Electronic Supplementary Material (ESI) for Dalton Transactions.

SUPPLEMENTARY INFORMATION

Computational insights into the inhibition of haemozoin crystallization by antimalarial drugs

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Notes: all energies in this document are raw values. Spins on Fe are for the method 1 vacuum job unless noted otherwise; the values did not vary by much for the method 3 solvent jobs. The zero-point energies given in this file were scaled by 0.981 before addition to the SMD solvent energies, to obtain the corrected values used throughout the main paper.

List of abbreviations:

m1 method 1 (B3LYP/LanL2DZ for geometry optimization and frequency calculations, followed by single point solvent energies using B3LYP/LanL2DZ and SMD implicit solvent model)

m3 method 3 (B3LYP/LanL2DZ for geometry optimization and frequency calculations, followed by single point solvent energies using B3LYP/6-311+G(d,p) and SMD implicit solvent model)

ZPE Zero-point energy

CONTENTS

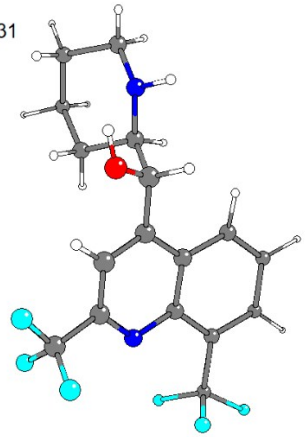
1. Mefloquine (MQ)

1.1 Free Mefloquine

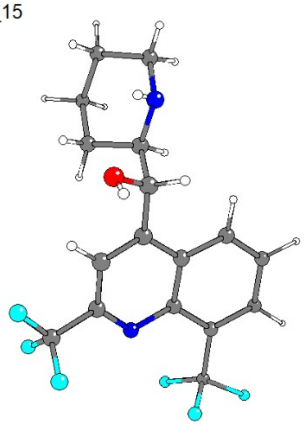
Minimum conformer in n-octanol (both methods) and water (method 1): MQ_31.
Minimum conformer in water (method 3): MQ_15. Energies:

conformer	ZPE	m1 (octanol)	m1 (water)	m3 (octanol)	m3 (water)
MQ_31	0.316636	-1441.167208	-1441.160693	-1441.674034	-1441.666191
MQ_15	0.316073	-1441.165438	-1441.160096	-1441.672860	-1441.666215

MQ_31



MQ_15



MQ_31 atomic coordinates:

1	6	0	2.650964	5.265256	0.842795
2	6	0	1.745453	5.617671	-0.348441
3	7	0	1.479773	4.410988	-1.175349
4	6	0	0.898660	3.242160	-0.459815
5	6	0	1.757140	2.891059	0.775300
6	6	0	2.017922	4.124618	1.666945
7	6	0	0.870757	2.087572	-1.522441
8	6	0	0.446495	0.743051	-0.960097
9	6	0	1.404094	-0.238117	-0.726138
10	6	0	0.996032	-1.472292	-0.159011
11	7	0	-0.258939	-1.775488	0.164016
12	6	0	-1.230176	-0.838706	-0.080127
13	6	0	-0.927184	0.451062	-0.652331
14	6	0	-2.004917	1.361257	-0.895247
15	6	0	-3.309572	1.017712	-0.578863
16	6	0	-3.606395	-0.249479	0.000082
17	6	0	-2.591327	-1.161794	0.245157
18	6	0	2.014524	-2.556321	0.136297
19	9	0	1.732672	-3.756020	-0.521078
20	9	0	3.307986	-2.174743	-0.264231
21	9	0	2.096694	-2.850427	1.503091
22	6	0	-2.923137	-2.501575	0.854091
23	9	0	-2.305331	-2.716775	2.091871
24	9	0	-4.309653	-2.619104	1.099434
25	9	0	-2.595374	-3.585636	0.033087
26	8	0	2.197177	1.954625	-2.095961
27	1	0	-0.136343	3.439377	-0.121077
28	1	0	2.799161	6.158687	1.464001
29	1	0	3.636047	4.952092	0.469773
30	1	0	2.224252	6.367829	-0.989748
31	1	0	0.804911	6.057474	0.037639
32	1	0	0.924870	4.650544	-2.001570
33	1	0	2.717289	2.479224	0.436761
34	1	0	1.251741	2.108855	1.355300
35	1	0	2.672665	3.844080	2.502184

36	1	0	1.071146	4.474911	2.108240
37	1	0	0.165806	2.384690	-2.319226
38	1	0	2.436090	-0.049971	-0.988101
39	1	0	-1.805113	2.328194	-1.345575
40	1	0	-4.120731	1.712829	-0.774525
41	1	0	-4.632053	-0.502881	0.244629
42	1	0	2.584004	2.866065	-2.098322

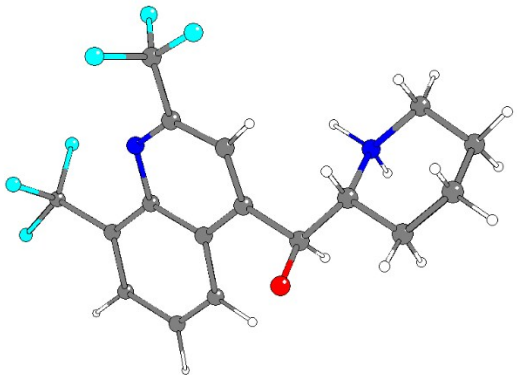
MQ_15 atomic coordinates:

1	6	0	-5.687847	-0.410900	1.346748
2	6	0	-5.403942	-1.471102	0.252725
3	7	0	-4.402885	-1.023879	-0.745331
4	6	0	-3.135288	-0.559106	-0.133340
5	6	0	-3.346036	0.539009	0.941968
6	6	0	-4.365551	0.052760	2.002315
7	6	0	-2.195123	-0.129844	-1.288353
8	6	0	-0.761114	0.125880	-0.840972
9	6	0	-0.317092	1.425863	-0.623212
10	6	0	1.018876	1.632450	-0.191061
11	7	0	1.898657	0.658648	0.024244
12	6	0	1.493835	-0.635413	-0.187478
13	6	0	0.157772	-0.959709	-0.624210
14	6	0	-0.184745	-2.335003	-0.826748
15	6	0	0.749524	-3.334756	-0.606756
16	6	0	2.068171	-3.015249	-0.172332
17	6	0	2.437492	-1.694601	0.034569
18	6	0	1.533533	3.035146	0.068513
19	9	0	2.657229	3.347513	-0.699736
20	9	0	0.559255	4.005215	-0.236987
21	9	0	1.884446	3.236651	1.407482
22	6	0	3.838234	-1.372739	0.492979
23	9	0	4.551343	-0.578349	-0.412060
24	9	0	3.882157	-0.727929	1.734412
25	9	0	4.604805	-2.548337	0.650039
26	8	0	-2.795989	1.070625	-1.876431
27	1	0	-2.675396	-1.430266	0.359031
28	1	0	-6.365997	-0.827471	2.105525
29	1	0	-6.198026	0.453040	0.893258
30	1	0	-6.324159	-1.740213	-0.280524
31	1	0	-5.024005	-2.388912	0.726245
32	1	0	-3.713654	1.451511	0.454511
33	1	0	-2.393935	0.786488	1.431516
34	1	0	-4.558483	0.855064	2.727035
35	1	0	-3.929555	-0.786451	2.568282
36	1	0	-2.219597	-0.940083	-2.030916
37	1	0	-0.986877	2.261274	-0.779796
38	1	0	-1.183451	-2.603301	-1.156500
39	1	0	0.482473	-4.375263	-0.765728
40	1	0	2.786753	-3.810044	-0.004636
41	1	0	-4.777805	-0.295895	-1.358227
42	1	0	-2.442700	1.234208	-2.775754

1.2 Mefloquine Zwitterion

Single conformer for all methods and solvents (designated MQZA_6). Energies:

ZPE	m1 (octanol)	m1 (water)	m3 (octanol)	m3 (water)
0.316059	-1441.137183	-1441.141522	-1441.641188	-1441.643884



Atomic coordinates:

1	6	0	4.289972	4.127723	1.380022
2	6	0	4.139272	2.646359	0.996352
3	7	0	2.681672	2.216887	1.129200
4	6	0	1.676761	3.093284	0.309183
5	6	0	1.862809	4.555306	0.721155
6	6	0	3.324474	5.026879	0.571314
7	6	0	0.213965	2.605240	0.568590
8	6	0	-0.010861	1.133389	0.162203
9	6	0	0.792207	0.439938	-0.749163
10	6	0	0.468776	-0.901200	-1.085736
11	7	0	-0.564253	-1.577673	-0.593397
12	6	0	-1.404485	-0.914694	0.273950
13	6	0	-1.178531	0.451977	0.664867
14	6	0	-2.127337	1.100828	1.513584
15	6	0	-3.228024	0.405129	1.993116
16	6	0	-3.431723	-0.959870	1.644533
17	6	0	-2.544536	-1.611426	0.797051
18	6	0	1.352667	-1.678627	-2.039615
19	9	0	2.461740	-0.902892	-2.460227
20	9	0	1.896552	-2.831441	-1.459116
21	9	0	0.695621	-2.080110	-3.201937
22	6	0	-2.786631	-3.049406	0.423835
23	9	0	-1.748774	-3.909554	0.816263
24	9	0	-3.946696	-3.555899	1.053052
25	9	0	-2.987319	-3.255058	-0.946606
26	8	0	-0.683600	3.408319	-0.095298
27	1	0	1.958776	2.960843	-0.742860
28	1	0	5.333991	4.416930	1.206358
29	1	0	4.102977	4.251357	2.457879
30	1	0	4.746295	1.989530	1.630214
31	1	0	4.415656	2.478925	-0.050200
32	1	0	2.377624	2.280629	2.111879
33	1	0	1.519841	4.688601	1.760688
34	1	0	1.172899	5.131707	0.098143
35	1	0	3.420891	6.065247	0.910732
36	1	0	3.612454	5.011661	-0.490582
37	1	0	0.134089	2.629358	1.707387
38	1	0	1.639240	0.905472	-1.240691
39	1	0	-2.003056	2.158436	1.717066
40	1	0	-3.956850	0.904048	2.625087
41	1	0	-4.295383	-1.490901	2.030266
42	1	0	2.554869	1.238668	0.830200

1.3 [(FePPIXH)(MQ)]

See Fig. 1 for image. Charge 0, overall spin 5/2. Calculated spin on Fe: +4.05.

Energies:

ZPE	m1 (octanol)	m1 (water)	m3 (octanol)	m3 (water)
0.903698	-3398.729206	-3398.717496	-4540.243260	-4540.228977

Atomic coordinates:

1	26	0	0.829791	-1.348094	-0.915461
2	8	0	3.930653	3.538279	-0.001886
3	7	0	0.856233	-3.371250	-0.386537
4	6	0	1.901899	-4.057900	0.232857
5	8	0	1.677069	3.474023	0.378856
6	7	0	-0.985721	-1.705244	-1.885036
7	6	0	1.448594	-5.367730	0.679764
8	8	0	8.294042	2.429281	-0.540584
9	7	0	1.055536	0.316071	-2.151695
10	6	0	0.104929	-5.472047	0.320731
11	8	0	7.767678	2.971016	1.629186
12	1	0	8.530708	3.586175	1.532414
13	7	0	2.913052	-1.363101	-0.711682
14	6	0	-0.242769	-4.222688	-0.363415
15	6	0	-1.488291	-3.938420	-0.933799
16	1	0	-2.265213	-4.685259	-0.818529
17	6	0	-1.832110	-2.791735	-1.655573
18	6	0	-3.128483	-2.563673	-2.284624
19	6	0	-3.057949	-1.317414	-2.901996
20	6	0	-1.711160	-0.797020	-2.648169
21	6	0	-1.239041	0.448318	-3.075407
22	1	0	-1.928325	1.073165	-3.633441
23	6	0	0.035017	0.972853	-2.838889
24	6	0	0.486701	2.295751	-3.260529
25	6	0	1.792631	2.434253	-2.821751
26	6	0	2.150607	1.180322	-2.160718
27	6	0	3.409603	0.881141	-1.635649
28	1	0	4.176795	1.639188	-1.734074
29	6	0	3.773142	-0.301636	-0.985322
30	6	0	5.115197	-0.599961	-0.486757
31	6	0	5.056475	-1.862218	0.081366
32	6	0	3.679024	-2.330195	-0.063258
33	6	0	3.204349	-3.565963	0.382260
34	1	0	3.921797	-4.211124	0.878548
35	6	0	2.308353	-6.400870	1.355114
36	6	0	-0.829338	-6.583328	0.507217
37	1	0	-1.702852	-6.579106	-0.144880
38	6	0	-0.737019	-7.604207	1.396699
39	1	0	0.066555	-7.686807	2.121321
40	1	0	-1.500259	-8.377562	1.430578
41	6	0	-4.277427	-3.533682	-2.282459
42	6	0	-4.070347	-0.613645	-3.695042
43	1	0	-3.688730	0.061562	-4.462446
44	6	0	-5.416104	-0.715076	-3.564002
45	1	0	-5.885354	-1.319012	-2.793240
46	1	0	-6.082013	-0.152993	-4.214126
47	6	0	-0.358387	3.296300	-4.002756
48	1	0	-1.221092	3.621925	-3.404457
49	1	0	-0.751603	2.876176	-4.938635
50	1	0	0.219599	4.189828	-4.260499
51	6	0	2.663459	3.665165	-2.870272
52	1	0	2.443031	4.251476	-3.771496
53	1	0	3.724125	3.393834	-2.923659
54	6	0	2.458815	4.597846	-1.626741
55	1	0	3.156796	5.439892	-1.708899
56	1	0	1.432866	4.978974	-1.610751
57	6	0	2.740725	3.845718	-0.325483
58	6	0	6.305375	0.321420	-0.590900
59	1	0	6.319378	0.831739	-1.560825
60	1	0	7.232848	-0.262095	-0.548835

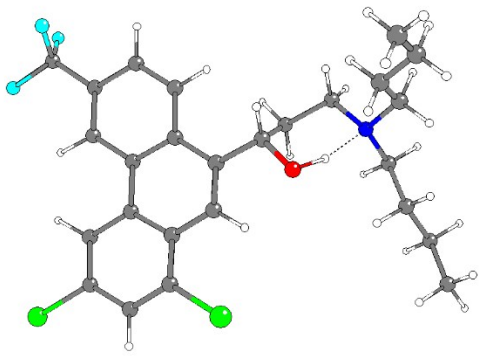
61	6	0	6.330636	1.392072	0.531435
62	1	0	6.316278	0.924942	1.524074
63	1	0	5.450898	2.051204	0.470025
64	6	0	7.548111	2.280301	0.440186
65	6	0	6.166707	-2.651208	0.723906
66	1	0	5.950491	-2.872983	1.778598
67	1	0	7.114290	-2.103975	0.690986
68	1	0	6.323231	-3.612400	0.215125
69	1	0	-4.956488	-3.352982	-1.437934
70	1	0	-3.932318	-4.571480	-2.212888
71	1	0	-4.866118	-3.436136	-3.202109
72	1	0	2.172179	-6.394355	2.446712
73	1	0	3.372984	-6.238332	1.157082
74	1	0	2.054274	-7.408095	1.002663
75	6	0	2.622681	0.917702	4.329185
76	6	0	2.743188	1.955986	3.201831
77	7	0	1.917210	1.572220	2.002046
78	6	0	0.461027	1.292992	2.310698
79	6	0	0.316340	0.272839	3.455167
80	6	0	1.140123	0.683058	4.697742
81	6	0	-0.190205	0.832209	0.964473
82	6	0	-1.712690	0.886786	1.045714
83	6	0	-2.445525	-0.281706	1.214463
84	6	0	-3.857620	-0.193814	1.307485
85	7	0	-4.548925	0.941674	1.245062
86	6	0	-3.853330	2.110444	1.063625
87	6	0	-2.415143	2.138291	0.946799
88	6	0	-1.760235	3.394973	0.725986
89	6	0	-2.502844	4.563482	0.649261
90	6	0	-3.920955	4.541258	0.783784
91	6	0	-4.588249	3.341565	0.982627
92	6	0	-4.694881	-1.441832	1.497734
93	9	0	-5.608874	-1.646075	0.452283
94	9	0	-3.899852	-2.603248	1.550329
95	9	0	-5.439011	-1.421290	2.680566
96	6	0	-6.089741	3.334685	1.111414
97	9	0	-6.617749	4.641891	1.011733
98	9	0	-6.735783	2.595879	0.111966
99	9	0	-6.542992	2.843459	2.342593
100	8	0	0.294732	-0.475742	0.653149
101	1	0	0.031747	2.258997	2.607731
102	1	0	3.188449	1.272349	5.200534
103	1	0	3.082513	-0.030404	4.011276
104	1	0	3.773619	2.088894	2.857594
105	1	0	2.377500	2.934983	3.535436
106	1	0	1.911791	2.475583	1.244967
107	1	0	0.640845	-0.709539	3.089293
108	1	0	-0.744752	0.182750	3.719104
109	1	0	1.060149	-0.096910	5.465613
110	1	0	0.724363	1.603905	5.135734
111	1	0	0.139327	1.537785	0.188037
112	1	0	-1.935489	-1.234703	1.263036
113	1	0	-0.681154	3.447024	0.598147
114	1	0	-2.001338	5.511899	0.480705
115	1	0	-4.482466	5.467300	0.724093
116	1	0	2.311672	0.743565	1.538105

2. Halofantrine (HN)

2.1 Free Halofantrine

Single conformer for all methods and solvents (designated HF19_1). Energies:

ZPE	m1 (octanol)	m1 (water)	m3 (octanol)	m3 (water)
0.515246	-1468.128602	-1468.110434	-2359.238439	-2359.219222



Atomic coordinates:

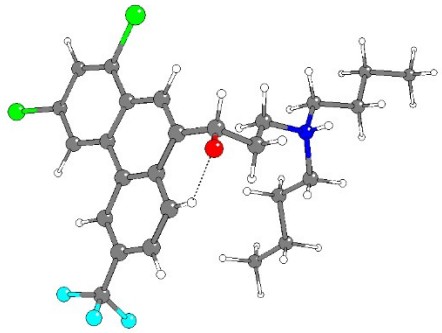
1	6	0	3.515350	-2.646740	-0.324068
2	6	0	3.669830	-1.275141	-0.154371
3	1	0	4.672228	-0.865857	-0.164545
4	6	0	2.546135	-0.425189	0.034923
5	6	0	2.706158	1.015346	0.231702
6	6	0	3.983543	1.644054	0.233363
7	1	0	4.891166	1.074182	0.081455
8	6	0	4.079740	3.011996	0.434114
9	6	0	2.946983	3.828965	0.640561
10	1	0	3.048139	4.896480	0.795389
11	6	0	1.703705	3.212222	0.636602
12	6	0	1.528218	1.811529	0.436535
13	6	0	0.232333	1.188860	0.430467
14	1	0	-0.653869	1.784878	0.606616
15	6	0	0.067401	-0.159809	0.223135
16	6	0	1.232870	-1.008202	0.036763
17	6	0	1.113077	-2.422561	-0.130104
18	1	0	0.132552	-2.883672	-0.104779
19	6	0	2.223956	-3.234336	-0.306776
20	1	0	2.111918	-4.308263	-0.422730
21	6	0	4.702793	-3.533413	-0.534688
22	6	0	-1.346480	-0.732754	0.179510
23	1	0	-1.376047	-1.672825	0.759005
24	6	0	-1.808584	-1.040975	-1.276686
25	1	0	-1.121507	-1.748868	-1.758732
26	1	0	-1.760331	-0.107843	-1.853285
27	6	0	-3.236401	-1.633794	-1.321025
28	1	0	-3.501776	-1.898745	-2.360450
29	1	0	-3.251829	-2.564011	-0.739437
30	6	0	-5.434841	-1.439953	-0.170859
31	1	0	-5.777603	-2.220770	-0.877883
32	1	0	-6.259337	-0.724539	-0.069307
33	6	0	-5.160614	-2.067215	1.210166
34	1	0	-4.841821	-1.276199	1.903352
35	1	0	-4.326813	-2.782909	1.148342
36	6	0	-6.401115	-2.792561	1.777924
37	1	0	-7.236804	-2.079567	1.853499
38	1	0	-6.723106	-3.576060	1.074006
39	6	0	-6.138808	-3.421932	3.161875
40	1	0	-5.330657	-4.164440	3.110777
41	1	0	-7.034422	-3.926675	3.546713

42	1	0	-5.843091	-2.656997	3.892375
43	6	0	-4.664437	0.362951	-1.698432
44	1	0	-3.784998	0.626576	-2.298585
45	1	0	-5.426984	-0.023006	-2.402098
46	6	0	-5.181299	1.639617	-1.007472
47	1	0	-4.388715	2.035308	-0.356552
48	1	0	-6.035787	1.402274	-0.356709
49	6	0	-5.609463	2.721299	-2.024197
50	1	0	-4.756150	2.968635	-2.674713
51	1	0	-6.395537	2.317049	-2.681332
52	6	0	-6.121455	4.006881	-1.342055
53	1	0	-6.997068	3.797396	-0.712421
54	1	0	-6.413635	4.762035	-2.083260
55	1	0	-5.346275	4.446987	-0.700561
56	7	0	-4.261357	-0.707742	-0.734754
57	1	0	-3.180951	0.006954	0.413243
58	8	0	-2.260463	0.221480	0.782613
59	9	0	5.925892	-2.859445	-0.432979
60	9	0	4.699940	-4.153096	-1.804733
61	9	0	4.755452	-4.596988	0.390292
62	17	0	5.717664	3.799194	0.434901
63	17	0	0.252878	4.281731	0.899235

2.2 Halofantrine Zwitterion

Single conformer for all methods and solvents (designated HFZ_5). Energies:

ZPE	m1 (octanol)	m1 (water)	m3 (octanol)	m3 (water)
0.514804	-1468.086104	-1468.079515	-2359.196041	-2359.188156



Atomic coordinates:

1	6	0	-3.182244	-2.223067	0.234555
2	6	0	-3.087506	-0.893385	-0.167948
3	1	0	-3.740464	-0.543807	-0.958610
4	6	0	-2.161015	-0.009502	0.451094
5	6	0	-2.068920	1.399476	0.062590
6	6	0	-2.909227	1.970207	-0.934158
7	1	0	-3.654305	1.373120	-1.444483
8	6	0	-2.788884	3.313348	-1.258104
9	6	0	-1.850374	4.160624	-0.631989
10	1	0	-1.774450	5.207830	-0.898882
11	6	0	-1.033462	3.596896	0.339009
12	6	0	-1.098886	2.228148	0.727911
13	6	0	-0.227548	1.651019	1.718112
14	1	0	0.500526	2.298377	2.198961
15	6	0	-0.286798	0.323790	2.085200
16	6	0	-1.305359	-0.526429	1.482175
17	6	0	-1.464886	-1.880329	1.916101
18	1	0	-0.873414	-2.166412	2.789236
19	6	0	-2.377550	-2.722215	1.294503
20	1	0	-2.502118	-3.747012	1.632867
21	6	0	-4.114895	-3.157019	-0.467961

22	6	0	0.737254	-0.239003	3.114862
23	1	0	1.260998	0.669453	3.526034
24	6	0	1.905925	-1.001566	2.280165
25	1	0	1.433714	-1.866238	1.800263
26	1	0	2.580787	-1.362544	3.070222
27	6	0	2.632871	-0.106735	1.287714
28	1	0	1.997835	0.199201	0.452560
29	1	0	2.997822	0.798933	1.790540
30	6	0	4.692637	0.270445	-0.166815
31	1	0	4.813251	1.144707	0.483371
32	1	0	4.056035	0.564404	-1.005885
33	6	0	6.066254	-0.225649	-0.646167
34	1	0	5.953258	-1.029342	-1.385790
35	1	0	6.634619	-0.641047	0.201596
36	6	0	6.880761	0.927589	-1.281158
37	1	0	6.307928	1.364451	-2.112704
38	1	0	7.019266	1.728214	-0.539580
39	6	0	8.256840	0.458373	-1.795234
40	1	0	8.863573	0.040871	-0.980665
41	1	0	8.815720	1.293711	-2.233670
42	1	0	8.150762	-0.314847	-2.567734
43	6	0	3.598252	-2.060370	-0.095729
44	1	0	4.561151	-2.492578	-0.387962
45	1	0	3.137441	-2.722821	0.642347
46	6	0	2.678831	-1.903143	-1.315994
47	1	0	3.122060	-1.225843	-2.059537
48	1	0	1.713041	-1.477612	-1.016893
49	6	0	2.430134	-3.280381	-1.979479
50	1	0	3.391883	-3.723505	-2.281125
51	1	0	1.983789	-3.963229	-1.242082
52	6	0	1.501464	-3.175492	-3.206279
53	1	0	0.518024	-2.778569	-2.924423
54	1	0	1.343669	-4.160172	-3.662221
55	1	0	1.927381	-2.514268	-3.973103
56	7	0	3.907306	-0.754778	0.653768
57	1	0	4.496096	-1.024084	1.454443
58	8	0	0.221567	-1.078025	4.058422
59	9	0	-4.818681	-4.001210	0.408794
60	9	0	-3.438631	-4.035978	-1.356650
61	9	0	-5.079117	-2.505441	-1.252667
62	17	0	-3.873307	4.026568	-2.535680
63	17	0	0.186617	4.708031	1.130504

2.3 [(FePPIXH)(HN)]

See Fig. 1 for image. Charge 0, overall spin 5/2. Calculated spin on Fe: +4.04.

Energies:

ZPE	m1 (octanol)	m1 (water)	m3 (octanol)	m3 (water)
1.102348	-3425.673700	-3425.653110	-5457.794700	-5457.771466

Atomic coordinates:

1	6	0	1.750735	-0.829563	-3.093494
2	6	0	3.167669	-0.827644	-3.434671
3	6	0	3.757444	-1.857289	-2.703726
4	6	0	2.682396	-2.490581	-1.931452
5	6	0	2.844207	-3.582459	-1.073896
6	1	0	3.849967	-3.967671	-0.947760
7	6	0	1.832432	-4.251807	-0.377247
8	6	0	2.040690	-5.444045	0.430905
9	6	0	0.788940	-5.855007	0.876168
10	6	0	-0.179634	-4.873748	0.370181
11	6	0	-1.552202	-4.869167	0.640224
12	1	0	-1.923139	-5.641609	1.303503
13	6	0	-2.490430	-3.964072	0.134651
14	6	0	-3.928510	-4.025515	0.389485

15	6	0	-4.507027	-2.979272	-0.308056
16	6	0	-3.416924	-2.275839	-0.986552
17	6	0	-3.575542	-1.152980	-1.803043
18	1	0	-4.580865	-0.762324	-1.901077
19	6	0	-2.560078	-0.475406	-2.481881
20	6	0	-2.769592	0.682138	-3.350892
21	6	0	-1.531721	1.015794	-3.876497
22	6	0	-0.564875	0.073621	-3.315449
23	6	0	0.802028	0.063169	-3.606239
24	1	0	1.157731	0.816072	-4.301912
25	6	0	3.819464	0.098695	-4.424645
26	1	0	4.593118	-0.426475	-4.998303
27	1	0	4.305318	0.951354	-3.927541
28	1	0	3.095523	0.506256	-5.138231
29	6	0	5.148484	-2.313438	-2.685209
30	1	0	5.304239	-3.333762	-2.333051
31	6	0	6.254588	-1.616663	-3.050303
32	1	0	6.219595	-0.582605	-3.378184
33	1	0	7.238955	-2.075577	-3.000842
34	6	0	3.374691	-6.100541	0.665344
35	1	0	3.292937	-6.935399	1.368542
36	1	0	4.104081	-5.387401	1.072325
37	1	0	3.793994	-6.502891	-0.267833
38	6	0	0.524063	-7.047010	1.692790
39	1	0	1.309191	-7.300660	2.407643
40	6	0	-0.549784	-7.871876	1.629666
41	1	0	-1.349150	-7.738873	0.905591
42	1	0	-0.628467	-8.732625	2.289257
43	6	0	-4.609132	-5.050852	1.256452
44	1	0	-5.698537	-4.984429	1.165877
45	1	0	-4.358495	-4.910354	2.317491
46	1	0	-4.314676	-6.073424	0.984386
47	6	0	-5.967373	-2.594916	-0.357726
48	1	0	-6.586267	-3.501282	-0.410358
49	1	0	-6.179915	-2.018567	-1.264278
50	6	0	-6.442932	-1.760894	0.870969
51	1	0	-7.505529	-1.517035	0.732207
52	1	0	-6.336691	-2.334229	1.796505
53	6	0	-5.659394	-0.453990	1.016323
54	6	0	-4.094381	1.374867	-3.561675
55	1	0	-4.890194	0.649583	-3.765247
56	1	0	-4.039743	2.022108	-4.444594
57	6	0	-4.495591	2.222694	-2.322446
58	1	0	-4.685290	1.567664	-1.458506
59	1	0	-3.684932	2.906779	-2.044441
60	6	0	-5.740060	3.062172	-2.481213
61	6	0	-1.188160	2.114606	-4.847745
62	1	0	-2.075345	2.690706	-5.129645
63	1	0	-0.751212	1.710299	-5.771403
64	1	0	-0.457522	2.819021	-4.425661
65	6	0	3.200711	4.691283	-0.543141
66	6	0	4.033029	3.755425	0.061115
67	1	0	5.069340	4.021212	0.228260
68	6	0	3.543767	2.479685	0.454018
69	6	0	4.415095	1.494276	1.092981
70	6	0	5.786443	1.760288	1.368174
71	1	0	6.237037	2.710491	1.111896
72	6	0	6.569377	0.793269	1.978037
73	6	0	6.058792	-0.468966	2.351014
74	1	0	6.689610	-1.207024	2.831671
75	6	0	4.722002	-0.723411	2.080823
76	6	0	3.857804	0.219494	1.451357
77	6	0	2.474503	-0.058117	1.177829
78	1	0	2.065861	-1.029731	1.428497
79	6	0	1.640282	0.865306	0.594033
80	6	0	2.162161	2.166821	0.212663
81	6	0	1.336411	3.152994	-0.410554
82	1	0	0.294207	2.931200	-0.609433
83	6	0	1.834755	4.391974	-0.785311
84	1	0	1.190603	5.127416	-1.258142
85	6	0	3.727026	6.027036	-0.966969
86	6	0	0.160697	0.506958	0.401475
87	1	0	-0.207061	0.946775	-0.539123
88	6	0	-0.681096	1.086816	1.577946
89	1	0	-0.621315	2.183425	1.548299
90	1	0	-0.220904	0.752794	2.515549
91	6	0	-2.139555	0.603939	1.498528

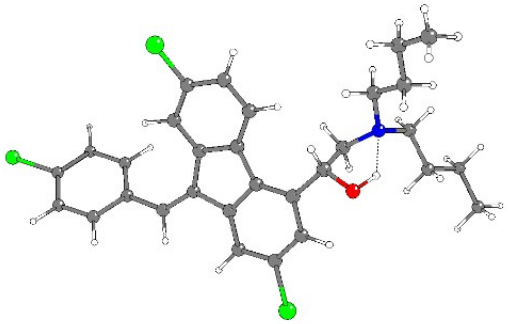
92	1	0	-2.523174	0.701732	0.476590
93	1	0	-2.182605	-0.459365	1.751180
94	6	0	-3.508241	2.689421	1.886731
95	1	0	-3.691890	2.578639	0.812611
96	1	0	-2.660903	3.373725	2.023456
97	6	0	-4.780247	3.255010	2.543897
98	1	0	-4.622870	3.417587	3.620364
99	1	0	-5.591961	2.523273	2.439375
100	6	0	-5.204283	4.589113	1.886413
101	1	0	-4.378098	5.314777	1.959652
102	1	0	-5.391093	4.428016	0.815473
103	6	0	-6.467392	5.185763	2.540530
104	1	0	-7.315083	4.492818	2.455383
105	1	0	-6.754710	6.126630	2.054368
106	1	0	-6.305952	5.391636	3.608191
107	6	0	-2.857050	1.214849	3.871864
108	1	0	-3.830329	1.243782	4.376526
109	1	0	-2.445178	0.212303	4.039772
110	6	0	-1.931565	2.280122	4.491737
111	1	0	-2.352393	3.284119	4.343140
112	1	0	-0.946149	2.271763	4.011120
113	6	0	-1.755226	2.036594	6.008810
114	1	0	-2.742407	2.039478	6.495950
115	1	0	-1.329931	1.034517	6.171620
116	6	0	-0.850525	3.093372	6.675664
117	1	0	0.154740	3.089643	6.232946
118	1	0	-0.743797	2.902227	7.751026
119	1	0	-1.266428	4.102802	6.553867
120	7	0	1.475932	-1.846377	-2.178713
121	7	0	0.480930	-3.912210	-0.388208
122	7	0	-2.199402	-2.888400	-0.700073
123	7	0	-1.208328	-0.815535	-2.455590
124	7	0	-3.144078	1.310778	2.386968
125	1	0	-4.117361	0.629124	2.253981
126	8	0	-5.068237	-0.269847	2.182934
127	8	0	-5.575339	0.363086	0.041453
128	8	0	-5.995201	4.104169	-1.853165
129	8	0	-6.641845	2.539809	-3.401944
130	1	0	-7.459704	3.087880	-3.426826
131	8	0	-0.021510	-0.913668	0.341792
132	26	0	-0.297218	-2.097075	-1.073683
133	9	0	5.062274	6.239976	-0.603289
134	9	0	2.989585	7.098282	-0.421634
135	9	0	3.666152	6.214480	-2.366208
136	17	0	8.318206	1.147357	2.321519
137	17	0	4.079175	-2.353720	2.583917

3. Lumefantrine (LM)

3.1 Free Lumefantrine

Single conformer for all methods and solvents (designated LFZ4). Energies:

ZPE	m1 (octanol)	m1 (water)	m3 (octanol)	m3 (water)
0.553073	-1337.101281	-1337.081035	-2673.480768	-2673.459623



Atomic coordinates:

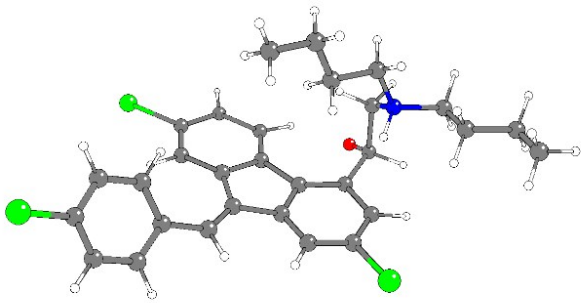
1	6	0	-0.456865	-3.428325	-1.147480
2	6	0	-1.567771	-2.577579	-1.174713
3	6	0	0.845060	-2.966932	-0.919013
4	6	0	1.014330	-1.588782	-0.728662
5	6	0	-0.095979	-0.693261	-0.746163
6	6	0	-1.402783	-1.191142	-0.960381
7	6	0	2.272087	-0.838218	-0.461828
8	6	0	1.860483	0.588946	-0.374913
9	6	0	0.439960	0.674520	-0.540867
10	6	0	-0.186072	1.933878	-0.534695
11	6	0	0.583992	3.104625	-0.390191
12	6	0	1.975373	2.992644	-0.262418
13	6	0	2.634103	1.755556	-0.253257
14	6	0	3.493792	-1.444894	-0.382997
15	6	0	4.813147	-0.921973	0.022376
16	6	0	4.985127	-0.027039	1.108831
17	6	0	6.264230	0.392719	1.509983
18	6	0	7.384935	-0.086743	0.816406
19	6	0	7.259207	-0.989140	-0.249528
20	6	0	5.974495	-1.410758	-0.628536
21	17	0	9.043039	0.457766	1.327085
22	6	0	-2.648299	-0.316568	-0.937974
23	8	0	-3.753322	-1.014457	-1.570276
24	6	0	-3.089406	0.024535	0.523314
25	7	0	-4.481928	0.538667	0.512976
26	6	0	-5.276325	0.128533	1.705254
27	6	0	-5.760424	-1.333434	1.646599
28	6	0	-6.564036	-1.734593	2.903794
29	6	0	-7.061161	-3.194207	2.850239
30	6	0	-4.569417	1.995054	0.212600
31	6	0	-5.891855	2.401816	-0.466672
32	6	0	-5.969018	3.920077	-0.742056
33	6	0	-7.285485	4.333100	-1.432500
34	17	0	-0.710808	-5.213391	-1.424414
35	17	0	2.969170	4.512393	-0.100939
36	1	0	-2.563041	-2.953321	-1.376996
37	1	0	1.677042	-3.662352	-0.897282
38	1	0	-1.257240	2.036801	-0.655650
39	1	0	0.111209	4.081332	-0.387767
40	1	0	3.712365	1.720860	-0.172864
41	1	0	3.513865	-2.504143	-0.644530
42	1	0	4.119736	0.314887	1.667918

43	1	0	6.385099	1.070276	2.349113
44	1	0	8.139716	-1.358117	-0.765550
45	1	0	5.870781	-2.117370	-1.448927
46	1	0	-2.454597	0.611952	-1.496351
47	1	0	-3.066393	-0.905706	1.099459
48	1	0	-2.380854	0.725930	0.993923
49	1	0	-4.697530	0.291686	2.635872
50	1	0	-6.154276	0.782854	1.764492
51	1	0	-6.382991	-1.464058	0.749534
52	1	0	-4.904751	-2.015053	1.535025
53	1	0	-5.937229	-1.594324	3.798336
54	1	0	-7.425491	-1.058135	3.018115
55	1	0	-7.628681	-3.456172	3.752712
56	1	0	-7.714865	-3.356234	1.982509
57	1	0	-6.218551	-3.894084	2.767745
58	1	0	-4.421090	2.594852	1.132661
59	1	0	-3.744066	2.252017	-0.465232
60	1	0	-5.989001	1.846136	-1.410454
61	1	0	-6.746256	2.108110	0.160612
62	1	0	-5.865662	4.469434	0.206757
63	1	0	-5.116843	4.221409	-1.371178
64	1	0	-7.317583	5.414972	-1.615520
65	1	0	-7.399615	3.824989	-2.399585
66	1	0	-8.154219	4.071253	-0.812940
67	1	0	-4.565276	-0.635270	-1.139329

3.2 Lumefantrine Zwitterion

Single conformer for all methods and solvents (designated LFZ2). Energies:

ZPE	m1 (octanol)	m1 (water)	m3 (octanol)	m3 (water)
0.553119	-1337.069458	-1337.058837	-2673.445156	-2673.433485



Atomic coordinates:

1	6	0	2.015529	-2.174677	-1.639859
2	6	0	2.760813	-0.990608	-1.742362
3	6	0	0.646135	-2.176475	-1.362317
4	6	0	0.020575	-0.926354	-1.220786
5	6	0	0.745568	0.297604	-1.345819
6	6	0	2.147171	0.277871	-1.578391
7	6	0	-1.405221	-0.642762	-0.884363
8	6	0	-1.512728	0.841654	-0.879511
9	6	0	-0.229948	1.401889	-1.176572
10	6	0	-0.066986	2.789114	-1.345002
11	6	0	-1.187024	3.630025	-1.184480
12	6	0	-2.436140	3.062518	-0.890511
13	6	0	-2.633055	1.681769	-0.745943
14	6	0	-2.324454	-1.636906	-0.696951
15	6	0	-3.718042	-1.595392	-0.214286
16	6	0	-4.652244	-2.524164	-0.740606
17	6	0	-5.979499	-2.569412	-0.284393
18	6	0	-6.371533	-1.689529	0.734410
19	6	0	-5.471139	-0.778766	1.305577

20	6	0	-4.150760	-0.736885	0.828057
21	17	0	-8.084703	-1.744419	1.344824
22	6	0	3.073488	1.534543	-1.622531
23	8	0	2.624354	2.633816	-2.306695
24	6	0	3.333320	1.996589	-0.129689
25	7	0	3.865190	0.877525	0.820694
26	6	0	5.372037	0.692325	0.648500
27	6	0	5.852958	-0.715178	1.037943
28	6	0	7.381111	-0.859938	0.845621
29	6	0	7.886672	-2.268897	1.216818
30	6	0	3.466602	1.095664	2.278523
31	6	0	2.007927	0.695969	2.558110
32	6	0	1.631542	0.952932	4.035563
33	6	0	0.177030	0.544249	4.346608
34	17	0	2.876610	-3.777294	-1.856657
35	17	0	-3.885634	4.164405	-0.704490
36	1	0	3.817635	-1.041558	-1.995102
37	1	0	0.104203	-3.111306	-1.268981
38	1	0	0.918590	3.150626	-1.664322
39	1	0	-1.092475	4.703499	-1.315102
40	1	0	-3.627592	1.295671	-0.567373
41	1	0	-1.983591	-2.647476	-0.928349
42	1	0	-4.340237	-3.208892	-1.526176
43	1	0	-6.688550	-3.274188	-0.706727
44	1	0	-5.789273	-0.121212	2.108275
45	1	0	-3.445231	-0.055133	1.292088
46	1	0	4.057237	1.139664	-2.000495
47	1	0	4.078222	2.797975	-0.139323
48	1	0	2.395984	2.368841	0.289965
49	1	0	5.590496	0.891806	-0.404717
50	1	0	5.857311	1.467127	1.253009
51	1	0	5.603355	-0.938038	2.085618
52	1	0	5.338775	-1.464347	0.417165
53	1	0	7.639074	-0.642208	-0.201196
54	1	0	7.900050	-0.108878	1.460449
55	1	0	8.971186	-2.347304	1.072848
56	1	0	7.669842	-2.504597	2.267558
57	1	0	7.409442	-3.036930	0.594176
58	1	0	4.143994	0.504132	2.904756
59	1	0	3.636581	2.156662	2.491904
60	1	0	1.323841	1.254832	1.906706
61	1	0	1.867113	-0.371428	2.327348
62	1	0	2.317802	0.397217	4.693014
63	1	0	1.768382	2.020232	4.266260
64	1	0	0.016371	-0.524965	4.155106
65	1	0	-0.069832	0.738256	5.397664
66	1	0	-0.531122	1.107697	3.725270
67	1	0	3.406360	0.012624	0.486721

3.3 [(FePPIXH)(LM)]

See Fig. 1 for image. Charge 0, overall spin 5/2. Calculated spin on Fe: +4.04.

Energies:

ZPE	m1 (octanol)	m1 (water)	m3 (octanol)	m3 (water)
1.141868	-3294.654212	-3294.631857	-5772.039599	-5772.014959

Atomic coordinates:

1	6	0	3.679305	-2.876999	0.166103
2	6	0	2.338742	-2.423662	-0.010931
3	6	0	2.393766	-1.010728	-0.467791
4	6	0	3.774348	-0.637544	-0.576582
5	6	0	4.631318	-1.797756	-0.208788
6	6	0	5.986895	-1.958256	-0.149270
7	6	0	7.094127	-1.098282	-0.612075
8	6	0	8.291604	-1.057823	0.146809
9	6	0	9.398745	-0.301038	-0.269614
10	6	0	9.316357	0.403333	-1.479217
11	6	0	8.164780	0.359627	-2.278423

12	6	0	7.060673	-0.390537	-1.840360
13	6	0	4.138697	0.676995	-0.906609
14	6	0	3.109655	1.590731	-1.159169
15	6	0	1.756618	1.248790	-1.096397
16	6	0	1.378820	-0.063965	-0.739332
17	6	0	3.955698	-4.180528	0.603483
18	6	0	2.868408	-5.022727	0.872123
19	6	0	1.539186	-4.607594	0.706484
20	6	0	1.267845	-3.297867	0.258317
21	17	0	10.746822	1.379203	-2.036193
22	17	0	3.568686	3.308314	-1.588445
23	17	0	3.199120	-6.721322	1.450578
24	6	0	-0.123005	-0.396053	-0.719158
25	6	0	-0.461315	-1.040606	-2.095451
26	7	0	-1.793473	-1.756575	-2.167113
27	6	0	-2.993538	-0.813390	-2.205874
28	6	0	-3.178680	-0.053298	-3.531338
29	6	0	-4.408580	0.880915	-3.470426
30	6	0	-4.634527	1.639524	-4.794363
31	6	0	-1.838701	-2.752347	-3.316489
32	6	0	-0.963120	-4.002428	-3.107402
33	6	0	-1.188167	-5.023440	-4.246345
34	6	0	-0.295184	-6.272596	-4.099199
35	1	0	6.331363	-2.889578	0.303356
36	1	0	8.352614	-1.614488	1.079326
37	1	0	10.304318	-0.265966	0.327379
38	1	0	8.131192	0.890127	-3.224684
39	1	0	6.182462	-0.453617	-2.475125
40	1	0	5.171645	0.994353	-0.946328
41	1	0	0.982301	1.982185	-1.288255
42	1	0	4.969979	-4.543477	0.732345
43	1	0	0.719634	-5.287901	0.913145
44	1	0	0.223017	-3.030038	0.148182
45	1	0	-0.429196	-0.258670	-2.861894
46	1	0	0.309163	-1.780666	-2.325849
47	1	0	-3.864955	-1.439687	-1.981029
48	1	0	-2.854595	-0.106491	-1.385815
49	1	0	-2.289416	0.554396	-3.752110
50	1	0	-3.313436	-0.751588	-4.369130
51	1	0	-5.304012	0.287193	-3.229959
52	1	0	-4.277442	1.599279	-2.649763
53	1	0	-5.511981	2.296552	-4.731904
54	1	0	-3.765743	2.263908	-5.044300
55	1	0	-4.798377	0.943054	-5.628266
56	1	0	-2.887413	-3.058731	-3.408834
57	1	0	-1.552803	-2.233786	-4.240209
58	1	0	0.102920	-3.735632	-3.079530
59	1	0	-1.205230	-4.460671	-2.140848
60	1	0	-2.245563	-5.328425	-4.257505
61	1	0	-0.988880	-4.544147	-5.218014
62	1	0	-0.473597	-6.986376	-4.913653
63	1	0	0.769034	-6.001193	-4.115874
64	1	0	-0.493096	-6.788243	-3.150149
65	8	0	-0.917179	0.781698	-0.510275
66	1	0	-0.334645	-1.117332	0.079368
67	1	0	-1.922087	-2.379872	-1.218767
68	26	0	-1.505770	1.696375	1.018145
69	8	0	-4.247242	-3.241263	0.077012
70	7	0	-1.599587	3.708557	0.433707
71	6	0	-2.656889	4.341163	-0.220624
72	8	0	-1.959756	-3.187777	-0.066934
73	7	0	-3.590591	1.656659	0.810809
74	6	0	-2.237374	5.646547	-0.711649
75	8	0	-8.207237	-2.993901	-1.338709
76	7	0	-1.694493	0.080961	2.321254
77	6	0	-0.907172	5.810989	-0.327761
78	8	0	-8.635646	-2.492178	0.860724
79	7	0	0.270708	2.162626	2.030394
80	6	0	-0.528889	4.594809	0.398109
81	6	0	0.701852	4.390023	1.029405
82	1	0	1.436484	5.181352	0.936213
83	6	0	1.068466	3.286124	1.805296
84	6	0	2.339917	3.150068	2.503513
85	6	0	2.307674	1.919671	3.157002
86	6	0	1.005240	1.317680	2.854152
87	6	0	0.575621	0.063712	3.303480
88	1	0	1.271432	-0.515888	3.900472

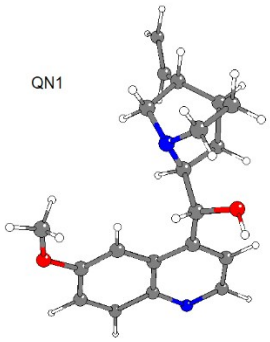
89	6	0	-0.667713	-0.519757	3.047974
90	6	0	-1.082511	-1.846917	3.498324
91	6	0	-2.372603	-2.040431	3.037155
92	6	0	-2.757768	-0.818309	2.334427
93	6	0	-4.019219	-0.575956	1.789585
94	1	0	-4.760625	-1.357312	1.900152
95	6	0	-4.416362	0.577233	1.110136
96	6	0	-5.766975	0.818494	0.605876
97	6	0	-5.751102	2.068446	0.011339
98	6	0	-4.387322	2.581912	0.139124
99	6	0	-3.947095	3.812157	-0.352453
100	1	0	-4.682573	4.424620	-0.863879
101	6	0	-3.097440	6.592675	-1.504204
102	6	0	0.012169	6.921439	-0.584580
103	6	0	3.434017	4.181195	2.517598
104	6	0	-0.217583	-2.801938	4.275988
105	1	0	-0.787477	-3.680463	4.596977
106	1	0	0.197060	-2.329821	5.177113
107	1	0	0.629807	-3.159885	3.674139
108	6	0	-3.210768	-3.292072	3.090377
109	1	0	-4.278468	-3.044904	3.106497
110	1	0	-3.004816	-3.853084	4.011285
111	6	0	-2.942013	-4.245314	1.876296
112	1	0	-3.664888	-5.069437	1.917479
113	1	0	-1.928093	-4.652364	1.948590
114	6	0	-3.092269	-3.521354	0.531755
115	6	0	-6.915454	-0.151634	0.725228
116	1	0	-6.938766	-0.607282	1.722162
117	1	0	-7.868171	0.380989	0.617612
118	6	0	-6.847719	-1.285706	-0.332865
119	1	0	-6.884707	-0.880460	-1.350885
120	1	0	-5.907795	-1.853394	-0.247958
121	6	0	-7.972020	-2.279069	-0.167011
122	6	0	-6.883941	2.802627	-0.655092
123	1	0	-7.823866	2.248003	-0.566980
124	1	0	-6.692451	2.957176	-1.726818
125	1	0	-7.041824	3.792978	-0.206595
126	6	0	3.305967	1.296687	4.028265
127	6	0	4.638956	1.547466	4.072578
128	6	0	-0.303438	8.205791	-0.888951
129	1	0	-8.900941	-3.676731	-1.188037
130	1	0	-3.542542	7.371024	-0.866820
131	1	0	-3.919435	6.071771	-2.006821
132	1	0	-2.505362	7.102933	-2.273940
133	1	0	1.072791	6.674622	-0.526008
134	1	0	3.943869	4.195199	3.488374
135	1	0	3.046117	5.188170	2.330254
136	1	0	4.191826	3.974831	1.747660
137	1	0	2.922885	0.544097	4.718440
138	1	0	5.129957	2.246183	3.402700
139	1	0	5.276849	1.024618	4.781094
140	1	0	-1.325832	8.567336	-0.935098
141	1	0	0.478193	8.937948	-1.076384

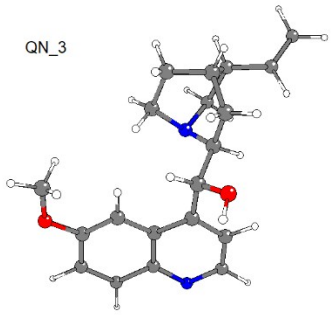
4. Quinine (QN)

4.1 Free Quinine

Minimum conformer in n-octanol (both methods): QN1. Minimum conformer in water (both methods): QN_3. Energies:

conformer	ZPE	m1 (octanol)	m1 (water)	m3 (octanol)	m3 (water)
QN1	0.411305	-1036.347902	-1036.345666	-1036.777606	-1036.773971
QN_3	0.410898	-1036.346846	-1036.346290	-1036.776953	-1036.774809





Atomic coordinates for QN1:

1	8	0	-0.565864	-1.738178	-2.257931
2	7	0	1.986660	-0.079168	-1.279072
3	8	0	0.901729	-0.962895	4.264670
4	7	0	-3.911051	-0.653923	1.428591
5	6	0	2.686143	1.230575	-1.148699
6	1	0	3.765975	1.045737	-1.188959
7	1	0	2.462180	1.644344	-0.157423
8	6	0	2.260027	2.247450	-2.285370
9	1	0	3.125141	2.445671	-2.935243
10	6	0	1.181591	1.518086	-3.153220
11	1	0	0.834148	2.194445	-3.943990
12	6	0	1.835985	0.257089	-3.777293
13	1	0	1.101662	-0.265238	-4.402741
14	1	0	2.676024	0.549760	-4.422571
15	6	0	2.316456	-0.676607	-2.610938
16	1	0	1.837587	-1.655197	-2.679840
17	1	0	3.402685	-0.827224	-2.640462
18	6	0	0.514084	0.157149	-1.127685
19	1	0	0.410570	0.696050	-0.177702
20	6	0	-0.026803	1.062386	-2.288980
21	1	0	-0.718958	0.500354	-2.923754
22	1	0	-0.572446	1.924293	-1.886770
23	6	0	1.789939	3.567711	-1.721078
24	1	0	0.947075	3.522903	-1.025466
25	6	0	2.335487	4.770949	-1.994663
26	1	0	3.180316	4.874380	-2.674896
27	1	0	1.954647	5.686931	-1.548303
28	6	0	-0.255168	-1.179190	-0.937473
29	1	0	0.431374	-1.863914	-0.418525
30	6	0	-1.519583	-0.997253	-0.102117
31	6	0	-2.770261	-0.902021	-0.704949
32	1	0	-2.858685	-0.955796	-1.784923
33	6	0	-3.937159	-0.730043	0.094523
34	1	0	-4.914486	-0.653318	-0.376752
35	6	0	-2.682630	-0.743499	2.054604
36	6	0	-2.651758	-0.662257	3.482777
37	1	0	-3.599661	-0.537242	3.996782
38	6	0	-1.456907	-0.739569	4.171962
39	1	0	-1.412014	-0.679636	5.254942

40	6	0	-0.229753	-0.902550	3.454872
41	6	0	-0.217027	-0.986412	2.065455
42	1	0	0.719699	-1.103176	1.532261
43	6	0	-1.446560	-0.911229	1.333666
44	6	0	2.205701	-1.129902	3.634034
45	1	0	2.258614	-2.077175	3.080113
46	1	0	2.923965	-1.141195	4.455782
47	1	0	2.427987	-0.294697	2.956004
48	1	0	-0.973991	-2.624163	-2.158231

Atomic coordinates for QN_3:

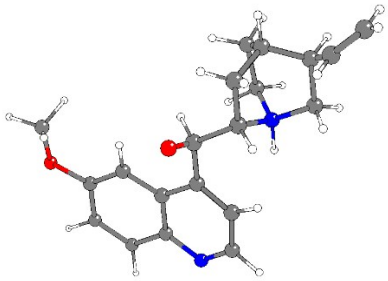
1	8	0	-0.485486	2.882408	0.371828
2	7	0	0.434253	-0.211333	-1.524630
3	8	0	-2.818447	-2.952070	2.332025
4	7	0	1.893077	-0.210324	3.575596
5	6	0	1.470994	-0.318021	-2.589437
6	1	0	1.561057	-1.372472	-2.875468
7	1	0	2.434339	-0.010512	-2.166954
8	6	0	1.101799	0.567888	-3.853404
9	1	0	1.037106	-0.079807	-4.739963
10	6	0	-0.328416	1.150950	-3.589740
11	1	0	-0.645122	1.739652	-4.459157
12	6	0	-1.295040	-0.039628	-3.362930
13	1	0	-2.325919	0.329672	-3.276744
14	1	0	-1.264742	-0.722942	-4.222681
15	6	0	-0.848962	-0.769060	-2.046545
16	1	0	-0.695901	-1.841070	-2.217479
17	1	0	-1.616195	-0.677943	-1.270342
18	6	0	0.307697	1.229668	-1.146182
19	1	0	1.332248	1.594380	-0.998433
20	6	0	-0.354683	2.036159	-2.313431
21	1	0	-1.394358	2.291156	-2.069872
22	1	0	0.164970	2.987477	-2.464446
23	6	0	2.138576	1.632500	-4.128874
24	1	0	2.329627	2.342301	-3.319365
25	6	0	2.843706	1.754539	-5.272431
26	1	0	3.585716	2.538575	-5.406326
27	1	0	2.699084	1.071859	-6.109188
28	6	0	-0.404911	1.418491	0.212712
29	1	0	-1.426887	1.020833	0.156740
30	6	0	0.354522	0.797943	1.381993
31	6	0	1.538588	1.405162	1.799444
32	1	0	1.897703	2.298039	1.296993
33	6	0	2.277608	0.871434	2.889661
34	1	0	3.204148	1.344323	3.207433
35	6	0	0.719069	-0.827685	3.196356
36	6	0	0.306700	-1.976968	3.943047
37	1	0	0.946687	-2.294445	4.760270
38	6	0	-0.859510	-2.646645	3.631531
39	1	0	-1.190579	-3.518905	4.186426
40	6	0	-1.668818	-2.190562	2.544433
41	6	0	-1.300063	-1.081120	1.791568
42	1	0	-1.919308	-0.758030	0.964496
43	6	0	-0.095981	-0.366942	2.096554
44	6	0	-3.709688	-2.585357	1.241382
45	1	0	-4.116976	-1.574286	1.383735
46	1	0	-3.194516	-2.644116	0.272152
47	1	0	-4.520473	-3.315646	1.272097
48	1	0	-0.813136	3.104216	1.269027

4.2 Quinine Zwitterion

Minimum conformer by method 3 (both solvents): QNZ31. Minima by method 1; n-octanol: QNZ_6, water: QNZ_3. Energies:

conformer	ZPE	m1 (octanol)	m1 (water)	m3 (octanol)	m3 (water)
QNZ31	0.411386	-1036.319630	-1036.326712	-1036.748034	-1036.753268
QNZ_6	0.411696	-1036.322194	-1036.325055	-1036.747425	-1036.748763
QNZ_3	0.411124	-1036.319169	-1036.326802	-1036.747354	-1036.752994

QNZ31:



Atomic coordinates:

1	8	0	1.396167	-1.398666	-1.154183
2	7	0	-0.270104	2.006983	-0.829920
3	8	0	0.832800	-3.663589	3.651018
4	7	0	-3.427617	-1.916137	0.463763
5	6	0	-0.258994	3.176948	-1.802014
6	1	0	-1.028829	3.893749	-1.494692
7	1	0	-0.529051	2.776516	-2.783970
8	6	0	1.166160	3.823467	-1.811429
9	1	0	1.119043	4.785162	-1.281602
10	6	0	2.124184	2.882593	-1.006839
11	1	0	3.145927	3.271457	-1.079376
12	6	0	1.670776	2.884823	0.476697
13	1	0	2.286047	2.179422	1.045501
14	1	0	1.802150	3.878612	0.921592
15	6	0	0.177448	2.464526	0.554325
16	1	0	0.011918	1.632794	1.241276
17	1	0	-0.477026	3.295105	0.842505
18	6	0	0.647735	0.842463	-1.381292
19	1	0	0.211172	0.591818	-2.355833
20	6	0	2.073139	1.429472	-1.541569
21	1	0	2.760297	0.782629	-0.987434
22	1	0	2.393258	1.382550	-2.586702
23	6	0	1.632092	4.092606	-3.226724
24	1	0	1.751440	3.218251	-3.870209
25	6	0	1.902493	5.315528	-3.723696
26	1	0	1.797195	6.217496	-3.121823
27	1	0	2.242657	5.451032	-4.747333
28	6	0	0.635203	-0.447721	-0.498974
29	1	0	1.068163	-0.126371	0.494973
30	6	0	-0.792752	-0.947089	-0.191289
31	6	0	-1.915249	-0.668313	-0.980299
32	1	0	-1.831047	-0.111255	-1.913077
33	6	0	-3.199999	-1.175334	-0.624369
34	1	0	-4.064733	-0.951927	-1.247411
35	6	0	-2.332871	-2.253400	1.243502
36	6	0	-2.549950	-3.085429	2.386239
37	1	0	-3.570195	-3.387322	2.602581
38	6	0	-1.487828	-3.505345	3.166777
39	1	0	-1.629458	-4.149857	4.029243

40	6	0	-0.153484	-3.122577	2.822604
41	6	0	0.095121	-2.294204	1.733779
42	1	0	1.101821	-2.054206	1.414438
43	6	0	-0.994390	-1.823247	0.937016
44	6	0	2.227620	-3.411420	3.311578
45	1	0	2.462568	-3.782729	2.305402
46	1	0	2.810319	-3.956588	4.057053
47	1	0	2.461475	-2.338816	3.367765
48	1	0	-1.213767	1.599908	-0.754412

4.3 [(FePPIXH)(QN1)]

See Fig. 1 for image. Charge 0, overall spin 5/2. Calculated spin on Fe: +4.04.

Energies:

ZPE	m1 (octanol)	m1 (water)	m3 (octanol)	m3 (water)
0.999615	-2993.909814	-2993.902156	-4135.346275	-4135.335844

Atomic coordinates:

1	26	0	-0.704737	1.416833	-0.822187
2	8	0	4.065097	-1.763370	-0.918760
3	7	0	-1.367454	3.270166	-0.100943
4	6	0	-0.570726	4.303683	0.392553
5	8	0	2.161320	-2.809565	-0.188491
6	7	0	1.185282	2.303122	-1.050148
7	6	0	-1.396571	5.301171	1.059146
8	8	0	7.742122	0.248764	-0.310062
9	7	0	-0.115541	0.023489	-2.257556
10	6	0	-2.717902	4.870015	0.944510
11	8	0	7.419543	0.903905	-2.487356
12	7	0	-2.677657	1.032808	-1.411670
13	6	0	-2.680866	3.601711	0.208945
14	8	0	-0.477018	0.389026	0.719057
15	7	0	1.960213	-1.321874	1.861868
16	6	0	-3.805754	2.868117	-0.184200
17	1	0	-4.773199	3.263483	0.104188
18	8	0	-0.692333	-6.321306	0.289207
19	7	0	-4.429078	-2.538212	2.024985
20	6	0	-3.814451	1.698845	-0.951873
21	6	0	-5.018270	1.003274	-1.391544
22	6	0	-4.596066	-0.105386	-2.121303
23	6	0	-3.129692	-0.069804	-2.126651
24	6	0	-2.306152	-1.021703	-2.737707
25	1	0	-2.791965	-1.866711	-3.213587
26	6	0	-0.909851	-0.991583	-2.787820
27	6	0	-0.068743	-2.013603	-3.406864
28	6	0	1.243329	-1.601232	-3.252166
29	6	0	1.201423	-0.312002	-2.564487
30	6	0	2.315409	0.482194	-2.288149
31	1	0	3.278163	0.107899	-2.613082
32	6	0	2.309415	1.703552	-1.610881
33	6	0	3.496222	2.518676	-1.357992
34	6	0	3.072626	3.624670	-0.640635
35	6	0	1.629156	3.480503	-0.451328
36	6	0	0.818178	4.389888	0.231540
37	1	0	1.310348	5.261777	0.650035
38	6	0	-0.880583	6.535124	1.747805
39	6	0	-3.949376	5.479306	1.449791
40	6	0	-6.427967	1.452782	-1.122260
41	6	0	-0.578533	-3.277213	-4.046480
42	1	0	0.239253	-3.851315	-4.494830
43	1	0	-1.306403	-3.063168	-4.841169
44	1	0	-1.078396	-3.927211	-3.314436
45	6	0	2.506958	-2.355716	-3.581384
46	1	0	3.330454	-1.663042	-3.789015
47	1	0	2.367254	-2.958643	-4.488341
48	6	0	2.951729	-3.317052	-2.427695

49	1	0	3.920551	-3.754820	-2.699676
50	1	0	2.216749	-4.120107	-2.312828
51	6	0	3.102753	-2.579714	-1.091166
52	6	0	4.894410	2.168016	-1.803011
53	1	0	4.887607	1.759357	-2.820300
54	1	0	5.509575	3.074921	-1.849868
55	6	0	5.579915	1.140270	-0.863233
56	1	0	5.650173	1.525561	0.161051
57	1	0	5.006606	0.201236	-0.815029
58	6	0	6.966982	0.780303	-1.337720
59	6	0	3.892375	4.782021	-0.134220
60	1	0	4.943106	4.682192	-0.425367
61	1	0	3.859995	4.853704	0.962253
62	1	0	3.528543	5.738780	-0.533689
63	6	0	2.744593	-1.984893	2.972687
64	1	0	3.792489	-2.000495	2.658530
65	1	0	2.401093	-3.022047	3.042182
66	6	0	2.548966	-1.211903	4.322851
67	1	0	3.527959	-0.848927	4.664273
68	6	0	1.664841	0.042192	4.017622
69	1	0	1.532421	0.621537	4.938636
70	6	0	2.395501	0.894759	2.948654
71	1	0	1.834955	1.818410	2.766010
72	1	0	3.393079	1.178104	3.309091
73	6	0	2.495288	0.076918	1.628662
74	1	0	1.895220	0.522502	0.838714
75	1	0	3.519235	-0.040809	1.265455
76	6	0	0.480923	-1.318420	2.236384
77	1	0	0.277155	-2.356167	2.524793
78	6	0	0.280499	-0.367896	3.450255
79	1	0	-0.249490	0.531131	3.119542
80	1	0	-0.335369	-0.853665	4.213977
81	6	0	1.976083	-2.100448	5.406601
82	1	0	1.022802	-2.585930	5.182506
83	6	0	2.556908	-2.330465	6.600941
84	1	0	3.510871	-1.878709	6.870832
85	1	0	2.096769	-2.977328	7.344033
86	6	0	-0.440998	-1.014930	1.006567
87	1	0	-0.022615	-1.550155	0.142150
88	6	0	-1.837760	-1.565842	1.314375
89	6	0	-2.850424	-0.712536	1.735362
90	1	0	-2.664070	0.353843	1.792945
91	6	0	-4.127822	-1.236693	2.079053
92	1	0	-4.919258	-0.569141	2.412815
93	6	0	-3.445433	-3.408129	1.595828
94	6	0	-3.769005	-4.800224	1.530102
95	1	0	-4.771415	-5.094094	1.825766
96	6	0	-2.836404	-5.726035	1.104420
97	1	0	-3.061669	-6.786605	1.047875
98	6	0	-1.530299	-5.292712	0.711974
99	6	0	-1.172548	-3.947293	0.761434
100	1	0	-0.185976	-3.634725	0.433201
101	6	0	-2.123823	-2.973961	1.215564
102	6	0	0.656482	-5.981571	-0.155928
103	1	0	0.627486	-5.306058	-1.019521
104	1	0	1.115706	-6.932702	-0.432321
105	1	0	1.232884	-5.498349	0.642319
106	6	0	-5.386024	-1.123373	-2.816714
107	1	0	2.104642	-1.955829	0.921595
108	6	0	-6.670597	-1.483234	-2.569776
109	6	0	-4.148843	6.770379	1.818238
110	1	0	8.619888	-0.034122	-0.655994
111	1	0	-0.978749	7.427804	1.112459
112	1	0	0.176778	6.439651	2.016460
113	1	0	-1.442683	6.730160	2.669746
114	1	0	-4.803420	4.806801	1.537965
115	1	0	-7.074069	1.239428	-1.982574
116	1	0	-6.482395	2.528681	-0.924062
117	1	0	-6.861097	0.934191	-0.254177
118	1	0	-4.872344	-1.648406	-3.622858
119	1	0	-7.257127	-1.058372	-1.761483
120	1	0	-7.154333	-2.252440	-3.166719
121	1	0	-3.381571	7.533299	1.736049
122	1	0	-5.116126	7.095046	2.193772

4.4 [(FePPIXH)(QN2)]

See Fig. 1 for image. Charge 0, overall spin 5/2. Calculated spin on Fe: +4.04.

Energies:

ZPE	m1 (octanol)	m1 (water)	m3 (octanol)	m3 (water)
0.999014	-2993.905199	-2993.897555	-4135.342735	-4135.332132

Atomic coordinates:

1	26	0	1.451155	0.759669	-0.932403
2	8	0	-1.208973	-4.820711	-1.193156
3	7	0	2.260547	2.624724	-0.387352
4	6	0	1.550974	3.809397	-0.194793
5	8	0	-2.013578	-2.935769	-0.164943
6	7	0	3.429548	0.085821	-1.141215
7	6	0	2.399582	4.809741	0.439321
8	8	0	-6.412223	0.524724	-3.105241
9	7	0	0.896455	-0.745786	-2.275684
10	6	0	3.646135	4.214727	0.628985
11	8	0	-7.293184	1.673387	-1.322049
12	1	0	-8.143430	1.296927	-1.647615
13	7	0	-0.265895	1.782929	-1.542409
14	6	0	3.547165	2.855431	0.085524
15	6	0	4.600021	1.938780	0.017030
16	1	0	5.550637	2.249344	0.435624
17	6	0	4.562598	0.671990	-0.576930
18	6	0	5.713468	-0.209468	-0.725894
19	6	0	5.263579	-1.343601	-1.400871
20	6	0	3.835007	-1.137592	-1.658659
21	6	0	2.997417	-2.053332	-2.307888
22	1	0	3.443850	-2.989747	-2.622803
23	6	0	1.637366	-1.888597	-2.578400
24	6	0	0.772892	-2.899076	-3.187146
25	6	0	-0.496387	-2.351859	-3.250088
26	6	0	-0.404287	-0.999522	-2.708088
27	6	0	-1.456364	-0.080693	-2.653417
28	1	0	-2.406826	-0.403566	-3.064738
29	6	0	-1.389493	1.220819	-2.145715
30	6	0	-2.479194	2.196351	-2.176689
31	6	0	-1.994750	3.356595	-1.599808
32	6	0	-0.615552	3.089963	-1.203173
33	6	0	0.219120	4.014134	-0.574832
34	1	0	-0.208628	4.988167	-0.362689
35	6	0	1.986690	6.219201	0.765572
36	6	0	4.872013	4.776248	1.198677
37	1	0	5.796501	4.270475	0.918388
38	6	0	4.986631	5.841707	2.031655
39	1	0	4.129884	6.393198	2.405347
40	1	0	5.963052	6.169738	2.379563
41	6	0	7.114113	0.105085	-0.275702
42	6	0	6.008160	-2.523495	-1.846034
43	1	0	5.558545	-3.079668	-2.669351
44	6	0	7.182046	-2.996228	-1.355648
45	1	0	7.695101	-2.542211	-0.513622
46	1	0	7.645698	-3.880482	-1.785955
47	6	0	1.170153	-4.297134	-3.579431
48	1	0	0.685556	-5.020799	-2.910010
49	1	0	2.252789	-4.453308	-3.531557
50	1	0	0.851495	-4.530203	-4.603901
51	6	0	-1.760381	-3.069738	-3.654293
52	1	0	-1.487684	-4.024962	-4.114276
53	1	0	-2.322801	-2.500503	-4.408079
54	6	0	-2.715072	-3.359366	-2.445133
55	1	0	-3.310336	-2.473549	-2.205276
56	1	0	-3.398100	-4.169948	-2.729580
57	6	0	-1.927724	-3.774421	-1.195186
58	6	0	-3.867540	1.952820	-2.713495
59	1	0	-3.888975	1.085773	-3.380912
60	1	0	-4.192130	2.809633	-3.319769
61	6	0	-4.901019	1.726634	-1.577594

62	1	0	-5.058335	2.632393	-0.984622
63	1	0	-4.528616	0.962961	-0.880317
64	6	0	-6.232468	1.240874	-2.106493
65	6	0	-2.717836	4.660822	-1.392696
66	1	0	-2.924910	4.841567	-0.328357
67	1	0	-3.676979	4.671204	-1.921622
68	1	0	-2.130012	5.511958	-1.761111
69	1	0	7.340381	-0.345318	0.702146
70	1	0	7.280138	1.183766	-0.184177
71	1	0	7.848608	-0.285427	-0.990673
72	1	0	1.696090	6.326039	1.821110
73	1	0	1.134710	6.544438	0.159403
74	1	0	2.812411	6.918190	0.583779
75	8	0	0.906648	-0.021238	0.672556
76	7	0	-0.157540	-2.946585	1.543518
77	8	0	-5.678453	-1.119682	1.445787
78	7	0	-2.296611	2.945955	3.267718
79	6	0	-0.391443	-4.033942	2.566258
80	1	0	-0.377974	-4.985543	2.026831
81	1	0	-1.399779	-3.893957	2.969995
82	6	0	0.700462	-3.975776	3.690155
83	1	0	1.255622	-4.923781	3.689851
84	6	0	1.708635	-2.844049	3.300479
85	1	0	2.502550	-2.794737	4.054778
86	6	0	2.308999	-3.193579	1.913920
87	1	0	3.075849	-2.458298	1.645931
88	1	0	2.793306	-4.177999	1.949363
89	6	0	1.171271	-3.174419	0.852162
90	1	0	1.304949	-2.363139	0.139319
91	1	0	1.074531	-4.112773	0.298135
92	6	0	-0.217676	-1.588879	2.233583
93	1	0	-1.154061	-1.620163	2.803226
94	6	0	0.999049	-1.467963	3.194416
95	1	0	1.703214	-0.733262	2.790972
96	1	0	0.673499	-1.111466	4.177078
97	6	0	0.093940	-3.791521	5.064897
98	1	0	-0.544423	-2.914855	5.201572
99	6	0	0.283283	-4.624919	6.107322
100	1	0	0.902821	-5.516967	6.021845
101	1	0	-0.175141	-4.441138	7.076091
102	6	0	-0.366775	-0.413926	1.204822
103	1	0	-1.003121	-0.776795	0.385371
104	6	0	-1.066212	0.756024	1.903555
105	6	0	-0.324165	1.821700	2.398835
106	1	0	0.750003	1.842762	2.253512
107	6	0	-0.974418	2.891519	3.074716
108	1	0	-0.392408	3.723492	3.465156
109	6	0	-3.059978	1.900564	2.783772
110	6	0	-4.475073	1.959792	2.987735
111	1	0	-4.868480	2.825755	3.511272
112	6	0	-5.300154	0.948079	2.536510
113	1	0	-6.375694	0.973729	2.680974
114	6	0	-4.739003	-0.176175	1.851995
115	6	0	-3.367367	-0.270615	1.623013
116	1	0	-2.966939	-1.116548	1.071892
117	6	0	-2.494863	0.769090	2.090407
118	6	0	-5.206317	-2.363405	0.838192
119	1	0	-4.642487	-2.174224	-0.081689
120	1	0	-6.109853	-2.936504	0.621635
121	1	0	-4.560736	-2.917122	1.531485
122	1	0	-1.005924	-3.007824	0.761396

4.5 [(FePPIXH)$_2$(μ-O)(QNH$_2$)]

See Fig. 6 for image. Charge 0, overall spin 0. Calculated spins on Fe: +4.04, -4.05.

Energies:

ZPE	m1 (octanol)	m1 (water)
1.613552	-5027.888045	-5027.884432

Atomic coordinates:

1	26	0	2.278174	0.361614	-1.852853
2	7	0	2.612278	2.436151	-1.712717
3	7	0	4.382234	0.153874	-1.748396
4	7	0	0.584805	0.868938	-3.030672
5	7	0	2.295145	-1.458905	-2.947478
6	6	0	1.661283	3.439796	-1.862524
7	6	0	2.197643	4.716813	-1.388400
8	6	0	3.500932	4.481916	-0.993779
9	6	0	3.754719	3.057344	-1.213993
10	6	0	5.301608	1.111814	-1.342497
11	6	0	6.647847	0.534286	-1.293107
12	6	0	6.523887	-0.796267	-1.688355
13	6	0	5.109579	-1.020505	-1.953475
14	6	0	3.274835	-2.441890	-2.863532
15	6	0	2.804523	-3.680264	-3.492079
16	6	0	1.535129	-3.407815	-4.000737
17	6	0	1.243516	-2.020488	-3.670209
18	6	0	-0.186072	0.013448	-3.824787
19	6	0	-0.035728	2.115151	-3.108844
20	6	0	-1.215012	2.047835	-3.973364
21	6	0	-1.316109	0.738359	-4.406733
22	6	0	0.097974	-1.326223	-4.077690
23	6	0	4.574139	-2.232171	-2.397422
24	6	0	4.993410	2.443025	-1.044363
25	6	0	0.428987	3.285096	-2.501242
26	1	0	-0.616316	-1.867491	-4.688447
27	1	0	5.258124	-3.070963	-2.457803
28	1	0	5.798610	3.072769	-0.682777
29	1	0	-0.183801	4.172846	-2.617698
30	6	0	4.511070	5.465185	-0.467650
31	6	0	-2.334840	0.148118	-5.346570
32	6	0	-2.072624	3.226318	-4.369241
33	6	0	1.433508	6.014089	-1.361696
34	6	0	7.845094	1.299622	-0.945538
35	6	0	7.619065	-1.803248	-1.907606
36	6	0	3.585033	-4.918302	-3.522204
37	6	0	0.611613	-4.336710	-4.741146
38	6	0	0.492715	6.107368	-0.118467
39	6	0	-3.091521	3.675196	-3.286649
40	6	0	-4.174688	2.620538	-3.056597
41	6	0	-0.320021	7.381235	-0.107863
42	8	0	-1.178751	7.446959	-1.203784
43	8	0	-0.269300	8.290188	0.733248
44	8	0	-4.808777	2.109730	-4.037103
45	1	0	5.449386	5.420874	-1.036924
46	1	0	4.138929	6.493281	-0.530272
47	1	0	4.751361	5.269111	0.585518
48	1	0	-1.931268	0.054681	-6.365638
49	1	0	-2.643000	-0.855818	-5.026015
50	1	0	-3.235928	0.767739	-5.383784
51	1	0	-1.429988	4.081364	-4.621978
52	1	0	-2.639728	2.978061	-5.272561
53	1	0	2.130167	6.860897	-1.339928
54	1	0	0.824928	6.129782	-2.265595
55	1	0	7.307166	-2.599662	-2.591073
56	1	0	-0.430391	-4.004801	-4.688072
57	1	0	-0.195246	5.253304	-0.124677
58	1	0	1.080450	6.073356	0.803071
59	1	0	-2.602638	3.894431	-2.332851
60	1	0	-3.584695	4.594631	-3.633070
61	8	0	1.571000	-0.122033	-0.205971

62	1	0	-1.706109	8.278261	-1.186318
63	8	0	-4.393079	2.288178	-1.793508
64	6	0	9.065465	0.824151	-0.584762
65	6	0	3.424119	-5.986131	-4.344804
66	1	0	0.659382	-5.350830	-4.324511
67	1	0	0.878995	-4.411966	-5.805554
68	1	0	7.934879	-2.275839	-0.967503
69	1	0	8.503302	-1.322091	-2.344542
70	1	0	4.390531	-4.980054	-2.788995
71	1	0	2.681222	-6.016660	-5.135078
72	1	0	4.068339	-6.857128	-4.252827
73	1	0	7.737985	2.384027	-0.988475
74	1	0	9.282907	-0.234554	-0.487902
75	1	0	9.883014	1.508171	-0.370540
76	8	0	-5.571035	-0.944357	1.794679
77	7	0	-6.338317	0.745934	-1.448888
78	8	0	-3.221467	-5.401344	-1.492172
79	7	0	-1.217168	-0.325458	-0.394716
80	6	0	-7.432045	1.771741	-1.701942
81	1	0	-7.180169	2.274596	-2.639680
82	1	0	-7.369724	2.508014	-0.894024
83	6	0	-8.835347	1.089188	-1.757728
84	1	0	-9.149320	0.996140	-2.806921
85	6	0	-8.651273	-0.350346	-1.181009
86	1	0	-9.629915	-0.828047	-1.058287
87	6	0	-7.785446	-1.153894	-2.189630
88	1	0	-7.569307	-2.148595	-1.777935
89	1	0	-8.333186	-1.303888	-3.128031
90	6	0	-6.465768	-0.368975	-2.460899
91	1	0	-5.578578	-1.004478	-2.384563
92	1	0	-6.435498	0.106041	-3.445223
93	6	0	-6.457362	0.227941	-0.026773
94	1	0	-6.251497	1.079602	0.629951
95	6	0	-7.919603	-0.284255	0.184641
96	1	0	-7.891430	-1.270483	0.657783
97	1	0	-8.454575	0.365942	0.883546
98	6	0	-9.880266	1.907082	-1.030643
99	1	0	-9.702787	2.087639	0.032356
100	6	0	-10.988393	2.419994	-1.601280
101	1	0	-11.208591	2.276783	-2.658569
102	1	0	-11.708042	2.999504	-1.028023
103	6	0	-5.447892	-0.890881	0.357073
104	1	0	-5.806556	-1.826949	-0.091093
105	6	0	-3.974455	-0.688770	-0.016189
106	6	0	-3.353450	0.536769	0.229299
107	1	0	-3.916030	1.383329	0.596250
108	6	0	-1.972980	0.699439	0.030130
109	1	0	-1.466137	1.634979	0.226178
110	6	0	-1.756302	-1.566803	-0.675116
111	6	0	-0.899531	-2.617078	-1.105448
112	1	0	0.164840	-2.431557	-1.191651
113	6	0	-1.429132	-3.860505	-1.380319
114	1	0	-0.801069	-4.684962	-1.701299
115	6	0	-2.827687	-4.098976	-1.214908
116	6	0	-3.678280	-3.085789	-0.785313
117	1	0	-4.725138	-3.294327	-0.615930
118	6	0	-3.165662	-1.781109	-0.502886
119	6	0	-4.613681	-5.779875	-1.262010
120	1	0	-4.895926	-5.617424	-0.213736
121	1	0	-4.664572	-6.843238	-1.501182
122	1	0	-5.287447	-5.218609	-1.924063
123	1	0	-5.166857	-1.802113	2.214169
124	1	0	-5.355580	1.382676	-1.618237
125	1	0	-0.168714	-0.212374	-0.431431
126	26	0	1.924445	-0.480748	1.598366
127	7	0	0.932820	-2.317973	1.982246
128	7	0	3.719728	-1.592352	1.674028
129	7	0	0.309227	0.415348	2.611951
130	7	0	3.073595	1.161207	2.279010
131	6	0	-0.395752	-2.522170	2.363071
132	6	0	-0.738039	-3.950400	2.275621
133	6	0	0.410445	-4.597151	1.849722
134	6	0	1.444219	-3.580214	1.686809
135	6	0	3.842153	-2.961371	1.440217
136	6	0	5.243786	-3.348559	1.393500
137	6	0	5.983150	-2.196569	1.648994
138	6	0	5.016818	-1.105304	1.800792

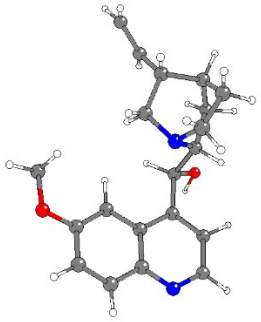
139	6	0	4.464436	1.271237	2.296688
140	6	0	4.862933	2.630667	2.633395
141	6	0	3.688998	3.352581	2.834590
142	6	0	2.582958	2.414008	2.622167
143	6	0	0.198970	1.772116	2.922221
144	6	0	-0.925886	-0.152676	2.932871
145	6	0	-1.840190	0.875458	3.438539
146	6	0	-1.139933	2.070273	3.420964
147	6	0	1.238100	2.701957	2.871935
148	6	0	5.354962	0.219695	2.075768
149	6	0	2.775220	-3.863734	1.384379
150	6	0	-1.252504	-1.503736	2.791594
151	1	0	0.991386	3.716565	3.165565
152	1	0	6.410555	0.451534	2.154701
153	1	0	3.019108	-4.903291	1.193120
154	1	0	-2.265590	-1.782678	3.042464
155	6	0	0.633800	-6.066090	1.602678
156	6	0	-1.607248	3.424468	3.885348
157	6	0	5.747583	-4.741290	1.129260
158	6	0	7.431206	-2.019786	1.769061
159	6	0	8.359707	-2.967886	2.054455
160	6	0	6.283203	3.118235	2.724272
161	6	0	3.500396	4.759208	3.194646
162	6	0	4.386966	5.587342	3.803230
163	1	0	-0.266579	-6.651531	1.809906
164	1	0	0.919633	-6.261762	0.559194
165	1	0	1.436476	-6.462930	2.239764
166	1	0	-1.069406	3.745257	4.788665
167	1	0	-1.449605	4.199092	3.121786
168	1	0	-2.672908	3.412210	4.133623
169	1	0	5.031096	-5.326701	0.541994
170	1	0	6.694237	-4.716430	0.575714
171	1	0	5.932716	-5.293538	2.062555
172	1	0	7.794732	-1.002183	1.624040
173	1	0	8.103294	-4.001730	2.263615
174	1	0	9.413886	-2.709048	2.119018
175	1	0	6.961306	2.514072	2.111680
176	1	0	6.362902	4.159346	2.386746
177	1	0	6.658721	3.085930	3.757688
178	6	0	-2.083093	-4.599182	2.524121
179	6	0	-2.766633	-4.343583	3.894913
180	6	0	-3.883652	-3.279770	3.850650
181	8	0	-4.199857	-2.730632	4.967282
182	8	0	-4.405979	-2.999987	2.693838
183	1	0	-2.798818	-4.265535	1.761803
184	1	0	-1.961006	-5.679116	2.383679
185	1	0	-3.239593	-5.270584	4.248647
186	1	0	-2.053260	-4.049371	4.671954
187	1	0	-5.040339	-1.538603	5.413146
188	6	0	-3.254646	0.665884	3.915191
189	6	0	-3.344859	0.350970	5.442483
190	6	0	-4.809031	0.421760	5.900937
191	8	0	-5.537883	-0.715116	5.779339
192	8	0	-5.308604	1.485481	6.320468
193	1	0	-3.831861	1.581337	3.730741
194	1	0	-3.752573	-0.126260	3.348428
195	1	0	-2.917732	-0.636786	5.644896
196	1	0	-2.784552	1.108395	5.999937
197	1	0	2.524932	5.180847	2.947198
198	1	0	5.365972	5.259333	4.138607
199	1	0	4.125070	6.622017	4.009914

5. Quinidine

5.1 Free Quinidine

Single conformer for all methods and solvents (designated QD_83). Energies:

ZPE	m1 (octanol)	m1 (water)	m3 (octanol)	m3 (water)
0.410791	-1036.347153	-1036.345957	-1036.777164	-1036.774410



Atomic coordinates:

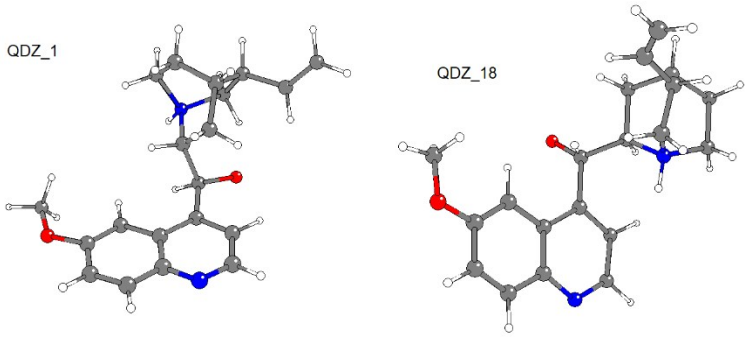
1	8	0	2.563644	-1.231964	-1.178210
2	7	0	0.610294	1.388633	0.641122
3	8	0	-4.076600	-0.958651	-0.731491
4	7	0	-0.211723	-3.714074	2.224513
5	6	0	-0.030363	2.176944	-0.450236
6	1	0	-0.968704	2.595831	-0.068126
7	1	0	-0.290109	1.501034	-1.273509
8	6	0	0.910915	3.330127	-0.978781
9	1	0	0.591062	4.287391	-0.541157
10	6	0	2.334815	2.999926	-0.424420
11	1	0	3.074523	3.672622	-0.874514
12	6	0	2.294256	3.195728	1.118008
13	1	0	3.251505	2.881740	1.556235
14	1	0	2.157293	4.257266	1.363713
15	6	0	1.109499	2.332961	1.686380
16	1	0	1.422473	1.751697	2.560915
17	1	0	0.269515	2.965960	1.996587
18	6	0	1.780973	0.603975	0.135461
19	1	0	2.346513	0.292346	1.022445
20	6	0	2.692716	1.521595	-0.745406
21	1	0	3.747539	1.321478	-0.528577
22	1	0	2.554339	1.305532	-1.810957
23	6	0	0.852678	3.463939	-2.481466
24	1	0	1.190252	2.598067	-3.057787
25	6	0	1.333181	-0.700860	-0.567016
26	1	0	0.619919	-0.468700	-1.369860
27	6	0	0.734119	-1.721998	0.398531
28	6	0	1.601258	-2.472095	1.193060
29	1	0	2.673521	-2.319626	1.118616
30	6	0	1.092126	-3.448268	2.092406
31	1	0	1.771591	-4.027656	2.713577
32	6	0	-1.096149	-2.991703	1.449768
33	6	0	-2.490150	-3.283497	1.591556
34	1	0	-2.766808	-4.058602	2.299315
35	6	0	-3.437279	-2.601243	0.854394
36	1	0	-4.499089	-2.807152	0.947111
37	6	0	-3.024457	-1.581749	-0.059726
38	6	0	-1.680058	-1.268338	-0.225465
39	1	0	-1.385219	-0.474033	-0.898404
40	6	0	-0.678124	-1.968971	0.519762

41	6	0	-3.770018	0.109229	-1.672449
42	1	0	-3.264057	0.945767	-1.170832
43	1	0	-4.735659	0.440466	-2.059018
44	1	0	-3.146232	-0.257778	-2.499791
45	6	0	0.408652	4.549170	-3.149301
46	1	0	0.060513	5.439652	-2.627046
47	1	0	0.384346	4.581762	-4.236349
48	1	0	2.393277	-2.120686	-1.556151

5.2 Quinidine Zwitterion

Minimum conformer in both solvents (method 1) and n-octanol (method 3): QDZ_1. Minimum conformer in water (method 3): QDZ_18. Energies:

conformer	ZPE	m1 (octanol)	m1 (water)	m3 (octanol)	m3 (water)
QDZ_1	0.411476	-1036.323757	-1036.327311	-1036.748396	-1036.750342
QDZ_18	0.411099	-1036.319543	-1036.326841	-1036.747963	-1036.753396



QDZ_1 atomic coordinates:

1	8	0	1.848728	0.096879	-1.755747
2	7	0	1.730408	1.967751	0.475289
3	8	0	-4.545480	1.566619	0.065952
4	7	0	-1.969650	-3.220085	-1.281807
5	6	0	3.200133	1.669718	0.101074
6	1	0	3.703209	2.639524	0.013432
7	1	0	3.097792	1.148841	-0.868991
8	6	0	3.829820	0.757143	1.192549
9	1	0	4.510497	1.340334	1.830845
10	6	0	2.667946	0.236438	2.101213
11	1	0	3.065043	-0.501645	2.806505
12	6	0	2.080011	1.444295	2.882812
13	1	0	1.214479	1.117268	3.471029
14	1	0	2.820945	1.846410	3.583718
15	6	0	1.656370	2.555546	1.875103
16	1	0	0.632759	2.903653	2.047060
17	1	0	2.331523	3.417787	1.903779
18	6	0	0.842417	0.691048	0.398474
19	1	0	-0.105425	0.996910	0.863052
20	6	0	1.555047	-0.399745	1.229844
21	1	0	0.822379	-0.912742	1.862970
22	1	0	1.981938	-1.137142	0.543923
23	6	0	4.625479	-0.356599	0.538343
24	1	0	4.118203	-0.884656	-0.270914
25	6	0	0.636391	0.335401	-1.135352
26	1	0	0.083783	1.226863	-1.551737
27	6	0	-0.350435	-0.858551	-1.195228
28	6	0	0.163111	-2.089419	-1.588289
29	1	0	1.206723	-2.120850	-1.886390
30	6	0	-0.672851	-3.240482	-1.616305

31	1	0	-0.268331	-4.205624	-1.914771
32	6	0	-2.517634	-2.002936	-0.924852
33	6	0	-3.910486	-1.969835	-0.598484
34	1	0	-4.453078	-2.909629	-0.635612
35	6	0	-4.537137	-0.784453	-0.262841
36	1	0	-5.594692	-0.739080	-0.021628
37	6	0	-3.788161	0.432416	-0.251859
38	6	0	-2.428933	0.440970	-0.547147
39	1	0	-1.877493	1.374431	-0.576409
40	6	0	-1.752716	-0.780929	-0.879120
41	6	0	-3.897188	2.865740	0.033170
42	1	0	-3.088840	2.927444	0.777516
43	1	0	-4.677897	3.587812	0.281353
44	1	0	-3.493754	3.085008	-0.965806
45	6	0	5.884738	-0.690910	0.883273
46	1	0	6.428351	-0.164754	1.668231
47	1	0	6.413274	-1.500246	0.385319
48	1	0	1.365053	2.626014	-0.224786

QDZ_18 atomic coordinates:

1	8	0	0.073505	0.857306	2.164199
2	7	0	1.862724	0.983121	-1.191942
3	8	0	-3.858327	-2.582038	1.810535
4	7	0	-3.290604	1.838343	-1.580252
5	6	0	2.246706	-0.461908	-1.488597
6	1	0	2.243755	-0.597331	-2.575553
7	1	0	1.465764	-1.090008	-1.053818
8	6	0	3.647027	-0.760004	-0.866745
9	1	0	4.406265	-0.731272	-1.661479
10	6	0	3.962355	0.393101	0.141969
11	1	0	4.870297	0.141713	0.700772
12	6	0	4.193822	1.692938	-0.677143
13	1	0	4.311946	2.541175	0.006595
14	1	0	5.111936	1.618762	-1.271921
15	6	0	2.977544	1.925923	-1.621063
16	1	0	2.589799	2.946943	-1.556022
17	1	0	3.216174	1.711124	-2.669198
18	6	0	1.560733	1.184950	0.350955
19	1	0	1.507918	2.273424	0.475814
20	6	0	2.773581	0.604901	1.114996
21	1	0	3.052817	1.291407	1.918264
22	1	0	2.475768	-0.326237	1.606735
23	6	0	3.678274	-2.138941	-0.242043
24	1	0	2.976384	-2.314752	0.575227
25	6	0	0.208220	0.568647	0.817697
26	1	0	0.297172	-0.539550	0.596205
27	6	0	-0.995843	1.050415	-0.023569
28	6	0	-1.005230	2.200466	-0.821104
29	1	0	-0.154571	2.880548	-0.852505
30	6	0	-2.166320	2.558609	-1.569875
31	1	0	-2.160226	3.456348	-2.186387
32	6	0	-3.335870	0.717936	-0.765516
33	6	0	-4.547833	-0.039947	-0.727156
34	1	0	-5.365450	0.284532	-1.363603
35	6	0	-4.671185	-1.132084	0.113108
36	1	0	-5.587849	-1.711709	0.169064
37	6	0	-3.585580	-1.502402	0.967503
38	6	0	-2.382857	-0.805117	0.940620
39	1	0	-1.576688	-1.017581	1.632713
40	6	0	-2.228460	0.305455	0.054772
41	6	0	-2.842008	-2.965104	2.782943
42	1	0	-3.279262	-3.790481	3.348714
43	1	0	-2.604922	-2.130843	3.456102
44	1	0	-1.922755	-3.301258	2.282940
45	6	0	4.503854	-3.132122	-0.626640
46	1	0	5.219013	-3.005395	-1.438754
47	1	0	4.491081	-4.102831	-0.137252
48	1	0	0.982305	1.210791	-1.677742

5.3 [(FePPIXH)(QD1)]

See Fig. 1 for image. Charge 0, overall spin 5/2. Calculated spin on Fe: +4.04.

Energies:

ZPE	m1 (octanol)	m1 (water)	m3 (octanol)	m3 (water)
0.999499	-2993.910550	-2993.903518	-4135.346867	-4135.337064

Atomic coordinates:

1	26	0	0.434683	1.278193	-0.939714
2	8	0	-3.623804	-2.768166	-0.435851
3	7	0	0.738440	3.314617	-0.535953
4	6	0	-0.239807	4.252403	-0.202219
5	8	0	-1.527456	-3.298921	0.324668
6	7	0	2.449318	1.181434	-1.514097
7	6	0	0.382117	5.479514	0.275600
8	8	0	-7.463770	-0.996543	-2.175237
9	7	0	0.125789	-0.402069	-2.138138
10	6	0	1.761314	5.279805	0.217587
11	8	0	-7.585331	-1.385837	0.084702
12	1	0	-8.401820	-1.874368	-0.169953
13	7	0	-1.584190	1.749630	-1.246095
14	6	0	1.965741	3.928316	-0.313517
15	8	0	0.383272	0.475204	0.752569
16	7	0	-1.611069	-1.578023	2.185106
17	6	0	3.210564	3.354128	-0.593801
18	1	0	4.087768	3.947849	-0.362943
19	8	0	2.050002	-6.025945	1.098528
20	7	0	4.878158	-1.352546	2.304054
21	6	0	3.441248	2.102513	-1.173821
22	6	0	4.756661	1.578787	-1.522205
23	6	0	4.550842	0.319683	-2.080745
24	6	0	3.103016	0.088337	-2.070857
25	6	0	2.474770	-1.075226	-2.527215
26	1	0	3.111799	-1.874117	-2.891147
27	6	0	1.098110	-1.312436	-2.548526
28	6	0	0.466558	-2.549008	-3.002202
29	6	0	-0.899650	-2.375101	-2.866704
30	6	0	-1.103379	-1.020653	-2.356645
31	6	0	-2.348215	-0.424335	-2.150098
32	1	0	-3.222134	-1.019787	-2.383098
33	6	0	-2.574444	0.863442	-1.659991
34	6	0	-3.894855	1.469118	-1.496371
35	6	0	-3.688623	2.739828	-0.988055
36	6	0	-2.243678	2.905504	-0.833979
37	6	0	-1.619483	4.052216	-0.339360
38	1	0	-2.269062	4.871564	-0.049403
39	6	0	-0.355621	6.721248	0.696457
40	6	0	2.852782	6.196418	0.550607
41	1	0	3.817900	5.961750	0.100684
42	6	0	2.803356	7.291920	1.350605
43	1	0	1.906542	7.597234	1.880054
44	1	0	3.689996	7.900697	1.509609
45	6	0	6.059495	2.306859	-1.337725
46	6	0	5.521273	-0.627406	-2.633598
47	1	0	5.125774	-1.334737	-3.363454
48	6	0	6.841963	-0.721183	-2.338243
49	1	0	7.324004	-0.098892	-1.590977
50	1	0	7.467099	-1.464837	-2.826360
51	6	0	1.206716	-3.768960	-3.481238
52	1	0	1.820085	-4.208605	-2.681791
53	1	0	1.881795	-3.531660	-4.314883
54	1	0	0.512662	-4.541455	-3.828835
55	6	0	-1.996054	-3.391762	-3.062845
56	1	0	-1.744787	-4.070894	-3.888153
57	1	0	-2.936899	-2.900808	-3.336360
58	6	0	-2.247870	-4.259755	-1.783494
59	1	0	-3.121691	-4.897673	-1.966174
60	1	0	-1.376207	-4.893041	-1.590241

61	6	0	-2.518420	-3.390710	-0.549631
62	6	0	-5.201664	0.789333	-1.820355
63	1	0	-5.128689	0.234720	-2.763294
64	1	0	-5.984601	1.541411	-1.976143
65	6	0	-5.656301	-0.189779	-0.705096
66	1	0	-5.772791	0.329893	0.253527
67	1	0	-4.914068	-0.988250	-0.549943
68	6	0	-6.960305	-0.868492	-1.047471
69	6	0	-4.713041	3.782637	-0.630746
70	1	0	-4.704955	3.996100	0.447540
71	1	0	-5.723789	3.453193	-0.892865
72	1	0	-4.527300	4.729590	-1.155950
73	6	0	-2.460422	-0.361237	1.877636
74	1	0	-3.402068	-0.725937	1.459824
75	1	0	-1.933886	0.208501	1.111180
76	6	0	-2.658923	0.484646	3.176824
77	1	0	-3.655439	0.285933	3.597827
78	6	0	-1.604010	-0.014562	4.221014
79	1	0	-1.599010	0.658713	5.085426
80	6	0	-2.012139	-1.446757	4.655889
81	1	0	-1.239781	-1.872796	5.308719
82	1	0	-2.946813	-1.423897	5.229118
83	6	0	-2.192104	-2.314489	3.376257
84	1	0	-1.683254	-3.280696	3.448860
85	1	0	-3.244405	-2.505956	3.144922
86	6	0	-0.169433	-1.190685	2.503013
87	1	0	0.268616	-2.103844	2.921924
88	6	0	-0.194931	-0.064087	3.574123
89	1	0	0.565865	-0.261326	4.337620
90	1	0	0.049158	0.892252	3.102565
91	6	0	-2.556409	1.969067	2.898529
92	1	0	-1.680735	2.295388	2.334354
93	6	0	0.656463	-0.854962	1.215213
94	1	0	0.360689	-1.572172	0.436568
95	6	0	2.140095	-1.049551	1.545789
96	6	0	2.943270	0.044895	1.841931
97	1	0	2.530934	1.045822	1.780237
98	6	0	4.302963	-0.148659	2.214312
99	1	0	4.930473	0.707761	2.451306
100	6	0	4.106521	-2.457701	2.001277
101	6	0	4.722009	-3.746200	2.090933
102	1	0	5.763241	-3.781831	2.396189
103	6	0	4.011822	-4.893793	1.796251
104	1	0	4.460491	-5.880575	1.857438
105	6	0	2.644903	-4.799418	1.384059
106	6	0	2.005486	-3.565762	1.286984
107	1	0	0.975416	-3.512828	0.948181
108	6	0	2.723545	-2.364882	1.604022
109	6	0	0.671353	-6.035555	0.616905
110	1	0	-0.014398	-5.588053	1.346406
111	1	0	0.427898	-7.088924	0.464704
112	1	0	0.581710	-5.482813	-0.326577
113	6	0	-3.457431	2.884924	3.307452
114	1	0	-4.352952	2.604334	3.861482
115	1	0	-3.324690	3.944676	3.101831
116	1	0	-1.627479	-2.315974	1.310100
117	1	0	6.560548	2.012340	-0.403848
118	1	0	5.919920	3.393010	-1.307639
119	1	0	6.749290	2.081628	-2.160174
120	1	0	-0.449640	6.788006	1.790545
121	1	0	-1.367218	6.755725	0.278725
122	1	0	0.174206	7.621401	0.361042

5.4 [(FePPIXH)(QD2)]

See Fig. 1 for image. Charge 0, overall spin 5/2. Calculated spin on Fe: +4.04.

Energies:

ZPE	m1 (octanol)	m1 (water)	m3 (octanol)	m3 (water)
0.999128	-2993.905455	-2993.898687	-4135.342290	-4135.332589

Atomic coordinates:

1	8	0	6.955645	1.006525	-3.073972
2	8	0	6.807500	-0.801593	-1.663641
3	1	0	7.738107	-0.954900	-1.948648
4	6	0	4.051441	1.390200	-2.849833
5	1	0	3.979020	0.758827	-3.745726
6	1	0	4.596792	2.288543	-3.156268
7	6	0	4.891108	0.646531	-1.777516
8	1	0	4.974755	1.266452	-0.873366
9	1	0	4.414076	-0.286516	-1.463973
10	6	0	6.292911	0.346125	-2.259436
11	1	0	1.667722	-4.694359	-3.249722
12	1	0	2.519848	-3.248884	-3.790243
13	6	0	1.933441	-3.672076	-2.961803
14	1	0	3.437888	-2.821607	-1.589867
15	6	0	2.849929	-3.738523	-1.692228
16	1	0	3.542132	-4.582743	-1.806564
17	8	0	2.089002	-2.930103	0.460490
18	6	0	2.024710	-3.931190	-0.412928
19	8	0	1.299798	-4.961611	-0.253199
20	7	0	-3.288295	-0.099561	-1.172591
21	6	0	-3.698771	-1.388317	-1.513085
22	7	0	-2.087643	2.504926	-0.768329
23	6	0	-5.133366	-1.530092	-1.316749
24	7	0	0.444833	1.463742	-1.702801
25	6	0	-5.595466	-0.304780	-0.836804
26	7	0	-0.735799	-1.136062	-2.073961
27	6	0	-4.429995	0.582909	-0.768726
28	6	0	-4.463725	1.923969	-0.372885
29	1	0	-5.421351	2.316203	-0.049665
30	6	0	-3.392572	2.822994	-0.387980
31	6	0	-3.489865	4.239280	-0.056817
32	6	0	-2.222102	4.784565	-0.255341
33	6	0	-1.363274	3.688282	-0.715396
34	6	0	-0.012859	3.814153	-1.061378
35	1	0	0.436110	4.796325	-0.963012
36	6	0	0.816781	2.796224	-1.532342
37	6	0	2.211323	2.983039	-1.931213
38	6	0	2.675347	1.749457	-2.350030
39	6	0	1.565519	0.806994	-2.206740
40	6	0	1.624707	-0.553413	-2.518145
41	1	0	2.573865	-0.940056	-2.873710
42	6	0	0.568167	-1.465456	-2.432743
43	6	0	0.663095	-2.891411	-2.728392
44	6	0	-0.610569	-3.415909	-2.596846
45	6	0	-1.480613	-2.311014	-2.195442
46	6	0	-2.851567	-2.410826	-1.960662
47	1	0	-3.307272	-3.378672	-2.137692
48	6	0	-5.929190	-2.768398	-1.623879
49	6	0	-6.955407	0.110804	-0.489509
50	1	0	-7.130766	1.187057	-0.481768
51	6	0	-8.011978	-0.681454	-0.175030
52	1	0	-7.943538	-1.763190	-0.118118
53	1	0	-8.981062	-0.245313	0.054457
54	6	0	-4.747131	4.950710	0.362474
55	6	0	-1.763678	6.166782	-0.104685
56	1	0	-0.853657	6.422297	-0.648266
57	6	0	-2.333365	7.154639	0.631359
58	1	0	-3.216438	7.001328	1.243463
59	1	0	-1.896542	8.149930	0.652716
60	6	0	2.950903	4.292505	-1.868445

61	1	0	3.020702	4.663166	-0.836411
62	1	0	2.448308	5.068249	-2.462313
63	1	0	3.971570	4.194214	-2.251904
64	6	0	-1.009392	-4.860176	-2.741612
65	1	0	-0.516592	-5.457340	-1.962471
66	1	0	-0.702652	-5.265275	-3.715068
67	1	0	-2.090922	-5.005098	-2.653107
68	1	0	-4.805957	5.065348	1.454942
69	1	0	-5.646040	4.413516	0.042170
70	1	0	-4.787501	5.956978	-0.072330
71	1	0	-6.074268	-3.388560	-0.726829
72	1	0	-5.433847	-3.392183	-2.375447
73	1	0	-6.922338	-2.508778	-2.009689
74	1	0	1.066730	-2.848318	1.367109
75	26	0	-1.303021	0.565491	-0.994132
76	8	0	-0.824738	0.043948	0.735400
77	1	0	1.113869	-0.690009	0.670463
78	1	0	1.552040	-3.396652	3.624613
79	6	0	0.509586	-3.559132	3.332470
80	1	0	0.417234	-4.592755	2.985837
81	6	0	-0.488713	-3.217145	4.477425
82	1	0	-0.911704	-4.138589	4.895791
83	1	0	0.023025	-2.693432	5.294927
84	7	0	0.223578	-2.672725	2.138723
85	1	0	-4.859228	-3.955260	2.771487
86	6	0	-4.722956	-2.979905	2.304382
87	1	0	-5.620359	-2.471549	1.959806
88	6	0	-3.503277	-2.422628	2.164416
89	1	0	-3.413585	-1.447747	1.681447
90	1	0	-2.430492	-4.085199	2.951240
91	6	0	-2.213358	-3.050179	2.648981
92	1	0	-0.719381	-0.375274	4.357053
93	6	0	-1.003937	-0.955381	3.471956
94	1	0	-1.731777	-0.364860	2.908604
95	6	0	-1.612238	-2.318002	3.895865
96	1	0	-2.399802	-2.163136	4.641771
97	1	0	-1.334216	-2.311653	0.764633
98	6	0	-1.114535	-3.049244	1.536785
99	1	0	-0.987747	-4.027054	1.062881
100	6	0	0.247986	-1.215425	2.588279
101	1	0	1.159312	-1.136831	3.191730
102	6	0	0.426701	-0.220788	1.388613
103	6	0	1.063828	1.061332	1.935608
104	1	0	0.257838	4.224514	2.958392
105	1	0	-0.776459	2.163006	1.962602
106	6	0	0.281695	2.179503	2.197781
107	6	0	0.869808	3.347713	2.759140
108	1	0	4.696294	3.374179	3.602077
109	6	0	4.354974	2.442066	3.162249
110	1	0	4.520896	-2.568356	2.096695
111	8	0	5.698056	-0.803473	2.179744
112	6	0	5.322120	-2.064504	1.542357
113	1	0	6.230051	-2.670186	1.552165
114	1	0	4.993326	-1.899125	0.510596
115	6	0	4.726348	0.176244	2.351370
116	6	0	5.215842	1.384171	2.943349
117	1	0	6.268976	1.435051	3.202515
118	6	0	2.969261	2.344642	2.819610
119	7	0	2.166953	3.441576	3.070231
120	6	0	2.471981	1.122299	2.237605
121	6	0	3.385369	0.041847	1.995055
122	1	0	3.040161	-0.868999	1.514865

5.5 [(FePPIXH)$_2$(μ-O)(QNH$_2$)], (00$\bar{1}$) face isomer

See Fig. 6 for image. Charge 0, overall spin 0. Calculated spins on Fe: +4.04, -4.06.

Energies:

ZPE	m1 (octanol)	m1 (water)
1.613720	-5027.886959	-5027.883568

Atomic coordinates:

1	26	0	-2.255623	0.121893	-1.876341
2	7	0	-2.771868	2.163595	-1.875411
3	7	0	-4.334432	-0.261720	-1.766087
4	7	0	-0.602386	0.697670	-3.078144
5	7	0	-2.103421	-1.760834	-2.848171
6	6	0	-1.913481	3.236025	-2.094019
7	6	0	-2.562712	4.488838	-1.704341
8	6	0	-3.841015	4.165517	-1.291020
9	6	0	-3.966974	2.712981	-1.417063
10	6	0	-5.337194	0.635745	-1.424611
11	6	0	-6.628461	-0.052687	-1.342664
12	6	0	-6.385906	-1.389368	-1.652731
13	6	0	-4.955069	-1.505648	-1.898567
14	6	0	-2.994672	-2.818217	-2.704729
15	6	0	-2.409562	-4.050315	-3.243004
16	6	0	-1.161525	-3.702213	-3.759111
17	6	0	-0.996794	-2.275454	-3.522219
18	6	0	0.253764	-0.139258	-3.801559
19	6	0	-0.093615	1.985664	-3.239541
20	6	0	1.100825	1.963181	-4.085077
21	6	0	1.326209	0.640666	-4.420580
22	6	0	0.090771	-1.512570	-3.964806
23	6	0	-4.312292	-2.692122	-2.260240
24	6	0	-5.148375	2.004680	-1.209650
25	6	0	-0.667630	3.148784	-2.718788
26	1	0	0.859803	-2.029130	-4.528651
27	1	0	-4.921034	-3.588986	-2.268298
28	1	0	-6.008017	2.582945	-0.889635
29	1	0	-0.135749	4.077850	-2.895010
30	6	0	-4.934079	5.088487	-0.825202
31	6	0	2.415596	0.077567	-5.295508
32	6	0	1.861574	3.182799	-4.548506
33	6	0	-1.916068	5.847737	-1.761150
34	6	0	-7.890810	0.626086	-1.048787
35	6	0	-7.385385	-2.502137	-1.807132
36	6	0	-3.078528	-5.351124	-3.192675
37	6	0	-0.150419	-4.593525	-4.427436
38	6	0	-1.018907	6.113202	-0.511041
39	6	0	2.812699	3.788848	-3.480631
40	6	0	3.977413	2.851246	-3.162294
41	6	0	-0.323576	7.453493	-0.573092
42	8	0	0.536944	7.532345	-1.666830
43	8	0	-0.462624	8.401540	0.213178
44	8	0	4.700885	2.368379	-4.093824
45	1	0	-5.862671	4.930432	-1.390198
46	1	0	-4.650444	6.138998	-0.949557
47	1	0	-5.161278	4.936099	0.237987
48	1	0	2.047332	-0.129101	-6.311220
49	1	0	2.805685	-0.866325	-4.892434
50	1	0	3.258238	0.772180	-5.365568
51	1	0	1.153418	3.960248	-4.867816
52	1	0	2.466850	2.926682	-5.424522
53	1	0	-2.684255	6.628703	-1.815375
54	1	0	-1.297856	5.951489	-2.659754
55	1	0	-7.001143	-3.307675	-2.441705
56	1	0	0.852231	-4.154373	-4.415019
57	1	0	-0.256740	5.327207	-0.443991
58	1	0	-1.623189	6.088538	0.400061
59	1	0	2.282162	4.022849	-2.553158
60	1	0	3.231964	4.723794	-3.878745
61	8	0	-1.523374	-0.188306	-0.198269

62	1	0	0.986948	8.407647	-1.695620
63	8	0	4.167472	2.588855	-1.878419
64	6	0	-9.065385	0.069908	-0.653327
65	6	0	-2.798396	-6.464569	-3.917253
66	1	0	-0.092699	-5.567579	-3.924959
67	1	0	-0.411979	-4.787450	-5.478110
68	1	0	-7.658350	-2.942472	-0.838386
69	1	0	-8.308710	-2.130901	-2.269510
70	1	0	-3.901697	-5.424431	-2.480566
71	1	0	-2.026810	-6.496513	-4.679316
72	1	0	-3.370270	-7.377520	-3.770297
73	1	0	-7.880217	1.709917	-1.169031
74	1	0	-9.186280	-0.994404	-0.479798
75	1	0	-9.942375	0.690953	-0.487837
76	1	0	0.223810	-0.150439	-0.398782
77	1	0	5.232227	1.829401	-1.607022
78	8	0	5.649803	-0.306046	1.908359
79	7	0	6.297525	1.373641	-1.366376
80	8	0	3.763691	-5.077844	-1.172345
81	7	0	1.277456	-0.165403	-0.343867
82	6	0	6.666392	0.289786	-2.350725
83	1	0	6.461587	0.693443	-3.346387
84	1	0	5.984609	-0.551768	-2.196966
85	6	0	8.167407	-0.131834	-2.161367
86	1	0	8.720682	0.141314	-3.070636
87	6	0	8.756477	0.716520	-0.984941
88	1	0	9.797912	0.420726	-0.813053
89	6	0	8.684741	2.207393	-1.394711
90	1	0	9.136702	2.829034	-0.612684
91	1	0	9.251781	2.380125	-2.317730
92	6	0	7.190970	2.585892	-1.593096
93	1	0	6.858242	3.357408	-0.892210
94	1	0	6.972699	2.935146	-2.606336
95	6	0	6.438132	0.900363	0.067879
96	1	0	6.140592	1.744341	0.699212
97	6	0	7.939072	0.536060	0.320330
98	1	0	8.354167	1.179848	1.102440
99	1	0	8.011554	-0.484275	0.707348
100	6	0	8.328328	-1.623373	-1.959278
101	1	0	7.888033	-2.043882	-1.051659
102	6	0	5.533536	-0.299205	0.468975
103	1	0	5.982650	-1.207477	0.046464
104	6	0	4.051411	-0.251368	0.078235
105	6	0	3.315489	0.919516	0.260354
106	1	0	3.791785	1.830864	0.592190
107	6	0	1.929409	0.944483	0.036893
108	1	0	1.336655	1.838296	0.178043
109	6	0	1.933156	-1.364704	-0.552064
110	6	0	1.183184	-2.513302	-0.925177
111	1	0	0.106432	-2.435849	-1.017510
112	6	0	1.829777	-3.713814	-1.133619
113	1	0	1.283951	-4.609473	-1.411273
114	6	0	3.243594	-3.808723	-0.956781
115	6	0	3.989814	-2.699384	-0.573748
116	1	0	5.049812	-2.800370	-0.390418
117	6	0	3.354388	-1.437019	-0.360449
118	6	0	5.188872	-5.302187	-0.940612
119	1	0	5.797506	-4.697248	-1.626826
120	1	0	5.348172	-6.362438	-1.143333
121	1	0	5.456216	-5.075460	0.099654
122	6	0	8.976453	-2.448243	-2.805719
123	1	0	9.437987	-2.081387	-3.721664
124	1	0	9.073029	-3.513147	-2.606420
125	1	0	5.311077	-1.180965	2.350990
126	26	0	-1.870694	-0.460321	1.622485
127	7	0	-0.744037	-2.189322	2.117083
128	7	0	-3.574629	-1.702047	1.758658
129	7	0	-0.342027	0.615832	2.595752
130	7	0	-3.150008	1.125007	2.198444
131	6	0	0.592250	-2.267189	2.516890
132	6	0	1.047904	-3.665940	2.504122
133	6	0	-0.041127	-4.423200	2.105023
134	6	0	-1.151177	-3.501787	1.884665
135	6	0	-3.588350	-3.086996	1.599220
136	6	0	-4.955089	-3.585247	1.575745
137	6	0	-5.783433	-2.483051	1.770573
138	6	0	-4.906399	-1.312154	1.859017

139	6	0	-4.545384	1.126808	2.206333
140	6	0	-5.050969	2.468762	2.458484
141	6	0	-3.938322	3.291247	2.617994
142	6	0	-2.761021	2.430510	2.467366
143	6	0	-0.339749	1.992643	2.827349
144	6	0	0.927740	0.163634	2.962298
145	6	0	1.753042	1.285991	3.418090
146	6	0	0.964534	2.420601	3.323165
147	6	0	-1.445372	2.835816	2.709956
148	6	0	-5.349109	-0.003703	2.052135
149	6	0	-2.453661	-3.904570	1.593433
150	6	0	1.360129	-1.163310	2.899381
151	1	0	-1.280876	3.882197	2.943527
152	1	0	-6.420085	0.148576	2.116648
153	1	0	-2.614223	-4.968845	1.457728
154	1	0	2.387446	-1.347755	3.177545
155	6	0	-0.142316	-5.916028	1.931258
156	6	0	1.320614	3.831191	3.712328
157	6	0	-5.347114	-5.025262	1.385875
158	6	0	-7.241068	-2.414649	1.884729
159	6	0	-8.093257	-3.416665	2.219899
160	6	0	-6.505620	2.847807	2.520390
161	6	0	-3.862105	4.727664	2.891024
162	6	0	-4.818573	5.523315	3.433687
163	1	0	0.799715	-6.414804	2.176610
164	1	0	-0.397095	-6.187185	0.896642
165	1	0	-0.918517	-6.344545	2.580519
166	1	0	0.723693	4.172579	4.569757
167	1	0	1.145397	4.541629	2.892125
168	1	0	2.372858	3.908318	4.002306
169	1	0	-4.585536	-5.582299	0.828465
170	1	0	-6.291477	-5.103272	0.833253
171	1	0	-5.490614	-5.541119	2.346866
172	1	0	-7.683187	-1.437902	1.687651
173	1	0	-7.757784	-4.415405	2.481251
174	1	0	-9.164563	-3.237801	2.272535
175	1	0	-7.133737	2.149453	1.956758
176	1	0	-6.668011	3.852341	2.109273
177	1	0	-6.877739	2.860641	3.555468
178	6	0	2.438715	-4.190775	2.791750
179	6	0	3.092552	-3.801803	4.145506
180	6	0	4.124684	-2.660000	4.039622
181	8	0	4.380777	-2.014915	5.119958
182	8	0	4.641208	-2.417265	2.871859
183	1	0	3.129897	-3.848024	2.010736
184	1	0	2.402895	-5.283344	2.715694
185	1	0	3.632838	-4.667160	4.554630
186	1	0	2.354499	-3.516787	4.902585
187	1	0	5.119397	-0.740391	5.515032
188	6	0	3.173254	1.214065	3.917727
189	6	0	3.271063	0.997912	5.461659
190	6	0	4.720042	1.210773	5.923466
191	8	0	5.543437	0.135996	5.848859
192	8	0	5.125028	2.328473	6.302808
193	1	0	3.680996	2.158621	3.682151
194	1	0	3.737072	0.430367	3.403310
195	1	0	2.921686	-0.007491	5.718974
196	1	0	2.646751	1.739230	5.970492
197	1	0	-2.916678	5.205836	2.630302
198	1	0	-5.776720	5.144761	3.775707
199	1	0	-4.637548	6.585570	3.577424

5.6 [(FePPIXH)$_2$(μ-O)(QNH$_2$)], (001) face isomer

See Fig. 6 for image. Charge 0, overall spin 0. Calculated spins on Fe: +4.04, -4.04.

Energies:

ZPE	m1 (octanol)	m1 (water)
1.615394	-5027.887394	-5027.883401

Atomic coordinates:

1	26	0	-1.927538	0.171702	-1.744546
2	7	0	-0.571886	-1.203413	-2.626254
3	7	0	-3.455209	-1.136967	-2.378391
4	7	0	-0.457642	1.626630	-2.147739
5	7	0	-3.327408	1.731666	-1.995254
6	8	0	-1.750891	-0.117220	0.087693
7	6	0	0.785665	-1.024554	-2.905430
8	6	0	1.398661	-2.302365	-3.291316
9	6	0	0.386499	-3.246333	-3.254479
10	6	0	-0.834642	-2.553508	-2.849532
11	6	0	-3.313623	-2.508831	-2.584258
12	6	0	-4.619971	-3.140101	-2.716991
13	6	0	-5.565136	-2.118326	-2.634174
14	6	0	-4.817131	-0.871931	-2.438771
15	6	0	-4.703052	1.607019	-2.192992
16	6	0	-5.338837	2.917727	-2.181660
17	6	0	-4.331990	3.847189	-1.930996
18	6	0	-3.079579	3.089625	-1.843964
19	6	0	-0.596187	2.991029	-1.895976
20	6	0	0.886745	1.424153	-2.454124
21	6	0	1.621168	2.686011	-2.344305
22	6	0	0.700904	3.654940	-1.983952
23	6	0	-1.808905	3.657584	-1.716254
24	6	0	-5.385078	0.401083	-2.368890
25	6	0	-2.088866	-3.160373	-2.767850
26	6	0	1.453676	0.199236	-2.818091
27	1	0	-1.751825	4.729130	-1.559225
28	1	0	-6.462597	0.468065	-2.464521
29	1	0	-2.121420	-4.228984	-2.949978
30	1	0	2.506147	0.208599	-3.068284
31	6	0	0.461554	-4.719466	-3.554752
32	6	0	0.939575	5.126071	-1.769704
33	6	0	-4.862693	-4.603923	-2.959585
34	6	0	-7.021447	-2.176699	-2.756264
35	6	0	-7.830016	-3.265133	-2.667945
36	6	0	-6.791291	3.180360	-2.468780
37	6	0	-4.407332	5.305173	-1.835888
38	6	0	-5.505573	6.067474	-1.596587
39	1	0	1.429990	-4.994323	-3.983486
40	1	0	0.325339	-5.322998	-2.645767
41	1	0	-0.312098	-5.024689	-4.271730
42	1	0	0.503685	5.726323	-2.581200
43	1	0	0.494180	5.478163	-0.829424
44	1	0	2.009583	5.356289	-1.738690
45	1	0	-3.956365	-5.122168	-3.288188
46	1	0	-5.216787	-5.107971	-2.048896
47	1	0	-5.627708	-4.750679	-3.733136
48	1	0	-7.513540	-1.222181	-2.945598
49	1	0	-7.459890	-4.263918	-2.462661
50	1	0	-8.904681	-3.164924	-2.799374
51	1	0	-7.248219	2.359039	-3.031163
52	1	0	-7.371626	3.316973	-1.545921
53	1	0	-6.907587	4.093777	-3.065589
54	6	0	2.861766	-2.565886	-3.577649
55	6	0	3.529098	-1.715150	-4.704172
56	6	0	4.568226	-0.707006	-4.186536
57	8	0	4.555180	0.468893	-4.719457
58	8	0	5.376271	-1.086461	-3.247342
59	1	0	3.453182	-2.425333	-2.663409
60	1	0	2.967905	-3.627563	-3.824221
61	1	0	4.064507	-2.385123	-5.390952
62	1	0	2.790818	-1.170591	-5.298847
63	1	0	5.285591	1.701413	-4.441622

64	6	0	3.096333	2.878589	-2.577653
65	6	0	3.450714	3.401154	-4.006611
66	6	0	4.952408	3.696995	-4.061589
67	8	0	5.758541	2.607873	-4.216689
68	8	0	5.419464	4.837761	-3.886238
69	1	0	3.484949	3.604123	-1.849061
70	1	0	3.630674	1.936404	-2.411110
71	1	0	3.169544	2.648250	-4.750082
72	1	0	2.908112	4.329902	-4.204951
73	1	0	-3.465356	5.835857	-1.977368
74	1	0	-6.488698	5.645278	-1.415663
75	1	0	-5.429989	7.151777	-1.569013
76	1	0	-0.124152	-0.531508	0.391852
77	1	0	6.474846	-0.514720	-2.264068
78	8	0	5.877280	-1.829806	0.994058
79	7	0	7.021181	-0.063328	-1.457586
80	8	0	3.017554	-5.811554	0.373967
81	7	0	0.924148	-0.655848	0.448358
82	6	0	8.107417	-0.970834	-0.902067
83	1	0	8.738841	-1.268266	-1.745103
84	1	0	7.621223	-1.852439	-0.482777
85	6	0	8.916394	-0.203050	0.198312
86	1	0	9.914656	0.038502	-0.194974
87	6	0	8.193786	1.161613	0.463778
88	1	0	8.694848	1.672762	1.293261
89	6	0	8.291902	2.011548	-0.826582
90	1	0	7.769765	2.965858	-0.690325
91	1	0	9.338391	2.246080	-1.054471
92	6	0	7.655317	1.215250	-1.998663
93	1	0	6.893301	1.781074	-2.539217
94	1	0	8.400863	0.896244	-2.734333
95	6	0	5.973482	0.260576	-0.377764
96	1	0	5.292657	0.947835	-0.891284
97	6	0	6.696562	0.955410	0.811872
98	1	0	6.239967	1.934720	1.003640
99	1	0	6.576094	0.364860	1.721296
100	6	0	9.093416	-1.045585	1.444864
101	1	0	8.179238	-1.453233	1.875940
102	6	0	5.209619	-1.062125	-0.027857
103	1	0	5.231476	-1.673266	-0.942488
104	6	0	3.715001	-0.888772	0.280120
105	6	0	3.089870	0.351512	0.427489
106	1	0	3.662116	1.269503	0.461135
107	6	0	1.689390	0.444183	0.515245
108	1	0	1.170276	1.391186	0.594014
109	6	0	1.468090	-1.924077	0.372697
110	6	0	0.616955	-3.062511	0.327803
111	1	0	-0.458457	-2.926470	0.321292
112	6	0	1.174675	-4.325577	0.303342
113	1	0	0.555446	-5.217162	0.289737
114	6	0	2.593886	-4.491826	0.330563
115	6	0	3.440698	-3.389606	0.323938
116	1	0	4.516264	-3.488625	0.398595
117	6	0	2.892928	-2.074112	0.331126
118	6	0	4.445030	-6.073229	0.568607
119	1	0	5.028119	-5.722154	-0.292984
120	1	0	4.527203	-7.157885	0.656417
121	1	0	4.804483	-5.588565	1.484495
122	6	0	10.286504	-1.306186	2.015684
123	1	0	11.220819	-0.927803	1.600346
124	1	0	10.363453	-1.907266	2.918727
125	1	0	5.520030	-1.517181	1.955204
126	26	0	-2.558594	-0.096402	1.767936
127	7	0	-1.992209	1.764481	2.580084
128	7	0	-4.481799	0.742530	1.533031
129	7	0	-1.100770	-0.930049	3.055525
130	7	0	-3.526609	-1.967101	1.871925
131	6	0	-0.803964	2.066774	3.238584
132	6	0	-0.659000	3.517457	3.373362
133	6	0	-1.789533	4.086212	2.815659
134	6	0	-2.628783	2.982485	2.350281
135	6	0	-4.811058	2.091859	1.552808
136	6	0	-6.233737	2.269149	1.251450
137	6	0	-6.752082	0.997533	1.018864
138	6	0	-5.652419	0.060245	1.194998
139	6	0	-4.784807	-2.269254	1.365764
140	6	0	-4.973596	-3.722046	1.315453

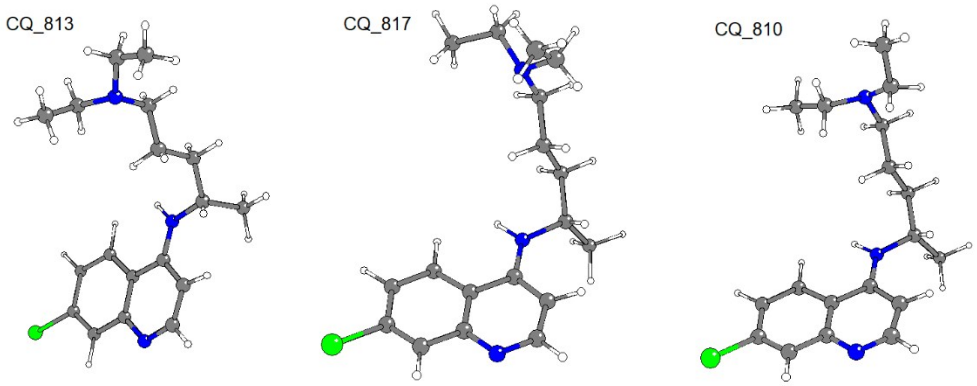
141	6	0	-3.809722	-4.290278	1.830031
142	6	0	-2.932199	-3.185947	2.191941
143	6	0	-0.886581	-2.291042	3.301851
144	6	0	-0.078773	-0.262598	3.736483
145	6	0	0.796970	-1.218240	4.414873
146	6	0	0.300957	-2.479513	4.133379
147	6	0	-1.707635	-3.324892	2.856573
148	6	0	-5.768617	-1.325944	1.065275
149	6	0	-3.929662	3.130240	1.871520
150	6	0	0.075669	1.125157	3.780392
151	1	0	-1.391283	-4.332900	3.101041
152	1	0	-6.734041	-1.706705	0.752088
153	1	0	-4.311085	4.143195	1.805169
154	1	0	0.926105	1.503703	4.337443
155	6	0	-2.159473	5.542443	2.719238
156	6	0	0.857478	-3.794932	4.605486
157	6	0	1.950971	-0.869843	5.327127
158	6	0	0.510904	4.204799	4.029660
159	6	0	-6.899992	3.572530	1.225766
160	6	0	-8.159782	0.619476	0.647212
161	6	0	-6.180205	-4.361925	0.789364
162	6	0	-3.479293	-5.749201	1.990145
163	6	0	1.768941	4.247250	3.107343
164	6	0	3.224734	-0.317014	4.640528
165	6	0	3.996122	-1.349108	3.794834
166	6	0	2.968927	4.870981	3.784359
167	8	0	3.309519	4.184465	4.946794
168	8	0	3.608861	5.860543	3.400241
169	8	0	3.717368	-2.587516	3.861468
170	1	0	-3.066757	5.766248	3.297647
171	1	0	-1.360021	6.185990	3.100939
172	1	0	-2.356946	5.839835	1.680257
173	1	0	0.571721	-4.000903	5.647823
174	1	0	0.504805	-4.635612	3.997303
175	1	0	1.951216	-3.762373	4.543390
176	1	0	1.609722	-0.130016	6.067988
177	1	0	2.238125	-1.768431	5.882909
178	1	0	0.238221	5.231587	4.301623
179	1	0	0.784555	3.696297	4.961165
180	1	0	-8.193423	-0.319684	0.083756
181	1	0	-2.399853	-5.917302	2.066069
182	1	0	2.036247	3.222325	2.820311
183	1	0	1.561080	4.818123	2.197712
184	1	0	3.003849	0.540747	3.993651
185	1	0	3.917315	0.054832	5.409666
186	1	0	4.104183	4.580902	5.371762
187	8	0	4.930394	-0.819262	3.031256
188	6	0	-8.220930	3.828230	1.403958
189	6	0	-6.607647	-5.632765	1.003103
190	1	0	-3.848713	-6.328951	1.134688
191	1	0	-3.940916	-6.174575	2.893435
192	1	0	-8.625989	1.398254	0.031350
193	1	0	-8.793539	0.487101	1.536518
194	1	0	-6.801339	-3.734245	0.149758
195	1	0	-6.087847	-6.331367	1.650860
196	1	0	-7.525919	-5.991483	0.544117
197	1	0	-6.249517	4.430049	1.050244
198	1	0	-8.945998	3.052885	1.631546
199	1	0	-8.599505	4.846547	1.358208

6. Chloroquine

6.1 Free Chloroquine

Minimum by method 3 in n-octanol: CQ_813. Minimum by method 3 in water and method 1 in n-octanol: CQ_817. Minimum by method 1 in water: CQ_810. Energies:

conformer	ZPE	m1 oct	m1 water	m3 oct	m3 water
CQ_813	0.416225	-880.658863	-880.650476	-1326.315713	-1326.306883
CQ_817	0.416306	-880.658982	-880.650843	-1326.315726	-1326.307172
CQ_810	0.416523	-880.658964	-880.651193	-1326.314385	-1326.306239



CQ_813 Atomic coordinates:

1	6	0	-2.647984	-1.293954	-2.982938
2	6	0	-2.741649	-2.584669	-2.401645
3	6	0	-1.566398	-0.487137	-2.646887
4	6	0	-0.557963	-0.928276	-1.738339
5	6	0	-0.680305	-2.242975	-1.162808
6	6	0	-1.796549	-3.063103	-1.515480
7	6	0	0.589863	-0.120461	-1.357399
8	6	0	1.503622	-0.692506	-0.453623
9	6	0	1.276101	-1.996284	0.052468
10	7	0	0.233619	-2.772825	-0.268925
11	7	0	0.744923	1.153913	-1.863635
12	6	0	1.875627	2.059795	-1.576167
13	6	0	3.121649	1.699233	-2.420609
14	6	0	1.428129	3.520960	-1.815354
15	6	0	0.385403	4.033585	-0.799015
16	6	0	-0.087099	5.467707	-1.115192
17	7	0	-1.079845	5.973946	-0.138755
18	6	0	-1.036076	7.447685	0.034578
19	6	0	0.157734	7.918063	0.885748
20	6	0	-2.450149	5.455775	-0.381285
21	6	0	-3.308013	5.396982	0.896031
22	17	0	-4.165790	-3.628468	-2.853521
23	1	0	-3.410077	-0.950577	-3.674601
24	1	0	-1.516995	0.498409	-3.104019
25	1	0	-1.862070	-4.047733	-1.066634
26	1	0	2.388316	-0.158093	-0.129094
27	1	0	1.990134	-2.422455	0.754781
28	1	0	2.124746	1.953740	-0.510441
29	1	0	3.386638	0.642138	-2.304228
30	1	0	3.984524	2.305538	-2.115205
31	1	0	2.931767	1.885398	-3.485888

32	1	0	2.321411	4.161015	-1.778235
33	1	0	1.033204	3.609681	-2.842751
34	1	0	-0.474273	3.350222	-0.772855
35	1	0	0.814453	4.028804	0.212257
36	1	0	0.786820	6.131426	-1.095522
37	1	0	-0.483692	5.506657	-2.153716
38	1	0	-1.960047	7.755217	0.538201
39	1	0	-1.025415	7.968126	-0.946725
40	1	0	0.132278	9.009097	1.013298
41	1	0	0.121627	7.446399	1.874535
42	1	0	1.118861	7.660258	0.423003
43	1	0	-2.361994	4.439008	-0.783294
44	1	0	-2.973656	6.054895	-1.156673
45	1	0	-2.828233	4.753460	1.642321
46	1	0	-4.304810	4.993433	0.670797
47	1	0	-3.444190	6.389348	1.343600
48	1	0	0.079729	1.482077	-2.550845

CQ_817 Atomic coordinates:

1	6	0	-2.761987	-1.905971	-0.631950
2	6	0	-2.939253	-3.167496	-0.007755
3	6	0	-1.480926	-1.369511	-0.701584
4	6	0	-0.352016	-2.056875	-0.162994
5	6	0	-0.563023	-3.334548	0.467717
6	6	0	-1.884089	-3.876234	0.532442
7	6	0	1.004967	-1.535613	-0.211784
8	6	0	2.015790	-2.327140	0.363641
9	6	0	1.687508	-3.568148	0.963393
10	7	0	0.454441	-4.085838	1.029647
11	7	0	1.261977	-0.310775	-0.792288
12	6	0	2.592375	0.319230	-0.908719
13	6	0	3.412270	-0.290921	-2.071332
14	6	0	2.419568	1.846310	-1.081908
15	6	0	1.799625	2.557920	0.139684
16	6	0	1.642256	4.075926	-0.087546
17	7	0	1.027957	4.770111	1.068161
18	6	0	1.986585	5.015482	2.175596
19	6	0	1.304842	5.106987	3.553246
20	6	0	0.260100	5.981699	0.684201
21	6	0	-1.101410	5.654362	0.043495
22	17	0	-4.624899	-3.855975	0.074087
23	1	0	-3.614582	-1.376193	-1.043589
24	1	0	-1.370345	-0.400659	-1.182939
25	1	0	-2.012455	-4.839599	1.012746
26	1	0	3.051990	-2.011363	0.360533
27	1	0	2.480786	-4.166300	1.408020
28	1	0	3.129163	0.144577	0.035825
29	1	0	3.468851	-1.382096	-1.988480
30	1	0	4.435459	0.107295	-2.073115
31	1	0	2.948018	-0.049442	-3.036409
32	1	0	3.409318	2.275833	-1.294016
33	1	0	1.806308	2.035542	-1.980167
34	1	0	0.812039	2.142118	0.375910
35	1	0	2.430611	2.371856	1.020974
36	1	0	2.629100	4.516509	-0.348863
37	1	0	0.996312	4.227192	-0.962069
38	1	0	2.584623	5.933381	1.991543
39	1	0	2.698702	4.181632	2.198120
40	1	0	2.053376	5.261440	4.342580
41	1	0	0.592544	5.939832	3.603450
42	1	0	0.756588	4.181402	3.763093
43	1	0	0.848547	6.632543	0.002787
44	1	0	0.080121	6.568118	1.592757
45	1	0	-0.990445	5.089633	-0.890950
46	1	0	-1.647461	6.578608	-0.190394
47	1	0	-1.705282	5.053131	0.732885
48	1	0	0.492775	0.194416	-1.210432

6.2 [(FePPIXH)(OH)(CQH)]

See Fig. 1 for image. Charge 0, overall spin 5/2. Calculated spin on Fe: +4.03.

Energies:

ZPE	m1 (octanol)	m1 (water)	m3 (octanol)	m3 (water)
1.027492	-2914.651088	-2914.639869	-4501.346989	-4501.332733

Atomic coordinates:

1	26	0	0.481718	0.242114	-1.538998
2	8	0	0.314708	-0.178154	0.240279
3	7	0	-1.029903	-0.902522	-2.429463
4	7	0	1.849811	-1.184184	-2.256351
5	7	0	-0.801600	1.886539	-1.720489
6	7	0	2.076980	1.613768	-1.543211
7	6	0	-2.384159	-0.587583	-2.434076
8	6	0	-3.170950	-1.759952	-2.819591
9	6	0	-2.267003	-2.777873	-3.071821
10	6	0	-0.934074	-2.234701	-2.819565
11	6	0	1.546974	-2.476671	-2.681226
12	6	0	2.768480	-3.265360	-2.802367
13	6	0	3.820810	-2.431996	-2.433250
14	6	0	3.229397	-1.131027	-2.103679
15	6	0	3.433668	1.287484	-1.514536
16	6	0	4.230460	2.473906	-1.226580
17	6	0	3.334576	3.533122	-1.086790
18	6	0	1.991883	2.978223	-1.293858
19	6	0	-0.491634	3.206881	-1.419483
20	6	0	-2.186475	1.818417	-1.820671
21	6	0	-2.773058	3.134031	-1.559680
22	6	0	-1.719545	3.999081	-1.320830
23	6	0	0.799439	3.708733	-1.227563
24	6	0	3.955664	0.010059	-1.749567
25	6	0	0.257366	-2.954872	-2.941316
26	6	0	-2.916106	0.670787	-2.137510
27	1	0	0.878342	4.766262	-0.998420
28	1	0	5.032709	-0.099268	-1.685419
29	1	0	0.172699	-3.985980	-3.269786
30	1	0	-3.996041	0.753367	-2.143810
31	6	0	-2.556552	-4.189243	-3.510734
32	6	0	-1.764741	5.473066	-1.014478
33	6	0	-4.252207	3.431136	-1.545596
34	6	0	-4.677774	-1.835757	-2.889158
35	6	0	2.828191	-4.713141	-3.208094
36	6	0	5.249969	-2.737496	-2.306654
37	6	0	5.958121	-3.630152	-3.041355
38	6	0	5.731943	2.512566	-1.145555
39	6	0	3.595320	4.950243	-0.827938
40	6	0	4.701832	5.503827	-0.269082
41	6	0	-5.321877	-2.490791	-1.635904
42	6	0	-4.943008	2.903457	-0.261773
43	6	0	-6.392742	3.311665	-0.178711
44	6	0	-5.227066	-1.638174	-0.368111
45	8	0	-5.356590	-0.374838	-0.404116
46	8	0	-5.037731	-2.325324	0.753339
47	8	0	-6.950287	2.987382	1.063707
48	8	0	-7.074660	3.866558	-1.053216
49	1	0	-1.963697	-4.469087	-4.392158
50	1	0	-3.613298	-4.313759	-3.770673
51	1	0	-2.325583	-4.915678	-2.718124
52	1	0	-1.202318	6.055852	-1.757232
53	1	0	-1.330379	5.696118	-0.029566
54	1	0	-2.793317	5.848719	-1.013254
55	1	0	-4.746190	2.986226	-2.418269
56	1	0	-4.420592	4.511128	-1.624461
57	1	0	-4.975116	-2.423887	-3.768619
58	1	0	-5.112314	-0.838808	-3.017441
59	1	0	1.923228	-5.255899	-2.910357
60	1	0	3.688639	-5.210613	-2.745299
61	1	0	2.933890	-4.827266	-4.297167

62	1	0	5.779224	-2.196424	-1.520645
63	1	0	5.521514	-4.187815	-3.865609
64	1	0	7.013383	-3.800772	-2.842621
65	1	0	6.190472	1.680043	-1.689426
66	1	0	6.084270	2.457075	-0.105071
67	1	0	6.121297	3.445110	-1.572418
68	1	0	2.799201	5.634933	-1.123427
69	1	0	5.537254	4.914498	0.095090
70	1	0	4.778700	6.581493	-0.145734
71	1	0	-4.877358	-3.468619	-1.427144
72	1	0	-6.393091	-2.652106	-1.832935
73	1	0	-4.430762	3.273220	0.636296
74	1	0	-4.910732	1.805710	-0.216100
75	1	0	-7.900243	3.248008	1.078810
76	6	0	4.944468	1.438093	3.502715
77	6	0	6.175764	0.940390	3.004475
78	6	0	3.801846	0.659519	3.357556
79	6	0	3.843920	-0.618762	2.723497
80	6	0	5.106741	-1.093291	2.218930
81	6	0	6.275625	-0.287199	2.379752
82	6	0	2.677707	-1.465197	2.540123
83	6	0	2.868687	-2.690182	1.881616
84	6	0	4.157851	-3.048344	1.414579
85	7	0	5.259595	-2.302234	1.563872
86	7	0	1.426872	-1.033770	2.964862
87	6	0	0.195172	-1.865107	2.978923
88	6	0	0.248366	-2.928794	4.101537
89	6	0	-1.014015	-0.906084	3.101049
90	6	0	-2.386409	-1.615001	3.052167
91	6	0	-3.518507	-0.570602	3.070529
92	7	0	-4.912328	-1.144182	2.952652
93	6	0	-5.234770	-2.209662	3.969062
94	6	0	-5.208919	-1.751205	5.437751
95	6	0	-5.917242	-0.008766	2.901490
96	6	0	-7.368332	-0.472350	2.715776
97	17	0	7.662770	1.978859	3.193785
98	1	0	4.901886	2.411639	3.979516
99	1	0	2.866985	1.068652	3.732839
100	1	0	7.213602	-0.672971	1.996397
101	1	0	2.042998	-3.366539	1.697956
102	1	0	4.288437	-3.993108	0.891454
103	1	0	0.122862	-2.360449	2.002592
104	1	0	-0.585879	-3.635496	4.015636
105	1	0	1.179233	-3.504966	4.052905
106	1	0	0.195999	-2.452595	5.090379
107	1	0	-0.931154	-0.343585	4.048567
108	1	0	-0.952340	-0.191531	2.270692
109	1	0	-2.462497	-2.215700	2.135611
110	1	0	-2.479935	-2.296836	3.906961
111	1	0	-3.457815	0.041954	3.982739
112	1	0	-3.397463	0.100575	2.211609
113	1	0	-6.222374	-2.603204	3.711511
114	1	0	-4.526624	-3.028559	3.810621
115	1	0	-5.464178	-2.599227	6.085470
116	1	0	-4.218305	-1.391104	5.739939
117	1	0	-5.937396	-0.955329	5.631776
118	1	0	-5.813980	0.604631	3.807450
119	1	0	-5.636224	0.601358	2.038281
120	1	0	-7.989447	0.411108	2.528454
121	1	0	-7.460446	-1.133076	1.846864
122	1	0	-7.771787	-0.984545	3.597610
123	1	0	-4.976764	-1.698532	1.838550
124	1	0	0.958037	-0.244386	0.974546
125	1	0	1.391058	-0.210552	3.554055

6.3 [(FePPIX)(OH)(CQH_2)]

See Fig. 1 for image. Charge 0, overall spin 5/2. Calculated spin on Fe: +4.07.

Energies:

ZPE	m1 (octanol)	m1 (water)	m3 (octanol)	m3 (water)
1.030062	-2914.658406	-2914.647772	-4501.343265	-4501.329629

Atomic coordinates:

1	26	0	2.728822	0.646889	0.511332
2	7	0	2.478323	2.696310	0.313960
3	7	0	4.784883	0.971778	0.274689
4	7	0	0.919536	0.591708	1.530947
5	7	0	3.201000	-1.160849	1.450714
6	6	0	1.252384	3.357596	0.368866
7	6	0	1.348651	4.654793	-0.299942
8	6	0	2.665430	4.794345	-0.705267
9	6	0	3.363401	3.572499	-0.316484
10	6	0	5.388858	2.119475	-0.246590
11	6	0	6.807196	1.885600	-0.463833
12	6	0	7.063078	0.569429	-0.075646
13	6	0	5.789799	0.013919	0.388174
14	6	0	4.418838	-1.839717	1.353243
15	6	0	4.283937	-3.189739	1.879737
16	6	0	2.965542	-3.321028	2.316254
17	6	0	2.307739	-2.039026	2.055638
18	6	0	0.349465	-0.502256	2.184009
19	6	0	-0.037152	1.609305	1.579971
20	6	0	-1.228258	1.152223	2.293932
21	6	0	-0.992760	-0.165196	2.655290
22	6	0	0.983243	-1.729945	2.386148
23	6	0	5.606142	-1.289584	0.858333
24	6	0	4.715351	3.312147	-0.543860
25	6	0	0.107368	2.872165	1.004033
26	1	0	0.398580	-2.502794	2.872634
27	1	0	6.473531	-1.939833	0.849554
28	1	0	5.294800	4.107209	-1.001377
29	1	0	-0.764137	3.515086	1.005368
30	6	0	3.293006	5.940798	-1.451914
31	6	0	-1.905112	-1.082175	3.426221
32	6	0	-2.395808	2.032960	2.686457
33	6	0	0.182505	5.559522	-0.603538
34	6	0	7.786607	2.908598	-0.971743
35	6	0	8.325293	-0.171525	-0.060864
36	6	0	9.456689	0.097204	-0.761347
37	6	0	5.388654	-4.207241	1.959257
38	6	0	2.303301	-4.457578	2.958731
39	6	0	2.657381	-5.766292	2.896735
40	6	0	-0.559086	5.139927	-1.915715
41	6	0	-3.457454	2.379091	1.603285
42	6	0	-4.605722	1.396120	1.525308
43	6	0	-1.224714	3.750516	-1.769037
44	8	0	-2.156447	3.649084	-0.880781
45	8	0	-0.763902	2.786037	-2.502320
46	8	0	-5.694421	1.894120	0.891007
47	8	0	-4.595002	0.227224	2.007451
48	1	0	4.192550	6.313421	-0.942222
49	1	0	2.594330	6.778322	-1.545420
50	1	0	3.590248	5.646001	-2.468491
51	1	0	-1.720724	-1.015513	4.509274
52	1	0	-1.763217	-2.131316	3.137006
53	1	0	-2.949456	-0.819004	3.232367
54	1	0	-1.985173	2.985759	3.049269
55	1	0	-2.905191	1.570501	3.540118
56	1	0	0.531757	6.595655	-0.709363
57	1	0	-0.551852	5.549203	0.210728
58	1	0	7.418531	3.929717	-0.827695
59	1	0	7.991273	2.780583	-2.045110
60	1	0	8.745868	2.822863	-0.446118
61	1	0	8.349971	-1.042882	0.594389

62	1	0	9.532617	0.915899	-1.469565
63	1	0	10.338098	-0.529540	-0.649550
64	1	0	6.377831	-3.736901	1.960697
65	1	0	5.357711	-4.904107	1.108683
66	1	0	5.301734	-4.805598	2.874475
67	1	0	1.421483	-4.213246	3.552269
68	1	0	3.490498	-6.123322	2.299923
69	1	0	2.087891	-6.519828	3.435542
70	1	0	0.140768	5.122735	-2.758533
71	1	0	-1.342396	5.884429	-2.113140
72	1	0	-3.010765	2.505711	0.602836
73	1	0	-3.900642	3.360083	1.819012
74	6	0	-0.101217	-4.993789	-2.284821
75	6	0	1.086263	-4.286222	-1.973899
76	6	0	1.116414	-2.908374	-1.854307
77	6	0	-0.090312	-2.182613	-2.060325
78	6	0	-1.312204	-2.856555	-2.367439
79	6	0	-1.278807	-4.277379	-2.473468
80	6	0	-2.522832	-2.057870	-2.534133
81	6	0	-2.406208	-0.654983	-2.414231
82	6	0	-1.170790	-0.049128	-2.154399
83	7	0	-0.063814	-0.800529	-1.966332
84	17	0	2.612759	-5.237135	-1.729066
85	7	0	-3.716214	-2.671473	-2.805992
86	6	0	-5.044537	-2.013933	-2.773660
87	6	0	-6.004533	-2.795878	-3.689340
88	6	0	-5.559998	-1.913216	-1.310817
89	6	0	-6.634437	-0.823991	-1.097428
90	6	0	-7.243069	-0.942363	0.319457
91	7	0	-7.762670	0.357797	0.854598
92	6	0	-8.841690	0.958865	0.009078
93	6	0	-9.230439	2.382691	0.444413
94	6	0	-8.096777	0.260397	2.317127
95	6	0	-9.300197	-0.633334	2.682623
96	1	0	-0.084816	-6.075011	-2.369153
97	1	0	2.022398	-2.363860	-1.607256
98	1	0	-2.177208	-4.842191	-2.707733
99	1	0	-3.257596	0.001829	-2.528222
100	1	0	-1.062531	1.055386	-2.137439
101	1	0	-3.735971	-3.680927	-2.878532
102	1	0	-4.928451	-1.002584	-3.181358
103	1	0	-7.003914	-2.347858	-3.668926
104	1	0	-5.650907	-2.794194	-4.727042
105	1	0	-6.103376	-3.839583	-3.355677
106	1	0	-5.952582	-2.897721	-1.009025
107	1	0	-4.715436	-1.689578	-0.646339
108	1	0	-6.164470	0.162576	-1.211153
109	1	0	-7.418789	-0.903183	-1.863108
110	1	0	-8.030313	-1.714805	0.321943
111	1	0	-6.452475	-1.252112	1.013187
112	1	0	-6.559023	1.239548	0.859337
113	1	0	-8.458219	1.002118	-1.015753
114	1	0	-9.731134	0.305439	-0.005082
115	1	0	-9.907055	2.820738	-0.300204
116	1	0	-9.749504	2.397622	1.409964
117	1	0	-8.342049	3.021149	0.516491
118	1	0	-7.188703	-0.103481	2.812647
119	1	0	-8.268904	1.278204	2.683934
120	1	0	-9.436194	-0.627892	3.771764
121	1	0	-10.233563	-0.273922	2.231598
122	1	0	-9.148092	-1.674800	2.374804
123	1	0	0.872986	-0.338328	-1.707293
124	8	0	2.273583	0.114573	-1.277409
125	1	0	2.754761	0.573282	-1.995743

6.4 [(FePPIXH)$_2$(μ-O)(CQH$_2$)]

See Fig. 6 for image. Charge 0, overall spin 0. Calculated spins on Fe: +4.03, -4.04.

Energies:

ZPE	m1 (octanol)	m1 (water)	m3 (octanol)	m3 (water)
1.622183	-4872.202457	-4872.195719	-7599.902922	-7599.891479

Atomic coordinates:

1	26	0	2.127544	0.519425	1.819328
2	7	0	2.304897	2.611965	1.692401
3	7	0	4.234027	0.457798	1.778955
4	7	0	0.299350	0.879170	2.835160
5	7	0	2.226749	-1.254999	2.991317
6	6	0	1.280778	3.542920	1.819381
7	6	0	1.770658	4.882087	1.493751
8	6	0	3.107122	4.749572	1.169114
9	6	0	3.433613	3.329426	1.299031
10	6	0	5.089906	1.466690	1.339681
11	6	0	6.452086	0.963009	1.226325
12	6	0	6.416271	-0.375778	1.611683
13	6	0	5.025536	-0.667347	1.973098
14	6	0	3.311601	-2.134324	3.040222
15	6	0	2.962139	-3.332227	3.793530
16	6	0	1.645388	-3.165059	4.217399
17	6	0	1.207054	-1.858594	3.719534
18	6	0	-0.479672	-0.035873	3.545972
19	6	0	-0.469620	2.039318	2.747804
20	6	0	-1.783523	1.831747	3.360393
21	6	0	-1.788832	0.541250	3.858929
22	6	0	-0.055344	-1.301010	3.949414
23	6	0	4.581879	-1.874484	2.518183
24	6	0	4.705587	2.792521	1.107952
25	6	0	-0.016067	3.263920	2.257544
26	1	0	-0.766570	-1.893117	4.514788
27	1	0	5.311598	-2.670908	2.607991
28	1	0	5.479372	3.479987	0.783511
29	1	0	-0.714072	4.093298	2.298479
30	6	0	4.087806	5.822799	0.782915
31	6	0	-2.895704	-0.148849	4.611086
32	6	0	-2.860258	2.884855	3.458369
33	6	0	0.939473	6.137473	1.566682
34	6	0	7.653379	1.777426	0.832977
35	6	0	7.508928	-1.339714	1.746921
36	6	0	8.734700	-1.295550	1.165379
37	6	0	3.898718	-4.467253	4.105151
38	6	0	0.815995	-4.041036	5.047602
39	6	0	0.935330	-5.384193	5.200132
40	6	0	-0.020398	6.295418	0.344601
41	6	0	-3.639575	3.143736	2.141992
42	6	0	-4.840056	2.207654	1.919629
43	6	0	-0.917915	7.502229	0.479868
44	8	0	-1.782330	7.379397	1.568420
45	8	0	-0.932499	8.508704	-0.244418
46	8	0	-5.407799	2.290753	0.732216
47	8	0	-5.267349	1.452336	2.861796
48	1	0	4.942913	5.857066	1.471987
49	1	0	3.619906	6.812504	0.785816
50	1	0	4.484470	5.651912	-0.226507
51	1	0	-2.746860	-0.077214	5.698982
52	1	0	-2.951234	-1.215897	4.359128
53	1	0	-3.860976	0.302757	4.359334
54	1	0	-2.408146	3.830259	3.790730
55	1	0	-3.588594	2.591831	4.221059
56	1	0	1.593713	7.016459	1.612100
57	1	0	0.338028	6.143481	2.483468
58	1	0	7.473419	2.852044	0.942653
59	1	0	7.940807	1.591229	-0.211161
60	1	0	8.518537	1.518448	1.456844

61	1	0	7.307554	-2.189084	2.400686
62	1	0	9.025827	-0.520650	0.464646
63	1	0	9.470832	-2.069803	1.369343
64	1	0	4.944979	-4.142352	4.101538
65	1	0	3.803082	-5.283940	3.376070
66	1	0	3.683380	-4.885293	5.095853
67	1	0	0.017382	-3.547691	5.603212
68	1	0	1.668979	-5.974004	4.659254
69	1	0	0.268275	-5.927851	5.864849
70	1	0	-0.649441	5.400955	0.262800
71	1	0	0.558411	6.401317	-0.575166
72	1	0	-2.989833	3.083609	1.260477
73	1	0	-4.048020	4.165260	2.147957
74	6	0	-0.658170	-5.922730	1.031295
75	6	0	0.553499	-5.199315	0.953939
76	6	0	0.595019	-3.822009	0.838305
77	6	0	-0.633729	-3.113105	0.784860
78	6	0	-1.884165	-3.803941	0.837536
79	6	0	-1.857030	-5.219588	0.970108
80	6	0	-3.124679	-3.038013	0.711218
81	6	0	-3.012422	-1.620749	0.695922
82	6	0	-1.764314	-1.016648	0.668294
83	7	0	-0.615583	-1.731677	0.675291
84	17	0	2.112431	-6.135780	1.004156
85	7	0	-4.320511	-3.663343	0.598425
86	6	0	-5.563006	-3.019509	0.071706
87	6	0	-6.473455	-4.130231	-0.476701
88	6	0	-6.287957	-2.116322	1.107590
89	6	0	-6.921775	-0.905411	0.383544
90	6	0	-7.738217	-0.016176	1.336411
91	7	0	-7.845335	1.410939	0.822407
92	6	0	-8.533921	1.506156	-0.530585
93	6	0	-8.506330	2.926563	-1.111544
94	6	0	-8.419469	2.335531	1.883750
95	6	0	-9.895087	2.093607	2.233140
96	1	0	-0.646813	-7.001984	1.135453
97	1	0	1.532769	-3.279888	0.783411
98	1	0	-2.780814	-5.786618	1.037176
99	1	0	-3.885047	-0.986211	0.666746
100	1	0	-1.657497	0.059123	0.614810
101	1	0	-4.303096	-4.668563	0.471284
102	1	0	-5.246576	-2.414785	-0.785716
103	1	0	-7.388341	-3.689979	-0.886898
104	1	0	-5.968588	-4.653218	-1.295470
105	1	0	-6.759446	-4.840320	0.313803
106	1	0	-7.054159	-2.702497	1.636258
107	1	0	-5.590818	-1.751723	1.872918
108	1	0	-6.115807	-0.300079	-0.049910
109	1	0	-7.533562	-1.249993	-0.458550
110	1	0	-8.746991	-0.415950	1.493227
111	1	0	-7.216134	0.063669	2.296016
112	1	0	-6.788728	1.756763	0.705875
113	1	0	-8.001673	0.849797	-1.222593
114	1	0	-9.560389	1.134778	-0.417863
115	1	0	-8.838525	2.874324	-2.154169
116	1	0	-9.161093	3.627506	-0.578765
117	1	0	-7.484009	3.322938	-1.112222
118	1	0	-7.778470	2.207035	2.762355
119	1	0	-8.276171	3.357564	1.520738
120	1	0	-10.194558	2.809395	3.008846
121	1	0	-10.556347	2.244803	1.372213
122	1	0	-10.068325	1.087639	2.631655
123	1	0	0.283850	-1.216272	0.541100
124	8	0	1.616378	-0.071492	0.143582
125	1	0	-2.360116	8.172942	1.645216
126	26	0	1.761097	0.025707	-1.713193
127	7	0	1.157485	-1.897849	-2.356838
128	7	0	3.729859	-0.582401	-2.199539
129	7	0	-0.169917	0.655118	-2.260599
130	7	0	2.379367	1.980401	-2.261625
131	6	0	-0.142712	-2.350717	-2.596897
132	6	0	-0.137336	-3.795908	-2.863775
133	6	0	1.183762	-4.202532	-2.770513
134	6	0	1.978274	-3.019948	-2.450587
135	6	0	4.191503	-1.898377	-2.226317
136	6	0	5.644276	-1.927290	-2.331633
137	6	0	6.061209	-0.601275	-2.436489

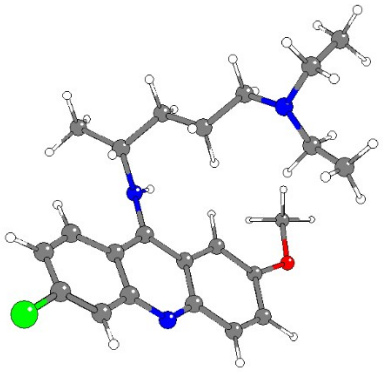
138	6	0	4.851228	0.223389	-2.357231
139	6	0	3.683589	2.421111	-2.490165
140	6	0	3.697951	3.851935	-2.759037
141	6	0	2.377462	4.287326	-2.672114
142	6	0	1.567151	3.103575	-2.369586
143	6	0	-0.639763	1.967224	-2.202647
144	6	0	-1.298173	-0.153073	-2.379223
145	6	0	-2.511997	0.662962	-2.320159
146	6	0	-2.101977	1.980800	-2.202766
147	6	0	0.173098	3.100806	-2.251199
148	6	0	4.821814	1.611429	-2.490382
149	6	0	3.366668	-3.025169	-2.310000
150	6	0	-1.278636	-1.538752	-2.556060
151	1	0	-0.331650	4.060396	-2.276566
152	1	0	5.771129	2.112907	-2.639039
153	1	0	3.854248	-3.992164	-2.363842
154	1	0	-2.235798	-2.031900	-2.645623
155	6	0	1.766393	-5.576385	-2.975245
156	6	0	-2.982951	3.198418	-2.099335
157	6	0	6.494210	-3.166127	-2.387143
158	6	0	7.396462	-0.057213	-2.680994
159	6	0	8.597367	-0.677485	-2.546745
160	6	0	4.911816	4.649360	-3.154202
161	6	0	1.816804	5.615822	-2.923342
162	6	0	2.456494	6.812392	-2.870773
163	1	0	2.529624	-5.572354	-3.765715
164	1	0	0.998089	-6.298928	-3.266810
165	1	0	2.243006	-5.955318	-2.060624
166	1	0	-3.335982	3.524754	-3.088245
167	1	0	-2.459128	4.046932	-1.643066
168	1	0	-3.868682	2.989913	-1.485249
169	1	0	5.897162	-4.070770	-2.537262
170	1	0	7.062975	-3.299130	-1.455630
171	1	0	7.222590	-3.106585	-3.207004
172	1	0	7.420736	0.974442	-3.034291
173	1	0	8.701560	-1.691617	-2.177432
174	1	0	9.518253	-0.156105	-2.797854
175	1	0	5.690981	4.013623	-3.588206
176	1	0	5.360765	5.180328	-2.301099
177	1	0	4.648212	5.407746	-3.901620
178	1	0	0.760387	5.635900	-3.193539
179	1	0	3.498919	6.911580	-2.583551
180	1	0	1.926438	7.733570	-3.098898
181	6	0	-1.332281	-4.686264	-3.130645
182	6	0	-2.342976	-4.230633	-4.217925
183	6	0	-3.637244	-3.620669	-3.639827
184	8	0	-4.407582	-3.021577	-4.509923
185	8	0	-3.876112	-3.697461	-2.382693
186	1	0	-1.911817	-4.800400	-2.203283
187	1	0	-0.955741	-5.683042	-3.387358
188	1	0	-2.650151	-5.089041	-4.830865
189	1	0	-1.909425	-3.503984	-4.914339
190	1	0	-5.473575	-2.294856	-4.095465
191	6	0	-3.926430	0.145102	-2.307164
192	6	0	-4.660866	0.148211	-3.684986
193	6	0	-6.085567	-0.386445	-3.465946
194	8	0	-6.315262	-1.671575	-3.751379
195	8	0	-6.967002	0.358286	-2.959306
196	1	0	-4.518327	0.760901	-1.616282
197	1	0	-3.934732	-0.881026	-1.924035
198	1	0	-4.116466	-0.464670	-4.409643
199	1	0	-4.730484	1.175268	-4.059104

7. Mepacrine

7.1 Free Mepacrine

Single conformer for all methods and solvents (designated QUN_10). Energies:

conformer	ZPE	m1 oct	m1 water	m3 oct	m3 water
QUN_10	0.495494	-1148.776217	-1148.768151	-1594.536427	-1594.527464



Atomic coordinates:

1	6	0	1.236686	3.292364	0.498901
2	6	0	0.557008	4.008096	-0.542329
3	6	0	-0.615169	3.508362	-1.062100
4	6	0	-1.191791	2.284205	-0.571391
5	6	0	-0.520847	1.580218	0.500340
6	6	0	0.719213	2.108575	1.003728
7	7	0	-2.332327	1.845038	-1.169473
8	6	0	-2.904195	0.710349	-0.685883
9	6	0	-2.363228	-0.047667	0.427672
10	6	0	-1.113639	0.368493	0.992567
11	6	0	-4.129539	0.278448	-1.303491
12	6	0	-4.803091	-0.804905	-0.792178
13	6	0	-4.342685	-1.513984	0.357254
14	6	0	-3.148063	-1.134780	0.943632
15	17	0	-6.361543	-1.352967	-1.563030
16	8	0	2.427967	3.889636	0.912956
17	6	0	3.202894	3.248450	1.964168
18	7	0	-0.492670	-0.341788	2.024008
19	6	0	-0.257752	-1.811575	2.088991
20	6	0	-0.689530	-2.367209	3.462534
21	6	0	1.234422	-2.136683	1.805234
22	6	0	1.684001	-1.827470	0.362149
23	6	0	3.192709	-2.085010	0.153647
24	7	0	3.640075	-1.810040	-1.229065
25	6	0	4.750021	-2.674750	-1.691635
26	6	0	3.791074	-0.366367	-1.523892
27	6	0	6.130843	-2.445835	-1.017812
28	6	0	3.898546	-0.052236	-3.026926
29	1	0	1.001721	4.930909	-0.901780
30	1	0	-1.148661	4.015910	-1.859448
31	1	0	1.269003	1.572184	1.769577
32	1	0	-4.491413	0.846703	-2.152675
33	1	0	-4.936204	-2.324347	0.767381
34	1	0	-2.828539	-1.646567	1.842699
35	1	0	3.535304	2.246270	1.657211
36	1	0	2.624265	3.178097	2.896337
37	1	0	4.071048	3.891949	2.118263
38	1	0	0.177992	0.184921	2.573070
39	1	0	-0.856851	-2.274524	1.298623
40	1	0	-1.734239	-2.119741	3.683266
41	1	0	-0.071489	-1.940064	4.264640
42	1	0	-0.575289	-3.458108	3.495557
43	1	0	1.399711	-3.204136	2.018181

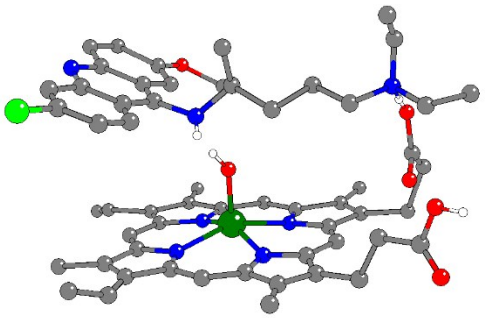
44	1	0	1.860751	-1.580639	2.525040
45	1	0	1.445130	-0.785421	0.115821
46	1	0	1.126579	-2.452817	-0.348734
47	1	0	3.397989	-3.142748	0.372221
48	1	0	3.765283	-1.494344	0.902369
49	1	0	4.855959	-2.550274	-2.775930
50	1	0	4.441906	-3.717033	-1.531536
51	1	0	4.663344	0.073686	-0.993673
52	1	0	2.902858	0.144678	-1.133665
53	1	0	6.076452	-2.593928	0.068736
54	1	0	6.509133	-1.432758	-1.204967
55	1	0	6.866989	-3.156467	-1.417634
56	1	0	3.056727	-0.501099	-3.567467
57	1	0	4.830842	-0.427936	-3.466518
58	1	0	3.873308	1.033985	-3.184475

7.2 [(FePPIXH)(OH)(MPH))]

Charge 0, overall spin 5/2. Calculated spin on Fe: +4.02.

Energies:

ZPE	m1 oct	m1 water	m3 oct	m3 water
1.108331	-3182.771403	-3182.759395	-4769.570722	-4769.555391



Atomic coordinates:

1	26	0	0.225745	-1.700889	-1.149951
2	8	0	0.375342	-0.570237	0.272976
3	7	0	-1.494275	-2.801807	-0.668124
4	7	0	1.337983	-3.398097	-0.565668
5	7	0	-0.972854	-0.631064	-2.511464
6	7	0	1.858520	-1.184945	-2.377362
7	6	0	-2.804610	-2.374268	-0.846875
8	6	0	-3.718954	-3.215424	-0.071216
9	6	0	-2.939208	-4.173388	0.554327
10	6	0	-1.552658	-3.907507	0.173755
11	6	0	0.885159	-4.449648	0.229313
12	6	0	2.005403	-5.286518	0.644356
13	6	0	3.152099	-4.724206	0.087502
14	6	0	2.714301	-3.542591	-0.666015
15	6	0	3.170018	-1.631147	-2.211804
16	6	0	4.078515	-0.841481	-3.036037
17	6	0	3.294193	0.085178	-3.719745
18	6	0	1.906480	-0.153611	-3.306647
19	6	0	-0.540550	0.314295	-3.433737
20	6	0	-2.360594	-0.537306	-2.471839
21	6	0	-2.819382	0.502539	-3.395778
22	6	0	-1.688668	1.029278	-3.995087
23	6	0	0.793015	0.547040	-3.784635
24	6	0	3.557170	-2.710102	-1.410058
25	6	0	-0.453059	-4.668005	0.580853
26	6	0	-3.200599	-1.324387	-1.681481
27	1	0	0.975274	1.333701	-4.509356

28	1	0	4.615462	-2.945227	-1.394164
29	1	0	-0.661553	-5.522246	1.217078
30	1	0	-4.260295	-1.101671	-1.705873
31	6	0	-3.387215	-5.290103	1.460352
32	6	0	-1.596022	2.108704	-5.041626
33	6	0	-4.261894	0.877010	-3.632362
34	6	0	-5.216724	-3.046101	0.029817
35	6	0	1.906068	-6.498631	1.530118
36	6	0	4.550810	-5.139466	0.206891
37	6	0	5.027603	-6.367331	0.534151
38	6	0	5.564276	-1.052789	-3.139205
39	6	0	3.686761	1.092602	-4.707533
40	6	0	4.902581	1.677878	-4.852202
41	6	0	-5.674721	-2.257300	1.287110
42	6	0	-4.847587	1.746098	-2.491633
43	6	0	-6.247542	2.220851	-2.793953
44	6	0	-5.427598	-0.748129	1.215685
45	8	0	-5.483992	-0.113611	0.113586
46	8	0	-5.198341	-0.161982	2.383101
47	8	0	-6.709725	3.117528	-1.822582
48	8	0	-6.963463	1.905737	-3.755624
49	1	0	-2.987112	-6.260420	1.136160
50	1	0	-4.479275	-5.372957	1.477109
51	1	0	-3.054743	-5.130187	2.496329
52	1	0	-1.107685	1.742216	-5.955282
53	1	0	-1.013403	2.970718	-4.686245
54	1	0	-2.587668	2.476605	-5.325163
55	1	0	-4.880396	-0.022577	-3.738908
56	1	0	-4.358316	1.418983	-4.579901
57	1	0	-5.691402	-4.036531	0.060189
58	1	0	-5.611351	-2.536037	-0.855386
59	1	0	0.992718	-6.489616	2.134886
60	1	0	2.761049	-6.549804	2.215757
61	1	0	1.900838	-7.430609	0.945544
62	1	0	5.289387	-4.361399	0.010228
63	1	0	4.382693	-7.221997	0.711711
64	1	0	6.097933	-6.544371	0.606556
65	1	0	5.846307	-2.083541	-2.898288
66	1	0	6.117138	-0.393212	-2.454034
67	1	0	5.918151	-0.838001	-4.154819
68	1	0	2.903572	1.400848	-5.401642
69	1	0	5.735689	1.474442	-4.186652
70	1	0	5.077806	2.406416	-5.640129
71	1	0	-5.197102	-2.640425	2.194409
72	1	0	-6.760734	-2.389741	1.413371
73	1	0	-4.219057	2.628692	-2.311595
74	1	0	-4.890688	1.184621	-1.547912
75	1	0	-7.629436	3.396562	-2.039156
76	7	0	1.311467	1.977938	1.134491
77	6	0	0.221848	2.222680	2.155318
78	6	0	0.495744	3.500991	2.979974
79	6	0	-1.131550	2.276832	1.405623
80	6	0	-2.352460	2.137383	2.348704
81	6	0	-3.637038	2.619343	1.650524
82	7	0	-4.913639	2.325916	2.409369
83	6	0	-4.888697	2.722389	3.863933
84	6	0	-4.744251	4.230130	4.134312
85	6	0	-6.093019	2.883749	1.635399
86	6	0	-7.453314	2.513696	2.243957
87	1	0	0.210935	1.362895	2.833203
88	1	0	-0.283561	3.655048	3.735953
89	1	0	1.454521	3.431991	3.506004
90	1	0	0.524109	4.388302	2.332370
91	1	0	-1.192991	3.234287	0.859412
92	1	0	-1.160754	1.466991	0.665850
93	1	0	-2.463925	1.085572	2.644256
94	1	0	-2.182660	2.720909	3.262409
95	1	0	-3.577598	3.699590	1.452432
96	1	0	-3.745623	2.104920	0.688437
97	1	0	-5.812417	2.342287	4.310595
98	1	0	-4.069282	2.169280	4.332286
99	1	0	-4.718948	4.401200	5.217705
100	1	0	-3.817188	4.637124	3.713339
101	1	0	-5.585763	4.803901	3.729117
102	1	0	-5.981582	3.973175	1.549847
103	1	0	-6.021950	2.458601	0.630377
104	1	0	-8.243437	2.800575	1.539713

105	1	0	-7.527376	1.432924	2.408742
106	1	0	-7.653354	3.028832	3.191348
107	1	0	-5.050051	1.109808	2.379324
108	1	0	0.820159	0.295465	0.477376
109	1	0	1.144002	2.545851	0.304962
110	6	0	2.951113	-1.035218	3.748992
111	6	0	4.278574	-0.863871	4.274702
112	6	0	5.054570	0.189990	3.849948
113	6	0	4.550854	1.148022	2.900672
114	6	0	3.181031	1.014587	2.436900
115	6	0	2.410636	-0.121929	2.858233
116	7	0	5.399341	2.117893	2.469308
117	6	0	4.939688	3.011269	1.553275
118	6	0	3.570259	3.016268	1.068769
119	6	0	2.679862	2.007343	1.547039
120	6	0	5.863851	4.004134	1.077682
121	6	0	5.438935	4.951345	0.176803
122	6	0	4.095351	4.996003	-0.302879
123	6	0	3.190277	4.049579	0.143872
124	17	0	6.602990	6.211475	-0.437314
125	8	0	2.306539	-2.182501	4.195035
126	6	0	0.976400	-2.479112	3.663486
127	1	0	4.646180	-1.602947	4.980150
128	1	0	6.072991	0.328612	4.198618
129	1	0	1.443170	-0.302966	2.408191
130	1	0	6.879292	3.968169	1.455636
131	1	0	3.798283	5.767330	-1.005829
132	1	0	2.171873	4.109844	-0.230715
133	1	0	0.256806	-1.704056	3.961903
134	1	0	0.994778	-2.558900	2.570886
135	1	0	0.697467	-3.435937	4.108550

7.3 [(FePPIXH)$_2$(μ-O)(MPH$_2$)]

See Fig. 6 for image. Charge 0, overall spin 0. Calculated spins on Fe: +4.03, -4.04.

Energies:

ZPE	m1 (octanol)	m1 (water)
1.699397	-5140.307367	-5140.297912

Atomic coordinates:

1	26	0	2.261383	0.250073	-1.903059
2	7	0	2.585370	2.333770	-1.815648
3	7	0	4.372268	0.050235	-1.976471
4	7	0	0.464289	0.747224	-2.924696
5	7	0	2.216129	-1.562201	-3.023759
6	6	0	1.623698	3.338964	-1.907749
7	6	0	2.224596	4.637544	-1.589208
8	6	0	3.561974	4.403256	-1.325406
9	6	0	3.778202	2.968063	-1.476169
10	6	0	5.315990	1.016476	-1.655964
11	6	0	6.666970	0.448881	-1.716049
12	6	0	6.516979	-0.888875	-2.074074
13	6	0	5.087607	-1.121237	-2.227569
14	6	0	3.202744	-2.541279	-3.020544
15	6	0	2.698848	-3.773157	-3.636973
16	6	0	1.398874	-3.499971	-4.058383
17	6	0	1.122710	-2.119663	-3.685366
18	6	0	-0.356684	-0.116290	-3.651875
19	6	0	-0.219674	1.962742	-2.870454
20	6	0	-1.519975	1.848159	-3.544650
21	6	0	-1.589494	0.560487	-4.046557
22	6	0	-0.058386	-1.434824	-3.985211
23	6	0	4.528428	-2.333926	-2.637651
24	6	0	5.027454	2.355917	-1.386180
25	6	0	0.309775	3.148435	-2.350581
26	1	0	-0.814714	-1.975385	-4.543230
27	1	0	5.210289	-3.168023	-2.754887

28	1	0	5.861612	3.002500	-1.139086
29	1	0	-0.332116	4.022386	-2.373932
30	6	0	4.632290	5.409651	-0.993226
31	6	0	-2.672721	-0.069674	-4.881853
32	6	0	-2.542742	2.953848	-3.682196
33	6	0	1.539507	5.982765	-1.628299
34	6	0	7.880502	1.217801	-1.437756
35	6	0	7.593250	-1.910728	-2.312361
36	6	0	3.480572	-5.006569	-3.734029
37	6	0	0.431440	-4.423512	-4.747751
38	6	0	1.436738	6.644408	-0.223999
39	6	0	-3.682612	2.919719	-2.623091
40	6	0	-4.937294	2.158000	-3.062473
41	6	0	0.783470	8.007783	-0.246959
42	8	0	-0.396745	8.015390	-0.987060
43	8	0	1.195113	9.032554	0.318314
44	8	0	-5.743346	1.787785	-2.062345
45	1	0	5.551899	5.223931	-1.562709
46	1	0	4.307195	6.429379	-1.226805
47	1	0	4.894158	5.381125	0.074449
48	1	0	-2.277151	-0.407766	-5.850255
49	1	0	-3.101895	-0.949820	-4.381199
50	1	0	-3.491940	0.629160	-5.068771
51	1	0	-2.040194	3.926670	-3.623883
52	1	0	-3.012411	2.904253	-4.671961
53	1	0	2.098736	6.657343	-2.293250
54	1	0	0.532732	5.906390	-2.046828
55	1	0	7.209267	-2.933729	-2.256221
56	1	0	-0.604905	-4.089951	-4.633254
57	1	0	0.843134	5.993928	0.429519
58	1	0	2.422805	6.765660	0.231451
59	1	0	-3.341360	2.509430	-1.668804
60	1	0	-4.018525	3.946981	-2.413742
61	8	0	1.706292	-0.236205	-0.205012
62	1	0	-0.812241	8.907787	-0.962993
63	1	0	-0.194364	0.082760	-0.170379
64	6	0	-3.493290	3.097952	1.547070
65	6	0	-2.141544	3.268922	1.174174
66	6	0	-1.381705	2.249921	0.639474
67	6	0	-1.989917	0.977499	0.434832
68	6	0	-3.373666	0.759534	0.769245
69	6	0	-4.079929	1.857087	1.348780
70	6	0	-3.934067	-0.573487	0.591641
71	6	0	-3.104760	-1.564581	-0.086401
72	6	0	-1.735744	-1.285169	-0.351695
73	7	0	-1.215387	-0.042118	-0.057566
74	6	0	-0.898742	-2.278992	-0.924751
75	6	0	-3.630880	-2.825981	-0.493636
76	6	0	-2.801283	-3.788697	-1.054324
77	6	0	-1.420836	-3.513111	-1.262365
78	8	0	-3.213907	-5.068557	-1.429327
79	6	0	-4.581079	-5.469656	-1.099613
80	17	0	-1.396147	4.907416	1.438814
81	1	0	-4.052302	3.916781	1.985378
82	1	0	-0.338433	2.390282	0.381420
83	1	0	-5.105812	1.743895	1.656215
84	1	0	0.151932	-2.061627	-1.066658
85	1	0	-4.677134	-3.036482	-0.333387
86	1	0	-0.793792	-4.287445	-1.692400
87	1	0	-4.640018	-6.528901	-1.357663
88	1	0	-5.309019	-4.904298	-1.699098
89	1	0	-4.784900	-5.322456	-0.031066
90	7	0	-5.131568	-1.013242	1.047238
91	6	0	-6.392672	-0.303922	1.385785
92	6	0	-6.580858	-0.143907	2.909641
93	6	0	-7.551354	-1.122390	0.748411
94	6	0	-7.599530	-0.963169	-0.792858
95	6	0	-8.391103	0.298396	-1.198282
96	7	0	-8.018455	0.867640	-2.547244
97	6	0	-8.872041	2.084734	-2.832518
98	6	0	-8.569330	2.762798	-4.177988
99	6	0	-7.990416	-0.139583	-3.668966
100	6	0	-9.353083	-0.755256	-4.031988
101	1	0	-5.135465	-2.021829	1.349481
102	1	0	-6.380925	0.672737	0.892441
103	1	0	-7.529032	0.368521	3.119922
104	1	0	-5.766457	0.428633	3.365218

105	1	0	-6.583333	-1.119960	3.403604
106	1	0	-8.502260	-0.795747	1.193762
107	1	0	-7.427698	-2.177937	1.024991
108	1	0	-8.054580	-1.851181	-1.250615
109	1	0	-6.570517	-0.895425	-1.168841
110	1	0	-8.193124	1.102644	-0.477979
111	1	0	-9.471287	0.093107	-1.169864
112	1	0	-6.838997	1.309222	-2.382947
113	1	0	-8.670439	2.787377	-2.014058
114	1	0	-9.933206	1.802854	-2.770336
115	1	0	-9.071647	3.737869	-4.204051
116	1	0	-8.939316	2.178709	-5.028612
117	1	0	-7.494805	2.918470	-4.316524
118	1	0	-7.288774	-0.925346	-3.372956
119	1	0	-7.539411	0.364188	-4.528371
120	1	0	-9.214907	-1.478667	-4.845249
121	1	0	-10.067922	-0.001357	-4.381823
122	1	0	-9.804250	-1.290937	-3.187559
123	8	0	-5.211944	1.947191	-4.281283
124	6	0	9.164725	0.906122	-1.750473
125	6	0	3.263156	-6.072588	-4.546096
126	1	0	0.499799	-5.438895	-4.337073
127	1	0	0.636923	-4.495597	-5.826053
128	1	0	8.394218	-1.823894	-1.569534
129	1	0	8.051307	-1.783569	-3.304644
130	1	0	4.341329	-5.066984	-3.066352
131	1	0	2.460785	-6.106183	-5.275689
132	1	0	3.918214	-6.939581	-4.507578
133	1	0	7.724720	2.165892	-0.922116
134	1	0	9.441651	0.013367	-2.300783
135	1	0	9.976623	1.574903	-1.475187
136	26	0	2.113418	-0.800561	1.525236
137	7	0	0.998888	-2.595653	1.863387
138	7	0	3.804528	-2.046629	1.340694
139	7	0	0.710690	0.100678	2.816728
140	7	0	3.458449	0.692344	2.191481
141	6	0	-0.287585	-2.747602	2.395064
142	6	0	-0.757886	-4.124815	2.198410
143	6	0	0.268312	-4.792411	1.546062
144	6	0	1.364419	-3.848546	1.374513
145	6	0	3.785382	-3.394880	0.989619
146	6	0	5.140773	-3.892458	0.805029
147	6	0	5.996040	-2.830210	1.085063
148	6	0	5.144125	-1.675236	1.383949
149	6	0	4.842756	0.712615	2.023936
150	6	0	5.370690	2.035539	2.329733
151	6	0	4.283804	2.824410	2.700954
152	6	0	3.103408	1.954936	2.642374
153	6	0	0.768242	1.408848	3.298765
154	6	0	-0.500266	-0.423621	3.276864
155	6	0	-1.216521	0.582228	4.066286
156	6	0	-0.426965	1.716650	4.079210
157	6	0	1.839585	2.289348	3.137570
158	6	0	5.617822	-0.394945	1.675755
159	6	0	2.640888	-4.196035	0.928712
160	6	0	-0.973049	-1.719477	3.052705
161	1	0	1.708706	3.287614	3.540090
162	1	0	6.691579	-0.250489	1.649865
163	1	0	2.783484	-5.222283	0.608621
164	1	0	-1.952300	-1.942627	3.455002
165	6	0	0.258084	-6.233119	1.106013
166	6	0	-0.669343	3.015034	4.800801
167	6	0	5.497600	-5.296355	0.397974
168	6	0	7.459666	-2.792515	1.111766
169	6	0	8.304958	-3.834199	1.313189
170	6	0	6.817554	2.436420	2.243111
171	6	0	4.224421	4.236586	3.077064
172	6	0	5.248443	5.066291	3.407027
173	1	0	0.153758	-6.915333	1.962062
174	1	0	-0.586770	-6.432438	0.432571
175	1	0	1.172714	-6.512561	0.574189
176	1	0	0.076445	3.174705	5.592271
177	1	0	-0.616656	3.876420	4.122527
178	1	0	-1.654605	3.026850	5.277318
179	1	0	4.720147	-5.743968	-0.232450
180	1	0	6.439198	-5.312814	-0.163826
181	1	0	5.628787	-5.954788	1.269527

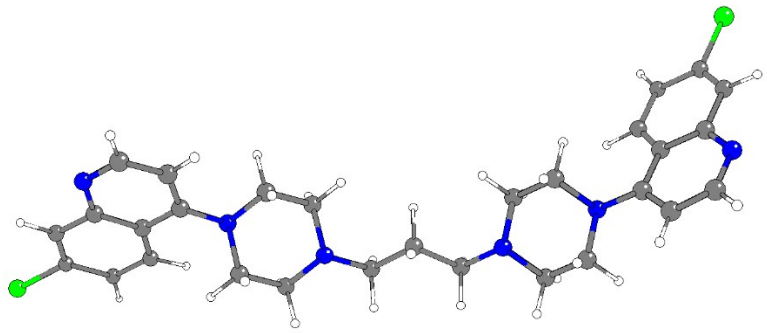
182	1	0	7.910885	-1.809680	0.969906
183	1	0	7.957324	-4.842848	1.514977
184	1	0	9.381858	-3.684265	1.310804
185	1	0	7.412503	1.709234	1.682489
186	1	0	6.925306	3.410628	1.746909
187	1	0	7.269665	2.533040	3.240959
188	6	0	-2.072840	-4.819749	2.522598
189	6	0	-2.983051	-4.322596	3.674592
190	6	0	-4.052674	-3.297526	3.246184
191	8	0	-4.256193	-2.276655	4.013494
192	8	0	-4.684243	-3.496802	2.133572
193	1	0	-2.696683	-4.835253	1.616714
194	1	0	-1.821676	-5.870071	2.723218
195	1	0	-3.538500	-5.191174	4.057225
196	1	0	-2.411200	-3.918998	4.516072
197	1	0	-4.488945	-1.668675	5.420326
198	6	0	-2.540982	0.376450	4.754698
199	6	0	-2.407417	-0.390514	6.108287
200	6	0	-3.740271	-0.440647	6.862568
201	8	0	-4.724165	-1.193430	6.289070
202	8	0	-3.936703	0.178348	7.923680
203	1	0	-3.000382	1.352442	4.956131
204	1	0	-3.227181	-0.177720	4.105811
205	1	0	-2.055989	-1.411000	5.910610
206	1	0	-1.677287	0.110190	6.750766
207	1	0	3.224397	4.671906	3.087953
208	1	0	6.281779	4.741315	3.465484
209	1	0	5.054608	6.106423	3.657359

8. Piperaquine

8.1 Free Piperaquine

Single conformer for all methods and solvents (designated PIP_80R2). Energies:

Raw ZPE	M1 octanol	M1 water	M3 Octanol	M3 Water
0.574968	-1482.516318	-1482.510070	-2373.704358	-2373.697552



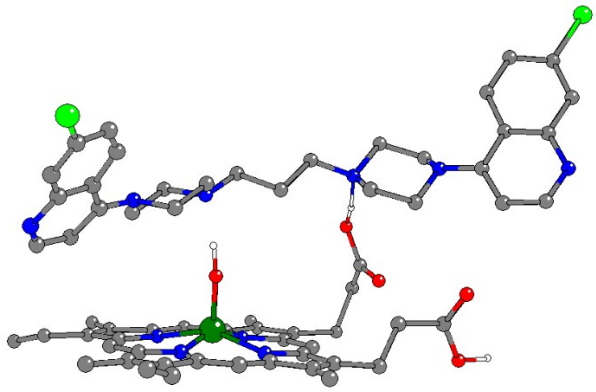
Atomic coordinates:

1	6	0	-1.256463	-1.513826	-0.836002
2	6	0	0.091695	-1.359455	-0.104516
3	6	0	4.869675	-2.736689	-0.022488
4	6	0	3.572833	-2.748530	-0.847774
5	7	0	2.566318	-1.830231	-0.269339
6	6	0	3.101382	-0.453337	-0.189612
7	6	0	4.393973	-0.429919	0.636499
8	7	0	5.400146	-1.359658	0.054764
9	1	0	4.657153	-3.143971	0.983053
10	1	0	5.612119	-3.379159	-0.508603
11	1	0	3.818198	-2.479684	-1.896547
12	1	0	3.161527	-3.765875	-0.846260
13	6	0	1.253083	-1.922345	-0.948028
14	1	0	3.306364	-0.041626	-1.201588
15	1	0	2.364008	0.195325	0.295644
16	1	0	4.799322	0.582815	0.678974
17	1	0	4.158361	-0.742851	1.669073
18	6	0	6.762391	-1.176038	0.381699
19	6	0	7.520016	-2.165741	1.021111
20	6	0	8.876243	-1.913760	1.366207
21	7	0	9.514473	-0.763519	1.129926
22	6	0	8.810280	0.216673	0.451152
23	6	0	7.444883	0.051133	0.022109
24	6	0	6.859775	1.069367	-0.791046
25	6	0	7.553740	2.231401	-1.104441
26	6	0	8.872208	2.399932	-0.604527
27	6	0	9.505876	1.426603	0.143068
28	17	0	9.752424	3.943355	-1.007058
29	1	0	-1.234951	-0.928421	-1.781930
30	1	0	-1.380547	-2.568776	-1.119520
31	1	0	1.057893	-2.986588	-1.140633
32	1	0	1.275420	-1.417062	-1.938785
33	1	0	7.079318	-3.114583	1.305095
34	1	0	9.446547	-2.682032	1.884635
35	1	0	5.871118	0.911567	-1.209091
36	1	0	7.111020	2.995458	-1.734958
37	1	0	10.525432	1.531811	0.496197
38	1	0	0.047671	-1.897224	0.850162
39	1	0	0.275851	-0.301898	0.124999
40	6	0	-3.674440	0.590980	1.265729
41	6	0	-2.510840	0.298245	0.304088
42	7	0	-2.424823	-1.146277	-0.003339

43	6	0	-3.698743	-1.636662	-0.576413
44	6	0	-4.860535	-1.356641	0.384642
45	7	0	-4.941434	0.098465	0.687187
46	1	0	-3.462587	0.111471	2.239021
47	1	0	-3.748976	1.673053	1.420062
48	1	0	-2.651474	0.899512	-0.619204
49	1	0	-1.579470	0.623094	0.780215
50	1	0	-3.916168	-1.161887	-1.557229
51	1	0	-3.617788	-2.719521	-0.735192
52	1	0	-5.801990	-1.704772	-0.044547
53	1	0	-4.688464	-1.917127	1.320506
54	6	0	-6.158983	0.626152	1.171164
55	6	0	-7.362018	0.553601	0.365855
56	6	0	-6.257714	1.269054	2.412038
57	6	0	-7.517405	1.742436	2.871400
58	7	0	-8.664159	1.614520	2.196883
59	6	0	-8.592508	1.032268	0.942543
60	6	0	-7.377783	0.099185	-0.988220
61	6	0	-8.558769	0.042909	-1.717751
62	6	0	-9.769361	0.450975	-1.097534
63	6	0	-9.805287	0.947030	0.191049
64	17	0	-11.308673	0.344312	-2.066100
65	1	0	-5.395582	1.374453	3.060808
66	1	0	-7.584852	2.217846	3.847970
67	1	0	-6.442333	-0.163798	-1.470769
68	1	0	-8.563545	-0.288754	-2.750888
69	1	0	-10.719230	1.295747	0.658419

8.2 [(FePPIXH)(OH)(PQH)]

Charge 0, overall spin 5/2. Calculated spin on Fe: +4.01.



Energies:

Raw ZPE	M1 octanol	M1 water	M3 Octanol	M3 Water
1.188073	-3516.512279	-3516.499113	-5548.732503	-5548.716392

Atomic coordinates:

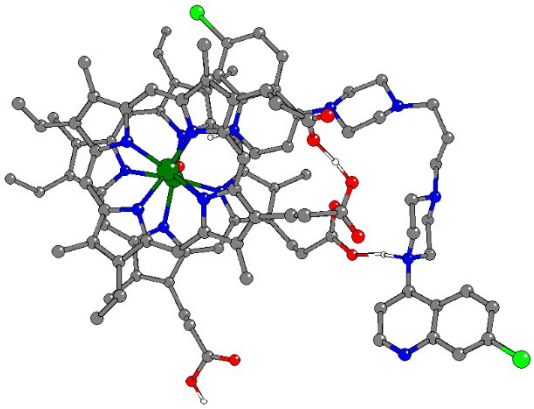
1	26	0	-2.223709	-2.162792	0.303319
2	8	0	-1.690083	-0.593211	-0.367579
3	1	0	-1.475214	0.193961	-0.966746
4	1	0	3.629363	-0.570095	-1.821139
5	7	0	-0.953120	-3.548237	-0.646239
6	7	0	-3.732251	-2.812056	-1.037318
7	7	0	-1.023958	-2.409026	2.015724
8	7	0	-3.791285	-1.659986	1.633404
9	6	0	0.351459	-3.840129	-0.270376
10	6	0	1.041035	-4.541946	-1.355870
11	6	0	0.122396	-4.688211	-2.380402

12	6	0	-1.120710	-4.064556	-1.926669
13	6	0	-3.521776	-3.454566	-2.256160
14	6	0	-4.757296	-3.484429	-3.030169
15	6	0	-5.732283	-2.859996	-2.253012
16	6	0	-5.069317	-2.442827	-1.009411
17	6	0	-5.121659	-1.441265	1.283757
18	6	0	-5.838145	-0.810346	2.389447
19	6	0	-4.916555	-0.650850	3.421046
20	6	0	-3.644836	-1.204927	2.935355
21	6	0	-1.257017	-1.851681	3.265702
22	6	0	0.281057	-2.883745	2.032202
23	6	0	0.898491	-2.610232	3.333361
24	6	0	-0.056919	-1.968462	4.099733
25	6	0	-2.462906	-1.279082	3.682125
26	6	0	-5.700908	-1.796361	0.060177
27	6	0	-2.304300	-4.013357	-2.667846
28	6	0	0.917312	-3.532504	0.971501
29	1	0	-2.485804	-0.874174	4.688426
30	1	0	-6.757522	-1.578957	-0.051915
31	1	0	-2.282920	-4.479663	-3.647766
32	1	0	1.950247	-3.823866	1.120168
33	6	0	0.317835	-5.353823	-3.717396
34	6	0	0.051526	-1.477166	5.519301
35	6	0	2.315318	-2.973879	3.704817
36	6	0	2.486856	-4.978650	-1.351627
37	6	0	-4.906545	-4.073283	-4.406718
38	6	0	-7.144971	-2.610488	-2.541869
39	6	0	-7.924325	-3.194233	-3.488441
40	6	0	-7.300875	-0.459055	2.388828
41	6	0	-5.103513	-0.097449	4.763773
42	6	0	-6.057995	0.776919	5.171920
43	6	0	3.433113	-3.997682	-2.102750
44	6	0	3.348695	-2.024685	3.042694
45	6	0	4.797944	-2.310878	3.357174
46	6	0	3.588061	-2.649305	-1.407407
47	8	0	3.796549	-2.538100	-0.169333
48	8	0	3.507438	-1.595336	-2.237830
49	8	0	5.028373	-3.604253	3.798986
50	8	0	5.737486	-1.506983	3.218105
51	1	0	-0.463902	-6.099878	-3.914547
52	1	0	1.283526	-5.868599	-3.768458
53	1	0	0.289080	-4.626566	-4.541758
54	1	0	-0.703754	-1.944539	6.166216
55	1	0	-0.093562	-0.389498	5.583827
56	1	0	1.034434	-1.703504	5.945777
57	1	0	2.541114	-4.003965	3.406622
58	1	0	2.438083	-2.939998	4.793629
59	1	0	2.577641	-5.961354	-1.833942
60	1	0	2.855888	-5.098880	-0.327470
61	1	0	-3.940816	-4.178611	-4.912141
62	1	0	-5.545021	-3.440173	-5.036071
63	1	0	-5.369699	-5.070693	-4.374754
64	1	0	-7.627799	-1.865093	-1.908599
65	1	0	-7.567378	-3.977843	-4.148190
66	1	0	-8.966583	-2.905527	-3.600347
67	1	0	-7.870615	-1.093452	1.700480
68	1	0	-7.469448	0.586137	2.089312
69	1	0	-7.731184	-0.584340	3.389613
70	1	0	-4.385439	-0.429918	5.514568
71	1	0	-6.793239	1.203880	4.496949
72	1	0	-6.101274	1.106887	6.207064
73	1	0	3.086738	-3.824462	-3.125349
74	1	0	4.435088	-4.449182	-2.157816
75	1	0	3.155283	-0.983260	3.327572
76	1	0	3.266445	-2.073093	1.947504
77	1	0	5.990950	-3.753954	3.945191
78	6	0	-1.468614	2.728770	-0.992105
79	6	0	-2.852084	2.662862	-0.331308
80	7	0	-1.269993	1.573955	-1.914731
81	7	0	-3.918099	2.632984	-1.372333
82	6	0	-2.362599	1.525790	-2.931614
83	6	0	-3.746602	1.466347	-2.266263
84	1	0	-0.702148	2.694315	-0.210656
85	1	0	-1.363558	3.681797	-1.544875
86	1	0	-2.990742	3.524988	0.323879
87	1	0	-2.911307	1.752199	0.286960
88	1	0	-2.221971	0.625316	-3.541073

89	1	0	-2.314263	2.409710	-3.593699
90	1	0	-3.846139	0.515504	-1.717804
91	1	0	-4.512480	1.499279	-3.048447
92	6	0	0.072996	1.575347	-2.558819
93	6	0	1.215519	1.134362	-1.617170
94	6	0	2.570334	1.451222	-2.279888
95	1	0	0.032654	0.880758	-3.407607
96	1	0	0.291334	2.580545	-2.972407
97	1	0	1.132846	1.657370	-0.657270
98	1	0	1.122467	0.061537	-1.412166
99	1	0	2.570955	1.064351	-3.308162
100	1	0	2.705481	2.546053	-2.336394
101	6	0	-7.606578	2.539095	-0.673213
102	6	0	-6.314157	2.125036	-1.095608
103	6	0	-5.230073	3.006572	-1.001418
104	6	0	-5.507389	4.352235	-0.541378
105	6	0	-6.846651	4.655823	-0.105110
106	7	0	-7.886386	3.743283	-0.164449
107	6	0	-7.151185	5.963845	0.383560
108	6	0	-6.165870	6.931765	0.386095
109	6	0	-4.856962	6.680544	-0.104537
110	6	0	-4.543637	5.406201	-0.560533
111	17	0	-6.547314	8.603863	1.000398
112	1	0	-8.437730	1.838811	-0.731990
113	1	0	-6.178427	1.105982	-1.438610
114	1	0	-8.162160	6.158161	0.723230
115	1	0	-4.126095	7.482100	-0.134722
116	1	0	-3.561133	5.218265	-0.980673
117	6	0	5.011718	1.238691	-2.338320
118	6	0	6.264666	0.681624	-1.653830
119	7	0	3.763954	0.843188	-1.599311
120	7	0	6.324233	1.152100	-0.247674
121	6	0	3.859194	1.216726	-0.149173
122	6	0	5.141381	0.673776	0.500936
123	1	0	4.934923	0.842359	-3.357935
124	1	0	5.076964	2.337865	-2.389380
125	1	0	7.152207	1.002789	-2.202124
126	1	0	6.240963	-0.422121	-1.682576
127	1	0	2.994903	0.793796	0.371394
128	1	0	3.831987	2.314971	-0.053347
129	1	0	5.098005	-0.426397	0.538263
130	1	0	5.190549	1.041584	1.530076
131	6	0	9.120416	0.443670	2.158661
132	6	0	7.824953	0.422977	1.570581
133	6	0	7.581745	1.163758	0.408673
134	6	0	8.655907	1.994632	-0.095476
135	6	0	9.937964	1.908122	0.557008
136	7	0	10.165038	1.124228	1.674553
137	6	0	11.033962	2.685311	0.068676
138	6	0	10.834573	3.545189	-0.993403
139	6	0	9.564467	3.706318	-1.607781
140	6	0	8.498039	2.938476	-1.156551
141	17	0	12.224284	4.544629	-1.619763
142	1	0	9.305464	-0.152211	3.049720
143	1	0	7.063690	-0.200691	2.024373
144	1	0	11.991260	2.583715	0.567265
145	1	0	9.435320	4.432746	-2.403483
146	1	0	7.514299	3.093337	-1.587809

8.3 [(FePPIXH)$_2$(μ-O)(PQH$_2$)]

See Fig. 6 for image; alternative view is shown below. Charge 0, overall spin 0. Calculated spins on Fe: +4.03, -4.04.



Energies:

ZPE	m1 (octanol)	m1 (water)
1.777939	-5474.021112	-5474.014931

Atomic coordinates:

1	1	0	3.483196	-5.446581	-4.009613
2	1	0	3.235148	-4.505074	-5.486553
3	1	0	9.305855	-0.159079	-0.370280
4	1	0	9.760771	0.562247	-1.921904
5	1	0	6.852272	-3.958684	-2.537902
6	1	0	5.586612	-5.335704	-4.987745
7	1	0	7.142126	-5.772443	-4.091695
8	1	0	7.954553	4.159503	-1.176978
9	1	0	10.114626	2.132082	-0.333982
10	1	0	10.209329	3.974532	-0.397497
11	26	0	3.296466	0.648729	-1.821413
12	7	0	3.011168	2.720804	-1.980865
13	7	0	5.365424	1.047722	-1.794632
14	7	0	1.439225	0.464379	-2.829713
15	7	0	3.798750	-1.197523	-2.742263
16	6	0	1.801598	3.379828	-2.180838
17	6	0	1.999233	4.826908	-2.085995
18	6	0	3.340821	5.033014	-1.826495
19	6	0	3.963265	3.712459	-1.753968
20	6	0	5.977125	2.261795	-1.521734
21	6	0	7.414391	2.065087	-1.301979
22	6	0	7.658814	0.703041	-1.473877
23	6	0	6.377347	0.088045	-1.795699
24	6	0	5.033779	-1.832641	-2.652624
25	6	0	4.959251	-3.168657	-3.252628
26	6	0	3.655747	-3.321092	-3.720591
27	6	0	2.947665	-2.090550	-3.396592
28	6	0	0.889440	-0.681547	-3.409216
29	6	0	0.413930	1.409480	-2.808333
30	6	0	-0.829937	0.821861	-3.309686
31	6	0	-0.529555	-0.471312	-3.698409
32	6	0	1.599487	-1.848761	-3.687792
33	6	0	6.206137	-1.249871	-2.163172
34	6	0	5.319425	3.496000	-1.510243
35	6	0	0.587093	2.759128	-2.487891
36	1	0	1.056351	-2.642689	-4.188755
37	1	0	7.091433	-1.875085	-2.149776
38	1	0	5.918245	4.378323	-1.313718
39	1	0	-0.288446	3.395147	-2.569213
40	6	0	4.061637	6.342917	-1.658642

41	6	0	-1.482657	-1.474328	-4.291403
42	6	0	-2.150291	1.542531	-3.434300
43	6	0	0.928802	5.872512	-2.263146
44	6	0	8.344140	3.155136	-1.008971
45	6	0	8.978961	-0.013320	-1.409482
46	6	0	6.083527	-4.106612	-3.297440
47	6	0	3.051406	-4.518003	-4.402127
48	6	0	0.267803	6.261973	-0.903647
49	6	0	-2.938062	1.783072	-2.104554
50	6	0	-3.954922	0.677648	-1.744886
51	6	0	-0.890055	7.215094	-1.079218
52	8	0	-0.482651	8.430306	-1.622649
53	8	0	-2.079472	6.993682	-0.803443
54	8	0	-5.139572	1.121902	-1.398820
55	8	0	-3.610875	-0.553334	-1.786148
56	1	0	4.994225	6.370036	-2.236982
57	1	0	3.442442	7.182779	-1.992575
58	1	0	4.313680	6.526765	-0.605325
59	1	0	-1.772011	-1.197706	-5.315564
60	1	0	-1.050931	-2.480216	-4.336682
61	1	0	-2.393902	-1.516996	-3.682238
62	1	0	-1.971094	2.526457	-3.892403
63	1	0	-2.794505	0.995695	-4.132291
64	1	0	1.347680	6.778892	-2.714095
65	1	0	0.152039	5.512634	-2.949101
66	6	0	9.623249	3.072841	-0.557735
67	1	0	8.934654	-1.000445	-1.880086
68	6	0	6.269883	-5.128240	-4.170093
69	1	0	1.966503	-4.565308	-4.257210
70	1	0	-0.108472	5.368780	-0.399046
71	1	0	1.025448	6.730318	-0.264403
72	1	0	-2.232745	1.877377	-1.266408
73	1	0	-3.493421	2.724232	-2.170614
74	8	0	2.909377	0.168302	-0.080662
75	1	0	-1.249847	9.037012	-1.737194
76	7	0	-7.611789	-2.369786	-1.444158
77	6	0	-7.062796	-3.684728	-1.895052
78	6	0	-6.953552	-1.856370	-0.209526
79	6	0	-7.624626	-0.575258	0.279337
80	7	0	-7.563037	0.490677	-0.822882
81	6	0	-8.157174	1.792058	-0.412374
82	6	0	-7.438543	-1.361687	-2.520840
83	6	0	-8.102134	-0.027498	-2.153192
84	6	0	-7.331253	-4.857438	-0.922990
85	1	0	-5.973081	-3.609962	-2.058096
86	1	0	-7.524281	-3.907746	-2.867341
87	1	0	-7.047481	-2.577462	0.605064
88	1	0	-5.876410	-1.675284	-0.374139
89	1	0	-8.670114	-0.767717	0.524857
90	1	0	-7.105104	-0.174870	1.158943
91	1	0	-6.367182	-1.193222	-2.743044
92	1	0	-7.919506	-1.727925	-3.437034
93	1	0	-7.875172	0.735053	-2.905560
94	1	0	-9.183194	-0.150098	-2.081577
95	1	0	-6.479449	0.667064	-1.017265
96	1	0	-7.418717	-4.488436	0.104678
97	1	0	-8.296972	-5.328544	-1.149713
98	6	0	-7.293274	2.871932	-0.318033
99	6	0	-7.804437	4.144229	0.070673
100	7	0	-9.087952	4.368743	0.350200
101	6	0	-9.963507	3.302488	0.265723
102	6	0	-9.555153	1.965753	-0.110645
103	6	0	-10.566895	0.950376	-0.145554
104	6	0	-11.890029	1.233901	0.161601
105	6	0	-12.257540	2.557566	0.519655
106	6	0	-11.330357	3.576966	0.577521
107	17	0	-13.999925	2.892968	0.912384
108	1	0	-6.240238	2.746745	-0.544094
109	1	0	-7.131476	4.993968	0.150541
110	1	0	-10.320807	-0.071971	-0.402982
111	1	0	-12.641811	0.451904	0.135437
112	1	0	-11.590584	4.591781	0.855679
113	7	0	-2.249502	-4.324554	-0.506636
114	6	0	-2.551092	-5.277828	-1.617962
115	6	0	-3.734898	-6.205218	-1.274661
116	7	0	-4.875687	-5.388623	-0.852169
117	6	0	-4.540980	-4.640546	0.371047

118	6	0	-3.448896	-3.619542	0.043081
119	1	0	-2.832861	-4.687150	-2.505421
120	1	0	-1.661249	-5.862018	-1.868381
121	1	0	-3.997503	-6.773632	-2.176406
122	1	0	-3.423642	-6.931933	-0.494195
123	1	0	-5.406888	-4.094198	0.745456
124	1	0	-4.199445	-5.308383	1.185135
125	1	0	-3.836828	-2.886766	-0.678521
126	1	0	-3.148632	-3.107548	0.961641
127	6	0	-6.229693	-5.952642	-0.979556
128	1	0	-6.455420	-6.713835	-0.204721
129	1	0	-6.276452	-6.464788	-1.952180
130	6	0	1.664410	-6.244726	-0.147687
131	6	0	2.805194	-5.405683	-0.175901
132	6	0	2.711292	-4.029267	-0.271895
133	6	0	1.420560	-3.446777	-0.370189
134	6	0	0.241671	-4.260028	-0.416545
135	6	0	0.404673	-5.667382	-0.261069
136	6	0	-1.059990	-3.609213	-0.498376
137	6	0	-1.090257	-2.195760	-0.503741
138	6	0	0.092351	-1.466987	-0.453039
139	7	0	1.297539	-2.068858	-0.385822
140	17	0	4.445492	-6.171970	-0.028777
141	1	0	1.778918	-7.315288	-0.015720
142	1	0	3.591511	-3.395756	-0.257089
143	1	0	-0.474423	-6.295754	-0.178734
144	1	0	-2.019461	-1.654282	-0.637261
145	1	0	0.105327	-0.386774	-0.493705
146	1	0	2.120128	-1.432117	-0.296839
147	26	0	2.923576	0.517987	1.751172
148	7	0	2.329021	-1.319321	2.615801
149	7	0	4.878885	0.004737	2.338576
150	7	0	0.962044	1.161455	2.153386
151	7	0	3.495863	2.532378	2.016450
152	6	0	1.022551	-1.770095	2.807265
153	6	0	1.024477	-3.172270	3.232693
154	6	0	2.350423	-3.557826	3.316759
155	6	0	3.155565	-2.402165	2.923034
156	6	0	5.356069	-1.277764	2.602325
157	6	0	6.811299	-1.276628	2.653388
158	6	0	7.216974	0.040788	2.449105
159	6	0	5.994763	0.829650	2.264012
160	6	0	4.804643	3.015791	2.087498
161	6	0	4.803767	4.469678	2.138360
162	6	0	3.467841	4.871670	2.103901
163	6	0	2.666490	3.646902	2.019996
164	6	0	0.476580	2.459494	2.002615
165	6	0	-0.160914	0.344415	2.273478
166	6	0	-1.382487	1.132119	2.092929
167	6	0	-0.986234	2.450072	1.953458
168	6	0	1.268161	3.606123	1.960871
169	6	0	5.952926	2.219912	2.147093
170	6	0	4.549234	-2.391377	2.868000
171	6	0	-0.134085	-1.013331	2.601444
172	1	0	0.740628	4.552401	1.916599
173	1	0	6.904412	2.738346	2.157830
174	1	0	5.053433	-3.321688	3.108043
175	1	0	-1.087970	-1.519785	2.740058
176	6	0	2.915921	-4.884801	3.747031
177	6	0	-1.863258	3.663151	1.794593
178	6	0	7.669524	-2.492139	2.875597
179	6	0	8.563167	0.613461	2.402322
180	6	0	9.707717	0.087788	2.909373
181	6	0	6.022768	5.341474	2.267969
182	6	0	2.884936	6.209047	2.200814
183	6	0	3.509427	7.415567	2.162748
184	1	0	3.534988	-4.779907	4.649090
185	1	0	2.118270	-5.597385	3.980059
186	1	0	3.548063	-5.334964	2.969105
187	1	0	-1.730436	4.365653	2.629482
188	1	0	-1.653835	4.216764	0.869373
189	1	0	-2.920946	3.382378	1.774232
190	1	0	7.146428	-3.414334	2.600821
191	1	0	8.586302	-2.437249	2.275313
192	1	0	7.976162	-2.588781	3.927753
193	1	0	8.644093	1.578579	1.901391
194	1	0	9.735475	-0.845665	3.462431

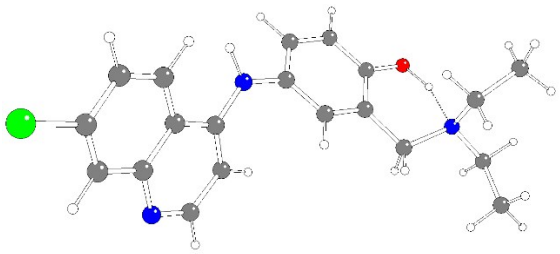
195	1	0	10.653003	0.614890	2.803337
196	1	0	6.934352	4.757924	2.425155
197	1	0	6.178861	5.958311	1.370431
198	1	0	5.922345	6.031135	3.117218
199	1	0	1.804371	6.233229	2.343215
200	1	0	4.579449	7.532075	2.029959
201	1	0	2.937016	8.333329	2.272622
202	6	0	-0.221624	-3.987306	3.473046
203	6	0	-1.056540	-3.578993	4.729357
204	6	0	-2.559621	-3.385903	4.444870
205	8	0	-3.426076	-3.804936	5.253148
206	8	0	-2.821578	-2.705054	3.319747
207	1	0	-0.879377	-3.890722	2.601043
208	1	0	0.046746	-5.047603	3.550871
209	1	0	-0.958470	-4.318852	5.529635
210	1	0	-0.687768	-2.623735	5.128433
211	1	0	-3.975607	-2.155100	3.097854
212	6	0	-2.770497	0.557929	1.969694
213	6	0	-3.583475	0.406606	3.293629
214	6	0	-4.918987	-0.256134	2.927967
215	8	0	-4.912795	-1.587286	2.792003
216	8	0	-5.932918	0.448172	2.668322
217	1	0	-3.360613	1.183151	1.287441
218	1	0	-2.704204	-0.432494	1.506296
219	1	0	-3.025135	-0.206586	4.007075
220	1	0	-3.780603	1.389403	3.732499

9. Amodiaquine

9.1 Free Amodiaquine

Single conformer for all methods and solvents (designated AQZ_39). Energies:

ZPE	m1 oct	m1 water	m3 oct	m3 water
0.388526	-1029.680369	-1029.673209	-1475.384030	-1475.375887



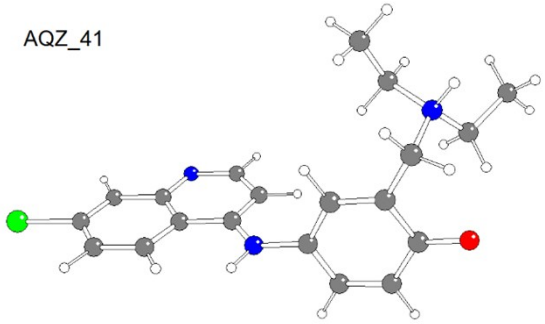
Atomic coordinates:

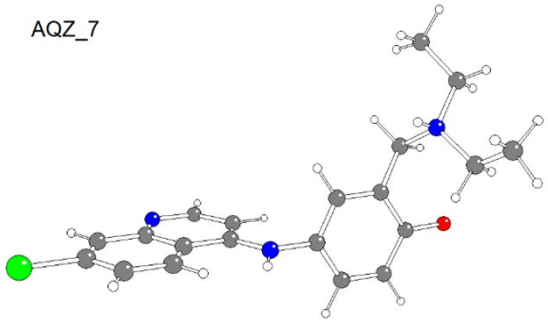
1	6	0	1.033307	-5.220472	1.008074
2	6	0	0.720403	-6.128821	-0.036429
3	6	0	-0.247593	-5.856580	-0.983258
4	6	0	-0.975348	-4.628406	-0.914576
5	6	0	-0.697222	-3.698555	0.150695
6	6	0	0.329130	-4.024385	1.088502
7	6	0	-1.475096	-2.474545	0.202841
8	6	0	-2.416883	-2.263254	-0.815788
9	6	0	-2.593858	-3.242076	-1.825519
10	7	0	-1.918878	-4.396733	-1.899033
11	7	0	-1.279872	-1.581594	1.251578
12	6	0	-1.774924	-0.242913	1.357449
13	6	0	-2.294750	0.203111	2.592314
14	6	0	-2.701479	1.535838	2.755288
15	6	0	-2.627233	2.435745	1.675817
16	6	0	-2.131198	1.993824	0.417437
17	6	0	-1.688492	0.667900	0.283024
18	8	0	-3.034627	3.748423	1.854401
19	6	0	-2.146094	2.938036	-0.778958
20	7	0	-1.834081	4.353670	-0.392452
21	6	0	-2.376341	5.352498	-1.360135
22	17	0	1.650384	-7.693190	-0.120538
23	1	0	1.816227	-5.458291	1.720528
24	1	0	-0.483286	-6.540165	-1.791033
25	1	0	0.605688	-3.327896	1.876119
26	1	0	-3.041537	-1.378553	-0.820887
27	1	0	-3.337169	-3.072931	-2.602136
28	1	0	-2.380394	-0.494181	3.423199
29	1	0	-3.089697	1.894399	3.703625
30	1	0	-1.263225	0.341464	-0.663045
31	1	0	-1.458715	2.567243	-1.557157
32	1	0	-3.155641	2.947948	-1.215194
33	6	0	-0.392206	4.530779	-0.039380
34	6	0	-0.091050	5.877726	0.638059
35	1	0	0.245849	4.404141	-0.931709
36	1	0	-0.135662	3.719078	0.651533
37	1	0	-0.742343	6.029885	1.507408
38	1	0	-0.217632	6.726925	-0.044165
39	1	0	0.949266	5.888656	0.986888
40	6	0	-1.759910	5.328615	-2.778175
41	1	0	-3.458366	5.178465	-1.429257
42	1	0	-2.247693	6.348572	-0.922897
43	1	0	-0.686151	5.551275	-2.761774
44	1	0	-1.901254	4.356990	-3.267420
45	1	0	-2.246610	6.088702	-3.402892
46	1	0	-0.799189	-1.931802	2.069850
47	1	0	-2.685507	4.276106	1.043534

9.2 Amodiaquine zwitterion

Minimum for method 1, n-octanol: AQZ_41. Minimum for all other conditions: AQZ_7. Energies:

conformer	ZPE	m1 oct	m1 water	m3 oct	m3 water
AQZ_7	0.389161	-1029.663605	-1029.661868	-1475.367202	-1475.364491
AQZ_41	0.389228	-1029.663797	-1029.661586	-1475.366663	-1475.363615





AQZ_41 Atomic coordinates:

1	6	0	-2.146068	-3.955940	1.836122
2	6	0	-3.564297	-3.975336	1.797546
3	6	0	-4.290632	-3.154181	0.957771
4	6	0	-3.605344	-2.247992	0.089544
5	6	0	-2.164406	-2.209796	0.103696
6	6	0	-1.467969	-3.079409	0.996031
7	6	0	-1.500334	-1.279507	-0.793343
8	6	0	-2.318020	-0.478410	-1.610583
9	6	0	-3.725758	-0.603496	-1.538357
10	7	0	-4.382260	-1.446205	-0.727010
11	7	0	-0.120409	-1.191299	-0.830231
12	6	0	0.616546	-0.237951	-1.626350
13	6	0	1.189712	-0.617004	-2.871809
14	6	0	1.939049	0.282135	-3.625975
15	6	0	2.146317	1.650908	-3.204188
16	6	0	1.540408	2.013490	-1.924799
17	6	0	0.816142	1.070909	-1.164471
18	8	0	2.821903	2.520389	-3.909003
19	6	0	1.842497	3.376908	-1.402305
20	7	0	0.833884	4.505923	-1.889506
21	6	0	-0.555898	4.349517	-1.281902
22	17	0	-4.437714	-5.130298	2.906926
23	1	0	-1.609334	-4.613681	2.511658
24	1	0	-5.374216	-3.164547	0.924615
25	1	0	-0.381701	-3.075155	1.045270
26	1	0	-1.871645	0.217781	-2.310704
27	1	0	-4.347122	0.015386	-2.183639
28	1	0	1.036102	-1.634531	-3.228128
29	1	0	2.390230	-0.018482	-4.568308
30	1	0	0.411257	1.345075	-0.188789
31	1	0	1.816269	3.442339	-0.310176
32	1	0	2.809152	3.717643	-1.790674
33	6	0	0.774714	4.589960	-3.429247
34	6	0	0.482349	6.020362	-3.895689
35	1	0	-0.004057	3.888931	-3.743686
36	1	0	1.728157	4.190994	-3.802599
37	1	0	1.285043	6.712888	-3.606733
38	1	0	-0.472544	6.413493	-3.520744
39	1	0	0.431313	6.026640	-4.990457
40	6	0	-0.611184	4.741586	0.200586
41	1	0	-1.235357	4.977107	-1.867707
42	1	0	-0.832643	3.302633	-1.434123
43	1	0	-1.643142	4.643070	0.556322

44	1	0	0.013095	4.095724	0.826909
45	1	0	-0.305594	5.784838	0.359172
46	1	0	0.417527	-1.847312	-0.278890
47	1	0	1.228130	5.396167	-1.554618

AQZ_7 Atomic coordinates:

1	6	0	0.062428	-5.043770	-1.858018
2	6	0	-0.541403	-5.908334	-0.908729
3	6	0	-1.272609	-5.433185	0.161873
4	6	0	-1.439311	-4.023117	0.333348
5	6	0	-0.842671	-3.120469	-0.619343
6	6	0	-0.093226	-3.670648	-1.702662
7	6	0	-1.037485	-1.695016	-0.418350
8	6	0	-1.786750	-1.298177	0.702877
9	6	0	-2.323567	-2.276753	1.573042
10	7	0	-2.175713	-3.602216	1.425089
11	7	0	-0.495622	-0.775925	-1.301397
12	6	0	-0.595855	0.657217	-1.157309
13	6	0	-1.560623	1.394815	-1.901531
14	6	0	-1.669704	2.777302	-1.780918
15	6	0	-0.810415	3.538667	-0.896740
16	6	0	0.157259	2.750983	-0.134349
17	6	0	0.243779	1.349257	-0.273498
18	8	0	-0.864087	4.836243	-0.777679
19	6	0	0.954511	3.493485	0.878709
20	7	0	2.324483	4.093199	0.320690
21	6	0	3.048715	4.900248	1.391871
22	17	0	-0.326701	-7.707218	-1.128612
23	1	0	0.633855	-5.454189	-2.683909
24	1	0	-1.734141	-6.089145	0.891354
25	1	0	0.383972	-3.024715	-2.435865
26	1	0	-1.967594	-0.247340	0.895350
27	1	0	-2.909495	-1.956550	2.432639
28	1	0	-2.228768	0.850586	-2.567684
29	1	0	-2.414303	3.331182	-2.347495
30	1	0	0.955338	0.778165	0.325916
31	1	0	0.405024	4.381336	1.210675
32	1	0	1.262587	2.867890	1.720300
33	6	0	2.100118	4.893521	-0.972573
34	6	0	3.405069	5.364995	-1.625137
35	1	0	1.407226	5.700505	-0.726290
36	1	0	1.556861	4.218829	-1.636468
37	1	0	4.111442	4.537527	-1.785731
38	1	0	3.914230	6.157402	-1.065075
39	1	0	3.159249	5.775483	-2.611450
40	6	0	3.491754	4.058046	2.597533
41	1	0	3.921635	5.359835	0.921166
42	1	0	2.359778	5.697496	1.689284
43	1	0	4.112271	4.680464	3.252673
44	1	0	2.648571	3.693553	3.191145
45	1	0	4.101349	3.197360	2.290153
46	1	0	-0.047531	-1.126576	-2.137683
47	1	0	2.905643	3.280173	0.072241

9.3 [(FePPIXH)(AQ)]

See Fig. 1 for image. Charge 0, overall spin 5/2. Calculated spin on Fe: +4.04.

Energies:

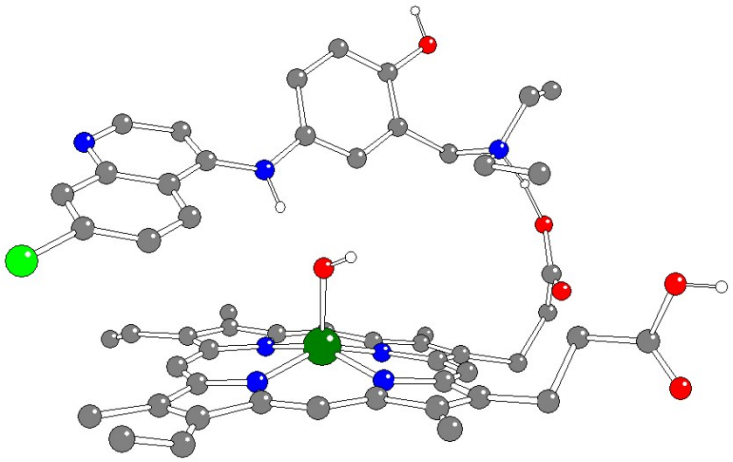
ZPE	m1 oct	m1 water	m3 oct	m3 water
0.975734	-2987.225493	-2987.214883	-4573.941146	-4573.928028

Atomic coordinates:

1	26	0	-2.312445	1.074051	0.537029
2	7	0	-3.796215	-0.377702	0.295196
3	7	0	-3.616570	2.427115	-0.382492
4	7	0	-1.544963	-0.096157	2.085688
5	7	0	-1.389005	2.712122	1.459824
6	6	0	-3.736145	-1.694159	0.745588
7	6	0	-4.803182	-2.486497	0.134570
8	6	0	-5.521757	-1.625363	-0.675964
9	6	0	-4.886502	-0.313530	-0.572094
10	6	0	-4.730508	2.107671	-1.159513
11	6	0	-5.224055	3.294652	-1.844469
12	6	0	-4.400455	4.351728	-1.459041
13	6	0	-3.403323	3.791300	-0.541430
14	6	0	-1.498278	4.045661	1.057177
15	6	0	-0.526534	4.866149	1.767853
16	6	0	0.182085	4.009496	2.609820
17	6	0	-0.375689	2.668978	2.411130
18	6	0	-0.479729	0.231276	2.920464
19	6	0	-1.782255	-1.456292	2.271821
20	6	0	-0.822219	-2.008873	3.226418
21	6	0	-0.016227	-0.959472	3.633315
22	6	0	0.058221	1.511797	3.068125
23	6	0	-2.417726	4.530163	0.120679
24	6	0	-5.307056	0.834192	-1.247074
25	6	0	-2.795967	-2.188787	1.653980
26	1	0	0.885849	1.614323	3.761678
27	1	0	-2.380136	5.593520	-0.087211
28	1	0	-6.177553	0.730215	-1.886306
29	1	0	-2.848690	-3.245602	1.884022
30	6	0	-6.713902	-1.944449	-1.537782
31	6	0	1.128505	-0.979062	4.610981
32	6	0	-0.752785	-3.460274	3.630010
33	6	0	-5.000418	-3.971603	0.322516
34	6	0	-6.386156	3.325534	-2.799218
35	6	0	-4.430314	5.758233	-1.864201
36	6	0	-5.472723	6.449229	-2.391432
37	6	0	-0.384607	6.357786	1.631242
38	6	0	1.248888	4.311586	3.566744
39	6	0	2.092299	5.374683	3.556620
40	6	0	-4.362914	-4.832046	-0.817139
41	6	0	-0.106587	-4.349237	2.525127
42	6	0	0.058312	-5.794808	2.928732
43	6	0	-2.888144	-4.473433	-1.029226
44	8	0	-2.033584	-4.683677	-0.110861
45	8	0	-2.614808	-3.892816	-2.185601
46	8	0	1.033184	-6.523471	2.685243
47	8	0	-1.049724	-6.285171	3.618859
48	1	0	-7.528841	-1.223513	-1.388824
49	1	0	-7.107945	-2.940951	-1.311588
50	1	0	-6.453020	-1.930493	-2.605746
51	1	0	0.954312	-0.291072	5.449975
52	1	0	2.072371	-0.680113	4.133977
53	1	0	1.276579	-1.979024	5.030971
54	1	0	-1.751853	-3.851802	3.851378
55	1	0	-0.172751	-3.558408	4.555604
56	1	0	-6.072821	-4.206253	0.364575
57	1	0	-4.572591	-4.295186	1.277268
58	1	0	-6.595065	2.336087	-3.219456
59	1	0	-6.184945	4.007043	-3.635144
60	1	0	-7.306976	3.674896	-2.309158
61	1	0	-3.498662	6.307436	-1.722712
62	1	0	-6.455593	6.013525	-2.538855
63	1	0	-5.360485	7.494954	-2.666945
64	1	0	-1.313810	6.824420	1.286718
65	1	0	0.405108	6.630877	0.915648
66	1	0	-0.121186	6.811541	2.594264
67	1	0	1.371204	3.592258	4.377392
68	1	0	2.082293	6.127986	2.774965
69	1	0	2.838652	5.497297	4.337587
70	1	0	-4.900258	-4.676901	-1.757518
71	1	0	-4.438224	-5.889863	-0.533813
72	1	0	0.886778	-3.972273	2.259526

73	1	0	-0.724180	-4.341485	1.614523
74	6	0	-0.100581	-2.058682	-1.243998
75	7	0	-0.608055	-2.463638	-2.628826
76	6	0	0.362182	-3.284221	-3.454375
77	6	0	1.379437	-2.504702	-4.305667
78	1	0	0.380213	-2.951145	-0.831987
79	1	0	-1.002210	-1.876055	-0.655690
80	1	0	0.876240	-3.949495	-2.751638
81	1	0	-0.248657	-3.923414	-4.102477
82	1	0	2.043386	-3.223487	-4.803351
83	1	0	0.889276	-1.914837	-5.087869
84	1	0	1.994142	-1.829664	-3.704242
85	1	0	-1.503437	-3.200936	-2.380753
86	6	0	8.617740	-0.611681	-2.325322
87	6	0	9.608621	-0.041003	-1.484664
88	6	0	7.278056	-0.428699	-2.001981
89	6	0	6.884665	0.312379	-0.846192
90	6	0	7.911942	0.904746	-0.027662
91	6	0	9.285320	0.704840	-0.368026
92	6	0	5.503578	0.509788	-0.448301
93	6	0	5.262236	1.304446	0.681668
94	6	0	6.353559	1.857481	1.398976
95	7	0	7.643091	1.677150	1.087845
96	7	0	4.490396	-0.113658	-1.175827
97	17	0	11.357580	-0.300443	-1.920865
98	1	0	8.909297	-1.170253	-3.208586
99	1	0	6.534011	-0.844377	-2.677072
100	1	0	10.036199	1.155464	0.271055
101	1	0	4.255984	1.475902	1.042509
102	1	0	6.153829	2.464994	2.279298
103	1	0	4.768149	-0.892895	-1.758303
104	6	0	3.084130	0.104544	-1.080273
105	6	0	2.527959	1.397046	-0.936697
106	6	0	1.141802	1.557636	-0.848819
107	6	0	0.267123	0.446182	-0.937799
108	6	0	0.813515	-0.852137	-1.160567
109	6	0	2.213607	-0.999566	-1.189394
110	8	0	-1.080268	0.620891	-0.815059
111	1	0	3.174880	2.267696	-0.897813
112	1	0	0.707984	2.543865	-0.712750
113	1	0	2.637502	-1.999717	-1.275387
114	6	0	-1.255548	-1.314058	-3.374560
115	1	0	-0.929298	-7.241855	3.817833
116	6	0	-2.087995	-1.791121	-4.575263
117	1	0	-0.481346	-0.601719	-3.679832
118	1	0	-1.893840	-0.804134	-2.648394
119	1	0	-2.833408	-2.527962	-4.257610
120	1	0	-1.470523	-2.233223	-5.366948
121	1	0	-2.611377	-0.929328	-5.007808

9.4 [(FePPIXH)(OH)(AQH)]



Charge 0, overall spin 5/2. Calculated spin on Fe: +4.06.

Energies:

ZPE	m1 oct	m1 water	m3 oct	m3 water
1.000787	-3063.657944	-3063.647787	-4650.405941	-4650.392502

Atomic coordinates:

1	26	0	-0.488216	1.068060	1.133344
2	7	0	0.625586	2.709784	0.489133
3	7	0	-2.196662	2.227297	0.776578
4	7	0	1.180159	0.517480	2.279017
5	7	0	-1.638834	-0.086549	2.427932
6	6	0	2.013730	2.844626	0.547623
7	6	0	2.445983	3.960478	-0.289888
8	6	0	1.299603	4.521465	-0.830472
9	6	0	0.168575	3.747543	-0.322966
10	6	0	-2.274547	3.366581	-0.017131
11	6	0	-3.677074	3.749624	-0.208388
12	6	0	-4.443401	2.827381	0.499992
13	6	0	-3.510631	1.875383	1.090069
14	6	0	-3.028092	-0.159931	2.451289
15	6	0	-3.456437	-1.289853	3.278267
16	6	0	-2.295903	-1.885147	3.771941
17	6	0	-1.176087	-1.114711	3.252467
18	6	0	1.251387	-0.547545	3.178198
19	6	0	2.478843	1.009569	2.160188
20	6	0	3.389645	0.252749	3.018990
21	6	0	2.625171	-0.718332	3.644762
22	6	0	0.166245	-1.324469	3.589774
23	6	0	-3.887140	0.758310	1.840350
24	6	0	-1.176862	4.042395	-0.561042
25	6	0	2.864191	2.064626	1.329832
26	1	0	0.381299	-2.139582	4.273079
27	1	0	-4.951306	0.601743	1.976096
28	1	0	-1.384756	4.892859	-1.201657
29	1	0	3.925212	2.272647	1.275205
30	6	0	1.178317	5.710223	-1.746794
31	6	0	3.076033	-1.753370	4.641383
32	6	0	4.865770	0.530105	3.197287
33	6	0	3.881712	4.380046	-0.486600
34	6	0	-4.106704	4.920918	-0.977582
35	6	0	-5.934695	2.807500	0.692049
36	6	0	-4.857502	-1.675012	3.464161
37	6	0	-2.177770	-3.101336	4.649195
38	6	0	4.671771	3.397206	-1.388365
39	6	0	5.806883	-0.459524	2.455727

40	6	0	5.606043	-0.457129	0.932577
41	6	0	6.084248	3.867621	-1.639072
42	8	0	6.682039	3.159500	-2.679256
43	8	0	6.697408	4.758922	-1.030677
44	8	0	5.420582	0.639717	0.309833
45	8	0	5.627596	-1.647302	0.367949
46	1	0	0.596611	6.518843	-1.282545
47	1	0	2.161565	6.118087	-2.001822
48	1	0	0.675719	5.446319	-2.687685
49	1	0	2.461602	-1.734106	5.551602
50	1	0	3.014121	-2.769630	4.226240
51	1	0	4.116165	-1.585899	4.939396
52	1	0	5.100968	1.543061	2.856871
53	1	0	5.113569	0.495743	4.268073
54	1	0	3.921281	5.382528	-0.927663
55	1	0	4.396919	4.458593	0.478636
56	1	0	4.746596	2.402095	-0.926656
57	1	0	4.174372	3.262557	-2.356970
58	1	0	6.847817	-0.170319	2.662519
59	1	0	5.670100	-1.484028	2.815810
60	6	0	-5.296195	5.087683	-1.608330
61	6	0	-5.385969	-2.393135	4.486583
62	1	0	-6.441634	2.231551	-0.094418
63	1	0	-6.341103	3.825262	0.661012
64	1	0	-6.210385	2.365420	1.656225
65	1	0	-2.960207	-3.830722	4.407020
66	1	0	-2.286527	-2.848851	5.714375
67	1	0	-1.208927	-3.597734	4.526874
68	1	0	-3.384360	5.735749	-1.045804
69	1	0	-5.542925	-1.347886	2.681527
70	1	0	-6.057263	4.313881	-1.638343
71	1	0	-5.517438	6.009813	-2.140456
72	1	0	-4.797899	-2.733819	5.333257
73	1	0	-6.445621	-2.635558	4.502947
74	1	0	7.618874	3.442150	-2.790494
75	6	0	-4.426431	0.552206	-2.378591
76	6	0	-5.782455	0.145597	-2.464765
77	6	0	-6.186731	-1.150809	-2.216490
78	6	0	-5.207849	-2.132014	-1.866735
79	6	0	-3.821040	-1.749036	-1.770732
80	6	0	-3.466117	-0.391339	-2.032039
81	6	0	-2.851282	-2.779441	-1.451377
82	6	0	-3.342323	-4.078918	-1.248907
83	6	0	-4.731491	-4.340909	-1.353670
84	7	0	-5.658656	-3.422696	-1.654072
85	7	0	-1.497112	-2.454792	-1.348607
86	6	0	-0.404514	-3.314197	-1.605628
87	6	0	-0.484829	-4.458802	-2.435893
88	6	0	0.658461	-5.231600	-2.689952
89	6	0	1.901199	-4.871020	-2.143704
90	6	0	2.022573	-3.711556	-1.347111
91	6	0	0.860534	-2.966823	-1.072688
92	8	0	3.066134	-5.638028	-2.365555
93	6	0	3.341704	-3.302473	-0.721496
94	7	0	4.282335	-2.453479	-1.586306
95	6	0	3.550300	-1.290390	-2.232929
96	6	0	5.113034	-3.251716	-2.571092
97	6	0	6.087263	-4.218257	-1.878515
98	6	0	4.483586	-0.253736	-2.876740
99	17	0	-7.031343	1.399269	-2.930273
100	1	0	-4.149854	1.581845	-2.578124
101	1	0	-7.221314	-1.467253	-2.285481
102	1	0	-2.431224	-0.075479	-1.952337
103	1	0	-2.676517	-4.886474	-0.968884
104	1	0	-5.097303	-5.350072	-1.174090
105	1	0	-1.424255	-4.737737	-2.898875
106	1	0	0.575101	-6.113014	-3.324807
107	1	0	0.923000	-2.091466	-0.430923
108	1	0	2.862390	-6.486088	-2.809061
109	1	0	3.156709	-2.694140	0.168851
110	1	0	3.916251	-4.176990	-0.413233
111	1	0	2.835025	-1.693820	-2.959242
112	1	0	2.983409	-0.808978	-1.427960
113	1	0	4.437944	-3.792184	-3.242249
114	1	0	5.681355	-2.521762	-3.153131
115	1	0	6.659500	-3.707026	-1.095762
116	1	0	5.565914	-5.075863	-1.443447

117	1	0	6.793152	-4.605559	-2.624045
118	1	0	3.879074	0.605635	-3.193387
119	1	0	5.222121	0.110909	-2.155883
120	1	0	4.992000	-0.633954	-3.769521
121	1	0	4.984125	-2.002790	-0.792746
122	1	0	-1.230144	-1.512077	-1.013144
123	8	0	-0.396667	0.003008	-0.446500
124	1	0	0.126714	0.386726	-1.181297

9.5 [(FePPIXH)$_2$(μ-O)(AQH$_2$)]

See Fig. 6 for picture. Charge 0, overall spin 0. Calculated spins on Fe: +4.04, -4.03.

Energies:

ZPE	m1 oct	m1 water
1.593274	-5021.198481	-5021.190932

Atomic coordinates:

1	26	0	-1.947585	-0.094756	-1.700206
2	7	0	-1.074047	-1.883694	-2.483069
3	7	0	-3.817334	-0.975279	-2.103015
4	7	0	-0.169327	0.825474	-2.288629
5	7	0	-2.890160	1.758230	-2.119700
6	6	0	0.265735	-2.127471	-2.818671
7	6	0	0.431980	-3.522066	-3.258660
8	6	0	-0.820591	-4.107336	-3.154056
9	6	0	-1.742702	-3.091479	-2.671025
10	6	0	-4.073956	-2.341127	-2.207971
11	6	0	-5.506981	-2.595294	-2.164869
12	6	0	-6.128985	-1.352075	-2.087586
13	6	0	-5.058013	-0.350405	-2.060150
14	6	0	-4.261438	2.005288	-2.198452
15	6	0	-4.509637	3.425754	-2.400063
16	6	0	-3.263389	4.049791	-2.428997
17	6	0	-2.264551	2.991684	-2.245919
18	6	0	0.092418	2.192035	-2.210878
19	6	0	1.067277	0.200846	-2.434917
20	6	0	2.139825	1.193836	-2.357675
21	6	0	1.533259	2.430262	-2.228738
22	6	0	-0.880694	3.192086	-2.211493
23	6	0	-5.258329	1.029435	-2.115393
24	6	0	-3.104790	-3.314901	-2.463031
25	6	0	1.267499	-1.154956	-2.715109
26	1	0	-0.522221	4.215209	-2.238524
27	1	0	-6.285451	1.374281	-2.143131
28	1	0	-3.453451	-4.333774	-2.591881
29	1	0	2.291922	-1.458016	-2.884829
30	6	0	-1.212290	-5.516895	-3.512867
31	6	0	2.199776	3.776820	-2.138006
32	6	0	-6.142295	-3.958584	-2.200197
33	6	0	-7.552753	-1.016540	-2.034823
34	6	0	-8.598025	-1.779719	-2.444398
35	6	0	-5.861959	4.050965	-2.609179
36	6	0	-2.918549	5.449936	-2.674794
37	6	0	-3.730039	6.538788	-2.640027
38	1	0	-1.819773	-5.542655	-4.429455
39	1	0	-0.333149	-6.145803	-3.682075
40	1	0	-1.801195	-5.987050	-2.715372
41	1	0	2.123707	4.330946	-3.085004
42	1	0	1.748654	4.403414	-1.356995
43	1	0	3.263094	3.670469	-1.899959
44	1	0	-5.458419	-4.732589	-1.835228
45	1	0	-7.042772	-3.985210	-1.574037
46	1	0	-6.447603	-4.241840	-3.218617
47	1	0	-7.789532	-0.038074	-1.616449

48	1	0	-8.472656	-2.751996	-2.910807
49	1	0	-9.619135	-1.418928	-2.344908
50	1	0	-6.626644	3.304225	-2.844402
51	1	0	-6.204024	4.600429	-1.719051
52	1	0	-5.834078	4.769181	-3.438943
53	1	0	-1.875986	5.632739	-2.937003
54	1	0	-4.782321	6.488314	-2.380237
55	1	0	-3.336255	7.525924	-2.868620
56	6	0	1.633250	-4.304806	-3.780653
57	6	0	2.962455	-3.601762	-4.140229
58	6	0	3.909015	-3.389664	-2.943285
59	8	0	4.508821	-2.241645	-2.855997
60	8	0	4.037458	-4.349555	-2.094522
61	1	0	1.886848	-5.085666	-3.048566
62	1	0	1.287889	-4.834030	-4.680139
63	1	0	3.502561	-4.262689	-4.833843
64	1	0	2.811071	-2.651521	-4.661113
65	1	0	5.540467	-1.210332	-3.182293
66	6	0	3.612241	0.889338	-2.361828
67	6	0	4.264428	0.919506	-3.781871
68	6	0	5.774512	0.773794	-3.632845
69	8	0	6.236263	-0.457775	-3.276377
70	8	0	6.564844	1.736495	-3.735280
71	1	0	4.128436	1.607451	-1.712840
72	1	0	3.778486	-0.102017	-1.929683
73	1	0	3.856449	0.105191	-4.391451
74	1	0	4.059999	1.874317	-4.274518
75	26	0	-2.279260	0.403459	1.831620
76	7	0	-2.520917	2.492014	1.778911
77	7	0	-4.385293	0.278623	1.818447
78	7	0	-0.465838	0.803861	2.859603
79	7	0	-2.315128	-1.411260	2.921853
80	6	0	-1.509887	3.443233	1.870269
81	6	0	-2.053869	4.780647	1.628972
82	6	0	-3.408513	4.626546	1.405705
83	6	0	-3.690006	3.194228	1.496186
84	6	0	-5.289587	1.283579	1.508457
85	6	0	-6.642987	0.729492	1.399081
86	6	0	-6.534331	-0.637305	1.655374
87	6	0	-5.127249	-0.898165	1.929459
88	6	0	-3.331760	-2.358241	2.861458
89	6	0	-2.914006	-3.590819	3.537584
90	6	0	-1.632805	-3.357538	4.031184
91	6	0	-1.276111	-1.998811	3.644002
92	6	0	0.321980	-0.084753	3.596054
93	6	0	0.295586	1.965548	2.728728
94	6	0	1.618715	1.780109	3.326506
95	6	0	1.621745	0.518408	3.898079
96	6	0	-0.064037	-1.373798	3.961104
97	6	0	-4.615377	-2.126748	2.359530
98	6	0	-4.958345	2.633580	1.354355
99	6	0	-0.187202	3.180673	2.235411
100	1	0	0.647270	-1.947929	4.544546
101	1	0	-5.310448	-2.957632	2.401008
102	1	0	-5.763728	3.320483	1.119224
103	1	0	0.502620	4.018384	2.240713
104	6	0	-4.442084	5.688695	1.147330
105	6	0	2.741126	-0.122645	4.673698
106	6	0	2.725870	2.807711	3.320472
107	6	0	-1.255645	6.057786	1.675602
108	6	0	-7.828189	1.543706	1.133022
109	6	0	-7.640512	-1.653242	1.721397
110	6	0	-3.742219	-4.796330	3.619226
111	6	0	-0.743188	-4.305827	4.787609
112	6	0	-0.492539	6.330062	0.340956
113	6	0	3.416020	3.025233	1.944568
114	6	0	4.495147	1.982175	1.581828
115	6	0	0.354037	7.578711	0.411870
116	8	0	1.363004	7.460169	1.367519
117	8	0	0.218221	8.612485	-0.259308
118	8	0	5.085535	2.172754	0.419180
119	8	0	4.781688	1.033076	2.387037
120	1	0	-5.251307	5.652495	1.889576
121	1	0	-4.004039	6.691389	1.182398
122	1	0	-4.896079	5.569407	0.154789
123	1	0	2.650495	-1.214465	4.703131
124	1	0	3.701022	0.125502	4.207228

125	1	0	2.757879	0.232383	5.714917
126	1	0	2.324582	3.775197	3.658136
127	1	0	3.495206	2.511116	4.040650
128	1	0	-1.920628	6.906422	1.877273
129	1	0	-0.526184	6.028021	2.492870
130	6	0	-9.078563	1.131951	0.795839
131	1	0	-7.322353	-2.575947	2.216229
132	6	0	-3.683505	-5.771403	4.560263
133	1	0	0.317355	-4.077350	4.635172
134	1	0	0.160670	5.476366	0.123859
135	1	0	-1.203251	6.445138	-0.480921
136	1	0	2.684048	3.051392	1.126244
137	1	0	3.913384	4.005779	1.932942
138	8	0	-1.747663	-0.149565	0.148970
139	1	0	1.905625	8.280914	1.404901
140	6	0	0.935047	-5.745330	0.226359
141	6	0	-0.319809	-5.096888	0.302884
142	6	0	-0.449621	-3.723879	0.413845
143	6	0	0.735300	-2.944793	0.465498
144	6	0	2.023000	-3.556119	0.400481
145	6	0	2.090418	-4.970921	0.270880
146	6	0	3.215275	-2.726119	0.559329
147	6	0	3.026508	-1.372509	0.941825
148	6	0	1.750651	-0.826933	0.883925
149	7	0	0.648489	-1.569811	0.617206
150	17	0	-1.821517	-6.128013	0.283414
151	7	0	4.440248	-3.278374	0.326294
152	6	0	5.687728	-2.656971	0.705951
153	6	0	6.205493	-1.537974	0.029967
154	6	0	7.450047	-0.979542	0.380253
155	6	0	8.188020	-1.605255	1.409587
156	6	0	7.686258	-2.726594	2.093691
157	6	0	6.431914	-3.247823	1.743470
158	6	0	8.017468	0.182415	-0.410921
159	7	0	7.596138	1.574424	0.079986
160	6	0	8.031709	2.608354	-0.958348
161	6	0	7.544904	4.028867	-0.641798
162	6	0	8.068311	1.897474	1.493404
163	6	0	9.574897	2.144248	1.640357
164	8	0	9.452634	-1.071005	1.715461
165	1	0	0.989275	-6.825444	0.145465
166	1	0	-1.418421	-3.241698	0.476103
167	1	0	3.058089	-5.455409	0.224102
168	1	0	3.859248	-0.726103	1.192843
169	1	0	1.590246	0.233346	1.020357
170	1	0	5.647727	-1.122186	-0.800447
171	1	0	8.268643	-3.191729	2.887640
172	1	0	6.031580	-4.116351	2.257994
173	1	0	7.676578	0.112005	-1.448179
174	1	0	9.110468	0.158643	-0.398290
175	1	0	7.617454	2.282837	-1.917386
176	1	0	9.124726	2.564141	-1.031717
177	1	0	7.775494	4.670996	-1.500484
178	1	0	8.033306	4.460875	0.240253
179	1	0	6.461207	4.035041	-0.485416
180	1	0	7.737803	1.067564	2.122007
181	1	0	7.496694	2.777094	1.803877
182	1	0	9.792297	2.317877	2.702076
183	1	0	9.910614	3.029342	1.087751
184	1	0	10.157858	1.274065	1.326782
185	1	0	9.923700	-1.609481	2.382997
186	1	0	-0.272151	-1.090890	0.503336
187	1	0	6.498306	1.654957	0.160650
188	1	0	4.468705	-3.922482	-0.508549
189	1	0	-0.913420	-5.338785	4.461547
190	1	0	-0.934043	-4.268686	5.870407
191	1	0	-7.997918	-1.922227	0.717663
192	1	0	-8.499582	-1.258264	2.279787
193	1	0	-4.482330	-4.913791	2.826559
194	1	0	-3.008100	-5.727895	5.409260
195	1	0	-4.340037	-6.636326	4.505679
196	1	0	-7.683549	2.620439	1.226331
197	1	0	-9.342691	0.089670	0.653795
198	1	0	-9.874908	1.857443	0.647875

10. Desethyl Amodiaquine

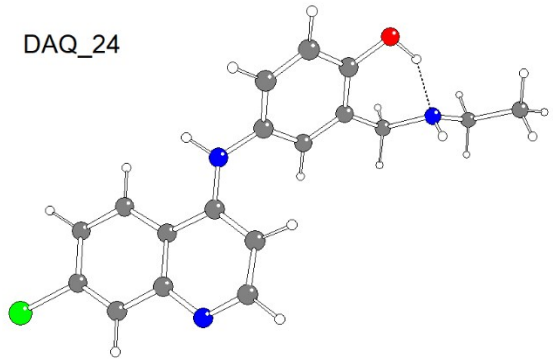
10.1 Free Desethyl Amodiaquine

Minimum in n-octanol, method 3; DAQ_24. Minimum for all other systems; DAQ_31.

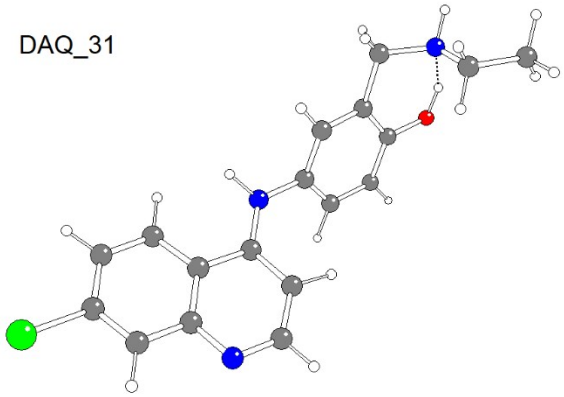
Energies:

conformer	ZPE	m1 (octanol)	m1 (water)	m3 (octanol)	m3 (water)
DAQ_24	0.332041	-951.075237	-951.069590	-1396.746499	-1396.739830
DAQ_31	0.332120	-951.075409	-951.070505	-1396.746122	-1396.740176

DAQ_24



DAQ_31



DAQ_24 Atomic coordinates:

1	6	0	-1.907941	-0.527562	4.534974
2	6	0	-3.212211	-1.060869	4.366478
3	6	0	-3.709061	-1.412455	3.126656
4	6	0	-2.889722	-1.250574	1.966921
5	6	0	-1.551801	-0.734795	2.110836
6	6	0	-1.099467	-0.369258	3.414994
7	6	0	-0.741113	-0.609592	0.913625
8	6	0	-1.333881	-0.962639	-0.308394
9	6	0	-2.666950	-1.443671	-0.331762
10	7	0	-3.443183	-1.600058	0.748370
11	7	0	0.576004	-0.174744	1.018926
12	6	0	1.454413	0.202398	-0.046287
13	6	0	2.795685	-0.238010	-0.020792
14	6	0	3.699270	0.166590	-1.014884
15	6	0	3.272499	1.008469	-2.058106
16	6	0	1.927060	1.471982	-2.089464
17	6	0	1.036648	1.063796	-1.083230
18	8	0	4.178129	1.388586	-3.036801
19	6	0	1.507213	2.465583	-3.162070
20	7	0	2.095241	2.106681	-4.489761
21	6	0	1.951258	3.155721	-5.533418
22	6	0	2.508868	2.673231	-6.880785
23	17	0	-4.253875	-1.265791	5.846826
24	1	0	-1.559485	-0.241690	5.521884
25	1	0	-4.708568	-1.809108	2.989006
26	1	0	-0.115914	0.070215	3.561469
27	1	0	-0.774062	-0.909832	-1.233931
28	1	0	-3.110929	-1.726957	-1.284141
29	1	0	3.126351	-0.909965	0.768442
30	1	0	4.731557	-0.169280	-1.008207
31	1	0	0.016720	1.440593	-1.087779
32	1	0	3.636325	1.750371	-3.822105
33	1	0	0.409065	2.549720	-3.204545

34	1	0	1.897921	3.463871	-2.913511
35	1	0	0.894778	3.459035	-5.650432
36	1	0	2.505117	4.040835	-5.193315
37	1	0	3.566078	2.397445	-6.788391
38	1	0	1.956920	1.797730	-7.250117
39	1	0	2.422547	3.464169	-7.635632
40	1	0	1.723419	1.211287	-4.819368
41	1	0	0.997387	-0.202110	1.938112

DAQ_31 Atomic coordinates:

1	6	0	3.168513	3.960480	-1.039072
2	6	0	2.603324	4.876861	-1.963608
3	6	0	1.433196	4.606822	-2.645839
4	6	0	0.750223	3.372916	-2.413548
5	6	0	1.286741	2.434677	-1.460400
6	6	0	2.511270	2.758714	-0.800993
7	6	0	0.549001	1.206578	-1.229619
8	6	0	-0.614250	0.998385	-1.986118
9	6	0	-1.037762	1.985105	-2.911514
10	7	0	-0.406639	3.144969	-3.136362
11	7	0	0.998767	0.305868	-0.269461
12	6	0	0.504387	-1.016341	-0.028879
13	6	0	0.327111	-1.944856	-1.079197
14	6	0	-0.123353	-3.243024	-0.805525
15	6	0	-0.371071	-3.648617	0.520919
16	6	0	-0.161548	-2.737301	1.591689
17	6	0	0.250634	-1.426055	1.296224
18	8	0	-0.811436	-4.941136	0.758584
19	6	0	-0.325017	-3.203256	3.033412
20	7	0	-1.450767	-4.177268	3.180401
21	6	0	-2.813443	-3.579447	3.111099
22	6	0	-3.893604	-4.655583	3.296350
23	17	0	3.476045	6.449553	-2.254741
24	1	0	4.102110	4.196930	-0.539534
25	1	0	1.002467	5.296185	-3.363204
26	1	0	2.977252	2.057462	-0.112820
27	1	0	-1.214362	0.106990	-1.851506
28	1	0	-1.947300	1.816941	-3.484775
29	1	0	0.550663	-1.653934	-2.101340
30	1	0	-0.273818	-3.964796	-1.602490
31	1	0	0.376441	-0.709787	2.107417
32	1	0	-1.135372	-4.973846	1.728747
33	1	0	0.588243	-3.728203	3.350757
34	1	0	-0.452003	-2.331897	3.697676
35	1	0	-2.932564	-2.785926	3.870400
36	1	0	-2.920488	-3.105090	2.128287
37	1	0	-3.807804	-5.429852	2.524769
38	1	0	-3.813167	-5.138659	4.280454
39	1	0	-4.892767	-4.209008	3.225388
40	1	0	-1.343587	-4.735996	4.029046
41	1	0	1.692222	0.640182	0.386424

10.2 [(FePPIXH)(DAQ)]

See Fig. 1 for image. Charge 0, overall spin 5/2. Calculated spin on Fe: +4.04.

Energies:

ZPE	m1 oct	m1 water	m3 oct	m3 water
0.918409	-2908.626117	-2908.615955	-4495.309125	-4495.296598

Atomic coordinates:

1	26	0	-1.765765	1.399971	0.443524
2	7	0	-2.987617	0.186269	1.626587
3	7	0	-0.892654	2.091640	2.218504
4	7	0	-3.247887	1.294411	-1.023510
5	7	0	-1.129323	3.178353	-0.455384
6	6	0	-4.032869	-0.615648	1.177666
7	6	0	-4.443410	-1.544934	2.229763
8	6	0	-3.641216	-1.282698	3.327400
9	6	0	-2.741632	-0.195157	2.943868
10	6	0	-0.951346	1.462945	3.465895
11	6	0	-0.025968	2.097136	4.392795
12	6	0	0.598916	3.130516	3.693993
13	6	0	0.037306	3.121040	2.340743
14	6	0	-0.153117	4.050542	0.030361
15	6	0	0.202826	5.027143	-0.990322
16	6	0	-0.579269	4.741440	-2.108482
17	6	0	-1.418303	3.593575	-1.751132
18	6	0	-3.232224	1.955206	-2.250319
19	6	0	-4.252183	0.332693	-1.114187
20	6	0	-4.871079	0.373402	-2.439656
21	6	0	-4.241639	1.386349	-3.140222
22	6	0	-2.378966	3.010178	-2.583988
23	6	0	0.388765	4.008601	1.319254
24	6	0	-1.794344	0.391339	3.784898
25	6	0	-4.612895	-0.546392	-0.090993
26	1	0	-2.485073	3.420361	-3.582411
27	1	0	1.149136	4.745811	1.550429
28	1	0	-1.722523	-0.009248	4.790656
29	1	0	-5.402117	-1.255003	-0.308333
30	6	0	-3.653562	-1.948532	4.677949
31	6	0	-4.489761	1.824277	-4.558312
32	6	0	-5.920393	-0.590698	-2.938825
33	6	0	-5.530759	-2.580327	2.089416
34	6	0	0.153954	1.715929	5.836921
35	6	0	1.590022	4.104731	4.155795
36	6	0	2.440033	3.986460	5.206951
37	6	0	1.195757	6.143411	-0.816005
38	6	0	-0.647760	5.426457	-3.400712
39	6	0	0.298401	6.214931	-3.970476
40	6	0	-5.057490	-3.836695	1.297685
41	6	0	-5.315850	-1.812726	-3.711081
42	6	0	-4.219977	-2.484552	-2.882575
43	6	0	-6.100305	-4.925647	1.221388
44	8	0	-5.910440	-6.143948	1.363623
45	8	0	-7.371500	-4.425263	0.941036
46	8	0	-4.511080	-3.147592	-1.834931
47	8	0	-2.982826	-2.248274	-3.288298
48	1	0	-3.855245	-1.227160	5.481992
49	1	0	-4.423513	-2.724832	4.731741
50	1	0	-2.689592	-2.426215	4.902316
51	1	0	-4.638603	2.910160	-4.629708
52	1	0	-3.645188	1.563221	-5.211640
53	1	0	-5.381956	1.340406	-4.969208
54	1	0	-6.517906	-0.973569	-2.104077
55	1	0	-6.616830	-0.074883	-3.613157
56	1	0	-5.872983	-2.889909	3.084626
57	1	0	-6.405452	-2.158777	1.581923
58	1	0	-0.724975	1.196554	6.233038
59	1	0	1.019207	1.051890	5.979548
60	1	0	0.322058	2.605907	6.455544
61	1	0	1.644464	5.029261	3.580002
62	1	0	2.497312	3.094158	5.822365
63	1	0	3.125465	4.792148	5.457859
64	1	0	1.336446	6.403329	0.238529
65	1	0	2.182644	5.877755	-1.222923
66	1	0	0.860942	7.046923	-1.339996
67	1	0	-1.569007	5.277364	-3.964709
68	1	0	1.266971	6.396787	-3.515753
69	1	0	0.122297	6.680205	-4.937137
70	1	0	-4.797967	-3.562998	0.264037
71	1	0	-4.167643	-4.273780	1.763056
72	1	0	-6.120278	-2.532417	-3.906203
73	1	0	-4.886865	-1.482967	-4.661943
74	6	0	0.044399	-1.733347	-2.268696

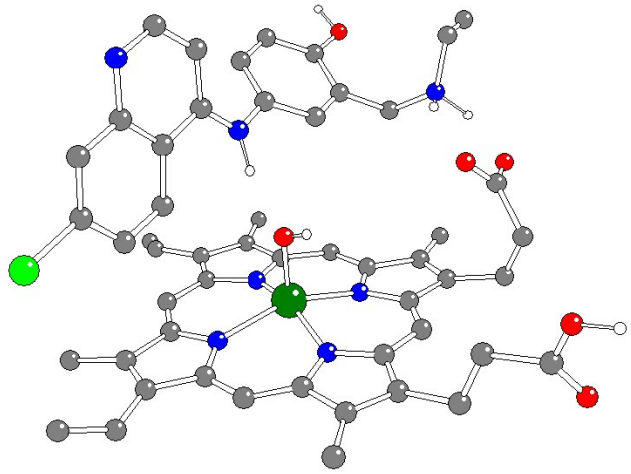
75	1	0	0.457897	-2.478719	-2.956373
76	1	0	-0.355829	-0.909593	-2.873570
77	6	0	8.594969	-3.547940	-0.470033
78	6	0	9.767695	-2.748400	-0.462496
79	6	0	7.355729	-2.920155	-0.523509
80	6	0	7.243386	-1.497353	-0.575655
81	6	0	8.449821	-0.710477	-0.536901
82	6	0	9.717425	-1.368310	-0.487645
83	6	0	5.978360	-0.793048	-0.657114
84	6	0	6.013833	0.608413	-0.644108
85	6	0	7.261750	1.279547	-0.581291
86	7	0	8.454232	0.672664	-0.536848
87	7	0	4.797357	-1.525448	-0.776211
88	17	0	11.380535	-3.591316	-0.400433
89	1	0	8.673148	-4.629052	-0.423113
90	1	0	6.468444	-3.547766	-0.492332
91	1	0	10.608193	-0.750705	-0.467758
92	1	0	5.104932	1.191851	-0.722222
93	1	0	7.278220	2.367496	-0.584023
94	1	0	4.888076	-2.480730	-1.097334
95	6	0	3.460013	-1.056810	-0.624716
96	6	0	3.092103	-0.137089	0.383258
97	6	0	1.757475	0.263307	0.522581
98	6	0	0.751679	-0.255186	-0.325974
99	6	0	1.108575	-1.206756	-1.325208
100	6	0	2.453772	-1.582408	-1.466084
101	8	0	-0.559093	0.107853	-0.205250
102	1	0	3.840387	0.246498	1.069559
103	1	0	2.730974	-2.283535	-2.252714
104	7	0	-1.155382	-2.349775	-1.593389
105	1	0	-1.449555	-1.697450	-0.852473
106	1	0	-2.045833	-2.366297	-2.405023
107	6	0	-1.014628	-3.747028	-1.050259
108	1	0	-2.035466	-4.142726	-0.985114
109	1	0	-0.481210	-4.336770	-1.805805
110	6	0	-0.313734	-3.837875	0.315537
111	1	0	0.724785	-3.494433	0.270235
112	1	0	-0.840719	-3.236801	1.067911
113	1	0	-0.317582	-4.880435	0.658137
114	1	0	1.477847	0.967541	1.298975
115	1	0	-8.014415	-5.165026	0.847750

10.3 [(FePPIXH)(OH)(DAQH)]

Charge 0, overall spin 5/2. Calculated spin on Fe: +4.06.

Energies:

ZPE	m1 oct	m1 water	m3 oct	m3 water
0.944713	-2985.056232	-2985.048250	-4571.774032	-4571.762779



Atomic coordinates:

1	26	0	-0.475328	0.656320	1.453830
2	8	0	-0.377345	0.005641	-0.322300
3	1	0	-0.183826	0.672579	-1.015095
4	7	0	1.532202	0.995416	1.922216
5	7	0	-0.381581	-1.060856	2.635156
6	7	0	-0.617669	2.707369	1.068355
7	7	0	-2.540831	0.690477	1.844565
8	6	0	2.301957	2.074577	1.495375
9	6	0	3.719293	1.802537	1.716956
10	6	0	3.800180	0.557783	2.316826
11	6	0	2.430015	0.056689	2.434090
12	6	0	0.778437	-1.710629	3.058502
13	6	0	0.449166	-3.005937	3.634415
14	6	0	-0.938158	-3.133567	3.567964
15	6	0	-1.441481	-1.904930	2.949328
16	6	0	-3.308837	-0.389351	2.284032
17	6	0	-4.728267	-0.069235	2.196054
18	6	0	-4.814525	1.230195	1.701016
19	6	0	-3.438582	1.690469	1.490422
20	6	0	-1.785018	3.421513	0.797777
21	6	0	0.441657	3.566337	0.777056
22	6	0	-0.071483	4.842639	0.281503
23	6	0	-1.452602	4.754080	0.299742
24	6	0	-3.083648	2.947272	0.989331
25	6	0	-2.792519	-1.594498	2.768545
26	6	0	2.073406	-1.186169	2.958786
27	6	0	1.791956	3.261315	0.961033
28	1	0	-3.891416	3.621766	0.726575
29	1	0	-3.514777	-2.343508	3.072745
30	1	0	2.880036	-1.802840	3.340354
31	1	0	2.512620	4.027239	0.695648
32	6	0	5.051860	-0.155677	2.759922
33	6	0	-2.461549	5.797119	-0.101301
34	6	0	0.781662	5.998208	-0.176400
35	6	0	4.865214	2.681770	1.279763
36	6	0	1.445603	-4.002515	4.160311
37	6	0	-1.797126	-4.245826	3.978319
38	6	0	-1.510504	-5.232028	4.865442
39	6	0	-5.851064	-0.978991	2.611634
40	6	0	-5.997825	2.058407	1.453470
41	6	0	-7.249991	1.629494	1.158680
42	6	0	5.051633	2.708945	-0.271098
43	6	0	1.210791	5.851344	-1.658053
44	6	0	2.168594	6.939954	-2.092499
45	6	0	5.107133	1.296217	-0.853349
46	8	0	4.207304	0.934615	-1.710053
47	8	0	6.055831	0.499622	-0.414359
48	8	0	2.304900	6.974599	-3.474724
49	8	0	2.790543	7.720838	-1.355764

50	1	0	5.432186	0.257999	3.704942
51	1	0	5.836852	-0.049106	2.002005
52	1	0	4.883035	-1.226405	2.921855
53	1	0	-3.149715	6.029858	0.722812
54	1	0	-3.072525	5.462246	-0.951117
55	1	0	-1.973742	6.732386	-0.395139
56	1	0	1.680005	6.094478	0.443761
57	1	0	0.236703	6.942169	-0.058057
58	1	0	5.793656	2.313129	1.727307
59	1	0	4.726400	3.714081	1.631852
60	1	0	2.444897	-3.839170	3.743498
61	1	0	1.141831	-5.025586	3.906298
62	1	0	1.534036	-3.950892	5.255506
63	1	0	-2.780495	-4.277726	3.508099
64	1	0	-0.578096	-5.275647	5.419022
65	1	0	-2.234731	-6.015592	5.074091
66	1	0	-5.537629	-1.683530	3.390040
67	1	0	-6.227693	-1.570891	1.764479
68	1	0	-6.694780	-0.399393	3.004263
69	1	0	-5.839981	3.136222	1.508752
70	1	0	-7.498215	0.580762	1.028919
71	1	0	-8.056938	2.340621	1.000774
72	1	0	5.991620	3.228419	-0.498764
73	1	0	4.230856	3.242914	-0.759412
74	1	0	0.343482	5.860390	-2.328676
75	1	0	1.709058	4.885515	-1.824638
76	6	0	-4.405926	-0.589418	-1.699747
77	6	0	-5.308919	-0.843827	-2.762911
78	6	0	-4.965753	-1.614136	-3.855931
79	6	0	-3.656616	-2.182761	-3.929165
80	6	0	-2.716227	-1.942805	-2.861640
81	6	0	-3.128227	-1.136694	-1.757124
82	6	0	-1.397972	-2.544352	-2.967751
83	6	0	-1.139434	-3.310594	-4.118185
84	6	0	-2.140494	-3.477089	-5.106120
85	7	0	-3.369827	-2.950588	-5.043998
86	7	0	-0.446554	-2.332027	-1.971376
87	6	0	0.746119	-3.079538	-1.789929
88	6	0	0.805154	-4.478621	-1.998562
89	6	0	1.993056	-5.185169	-1.763985
90	6	0	3.136571	-4.510852	-1.301614
91	6	0	3.099173	-3.122386	-1.056906
92	6	0	1.901293	-2.424636	-1.305549
93	8	0	4.355337	-5.179959	-1.057403
94	6	0	4.311546	-2.398520	-0.507886
95	7	0	5.069872	-1.601735	-1.551445
96	1	0	5.738073	-0.907013	-1.030620
97	1	0	4.436186	-0.862155	-1.951760
98	17	0	-6.985158	-0.122827	-2.664201
99	1	0	-4.709111	0.023424	-0.858270
100	1	0	-5.650400	-1.812440	-4.672611
101	1	0	-2.442906	-0.927950	-0.942317
102	1	0	-0.165928	-3.754038	-4.286028
103	1	0	-1.915917	-4.065798	-5.993779
104	1	0	-0.079917	-5.017285	-2.319032
105	1	0	2.018233	-6.261696	-1.928428
106	1	0	1.853334	-1.356725	-1.103908
107	1	0	4.267702	-6.147605	-1.171926
108	1	0	4.005251	-1.664046	0.243980
109	1	0	5.009901	-3.101674	-0.051059
110	6	0	5.771184	-2.378975	-2.632619
111	1	0	-0.541929	-1.517295	-1.343564
112	6	0	6.980329	-3.162119	-2.100756
113	1	0	6.088130	-1.642639	-3.380627
114	1	0	5.044792	-3.051077	-3.101673
115	1	0	6.667539	-3.954841	-1.414203
116	1	0	7.688236	-2.497153	-1.590356
117	1	0	7.505535	-3.634803	-2.939755
118	1	0	2.953431	7.664734	-3.745683

10.4 [(FePPIXH)$_2$(μ-O)(DAQH$_2$)]

See Fig. 6 for picture. Charge 0, overall spin 0. Calculated spins on Fe: +4.04, -4.03.

Energies:

ZPE	m1 oct	m1 water
1.536433	-4942.605165	-4942.596613

Atomic coordinates:

1	26	0	-1.758300	-0.118794	-1.711212
2	7	0	-1.021302	-2.002794	-2.396041
3	7	0	-3.685109	-0.862886	-2.124953
4	7	0	0.110643	0.626955	-2.280269
5	7	0	-2.533296	1.782052	-2.215930
6	6	0	0.305238	-2.370880	-2.661591
7	6	0	0.376283	-3.801260	-3.006660
8	6	0	-0.926258	-4.273756	-2.954404
9	6	0	-1.779797	-3.159816	-2.561574
10	6	0	-4.052027	-2.204757	-2.195565
11	6	0	-5.502146	-2.339516	-2.170624
12	6	0	-6.020238	-1.048160	-2.133131
13	6	0	-4.870850	-0.137090	-2.119434
14	6	0	-3.877849	2.137191	-2.331645
15	6	0	-4.003252	3.562122	-2.601540
16	6	0	-2.708548	4.078475	-2.632684
17	6	0	-1.804315	2.952645	-2.382239
18	6	0	0.480754	1.971067	-2.246397
19	6	0	1.296109	-0.099276	-2.373339
20	6	0	2.444377	0.806722	-2.298310
21	6	0	1.936206	2.092364	-2.227011
22	6	0	-0.409536	3.043368	-2.316673
23	6	0	-4.954777	1.251258	-2.226683
24	6	0	-3.161664	-3.263442	-2.394724
25	6	0	1.381429	-1.480017	-2.588785
26	1	0	0.029234	4.033631	-2.372185
27	1	0	-5.949471	1.678141	-2.287073
28	1	0	-3.590788	-4.253528	-2.505006
29	1	0	2.374693	-1.874449	-2.753769
30	6	0	-1.442393	-5.659354	-3.242940
31	6	0	2.714320	3.379159	-2.151051
32	6	0	-6.247657	-3.646281	-2.181214
33	6	0	-7.413138	-0.598143	-2.099073
34	6	0	-8.507875	-1.275622	-2.528691
35	6	0	-5.294329	4.282771	-2.879808
36	6	0	-2.248583	5.431564	-2.946882
37	6	0	-2.958883	6.588618	-2.907170
38	1	0	-2.259833	-5.633653	-3.976055
39	1	0	-0.659951	-6.307512	-3.648581
40	1	0	-1.829130	-6.146160	-2.336972
41	1	0	2.855321	3.825108	-3.146580
42	1	0	2.211682	4.128824	-1.527357
43	1	0	3.708630	3.210372	-1.722428
44	1	0	-5.647767	-4.458050	-1.755334
45	1	0	-7.172905	-3.571880	-1.596916
46	1	0	-6.532231	-3.946733	-3.200685
47	1	0	-7.577820	0.392639	-1.675407
48	1	0	-8.449588	-2.250919	-3.002264
49	1	0	-9.499803	-0.838724	-2.440000
50	1	0	-6.091748	3.591818	-3.171132
51	1	0	-5.652524	4.845860	-2.004707
52	1	0	-5.166863	5.004919	-3.696183
53	1	0	-1.209148	5.506057	-3.269413
54	1	0	-3.992828	6.637061	-2.581174
55	1	0	-2.499807	7.530320	-3.197895
56	6	0	1.583661	-4.679123	-3.285918
57	6	0	2.775121	-4.105766	-4.092841
58	6	0	3.959950	-3.641665	-3.220403
59	8	0	4.629488	-2.638012	-3.703744
60	8	0	4.201834	-4.244604	-2.112909
61	1	0	2.000564	-5.038744	-2.335014

62	1	0	1.214680	-5.573348	-3.801313
63	1	0	3.175450	-4.898363	-4.741204
64	1	0	2.485306	-3.282649	-4.752400
65	1	0	5.697393	-1.821955	-3.355527
66	6	0	3.892662	0.401352	-2.231962
67	6	0	4.661435	0.512085	-3.588588
68	6	0	6.133743	0.201567	-3.326487
69	8	0	6.459590	-1.097448	-3.152440
70	8	0	6.987291	1.108020	-3.170196
71	1	0	4.399477	1.036260	-1.491526
72	1	0	3.974780	-0.630254	-1.874741
73	1	0	4.237880	-0.194890	-4.308997
74	1	0	4.586762	1.529936	-3.981608
75	26	0	-2.044835	0.553693	1.802342
76	7	0	-2.214147	2.649321	1.668846
77	7	0	-4.150690	0.504074	1.823512
78	7	0	-0.195249	0.939356	2.792889
79	7	0	-2.117328	-1.212432	2.968848
80	6	0	-1.179018	3.577177	1.734105
81	6	0	-1.683029	4.918819	1.436455
82	6	0	-3.039109	4.792929	1.205910
83	6	0	-3.361808	3.374154	1.353638
84	6	0	-5.022761	1.520190	1.464117
85	6	0	-6.392390	1.003565	1.375430
86	6	0	-6.323948	-0.355024	1.683864
87	6	0	-4.926647	-0.644388	1.980775
88	6	0	-3.172214	-2.119724	2.970977
89	6	0	-2.776713	-3.349003	3.666849
90	6	0	-1.475415	-3.145299	4.123485
91	6	0	-1.080110	-1.814466	3.682354
92	6	0	0.575955	0.045469	3.539947
93	6	0	0.584857	2.086453	2.654462
94	6	0	1.900159	1.895192	3.276339
95	6	0	1.885300	0.631363	3.839276
96	6	0	0.162117	-1.222514	3.945612
97	6	0	-4.450112	-1.867998	2.463216
98	6	0	-4.647843	2.848946	1.240928
99	6	0	0.132355	3.296906	2.125275
100	1	0	0.873471	-1.804462	4.522102
101	1	0	-5.165223	-2.680714	2.519102
102	1	0	-5.431247	3.549518	0.974229
103	1	0	0.840585	4.118608	2.113214
104	6	0	-4.039584	5.873011	0.896403
105	6	0	2.969902	-0.040781	4.637023
106	6	0	2.987207	2.944572	3.334351
107	6	0	-0.854117	6.177535	1.445457
108	6	0	-7.552108	1.844620	1.081244
109	6	0	-7.458992	-1.337040	1.765495
110	6	0	-3.665229	-4.495995	3.867550
111	6	0	-0.631192	-4.070990	4.955807
112	6	0	-0.048428	6.369357	0.123142
113	6	0	3.737583	3.199555	1.994125
114	6	0	5.063459	2.435616	1.828230
115	6	0	0.832806	7.595336	0.157919
116	8	0	0.092915	8.760701	0.347612
117	8	0	2.067562	7.625075	0.042846
118	8	0	5.715997	2.096765	2.899165
119	8	0	5.469525	2.224089	0.614360
120	1	0	-4.840837	5.908183	1.647391
121	1	0	-3.567046	6.859993	0.869337
122	1	0	-4.511257	5.710411	-0.081935
123	1	0	3.178712	-1.050763	4.259751
124	1	0	3.903787	0.526707	4.583067
125	1	0	2.687886	-0.136940	5.695389
126	1	0	2.542198	3.890734	3.673851
127	1	0	3.739422	2.669852	4.080379
128	1	0	-1.492944	7.054818	1.587945
129	1	0	-0.152710	6.161430	2.290418
130	6	0	-8.820895	1.462781	0.780064
131	1	0	-7.162749	-2.272347	2.250002
132	6	0	-3.307759	-5.781135	4.113529
133	1	0	-1.255736	-4.646090	5.649925
134	1	0	0.594288	5.504948	-0.065460
135	1	0	-0.757236	6.463877	-0.707831
136	1	0	3.112450	2.979144	1.122455
137	1	0	4.004579	4.264925	1.924225
138	8	0	-1.615888	-0.134596	0.143713

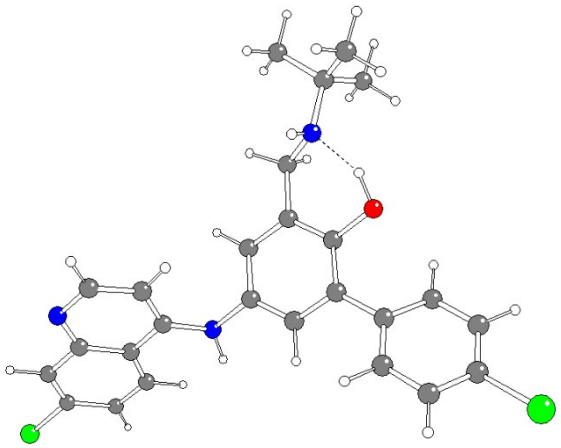
139	1	0	0.684280	9.547753	0.370535
140	6	0	1.152219	-6.128598	0.475973
141	6	0	-0.162821	-5.608864	0.538238
142	6	0	-0.432178	-4.250293	0.582612
143	6	0	0.663804	-3.350350	0.569571
144	6	0	2.008820	-3.834154	0.509005
145	6	0	2.222290	-5.238608	0.459065
146	6	0	3.110345	-2.885871	0.588769
147	6	0	2.787178	-1.525925	0.833257
148	6	0	1.466040	-1.110008	0.780876
149	7	0	0.442008	-1.984103	0.639052
150	17	0	-1.549699	-6.784412	0.582043
151	7	0	4.410599	-3.301565	0.415266
152	6	0	5.466636	-2.488315	0.954219
153	6	0	6.374647	-1.796044	0.131685
154	6	0	7.212402	-0.802569	0.679520
155	6	0	7.120459	-0.508478	2.062846
156	6	0	6.310653	-1.297638	2.901536
157	6	0	5.488449	-2.285626	2.350666
158	6	0	8.121776	0.004387	-0.230686
159	7	0	7.993545	1.493981	0.053345
160	6	0	8.742594	2.372252	-0.924053
161	6	0	8.600658	3.850911	-0.538070
162	1	0	8.326549	1.612433	1.027458
163	8	0	7.746000	0.630381	2.583093
164	1	0	1.315458	-7.200449	0.451211
165	1	0	-1.447560	-3.871737	0.634216
166	1	0	3.238266	-5.615571	0.427415
167	1	0	3.563939	-0.782058	0.941347
168	1	0	1.192480	-0.064129	0.810060
169	1	0	6.379451	-1.960463	-0.942058
170	1	0	6.302527	-1.087375	3.966933
171	1	0	4.826836	-2.871252	2.983588
172	1	0	7.881996	-0.159853	-1.282655
173	1	0	9.176570	-0.254209	-0.068652
174	1	0	8.324819	2.167945	-1.912506
175	1	0	9.793879	2.057270	-0.911005
176	1	0	9.134039	4.470891	-1.268181
177	1	0	9.022120	4.058801	0.454756
178	1	0	7.547716	4.155724	-0.538462
179	1	0	6.975532	1.301840	2.853497
180	1	0	-0.501938	-1.567040	0.522286
181	1	0	6.958473	1.770791	0.122367
182	1	0	4.576738	-3.877449	-0.437287
183	1	0	-0.084985	-4.795632	4.333809
184	1	0	0.110001	-3.523767	5.548477
185	1	0	-7.838727	-1.589152	0.765397
186	1	0	-8.298339	-0.918956	2.337399
187	1	0	-4.732942	-4.282335	3.808437
188	1	0	-2.273755	-6.109234	4.144358
189	1	0	-4.063789	-6.549143	4.257035
190	1	0	-7.369016	2.918636	1.122328
191	1	0	-9.124546	0.425633	0.690268
192	1	0	-9.592476	2.209280	0.607413

11. Tebuquine

11.1 Free Tebuquine

Single conformer for all methods and solvents (designated TQ_27). Energies:

conformer	ZPE	m1 (octanol)	m1 (water)	m3 (octanol)	m3 (water)
TQ_27	0.459499	-1275.055005	-1275.043617	-2166.130852	-2166.118565



Atomic coordinates:

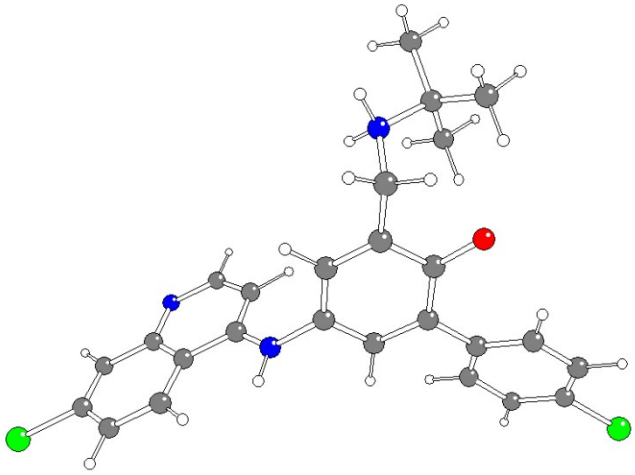
1	6	0	-3.837471	1.560099	2.142305
2	6	0	-2.717680	1.030918	1.452417
3	6	0	-2.911953	0.111442	0.410648
4	6	0	-4.278673	-0.235268	0.069693
5	6	0	-5.336776	0.352314	0.851663
6	7	0	-5.113432	1.248211	1.881680
7	6	0	-6.694751	0.013516	0.563025
8	6	0	-6.974122	-0.860408	-0.469435
9	6	0	-5.953891	-1.432800	-1.273167
10	6	0	-4.628354	-1.115519	-0.999048
11	17	0	-8.703702	-1.295369	-0.838958
12	7	0	-1.859463	-0.484522	-0.277860
13	6	0	-0.480003	-0.106810	-0.237557
14	6	0	-0.079650	1.238236	-0.376757
15	6	0	1.280506	1.570805	-0.415384
16	6	0	2.266960	0.549546	-0.308823
17	6	0	1.886902	-0.812307	-0.171329
18	6	0	0.503572	-1.106164	-0.140444
19	6	0	2.881283	-1.915186	-0.039438
20	6	0	2.585280	-3.052530	0.753033
21	6	0	3.486526	-4.124597	0.868378
22	6	0	4.704335	-4.055720	0.179748
23	6	0	5.040837	-2.945334	-0.605084
24	6	0	4.130682	-1.879255	-0.706236
25	17	0	5.884624	-5.439514	0.319232
26	8	0	3.606857	0.908502	-0.337912
27	6	0	1.720314	3.010036	-0.656091
28	7	0	2.905754	3.353268	0.192827
29	6	0	3.665453	4.620122	-0.118923
30	6	0	4.711681	4.779748	1.008602
31	6	0	4.389639	4.461312	-1.476967
32	6	0	2.730464	5.858135	-0.148002
33	1	0	-3.674098	2.262132	2.957648
34	1	0	-1.720323	1.314950	1.765213
35	1	0	-7.469808	0.464280	1.172352
36	1	0	-6.213125	-2.096781	-2.091107
37	1	0	-3.863031	-1.538495	-1.645144

38	1	0	-2.067758	-1.322553	-0.804748
39	1	0	-0.829840	2.016584	-0.489924
40	1	0	0.186726	-2.142441	-0.051648
41	1	0	1.655132	-3.096519	1.313341
42	1	0	3.249364	-4.984250	1.487057
43	1	0	5.992275	-2.908148	-1.125993
44	1	0	4.394503	-1.009279	-1.294218
45	1	0	3.646453	1.915765	-0.113745
46	1	0	2.032605	3.120448	-1.702562
47	1	0	0.875083	3.693549	-0.492472
48	1	0	2.637993	3.344550	1.181601
49	1	0	5.328668	5.669128	0.835215
50	1	0	4.225938	4.895789	1.988028
51	1	0	5.371354	3.904728	1.053147
52	1	0	5.019480	5.338930	-1.666876
53	1	0	5.030665	3.571701	-1.474569
54	1	0	3.686852	4.376238	-2.314706
55	1	0	3.312857	6.770830	-0.325922
56	1	0	1.982592	5.782952	-0.947016
57	1	0	2.202272	5.976211	0.808200

11.2 Tebuquine Zwitterion

Single conformer for all methods and solvents (designated TQZ_8). Energies:

conformer	ZPE	m1 (octanol)	m1 (water)	m3 (octanol)	m3 (water)
TQZ_8	0.460277	-1275.035365	-1275.029280	-2166.109286	-2166.102179



Atomic coordinates:

1	6	0	6.066691	-1.035173	-1.361184
2	6	0	6.890507	-0.799822	-0.229952
3	6	0	6.386967	-0.314214	0.960803
4	6	0	4.989397	-0.035687	1.075132
5	6	0	4.127525	-0.270608	-0.055984
6	6	0	4.705449	-0.769113	-1.262448
7	6	0	2.712789	0.019288	0.097448
8	6	0	2.287103	0.517198	1.341122
9	6	0	3.226897	0.708683	2.382624
10	7	0	4.539694	0.453267	2.288480
11	7	0	1.829694	-0.187813	-0.948942
12	6	0	0.426688	0.148129	-0.908532
13	6	0	-0.542122	-0.841839	-0.627446
14	6	0	-1.924321	-0.587962	-0.624069
15	6	0	-2.395229	0.763310	-0.931920
16	6	0	-1.372391	1.765057	-1.190917

17	6	0	-0.000481	1.452193	-1.195185
18	8	0	-3.657366	1.113332	-0.954124
19	6	0	-1.847499	3.132641	-1.552002
20	7	0	-1.962824	4.113072	-0.307053
21	6	0	-3.279814	4.218254	0.557376
22	17	0	8.672898	-1.154440	-0.376711
23	1	0	6.498830	-1.413658	-2.281576
24	1	0	7.011932	-0.131655	1.827598
25	1	0	4.092729	-0.949300	-2.142469
26	1	0	1.239648	0.735927	1.512274
27	1	0	2.883501	1.084991	3.344806
28	1	0	-0.181906	-1.849641	-0.433802
29	1	0	0.744372	2.208887	-1.445276
30	1	0	-1.144040	3.653865	-2.211991
31	1	0	-2.842530	3.094431	-1.995539
32	1	0	-1.770858	5.062774	-0.652304
33	6	0	-4.498344	4.209523	-0.382437
34	6	0	-3.321034	3.034353	1.540995
35	6	0	-3.141238	5.564742	1.306929
36	1	0	-4.422421	4.976579	-1.166306
37	1	0	-4.620410	3.217909	-0.830554
38	1	0	-5.394452	4.430869	0.209272
39	1	0	2.176753	-0.626567	-1.791684
40	1	0	-1.199767	3.842261	0.329071
41	6	0	-2.878967	-1.684489	-0.300708
42	6	0	-4.206496	-1.691413	-0.803427
43	6	0	-5.088699	-2.750033	-0.524510
44	6	0	-4.649254	-3.811485	0.275899
45	6	0	-3.354350	-3.838141	0.809571
46	6	0	-2.483831	-2.774131	0.519662
47	17	0	-5.795406	-5.186275	0.649911
48	1	0	-2.427869	3.002969	2.181169
49	1	0	-3.436394	2.091184	1.000701
50	1	0	-4.192131	3.155500	2.195909
51	1	0	-3.130289	6.420720	0.616652
52	1	0	-2.236759	5.597869	1.930313
53	1	0	-4.000585	5.693963	1.973066
54	1	0	-4.541896	-0.849122	-1.394869
55	1	0	-6.098793	-2.742703	-0.922368
56	1	0	-3.034363	-4.658986	1.443789
57	1	0	-1.492351	-2.788806	0.964264

11.3 [(FePPIXH)(TQ)]

See Fig. 1 for image. Charge 0, overall spin 5/2. Calculated spin on Fe: +4.05.

Energies:

ZPE	m1 oct	m1 water	m3 oct	m3 water
1.046687	-3232.595946	-3232.583238	-5264.684103	-5264.668964

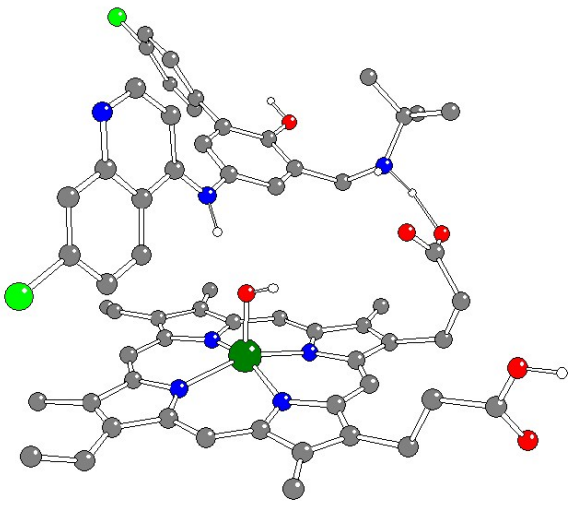
Atomic coordinates:

1	26	0	-1.674991	0.768193	1.164727
2	7	0	-3.551408	1.011005	0.288406
3	7	0	-1.456407	2.843423	1.038191
4	7	0	-2.463558	-0.935209	2.108557
5	7	0	-0.239436	0.803338	2.687238
6	6	0	-4.531069	0.032946	0.132362
7	6	0	-5.550424	0.484570	-0.813048
8	6	0	-5.195148	1.767993	-1.196204
9	6	0	-3.962813	2.096779	-0.482928
10	6	0	-2.211133	3.711933	0.246287
11	6	0	-1.651647	5.055640	0.293440
12	6	0	-0.527893	4.992060	1.113194
13	6	0	-0.419413	3.604328	1.569818
14	6	0	0.688608	1.822328	2.918608
15	6	0	1.714040	1.368939	3.846295

16	6	0	1.381198	0.062267	4.205703
17	6	0	0.141486	-0.262876	3.497080
18	6	0	-1.826038	-1.729128	3.064458
19	6	0	-3.642472	-1.606798	1.778305
20	6	0	-3.751613	-2.845096	2.548326
21	6	0	-2.624167	-2.918306	3.345572
22	6	0	-0.598814	-1.437164	3.664530
23	6	0	0.593695	3.116615	2.397636
24	6	0	-3.340489	3.346548	-0.493781
25	6	0	-4.576826	-1.171502	0.836358
26	1	0	-0.209720	-2.179002	4.353252
27	1	0	1.370608	3.817220	2.682045
28	1	0	-3.799195	4.116818	-1.104969
29	1	0	-5.413825	-1.827973	0.633618
30	6	0	-5.911605	2.698373	-2.138666
31	6	0	-2.242579	-4.005963	4.313086
32	6	0	-4.861284	-3.859098	2.411177
33	6	0	-6.747711	-0.323844	-1.246550
34	6	0	-2.239444	6.262887	-0.383606
35	6	0	0.381516	6.061521	1.531490
36	6	0	0.663722	7.206009	0.859925
37	6	0	2.866578	2.196732	4.345130
38	6	0	2.047478	-0.850906	5.135242
39	6	0	3.329879	-0.798767	5.576697
40	6	0	-6.379831	-1.448203	-2.259292
41	6	0	-4.534352	-5.002357	1.390130
42	6	0	-4.047504	-4.399565	0.069369
43	6	0	-7.578710	-2.184471	-2.807401
44	8	0	-7.729182	-2.586523	-3.971910
45	8	0	-8.554907	-2.411923	-1.837820
46	8	0	-4.880622	-3.900909	-0.755461
47	8	0	-2.737071	-4.359325	-0.072826
48	1	0	-6.206425	3.631566	-1.638777
49	1	0	-6.820784	2.238286	-2.538331
50	1	0	-5.278758	2.972725	-2.994145
51	1	0	-1.989716	-3.600756	5.302114
52	1	0	-1.371595	-4.574441	3.956887
53	1	0	-3.062801	-4.718767	4.447194
54	1	0	-5.788717	-3.369127	2.093543
55	1	0	-5.069659	-4.321036	3.385385
56	1	0	-7.491358	0.341390	-1.701609
57	1	0	-7.239677	-0.783902	-0.382162
58	1	0	-3.321653	6.163160	-0.522657
59	1	0	-1.790232	6.434250	-1.372049
60	1	0	-2.060762	7.165337	0.213212
61	1	0	0.878003	5.910934	2.491313
62	1	0	0.257891	7.426033	-0.122609
63	1	0	1.343854	7.942513	1.281312
64	1	0	2.694134	3.268263	4.201813
65	1	0	3.803646	1.943862	3.827292
66	1	0	3.034091	2.026181	5.415950
67	1	0	1.434772	-1.671745	5.508688
68	1	0	4.041373	-0.050638	5.243032
69	1	0	3.702692	-1.540106	6.279039
70	1	0	-5.737939	-2.202944	-1.779937
71	1	0	-5.833054	-1.037810	-3.114973
72	1	0	-5.444645	-5.588733	1.219360
73	1	0	-3.750735	-5.651237	1.793969
74	6	0	-0.138671	-2.733041	-0.241092
75	1	0	0.263978	-3.747608	-0.282495
76	1	0	-0.602459	-2.610018	0.743145
77	6	0	8.525411	-3.071159	-2.154918
78	6	0	9.671824	-2.439430	-1.606027
79	6	0	7.266193	-2.598264	-1.804151
80	6	0	7.107121	-1.500065	-0.905088
81	6	0	8.289036	-0.859438	-0.386724
82	6	0	9.577332	-1.358761	-0.750939
83	6	0	5.818317	-0.984299	-0.485846
84	6	0	5.811296	0.135815	0.357302
85	6	0	7.039311	0.698989	0.788926
86	7	0	8.250498	0.237799	0.454751
87	7	0	4.656506	-1.632307	-0.904526
88	17	0	11.310245	-3.081529	-2.071588
89	1	0	8.639613	-3.900942	-2.844419
90	1	0	6.401843	-3.072010	-2.262935
91	1	0	10.448363	-0.861556	-0.339417
92	1	0	4.881190	0.554848	0.720346

93	1	0	7.022807	1.561215	1.452744
94	1	0	4.762879	-2.584440	-1.230285
95	6	0	3.313166	-1.173108	-0.791997
96	6	0	2.955869	0.165771	-1.038519
97	6	0	1.620210	0.612244	-0.943906
98	6	0	0.611774	-0.323851	-0.558915
99	6	0	0.949414	-1.702828	-0.456900
100	6	0	2.288429	-2.108537	-0.542965
101	8	0	-0.689296	0.050635	-0.327099
102	1	0	3.718371	0.859769	-1.376289
103	1	0	2.538417	-3.160952	-0.414873
104	7	0	-1.298046	-2.655769	-1.216056
105	1	0	-1.655279	-1.690526	-1.169608
106	1	0	-2.069666	-3.386342	-0.769414
107	6	0	-1.131152	-3.073432	-2.688489
108	6	0	-2.543403	-2.916886	-3.305662
109	6	0	-0.686530	-4.552407	-2.730056
110	6	0	-0.128371	-2.171333	-3.440622
111	1	0	-2.851332	-1.861525	-3.312844
112	1	0	-3.295400	-3.487715	-2.749684
113	1	0	-2.532063	-3.266824	-4.344341
114	1	0	-1.358298	-5.178711	-2.133162
115	1	0	0.339538	-4.682671	-2.363000
116	1	0	-0.710329	-4.906740	-3.767202
117	1	0	0.894881	-2.286966	-3.071858
118	1	0	-0.405037	-1.112269	-3.364204
119	1	0	-0.139008	-2.443465	-4.503537
120	6	0	-0.040933	3.549163	-2.728508
121	6	0	0.170052	2.278048	-2.170325
122	6	0	1.312104	2.004739	-1.380116
123	6	0	2.219812	3.061856	-1.133947
124	6	0	2.018969	4.343145	-1.674264
125	6	0	0.892724	4.561600	-2.475483
126	17	0	0.624975	6.217419	-3.202241
127	1	0	-0.911174	3.741249	-3.347978
128	1	0	-0.552819	1.491099	-2.355226
129	1	0	3.089366	2.892444	-0.503966
130	1	0	2.717475	5.147610	-1.469377
131	1	0	-9.290216	-2.945775	-2.216790

11.4 [(FePPIXH)(OH)(TQH)]



Charge 0, overall spin 5/2. Calculated spin on Fe: +4.06.

Energies:

ZPE	m1 oct	m1 water	m3 oct	m3 water
1.071817	-3309.033686	-3309.020034	-5341.157783	-5341.141017

Atomic coordinates:

1	26	0	-1.971522	-0.351647	1.463752
2	8	0	-1.141483	-0.324789	-0.237694
3	1	0	-1.577003	0.219337	-0.927605
4	7	0	-1.734029	1.632554	2.062698
5	7	0	-0.428994	-0.854445	2.778361
6	7	0	-3.924958	0.158895	0.917565
7	7	0	-2.652333	-2.328354	1.667761
8	6	0	-2.478978	2.716058	1.605304
9	6	0	-1.799451	3.966620	1.928816
10	6	0	-0.651909	3.632029	2.626195
11	6	0	-0.613802	2.171042	2.697880
12	6	0	0.497119	0.027115	3.336973
13	6	0	1.569977	-0.712907	3.984414
14	6	0	1.278690	-2.066998	3.822125
15	6	0	0.023001	-2.136658	3.070804
16	6	0	-1.899770	-3.412865	2.122544
17	6	0	-2.613918	-4.660572	1.881197
18	6	0	-3.822268	-4.318738	1.278480
19	6	0	-3.832859	-2.857851	1.159532
20	6	0	-4.923457	-0.718155	0.494696
21	6	0	-4.394478	1.443808	0.648860
22	6	0	-5.711655	1.372985	0.017957
23	6	0	-6.041727	0.032056	-0.072013
24	6	0	-4.874692	-2.108794	0.602935
25	6	0	-0.654380	-3.316604	2.749529
26	6	0	0.404736	1.423900	3.290500
27	6	0	-3.712355	2.623498	0.953638
28	1	0	-5.728619	-2.657147	0.220109
29	1	0	-0.189203	-4.248830	3.049231
30	1	0	1.201190	1.982114	3.770622
31	1	0	-4.194765	3.556909	0.684177
32	6	0	0.372176	4.579008	3.197197
33	6	0	-7.293025	-0.586502	-0.636287
34	6	0	-6.506442	2.561516	-0.460674
35	6	0	-2.226180	5.339541	1.472654
36	6	0	2.766114	-0.097519	4.657459
37	6	0	2.035055	-3.245217	4.250471
38	6	0	2.957792	-3.322058	5.242594
39	6	0	-2.123466	-6.029151	2.265163
40	6	0	-4.929995	-5.180577	0.855558
41	6	0	-4.850186	-6.474061	0.456885
42	6	0	-2.061961	5.534104	-0.069344
43	6	0	-6.104122	2.985637	-1.895639
44	6	0	-6.802258	4.252352	-2.341956
45	6	0	-0.673110	5.107965	-0.545426
46	8	0	-0.545724	4.141539	-1.382060
47	8	0	0.354926	5.761318	-0.028371
48	8	0	-6.660447	4.455579	-3.709236
49	8	0	-7.423936	5.051543	-1.624920
50	1	0	0.023237	5.020181	4.141917
51	1	0	0.568632	5.395700	2.493164
52	1	0	1.325520	4.080544	3.407030
53	1	0	-7.789448	-1.233880	0.099260
54	1	0	-7.076015	-1.203563	-1.519417
55	1	0	-8.014546	0.179393	-0.939442
56	1	0	-6.377746	3.417952	0.210615
57	1	0	-7.578504	2.331932	-0.447117
58	1	0	-1.618043	6.095261	1.979522
59	1	0	-3.274040	5.538516	1.739603
60	1	0	2.968920	0.911776	4.283609
61	1	0	3.662468	-0.705630	4.484170
62	1	0	2.628255	-0.022786	5.746214
63	1	0	1.825719	-4.163334	3.700483
64	1	0	3.212805	-2.480108	5.878445
65	1	0	3.464787	-4.260090	5.454801
66	1	0	-1.465681	-5.994346	3.140886

67	1	0	-1.558519	-6.501138	1.447920
68	1	0	-2.964737	-6.689927	2.503920
69	1	0	-5.918109	-4.718467	0.859190
70	1	0	-3.907175	-7.004405	0.368121
71	1	0	-5.743476	-7.022893	0.169409
72	1	0	-2.211415	6.595892	-0.304508
73	1	0	-2.801523	4.946653	-0.621744
74	1	0	-6.319962	2.193222	-2.621987
75	1	0	-5.020988	3.163594	-1.958942
76	1	0	-7.092990	5.296522	-3.984961
77	1	0	1.779883	6.700590	-2.304508
78	1	0	1.692448	5.381219	-3.487672
79	1	0	3.032397	6.545026	-3.559972
80	1	0	3.408035	3.420731	-3.360596
81	1	0	4.710876	3.481039	-2.146612
82	1	0	4.692316	4.638004	-3.488508
83	6	0	7.969290	-1.571119	-1.417609
84	6	0	6.669376	-1.049496	-1.534791
85	6	0	6.073093	-0.318045	-0.480286
86	6	0	6.820305	-0.130601	0.710114
87	6	0	8.123963	-0.643491	0.840981
88	6	0	8.682055	-1.353898	-0.229921
89	17	0	10.368195	-2.017555	-0.071725
90	1	0	8.417011	-2.129193	-2.233684
91	1	0	6.117809	-1.203937	-2.458200
92	1	0	6.366168	0.367804	1.563341
93	1	0	8.683449	-0.504609	1.760719
94	6	0	-1.688589	-4.195887	-1.979866
95	6	0	-1.537693	-5.094489	-3.066282
96	6	0	-0.501071	-4.991378	-3.972267
97	6	0	0.461754	-3.946269	-3.819553
98	6	0	0.334195	-3.016484	-2.723609
99	6	0	-0.759511	-3.172985	-1.818846
100	6	0	1.336059	-1.972087	-2.597451
101	6	0	2.353770	-1.947121	-3.568457
102	6	0	2.378033	-2.911444	-4.604887
103	7	0	1.481898	-3.895081	-4.753267
104	7	0	1.258345	-1.035429	-1.569191
105	6	0	2.314161	-0.171351	-1.170940
106	6	0	3.644679	-0.630359	-1.057735
107	6	0	4.681676	0.209228	-0.610042
108	6	0	4.366029	1.551779	-0.280853
109	6	0	3.042642	2.029751	-0.359027
110	6	0	2.025722	1.158378	-0.794636
111	8	0	5.353195	2.484871	0.101730
112	6	0	2.712478	3.450686	0.061298
113	7	0	2.234956	4.372609	-1.045046
114	1	0	1.544420	5.122668	-0.552234
115	1	0	1.522904	3.878642	-1.614980
116	17	0	-2.767130	-6.432789	-3.257660
117	1	0	-2.516875	-4.306803	-1.288932
118	1	0	-0.379547	-5.673864	-4.805605
119	1	0	-0.891297	-2.484448	-0.990714
120	1	0	3.110671	-1.172435	-3.558650
121	1	0	3.167841	-2.866996	-5.352908
122	1	0	3.867976	-1.670238	-1.273752
123	1	0	0.996938	1.510803	-0.834562
124	1	0	6.253001	2.097524	0.059831
125	1	0	1.881048	3.428642	0.775315
126	1	0	3.568217	3.917319	0.547428
127	6	0	3.237500	5.094764	-1.949443
128	1	0	0.362212	-0.884026	-1.074542
129	6	0	4.159018	5.970473	-1.072445
130	6	0	2.378515	5.985872	-2.880870
131	6	0	4.059577	4.087357	-2.781139
132	1	0	4.828291	5.364822	-0.451245
133	1	0	3.573118	6.634772	-0.424693
134	1	0	4.785213	6.596225	-1.719289

11.5 [(FePPIXH)$_2$(μ-O)(TQH$_2$)]

See Fig. 6 for picture. Charge 0, overall spin 0. Calculated spins on Fe: +4.04, -4.03.

Energies:

ZPE	m1 oct	m1 water
1.663074	-5266.581710	-5266.568452

Atomic coordinates:

1	26	0	-2.732071	-0.218777	1.586472
2	7	0	-2.185667	1.488080	2.749446
3	7	0	-4.716553	0.471338	1.745952
4	7	0	-1.006104	-1.102797	2.382713
5	7	0	-3.553967	-2.167802	1.548915
6	6	0	-0.948793	1.772222	3.342424
7	6	0	-0.965127	3.119642	3.936533
8	6	0	-2.234427	3.625769	3.705037
9	6	0	-2.976806	2.615839	2.959389
10	6	0	-5.116042	1.782271	1.994125
11	6	0	-6.539544	1.941684	1.729326
12	6	0	-7.017329	0.687897	1.359800
13	6	0	-5.866788	-0.221577	1.384655
14	6	0	-4.887820	-2.511929	1.327465
15	6	0	-5.035436	-3.959044	1.273477
16	6	0	-3.761618	-4.497722	1.450863
17	6	0	-2.849291	-3.362807	1.618492
18	6	0	-0.609866	-2.424217	2.172791
19	6	0	0.111945	-0.437946	2.881720
20	6	0	1.261014	-1.342293	2.907456
21	6	0	0.813546	-2.575841	2.465736
22	6	0	-1.470320	-3.468264	1.830865
23	6	0	-5.941954	-1.601863	1.200703
24	6	0	-4.300133	2.773199	2.546991
25	6	0	0.127277	0.880496	3.350927
26	1	0	-1.033810	-4.459842	1.785926
27	1	0	-6.922019	-2.013947	0.989314
28	1	0	-4.759977	3.734923	2.747158
29	1	0	1.054474	1.221066	3.790318
30	6	0	-2.815679	4.952010	4.120816
31	6	0	1.628345	-3.833576	2.311408
32	6	0	-7.298762	3.235406	1.844845
33	6	0	-8.373002	0.272025	0.995182
34	6	0	-9.539400	0.874774	1.338880
35	6	0	-6.340774	-4.694987	1.138403
36	6	0	-3.343203	-5.895527	1.562217
37	6	0	-4.015336	-7.007217	1.165076
38	1	0	-3.760947	4.817852	4.663782
39	1	0	-2.136875	5.503217	4.778275
40	1	0	-3.021577	5.595206	3.254257
41	1	0	1.776658	-4.338883	3.276471
42	1	0	1.156345	-4.555952	1.636356
43	1	0	2.623539	-3.607073	1.906817
44	1	0	-6.645862	4.102155	1.693617
45	1	0	-8.099980	3.285314	1.097397
46	1	0	-7.770376	3.346419	2.832667
47	1	0	-8.441140	-0.622399	0.375937
48	1	0	-9.585333	1.746431	1.984641
49	1	0	-10.491168	0.474787	0.997126
50	1	0	-7.196089	-4.057625	1.383730
51	1	0	-6.498357	-5.074886	0.117673
52	1	0	-6.369398	-5.561077	1.811798
53	1	0	-2.376728	-6.056338	2.041354
54	1	0	-4.975536	-6.971645	0.660778
55	1	0	-3.597089	-7.995864	1.337791
56	6	0	0.163981	3.898354	4.586144
57	6	0	1.112543	3.176174	5.575497
58	6	0	2.472721	2.773274	4.970479
59	8	0	3.033101	1.748727	5.544913
60	8	0	2.954132	3.429522	3.978036
61	1	0	0.803897	4.327631	3.803872

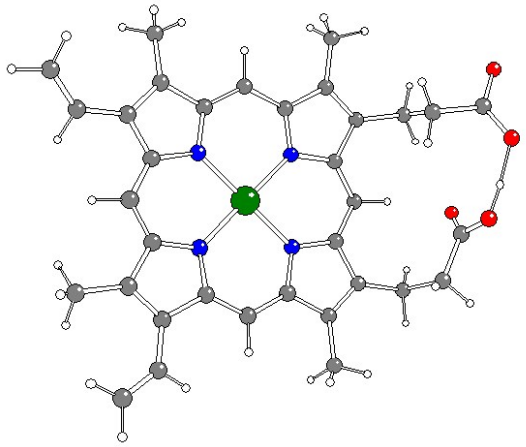
62	1	0	-0.289225	4.754177	5.099059
63	1	0	1.345335	3.854445	6.408818
64	1	0	0.661004	2.285870	6.023479
65	1	0	4.129416	1.009322	5.237302
66	6	0	2.674254	-0.969223	3.263969
67	6	0	3.104292	-1.299990	4.730796
68	6	0	4.596639	-0.980631	4.851640
69	8	0	4.932628	0.308822	5.022740
70	8	0	5.469791	-1.866614	4.667562
71	1	0	3.354053	-1.503269	2.584765
72	1	0	2.830229	0.101031	3.091807
73	1	0	2.515864	-0.703481	5.434422
74	1	0	2.957028	-2.364704	4.933381
75	26	0	-2.375472	-0.134487	-1.987094
76	7	0	-2.501208	-2.203972	-2.350265
77	7	0	-4.449145	-0.066046	-2.359705
78	7	0	-0.378267	-0.303497	-2.716323
79	7	0	-2.306763	1.854603	-2.712355
80	6	0	-1.441109	-3.102706	-2.426580
81	6	0	-1.943993	-4.476782	-2.471856
82	6	0	-3.322400	-4.396030	-2.458687
83	6	0	-3.661320	-2.975034	-2.383092
84	6	0	-5.336426	-1.131188	-2.395444
85	6	0	-6.716457	-0.638624	-2.457207
86	6	0	-6.640479	0.753893	-2.452858
87	6	0	-5.223866	1.093297	-2.408512
88	6	0	-3.374859	2.745570	-2.699008
89	6	0	-2.905700	4.099454	-3.013972
90	6	0	-1.537696	3.997132	-3.262765
91	6	0	-1.181827	2.597126	-3.073561
92	6	0	0.474997	0.733034	-3.100832
93	6	0	0.400646	-1.460062	-2.733126
94	6	0	1.788364	-1.143265	-3.090260
95	6	0	1.827126	0.219857	-3.328803
96	6	0	0.101792	2.067559	-3.254934
97	6	0	-4.713406	2.391400	-2.508576
98	6	0	-4.963717	-2.479147	-2.393070
99	6	0	-0.094861	-2.753849	-2.553502
100	1	0	0.883086	2.758820	-3.552722
101	1	0	-5.436648	3.198553	-2.514210
102	1	0	-5.758771	-3.215814	-2.422342
103	1	0	0.621918	-3.565465	-2.617772
104	6	0	-4.326290	-5.514070	-2.531969
105	6	0	2.995117	1.062519	-3.760920
106	6	0	2.893913	-2.162933	-3.260507
107	6	0	-1.077926	-5.709955	-2.520191
108	6	0	-7.880769	-1.516406	-2.571686
109	6	0	-7.772885	1.737886	-2.547048
110	6	0	-3.785413	5.266454	-3.111032
111	6	0	-0.592924	5.082177	-3.701425
112	6	0	-0.535304	-6.073051	-1.117694
113	6	0	3.334784	-2.910205	-1.966044
114	6	0	4.666861	-2.456269	-1.344508
115	6	0	0.398359	-7.261175	-1.130544
116	8	0	0.854001	-7.550300	0.154250
117	8	0	0.753052	-7.929325	-2.112491
118	8	0	5.555916	-1.882388	-2.097489
119	8	0	4.837875	-2.725106	-0.087364
120	1	0	-4.996117	-5.398046	-3.395132
121	1	0	-3.834073	-6.487337	-2.625287
122	1	0	-4.951926	-5.549271	-1.630240
123	1	0	3.217341	1.849075	-3.026402
124	1	0	3.901438	0.462579	-3.872078
125	1	0	2.802348	1.557397	-4.722724
126	1	0	2.564979	-2.906597	-4.000747
127	1	0	3.784051	-1.686073	-3.682413
128	1	0	-1.644641	-6.561248	-2.913145
129	1	0	-0.234747	-5.570962	-3.207743
130	6	0	-9.194341	-1.201106	-2.425590
131	1	0	-7.424246	2.746913	-2.787559
132	6	0	-3.436642	6.573009	-3.004457
133	1	0	-1.102247	5.797367	-4.358677
134	1	0	0.003610	-5.225173	-0.674749
135	1	0	-1.363228	-6.294697	-0.432819
136	1	0	2.576257	-2.853257	-1.178205
137	1	0	3.470766	-3.979883	-2.186977
138	8	0	-2.223273	0.144515	-0.166242

139	1	0	1.468268	-8.320135	0.143520
140	6	0	0.790247	5.802200	1.237601
141	6	0	-0.492587	5.392901	0.801755
142	6	0	-0.782585	4.087188	0.440506
143	6	0	0.260801	3.128860	0.506038
144	6	0	1.568966	3.498726	0.950783
145	6	0	1.804032	4.852360	1.314926
146	6	0	2.633566	2.506670	0.932165
147	6	0	2.350163	1.256981	0.322188
148	6	0	1.042846	0.932153	-0.007220
149	7	0	0.028827	1.820813	0.109218
150	17	0	-1.803804	6.647593	0.693487
151	7	0	3.860730	2.774229	1.490803
152	6	0	5.000605	2.029448	1.014642
153	6	0	5.598310	0.992628	1.753466
154	6	0	6.492770	0.108635	1.115139
155	6	0	6.781424	0.281502	-0.264369
156	6	0	6.322188	1.427003	-0.966998
157	6	0	5.417642	2.279383	-0.304344
158	6	0	7.117851	-1.021224	1.931262
159	7	0	7.170480	-2.320817	1.144089
160	1	0	7.752416	-2.096427	0.316876
161	8	0	7.502195	-0.716066	-0.938213
162	1	0	0.973180	6.838136	1.500889
163	1	0	-1.772199	3.796058	0.104712
164	1	0	2.794574	5.145476	1.642534
165	1	0	3.116443	0.500301	0.227622
166	1	0	0.766821	-0.061601	-0.331655
167	1	0	5.339392	0.841582	2.798313
168	1	0	4.985955	3.121617	-0.838038
169	1	0	6.568556	-1.192796	2.859731
170	1	0	8.149581	-0.759654	2.192710
171	1	0	6.815138	-1.250604	-1.520206
172	1	0	-0.931145	1.455244	-0.056070
173	1	0	6.196522	-2.513177	0.721170
174	1	0	3.834914	3.200464	2.439591
175	1	0	-0.198655	5.650779	-2.846366
176	1	0	0.265069	4.678027	-4.249363
177	1	0	-8.329450	1.797185	-1.601251
178	1	0	-8.485623	1.439371	-3.327281
179	1	0	-4.839030	5.049442	-3.289678
180	1	0	-2.425454	6.896404	-2.780011
181	1	0	-4.183609	7.356035	-3.109892
182	1	0	-7.657737	-2.554998	-2.817309
183	1	0	-9.541339	-0.207932	-2.162316
184	1	0	-9.960333	-1.960122	-2.565298
185	6	0	7.684742	-3.594049	1.844270
186	6	0	6.554376	-4.171636	2.720750
187	6	0	8.937705	-3.269749	2.684299
188	6	0	8.036754	-4.571990	0.697568
189	1	0	6.906305	-5.098234	3.191550
190	1	0	5.676525	-4.412781	2.107575
191	1	0	6.248712	-3.480988	3.511859
192	1	0	9.355208	-4.205605	3.073918
193	1	0	8.697911	-2.634763	3.543618
194	1	0	9.716644	-2.780500	2.083530
195	1	0	8.345565	-5.535458	1.118338
196	1	0	8.862727	-4.192406	0.080443
197	1	0	7.168511	-4.746592	0.050319
198	6	0	7.217144	1.254434	-4.704384
199	6	0	6.787835	0.860654	-3.423985
200	6	0	6.771502	1.780268	-2.348571
201	6	0	7.192432	3.109639	-2.598408
202	6	0	7.623658	3.517813	-3.872848
203	6	0	7.630235	2.576730	-4.909946
204	17	0	8.190788	3.088037	-6.569685
205	1	0	7.224924	0.541929	-5.523174
206	1	0	6.440841	-0.155903	-3.281461
207	1	0	7.210139	3.827869	-1.782620
208	1	0	7.955314	4.536407	-4.047330

12. Miscellaneous

12.1 FePPIXH

Ground state; overall *S* = 3/2. Spin on Fe (method 3, n-octanol): +3.01.



Energies:

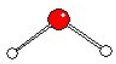
ZPE	m1 oct	m1 water	m3 oct	m3 water
0.584315	-1957.522952	-1957.529324	-3098.544210	-3098.548643

Atomic coordinates:

1	26	0	1.066900	-0.039951	-0.221654
2	7	0	-0.519164	-1.241684	-0.406649
3	7	0	2.267918	-1.645556	-0.111390
4	7	0	-0.130962	1.560297	-0.354609
5	7	0	2.653603	1.167968	0.001319
6	6	0	-1.845954	-0.865230	-0.564911
7	6	0	-2.731059	-2.043096	-0.567452
8	6	0	-1.911443	-3.145094	-0.437408
9	6	0	-0.543198	-2.641885	-0.352803
10	6	0	1.891801	-2.991934	-0.153658
11	6	0	3.059955	-3.865577	-0.065912
12	6	0	4.164923	-3.035597	0.042010
13	6	0	3.652807	-1.655148	0.011904
14	6	0	3.989721	0.788999	0.137033
15	6	0	4.854448	1.957596	0.295995
16	6	0	4.025184	3.067624	0.265421
17	6	0	2.656968	2.559628	0.066609
18	6	0	0.235063	2.897282	-0.259563
19	6	0	-1.509790	1.575154	-0.594434
20	6	0	-2.014072	2.958441	-0.660009
21	6	0	-0.925539	3.774714	-0.436010
22	6	0	1.531678	3.366924	-0.043798
23	6	0	4.455991	-0.524627	0.130939
24	6	0	0.581200	-3.454674	-0.250518
25	6	0	-2.306252	0.445070	-0.710663
26	1	0	1.663386	4.439435	0.033450
27	1	0	5.521363	-0.675204	0.254203
28	1	0	0.421310	-4.526705	-0.242892
29	1	0	-3.360326	0.587330	-0.912378
30	6	0	-2.300845	-4.597280	-0.373182
31	6	0	-0.865540	5.277254	-0.379991
32	6	0	-3.437425	3.383320	-0.941832
33	6	0	-4.235457	-1.991694	-0.565281
34	6	0	3.021953	-5.367128	-0.128946
35	6	0	5.586618	-3.372721	0.129990

36	6	0	6.126831	-4.528392	0.592131
37	6	0	6.351551	1.913676	0.424489
38	6	0	4.357153	4.490098	0.358162
39	6	0	5.451795	5.039341	0.942274
40	6	0	-4.741568	-1.791309	0.896037
41	6	0	-4.438811	3.234370	0.243101
42	6	0	-5.235163	1.930471	0.197349
43	6	0	-6.291622	-1.734096	0.981828
44	8	0	-6.878217	-0.652721	1.345327
45	8	0	-6.885074	-2.844077	0.682088
46	8	0	-5.789746	1.599292	1.373899
47	8	0	-5.342088	1.235352	-0.846620
48	1	0	-1.837418	-5.175852	-1.184331
49	1	0	-3.384712	-4.717929	-0.461047
50	1	0	-1.993270	-5.057727	0.575909
51	1	0	-0.181295	5.683683	-1.137731
52	1	0	-0.515297	5.628899	0.600485
53	1	0	-1.850092	5.721834	-0.552919
54	1	0	-3.843091	2.810464	-1.785225
55	1	0	-3.422515	4.433482	-1.253939
56	1	0	-4.655517	-2.924513	-0.956519
57	1	0	-4.615405	-1.173388	-1.185600
58	1	0	2.157340	-5.728823	-0.695688
59	1	0	2.968410	-5.815603	0.873980
60	1	0	3.925111	-5.757384	-0.612531
61	1	0	6.278611	-2.604992	-0.217412
62	1	0	5.527435	-5.335683	1.001539
63	1	0	7.203918	-4.675275	0.593906
64	1	0	6.776652	1.032072	-0.067361
65	1	0	6.669283	1.887469	1.477226
66	1	0	6.805508	2.801206	-0.031495
67	1	0	3.639007	5.175677	-0.092032
68	1	0	6.202639	4.449083	1.458414
69	1	0	5.600642	6.116121	0.937782
70	1	0	-4.343453	-0.864390	1.324115
71	1	0	-4.397749	-2.631705	1.511483
72	1	0	-5.175187	4.049600	0.204486
73	1	0	-3.946095	3.309736	1.218187
74	1	0	-6.288758	0.660978	1.375273

12.2 Water



Energies:

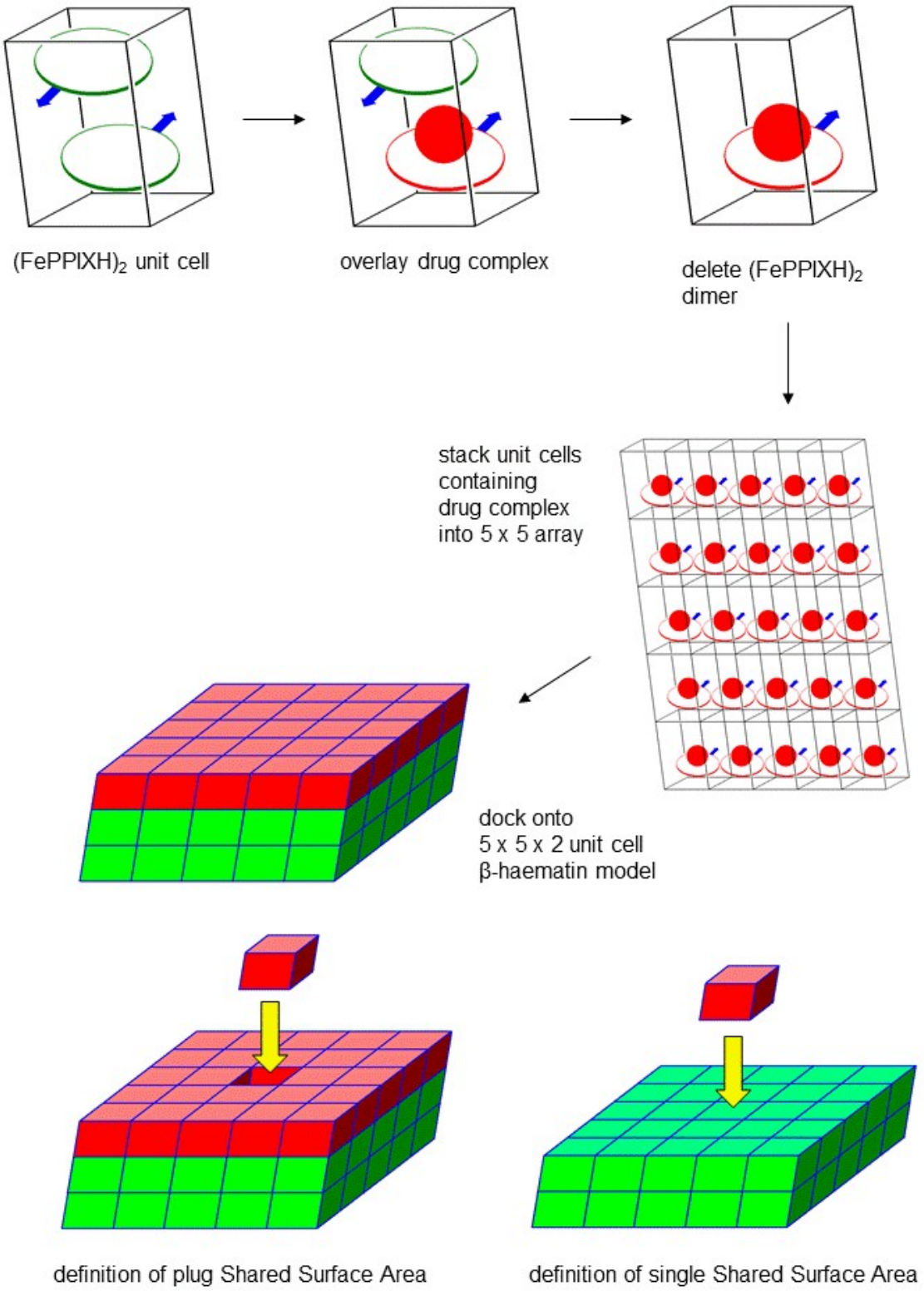
ZPE	m1 oct	m1 water	m3 oct	m3 water
0.020764	-76.429402	-76.432623	-76.469064	-76.470876

Atomic coordinates:

1	1	0	-0.057636	0.000000	-0.142236
2	8	0	-0.062648	0.000000	0.834815
3	1	0	0.853244	0.000000	1.174196

13. Fig. S1. Methodology for haemozoin surface modelling

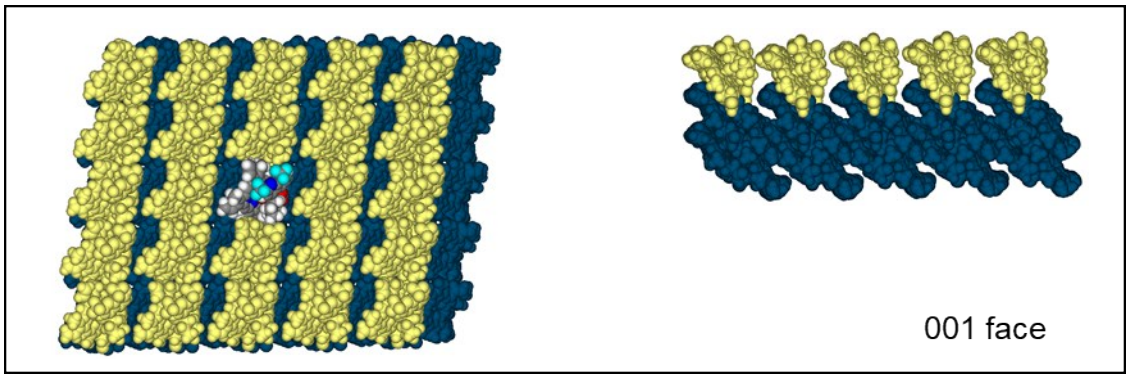
In this figure, FePPIXH molecules and native [$(FePPIXH)_2$] unit cells are coloured green. Drug complexes and their unit cells are coloured red. The blue arrows denote the propionic acid groups used for hydrogen bonding to the next layer.

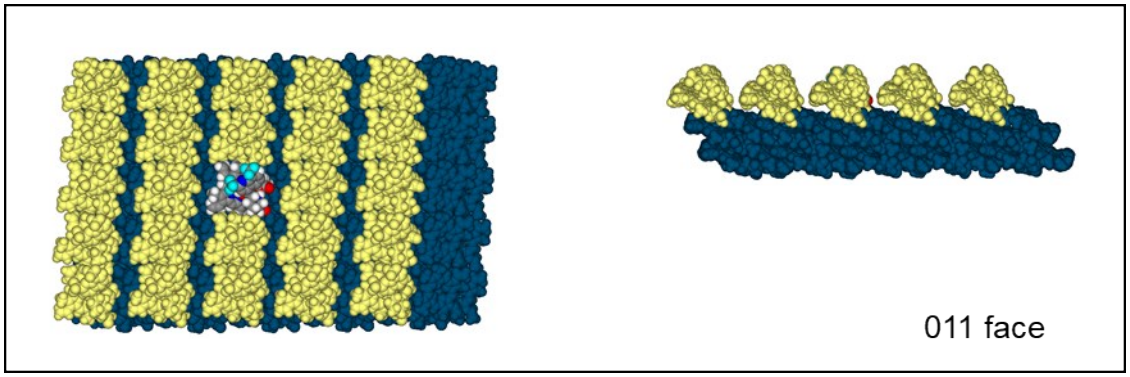


14. Images of drug complex coated haemozoin crystal surfaces

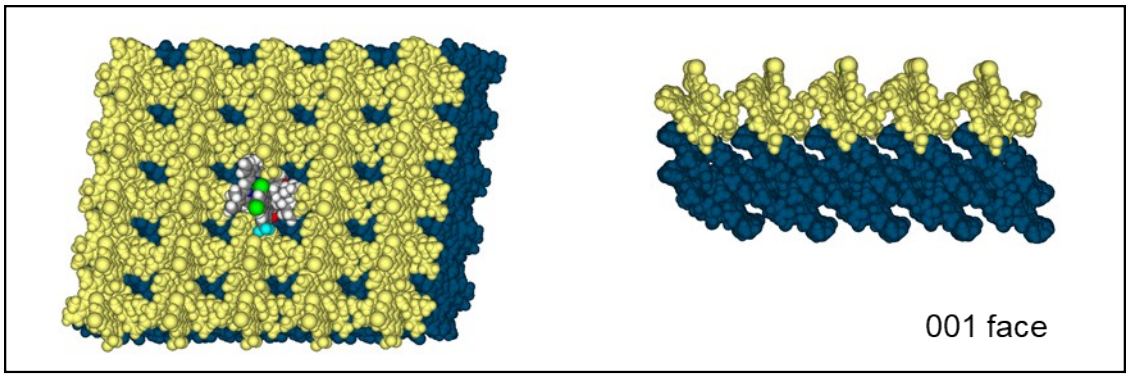
The colour coding in the following pictures is as used in Fig. 3.

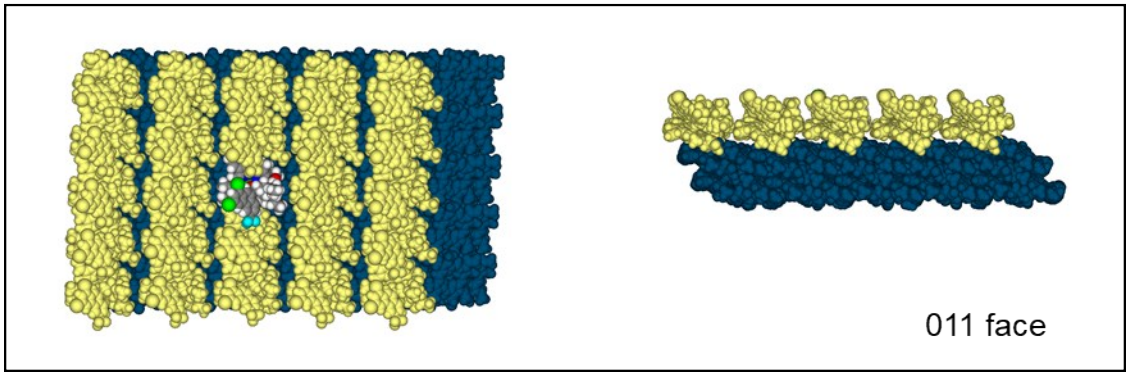
14.1 Mefloquine



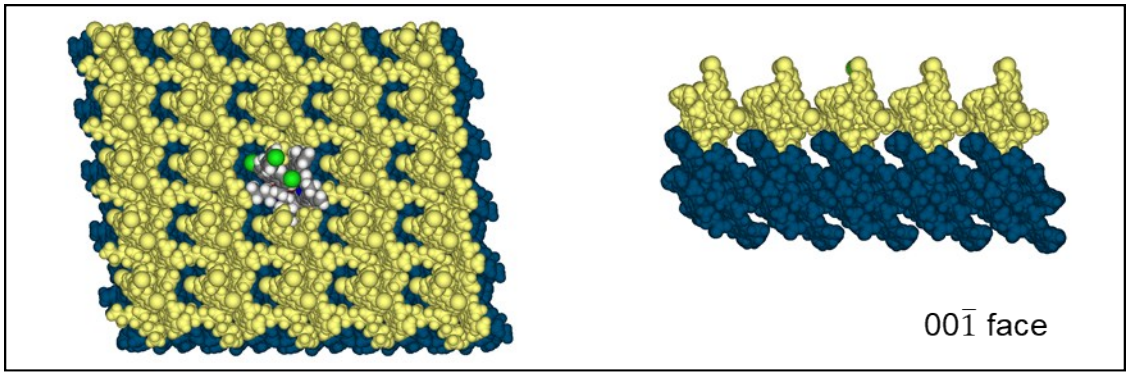


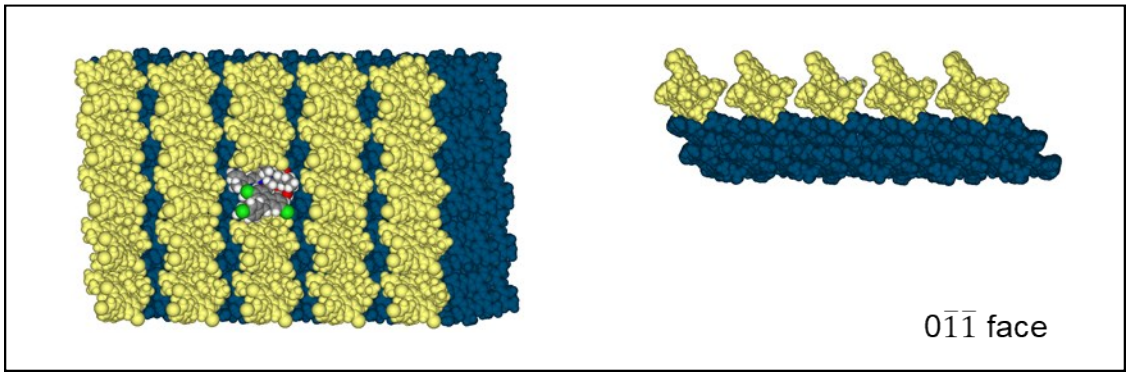
14.2 Halofantrine





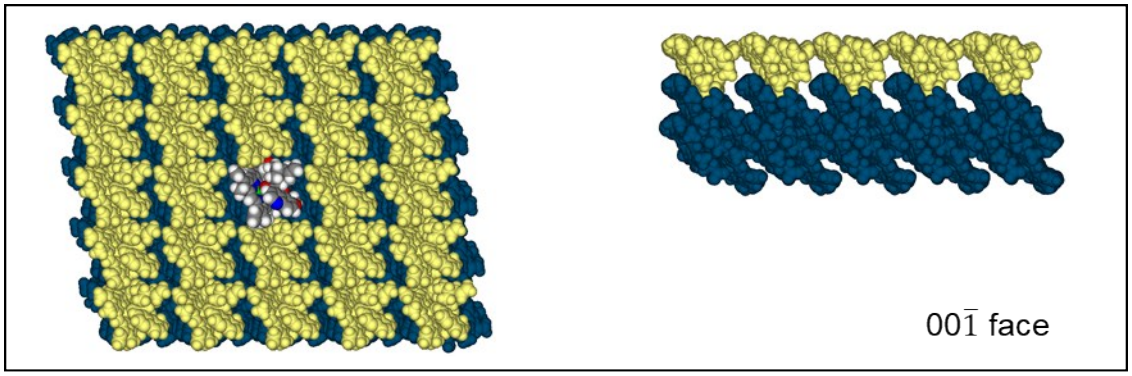
14.3 Lumefantrine

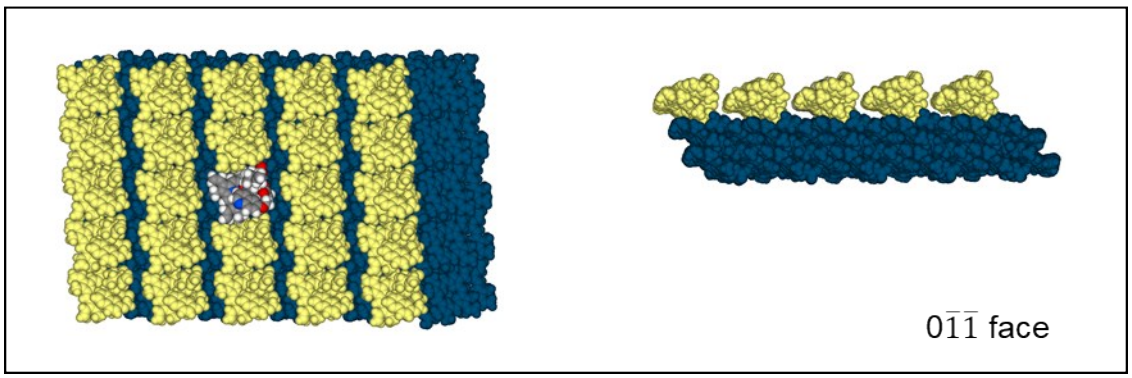




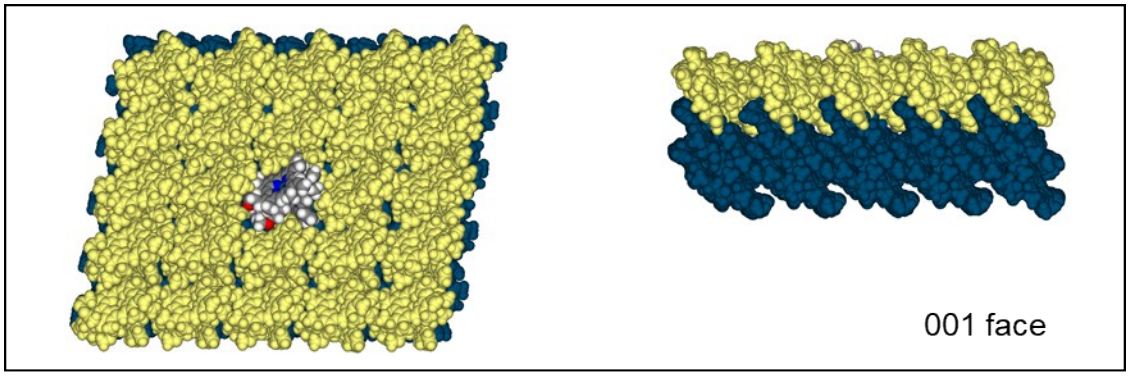
14.4 Quinine

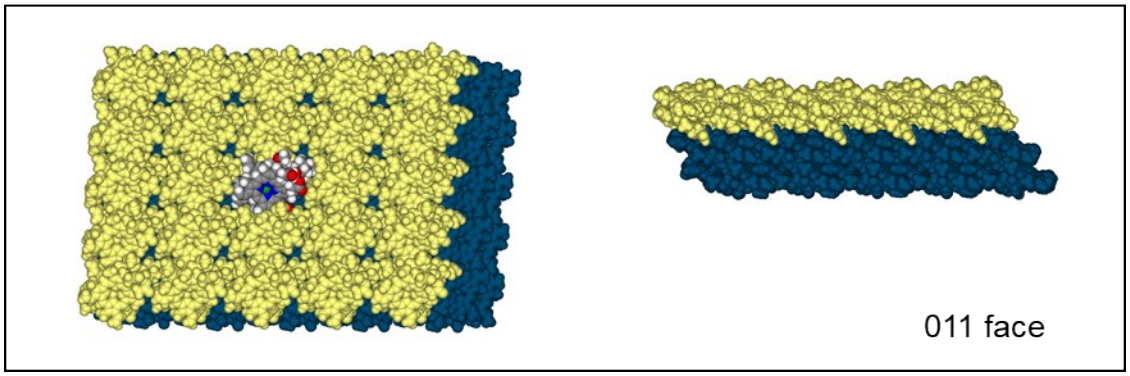
[(FePPIXH)(QN1)];





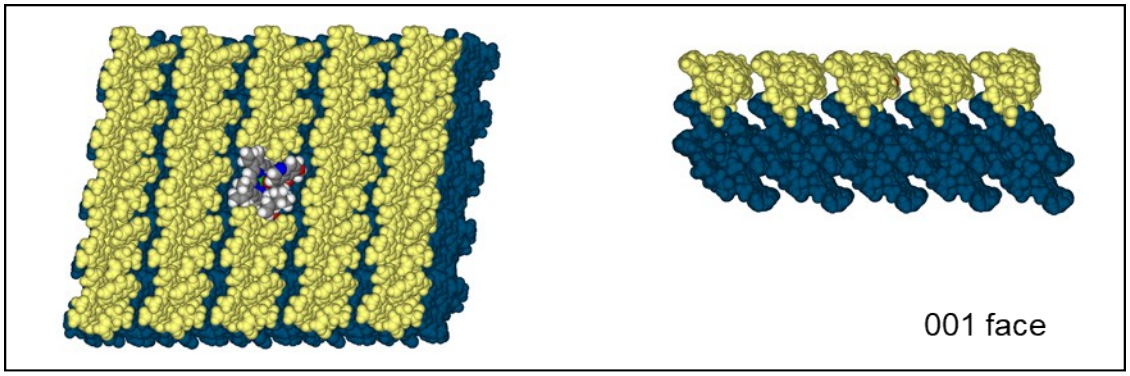
[$(FePPIXH)_2(\mu\text{-}O)(QNH_2)$];

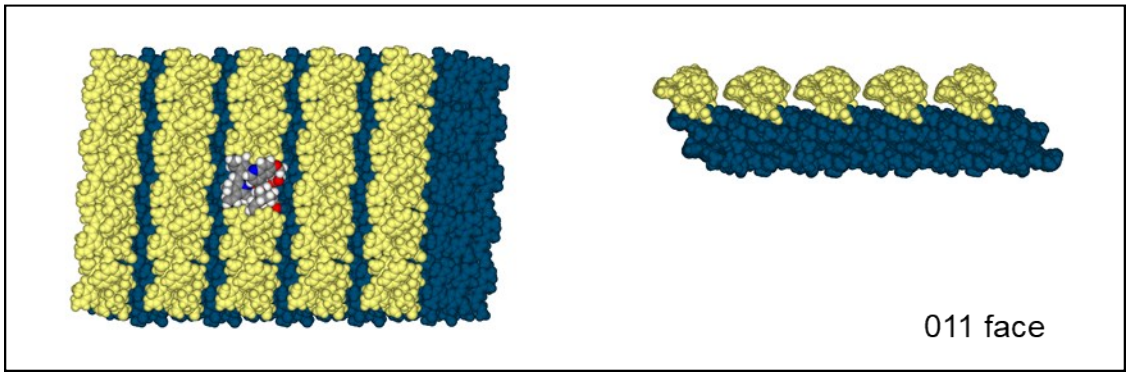




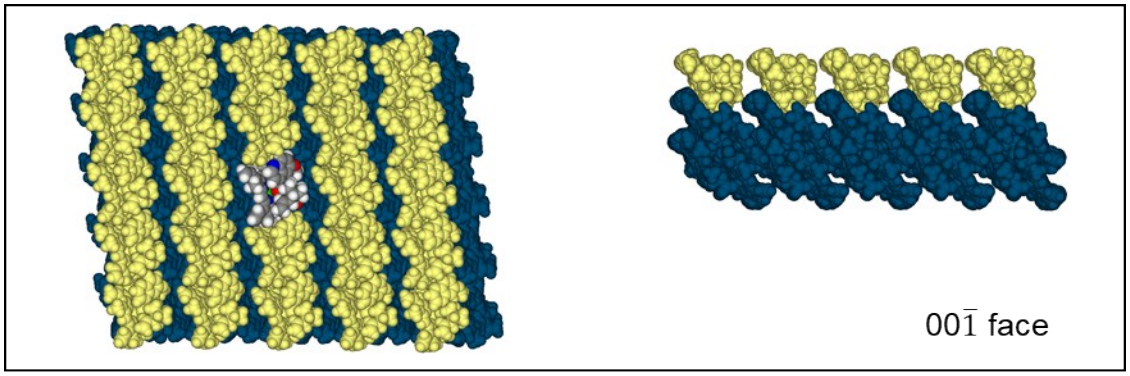
14.5 Quinidine

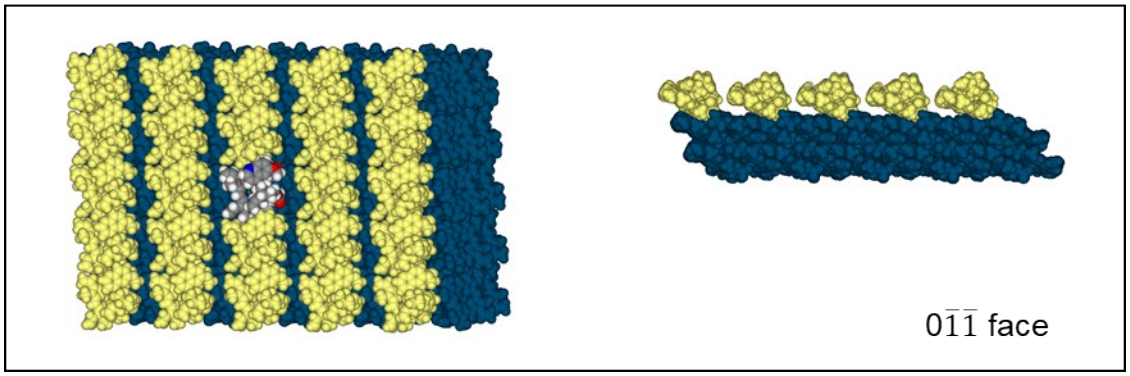
[(FePPIXH)(QD1)];



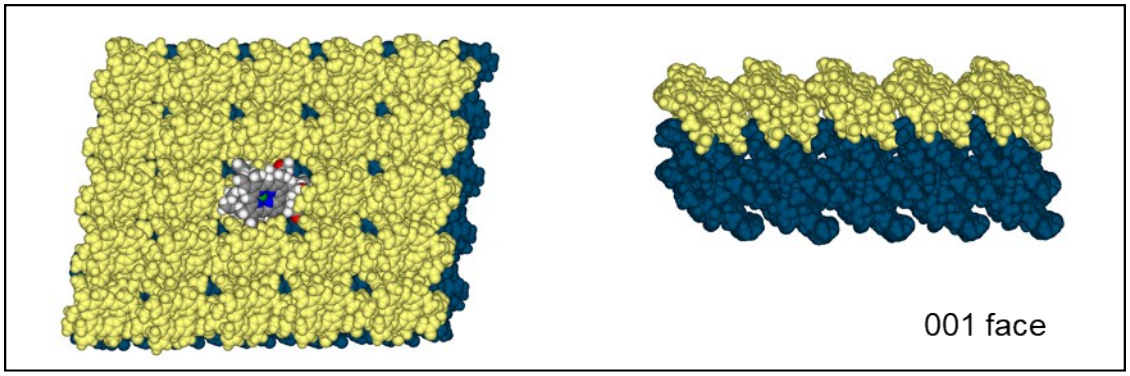


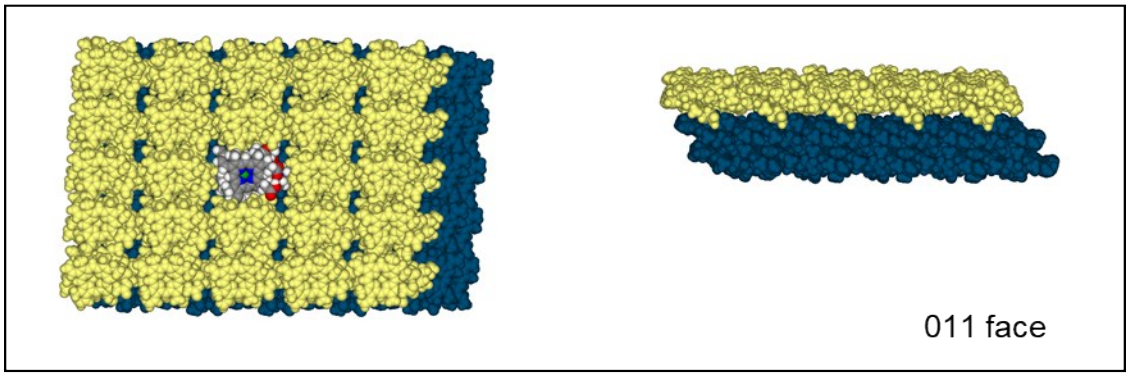
[(FePPIXH)(QD2)];

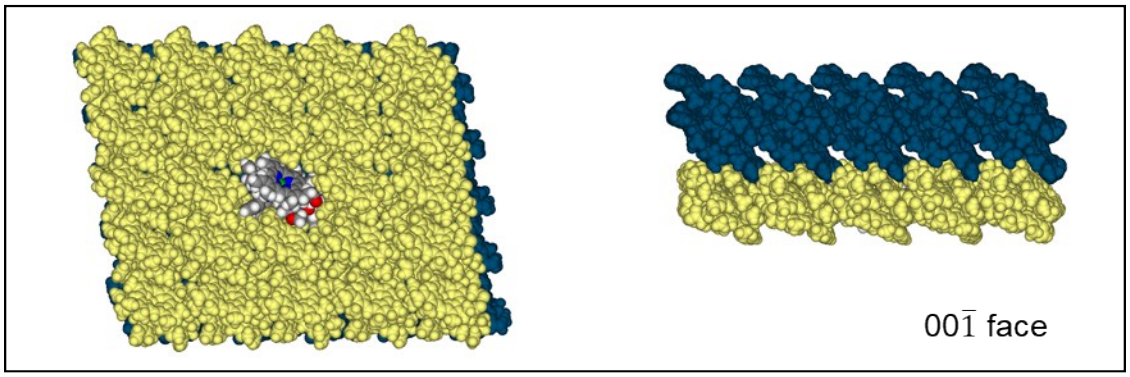


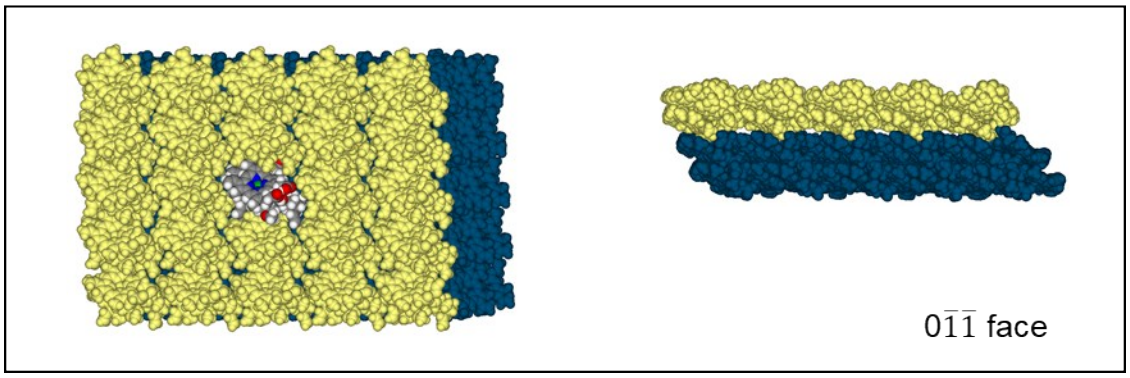


$[(FePPIXH)_2(\mu\text{-}O)(QDH_2)]$;



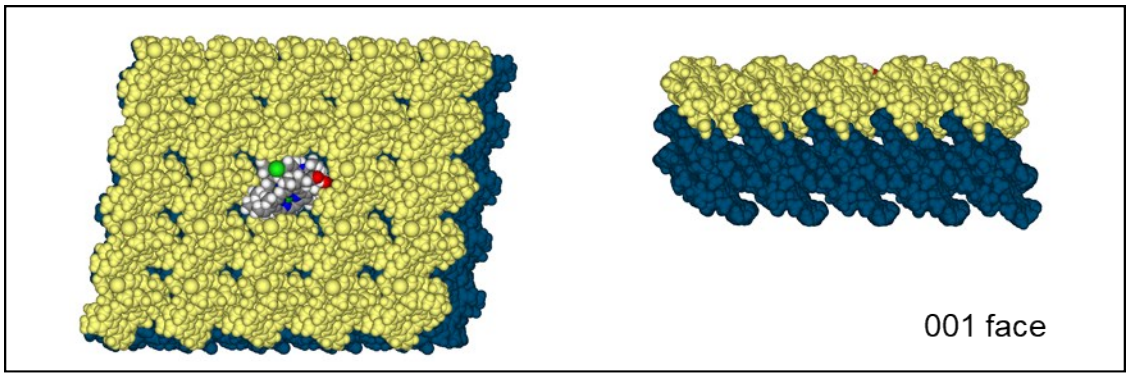


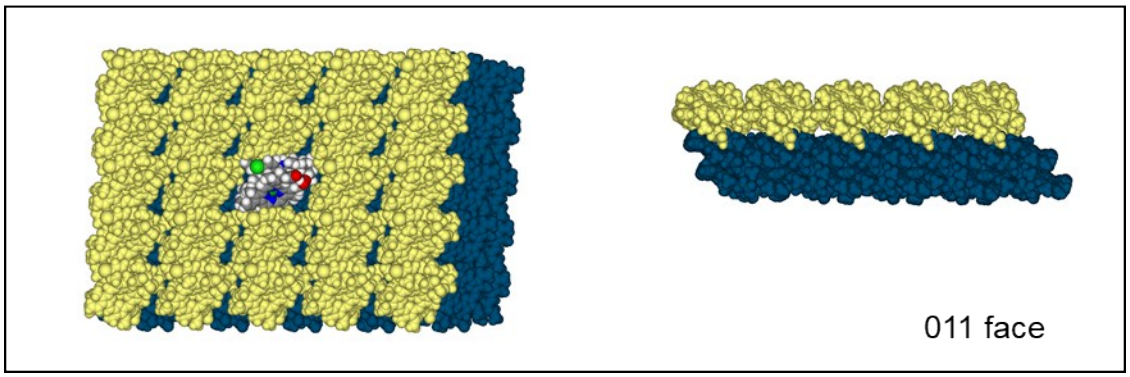




14.6 Chloroquine

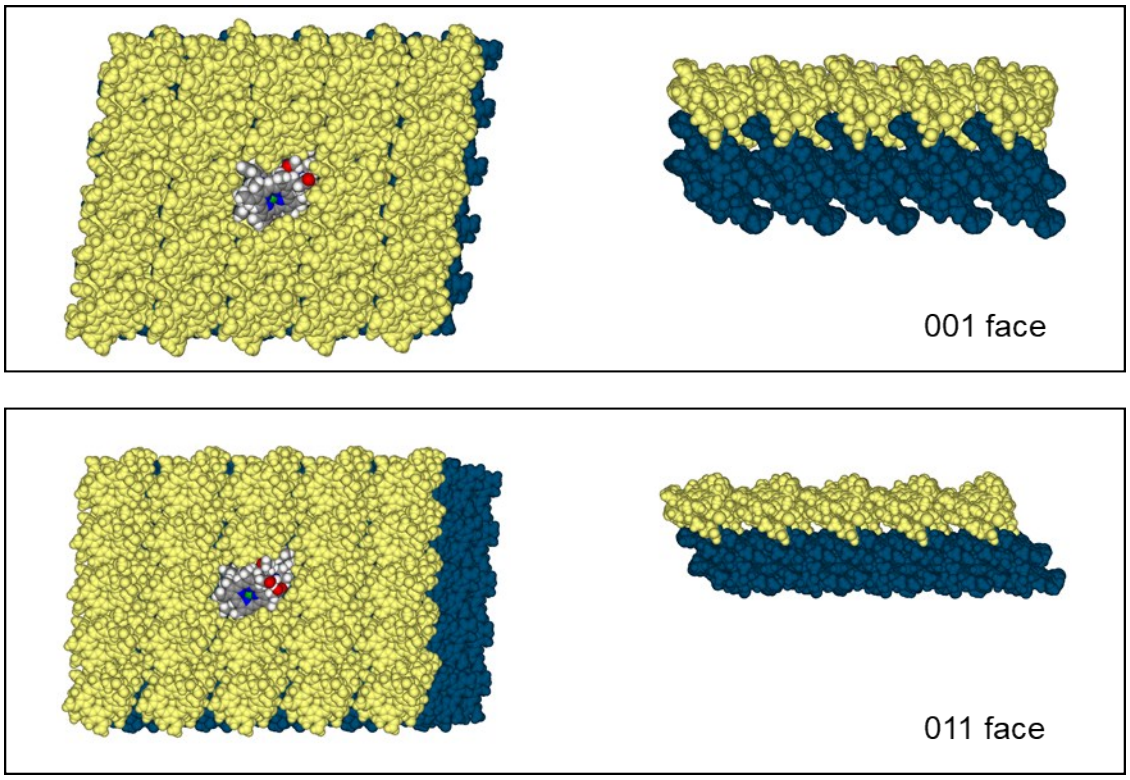
$[(FePPIXH)_2(\mu\text{-}O)(CQH_2)]$;





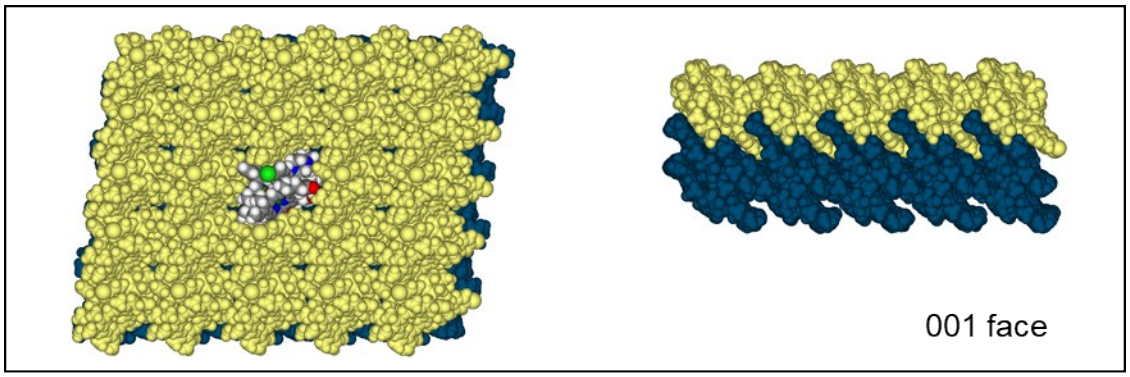
14.7 Mepacrine

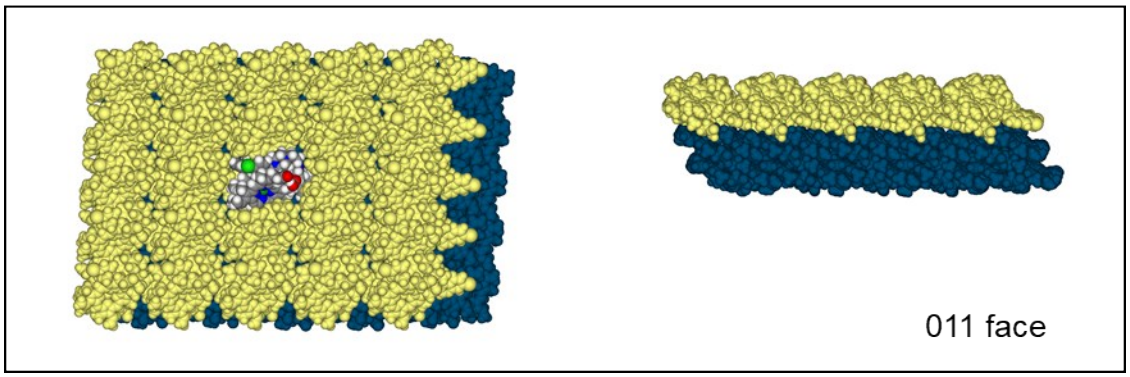
$[(FePPIXH)_2(\mu\text{-}O)(MPH_2)]$;



14.8 Piperaquine

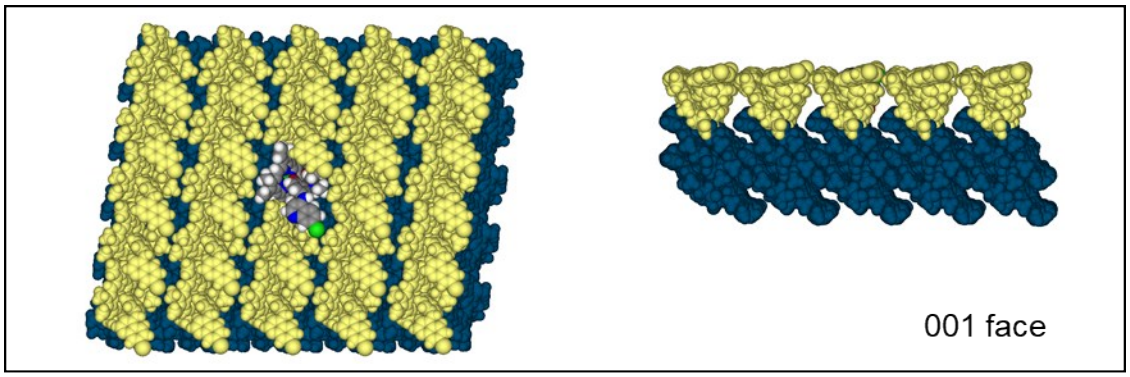
$[(FePPIXH)_2(\mu\text{-}O)(PQH_2)]$;

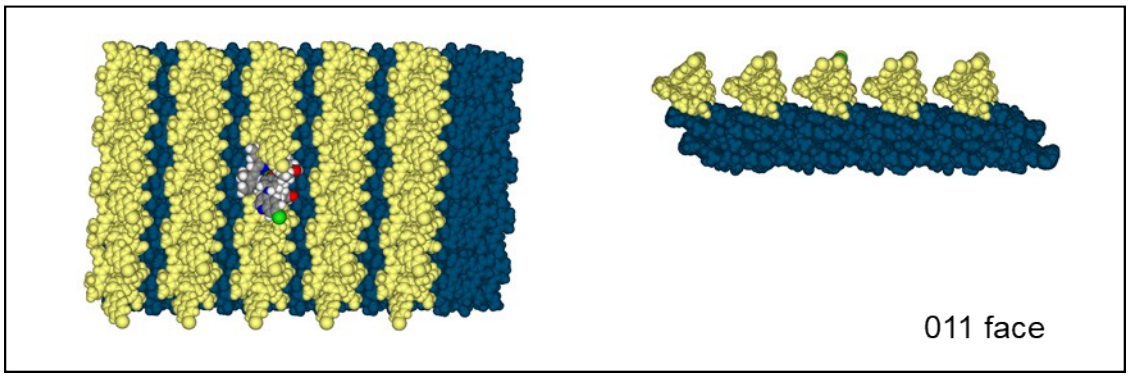




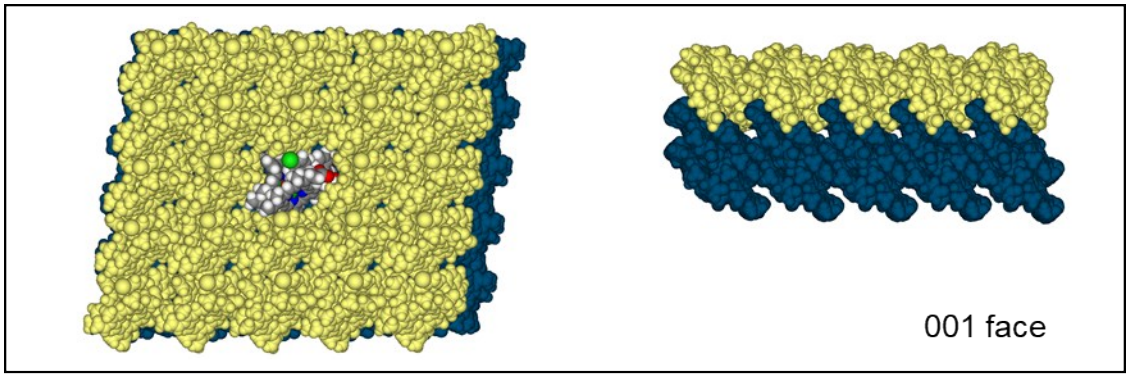
14.9 Amodiaquine

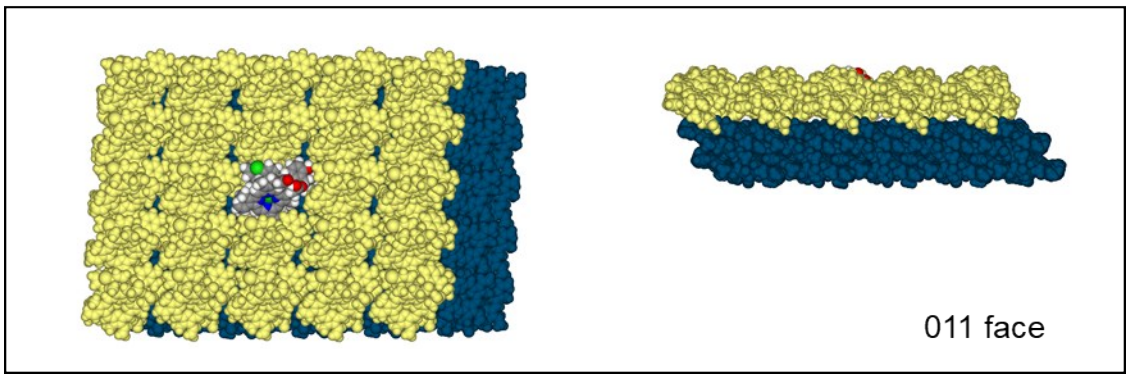
[(FePPIXH)(AQ)];





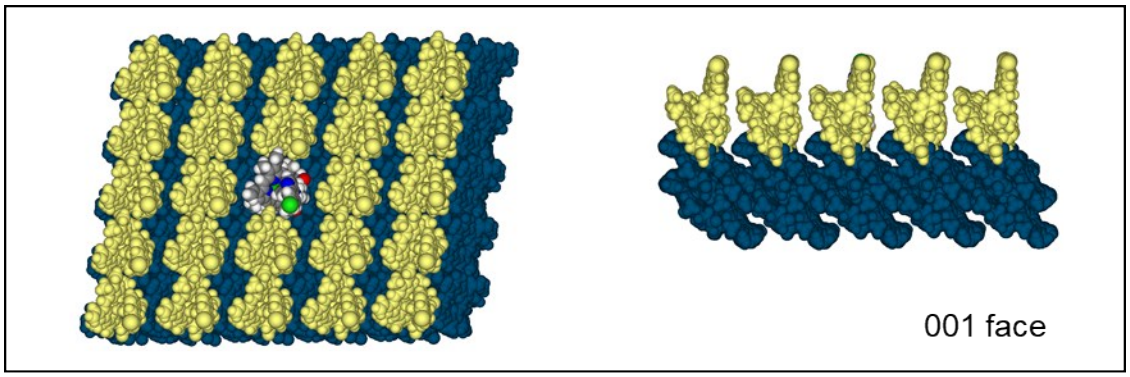
[$(FePPIXH)_2(\mu\text{-}O)(AQH_2)$];

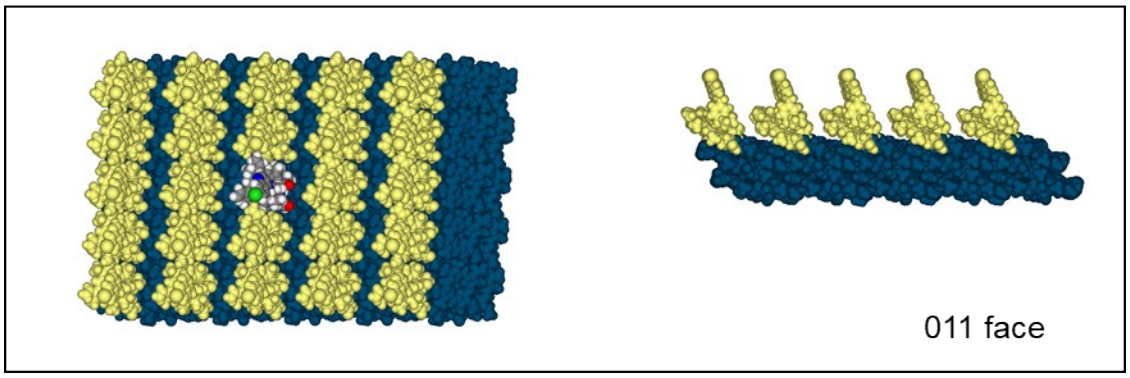




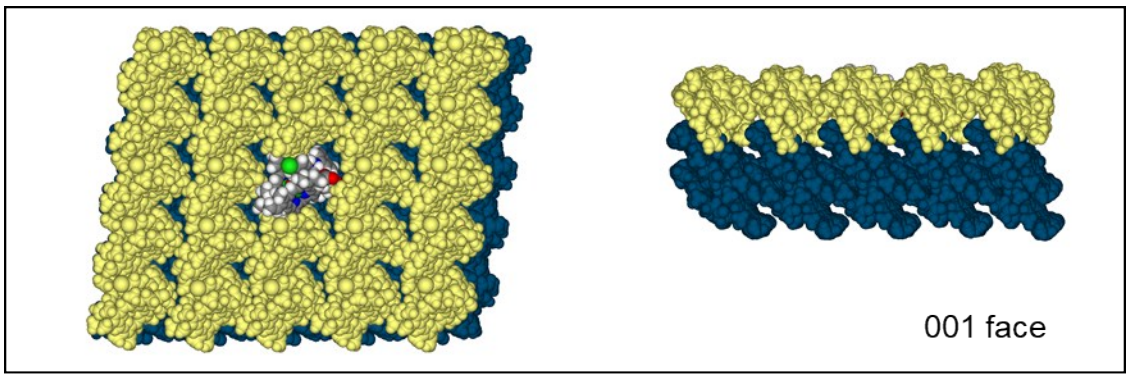
14.10 Desethyl Amodiaquine

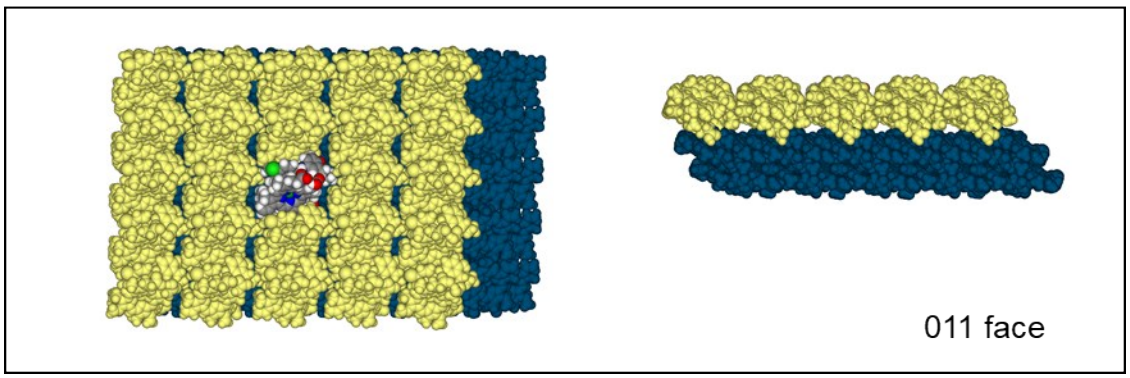
[(FePPIXH)(DAQ)];





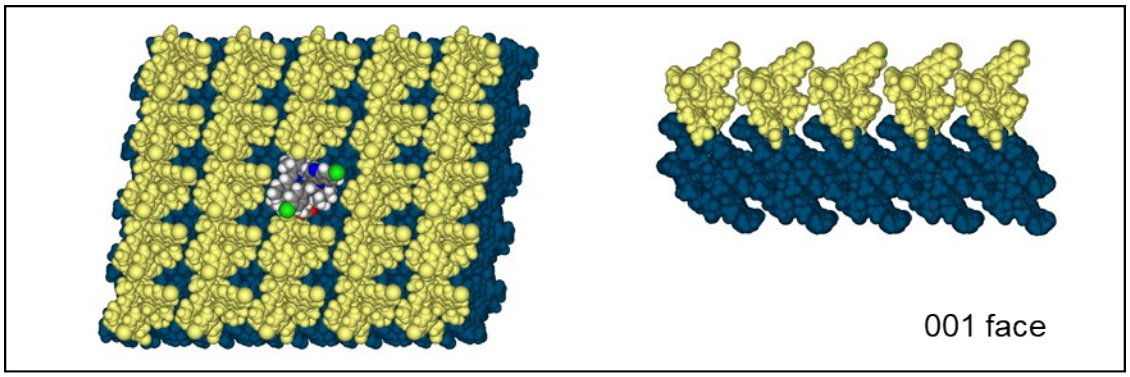
[$(FePPIXH)_2(\mu\text{-}O)(DAQH_2)$];

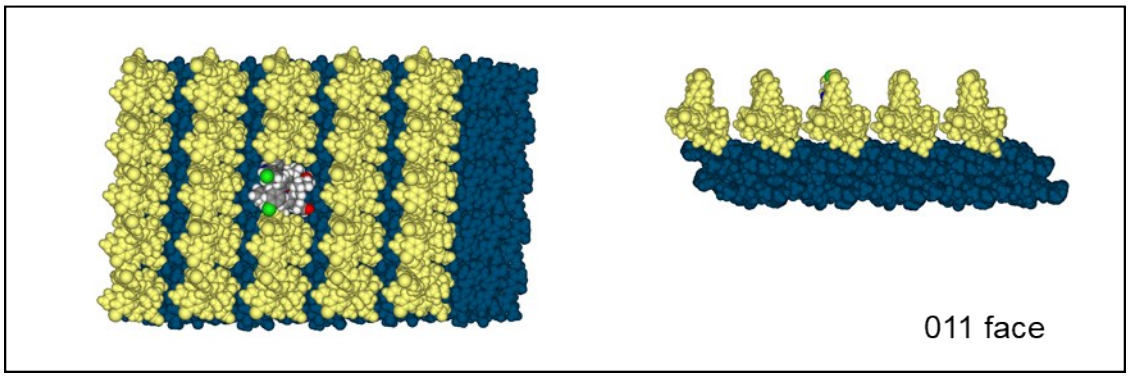




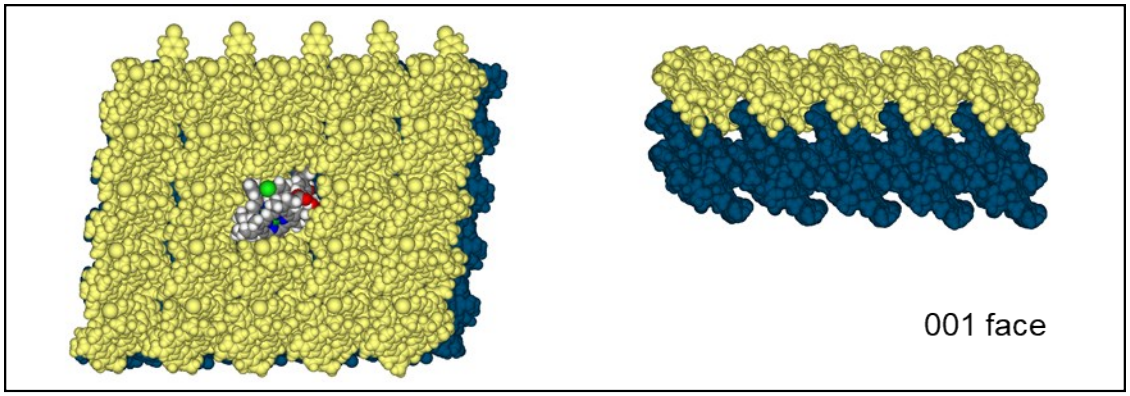
14.11 Tebuquine

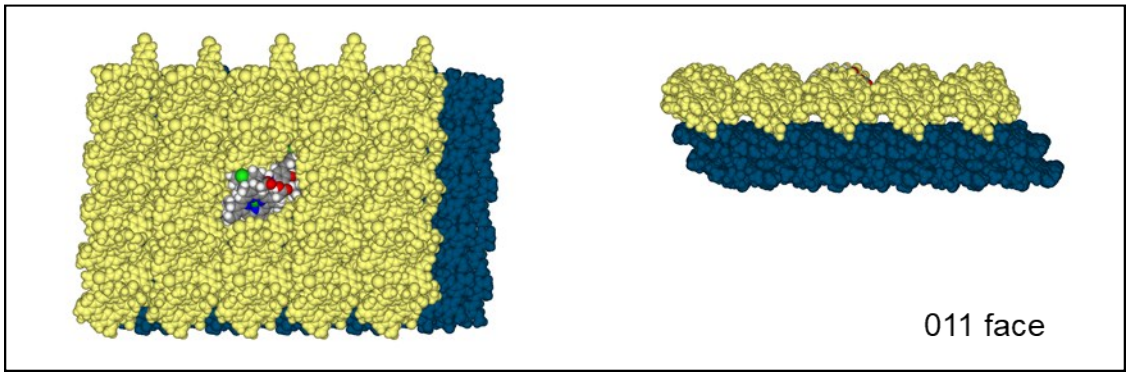
[(FePPIXH)(TQ)];





[$(FePPIXH)_2(\mu\text{-}O)(TQH_2)$];





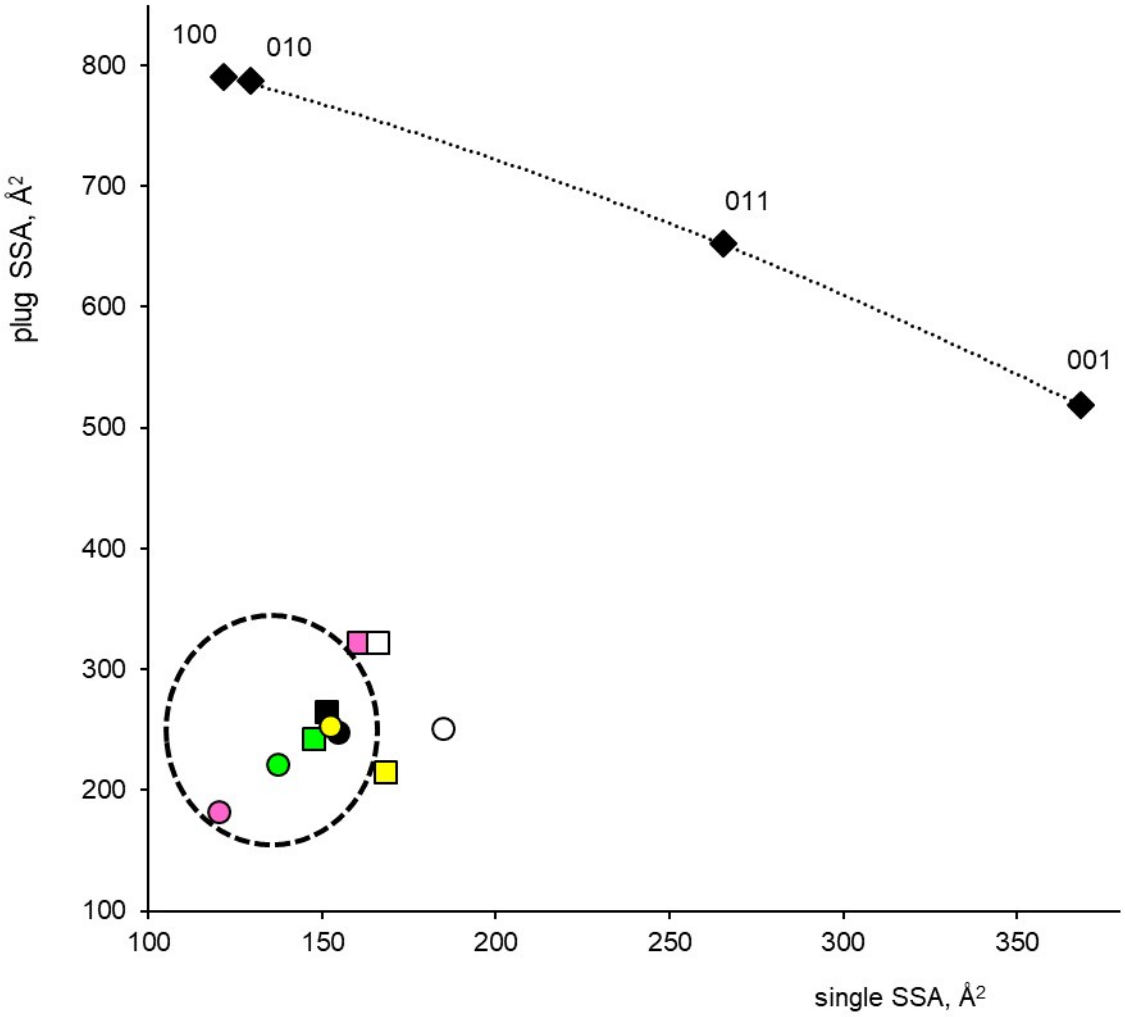
15. Surface area data for Fig. 2

15.1 Data included in Fig. 2

Drug	Face	Single SSA, Å^2	Plug SSA, Å^2	Face	Single SSA, Å^2	Plug SSA, Å^2
haematin	001	368.6	518.0	100	121.7	789.4
	010	129.6	786.4	011	265.5	651.4
1. zwitterionic complexes						
[(FePPIXH)(MQ)]	001	138.0	242.8	011	144.9	229.7
[(FePPIXH)(HN)]	001	130.7	312.7	011	148.6	314.7
[(FePPIXH)(LM)]	001	155.8	289.9	011	145.3	295.0
[(FePPIXH)(QN(1))]	001	128.3	235.2	011	139.9	219.2
[(FePPIXH)(QN(2))]	001	130.2	274.4	011	142.8	245.8
[(FePPIXH)(QD(1))]	001	110.5	251.3	011	152.9	283.3
[(FePPIXH)(QD(2))]	001	127.4	269.3	011	147.8	273.0
[(FePPIXH)(AQ)]	001	139.7	260.8	011	135.7	230.9
[(FePPIXH)(DAQ)]	001	140.7	180.0	011	153.4	211.4
[(FePPIXH)(TQ)]	001	124.7	185.7	011	132.6	230.4
2. dinuclear complexes						
[(FePPIXH)$_2$(μ-O)(QNH$_2$)]	001	201.3	622.1	011	170.2	497.2
[(FePPIXH)$_2$(μ-O)(QDH$_2$)] #1	001	152.7	460.9	011	163.0	485.9
[(FePPIXH)$_2$(μ-O)(QDH$_2$)] #2	001	185.1	554.6	011	143.5	456.7
[(FePPIXH)$_2$(μ-O)(CQH$_2$)]	001	183.9	533.7	011	150.5	455.0
[(FePPIXH)$_2$(μ-O)(MPH$_2$)]	001	225.1	617.9	011	180.2	558.2
[(FePPIXH)$_2$(μ-O)(PQH$_2$)]	001	295.8	776.9	011	199.9	718.0
[(FePPIXH)$_2$(μ-O)(AQH$_2$)]	001	173.3	515.2	011	162.3	469.1
[(FePPIXH)$_2$(μ-O)(DAQH$_2$)]	001	144.4	428.2	011	150.1	434.6
[(FePPIXH)$_2$(μ-O)(TQH$_2$)]	001	204.2	631.9	011	152.9	601.1

15.2 Data not included in Fig. 2

Data points for the hydroxy-bound, [(FePPIXH)(OH)(drugH)] type complexes were omitted from Fig. 2 for clarity. The equivalent plot for these complexes, together with the original data, are given below. The colour coding is as used in Fig. 2.

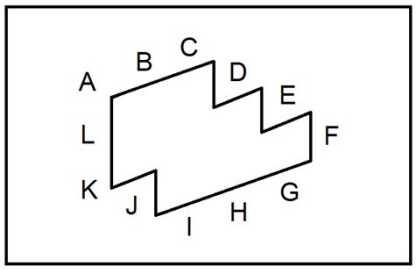


Drug	Face	Single SSA, Å²	Plug SSA, Å²	Face	Single SSA, Å²	Plug SSA, Å²
[(FePPIXH)(OH)(CQ)]	001	152.5	252.5	011	168.2	214.7
[(FePPIXH)(OH)(MP)]	001	154.6	247.9	011	151.4	264.7
[(FePPIXH)(OH)(PQ)]	001	184.7	250.5	011	166.2	322.3
[(FePPIXH)(OH)(AQ)]	001	137.4	221.6	011	147.7	242.0
[(FePPIXH)(OH)(TQ)]	001	120.3	181.4	011	160.4	321.5

16. Surface area data for Fig. 5

The diagram shows the positions of molecules A – L around the central island; molecules G, H and I have the alternative conformation required to hydrogen bond to the propionate group in the layer below.

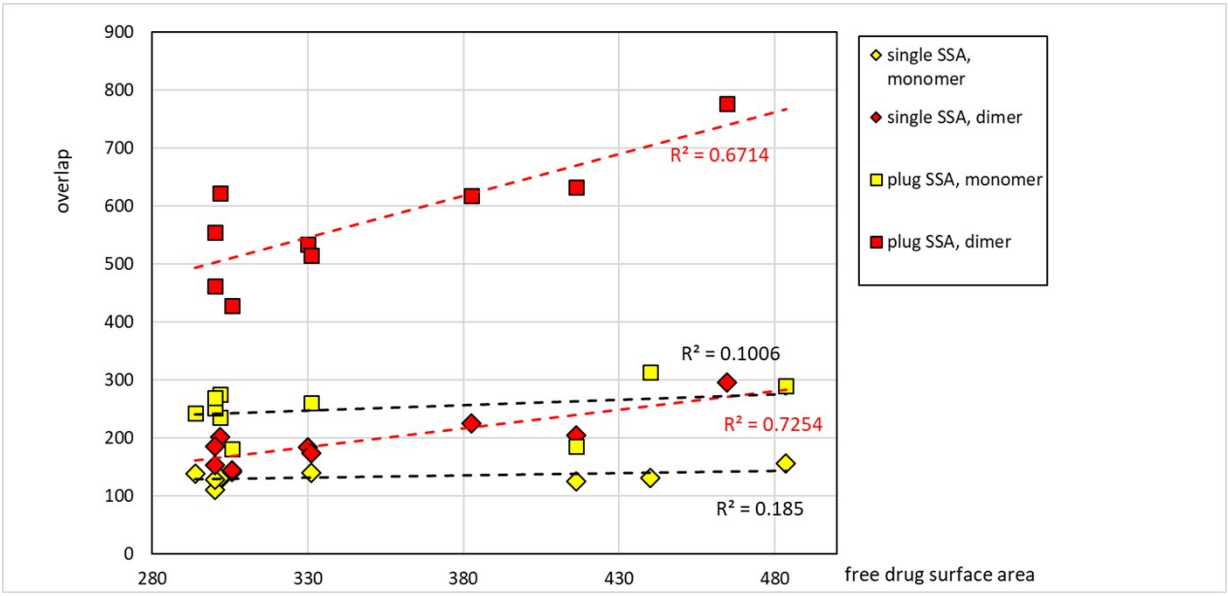
	[(FePPIXH)$_2$] dimers		[(FePPIXH)(μ-O)(CQH$_2$)]		[(FePPIXH)(QD)]	
#	Single SSA, Å^2	Plug SSA, Å^2	Single SSA, Å^2	Plug SSA, Å^2	Single SSA, Å^2	Plug SSA, Å^2
A	131.9	222.4	124.9	190.7	139.4	140.3
B	329.1	507.1	276.1	376.9	218.3	221.6
C	351.8	455.0	284.3	390.5	222.9	230.7
D	438.1	454.0	350.2	397.8	255.4	266.0
E	435.4	453.6	350.9	355.4	256.8	258.8
F	207.5	255.6	173.2	185.3	139.9	145.4
G	337.1	466.7	190.5	204.7	156.6	158.6
H	350.8	541.0	228.5	234.0	190.9	194.4
I	362.2	463.5	234.5	240.4	183.0	187.5
J	230.4	241.4	213.1	223.0	231.3	243.2
K	130.5	143.6	129.8	163.4	141.1	156.6
L	247.8	260.2	200.7	256.9	225.5	229.4



17. Free drug surface areas versus complex surface coverage

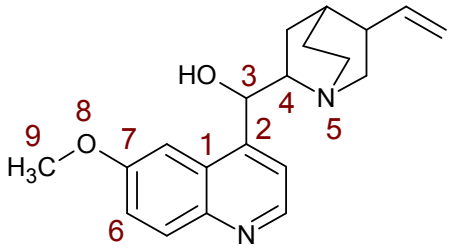
This analysis is for the {001} face of β-haematin. Surface area (SA) and shared surface area (SSA) values were obtained in Discovery Studio using a 1.4 Å solvent surface probe. The graph shows no correlation except for the dimer plug SSA values; the weak correlation in this case is lost if the data point for PQ is deleted.

Drug	free drug SA, Å²	single SSA, monomer, Å²	single SSA, dimer, Å²	plug SSA, monomer, Å²	plug SSA, dimer, Å²
[(FePPIXH)(MQ)]	293.9	138.0		242.8	
[(FePPIXH)(HN)]	439.9	130.7		312.7	
[(FePPIXH)(LM)]	483.6	155.8		289.9	
[(FePPIXH)(QN(1))]	301.8	128.3		235.2	
[(FePPIXH)(QN(2))]	301.8	130.2		274.4	
[(FePPIXH)(QD(1))]	300.3	110.5		251.3	
[(FePPIXH)(QD(2))]	300.3	127.4		269.3	
[(FePPIXH)(AQ)]	331.1	139.7		260.8	
[(FePPIXH)(DAQ)]	305.8	140.7		180.0	
[(FePPIXH)(TQ)]	416.3	124.7		185.7	
$[(FePPIXH)_2(\mu\text{-}O)(QNH_2)]$	301.8		201.3		622.1
$[(FePPIXH)_2(\mu\text{-}O)(QDH_2)]$ #1	300.3		152.7		460.9
$[(FePPIXH)_2(\mu\text{-}O)(QDH_2)]$ #2	300.3		185.1		554.6
$[(FePPIXH)_2(\mu\text{-}O)(CQH_2)]$	329.9		183.9		533.7
$[(FePPIXH)_2(\mu\text{-}O)(MPH_2)]$	382.6		225.1		617.9
$[(FePPIXH)_2(\mu\text{-}O)(PQH_2)]$	464.6		295.8		776.9
$[(FePPIXH)_2(\mu\text{-}O)(AQH_2)]$	331.1		173.3		515.2
$[(FePPIXH)_2(\mu\text{-}O)(DAQH_2)]$	305.8		144.4		428.2
$[(FePPIXH)_2(\mu\text{-}O)(TQH_2)]$	416.3		204.2		631.9



18. Comparison of torsion angles for quinine and quinidine

Definition of torsion angles (generic structure):



molecule	C1-C2-C3-C4 /°	C2-C3-C4-N5 /°	C6-C7-O8-C9 /°
QN, X-ray #1[a]	-77.3	156.1	-178.4
QN, X-ray #2	-75.9	158.9	179.4
QN, X-ray #3	-69.9	149.7	-174.5
QN1 (calc. min. in octanol)	-79.5	150.5	179.9
QN_3 (calc. min. in water)	-110.2	62.8	-179.4
QD, X-ray	79.0	-161.8	-1.6
QD_83 (calc. min. in octanol and water)	103.2	-68.5	179.1

[a]Crystal structure includes three independent molecules.