C	3.262801	-0.011721	0.675254
C	2.318642	0.027485	1.744926
N	1.033386	0.024838	1.549040
C	0.276537	0.257693	2.799119
C	1.276600	-0.158869	3.890674
C	2.644333	0.132235	3.222371
C	-1.042476	-0.494870	2.617958
N	-1.414734	-0.288256	1.197882
C	-2.701973	-0.186700	1.032903
C	-3.434848	-0.265802	2.357651
C	-2.297446	-0.038851	3.384429
C	-3.306523	-0.051302	-0.251480
C	-2.602409	-0.037614	-1.423467
N	-1.222862	-0.143324	-1.537038
C	-0.846420	-0.054265	-2.830199
C	-2.040342	0.001404	-3.757416
C	-3.232745	0.121057	-2.792343
C	0.468770	-0.005836	-3.283318
C	-0.137816	1.772460	-0.023491
H	0.059834	1.334417	2.850550
H	-0.856104	-1.569639	2.759936
H	-2.220634	1.027604	3.624243
H	-2.448970	-0.587654	4.316664
H	-4.239215	0.473018	2.424083
H	-3.897766	-1.256308	2.465742
H	4.585525	0.877539	-1.690001
H	4.515832	-0.877059	-1.793241
H	3.122398	1.090849	-3.559746
H	3.201844	-0.652079	-3.781601
H	-4.384753	0.053383	-0.299282
H	4.317958	-0.002658	0.925357
H	0.618879	0.058461	-4.355774
H	1.136431	0.386209	4.826719
H	1.181133	-1.230663	4.100747
H	-3.718355	1.100493	-2.863944
H	-4.006210	-0.633338	-2.965428
H	2.997514	1.149161	3.441516
H	3.439689	-0.556449	3.523574
H	-1.956493	0.846920	-4.447109
H	-2.084409	-0.905859	-4.372164
H	0.988531	-2.527717	-0.450150
H	-0.556466	-2.622841	-0.525680
N	-0.233420	2.934486	-0.003555

H_2O-[Co^{III}-corrin]-Me

E= -2454.703789

Co	0.032829	-0.001595	-0.075673
N	-1.387020	1.234613	-0.162866
N	-1.381636	-1.239019	0.096112
N	1.342285	-1.428811	0.039921
N	1.343744	1.427970	-0.023135
C	-2.740704	0.672640	-0.366261
H	-2.867429	0.490310	-1.444448
C	1.045047	-2.780822	-0.058448

C	-1.407205	2.534387	-0.095556
C	2.678622	-1.241265	0.036986
C	-3.671852	1.801585	0.108557
C	2.318854	-3.599425	-0.149545
C	-2.824882	3.071878	-0.153304
C	3.433205	-2.553967	0.034111
C	-0.213803	-3.317128	-0.083963
C	-0.215409	3.316323	-0.014326
C	3.312247	-0.000811	0.033917
C	-3.676690	-1.805572	-0.081028
C	-2.819147	-3.076637	0.141707
C	2.316924	3.607867	0.033764
C	3.436142	2.551421	0.010869
C	-2.726273	-0.676230	0.354466
H	-2.802632	-0.490661	1.435951
C	-1.404723	-2.538519	0.030439
C	1.044688	2.781838	-0.010309
C	2.679212	1.239834	0.007048
H	-3.920594	-1.700899	-1.144790
H	-4.612948	-1.818168	0.481867
H	-3.017302	-3.873234	-0.582228
H	-2.974820	-3.506089	1.140971
H	2.363205	4.289802	-0.821345
H	2.345584	4.229424	0.935308
H	4.068239	2.625805	-0.881281
H	4.105576	2.614421	0.875666
H	-0.311870	-4.393931	-0.170752
H	-0.314892	4.395909	0.022080
H	4.397398	-0.000845	0.041840
H	-4.631439	1.812637	-0.413533
H	-3.869185	1.697469	1.181987
H	2.378567	-4.092176	-1.126567
H	2.340280	-4.389739	0.606904
H	-3.017474	3.492914	-1.149795
H	-2.997580	3.873820	-0.571151
H	4.182703	-2.575150	-0.763231
H	3.974885	-2.680937	0.979396
C	0.119065	-0.125727	-2.017727
H	-0.316252	-1.074734	-2.342672
H	-0.424372	0.706846	-2.472531
H	1.169277	-0.079945	-2.319543
O	-0.053630	0.124778	2.240850
H	0.316763	0.946613	2.600797
H	0.457463	-0.587922	2.656563

H_2O-[Co^{III}-corrin]-Et

E= -2494.014239

C	2.592970	-1.397462	-0.135840
N	1.247195	-1.484661	-0.095371
C	0.846268	-2.809663	-0.174836
C	2.051808	-3.728068	-0.255762
C	3.248132	-2.761675	-0.189918
Co	0.047887	0.034229	0.016569
O	-0.071748	-0.032185	-2.357354

C	-0.451453	-3.244418	-0.207681
C	-1.582540	-2.378373	-0.108072
N	-1.467287	-1.090445	0.043128
C	-2.784403	-0.435338	0.207519
C	-3.776628	-1.469178	-0.354301
C	-3.036221	-2.810435	-0.129239
C	-2.638710	0.930747	-0.462113
N	-1.265465	1.380582	-0.141074
C	-1.190958	2.677933	-0.064448
C	-2.557509	3.323850	-0.200655
C	-3.514461	2.118058	-0.025442
C	0.054372	3.361869	0.071069
C	1.268499	2.731746	0.026485
N	1.461008	1.363284	-0.100809
C	2.779627	1.076425	-0.118215
C	3.630454	2.328984	-0.108808
C	2.601489	3.448557	0.127516
C	3.317921	-0.207990	-0.139091
C	0.206118	0.149386	1.981566
H	-2.950312	-0.281179	1.284442
H	-2.687261	0.786247	-1.551363
H	-3.793381	2.010802	1.029498
H	-4.431749	2.212395	-0.611315
H	-2.713825	4.120660	0.533365
H	-2.653642	3.781473	-1.194933
H	2.044694	-4.448107	0.568770
H	2.034976	-4.310321	-1.183438
H	3.867894	-2.918450	0.700344
H	3.915277	-2.842678	-1.054827
H	0.038788	4.441179	0.178335
H	-0.632459	-4.309787	-0.303003
H	4.399857	-0.289820	-0.159156
H	-4.753172	-1.433101	0.134200
H	-3.926683	-1.299408	-1.427026
H	2.709844	3.896929	1.121837
H	2.674554	4.263669	-0.598620
H	-3.297798	-3.264257	0.836728
H	-3.238924	-3.560334	-0.900117
H	4.401865	2.277316	0.665749
H	4.152376	2.437595	-1.067550
H	-0.233887	1.115097	2.251954
C	-0.381133	-0.973809	2.822805
H	1.286462	0.208422	2.149174
H	0.214718	-0.876328	-2.740704
H	0.504167	0.636751	-2.760362
H	-0.106508	-0.819556	3.876650
H	-1.474616	-1.011496	2.783708
H	-0.000236	-1.958616	2.532767

H_2O-[Co^{III}-corrin]-iProp

E= -2533.321868

C	2.274375	3.651195	-0.149403
C	1.018248	2.802317	-0.191361
N	1.335929	1.455365	-0.159066

C	2.677182	1.292514	-0.155618
C	3.410029	2.615829	-0.214733
C	-0.250511	3.319975	-0.247212
C	-1.420648	2.511687	-0.319507
N	-1.373206	1.209435	-0.261543
C	-2.694050	0.614705	-0.567096
C	-3.680412	1.739686	-0.217647
C	-2.842454	3.009122	-0.512815
C	-2.718505	-0.732760	0.153092
N	-1.345335	-1.262218	-0.000622
C	-1.337462	-2.554980	-0.170881
C	-2.742255	-3.126061	-0.186111
C	-3.614568	-1.863109	-0.387744
Co	0.057682	0.000592	-0.002620
N	1.392665	-1.398410	-0.117720
C	1.119345	-2.748084	-0.255020
C	2.404202	-3.543993	-0.384778
C	3.503918	-2.479660	-0.225841
C	2.723677	-1.185194	-0.146303
C	-0.131862	-3.305574	-0.295694
C	3.333701	0.066641	-0.124011
O	0.122623	-0.137069	-2.497808
H	-0.072468	0.651355	-3.027120
C	0.226592	0.068500	2.004248
C	-0.156336	-1.228616	2.711513
C	-0.468776	1.258359	2.655263
H	-2.901938	-0.563146	1.224455
H	-2.718011	0.411119	-1.649930
H	-3.936426	1.697536	0.847535
H	-4.608073	1.694499	-0.793270
H	-3.076000	3.853266	0.143596
H	-2.981575	3.359769	-1.545022
H	2.456630	-4.330363	0.374634
H	2.448824	-4.040772	-1.360348
H	4.094388	-2.619920	0.687379
H	4.212013	-2.462168	-1.060522
H	-0.366506	4.398411	-0.262530
H	-0.210795	-4.379765	-0.424914
H	4.418684	0.087356	-0.132677
H	-4.578348	-1.923275	0.123022
H	-3.809510	-1.708560	-1.455933
H	2.302403	4.236245	0.776834
H	2.297701	4.366606	-0.977214
H	-2.947554	-3.614766	0.776295
H	-2.879150	-3.884276	-0.963436
H	4.124257	2.705171	0.610437
H	3.989543	2.686187	-1.142671
H	1.311605	0.201080	2.082504
H	0.167245	-1.168590	3.761582
H	-1.240443	-1.388657	2.727235
H	0.312793	-2.115506	2.279338
H	-0.184830	1.299850	3.717801
H	-0.194603	2.217157	2.210005
H	-1.560930	1.166762	2.624988
H	-0.278269	-0.876239	-2.980233

H_2O-[Co^{III}-corrin]-tBut

E = -2572.626762

C	-2.520761	-3.442947	-0.244601
C	-1.194678	-2.709767	-0.246298
N	-1.401664	-1.335845	-0.267529
C	-2.713082	-1.072824	-0.454143
C	-3.528235	-2.339691	-0.608401
C	0.026380	-3.327082	-0.248813
C	1.254711	-2.608848	-0.346549
N	1.305144	-1.309769	-0.275961
C	2.650857	-0.812392	-0.647566
C	3.567655	-2.008452	-0.347465
C	2.624596	-3.210893	-0.601617
C	2.814302	0.522801	0.073020
N	1.478423	1.159344	-0.005715
C	1.569416	2.446734	-0.183601
C	3.011688	2.905884	-0.263237
C	3.767460	1.579904	-0.514545
Co	-0.024971	0.006371	0.010879
N	-1.243797	1.506545	-0.195727
C	-0.862929	2.840449	-0.258301
C	-2.080791	3.738143	-0.354592
C	-3.228557	2.749183	-0.616347
C	-2.569876	1.398379	-0.426663
C	0.426193	3.296422	-0.267020
C	-3.270674	0.199656	-0.524611
C	-0.137252	-0.066313	2.089662
C	-1.596843	-0.251015	2.517288
C	0.689163	-1.235785	2.626464
C	0.383961	1.245885	2.684224
O	0.209921	0.137411	-2.647696
H	3.040399	0.338471	1.133664
H	2.625086	-0.607234	-1.727574
H	3.882470	-1.991703	0.702665
H	4.464389	-2.029457	-0.971416
H	2.822569	-4.071618	0.045250
H	2.688818	-3.568319	-1.638668
H	-2.217630	4.278084	0.589939
H	-1.969168	4.492163	-1.138974
H	-4.075635	2.874306	0.065797
H	-3.628537	2.833946	-1.634043
H	0.058602	-4.411325	-0.245084
H	0.591397	4.364596	-0.359780
H	-4.340222	0.263777	-0.697036
H	4.759209	1.559558	-0.056748
H	3.888187	1.416280	-1.591798
H	-2.716871	-3.847169	0.756442
H	-2.524078	-4.287892	-0.938306
H	3.300955	3.366762	0.691620
H	3.170554	3.658152	-1.041978
H	-4.416047	-2.325832	0.030937
H	-3.882804	-2.432539	-1.642837
H	0.204008	1.231827	3.769892
H	1.460199	1.377795	2.545243
H	-0.125380	2.128213	2.287942

H	0.579537	-1.265496	3.721779
H	0.348583	-2.201823	2.244368
H	1.757841	-1.135329	2.416500
H	-1.647752	-0.182883	3.614493
H	-2.261951	0.519342	2.120842
H	-1.996484	-1.230334	2.243617
H	-0.001888	0.976580	-3.085032
H	-0.306460	-0.528720	-3.127098