
H	0	1.562241	4.444729	0.094671
H	0	5.570887	-0.564291	0.151092
H	0	0.549051	-4.540047	-0.061812
H	0	-3.326088	0.461404	-0.997495
C	0	-2.165228	-4.645865	-0.103068
C	0	-0.956035	5.196841	-0.490434
C	0	-3.431821	3.230782	-1.173097
C	0	-4.146503	-2.093560	-0.484380
C	0	3.172349	-5.298675	-0.135926
C	0	5.691566	-3.236732	-0.068462
C	0	6.279573	-4.381736	0.359337
C	0	6.300104	2.031418	0.473891
C	0	4.228596	4.540348	0.523516
C	0	5.315794	5.082621	1.126798
C	0	-4.719026	-1.797557	0.940342
C	0	-4.460416	3.250830	-0.003540
C	0	-5.223615	1.944444	0.154693
C	0	-6.221990	-1.641105	0.963431
O	0	-6.851422	-0.649113	1.385583
O	0	-6.876394	-2.743414	0.478310
O	0	-5.866463	1.841680	1.345280
O	0	-5.265537	1.042790	-0.714923
H	0	-1.697726	-5.259920	-0.884502
H	0	-3.246735	-4.790575	-0.179114
H	0	-1.844248	-5.049543	0.866543
H	0	-0.247413	5.618882	-1.215475
H	0	-0.673345	5.572212	0.502383
H	0	-1.943867	5.604727	-0.721819
H	0	-3.819226	2.564997	-1.952994
H	0	-3.399189	4.233557	-1.612317

H	0	-4.535826	-3.056082	-0.830092
H	0	-4.516053	-1.327764	-1.173117
H	0	2.263295	-5.703036	-0.591621
H	0	3.257970	-5.731961	0.870804
H	0	4.025137	-5.662876	-0.720036
H	0	6.344388	-2.457566	-0.460821
H	0	5.724985	-5.202870	0.802402
H	0	7.357141	-4.506590	0.295466
H	0	6.760551	1.163812	-0.008745
H	0	6.615337	2.026319	1.527099
H	0	6.722621	2.930221	0.010957
H	0	3.490713	5.231979	0.119103
H	0	6.090039	4.487895	1.600772
H	0	5.435942	6.161241	1.180961
H	0	-4.283864	-0.880206	1.344057
H	0	-4.457038	-2.623789	1.614665
H	0	-5.215363	4.027016	-0.193212
H	0	-3.997842	3.505364	0.956191
H	0	-7.855521	-2.633168	0.498673
H	0	-6.345911	0.959082	1.448201

2. [Fe(PPIXH)] (m=4)

Fe	0	1.066927	-0.039952	-0.221758
N	0	-0.519088	-1.241788	-0.406699
N	0	2.268053	-1.645471	-0.111454
N	0	-0.131075	1.560233	-0.354722
N	0	2.653562	1.168049	0.001220
C	0	-1.845882	-0.865410	-0.564952
C	0	-2.730923	-2.043314	-0.567420
C	0	-1.911251	-3.145276	-0.437285
C	0	-0.543044	-2.641992	-0.352695
C	0	1.891987	-2.991870	-0.153589
C	0	3.060196	-3.865444	-0.065835
C	0	4.165127	-3.035384	0.041947
C	0	3.652941	-1.654976	0.011791
C	0	3.989695	0.789178	0.136956
C	0	4.854326	1.957846	0.295980
C	0	4.024962	3.067800	0.265478
C	0	2.656788	2.559710	0.066593
C	0	0.234876	2.897227	-0.259683
C	0	-1.509900	1.574991	-0.594576
C	0	-2.014257	2.958226	-0.660223
C	0	-0.925791	3.774586	-0.436206
C	0	1.531458	3.366930	-0.043857
C	0	4.456064	-0.524404	0.130792
C	0	0.581414	-3.454692	-0.250364
C	0	-2.306276	0.444850	-0.710757
H	0	1.663110	4.439449	0.033399
H	0	5.521452	-0.674926	0.253998
H	0	0.421602	-4.526736	-0.242639
H	0	-3.360373	0.587015	-0.912453
C	0	-2.300606	-4.597465	-0.372887
C	0	-0.865872	5.277123	-0.380257
C	0	-3.437651	3.383005	-0.942087
C	0	-4.235320	-1.991949	-0.565290
C	0	3.022272	-5.367000	-0.128760
C	0	5.586853	-3.372443	0.129806

C	0	6.127150	-4.527964	0.592214
C	0	6.351433	1.913993	0.424473
C	0	4.356829	4.490293	0.358347
C	0	5.451254	5.039561	0.942833
C	0	-4.741439	-1.791248	0.895933
C	0	-4.438977	3.234272	0.242917
C	0	-5.235243	1.930333	0.197518
C	0	-6.291596	-1.734117	0.981779
O	0	-6.878135	-0.652906	1.345718
O	0	-6.884818	-2.844116	0.681640
O	0	-5.789820	1.599464	1.374232
O	0	-5.342162	1.234877	-0.846206
H	0	-1.836936	-5.176182	-1.183793
H	0	-3.384442	-4.718182	-0.461017
H	0	-1.993257	-5.057711	0.576376
H	0	-0.181043	5.683501	-1.137490
H	0	-0.516410	5.628860	0.600467
H	0	-1.850293	5.721677	-0.553996
H	0	-3.843297	2.809919	-1.785336
H	0	-3.422819	4.433079	-1.254462
H	0	-4.655370	-2.924829	-0.956389
H	0	-4.615241	-1.173759	-1.185781
H	0	2.157763	-5.728768	-0.695617
H	0	2.968581	-5.815402	0.874189
H	0	3.925530	-5.757245	-0.612163
H	0	6.278760	-2.604790	-0.217942
H	0	5.527809	-5.335121	1.001974
H	0	7.204237	-4.674842	0.593874
H	0	6.776596	1.032675	-0.067842
H	0	6.669147	1.887244	1.477201
H	0	6.805324	2.801796	-0.031033
H	0	3.638792	5.175847	-0.092064
H	0	6.201931	4.449309	1.459228
H	0	5.600070	6.116345	0.938410
H	0	-4.343483	-0.864170	1.323811
H	0	-4.397629	-2.631438	1.511674
H	0	-5.175425	4.049441	0.204125
H	0	-3.946261	3.309901	1.217976
H	0	-6.288791	0.661231	1.375721

3. [Fe(PPIX)]$^{-}$ (m=4)

Fe	0	0.993913	0.053565	-0.212032
N	0	-0.375449	-1.393586	-0.435318
N	0	2.454165	-1.334624	-0.109830
N	0	-0.455124	1.432181	-0.330807
N	0	2.366634	1.515003	0.013547
C	0	-1.755065	-1.248848	-0.588690
C	0	-2.408441	-2.552843	-0.724597
C	0	-1.408016	-3.501407	-0.656092
C	0	-0.151713	-2.771864	-0.475353
C	0	2.306147	-2.720185	-0.195782
C	0	3.591486	-3.387453	-0.078412
C	0	4.546654	-2.387366	0.088513
C	0	3.820527	-1.116235	0.060008
C	0	3.748931	1.357430	0.173948
C	0	4.403212	2.647307	0.314990
C	0	3.400337	3.610778	0.243134

C	0	2.142683	2.886168	0.047825
C	0	-0.309471	2.818120	-0.259310
C	0	-1.823239	1.218282	-0.514145
C	0	-2.547090	2.489288	-0.570096
C	0	-1.602775	3.482311	-0.406146
C	0	0.891748	3.492553	-0.077514
C	0	4.416726	0.134549	0.196863
C	0	1.088700	-3.384167	-0.366316
C	0	-2.427590	-0.029644	-0.627898
H	0	0.843326	4.574194	-0.024123
H	0	5.489942	0.162661	0.343545
H	0	1.106433	-4.467136	-0.410371
H	0	-3.503446	-0.053993	-0.759110
C	0	-1.527993	-4.998810	-0.759426
C	0	-1.815290	4.972560	-0.374422
C	0	-4.032455	2.653537	-0.762183
C	0	-3.893007	-2.757301	-0.903468
C	0	3.811182	-4.873771	-0.158520
C	0	5.998015	-2.491332	0.231929
C	0	6.736143	-3.584820	0.557501
C	0	5.884568	2.862592	0.470073
C	0	3.495065	5.068956	0.303199
C	0	4.520135	5.825716	0.774998
C	0	-4.709362	-2.734760	0.419567
C	0	-4.839597	2.611861	0.564121
C	0	-6.268156	3.150049	0.379301
C	0	-4.731134	-4.098548	1.136235
O	0	-5.023981	-4.079319	2.410062
O	0	-4.512317	-5.186728	0.497323
O	0	-7.182303	2.691191	1.196133
O	0	-6.531683	4.029860	-0.512137
H	0	-1.185907	-5.358534	-1.742037
H	0	-2.563481	-5.316976	-0.605435
H	0	-0.920557	-5.502383	0.004656
H	0	-1.204364	5.485963	-1.130484
H	0	-1.548122	5.396777	0.604312
H	0	-2.863165	5.224475	-0.566068
H	0	-4.424648	1.883769	-1.439461
H	0	-4.250069	3.612510	-1.244739
H	0	-4.076018	-3.723968	-1.385402
H	0	-4.290961	-1.984103	-1.575296
H	0	2.965798	-5.386513	-0.628282
H	0	3.950497	-5.317931	0.838553
H	0	4.709969	-5.103480	-0.745433
H	0	6.552146	-1.569030	0.052625
H	0	6.294399	-4.547451	0.792590
H	0	7.820402	-3.521611	0.616137
H	0	6.460296	1.993659	0.134142
H	0	6.161864	3.055431	1.517454
H	0	6.214910	3.728524	-0.118046
H	0	2.628406	5.609266	-0.079102
H	0	5.415780	5.399851	1.215445
H	0	4.461943	6.911475	0.749155
H	0	-5.757515	-2.480698	0.201991
H	0	-4.338188	-1.975031	1.116901
H	0	-4.347222	3.247334	1.314876
H	0	-4.884693	1.601187	0.986626

4. $[Fe(OH_2)(PPIXH_2)]^+$ (m=4)

Fe	0	1.056882	-0.046904	-0.067249
O	0	0.868948	-0.049444	2.057842
H	0	1.418903	-0.604975	2.639804
H	0	0.286900	0.561113	2.545741
N	0	-0.498013	-1.249824	-0.398996
N	0	2.272475	-1.631539	-0.090841
N	0	-0.135042	1.533609	-0.313822
N	0	2.647859	1.163627	-0.094423
C	0	-1.834017	-0.882936	-0.605231
C	0	-2.695809	-2.054646	-0.614400
C	0	-1.876334	-3.154660	-0.424736
C	0	-0.519021	-2.649825	-0.304494
C	0	1.903921	-2.990800	-0.092195
C	0	3.070889	-3.844996	-0.057929
C	0	4.183998	-3.002927	-0.051222
C	0	3.675206	-1.639256	-0.075856
C	0	4.003010	0.797132	-0.045211
C	0	4.855221	1.965378	0.048969
C	0	4.010575	3.073065	0.090647
C	0	2.649532	2.561709	-0.010205
C	0	0.225048	2.886598	-0.217720
C	0	-1.511891	1.547544	-0.602004
C	0	-2.011466	2.912742	-0.673772
C	0	-0.930624	3.742703	-0.410860
C	0	1.515953	3.363185	-0.034896
C	0	4.478662	-0.507778	-0.052289
C	0	0.596257	-3.459399	-0.152710
C	0	-2.298762	0.416204	-0.758625
H	0	1.646125	4.434887	0.048093
H	0	5.550798	-0.649397	-0.008367
H	0	0.438024	-4.530260	-0.116251
H	0	-3.345960	0.558040	-0.991681
C	0	-2.264140	-4.606710	-0.351913
C	0	-0.891764	5.246419	-0.364303
C	0	-3.423026	3.340493	-1.016702
C	0	-4.202189	-2.018380	-0.702114
C	0	3.049885	-5.347861	-0.087407
C	0	5.609353	-3.340798	-0.065809
C	0	6.178082	-4.488400	0.379660
C	0	6.358187	1.943155	0.060100
C	0	4.343316	4.497969	0.167826
C	0	5.469434	5.041150	0.692304
C	0	-4.822820	-1.803467	0.716337
C	0	-4.457218	3.282530	0.146189
C	0	-5.248580	1.984180	0.190993
C	0	-6.323113	-1.624769	0.703473
O	0	-6.951414	-0.660648	1.188621
O	0	-6.977812	-2.670886	0.107804
O	0	-5.898136	1.794906	1.369323
O	0	-5.307003	1.159845	-0.750516
H	0	-1.767844	-5.195091	-1.135249
H	0	-3.342628	-4.736037	-0.482614
H	0	-1.992316	-5.052738	0.614354
H	0	-0.264593	5.658376	-1.166631
H	0	-0.486124	5.610689	0.588900
H	0	-1.891102	5.676011	-0.477024
H	0	-3.811124	2.733496	-1.843292
H	0	-3.383655	4.370919	-1.385039
H	0	-4.587742	-2.953605	-1.119735

H	0	-4.539218	-1.209010	-1.356851
H	0	2.131488	-5.738665	-0.536368
H	0	3.130599	-5.775552	0.922141
H	0	3.893385	-5.733608	-0.671342
H	0	6.274455	-2.585074	-0.482728
H	0	5.610925	-5.288303	0.845377
H	0	7.251748	-4.638586	0.305027
H	0	6.759218	1.065313	-0.456994
H	0	6.758102	1.933751	1.084222
H	0	6.760235	2.832589	-0.437813
H	0	3.603311	5.185182	-0.241515
H	0	6.249628	4.448281	1.159651
H	0	5.620550	6.117255	0.684046
H	0	-4.388884	-0.920390	1.191770
H	0	-4.594552	-2.674801	1.344937
H	0	-5.195814	4.087119	0.021116
H	0	-3.994895	3.446194	1.125762
H	0	-7.955030	-2.543338	0.103923
H	0	-6.403991	0.921135	1.391736

5. [Fe(OH$_2$)(PPIXH)] (m=4)

Fe	0	-1.023012	0.040413	-0.098970
O	0	-0.746147	0.052076	2.021213
H	0	-1.216193	0.652304	2.627473
H	0	0.020295	-0.389559	2.431210
N	0	0.543228	1.205125	-0.454036
N	0	-2.215038	1.651484	-0.116286
N	0	0.129910	-1.560637	-0.344071
N	0	-2.644437	-1.137154	-0.084870
C	0	1.876711	0.812339	-0.654854
C	0	2.767719	1.962829	-0.647787
C	0	1.965082	3.079145	-0.460557
C	0	0.598042	2.606240	-0.354696
C	0	-1.816694	3.001749	-0.130693
C	0	-2.964738	3.879613	-0.088092
C	0	-4.094761	3.061441	-0.060764
C	0	-3.616008	1.686998	-0.082226
C	0	-3.990742	-0.742610	-0.022883
C	0	-4.862430	-1.893597	0.094624
C	0	-4.038839	-3.016597	0.135949
C	0	-2.669875	-2.533329	0.012477
C	0	-0.253111	-2.904593	-0.218628
C	0	1.509143	-1.606361	-0.629637
C	0	1.987573	-2.982093	-0.666623
C	0	0.887065	-3.783424	-0.389122
C	0	-1.550834	-3.354834	-0.017457
C	0	-4.441281	0.571415	-0.037023
C	0	-0.498887	3.440250	-0.201898
C	0	2.320230	-0.494608	-0.803545
H	0	-1.696747	-4.423165	0.082182
H	0	-5.509826	0.734109	0.021077
H	0	-0.313191	4.506862	-0.167194
H	0	3.373604	-0.662362	-1.020512
C	0	2.391656	4.518579	-0.362748
C	0	0.824673	-5.284372	-0.297847
C	0	3.397700	-3.435920	-0.960376
C	0	4.270876	1.898043	-0.679232
C	0	-2.911359	5.382089	-0.127413

C	0	-5.512730	3.428503	-0.056448
C	0	-6.056347	4.598482	0.362653
C	0	-6.365041	-1.843158	0.128164
C	0	-4.396456	-4.433997	0.232506
C	0	-5.535623	-4.957838	0.749571
C	0	4.831997	1.630834	0.751828
C	0	4.421637	-3.257196	0.202022
C	0	5.189244	-1.914278	0.139547
C	0	6.369705	1.727985	0.776245
O	0	7.043843	0.631981	1.163469
O	0	6.928239	2.806824	0.474742
O	0	5.743834	-1.522731	1.251579
O	0	5.218126	-1.271765	-0.971446
H	0	1.968369	5.121246	-1.178682
H	0	3.480237	4.606170	-0.417386
H	0	2.071805	4.974596	0.584245
H	0	0.202545	-5.713273	-1.096092
H	0	0.402386	-5.613429	0.661340
H	0	1.821657	-5.725000	-0.384047
H	0	3.804344	-2.878856	-1.814120
H	0	3.360736	-4.492997	-1.249191
H	0	4.688838	2.844278	-1.038965
H	0	4.630268	1.100333	-1.337546
H	0	-1.980615	5.747711	-0.572133
H	0	-2.988732	5.818970	0.878769
H	0	-3.742246	5.782470	-0.720270
H	0	-6.199217	2.671734	-0.436157
H	0	-5.467866	5.403348	0.791603
H	0	-7.129135	4.762914	0.302533
H	0	-6.755192	-0.951296	-0.373389
H	0	-6.750024	-1.836835	1.158360
H	0	-6.791490	-2.719597	-0.373409
H	0	-3.659888	-5.137406	-0.155526
H	0	-6.314794	-4.349603	1.198314
H	0	-5.697670	-6.032634	0.754789
H	0	4.496220	0.656227	1.116224
H	0	4.454806	2.407386	1.432001
H	0	5.178029	-4.051845	0.135075
H	0	3.957004	-3.350676	1.190363
H	0	6.501416	-0.282054	1.210436

6. [Fe(OH_2)(PPIX)]$^-$ (m=4)

Fe	0	0.940075	0.092300	-0.186240
O	0	0.686892	-0.294191	2.085088
H	0	1.380065	-0.935281	2.339135
H	0	-0.203272	-0.666972	2.245288
N	0	-0.363098	-1.416000	-0.517193
N	0	2.481592	-1.232324	-0.182698
N	0	-0.567589	1.404388	-0.371534
N	0	2.263488	1.611511	-0.030191
C	0	-1.745260	-1.330953	-0.681191
C	0	-2.338458	-2.662578	-0.817485
C	0	-1.295856	-3.566660	-0.754687
C	0	-0.072961	-2.781841	-0.566941
C	0	2.391529	-2.621660	-0.299591
C	0	3.709584	-3.231051	-0.235763
C	0	4.624282	-2.190542	-0.077051
C	0	3.840338	-0.953061	-0.054526

C	0	3.652013	1.515807	0.102931
C	0	4.247323	2.834839	0.257746
C	0	3.197974	3.749095	0.222490
C	0	1.972484	2.966005	0.032558
C	0	-0.479309	2.791968	-0.281664
C	0	-1.918589	1.134397	-0.592268
C	0	-2.694337	2.376299	-0.653920
C	0	-1.796756	3.405082	-0.451676
C	0	0.691881	3.513614	-0.076983
C	0	4.378314	0.325170	0.091292
C	0	1.198257	-3.334569	-0.463781
C	0	-2.468079	-0.138463	-0.723523
H	0	0.594568	4.591313	-0.007097
H	0	5.452682	0.403708	0.210890
H	0	1.266158	-4.415002	-0.525108
H	0	-3.539841	-0.207387	-0.873672
C	0	-1.361935	-5.067283	-0.866050
C	0	-2.072375	4.884691	-0.407313
C	0	-4.179410	2.480264	-0.884408
C	0	-3.813952	-2.941200	-0.960048
C	0	3.997666	-4.702994	-0.359842
C	0	6.082420	-2.229906	0.016190
C	0	6.884611	-3.296909	0.272660
C	0	5.719209	3.118774	0.391225
C	0	3.223211	5.208460	0.310890
C	0	4.219673	6.006010	0.777342
C	0	-4.598014	-2.861942	0.380952
C	0	-5.017446	2.380605	0.420240
C	0	-6.467138	2.850108	0.204398
C	0	-4.360146	-4.088780	1.280561
O	0	-4.412366	-3.889748	2.569986
O	0	-4.154063	-5.244234	0.764125
O	0	-7.371157	2.322710	0.993965
O	0	-6.752799	3.730084	-0.676826
H	0	-1.180612	-5.397647	-1.900602
H	0	-2.343285	-5.432799	-0.545796
H	0	-0.611475	-5.553347	-0.229714
H	0	-1.468125	5.432534	-1.144431
H	0	-1.842389	5.307158	0.581584
H	0	-3.125865	5.095103	-0.617656
H	0	-4.519824	1.705363	-1.583493
H	0	-4.427016	3.436930	-1.356578
H	0	-3.962328	-3.945800	-1.370189
H	0	-4.263273	-2.232852	-1.670853
H	0	3.151112	-5.250038	-0.786620
H	0	4.223614	-5.157889	0.616444
H	0	4.867834	-4.876286	-1.006679
H	0	6.584806	-1.274656	-0.142086
H	0	6.499872	-4.290256	0.478071
H	0	7.965721	-3.180619	0.300018
H	0	6.329827	2.284533	0.029476
H	0	6.006000	3.306206	1.437185
H	0	5.997631	4.010080	-0.185994
H	0	2.322853	5.712842	-0.041594
H	0	5.144543	5.616500	1.190208
H	0	4.107282	7.087855	0.775545
H	0	-5.676887	-2.826190	0.167424
H	0	-4.350636	-1.954523	0.943461
H	0	-4.576810	3.029804	1.191163
H	0	-5.022156	1.363057	0.828542

7. [Fe(OH)(PPIXH$_2$)] (m=6)

Fe	0	1.021487	-0.050150	0.247727
O	0	0.803408	-0.083215	2.062419
H	0	1.304167	0.252750	2.828474
N	0	-0.545033	-1.274910	-0.405794
N	0	2.304087	-1.686920	-0.116831
N	0	-0.148356	1.591943	-0.358042
N	0	2.698254	1.189760	-0.019000
C	0	-1.863680	-0.880702	-0.580352
C	0	-2.733825	-2.056955	-0.638266
C	0	-1.914642	-3.166529	-0.526955
C	0	-0.545966	-2.666245	-0.393638
C	0	1.916182	-3.023337	-0.191015
C	0	3.087638	-3.890872	-0.152498
C	0	4.199633	-3.057314	-0.051074
C	0	3.688995	-1.680531	-0.035568
C	0	4.034452	0.794109	0.061330
C	0	4.901288	1.964366	0.128102
C	0	4.069945	3.082627	0.083506
C	0	2.696228	2.579224	-0.026480
C	0	0.242220	2.924165	-0.321375
C	0	-1.518350	1.588468	-0.598548
C	0	-2.012737	2.966254	-0.714231
C	0	-0.917581	3.793108	-0.532578
C	0	1.552394	3.377719	-0.143605
C	0	4.481613	-0.531794	0.061607
C	0	0.592467	-3.469333	-0.296193
C	0	-2.307013	0.440579	-0.701647
H	0	1.693752	4.452952	-0.121999
H	0	5.552581	-0.680782	0.142263
H	0	0.434724	-4.542808	-0.319519
H	0	-3.358995	0.586514	-0.911847
C	0	-2.304359	-4.621214	-0.526256
C	0	-0.858509	5.297897	-0.551043
C	0	-3.437974	3.384626	-1.005944
C	0	-4.240933	-2.008302	-0.693163
C	0	3.061644	-5.391764	-0.252209
C	0	5.622694	-3.396812	-0.008119
C	0	6.184877	-4.581321	0.343574
C	0	6.404229	1.930654	0.186628
C	0	4.415464	4.505190	0.092587
C	0	5.557958	5.079191	0.548419
C	0	-4.826748	-1.807653	0.744361
C	0	-4.426017	3.289801	0.195215
C	0	-5.269618	2.024519	0.195883
C	0	-6.324484	-1.641042	0.769543
O	0	-6.957457	-0.667168	1.232500
O	0	-6.996743	-2.711557	0.226137
O	0	-5.853875	1.778046	1.404018
O	0	-5.431899	1.271520	-0.790535
H	0	-1.807042	-5.171534	-1.336993
H	0	-3.384311	-4.744915	-0.660573
H	0	-2.028962	-5.113062	0.417193
H	0	-0.162815	5.665428	-1.318125
H	0	-0.520359	5.698789	0.414898
H	0	-1.839800	5.736028	-0.760317
H	0	-3.849081	2.785128	-1.827827
H	0	-3.426847	4.422290	-1.357699
H	0	-4.647426	-2.934151	-1.113641
H	0	-4.584674	-1.183589	-1.326940

H	0	2.140110	-5.752979	-0.720982
H	0	3.134980	-5.867163	0.737177
H	0	3.905483	-5.756534	-0.851038
H	0	6.305204	-2.595391	-0.293600
H	0	5.603720	-5.432873	0.682680
H	0	7.264314	-4.709904	0.320924
H	0	6.806245	0.993796	-0.213626
H	0	6.774483	2.032090	1.217614
H	0	6.834694	2.754339	-0.396006
H	0	3.657140	5.175475	-0.313552
H	0	6.360102	4.511533	1.009281
H	0	5.698725	6.155648	0.488496
H	0	-4.380340	-0.927937	1.214263
H	0	-4.571144	-2.683606	1.355107
H	0	-5.135474	4.129802	0.163727
H	0	-3.909163	3.362100	1.158032
H	0	-6.366485	0.910000	1.409802
H	0	-7.971224	-2.568309	0.244813

8. [Fe(OH)(PPIXH)]$^{-}$ (m=6)

Fe	0	-1.018583	0.043785	0.273488
N	0	0.589852	1.222921	-0.354112
N	0	-2.257235	1.710919	-0.110993
N	0	0.129882	-1.619619	-0.290615
N	0	-2.722505	-1.157570	-0.033460
C	0	1.904032	0.802678	-0.533445
C	0	2.804442	1.959019	-0.598983
C	0	2.005988	3.083723	-0.482586
C	0	0.625477	2.617475	-0.345537
C	0	-1.832218	3.035856	-0.169680
C	0	-2.979370	3.931713	-0.146812
C	0	-4.117185	3.126154	-0.074204
C	0	-3.643248	1.737161	-0.056508
C	0	-4.048477	-0.730398	0.023264
C	0	-4.941080	-1.879686	0.087572
C	0	-4.133132	-3.017213	0.073395
C	0	-2.747010	-2.542873	-0.014998
C	0	-0.291465	-2.944698	-0.239294
C	0	1.504374	-1.653428	-0.518149
C	0	1.971806	-3.045129	-0.598751
C	0	0.853117	-3.840522	-0.413830
C	0	-1.614460	-3.366078	-0.087932
C	0	-4.464226	0.606247	0.015407
C	0	-0.492575	3.446429	-0.254719
C	0	2.321668	-0.527222	-0.640884
H	0	-1.776006	-4.438253	-0.051875
H	0	-5.533023	0.779019	0.077047
H	0	-0.303687	4.514968	-0.273925
H	0	3.372611	-0.700441	-0.848111
C	0	2.431329	4.528455	-0.479502
C	0	0.761146	-5.344084	-0.399007
C	0	3.393390	-3.491873	-0.855542
C	0	4.309407	1.883935	-0.672625
C	0	-2.914848	5.433065	-0.225675
C	0	-5.530057	3.499326	-0.051025
C	0	-6.080526	4.718976	0.187828
C	0	-6.443951	-1.815314	0.126961

C	0	-4.505416	-4.430872	0.098871
C	0	-5.690412	-4.984197	0.468366
C	0	4.939138	1.640878	0.734369
C	0	4.410626	-3.221348	0.293914
C	0	5.281479	-1.959798	0.070134
C	0	6.475352	1.735556	0.690384
O	0	7.168845	0.621082	0.973048
O	0	7.027423	2.830557	0.419198
O	0	5.904116	-1.517476	1.133599
O	0	5.329205	-1.424169	-1.090787
H	0	1.984237	5.084381	-1.316666
H	0	3.518956	4.615658	-0.564488
H	0	2.130915	5.036326	0.448152
H	0	0.113887	-5.719591	-1.205107
H	0	0.347041	-5.712263	0.550666
H	0	1.747477	-5.801400	-0.526633
H	0	3.791895	-2.980323	-1.742575
H	0	3.379624	-4.565344	-1.082245
H	0	4.717759	2.820739	-1.068806
H	0	4.633760	1.074004	-1.336772
H	0	-1.935803	5.781024	-0.570281
H	0	-3.103169	5.899108	0.753229
H	0	-3.670868	5.821553	-0.921079
H	0	-6.228159	2.685423	-0.251081
H	0	-5.491948	5.597229	0.430623
H	0	-7.159981	4.850773	0.163851
H	0	-6.818962	-0.846373	-0.219390
H	0	-6.830795	-1.971931	1.145278
H	0	-6.884921	-2.592016	-0.511381
H	0	-3.723787	-5.123185	-0.216404
H	0	-6.526608	-4.399192	0.837110
H	0	-5.832220	-6.061925	0.429986
H	0	4.617356	0.673950	1.131159
H	0	4.587608	2.429174	1.413787
H	0	5.107274	-4.068070	0.377810
H	0	3.918574	-3.128157	1.268981
H	0	6.623624	-0.310688	1.031249
O	0	-0.870116	0.062826	2.104700
H	0	-0.083945	-0.013188	2.678738

9. [Fe(OH)(PPIX)]$^{2-}$ (m=6)

Fe	0	0.866534	-0.050706	0.329440
O	0	0.769017	-0.042438	2.171452
H	0	-0.033993	0.040370	2.722077
N	0	-0.575710	-1.448298	-0.245198
N	0	2.332544	-1.539198	-0.034090
N	0	-0.501934	1.414617	-0.247925
N	0	2.400950	1.361732	-0.050835
C	0	-1.944746	-1.230760	-0.389392
C	0	-2.656941	-2.512118	-0.530922
C	0	-1.689432	-3.503052	-0.479110
C	0	-0.401426	-2.833992	-0.297394
C	0	2.091279	-2.909389	-0.089437
C	0	3.345153	-3.641649	-0.032203
C	0	4.365460	-2.689060	0.052381
C	0	3.708443	-1.376917	0.046632
C	0	3.773925	1.123779	0.027017

C	0	4.499270	2.384434	0.015462
C	0	3.543145	3.399586	-0.074935
C	0	2.235517	2.734520	-0.120588
C	0	-0.257628	2.787906	-0.306883
C	0	-1.882477	1.265634	-0.389271
C	0	-2.527901	2.581999	-0.530943
C	0	-1.510681	3.522064	-0.484294
C	0	0.998380	3.388135	-0.231743
C	0	4.367465	-0.143019	0.084757
C	0	0.820061	-3.496197	-0.208386
C	0	-2.545068	0.034331	-0.430106
H	0	1.004677	4.471578	-0.279297
H	0	5.449963	-0.166316	0.144771
H	0	0.774302	-4.579186	-0.254431
H	0	-3.623864	0.061749	-0.533734
C	0	-1.881373	-4.991651	-0.606159
C	0	-1.625785	5.018237	-0.614436
C	0	-4.003807	2.843443	-0.696075
C	0	-4.143730	-2.698933	-0.702197
C	0	3.483508	-5.140072	-0.052309
C	0	5.811347	-2.865742	0.141396
C	0	6.546080	-4.009965	0.076535
C	0	5.995742	2.534707	0.072951
C	0	3.711499	4.848734	-0.135429
C	0	4.843458	5.589005	0.015252
C	0	-4.883331	-3.287500	0.540751
C	0	-4.713309	3.437275	0.561942
C	0	-5.155445	4.942822	0.408600
C	0	-5.408268	-4.761525	0.347241
O	0	-6.115714	-5.210485	1.322194
O	0	-5.076797	-5.374801	-0.746521
O	0	-5.829285	5.406312	1.400358
O	0	-4.799689	5.562640	-0.673662
H	0	-1.287492	-5.398410	-1.439684
H	0	-2.937774	-5.239242	-0.775852
H	0	-1.561953	-5.514418	0.308704
H	0	-1.039759	5.387699	-1.470708
H	0	-1.246886	5.527292	0.285179
H	0	-2.672394	5.322049	-0.750077
H	0	-4.508789	1.920512	-1.009265
H	0	-4.152802	3.591824	-1.487497
H	0	-4.327118	-3.420512	-1.511325
H	0	-4.603549	-1.746103	-0.994232
H	0	2.510401	-5.639214	-0.026854
H	0	4.060466	-5.495217	0.813714
H	0	4.008411	-5.484675	-0.956050
H	0	6.378332	-1.944484	0.281991
H	0	6.107594	-4.990805	-0.069556
H	0	7.629854	-3.972248	0.167327
H	0	6.507100	1.570231	-0.009621
H	0	6.316725	2.998351	1.018057
H	0	6.360666	3.175598	-0.742368
H	0	2.795977	5.409675	-0.324151
H	0	5.814974	5.155700	0.226977
H	0	4.802455	6.673637	-0.059220
H	0	-5.754914	-2.672906	0.802322
H	0	-4.234290	-3.289494	1.427360
H	0	-4.068861	3.378203	1.449872
H	0	-5.618865	2.864913	0.803653

10. [Fe(OAc)(PPIXH$_2$)] (m=6)

Fe	0	-0.988597	0.105509	-0.033510
O	0	-0.812453	0.116824	1.846197
C	0	-0.721840	-0.786573	2.852768
C	0	-0.645022	-0.137016	4.226212
O	0	-0.704318	-2.023180	2.670972
H	0	-1.542499	0.470069	4.395442
H	0	0.218984	0.536861	4.268023
H	0	-0.560756	-0.902745	5.001237
N	0	0.605086	1.336496	-0.599674
N	0	-2.234781	1.772492	-0.327074
N	0	0.172518	-1.515140	-0.634010
N	0	-2.667657	-1.095066	-0.337937
C	0	1.923957	0.933662	-0.773146
C	0	2.805281	2.100311	-0.796450
C	0	1.996832	3.216231	-0.663428
C	0	0.623326	2.729631	-0.552014
C	0	-1.832492	3.108295	-0.351645
C	0	-2.992343	3.985914	-0.285799
C	0	-4.115032	3.161869	-0.219466
C	0	-3.622225	1.781456	-0.253068
C	0	-4.000414	-0.687304	-0.250472
C	0	-4.880255	-1.847996	-0.222144
C	0	-4.061435	-2.973862	-0.292296
C	0	-2.682516	-2.483847	-0.377238
C	0	-0.232627	-2.846270	-0.629094
C	0	1.550589	-1.526483	-0.844943
C	0	2.029754	-2.905957	-0.967135
C	0	0.920901	-3.722307	-0.822378
C	0	-1.547822	-3.290701	-0.496034
C	0	-4.430977	0.641612	-0.205611
C	0	-0.504419	3.543280	-0.437380
C	0	2.354910	-0.388719	-0.915980
H	0	-1.698089	-4.364354	-0.489168
H	0	-5.499971	0.802066	-0.124025
H	0	-0.334449	4.614870	-0.428144
H	0	3.407982	-0.544015	-1.112932
C	0	2.402940	4.665914	-0.625580
C	0	0.848517	-5.225658	-0.843119
C	0	3.457815	-3.337033	-1.222441
C	0	4.312282	2.038252	-0.847069
C	0	-2.948885	5.489085	-0.326871
C	0	-5.533952	3.517861	-0.166938
C	0	-6.080507	4.693877	0.233769
C	0	-6.382288	-1.798675	-0.163996
C	0	-4.420876	-4.392274	-0.319777
C	0	-5.580735	-4.963579	0.093053
C	0	4.893940	1.813977	0.588155
C	0	4.414183	-3.254254	0.004927
C	0	5.283906	-2.007073	0.020252
C	0	6.390067	1.629745	0.614538
O	0	7.010488	0.649151	1.079324
O	0	7.074354	2.692915	0.071858
O	0	5.873014	-1.786884	1.231221
O	0	5.461188	-1.243862	-0.955978
H	0	1.916602	5.240891	-1.425692
H	0	3.484881	4.780275	-0.751055
H	0	2.127747	5.138536	0.327724
H	0	0.152190	-5.587474	-1.612124
H	0	0.503109	-5.618616	0.123125

H	0	1.826499	-5.672838	-1.048190
H	0	3.895556	-2.739487	-2.031950
H	0	3.445465	-4.373540	-1.577018
H	0	4.728040	2.965452	-1.255264
H	0	4.649771	1.218817	-1.490709
H	0	-2.023144	5.858064	-0.781008
H	0	-3.017450	5.925818	0.680458
H	0	-3.788193	5.886567	-0.910846
H	0	-6.226240	2.738914	-0.488273
H	0	-5.488670	5.521658	0.611113
H	0	-7.157926	4.838443	0.214039
H	0	-6.773482	-0.837016	-0.512422
H	0	-6.753878	-1.952561	0.859863
H	0	-6.821671	-2.584218	-0.791136
H	0	-3.657573	-5.062841	-0.715235
H	0	-6.390779	-4.398497	0.542636
H	0	-5.727127	-6.037824	0.011620
H	0	4.437829	0.933445	1.047188
H	0	4.648333	2.685443	1.209608
H	0	5.105345	-4.109684	0.001875
H	0	3.868783	-3.307656	0.953404
H	0	6.401411	-0.929160	1.246810
H	0	8.047290	2.539558	0.091422

11. [Fe(OAc)(PPIXH)]$^{-}$ (m=6)

Fe	0	-0.956781	0.099150	-0.012927
O	0	-0.807041	0.116403	1.870990
C	0	-0.995401	-0.695659	2.934411
C	0	-0.471779	-0.096643	4.233152
O	0	-1.538803	-1.820683	2.867210
H	0	-0.930638	0.885344	4.398436
H	0	0.611266	0.056454	4.151674
H	0	-0.690545	-0.763002	5.071624
N	0	0.672543	1.274729	-0.566750
N	0	-2.158156	1.798939	-0.340168
N	0	0.167746	-1.559433	-0.565762
N	0	-2.666987	-1.057297	-0.353745
C	0	1.984410	0.837049	-0.727231
C	0	2.904270	1.977497	-0.753500
C	0	2.122651	3.113198	-0.626563
C	0	0.733902	2.668106	-0.523650
C	0	-1.713968	3.121623	-0.360502
C	0	-2.846382	4.031847	-0.320755
C	0	-3.997255	3.241640	-0.277496
C	0	-3.546266	1.847563	-0.296498
C	0	-3.989934	-0.611474	-0.295927
C	0	-4.899639	-1.746686	-0.273538
C	0	-4.110292	-2.896038	-0.313297
C	0	-2.717516	-2.444604	-0.371578
C	0	-0.271073	-2.880755	-0.549358
C	0	1.549626	-1.610183	-0.759406
C	0	1.998717	-3.004854	-0.849113
C	0	0.864113	-3.787513	-0.706619
C	0	-1.601901	-3.284910	-0.444859
C	0	-4.385679	0.729127	-0.266096

C	0	-0.369242	3.514258	-0.424958
C	0	2.384914	-0.496205	-0.848480
H	0	-1.780295	-4.354223	-0.426565
H	0	-5.451794	0.917013	-0.207815
H	0	-0.163090	4.579511	-0.414575
H	0	3.437334	-0.682313	-1.036981
C	0	2.572245	4.549574	-0.580399
C	0	0.751723	-5.289205	-0.706040
C	0	3.420646	-3.467402	-1.072288
C	0	4.408564	1.880706	-0.806987
C	0	-2.758630	5.533615	-0.358249
C	0	-5.404394	3.637106	-0.251891
C	0	-5.934714	4.853820	0.040071
C	0	-6.401046	-1.659320	-0.237590
C	0	-4.504409	-4.303679	-0.327611
C	0	-5.710185	-4.845960	-0.014521
C	0	5.017788	1.614202	0.604775
C	0	4.413383	-3.211936	0.101843
C	0	5.316369	-1.970214	-0.105910
C	0	6.555245	1.695515	0.577319
O	0	7.236435	0.570023	0.844968
O	0	7.119043	2.790353	0.330519
O	0	5.949257	-1.557948	0.962767
O	0	5.376179	-1.418705	-1.259403
H	0	2.137656	5.137306	-1.402178
H	0	3.661442	4.620687	-0.658946
H	0	2.277239	5.034596	0.361122
H	0	0.111527	-5.649612	-1.524444
H	0	0.318103	-5.655820	0.235135
H	0	1.733314	-5.759357	-0.821953
H	0	3.845796	-2.957258	-1.947828
H	0	3.399489	-4.539759	-1.302805
H	0	4.834626	2.816205	-1.187432
H	0	4.730505	1.073771	-1.475761
H	0	-1.778416	5.875543	-0.705561
H	0	-2.927207	5.975160	0.635475
H	0	-3.516812	5.952846	-1.032781
H	0	-6.114056	2.846274	-0.498077
H	0	-5.332348	5.707288	0.332670
H	0	-7.011054	5.007707	0.010973
H	0	-6.759767	-0.665390	-0.524704
H	0	-6.793742	-1.872892	0.767872
H	0	-6.851666	-2.387908	-0.924301
H	0	-3.721604	-5.002614	-0.623443
H	0	-6.553121	-4.257395	0.331690
H	0	-5.862716	-5.921180	-0.074557
H	0	4.682559	0.645682	0.986158
H	0	4.666015	2.397141	1.290033
H	0	5.088284	-4.072880	0.211382
H	0	3.897636	-3.100811	1.062758
H	0	6.682648	-0.357356	0.884405

12. [Fe(OAc)(PPIX)]$^{2-}$ (m=6)

Fe	0	-0.772622	0.046778	0.036667
O	0	-0.682886	0.036769	1.929468
C	0	-1.447636	0.013974	3.035059
C	0	-0.623334	-0.007387	4.318062
O	0	-2.701445	0.010634	3.029629
H	0	0.027662	0.874552	4.348503
H	0	0.026548	-0.890701	4.319250
H	0	-1.280829	-0.021833	5.191830
N	0	0.670347	1.454280	-0.467177
N	0	-2.224949	1.524940	-0.346282
N	0	0.611883	-1.411343	-0.478234
N	0	-2.278375	-1.370867	-0.359946
C	0	2.047057	1.241782	-0.557580
C	0	2.759343	2.523094	-0.668584
C	0	1.787103	3.512226	-0.653854
C	0	0.496950	2.840634	-0.524187
C	0	-1.995462	2.900203	-0.398267
C	0	-3.255832	3.620466	-0.379040
C	0	-4.268605	2.659134	-0.322089
C	0	-3.604378	1.354448	-0.302782
C	0	-3.656463	-1.140152	-0.319827
C	0	-4.374604	-2.402178	-0.345190
C	0	-3.413109	-3.413923	-0.406372
C	0	-2.108584	-2.747115	-0.424288
C	0	0.383164	-2.787428	-0.543953
C	0	1.997453	-1.252784	-0.568228
C	0	2.656641	-2.561771	-0.689212
C	0	1.645171	-3.510528	-0.678744
C	0	-0.869512	-3.397049	-0.503150
C	0	-4.258247	0.120543	-0.286357
C	0	-0.728972	3.498437	-0.478598
C	0	2.653844	-0.019097	-0.580921
H	0	-0.869932	-4.480582	-0.544839
H	0	-5.341675	0.139731	-0.252692
H	0	-0.690528	4.581554	-0.526071
H	0	3.735758	-0.040776	-0.643294
C	0	1.981078	5.001371	-0.766860
C	0	1.777931	-5.005466	-0.802976
C	0	4.137745	-2.815512	-0.807939
C	0	4.250047	2.718144	-0.782136
C	0	-3.401761	5.118372	-0.384565
C	0	-5.717750	2.830142	-0.255436
C	0	-6.455235	3.941546	-0.521682
C	0	-5.871350	-2.554865	-0.325932
C	0	-3.577510	-4.864202	-0.467271
C	0	-4.695066	-5.605319	-0.239572
C	0	4.933888	3.334460	0.479398
C	0	4.803229	-3.447786	0.455678
C	0	5.289162	-4.934019	0.254630
C	0	5.475293	4.800363	0.271043
O	0	6.158074	5.264853	1.255855
O	0	5.176109	5.393720	-0.843058
O	0	5.962199	-5.415586	1.237886
O	0	4.959691	-5.524111	-0.852542
H	0	1.399482	5.415134	-1.605313
H	0	3.040031	5.250147	-0.918665
H	0	1.648884	5.516711	0.147695
H	0	1.197234	-5.385581	-1.657934
H	0	1.404585	-5.515163	0.098674

H	0	2.828212	-5.297578	-0.936620
H	0	4.653031	-1.884147	-1.075165
H	0	4.315820	-3.540223	-1.615719
H	0	4.459998	3.428544	-1.595066
H	0	4.729731	1.765262	-1.039187
H	0	-2.461544	5.616981	-0.128904
H	0	-4.159334	5.439071	0.343203
H	0	-3.716196	5.494551	-1.370247
H	0	-6.273587	1.943893	0.053970
H	0	-6.016886	4.873501	-0.862996
H	0	-7.537745	3.924754	-0.412500
H	0	-6.380043	-1.611175	-0.548608
H	0	-6.226878	-2.895488	0.658348
H	0	-6.201001	-3.296028	-1.066759
H	0	-2.675729	-5.420499	-0.724601
H	0	-5.643920	-5.171886	0.058362
H	0	-4.662348	-6.689275	-0.326514
H	0	5.786899	2.721882	0.799226
H	0	4.242533	3.364078	1.332998
H	0	4.114282	-3.446725	1.311736
H	0	5.679266	-2.864778	0.768450

13. $[Fe(MeNH_2)(PPIXH_2)]^+$ (m=4)

N	0	0.742756	-0.033604	2.057464
H	0	0.251589	0.847307	2.234690
C	0	1.974012	-0.153815	2.902122
H	0	0.096551	-0.809098	2.228177
H	0	2.640727	0.683258	2.683476
H	0	2.491302	-1.082643	2.650191
H	0	1.733910	-0.153039	3.973122
Fe	0	1.012255	-0.043531	-0.116779
N	0	-0.548592	-1.256780	-0.410373
N	0	2.233905	-1.624858	-0.212138
N	0	-0.189532	1.535551	-0.400973
N	0	2.592780	1.176898	-0.144627
C	0	-1.887829	-0.895378	-0.611586
C	0	-2.744497	-2.070878	-0.609635
C	0	-1.917889	-3.168581	-0.432581
C	0	-0.560635	-2.658924	-0.331216
C	0	1.873347	-2.983868	-0.213288
C	0	3.047202	-3.832757	-0.221216
C	0	4.153745	-2.984416	-0.228394
C	0	3.634508	-1.622606	-0.218821
C	0	3.950529	0.816560	-0.122609
C	0	4.797447	1.988454	-0.027953
C	0	3.947528	3.092676	0.026519
C	0	2.588004	2.575830	-0.068565
C	0	0.163404	2.889550	-0.317020
C	0	-1.566974	1.538125	-0.676224
C	0	-2.073426	2.901242	-0.772302
C	0	-0.996301	3.739390	-0.525825
C	0	1.450202	3.372188	-0.115950
C	0	4.431272	-0.486539	-0.171564
C	0	0.566612	-3.461388	-0.226323
C	0	-2.353891	0.400735	-0.790551
H	0	1.574720	4.445273	-0.041637
H	0	5.504673	-0.624357	-0.146709

H	0	0.417960	-4.533991	-0.195495
H	0	-3.403323	0.535442	-1.017888
C	0	-2.297824	-4.623178	-0.367001
C	0	-0.962603	5.243824	-0.502250
C	0	-3.488370	3.315712	-1.118231
C	0	-4.251654	-2.039807	-0.689488
C	0	3.032753	-5.335227	-0.272041
C	0	5.581055	-3.311914	-0.281225
C	0	6.168313	-4.457675	0.143955
C	0	6.300728	1.975846	-0.035270
C	0	4.274847	4.518633	0.105658
C	0	5.407487	5.065437	0.612192
C	0	-4.867610	-1.801737	0.727260
C	0	-4.517852	3.279393	0.049747
C	0	-5.304943	1.980037	0.126524
C	0	-6.368125	-1.623194	0.716325
O	0	-6.994503	-0.650781	1.186831
O	0	-7.024473	-2.679551	0.140865
O	0	-5.949122	1.814597	1.311637
O	0	-5.365027	1.134489	-0.795916
H	0	-1.826978	-5.197647	-1.176058
H	0	-3.379704	-4.755224	-0.461859
H	0	-1.990493	-5.082689	0.582069
H	0	-0.316581	5.645028	-1.294887
H	0	-0.582534	5.624847	0.455116
H	0	-1.959957	5.668539	-0.646927
H	0	-3.877148	2.689805	-1.930288
H	0	-3.454704	4.338189	-1.508742
H	0	-4.637252	-2.982479	-1.089808
H	0	-4.593190	-1.242177	-1.356354
H	0	2.111574	-5.723111	-0.718316
H	0	3.125281	-5.778045	0.729982
H	0	3.872080	-5.708172	-0.870037
H	0	6.229422	-2.549830	-0.713103
H	0	5.617810	-5.262484	0.621314
H	0	7.240390	-4.601678	0.039949
H	0	6.701321	1.095190	-0.547572
H	0	6.713884	1.980020	0.983585
H	0	6.690970	2.862530	-0.547542
H	0	3.523542	5.204529	-0.284593
H	0	6.200642	4.475025	1.060276
H	0	5.551456	6.142533	0.608062
H	0	-4.433368	-0.910227	1.186612
H	0	-4.637406	-2.662665	1.369439
H	0	-5.259744	4.078636	-0.089586
H	0	-4.051953	3.465980	1.023526
H	0	-8.001706	-2.552114	0.137417
H	0	-6.452050	0.940343	1.354805

14. [Fe(MeNH$_2$)(PPIXH)] (m=4)

N	0	0.636925	-0.037292	2.014010
H	0	0.170316	0.859157	2.178017
C	0	1.831139	-0.210997	2.896495
H	0	-0.045095	-0.789004	2.147110
H	0	2.536019	0.602219	2.707380
H	0	2.322355	-1.155753	2.650483
H	0	1.557352	-0.211768	3.959970
Fe	0	0.976797	-0.036924	-0.152873
N	0	-0.592617	-1.211168	-0.479716
N	0	2.176579	-1.644445	-0.236879
N	0	-0.182128	1.566184	-0.435716
N	0	2.590157	1.152483	-0.134161
C	0	-1.929575	-0.822294	-0.666854
C	0	-2.816071	-1.976641	-0.653129
C	0	-2.006150	-3.091848	-0.490865
C	0	-0.638483	-2.614635	-0.404655
C	0	1.786846	-2.994685	-0.264614
C	0	2.942050	-3.866795	-0.257557
C	0	4.065965	-3.042068	-0.225382
C	0	3.576185	-1.669879	-0.210282
C	0	3.939029	0.762492	-0.084895
C	0	4.806175	1.916549	0.032712
C	0	3.978445	3.037895	0.070484
C	0	2.611203	2.550406	-0.053942
C	0	0.194959	2.912413	-0.329876
C	0	-1.563214	1.600373	-0.703245
C	0	-2.048394	2.974900	-0.766443
C	0	-0.949804	3.785252	-0.514915
C	0	1.489096	3.368493	-0.114376
C	0	4.394160	-0.550171	-0.131629
C	0	0.469781	-3.442568	-0.301788
C	0	-2.375012	0.482300	-0.833224
H	0	1.630733	4.438786	-0.029993
H	0	5.463793	-0.709533	-0.082200
H	0	0.293718	-4.511314	-0.281046
H	0	-3.431198	0.643540	-1.041065
C	0	-2.423990	-4.534857	-0.408093
C	0	-0.890781	5.288014	-0.454098
C	0	-3.463773	3.415731	-1.056372
C	0	-4.319761	-1.915015	-0.667212
C	0	2.896462	-5.368388	-0.328943
C	0	5.486705	-3.398845	-0.244695
C	0	6.043257	-4.570539	0.151699
C	0	6.309336	1.873877	0.061091
C	0	4.332097	4.456709	0.160084
C	0	5.473198	4.986880	0.666537
C	0	-4.866597	-1.629378	0.765872
C	0	-4.477319	3.253369	0.117441
C	0	-5.241874	1.907674	0.084729
C	0	-6.403952	-1.728729	0.806634
O	0	-7.077048	-0.626006	1.175167
O	0	-6.962516	-2.815158	0.533367
O	0	-5.785875	1.533936	1.208114
O	0	-5.278035	1.245276	-1.014389
H	0	-2.024192	-5.119097	-1.248952
H	0	-3.513392	-4.626198	-0.430684
H	0	-2.072617	-5.008556	0.518801
H	0	-0.255382	5.701061	-1.250167
H	0	-0.486200	5.638692	0.505284

H	0	-1.886674	5.725095	-0.566964
H	0	-3.874156	2.841410	-1.896809
H	0	-3.434830	4.467532	-1.364769
H	0	-4.740231	-2.866315	-1.010010
H	0	-4.687549	-1.126259	-1.331992
H	0	1.967574	-5.728490	-0.782361
H	0	2.975594	-5.827170	0.667360
H	0	3.729501	-5.751367	-0.930119
H	0	6.162554	-2.632470	-0.624611
H	0	5.465118	-5.384165	0.578424
H	0	7.115997	-4.728037	0.074389
H	0	6.702123	0.976107	-0.427354
H	0	6.699015	1.886046	1.089442
H	0	6.729686	2.744222	-0.456187
H	0	3.589739	5.156342	-0.223498
H	0	6.259416	4.383607	1.109562
H	0	5.630305	6.062405	0.667589
H	0	-4.529151	-0.649244	1.113889
H	0	-4.481613	-2.396520	1.452390
H	0	-5.236633	4.044671	0.044106
H	0	-4.004316	3.364552	1.099993
H	0	-6.537027	0.291166	1.198283

15. [Fe(MeNH$_2$)(PPIX)]$^-$ (m=4)

N	0	0.532835	-0.121040	2.035328
H	0	-0.204031	0.570395	2.185416
C	0	1.696424	0.073337	2.936915
H	0	0.136024	-1.060416	2.099426
H	0	2.101699	1.078028	2.781601
H	0	2.476755	-0.644932	2.667138
H	0	1.449599	-0.051478	4.003593
Fe	0	0.892463	0.071854	-0.217140
N	0	-0.379536	-1.454166	-0.564993
N	0	2.462025	-1.210431	-0.280442
N	0	-0.642479	1.361438	-0.425317
N	0	2.187886	1.626062	-0.102414
C	0	-1.764733	-1.396675	-0.719358
C	0	-2.332918	-2.739645	-0.849885
C	0	-1.271901	-3.623358	-0.793995
C	0	-0.063670	-2.814586	-0.617644
C	0	2.399563	-2.600304	-0.394673
C	0	3.730801	-3.182181	-0.355652
C	0	4.626047	-2.122757	-0.214491
C	0	3.815891	-0.902351	-0.176050
C	0	3.581816	1.560875	-0.004658
C	0	4.151953	2.892302	0.131167
C	0	3.082648	3.785213	0.115159
C	0	1.870149	2.977446	-0.045879
C	0	-0.581088	2.753759	-0.346348
C	0	-1.989224	1.064830	-0.645560
C	0	-2.787093	2.291138	-0.719402
C	0	-1.907802	3.339166	-0.523340
C	0	0.577408	3.498702	-0.145441
C	0	4.331654	0.385261	-0.034999
C	0	1.220054	-3.339966	-0.533445
C	0	-2.512734	-0.220100	-0.763822
H	0	0.459164	4.574831	-0.083693

H	0	5.406608	0.484612	0.061062
H	0	1.310140	-4.418718	-0.593270
H	0	-3.583556	-0.312489	-0.907319
C	0	-1.313192	-5.124587	-0.903740
C	0	-2.214901	4.813162	-0.496856
C	0	-4.272164	2.374871	-0.949863
C	0	-3.802369	-3.048571	-0.983887
C	0	4.047034	-4.647757	-0.484576
C	0	6.086183	-2.131420	-0.149957
C	0	6.914361	-3.180072	0.099515
C	0	5.620566	3.207906	0.224971
C	0	3.080689	5.245489	0.194400
C	0	4.070116	6.064553	0.637910
C	0	-4.583179	-2.986976	0.360467
C	0	-5.103462	2.352715	0.363834
C	0	-6.526707	2.920243	0.146715
C	0	-4.342435	-4.225924	1.249084
O	0	-4.463844	-4.042282	2.534845
O	0	-4.074318	-5.361028	0.716635
O	0	-7.435049	2.463922	0.973961
O	0	-6.746828	3.794000	-0.755524
H	0	-1.181518	-5.450094	-1.947365
H	0	-2.271586	-5.506644	-0.534693
H	0	-0.520761	-5.596610	-0.309441
H	0	-1.630514	5.362642	-1.248701
H	0	-1.984086	5.256184	0.482908
H	0	-3.274856	4.996891	-0.698707
H	0	-4.614544	1.560418	-1.600874
H	0	-4.527950	3.303503	-1.471419
H	0	-3.931231	-4.056705	-1.391583
H	0	-4.269126	-2.349373	-1.692784
H	0	3.207122	-5.211454	-0.902620
H	0	4.292278	-5.098349	0.488979
H	0	4.913551	-4.802780	-1.140777
H	0	6.566059	-1.167793	-0.326550
H	0	6.553274	-4.178689	0.321721
H	0	7.993312	-3.042538	0.103899
H	0	6.238550	2.384392	-0.148432
H	0	5.931426	3.407435	1.261816
H	0	5.865014	4.101382	-0.364055
H	0	2.164433	5.730106	-0.144397
H	0	5.010370	5.695089	1.034246
H	0	3.937366	7.144021	0.631708
H	0	-5.662759	-2.950395	0.150488
H	0	-4.336988	-2.085683	0.933314
H	0	-4.619160	2.988873	1.119317
H	0	-5.171614	1.345742	0.791534

16. [FeCl(PPIXH_2)] (m=4)

Fe	0	1.027077	-0.042911	-0.088935
Cl	0	0.740893	-0.061799	2.264295
N	0	-0.517868	-1.255446	-0.520796
N	0	2.266350	-1.635469	-0.247209
N	0	-0.147482	1.545893	-0.499999
N	0	2.630677	1.177683	-0.145037
C	0	-1.851112	-0.885279	-0.681349
C	0	-2.716070	-2.058538	-0.665972
C	0	-1.891661	-3.158145	-0.522120
C	0	-0.529195	-2.649895	-0.445667
C	0	1.900834	-2.984718	-0.276514
C	0	3.071600	-3.841274	-0.220336
C	0	4.175882	-2.998931	-0.144010
C	0	3.655890	-1.633160	-0.156228
C	0	3.973147	0.806345	-0.023242
C	0	4.822923	1.975024	0.126383
C	0	3.981890	3.082394	0.104224
C	0	2.626060	2.568677	-0.079785
C	0	0.212343	2.889912	-0.416518
C	0	-1.522198	1.548342	-0.745030
C	0	-2.029744	2.915601	-0.834006
C	0	-0.948003	3.748320	-0.615220
C	0	1.495997	3.369434	-0.193966
C	0	4.449633	-0.498694	-0.042249
C	0	0.593999	-3.457026	-0.341753
C	0	-2.316509	0.414433	-0.840012
H	0	1.621039	4.442722	-0.118751
H	0	5.517594	-0.640831	0.066139
H	0	0.440466	-4.529513	-0.316214
H	0	-3.370827	0.553270	-1.038104
C	0	-2.274048	-4.611764	-0.438057
C	0	-0.907904	5.252862	-0.580530
C	0	-3.457425	3.325776	-1.124056
C	0	-4.224021	-2.017847	-0.680080
C	0	3.051623	-5.344047	-0.276779
C	0	5.602149	-3.327536	-0.098102
C	0	6.167027	-4.488157	0.319749
C	0	6.321758	1.948844	0.244420
C	0	4.308363	4.506934	0.194605
C	0	5.413552	5.064881	0.749463
C	0	-4.769881	-1.786180	0.768238
C	0	-4.432554	3.267683	0.089625
C	0	-5.265645	1.996662	0.143767
C	0	-6.269378	-1.644745	0.831268
O	0	-6.907983	-0.669561	1.282784
O	0	-6.935300	-2.743892	0.339564
O	0	-5.851166	1.798105	1.358183
O	0	-5.417454	1.200683	-0.810748
H	0	-1.784904	-5.203918	-1.223677
H	0	-3.354870	-4.744932	-0.552477
H	0	-1.985859	-5.049414	0.527733
H	0	-0.199215	5.656630	-1.316535
H	0	-0.600357	5.622709	0.407473
H	0	-1.890205	5.683974	-0.798627
H	0	-3.877263	2.705473	-1.925247
H	0	-3.446855	4.353573	-1.503887
H	0	-4.634272	-2.957032	-1.065875
H	0	-4.592505	-1.212008	-1.323310
H	0	2.151423	-5.722554	-0.772529

H	0	3.085119	-5.787973	0.729021
H	0	3.920427	-5.722443	-0.828801
H	0	6.278852	-2.544598	-0.441977
H	0	5.588167	-5.313985	0.721203
H	0	7.245844	-4.620326	0.292999
H	0	6.752812	1.055989	-0.221018
H	0	6.645184	1.959454	1.295636
H	0	6.764323	2.825776	-0.242792
H	0	3.572901	5.189587	-0.231878
H	0	6.184829	4.480678	1.241415
H	0	5.550505	6.143420	0.746175
H	0	-4.324921	-0.887019	1.200953
H	0	-4.482691	-2.639862	1.396165
H	0	-5.148263	4.101055	0.035573
H	0	-3.906816	3.377819	1.044095
H	0	-7.911644	-2.620692	0.385067
H	0	-6.349637	0.922783	1.403437

17. [FeCl(PPIXH)]$^{-}$ (m=4)

Fe	0	-1.016803	0.037600	-0.026879
Cl	0	-0.882927	0.061842	2.345769
N	0	0.574234	1.190678	-0.423284
N	0	-2.201505	1.671333	-0.228552
N	0	0.116415	-1.585333	-0.382952
N	0	-2.662065	-1.132957	-0.154459
C	0	1.896442	0.782107	-0.603592
C	0	2.803657	1.926976	-0.603396
C	0	2.013698	3.047045	-0.423300
C	0	0.635403	2.584688	-0.332327
C	0	-1.786077	3.005460	-0.208328
C	0	-2.925757	3.900921	-0.184445
C	0	-4.063948	3.097406	-0.189545
C	0	-3.593257	1.714353	-0.209713
C	0	-3.997420	-0.716979	-0.122590
C	0	-4.888589	-1.856606	-0.014645
C	0	-4.081422	-2.990202	0.039115
C	0	-2.701822	-2.520458	-0.062429
C	0	-0.282593	-2.916486	-0.264632
C	0	1.494975	-1.636035	-0.609971
C	0	1.968929	-3.020682	-0.640910
C	0	0.859052	-3.811243	-0.404850
C	0	-1.587457	-3.353800	-0.086545
C	0	-4.428595	0.604324	-0.164411
C	0	-0.458424	3.428452	-0.223710
C	0	2.324517	-0.531809	-0.745369
H	0	-1.743622	-4.421232	0.012116
H	0	-5.496371	0.779435	-0.119222
H	0	-0.262482	4.493020	-0.171243
H	0	3.375232	-0.708742	-0.950210
C	0	2.448989	4.484479	-0.322292
C	0	0.776307	-5.311606	-0.308137
C	0	3.390149	-3.468710	-0.893908
C	0	4.307271	1.853183	-0.688962
C	0	-2.852241	5.403462	-0.193130
C	0	-5.476897	3.474535	-0.206230
C	0	-6.029408	4.667873	0.134071
C	0	-6.391277	-1.787482	0.006158

C	0	-4.453959	-4.401552	0.133942
C	0	-5.630974	-4.928272	0.560355
C	0	4.956069	1.602620	0.708037
C	0	4.408689	-3.186492	0.251799
C	0	5.306144	-1.949401	-0.003798
C	0	6.489116	1.730535	0.637711
O	0	7.213278	0.626086	0.879478
O	0	7.011393	2.842782	0.377832
O	0	5.991306	-1.539031	1.031200
O	0	5.309801	-1.399555	-1.160390
H	0	2.002126	5.101995	-1.115008
H	0	3.536689	4.568269	-0.407176
H	0	2.158323	4.925283	0.641686
H	0	0.119510	-5.734953	-1.081986
H	0	0.381354	-5.628536	0.667414
H	0	1.764226	-5.767524	-0.426113
H	0	3.786667	-2.966915	-1.787096
H	0	3.374450	-4.544575	-1.108505
H	0	4.706646	2.795997	-1.080449
H	0	4.628808	1.051472	-1.363627
H	0	-1.884370	5.762635	-0.557323
H	0	-2.999845	5.821558	0.813794
H	0	-3.631087	5.827444	-0.839834
H	0	-6.165308	2.694943	-0.534797
H	0	-5.446931	5.501818	0.511736
H	0	-7.104032	4.819714	0.062684
H	0	-6.763158	-0.858774	-0.439655
H	0	-6.785113	-1.840267	1.032190
H	0	-6.826468	-2.624619	-0.554072
H	0	-3.685000	-5.110993	-0.173326
H	0	-6.449771	-4.320467	0.931560
H	0	-5.782050	-6.005247	0.572681
H	0	4.657684	0.625328	1.096713
H	0	4.599667	2.373892	1.403606
H	0	5.085281	-4.044725	0.369743
H	0	3.913482	-3.049759	1.220260
H	0	6.690596	-0.316314	0.933865

18. [FeCl(PPIX)]$^{2-}$ (m=4)

Fe	0	0.861710	-0.045066	0.034900
Cl	0	0.834601	-0.062696	2.420465
N	0	-0.549884	-1.419689	-0.329272
N	0	2.287362	-1.489067	-0.174330
N	0	-0.501739	1.378810	-0.317554
N	0	2.328115	1.354587	-0.148975
C	0	-1.933359	-1.226790	-0.405825
C	0	-2.641007	-2.505148	-0.515069
C	0	-1.665851	-3.488155	-0.501236
C	0	-0.383613	-2.810482	-0.375588
C	0	2.075417	-2.868712	-0.223316
C	0	3.330705	-3.587181	-0.161213
C	0	4.336681	-2.625401	-0.063623
C	0	3.667301	-1.326519	-0.076799
C	0	3.707146	1.139921	-0.040164
C	0	4.420863	2.400743	0.000998
C	0	3.460740	3.406792	-0.095635

C	0	2.166612	2.734383	-0.176838
C	0	-0.288855	2.761894	-0.353629
C	0	-1.892275	1.232620	-0.399207
C	0	-2.554853	2.535881	-0.503572
C	0	-1.546513	3.484339	-0.481203
C	0	0.943452	3.391328	-0.283883
C	0	4.325764	-0.104880	0.001125
C	0	0.826099	-3.480097	-0.320385
C	0	-2.559293	0.014859	-0.417081
H	0	0.938336	4.473837	-0.317924
H	0	5.404893	-0.118684	0.091688
H	0	0.785565	-4.562380	-0.349286
H	0	-3.640547	0.033391	-0.466073
C	0	-1.853202	-4.977816	-0.613198
C	0	-1.681470	4.980245	-0.584637
C	0	-4.034160	2.790874	-0.633177
C	0	-4.128812	-2.708505	-0.642710
C	0	3.482360	-5.083135	-0.214817
C	0	5.786072	-2.788712	0.009992
C	0	6.503735	-3.918482	0.252193
C	0	5.909772	2.556717	0.155289
C	0	3.618332	4.859650	-0.088335
C	0	4.748845	5.587605	-0.289848
C	0	-4.815502	-3.383339	0.587191
C	0	-4.701818	3.470822	0.604543
C	0	-5.225585	4.931434	0.327357
C	0	-5.386283	-4.822773	0.292651
O	0	-6.126923	-5.309653	1.222688
O	0	-5.044060	-5.379131	-0.828782
O	0	-5.952994	5.429308	1.262017
O	0	-4.862669	5.490835	-0.785874
H	0	-1.245282	-5.395744	-1.430287
H	0	-2.906584	-5.227373	-0.800379
H	0	-1.551637	-5.487577	0.314840
H	0	-1.062803	5.380633	-1.402392
H	0	-1.358077	5.474345	0.344523
H	0	-2.726167	5.267789	-0.765492
H	0	-4.556230	1.856262	-0.872429
H	0	-4.203213	3.490619	-1.465115
H	0	-4.323858	-3.389767	-1.484266
H	0	-4.619617	-1.753397	-0.866460
H	0	2.567073	-5.573708	-0.559471
H	0	3.723787	-5.499053	0.775081
H	0	4.294133	-5.371048	-0.896691
H	0	6.364383	-1.877967	-0.150552
H	0	6.043815	-4.878799	0.458656
H	0	7.591240	-3.887077	0.269555
H	0	6.376088	1.646280	0.546136
H	0	6.141749	3.374052	0.850672
H	0	6.398413	2.794720	-0.802259
H	0	2.706086	5.424683	0.103523
H	0	5.708753	5.138206	-0.523271
H	0	4.719473	6.674049	-0.243310
H	0	-5.649699	-2.772690	0.954883
H	0	-4.115048	-3.480726	1.428414
H	0	-4.000365	3.535162	1.448093
H	0	-5.555797	2.882254	0.962697

19. FePPIX dimer (from X-ray crystal structure), [{Fe(PPIXH)}$_2$] (m=7)

Method 1 (B3LYP/LanL2DZ)

Energies (Hartrees):	vacuum	-3915.012129
	water	-3915.088688
	n-octanol	-3915.098392
	ZPE	1.177175

S = 416.858 cal mol^{-1} K^{-1}

Method 2 [OPBE/6-311+G(d,p)]

Energies (Hartrees):	vacuum	-6195.816992
	water	-6195.877437
	n-octanol	-6195.891418

Method 3 [B3LYP/6-311+G(d,p)]

Energies (Hartrees):	vacuum	-6197.045792
	water	-6197.111068
	n-octanol	-6197.123876

C	0	6.694219	2.156755	0.370073
C	0	5.949915	3.287046	0.050382
C	0	4.735865	3.263654	-0.622935
C	0	3.995188	4.457298	-1.005515
C	0	2.839719	4.029215	-1.634726
C	0	2.876341	2.572660	-1.617103
C	0	1.853433	1.766402	-2.096741
C	0	1.911168	0.380130	-2.140053
C	0	0.831352	-0.459852	-2.636246
C	0	1.306149	-1.758450	-2.643623
C	0	2.655841	-1.710477	-2.100360
C	0	3.450069	-2.828633	-1.904970
C	0	4.713782	-2.804714	-1.326327
C	0	4.452480	5.869281	-0.753149
C	0	1.777541	4.883012	-2.291776
C	0	-0.576097	0.027434	-2.874131
C	0	0.598748	-3.015546	-3.067243
C	0	0.643273	5.396676	-1.357896
C	0	-0.468386	4.400335	-1.040683
C	0	-1.338996	0.029859	-1.513301
C	0	-2.681301	0.763323	-1.518140
Fe	0	4.581922	0.192645	-0.664787
N	0	6.349357	0.848689	0.033928
N	0	4.054880	2.111808	-1.022874
N	0	3.014986	-0.396223	-1.774530
N	0	5.360994	-1.661717	-0.847316
O	0	-0.994229	4.313170	0.091796
O	0	-0.855677	3.664859	-2.111090
O	0	-3.722553	0.088826	-1.085879
C	0	-6.693745	-2.156929	-0.370879
C	0	-5.949163	-3.287145	-0.051568
C	0	-4.735278	-3.263704	0.622039
C	0	-3.994547	-4.457317	1.004610
C	0	-2.839408	-4.029195	1.634397

C	0	-2.876215	-2.572643	1.617024
C	0	-1.853500	-1.766333	2.096992
C	0	-1.911298	-0.380062	2.140232
C	0	-0.831567	0.459994	2.636494
C	0	-1.306383	1.758586	2.643651
C	0	-2.656012	1.710529	2.100246
C	0	-3.450300	2.828627	1.904781
C	0	-4.714109	2.804566	1.326353
C	0	-4.451538	-5.869314	0.751768
C	0	-1.777408	-4.882945	2.291798
C	0	0.575891	-0.027190	2.874543
C	0	-0.599061	3.015736	3.067243
C	0	-0.642700	-5.396416	1.358340
C	0	0.468624	-4.399723	1.041162
C	0	1.339068	-0.029124	1.513882
C	0	2.681302	-0.762741	1.518573
Fe	0	-4.581972	-0.192706	0.664704
N	0	-6.349263	-0.848901	-0.034194
N	0	-4.054612	-2.111838	1.022476
N	0	-3.015079	0.396234	1.774468
N	0	-5.361314	1.661500	0.847502
O	0	0.994210	-4.312003	-0.091379
O	0	0.855927	-3.664519	2.111790
O	0	3.722435	-0.088424	1.085730
C	0	9.675362	0.345084	1.778591
C	0	9.914254	3.619378	1.845250
O	0	-2.742441	1.979425	-1.897297
C	0	-7.408977	-0.055961	-0.488757
C	0	-8.423161	-0.870181	-1.131735
C	0	-7.983063	-2.188764	-1.054717
C	0	-5.523439	3.989137	1.106846
C	0	-6.688653	3.561913	0.479393
C	0	-6.560516	2.116858	0.305056
C	0	-7.509396	1.320693	-0.322849
C	0	-8.602301	-3.414141	-1.564033
C	0	-5.102864	5.392456	1.445476
C	0	-7.833633	4.343719	0.006375
C	0	-8.263524	5.536266	0.488508
C	0	7.408779	0.055613	0.488927
C	0	8.423162	0.869794	1.131647
C	0	7.983503	2.188483	1.053988
C	0	5.522908	-3.989377	-1.106571
C	0	6.687974	-3.562290	-0.478747
C	0	6.559982	-2.117209	-0.304516
C	0	7.508870	-1.321118	0.323475
C	0	8.603119	3.413891	1.562770
C	0	5.102294	-5.392655	-1.445329
C	0	7.832705	-4.344227	-0.005340
C	0	8.262626	-5.536837	-0.487296
O	0	2.742462	-1.978730	1.898040
C	0	-9.675601	-0.345605	-1.778326
C	0	-9.913377	-3.619927	-1.846568
H	0	6.350511	4.255901	0.322989
H	0	0.958096	2.254528	-2.461705
H	0	3.037804	-3.787332	-2.190893
H	0	5.463821	6.045256	-1.143607
H	0	4.471819	6.100304	0.321459
H	0	3.782910	6.592704	-1.230021
H	0	1.313155	4.347808	-3.126015
H	0	2.268415	5.764820	-2.724637
H	0	-1.101189	-0.622257	-3.584151

H	0	-0.587277	1.037482	-3.297468
H	0	1.121043	-3.504825	-3.901868
H	0	-0.422574	-2.800945	-3.399416
H	0	0.549681	-3.728796	-2.235752
H	0	0.152036	6.247162	-1.854404
H	0	1.043457	5.758649	-0.405552
H	0	-0.713774	0.541568	-0.769272
H	0	-1.493751	-0.996872	-1.170819
H	0	-1.652403	3.000091	-1.985390
H	0	-6.349475	-4.256000	-0.324596
H	0	-0.958221	-2.254401	2.462176
H	0	-3.038066	3.787376	2.190580
H	0	-4.470826	-6.099974	-0.322917
H	0	-5.462846	-6.045628	1.142162
H	0	-3.781818	-6.592755	1.228398
H	0	-2.268346	-5.764855	2.724376
H	0	-1.313432	-4.347757	3.126276
H	0	0.587113	-1.037354	3.297591
H	0	1.100757	0.622355	3.584866
H	0	0.422252	2.801197	3.399481
H	0	-1.121424	3.505022	3.901824
H	0	-0.549998	3.728970	2.235738
H	0	-1.042546	-5.758735	0.405985
H	0	-0.151279	-6.246595	1.855186
H	0	1.493994	0.997718	1.171812
H	0	0.713956	-0.540459	0.769496
H	0	1.652458	-2.999606	1.986179
H	0	10.539813	0.400752	1.100554
H	0	9.567105	-0.699565	2.088151
H	0	9.923121	0.931890	2.671348
H	0	10.678469	2.867522	1.675494
H	0	10.253085	4.575045	2.237583
H	0	-8.402643	1.803979	-0.698292
H	0	-7.923070	-4.249681	-1.735788
H	0	-4.016127	5.511042	1.379102
H	0	-5.408806	5.678999	2.462637
H	0	-5.559068	6.107809	0.751898
H	0	-8.392745	3.912946	-0.824901
H	0	-7.800006	6.026057	1.339626
H	0	-9.119468	6.039061	0.045044
H	0	8.401923	-1.804513	0.699241
H	0	7.924161	4.249737	1.734105
H	0	5.408625	-5.679263	-2.462354
H	0	4.015517	-5.511111	-1.379397
H	0	5.558127	-6.108041	-0.751540
H	0	8.391594	-3.913504	0.826112
H	0	7.799345	-6.026605	-1.338557
H	0	9.118366	-6.039711	-0.043529
H	0	-9.567781	0.699258	-2.087311
H	0	-10.539996	-0.401995	-1.100278
H	0	-9.923172	-0.932013	-2.671398
H	0	-10.677834	-2.868401	-1.676440
H	0	-10.251906	-4.575522	-2.239336

20. FePPIX dimer (no internal hydrogen bonds), [{Fe(PPIXH)}$_2$] (m=7)

Method 1 (B3LYP/LanL2DZ)

Energies (Hartrees):	vacuum	-3914.984625
	water	-3915.068605
	n-octanol	-3915.078675
	ZPE	1.176175

S = 427.019 cal mol^{-1} K^{-1}

Method 2 [OPBE/6-311+G(d,p)]

Energies (Hartrees):	vacuum	-6195.817224
	water	-6195.884786
	n-octanol	-6195.899484

Method 3 [B3LYP/6-311+G(d,p)]

Energies (Hartrees):	vacuum	-6197.033929
	water	-6197.105346
	n-octanol	-6197.119169

Fe	0	4.056777	-0.417185	-0.796075
O	0	3.274992	-0.238647	0.956837
N	0	2.592344	0.358135	-1.940060
N	0	5.047064	1.339858	-0.933450
N	0	3.313359	-2.258923	-1.165424
N	0	5.774808	-1.293682	-0.158576
C	0	1.455304	-0.296414	-2.420209
C	0	0.548753	0.643748	-3.064848
C	0	1.139783	1.889911	-2.962344
C	0	2.402421	1.703989	-2.264492
C	0	4.537218	2.557390	-1.393184
C	0	5.488912	3.632334	-1.178192
C	0	6.601934	3.060891	-0.571382
C	0	6.306391	1.638050	-0.416761
C	0	6.940199	-0.645031	0.259228
C	0	7.879770	-1.589582	0.837179
C	0	7.269803	-2.839154	0.783375
C	0	5.965080	-2.636632	0.156839
C	0	3.817706	-3.474212	-0.703011
C	0	2.072025	-2.565549	-1.723271
C	0	1.793318	-3.991607	-1.613017
C	0	2.881289	-4.557799	-0.976401
C	0	5.046168	-3.652977	-0.080902
C	0	7.185602	0.718473	0.140190
C	0	3.297797	2.729423	-1.998471
C	0	1.204945	-1.656908	-2.309993
H	0	5.302635	-4.656825	0.235585
H	0	8.139023	1.087228	0.497436
H	0	3.016076	3.733229	-2.292873
H	0	0.249717	-2.015461	-2.667857
C	0	0.622035	3.208355	-3.471594
C	0	3.114673	-6.001335	-0.618093
C	0	0.547326	-4.666136	-2.127977
C	0	-0.755880	0.300793	-3.746476
C	0	5.252595	5.074174	-1.534724

C	0	7.843069	3.691666	-0.113150
C	0	8.421309	4.815415	-0.605993
C	0	9.253191	-1.248610	1.346557
C	0	7.777032	-4.146686	1.204419
C	0	8.753892	-4.400281	2.111732
C	0	-2.027256	0.666070	-2.940128
C	0	-0.680729	-4.469725	-1.200574
C	0	-1.908179	-5.148607	-1.757357
C	0	-2.361802	-0.276601	-1.770977
O	0	-1.845537	-1.419729	-1.655960
O	0	-2.856835	-5.406159	-0.767607
O	0	-2.119537	-5.459078	-2.939868
H	0	1.371424	3.732826	-4.079337
H	0	-0.268837	3.067958	-4.092516
H	0	0.344673	3.878044	-2.644870
H	0	4.023136	-6.394836	-1.094800
H	0	3.230795	-6.135434	0.466554
H	0	2.276990	-6.628941	-0.939005
H	0	0.289201	-4.292034	-3.125535
H	0	0.733375	-5.740015	-2.250425
H	0	-0.801270	0.838893	-4.704337
H	0	-0.795151	-0.765922	-3.988455
H	0	4.197526	5.344059	-1.424693
H	0	5.841253	5.734432	-0.886612
H	0	5.550374	5.290699	-2.571389
H	0	8.348141	3.196245	0.717194
H	0	8.022003	5.353762	-1.460445
H	0	9.338766	5.204928	-0.171530
H	0	9.647669	-0.338648	0.882118
H	0	9.255498	-1.089871	2.435137
H	0	9.956984	-2.062469	1.134488
H	0	7.311032	-5.010009	0.728499
H	0	9.255128	-3.617766	2.672614
H	0	9.055293	-5.421887	2.329874
H	0	-1.967667	1.684178	-2.538784
H	0	-2.901112	0.647523	-3.608621
H	0	-0.486362	-4.855338	-0.193029
H	0	-0.934164	-3.404408	-1.095409
H	0	-3.679664	-5.763688	-1.174461
Fe	0	-4.056806	0.417207	0.796054
O	0	-3.275195	0.238706	-0.957000
N	0	-2.592302	-0.358184	1.939882
N	0	-5.047212	-1.339768	0.933606
N	0	-3.313276	2.258911	1.165362
N	0	-5.774787	1.293741	0.158624
C	0	-1.455333	0.296356	2.420217
C	0	-0.548744	-0.643862	3.064712
C	0	-1.139652	-1.890063	2.961894
C	0	-2.402293	-1.704088	2.264082
C	0	-4.537294	-2.557351	1.393142
C	0	-5.489150	-3.632215	1.178471
C	0	-6.602343	-3.060675	0.572067
C	0	-6.306726	-1.637867	0.417324
C	0	-6.940317	0.645183	-0.258935
C	0	-7.879757	1.589734	-0.837089
C	0	-7.269578	2.839216	-0.783647
C	0	-5.964861	2.636652	-0.157126
C	0	-3.817474	3.474182	0.702733
C	0	-2.072012	2.565531	1.723374
C	0	-1.793222	3.991559	1.613039
C	0	-2.881044	4.557740	0.976154

C	0	-5.045850	3.652942	0.080445
C	0	-7.185945	-0.718249	-0.139551
C	0	-3.297708	-2.729490	1.998046
C	0	-1.205021	1.656872	2.310199
H	0	-5.302200	4.656754	-0.236258
H	0	-8.139493	-1.086912	-0.496550
H	0	-3.015932	-3.733344	2.292231
H	0	-0.249862	2.015433	2.668232
C	0	-0.621790	-3.208588	3.470819
C	0	-3.114232	6.001250	0.617610
C	0	-0.547245	4.666041	2.128104
C	0	0.755848	-0.300929	3.746422
C	0	-5.252866	-5.074081	1.534913
C	0	-7.843697	-3.691353	0.114291
C	0	-8.421812	-4.815083	0.607329
C	0	-9.253266	1.248858	-1.346293
C	0	-7.776664	4.146717	-1.204984
C	0	-8.753282	4.400164	-2.112592
C	0	2.027214	-0.666202	2.940063
C	0	0.680794	4.469659	1.200680
C	0	1.908289	5.148470	1.757445
C	0	2.361614	0.276520	1.770916
O	0	1.845247	1.419610	1.655992
O	0	2.856906	5.406008	0.767665
O	0	2.119695	5.458884	2.939963
H	0	-1.371270	-3.733455	4.078103
H	0	0.268834	-3.068244	4.092109
H	0	-0.344007	-3.877892	2.643923
H	0	-4.022803	6.394876	1.094006
H	0	-3.230036	6.135223	-0.467086
H	0	-2.276595	6.628832	0.938690
H	0	-0.289155	4.291872	3.125647
H	0	-0.733278	5.739914	2.250632
H	0	0.801187	-0.839084	4.704258
H	0	0.795142	0.765777	3.988417
H	0	-4.197849	-5.344056	1.424603
H	0	-5.841758	-5.734272	0.886944
H	0	-5.550376	-5.290594	2.571658
H	0	-8.349063	-3.195875	-0.715838
H	0	-8.022191	-5.353489	1.461596
H	0	-9.339468	-5.204522	0.173220
H	0	-9.647994	0.339264	-0.881341
H	0	-9.255609	1.089491	-2.434781
H	0	-9.956830	2.063036	-1.134699
H	0	-7.310777	5.010096	-0.729053
H	0	-9.254337	3.617539	-2.673489
H	0	-9.054647	5.421728	-2.330982
H	0	1.967630	-1.684305	2.538709
H	0	2.901093	-0.647635	3.608519
H	0	0.486423	4.855324	0.193153
H	0	0.934192	3.404341	1.095426
H	0	3.679785	5.763466	1.174480

21. FePPIX dimer (single Fe-O bond), [{Fe(PPIXH)}$_2$] (m=7)

Method 1 (B3LYP/LanL2DZ)

Energies (Hartrees):	vacuum	-3914.953259
	water	-3915.070454
	n-octanol	-3915.073261
	ZPE	1.171878

S = 417.955 cal mol^{-1} K^{-1}

Method 3 [B3LYP/6-311+G(d,p)]

Energies (Hartrees):	vacuum	-6196.986524
	water	-6197.096882
	n-octanol	-6197.102826

C	0	7.940479	-2.075906	-0.329356
C	0	7.153198	-3.099299	0.182521
C	0	5.790271	-2.982600	0.467034
C	0	4.978414	-4.069326	1.028381
C	0	3.692920	-3.586799	1.138609
C	0	3.722979	-2.206082	0.630697
C	0	2.607327	-1.389280	0.536829
C	0	2.639646	-0.045838	0.154669
C	0	1.456151	0.821142	0.142635
C	0	1.901181	2.091536	-0.154469
C	0	3.350807	1.979518	-0.376164
C	0	4.166254	3.041323	-0.744285
C	0	5.531755	2.940691	-1.016457
C	0	5.511773	-5.423805	1.407666
C	0	2.486782	-4.265088	1.745123
C	0	0.042986	0.374351	0.406854
C	0	1.085988	3.352851	-0.222981
C	0	1.530343	-5.003807	0.735028
C	0	0.099214	-4.475043	0.789622
C	0	-0.699484	-0.027987	-0.913365
C	0	-2.023641	-0.723069	-0.603881
Fe	0	5.644665	-0.048055	-0.366692
N	0	7.501334	-0.777828	-0.587002
N	0	5.021707	-1.846555	0.253232
N	0	3.788909	0.664526	-0.182935
N	0	6.282165	1.765525	-0.937270
O	0	-0.886229	-5.150998	1.159182
O	0	0.032814	-3.182003	0.399235
O	0	-3.127815	-0.097821	-0.921943
C	0	-4.652014	-3.149296	0.859448
C	0	-4.154689	-2.753638	2.090214
C	0	-4.034829	-1.428560	2.488412
C	0	-3.458509	-1.012566	3.762022
C	0	-3.455472	0.369038	3.770866
C	0	-4.053764	0.790150	2.503758
C	0	-4.229638	2.116238	2.135665
C	0	-4.778242	2.521542	0.926873
C	0	-4.918705	3.924292	0.535895
C	0	-5.522647	3.926626	-0.705301
C	0	-5.727675	2.532064	-1.075325
C	0	-6.295716	2.129516	-2.276671
C	0	-6.451869	0.805682	-2.666732

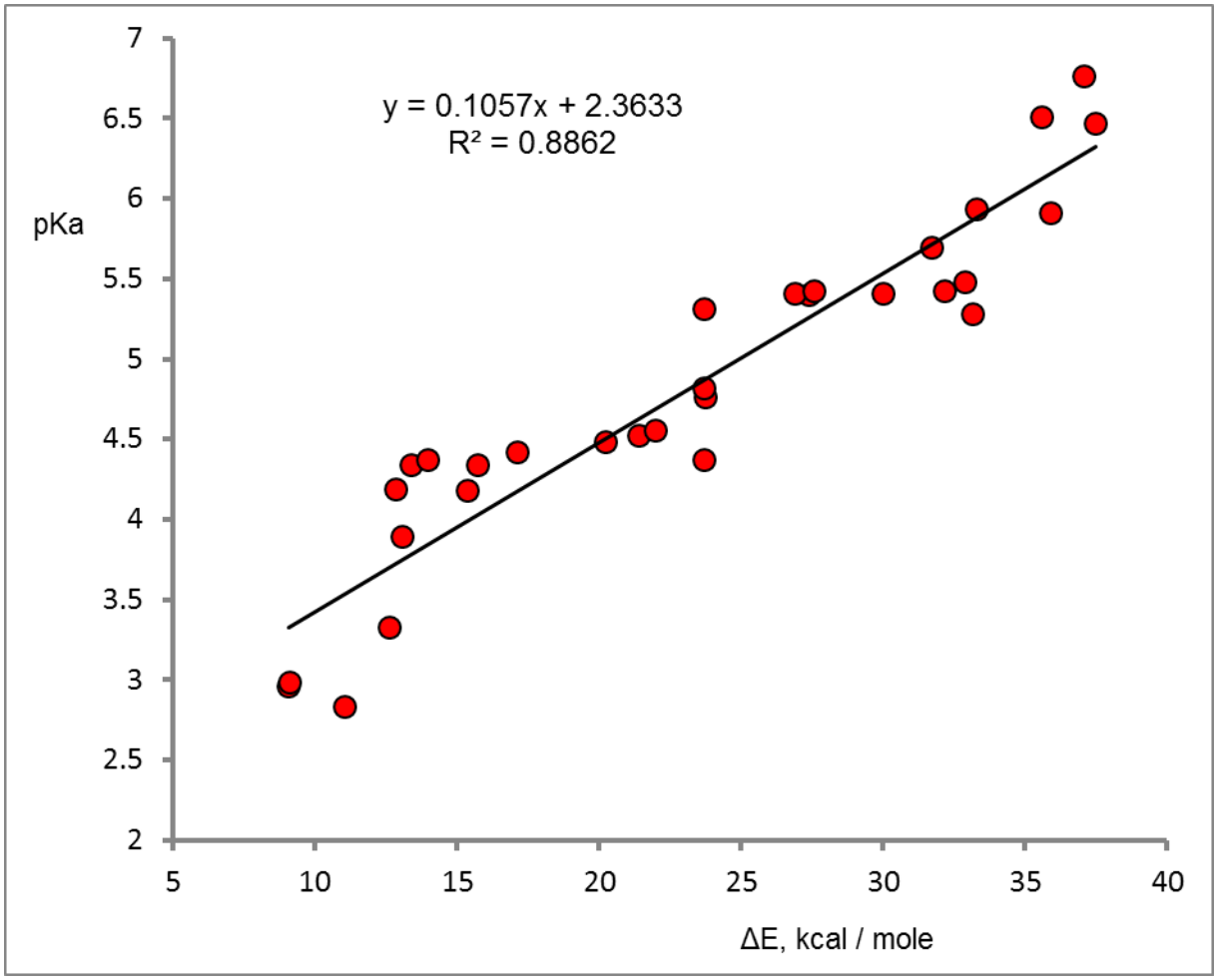
C	0	-2.951730	-1.962189	4.812590
C	0	-2.898175	1.288487	4.828231
C	0	-4.384618	5.094313	1.314804
C	0	-5.885063	5.107961	-1.563285
C	0	-1.461529	1.815827	4.507357
C	0	-1.465447	2.972596	3.490632
C	0	-2.900930	5.388403	0.916198
C	0	-2.352380	6.586255	1.705477
Fe	0	-4.988676	-0.305172	-0.195251
N	0	-5.161250	-2.300061	-0.123756
N	0	-4.400806	-0.318796	1.724483
N	0	-5.267608	1.676273	-0.070523
N	0	-6.041075	-0.308908	-1.922338
O	0	-0.820723	2.862517	2.393358
O	0	-2.194552	4.005174	3.841313
O	0	-2.242880	7.717317	1.181064
C	0	11.156879	-0.565662	-1.585958
C	0	11.460321	-3.602023	-0.334639
O	0	-2.019973	-1.869594	-0.029022
C	0	-5.589545	-3.147750	-1.149876
C	0	-5.346774	-4.544431	-0.809462
C	0	-4.749009	-4.547357	0.438937
C	0	-7.067153	0.395979	-3.919371
C	0	-7.037662	-0.992477	-3.940463
C	0	-6.388660	-1.414024	-2.696372
C	0	-6.172193	-2.740012	-2.342557
C	0	-4.194650	-5.677498	1.199374
C	0	-7.583956	1.332788	-4.975479
C	0	-7.499421	-1.923997	-4.970895
C	0	-8.446764	-1.698281	-5.915656
C	0	8.626455	-0.091279	-1.042751
C	0	9.795266	-0.968962	-1.092623
C	0	9.375333	-2.209002	-0.638557
C	0	6.360070	4.066339	-1.446328
C	0	7.637728	3.563732	-1.637047
C	0	7.570881	2.125327	-1.321408
C	0	8.659167	1.262171	-1.382981
C	0	10.120793	-3.460697	-0.499796
C	0	5.864257	5.468030	-1.666198
C	0	8.853436	4.238496	-2.092871
C	0	9.140929	5.561302	-1.996845
O	0	-2.033648	6.344072	2.991266
C	0	-5.641413	-5.712192	-1.708901
C	0	-4.796233	-6.879896	1.358837
H	0	7.623486	-4.054419	0.383912
H	0	1.645358	-1.831544	0.764327
H	0	3.702111	4.015406	-0.839441
H	0	6.339452	-5.347099	2.125902
H	0	5.889384	-5.967519	0.530114
H	0	4.732523	-6.042728	1.863658
H	0	1.907532	-3.520369	2.302367
H	0	2.830727	-4.996337	2.485578
H	0	-0.500135	1.178658	0.916155
H	0	0.040438	-0.488704	1.081594
H	0	1.701467	4.250631	-0.098209
H	0	0.331898	3.358470	0.573518
H	0	0.565298	3.443027	-1.187956
H	0	1.502561	-6.075565	0.950725
H	0	1.897064	-4.867778	-0.288875
H	0	-0.073472	-0.728608	-1.481701
H	0	-0.889071	0.855881	-1.528093

H	0	-0.897514	-2.690562	0.263852
H	0	-3.814389	-3.525482	2.769703
H	0	-3.891704	2.883551	2.821961
H	0	-6.636395	2.904453	-2.952483
H	0	-2.123697	-2.576135	4.432135
H	0	-3.739341	-2.650261	5.148864
H	0	-2.585612	-1.421188	5.690286
H	0	-2.867309	0.749976	5.783541
H	0	-3.540568	2.164184	4.978752
H	0	-4.431897	4.903894	2.391816
H	0	-4.989454	5.987913	1.117514
H	0	-5.661364	6.047792	-1.049845
H	0	-6.954379	5.113010	-1.816225
H	0	-5.323087	5.108765	-2.507692
H	0	-0.821537	1.007358	4.137921
H	0	-1.032055	2.204759	5.440179
H	0	-2.853248	5.630006	-0.150607
H	0	-2.285573	4.502690	1.115009
H	0	-2.087012	5.333692	3.317811
H	0	11.800153	-0.213729	-0.766022
H	0	11.098856	0.240358	-2.325519
H	0	11.664641	-1.414856	-2.057895
H	0	12.134355	-2.755973	-0.242425
H	0	11.908353	-4.589512	-0.258270
H	0	-6.490322	-3.512061	-3.031530
H	0	-3.198139	-5.521821	1.614049
H	0	-7.077720	2.303191	-4.943065
H	0	-8.661650	1.520637	-4.861280
H	0	-7.430207	0.909973	-5.975227
H	0	-7.023575	-2.904785	-4.971491
H	0	-9.011155	-0.772933	-5.974826
H	0	-8.696346	-2.465635	-6.644090
H	0	9.612521	1.674147	-1.689970
H	0	9.525163	-4.373324	-0.533465
H	0	5.991072	6.088901	-0.767399
H	0	4.801178	5.489034	-1.927398
H	0	6.417663	5.952325	-2.479173
H	0	9.604923	3.600281	-2.558562
H	0	8.481500	6.273254	-1.510518
H	0	10.075816	5.954980	-2.387663
H	0	-5.366492	-5.499552	-2.749666
H	0	-6.708771	-5.977037	-1.697272
H	0	-5.079351	-6.593816	-1.385099
H	0	-5.794357	-7.087230	0.978142
H	0	-4.302598	-7.682393	1.901492

Table S9. Calculated deprotonation energies (ΔE_p, kcal mol^{-1}) and experimentally determined pK_a values for simple organic acids and diacids.

pK_a values were obtained from standard literature sources and from the compilation of R. Williams, http://research.chem.psu.edu/brpgroup/pka_compilation.pdf (accessed 8 July 2013). DFT calculations used the B3LYP/LanL2DZ level of theory with SMD solvent corrections.

acid, ionization	ΔE_p	pK_a
malonic, pK_a 1	11.04	2.83
tartaric, pK_a 1	9.07	2.96
phthalic, pK_a 1	9.14	2.98
1,2-*cis*-cyclopropane-dicarboxylic, pK_a 1	12.66	3.33
1,2-*trans*-cyclopentane-dicarboxylic, pK_a 1	13.1	3.89
1,2-*trans*-cyclohexane-dicarboxylic, pK_a 1	15.4	4.18
succinic, pK_a 1	12.86	4.19
1,2-*cis*-cyclohexane-dicarboxylic, pK_a 1	13.4	4.34
glutaric, pK_a 1	15.73	4.34
1,2-*cis*-cyclopentane-dicarboxylic, pK_a 1	14	4.37
tartaric, pK_a 2	23.72	4.37
adipic, pK_a 1	17.16	4.42
pimelic, pK_a 1	20.26	4.48
suberic, pK_a 1	21.4	4.52
azelaic, pK_a 1	22	4.55
acetic	23.74	4.76
butyric	23.72	4.82
phthalic, pK_a 2	33.16	5.28
lauric	23.7	5.31
suberic, pK_a 2	27.4	5.40
azelaic, pK_a 2	26.9	5.41
adipic, pK_a 2	30	5.41
glutaric, pK_a 2	32.19	5.42
pimelic, pK_a 2	27.59	5.42
succinic, pK_a 2	32.9	5.48
malonic, pK_a 2	31.71	5.69
1,2-*trans*-cyclopentane-dicarboxylic, pK_a 2	35.9	5.91
1,2-*trans*-cyclohexane-dicarboxylic, pK_a 2	33.3	5.93
1,2-*cis*-cyclopropane-dicarboxylic, pK_a 2	37.5	6.47
1,2-*cis*-cyclopentane-dicarboxylic, pK_a 2	35.6	6.51
1,2-*cis*-cyclohexane-dicarboxylic, pK_a 2	37.1	6.76



Graph of experimental pK_a against calculated deprotonation energy, ΔE_p, where ΔE_p is calculated in water for the following reaction;

$HA^n + H_2O \rightarrow A^{n-1} + H_3O^+$

The calculated energies of H_2O and H_3O^+ in water (SMD implicit solvent method) were -76.432623 and -76.854229 Hartrees respectively.