

Histone Deacetylase 8:

Characterization of Physiological Divalent Metal Catalysis

Michael R. Nechay,¹ Nathan M. Gallup,¹ Amanda Morgenstern,² Quentin A. Smith,¹

Mark E. Eberhart,² Anastassia N. Alexandrova^{1,3,*}

¹*Department of Chemistry and Biochemistry, University of California, Los Angeles, Los Angeles, CA, 90095*

²*Molecular Theory Group, Colorado School of Mines, Golden, Colorado 80401*

³*California NanoSystems Institute, Los Angeles, CA, 90095*

*Electronic mail: ana@chem.ucla.edu

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Supporting Information

I. XYZ coordinates of equilibrated reactant states (lowest QM-energy structures obtained from QM/DMD trajectories)

Co²⁺

H	-0.7091596	-4.8591872	3.2845582
C	-0.5230898	-4.5844874	2.2532488
C	0.7945745	-3.9053774	2.0520402
N	1.3776761	-3.8204424	0.7997691
C	1.6612764	-3.2392696	2.9064872
C	2.5356204	-3.1334002	0.9262125
N	2.7348784	-2.7560500	2.1873146
H	0.9499303	-4.1016441	-0.1416903
H	-0.5727643	-5.5101475	1.6509742
H	-1.3627817	-3.9441726	1.9184819
H	1.5855286	-3.1009981	3.9860068
H	3.2222642	-2.9556115	0.0980455
H	2.3080388	-6.7834862	5.7034268
C	3.2847382	-6.4432764	6.0167766
C	4.0129441	-5.6464905	4.9789997
N	4.1121425	-6.0802458	3.6764314
C	4.7820615	-4.4913550	5.0406013
C	4.9096456	-5.2157983	3.0054639
N	5.3479505	-4.2338354	3.8015781
H	3.6448620	-6.9788532	3.3442653
H	3.1796968	-5.8567207	6.9454451
H	3.8541723	-7.3651506	6.2462303
H	4.9400029	-3.8383361	5.8997841
H	5.1105963	-5.3330057	1.9408551

H	-0.5415696	-3.3970680	-4.4447576
C	-0.1808598	-4.1972076	-3.8231578
C	0.5305633	-3.7297752	-2.5550814
O	1.3658347	-2.7726287	-2.6485193
O	0.2698709	-4.4027967	-1.5147827
H	0.5437115	-4.7693030	-4.4337465
H	-1.0119751	-4.8751872	-3.5725673
H	1.8977490	-0.1090000	-5.5861568
C	2.6112586	0.2730698	-4.8524872
O	3.4447946	1.1197679	-5.1907918
N	2.4974311	-0.1891340	-3.5764710
C	3.5004374	0.2135437	-2.5807378
C	4.8788034	-0.3893573	-2.9806205
O	4.9471635	-1.3649877	-3.7455573
C	2.9666251	-0.1857498	-1.1755791
C	3.9335948	-0.0515756	-0.0033090
O	3.7090033	0.7109920	0.9705822
O	4.9852283	-0.7929508	-0.0083162
H	1.8975082	-1.0032266	-3.3610853
H	3.6104940	1.3109298	-2.6278894
H	2.6390872	-1.2400603	-1.2215028
H	2.0774910	0.4294579	-0.9679962
H	8.0447554	0.1959598	-2.2970188
N	5.9897750	0.1940099	-2.4887833
O	8.3515790	-2.5133408	-3.1035625
C	7.5209081	-1.8374516	-2.4794493
H	5.9608254	0.9562405	-1.7745632
C	7.2898360	-0.3556098	-2.8349784
H	7.4876863	-0.2656621	-3.9170205
N	6.8550981	-2.2767107	-1.3855164
C	7.0865682	-3.5834286	-0.8188773
C	6.0267825	-4.5899866	-1.3241768
O	4.9461189	-4.2209592	-1.8032002
C	7.0932433	-3.4823466	0.7333446
C	8.0893554	-2.4721731	1.2327524
N	7.7519532	-1.1566601	1.5473461
C	9.4552115	-2.6189205	1.3992840
C	8.8784055	-0.5328346	1.8862116
N	9.9300542	-1.3869398	1.8115783
H	6.0975370	-1.6987887	-0.9752488
H	10.8991805	-1.1572599	2.0249494
H	8.0729272	-3.9235021	-1.1827692
H	7.3174840	-4.4725024	1.1638384
H	6.0937927	-3.1780094	1.0803466
H	10.1140604	-3.4738679	1.2562796
H	8.9444511	0.5143238	2.1792408
H	5.9194366	-7.8607456	-1.7443490
N	6.3393584	-5.9093764	-1.2496469
O	4.2034172	-6.9189760	0.3874693
C	4.1340423	-6.9552884	-0.8427208
H	7.2014962	-6.2080203	-0.7987956
C	5.3901570	-6.9192562	-1.7193990

H	5.1076457	-6.6792173	-2.7605016
N	2.9766983	-7.0334977	-1.5479761
C	1.7013021	-7.3000387	-0.8862991
C	1.6641628	-8.8022081	-0.5440940
O	1.2961524	-9.6536700	-1.3722133
H	3.0220609	-7.0032906	-2.5704433
H	0.8815326	-7.0283623	-1.5645196
H	1.6404394	-6.6687850	0.0153136
H	1.6063490	-10.6777240	1.8256590
N	2.1782282	-9.0675794	0.6716102
C	2.4445686	-10.3905942	1.2221494
C	3.7291212	-10.3794195	2.0633152
C	3.7180025	-9.3869325	3.2586587
O	4.4814795	-9.6039148	4.2197504
O	2.9309143	-8.3732425	3.1232629
H	2.4287540	-8.3193951	1.3407244
H	2.5111270	-11.1024046	0.3804751
H	4.5814027	-10.0872801	1.4184993
H	3.9439331	-11.3927444	2.4456046
H	1.7735990	-6.6652562	-6.1462066
C	2.0946388	-7.1276260	-5.2265470
O	3.1891161	-6.4140984	-4.6146198
H	4.0067446	-6.6788004	-5.0747467
H	2.3618081	-8.1833115	-5.4123312
H	1.2594966	-7.1056597	-4.5087185
H	4.6767974	-4.3759876	-7.9091156
C	5.2893070	-3.9249578	-7.1434560
O	4.8171485	-3.0619135	-6.3955753
H	7.0954860	-4.2313176	-6.2052966
N	6.5004164	-4.4741174	-7.0133760
H	6.8211599	-5.2089808	-7.6409324
H	7.4986058	4.4701774	-0.2574698
C	7.7040756	3.7413378	0.5462596
C	6.8586584	2.4624951	0.3520638
O	6.3122645	2.2795463	-0.7596784
O	6.8058312	1.6632952	1.3651719
H	8.7761305	3.4736152	0.5357913
H	7.4818988	4.1992997	1.5234162
H	0.7360996	2.7154584	2.9971984
C	1.6626890	3.1528582	3.3529482
O	1.6498298	4.0052759	4.2541664
H	4.2115176	4.2583576	2.7577484
N	2.7809913	2.7162755	2.7451105
C	4.0717578	3.2580982	3.1365382
H	2.7708207	1.9917231	2.0141178
H	4.8608334	2.6043533	2.7386542
H	4.1527528	3.2922787	4.2363838
H	8.8453850	7.5318458	4.9068372
C	9.5478446	6.7386462	5.0986072
C	8.8117203	5.4345447	5.2932816
C	8.5378925	4.5851420	4.2036962
C	8.3035501	5.0688763	6.5559349

C	7.7640546	3.4261996	4.3467065
C	7.5322994	3.9141421	6.7238502
C	7.2442616	3.0931070	5.6155084
O	6.4688775	1.9998976	5.8143086
H	6.3002941	1.5463119	4.9398150
H	10.2411394	6.6910747	4.2403996
H	10.1297758	7.0176578	5.9951012
H	8.9308306	4.8432962	3.2128133
H	8.5054429	5.7080056	7.4246242
H	7.5399214	2.7869813	3.4823613
H	7.1297920	3.6360326	7.7037094
H	8.8968350	-2.3677186	6.2765764
C	7.8532056	-2.1791488	6.4094064
O	5.7706477	0.4380241	3.7987952
C	5.1618012	-0.3305869	4.6181889
C	3.6631903	-0.2771412	4.7489046
N	5.8598925	-1.1101805	5.4435475
H	5.3807472	-1.6601134	6.1700495
C	7.3143136	-1.2611506	5.3167256
H	3.2304088	-0.2530273	3.7382651
H	3.2613187	-1.1314456	5.3148710
H	3.3933252	0.6649017	5.2591573
H	7.7790245	-0.2612116	5.3666064
H	7.5262930	-1.6706496	4.3121614
H	7.7020622	-1.7366399	7.4090854
H	7.3354413	-3.1533360	6.3808491
O	5.1300828	-1.8604183	2.5710437
H	4.1381604	-2.1285322	2.4485804
H	5.4820274	-2.6601844	3.0787317
Co	5.9252621	-0.1529061	1.7017240
K	3.6160630	-3.5281105	-3.9350245
C	5.4175302	-3.1939191	8.7233546
O	4.9405269	-2.5469627	7.8085429
N	5.3349970	-2.8549984	10.0039944
H	5.7378873	-3.4495743	10.7282207
H	5.9559966	-4.1099976	8.5299952
H	4.8371564	-2.0093200	10.2830672

Fe²⁺

H	-5.4987569	-2.4957286	2.0776899
C	-5.3126870	-2.2210288	1.0463805
C	-3.9817093	-1.5684677	0.8543183
N	-3.3973797	-1.4599479	-0.3957346
C	-3.0992219	-0.9515022	1.7283794
C	-2.2220296	-0.8064257	-0.2482908
N	-2.0145475	-0.4738033	1.0240591
H	-3.8283951	-1.7176546	-1.3421310
H	-5.3822205	-3.1423844	0.4393702
H	-6.1390907	-1.5612317	0.7167756
H	-3.1718434	-0.8450081	2.8116908
H	-1.5311661	-0.6188362	-1.0707971
H	-2.4815585	-4.4200276	4.4965585
C	-1.5048591	-4.0798178	4.8099083
C	-0.7511629	-3.3090751	3.7715711
N	-0.6370546	-3.7608636	2.4768435
C	0.0423137	-2.1705483	3.8343198
C	0.1923834	-2.9230022	1.8108683
N	0.6377514	-1.9415011	2.6037822
H	-1.1185744	-4.6532656	2.1475392
H	-1.6147691	-3.4757816	5.7269351
H	-0.9458787	-5.0014764	5.0654798
H	0.1967359	-1.5087980	4.6874905
H	0.4085861	-3.0559501	0.7509878
H	-5.3311669	-1.0336095	-5.6516259
C	-4.9704571	-1.8337490	-5.0300261
C	-4.2548283	-1.3605252	-3.7656554
O	-3.4102585	-0.4128683	-3.8718860
O	-4.5217050	-2.0154548	-2.7157908
H	-4.2488883	-2.4086116	-5.6412722
H	-5.8028626	-2.5083879	-4.7745487
H	-2.8918483	2.2544586	-6.7930251
C	-2.1783387	2.6365284	-6.0593555
O	-1.3478883	3.4878109	-6.3936366
N	-2.2898685	2.1649321	-4.7866500
C	-1.2902902	2.5594201	-3.7831207
C	0.0913407	1.9680573	-4.1873461
O	0.1640800	0.9957288	-4.9565506
C	-1.8276505	2.1314933	-2.3878143
C	-0.8862468	2.2693676	-1.1952416
O	-1.1816385	2.9650715	-0.1914639
O	0.2128391	1.5963873	-1.2158395
H	-2.8905663	1.3495257	-4.5777511
H	-1.1865713	3.6581748	-3.8121425
H	-2.1334543	1.0711421	-2.4522406
H	-2.7339411	2.7222969	-2.1827764
H	3.2551582	2.5594184	-3.5038871
N	1.1997739	2.5551120	-3.6942408
O	3.5620873	-0.1474078	-4.3226539
C	2.7330301	0.5256972	-3.6930664

H	1.1690720	3.3048533	-2.9668357
C	2.5002387	2.0078488	-4.0418467
H	2.6966565	2.1011054	-5.1239301
N	2.0696349	0.0806623	-2.5999327
C	2.3084696	-1.2282938	-2.0429189
C	1.2422128	-2.2299930	-2.5365573
O	0.1584373	-1.8600022	-3.0079085
C	2.3432497	-1.1408491	-0.4902490
C	3.3358758	-0.1204790	-0.0089677
N	2.9875048	1.2033839	0.2512541
C	4.7008749	-0.2555266	0.1732278
C	4.1087397	1.8454917	0.5742651
N	5.1661535	0.9930903	0.5443456
H	1.3181619	0.6607568	-2.1821457
H	6.1317457	1.2344399	0.7604643
H	3.2887871	-1.5654404	-2.4251704
H	2.5868711	-2.1312651	-0.0714986
H	1.3465194	-0.8516714	-0.1221051
H	5.3653305	-1.1115704	0.0670575
H	4.1664332	2.9037213	0.8277047
H	1.1298394	-5.4972870	-2.9512173
N	1.5522130	-3.5490834	-2.4595480
O	-0.5822603	-4.5616830	-0.8175585
C	-0.6535675	-4.5918320	-2.0477791
H	2.4195080	-3.8488491	-2.0194223
C	0.6005597	-4.5557976	-2.9262673
H	0.3161651	-4.3165613	-3.9671308
N	-1.8123977	-4.6636278	-2.7512714
C	-3.0864054	-4.9313761	-2.0875099
C	-3.1218848	-6.4340339	-1.7471423
O	-3.4872517	-7.2842177	-2.5776861
H	-1.7683264	-4.6345763	-3.7737843
H	-3.9074361	-4.6604679	-2.7646066
H	-3.1465029	-4.3006315	-1.1855458
H	-3.1832482	-8.3142654	0.6187907
N	-2.6099852	-6.7019229	-0.5308313
C	-2.3450287	-8.0271356	0.0152810
C	-1.0579268	-8.0268395	0.8514658
C	-1.0654004	-7.0465325	2.0557514
O	-0.2991810	-7.2708771	3.0128402
O	-1.8535956	-6.0321546	1.9308706
H	-2.3584449	-5.9551833	0.1385721
H	-2.2838468	-8.7352972	-0.8299736
H	-0.2073175	-7.7295654	0.2067874
H	-0.8437701	-9.0445619	1.2223550
H	-3.0159983	-4.3017976	-7.3530749
C	-2.6949585	-4.7641674	-6.4334153
O	-1.5966740	-4.0546751	-5.8239518
H	-0.7807136	-4.3245405	-6.2839970
H	-2.4326241	-5.8211965	-6.6184357
H	-3.5290620	-4.7382811	-5.7144836
H	-0.1127999	-2.0125290	-9.1159839

C	0.4997098	-1.5614992	-8.3503243
O	0.0277744	-0.6975110	-7.6035686
H	2.3058887	-1.8678590	-7.4121649
N	1.7108191	-2.1106589	-8.2202443
H	2.0307539	-2.8464974	-8.8471358
H	2.7090085	6.8336360	-1.4643381
C	2.9144784	6.1047964	-0.6606087
C	2.0656698	4.8274887	-0.8273554
O	1.5195791	4.6199023	-1.9363252
O	2.0105401	4.0539196	0.2032743
H	3.9858023	5.8333349	-0.6820750
H	2.7088085	6.5714234	0.3160283
H	-4.0534977	5.0789170	1.7903300
C	-3.1269082	5.5163168	2.1460798
O	-3.1391597	6.3755022	3.0404493
H	-0.5780796	6.6218162	1.5508801
N	-2.0080619	5.0757568	1.5404874
C	-0.7178395	5.6215568	1.9296699
H	-2.0212765	4.3356844	0.8247482
H	0.0729925	4.9719754	1.5277954
H	-0.6328364	5.6551212	3.0293021
H	4.0557878	9.8953044	3.6999689
C	4.7582474	9.1021048	3.8917389
C	4.0225921	7.7973114	4.0827388
C	3.7503222	6.9505908	2.9907208
C	3.5132494	7.4283845	5.3438361
C	2.9754824	5.7918714	3.1292810
C	2.7410412	6.2735599	5.5075508
C	2.4538361	5.4567868	4.3962697
O	1.6761425	4.3629829	4.5908215
H	1.5105232	3.9132680	3.7160916
H	5.4530260	9.0561536	3.0345560
H	5.3388748	9.3797775	4.7894889
H	4.1452614	7.2105428	2.0011090
H	3.7150123	8.0648158	6.2144851
H	2.7523745	5.1552562	2.2623073
H	2.3375780	5.9926925	6.4861139
H	4.1072377	-0.0042600	5.0697081
C	3.0636083	0.1843098	5.2025381
O	0.9720216	2.7834962	2.5837898
C	0.3625311	2.0182340	3.4146814
C	-1.1344755	2.0710338	3.5378941
N	1.0676194	1.2573000	4.2468849
H	0.5918314	0.7079927	4.9771558
C	2.5221207	1.1035882	4.1117041
H	-1.5618823	2.0769413	2.5241235
H	-1.5359994	1.2252825	4.1163946
H	-1.4089107	3.0213340	4.0298944
H	2.9880069	2.1029297	4.1590123
H	2.7257621	0.6931759	3.1054297
H	2.9127251	0.6254501	6.2027870
H	2.5466621	-0.7901636	5.1722253

O	0.3682426	0.4359319	1.4122288
H	-0.6234963	0.1528227	1.3093235
H	0.7445611	-0.3709078	1.8904265
Fe	1.1142851	2.1944183	0.5542483
K	-1.1614471	-1.1735171	-5.1459663
C	0.6280834	-0.8304768	7.5166628
O	0.1509296	-0.1835041	6.6016746
N	0.5453997	-0.4915398	8.7971261
H	0.9482900	-1.0861157	9.5213524
H	1.1663994	-1.7465391	7.3231269
H	0.0482839	0.3546028	9.0759754

Mg²⁺

H	-0.7091598	-4.8591886	3.2845591
C	-0.5230899	-4.5844887	2.2532494
C	0.7996937	-3.9194359	2.0562258
N	1.3793377	-3.8165491	0.8039423
C	1.6767061	-3.2842015	2.9223606
C	2.5473309	-3.1486806	0.9411060
N	2.7539705	-2.8018177	2.2099793
H	0.9486331	-4.0854157	-0.1399161
H	-0.5832249	-5.5084942	1.6491831
H	-1.3567542	-3.9351234	1.9209194
H	1.6064128	-3.1682401	4.0048652
H	3.2349278	-2.9626102	0.1153722
H	2.3080394	-6.7834881	5.7034284
C	3.2847391	-6.4432782	6.0167783
C	4.0261536	-5.6574718	4.9812708
N	4.1359438	-6.0962300	3.6813805
C	4.8078093	-4.5112808	5.0495430
C	4.9518565	-5.2428746	3.0179114
N	5.3917690	-4.2641663	3.8172049
H	3.6590092	-6.9879770	3.3457051
H	3.1775893	-5.8501562	6.9411762
H	3.8484450	-7.3661876	6.2568427
H	4.9603943	-3.8554099	5.9077753
H	5.1638835	-5.3641848	1.9557877
H	-0.5415698	-3.3970690	-4.4447588
C	-0.1808599	-4.1972088	-3.8231589
C	0.5270477	-3.7235428	-2.5546224
O	1.3614563	-2.7657130	-2.6503794
O	0.2636697	-4.3903103	-1.5110574
H	0.5457080	-4.7684382	-4.4320067
H	-1.0114105	-4.8757782	-3.5724025
H	1.8977495	-0.1090000	-5.5861584
C	2.6112593	0.2730699	-4.8524886
O	3.4468844	1.1165397	-5.1940085
N	2.4955955	-0.1821692	-3.5731699
C	3.4992329	0.2220316	-2.5763830
C	4.8772263	-0.3864772	-2.9748334
O	4.9411125	-1.3648330	-3.7367385
C	2.9586278	-0.1597504	-1.1665150
C	3.9391936	-0.0868677	0.0000708
O	3.7024459	0.6023205	1.0381860
O	5.0045422	-0.7907406	-0.0555772
H	1.8960338	-0.9961319	-3.3566713
H	3.6145066	1.3184033	-2.6331146
H	2.5929823	-1.2024702	-1.2142783
H	2.0932292	0.4848891	-0.9485082
H	8.0447577	0.1959599	-2.2970194
N	5.9909946	0.2005835	-2.4938995
O	8.3611147	-2.5058774	-3.1088828
C	7.5244693	-1.8376010	-2.4833354

H	5.9613514	0.9579183	-1.7753966
C	7.2898380	-0.3556099	-2.8349792
H	7.4905900	-0.2648610	-3.9166417
N	6.8568425	-2.2831933	-1.3951392
C	7.0961703	-3.5866930	-0.8255053
C	6.0299381	-4.5928127	-1.3174312
O	4.9448244	-4.2239616	-1.7869065
C	7.1254801	-3.4782711	0.7270167
C	8.1167255	-2.4501649	1.2028256
N	7.7620990	-1.1389838	1.5124695
C	9.4884089	-2.5766476	1.3416575
C	8.8851191	-0.4974946	1.8233467
N	9.9516694	-1.3338084	1.7347012
H	6.0980417	-1.7052020	-0.9841279
H	10.9210442	-1.0865092	1.9256528
H	8.0780358	-3.9279305	-1.2004601
H	7.3681208	-4.4639190	1.1585193
H	6.1275969	-3.1853969	1.0889045
H	10.1583994	-3.4216981	1.1914998
H	8.9436924	0.5536708	2.1058863
H	5.9194383	-7.8607478	-1.7443495
N	6.3412930	-5.9126056	-1.2472225
O	4.2005551	-6.9208979	0.3863183
C	4.1333179	-6.9558821	-0.8439214
H	7.2089555	-6.2137020	-0.8086808
C	5.3901585	-6.9192581	-1.7193995
H	5.1086642	-6.6778248	-2.7605385
N	2.9770825	-7.0350284	-1.5513251
C	1.7007800	-7.3040520	-0.8925559
C	1.6664842	-8.8059035	-0.5481372
O	1.3034486	-9.6594785	-1.3762825
H	3.0244146	-7.0035508	-2.5736649
H	0.8821675	-7.0365446	-1.5739204
H	1.6348536	-6.6715229	0.0078134
H	1.6063495	-10.6777270	1.8256595
N	2.1766927	-9.0685562	0.6698460
C	2.4445693	-10.3905971	1.2221497
C	3.7280220	-10.3774094	2.0651681
C	3.7109174	-9.3884819	3.2629681
O	4.4684101	-9.6084355	4.2282666
O	2.9263047	-8.3732383	3.1249266
H	2.4254663	-8.3187437	1.3376480
H	2.5129994	-11.1032696	0.3814042
H	4.5800747	-10.0796406	1.4226502
H	3.9459747	-11.3910247	2.4448508
H	1.7735995	-6.6652581	-6.1462083
C	2.0946394	-7.1276280	-5.2265485
O	3.1890584	-6.4142197	-4.6145358
H	4.0063891	-6.6767520	-5.0765048
H	2.3616188	-8.1833775	-5.4123464
H	1.2594751	-7.1055461	-4.5087580
H	4.6767987	-4.3759888	-7.9091178

C	5.2893085	-3.9249589	-7.1434580
O	4.8166330	-3.0631555	-6.3944426
H	7.0954880	-4.2313188	-6.2052983
N	6.5004182	-4.4741187	-7.0133780
H	6.8220257	-5.2076529	-7.6420349
H	7.4986079	4.4701787	-0.2574699
C	7.7040778	3.7413389	0.5462598
C	6.8399023	2.4724568	0.3680613
O	6.2914267	2.2909716	-0.7447294
O	6.7624211	1.6826511	1.3838574
H	8.7727251	3.4601482	0.5239222
H	7.4994281	4.2050222	1.5243685
H	0.7360998	2.7154592	2.9971992
C	1.6626895	3.1528591	3.3529491
O	1.6507769	4.0148846	4.2443046
H	4.2115188	4.2583588	2.7577492
N	2.7822709	2.7096909	2.7493453
C	4.0717589	3.2580991	3.1365391
H	2.7723540	1.9660537	2.0368874
H	4.8643445	2.6134049	2.7321577
H	4.1603425	3.2903653	4.2357978
H	8.8453875	7.5318479	4.9068386
C	9.5478473	6.7386481	5.0986086
C	8.8082513	5.4360313	5.2930870
C	8.5190305	4.5955071	4.2005501
C	8.3101707	5.0645913	6.5580563
C	7.7390326	3.4404011	4.3425345
C	7.5329240	3.9136028	6.7251541
C	7.2293282	3.1023012	5.6139094
O	6.4481387	2.0127052	5.8140554
H	6.2709168	1.5596217	4.9421560
H	10.2405164	6.6906408	4.2398898
H	10.1301742	7.0171835	5.9949378
H	8.9046574	4.8579462	3.2078964
H	8.5251986	5.6959381	7.4292815
H	7.5039624	2.8078968	3.4756694
H	7.1383317	3.6310791	7.7069769
H	8.8968375	-2.3677193	6.2765782
C	7.8532078	-2.1791494	6.4094082
O	5.7112049	0.4284250	3.8283841
C	5.1292939	-0.3352688	4.6756722
C	3.6350297	-0.2894956	4.8443653
N	5.8503433	-1.1061343	5.4830668
H	5.3899965	-1.6564274	6.2245205
C	7.3029537	-1.2554197	5.3271595
H	3.1730374	-0.4013198	3.8512868
H	3.2648091	-1.0726130	5.5236278
H	3.3606876	0.7056581	5.2361318
H	7.7668745	-0.2550182	5.3747927
H	7.4974170	-1.6607741	4.3174704
H	7.7039636	-1.7428722	7.4121863
H	7.3363067	-3.1535886	6.3772318

O	5.1340204	-1.8936593	2.6004590
H	4.1450790	-2.1838020	2.4876891
H	5.4908064	-2.6903869	3.1074542
Mg	5.8151256	-0.1228802	1.7844067
K	3.6195172	-3.5286447	-3.9231256
C	5.4339985	-3.2089991	8.7399975
O	4.9405283	-2.5469634	7.8085451
N	5.3349985	-2.8549992	10.0039972
H	5.7378889	-3.4495753	10.7282237
H	5.9559983	-4.1099988	8.5299976
H	4.8299986	-2.0139994	10.3499971

Mn²⁺

H	-0.7091598	-4.8591886	3.2845591
C	-0.5230899	-4.5844887	2.2532494
C	0.8129946	-3.9367611	2.0648712
N	1.3914210	-3.8107703	0.8132734
C	1.7067507	-3.3417432	2.9435297
C	2.5730445	-3.1691934	0.9636290
N	2.7919920	-2.8604383	2.2405317
H	0.9566205	-4.0600312	-0.1331661
H	-0.5955474	-5.5046145	1.6447306
H	-1.3456927	-3.9200153	1.9240532
H	1.6426638	-3.2531886	4.0289272
H	3.2596175	-2.9685944	0.1404869
H	2.3080394	-6.7834881	5.7034284
C	3.2847391	-6.4432782	6.0167783
C	4.0461992	-5.6775230	4.9822394
N	4.1719022	-6.1301152	3.6887514
C	4.8414406	-4.5414220	5.0538906
C	5.0093303	-5.2939082	3.0309219
N	5.4493679	-4.3145879	3.8296145
H	3.6891334	-7.0195839	3.3545801
H	3.1728310	-5.8358629	6.9314265
H	3.8403348	-7.3654117	6.2786013
H	4.9864301	-3.8773818	5.9069595
H	5.2340360	-5.4242123	1.9725031
H	-0.5415698	-3.3970690	-4.4447588
C	-0.1808599	-4.1972088	-3.8231589
C	0.5284062	-3.7161534	-2.5580798
O	1.3701379	-2.7658314	-2.6668246
O	0.2592469	-4.3644279	-1.5050275
H	0.5445377	-4.7699742	-4.4316915
H	-1.0119826	-4.8737778	-3.5687789
H	1.8977495	-0.1090000	-5.5861584
C	2.6112593	0.2730699	-4.8524886
O	3.4418940	1.1246452	-5.1863311
N	2.4975879	-0.1984172	-3.5821918
C	3.4910707	0.2013357	-2.5778133
C	4.8755805	-0.3980989	-2.9710439
O	4.9486564	-1.3664681	-3.7443763
C	2.9288929	-0.1994865	-1.1848366
C	3.8909228	-0.1157372	-0.0085685
O	3.6603749	0.6216411	0.9914368
O	4.9340687	-0.8594218	-0.0375857
H	1.8967108	-1.0134736	-3.3725488
H	3.6028840	1.2988052	-2.6218119
H	2.5749553	-1.2450176	-1.2487962
H	2.0540658	0.4369115	-0.9802977
H	8.0447577	0.1959599	-2.2970194
N	5.9871593	0.1868509	-2.4788220
O	8.3690665	-2.5016032	-3.1097890
C	7.5288813	-1.8362478	-2.4863516

H	5.9551294	0.9357394	-1.7533254
C	7.2898380	-0.3556099	-2.8349792
H	7.4807714	-0.2581676	-3.9174749
N	6.8590979	-2.2856819	-1.3998813
C	7.1015334	-3.5929128	-0.8409334
C	6.0335367	-4.5950063	-1.3301525
O	4.9514752	-4.2266818	-1.8064264
C	7.1542177	-3.4987861	0.7112511
C	8.1621763	-2.4813497	1.1692477
N	7.8187737	-1.1664093	1.4697301
C	9.5350740	-2.6125265	1.2868935
C	8.9485711	-0.5257022	1.7586110
N	10.0095973	-1.3679235	1.6604860
H	6.0913431	-1.7188128	-0.9921669
H	10.9828065	-1.1238758	1.8363667
H	8.0789684	-3.9307658	-1.2300586
H	7.3976768	-4.4887456	1.1318355
H	6.1652673	-3.2010674	1.0939186
H	10.1993337	-3.4615088	1.1334108
H	9.0143251	0.5271757	2.0328342
H	5.9194383	-7.8607478	-1.7443495
N	6.3429747	-5.9142141	-1.2515684
O	4.2114608	-6.9225505	0.3919054
C	4.1372353	-6.9537088	-0.8381410
H	7.2071244	-6.2150023	-0.8060121
C	5.3901585	-6.9192581	-1.7193995
H	5.1051802	-6.6786500	-2.7596407
N	2.9763923	-7.0243516	-1.5386822
C	1.7031686	-7.2889748	-0.8719418
C	1.6638285	-8.7919869	-0.5333030
O	1.2901730	-9.6398232	-1.3625884
H	3.0176091	-6.9930210	-2.5612680
H	0.8811725	-7.0148334	-1.5466214
H	1.6470402	-6.6594667	0.0312576
H	1.6063495	-10.6777270	1.8256595
N	2.1824913	-9.0634540	0.6793098
C	2.4445693	-10.3905971	1.2221497
C	3.7312548	-10.3934166	2.0593822
C	3.7236931	-9.4159107	3.2662136
O	4.4827344	-9.6480056	4.2271698
O	2.9436649	-8.3954684	3.1392691
H	2.4377952	-8.3188545	1.3500416
H	2.5047698	-11.0973215	0.3756775
H	4.5823497	-10.0947542	1.4159651
H	3.9444172	-11.4121657	2.4279068
H	1.7735995	-6.6652581	-6.1462083
C	2.0946394	-7.1276280	-5.2265485
O	3.1854022	-6.4111987	-4.6114998
H	4.0051330	-6.6747652	-5.0684831
H	2.3660705	-8.1820227	-5.4134733
H	1.2580068	-7.1100315	-4.5103232
H	4.6767987	-4.3759888	-7.9091178

C	5.2893085	-3.9249589	-7.1434580
O	4.8174568	-3.0614241	-6.3960171
H	7.0954880	-4.2313188	-6.2052983
N	6.5004182	-4.4741187	-7.0133780
H	6.8209039	-5.2094473	-7.6405217
H	7.4986079	4.4701787	-0.2574699
C	7.7040778	3.7413389	0.5462598
C	6.8555446	2.4679137	0.3925851
O	6.2899876	2.2539781	-0.7033667
O	6.8156043	1.6979542	1.4291438
H	8.7740722	3.4650124	0.5199532
H	7.5072705	4.2100562	1.5239838
H	0.7360998	2.7154592	2.9971992
C	1.6626895	3.1528591	3.3529491
O	1.6505021	4.0128744	4.2464734
H	4.2115188	4.2583588	2.7577492
N	2.7818794	2.7107134	2.7485337
C	4.0717589	3.2580991	3.1365391
H	2.7696482	1.9727887	2.0306940
H	4.8632107	2.6108517	2.7342214
H	4.1588738	3.2897562	4.2357127
H	8.8453850	7.5318458	4.9068372
C	9.5478446	6.7386462	5.0986072
C	8.7945532	5.4458137	5.3085539
C	8.5238721	4.5763969	4.2342472
C	8.2529608	5.1207760	6.5685085
C	7.7189956	3.4392145	4.3870715
C	7.4507876	3.9891231	6.7462405
C	7.1636945	3.1494536	5.6514470
O	6.3537105	2.0836235	5.8636012
H	6.1830936	1.6073747	5.0021834
H	10.2330638	6.6770783	4.2351733
H	10.1378830	7.0195690	5.9891594
H	8.9421313	4.8014733	3.2455429
H	8.4507183	5.7756887	7.4262756
H	7.4995315	2.7876569	3.5306994
H	7.0207215	3.7447280	7.7232703
H	8.8968375	-2.3677193	6.2765782
C	7.8532078	-2.1791494	6.4094082
O	5.6473006	0.4567012	3.9092527
C	5.0912621	-0.3343747	4.7461423
C	3.5950561	-0.3453553	4.9050700
N	5.8375440	-1.1012255	5.5377008
H	5.3934070	-1.6766210	6.2702720
C	7.2914380	-1.2118556	5.3714315
H	3.1472883	-0.4819265	3.9081009
H	3.2497768	-1.1396019	5.5845118
H	3.2760015	0.6400461	5.2872420
H	7.7393295	-0.2068774	5.4668287
H	7.4914757	-1.5642942	4.3427506
H	7.7016837	-1.7880919	7.4305908
H	7.3365853	-3.1518926	6.3358884

O	5.1751821	-1.9426256	2.6749455
H	4.1891370	-2.2395245	2.5413785
H	5.5422665	-2.7552829	3.1566321
Mn	5.8542129	-0.1397228	1.7991159
K	3.6211494	-3.5297471	-3.9348052
C	5.4339985	-3.2089991	8.7399975
O	4.9274550	-2.5545853	7.8105118
N	5.3349985	-2.8549992	10.0039972
H	5.7511467	-3.4415819	10.7272350
H	5.9559983	-4.1099988	8.5299976
H	4.8299986	-2.0139994	10.3499971

Ni²⁺

H	-0.7091598	-4.8591886	3.2845591
C	-0.5230899	-4.5844887	2.2532494
C	0.7717022	-3.8720859	2.0467229
N	1.3712196	-3.8091790	0.8011368
C	1.5978601	-3.1484156	2.8924435
C	2.5021949	-3.0783703	0.9229440
N	2.6636872	-2.6528853	2.1735963
H	0.9651396	-4.1187760	-0.1414455
H	-0.5462149	-5.5157400	1.6579076
H	-1.3802518	-3.9715525	1.9107682
H	1.4989205	-2.9767447	3.9651475
H	3.1988020	-2.9096144	0.1013423
H	2.3080394	-6.7834881	5.7034284
C	3.2847391	-6.4432782	6.0167783
C	3.9829943	-5.6263548	4.9716827
N	4.0485486	-6.0480102	3.6624718
C	4.7306099	-4.4559274	5.0177825
C	4.8060313	-5.1626207	2.9728130
N	5.2497625	-4.1776039	3.7619556
H	3.5879582	-6.9525562	3.3362255
H	3.1855848	-5.8683005	6.9530463
H	3.8645514	-7.3634298	6.2239746
H	4.9036733	-3.8059904	5.8767413
H	4.9773226	-5.2705935	1.9020900
H	-0.5415698	-3.3970690	-4.4447588
C	-0.1808599	-4.1972088	-3.8231589
C	0.5449729	-3.7355847	-2.5599959
O	1.3670437	-2.7669690	-2.6521966
O	0.3096417	-4.4276271	-1.5258398
H	0.5352752	-4.7759796	-4.4375023
H	-1.0135562	-4.8703153	-3.5647096
H	1.8977495	-0.1090000	-5.5861584
C	2.6112593	0.2730699	-4.8524886
O	3.4476111	1.1149468	-5.1960138
N	2.4958284	-0.1776634	-3.5714425
C	3.5047402	0.2303731	-2.5822503
C	4.8800048	-0.3779648	-2.9853423
O	4.9415589	-1.3607761	-3.7419927
C	2.9786444	-0.1556403	-1.1693148
C	3.9497277	-0.0330561	0.0005704
O	3.6928345	0.6605816	1.0224041
O	5.0373453	-0.7124421	-0.0390861
H	1.8996339	-0.9935808	-3.3521276
H	3.6170121	1.3269879	-2.6391640
H	2.6412202	-1.2077159	-1.2072897
H	2.0947568	0.4648476	-0.9551699
H	8.0447577	0.1959599	-2.2970194
N	5.9930232	0.2089611	-2.5047164
O	8.3334368	-2.5290434	-3.0888222
C	7.5080376	-1.8409029	-2.4712356

H	5.9655127	0.9642358	-1.7821757
C	7.2898380	-0.3556099	-2.8349792
H	7.4969206	-0.2754102	-3.9162474
N	6.8314247	-2.2664251	-1.3797821
C	7.0439295	-3.5614609	-0.7781194
C	6.0002151	-4.5832942	-1.2960193
O	4.9123560	-4.2220521	-1.7653936
C	6.9809342	-3.4117042	0.7696320
C	7.9633038	-2.3952583	1.2883910
N	7.6245177	-1.0806654	1.6053690
C	9.3254898	-2.5452071	1.4846000
C	8.7420967	-0.4616193	1.9758601
N	9.7934398	-1.3181047	1.9165584
H	6.0959344	-1.6611909	-0.9689141
H	10.7577989	-1.0923242	2.1538110
H	8.0453392	-3.9100614	-1.0894395
H	7.1720228	-4.3897837	1.2410299
H	5.9684463	-3.0910601	1.0591691
H	9.9848875	-3.4009995	1.3499702
H	8.7990716	0.5817444	2.2822212
H	5.9194383	-7.8607478	-1.7443495
N	6.3290042	-5.9008072	-1.2394913
O	4.1832788	-6.9271003	0.3762524
C	4.1261652	-6.9640347	-0.8546246
H	7.1974357	-6.1937903	-0.7966842
C	5.3901585	-6.9192581	-1.7193995
H	5.1144354	-6.6779233	-2.7622523
N	2.9771818	-7.0540515	-1.5715690
C	1.6966481	-7.3275928	-0.9232185
C	1.6695853	-8.8270871	-0.5686659
O	1.3213341	-9.6893637	-1.3939974
H	3.0321470	-7.0164689	-2.5933820
H	0.8829620	-7.0702222	-1.6140637
H	1.6172758	-6.6894254	-0.0279762
H	1.6063495	-10.6777270	1.8256595
N	2.1684417	-9.0761290	0.6565878
C	2.4445693	-10.3905971	1.2221497
C	3.7254234	-10.3587972	2.0683274
C	3.6988098	-9.3561046	3.2547141
O	4.4671899	-9.5524008	4.2166027
O	2.8948908	-8.3568219	3.1119160
H	2.4066159	-8.3185744	1.3191782
H	2.5205912	-11.1105298	0.3882830
H	4.5774118	-10.0634130	1.4246830
H	3.9490889	-11.3664180	2.4605554
H	1.7735995	-6.6652581	-6.1462083
C	2.0946394	-7.1276280	-5.2265485
O	3.1961288	-6.4199621	-4.6203622
H	4.0096044	-6.6868733	-5.0865578
H	2.3538153	-8.1856364	-5.4104731
H	1.2622557	-7.0977982	-4.5058704
H	4.6767987	-4.3759888	-7.9091178

C	5.2893085	-3.9249589	-7.1434580
O	4.8168503	-3.0628724	-6.3945671
H	7.0954880	-4.2313188	-6.2052983
N	6.5004182	-4.4741187	-7.0133780
H	6.8218036	-5.2080564	-7.6416889
H	7.4986079	4.4701787	-0.2574699
C	7.7040778	3.7413389	0.5462598
C	6.8347728	2.4704274	0.3618692
O	6.3084830	2.2794177	-0.7591026
O	6.7455938	1.6990578	1.3912914
H	8.7716385	3.4570793	0.5190600
H	7.5018055	4.2034074	1.5254711
H	0.7360998	2.7154592	2.9971992
C	1.6626895	3.1528591	3.3529491
O	1.6494754	4.0078153	4.2515190
H	4.2115188	4.2583588	2.7577492
N	2.7810400	2.7166175	2.7449336
C	4.0717589	3.2580991	3.1365391
H	2.7704616	1.9822220	2.0239558
H	4.8624573	2.6056239	2.7400068
H	4.1525792	3.2931772	4.2364863
H	8.8453875	7.5318479	4.9068386
C	9.5478473	6.7386481	5.0986086
C	8.8157590	5.4367727	5.3134831
C	8.4978257	4.5985596	4.2273103
C	8.3601901	5.0596348	6.5922646
C	7.7339206	3.4366888	4.3904800
C	7.5998340	3.9007308	6.7809701
C	7.2713730	3.0883772	5.6777867
O	6.5144858	1.9865921	5.8945501
H	6.3346515	1.5406767	5.0173568
H	10.2318749	6.6837755	4.2332218
H	10.1402434	7.0258768	5.9855944
H	8.8493289	4.8681923	3.2240513
H	8.5972253	5.6911872	7.4576193
H	7.4749088	2.8049234	3.5301874
H	7.2397796	3.6112895	7.7739403
H	8.8968375	-2.3677193	6.2765782
C	7.8532078	-2.1791494	6.4094082
O	5.8196489	0.4846556	3.8402340
C	5.1860546	-0.2798963	4.6469547
C	3.6938276	-0.1623660	4.8100591
N	5.8655490	-1.0968461	5.4522495
H	5.3809177	-1.6450645	6.1771946
C	7.3099955	-1.2935711	5.2950772
H	3.2445649	-0.0506081	3.8130384
H	3.2613066	-1.0317366	5.3288246
H	3.4799959	0.7549463	5.3881167
H	7.7999871	-0.3047833	5.2908957
H	7.4872089	-1.7494695	4.3039070
H	7.7067349	-1.7062171	7.3959300
H	7.3352864	-3.1534922	6.4141892

O	5.0099865	-1.7526355	2.6274027
H	4.0153422	-2.0201781	2.4768138
H	5.3749428	-2.5861273	3.0690629
Ni	5.8256083	-0.1142704	1.7502264
K	3.6246357	-3.5293963	-3.9270980
C	5.4339985	-3.2089991	8.7399975
O	4.9427023	-2.5474247	7.8076568
N	5.3349985	-2.8549992	10.0039972
H	5.7401707	-3.4479817	10.7281928
H	5.9559983	-4.1099988	8.5299976
H	4.8299986	-2.0139994	10.3499971

Zn²⁺

H	-0.7091596	-4.8591872	3.2845582
C	-0.5230898	-4.5844874	2.2532488
C	0.8090100	-3.9282925	2.0564669
N	1.3945751	-3.8397606	0.8051358
C	1.6908951	-3.2913984	2.9185825
C	2.5673976	-3.1793857	0.9403274
N	2.7758361	-2.8225997	2.2058877
H	0.9636896	-4.1046089	-0.1389627
H	-0.5896700	-5.5065239	1.6471695
H	-1.3508113	-3.9268782	1.9227727
H	1.6175375	-3.1647088	3.9996824
H	3.2555302	-3.0047227	0.1127349
H	2.3080388	-6.7834862	5.7034268
C	3.2847382	-6.4432764	6.0167766
C	4.0276638	-5.6586299	4.9814380
N	4.1391412	-6.0998221	3.6825986
C	4.8090327	-4.5123337	5.0486479
C	4.9551958	-5.2479782	3.0183218
N	5.3942780	-4.2676122	3.8162910
H	3.6634484	-6.9934635	3.3483281
H	3.1769997	-5.8495066	6.9406497
H	3.8482087	-7.3659101	6.2584376
H	4.9623222	-3.8560829	5.9062725
H	5.1668909	-5.3705526	1.9562851
H	-0.5415696	-3.3970680	-4.4447576
C	-0.1808598	-4.1972076	-3.8231578
C	0.5405320	-3.7317561	-2.5606256
O	1.3854876	-2.7845751	-2.6647636
O	0.2779934	-4.3951829	-1.5149135
H	0.5367569	-4.7743123	-4.4371436
H	-1.0144940	-4.8699349	-3.5664152
H	1.8977490	-0.1090000	-5.5861568
C	2.6112586	0.2730698	-4.8524872
O	3.4390371	1.1282852	-5.1834652
N	2.5017705	-0.2065921	-3.5840564
C	3.4975398	0.1877933	-2.5782374
C	4.8818389	-0.3940295	-2.9843266
O	4.9596867	-1.3667438	-3.7527461
C	2.9592182	-0.2559938	-1.1909321
C	3.8755295	-0.0594732	0.0150824
O	3.5265634	0.6485321	0.9861650
O	4.9962277	-0.6991067	0.0099094
H	1.9008660	-1.0222941	-3.3766519
H	3.5936561	1.2874886	-2.5983986
H	2.6984702	-1.3277136	-1.2510642
H	2.0253958	0.2975327	-1.0065889
H	8.0447554	0.1959598	-2.2970188
N	5.9895191	0.1975748	-2.4935470
O	8.3339489	-2.5199783	-3.0992972
C	7.5102365	-1.8363018	-2.4744983

H	5.9540716	0.9372613	-1.7583264
C	7.2898360	-0.3556098	-2.8349784
H	7.4896672	-0.2706235	-3.9168044
N	6.8439066	-2.2732711	-1.3775951
C	7.0864559	-3.5842063	-0.8234939
C	6.0192927	-4.5896685	-1.3135561
O	4.9317441	-4.2211562	-1.7772858
C	7.1419033	-3.4987114	0.7275057
C	8.1589428	-2.4973542	1.2000499
N	7.8380907	-1.1748811	1.4939735
C	9.5252251	-2.6526619	1.3541771
C	8.9704525	-0.5536157	1.8134194
N	10.0136861	-1.4177427	1.7416733
H	6.0950924	-1.6894103	-0.9579173
H	10.9865722	-1.1933459	1.9433488
H	8.0627544	-3.9187642	-1.2180309
H	7.3741664	-4.4933745	1.1427279
H	6.1560926	-3.1914585	1.1103597
H	10.1759728	-3.5148635	1.2187902
H	9.0452688	0.4970805	2.0921683
H	5.9194366	-7.8607456	-1.7443490
N	6.3374528	-5.9081909	-1.2493271
O	4.2031187	-6.9182071	0.3873622
C	4.1339293	-6.9555917	-0.8427330
H	7.2073196	-6.2061191	-0.8128660
C	5.3901570	-6.9192562	-1.7193990
H	5.1072207	-6.6795672	-2.7606396
N	2.9769194	-7.0349077	-1.5483607
C	1.7013634	-7.3008627	-0.8867879
C	1.6648668	-8.8027319	-0.5438217
O	1.2980814	-9.6548437	-1.3717928
H	3.0231297	-7.0074402	-2.5707494
H	0.8816759	-7.0297838	-1.5653733
H	1.6402573	-6.6690867	0.0144165
H	1.6063490	-10.6777240	1.8256590
N	2.1786413	-9.0673874	0.6722196
C	2.4445686	-10.3905942	1.2221494
C	3.7292947	-10.3826056	2.0629476
C	3.7194116	-9.3924990	3.2598034
O	4.4821534	-9.6116782	4.2209616
O	2.9343977	-8.3769829	3.1251888
H	2.4292805	-8.3189822	1.3409102
H	2.5101399	-11.1019111	0.3799709
H	4.5819709	-10.0902946	1.4187211
H	3.9427224	-11.3969920	2.4432291
H	1.7735990	-6.6652562	-6.1462066
C	2.0946388	-7.1276260	-5.2265470
O	3.1962227	-6.4204549	-4.6199759
H	4.0100312	-6.6908504	-5.0834877
H	2.3536264	-8.1856419	-5.4107633
H	1.2621681	-7.0981450	-4.5059031
H	4.6767974	-4.3759876	-7.9091156

C	5.2893070	-3.9249578	-7.1434560
O	4.8178748	-3.0607116	-6.3966700
H	7.0954860	-4.2313176	-6.2052966
N	6.5004164	-4.4741174	-7.0133760
H	6.8200863	-5.2107200	-7.6394514
H	7.4986058	4.4701774	-0.2574698
C	7.7040756	3.7413378	0.5462596
C	6.8724319	2.4485358	0.3880675
O	6.2885967	2.2455212	-0.6989124
O	6.8688104	1.6640423	1.4165864
H	8.7783984	3.4818637	0.5384563
H	7.4852189	4.2072435	1.5207902
H	0.7360996	2.7154584	2.9971984
C	1.6626890	3.1528582	3.3529482
O	1.6485392	4.0079064	4.2520878
H	4.2115176	4.2583576	2.7577484
N	2.7805700	2.7156117	2.7458086
C	4.0717578	3.2580982	3.1365382
H	2.7644640	1.9815707	2.0233548
H	4.8616511	2.6050358	2.7386866
H	4.1543419	3.2925167	4.2363874
H	8.8453850	7.5318458	4.9068372
C	9.5478446	6.7386462	5.0986072
C	8.8145496	5.4327780	5.2885385
C	8.5498459	4.5834174	4.1967951
C	8.3018623	5.0642407	6.5483478
C	7.7798539	3.4214476	4.3344671
C	7.5341847	3.9063287	6.7112663
C	7.2552063	3.0858816	5.6003647
O	6.4833047	1.9886290	5.7929261
H	6.3256119	1.5352871	4.9164316
H	10.2434808	6.6944490	4.2420795
H	10.1272313	7.0168641	5.9970777
H	8.9474852	4.8439881	3.2084348
H	8.4980502	5.7033292	7.4184197
H	7.5629349	2.7812973	3.4686562
H	7.1284136	3.6251465	7.6888501
H	8.8968350	-2.3677186	6.2765764
C	7.8532056	-2.1791488	6.4094064
O	5.8010045	0.4260424	3.7734926
C	5.1754559	-0.3344161	4.5913806
C	3.6761020	-0.2776606	4.6954581
N	5.8644121	-1.0962701	5.4397715
H	5.3786869	-1.6420291	6.1650117
C	7.3213296	-1.2441479	5.3278576
H	3.2622295	-0.2382514	3.6771942
H	3.2611652	-1.1362978	5.2452108
H	3.4016867	0.6597862	5.2120154
H	7.7839396	-0.2446941	5.3991089
H	7.5435658	-1.6366749	4.3187933
H	7.6995953	-1.7513510	7.4149943
H	7.3341483	-3.1519629	6.3641841

O	5.1752338	-1.9108972	2.5886329
H	4.1828664	-2.1787583	2.4656286
H	5.5186742	-2.7124435	3.1039359
Zn	5.9845079	-0.1858163	1.7199748
K	3.6324410	-3.5344487	-3.9369009
C	5.4174575	-3.1939005	8.7232910
O	4.9405269	-2.5469627	7.8085429
N	5.3349970	-2.8549984	10.0039944
H	5.7378873	-3.4495743	10.7282207
H	5.9559966	-4.1099976	8.5299952
H	4.8384652	-2.0084016	10.2825828

TABLE S1. List of literature binding energies with regards to a series of chelating agents for all of the relevant metal ions studied in HDAC8 (in kcal/mol).

	DTPA Stability constant	DTPA ΔG binding (kcal/mol)	GEDTA Stability Constant	GEDTA ΔG binding (kcal/mol)
²⁺ Co	18.4	-25.	12.5	-17.
²⁺ Fe	16.55	-23.	11.92	-16.
²⁺ Mg	9.3	-13.	5.21	-7.1
²⁺ Mn	15.6	-21.	12.3	-17.
²⁺ Ni	20.32	-28.	13.6	-19.
²⁺ Zn	18.75	-26.	14.5	-20.

TABLE S2.

Calculated ΔG (kcal/mol)
DTPA metal swapped with EGTA

	Co^{2+}	Fe^{2+}	Mg^{2+}	Mn^{2+}	Ni^{2+}	Zn^{2+}
Co^{2+}	0	-2.25	-3.41	-1.96	1.31	-2.37
Fe^{2+}		0	-1.16	0.29	3.56	-0.12
Mg^{2+}			0	1.45	4.72	1.03
Mn^{2+}				0	3.27	-0.41
Ni^{2+}					0	-3.68
Zn^{2+}						0

Experimental ΔG (kcal/mol)

DTPA metal swapped with EGTA

	Co^{2+}	Fe^{2+}	Mg^{2+}	Mn^{2+}	Ni^{2+}	Zn^{2+}
Co^{2+}	0	-1.73	-2.47	-3.55	1.12	-2.25
Fe^{2+}		0	-0.74	-1.81	2.85	-0.52
Mg^{2+}			0	-1.08	3.59	0.22
Mn^{2+}				0	4.66	1.30
Ni^{2+}					0	-3.37
Zn^{2+}						0

TABLE S3.

Calculated ΔG – Experimental ΔG (kcal/mol)
DTPA metal swapped with EGTA

	Co²⁺	Fe²⁺	Mg²⁺	Mn²⁺	Ni²⁺	Zn²⁺
Co²⁺	0	-0.52	-0.94	1.59	0.19	-0.12
Fe²⁺		0	-0.42	2.11	0.71	0.40
Mg²⁺			0	2.53	1.13	0.82
Mn²⁺				0	-1.40	-1.71
Ni²⁺					0	-0.31
Zn²⁺						0

TABLE S4

**Original ($\epsilon = 4$) converged Energy + COSMO correction compared with
recomputed single point Energy + COSMO correction at different values of ϵ
(All energies relative to respective reactant state, kcal/mol)**

	$\epsilon = 4$	$\epsilon = 8$	$\epsilon = 20$
TS1	10.43	10.96	11.32
Intermediate	7.07	7.73	8.17
TS2	13.81	14.20	14.45

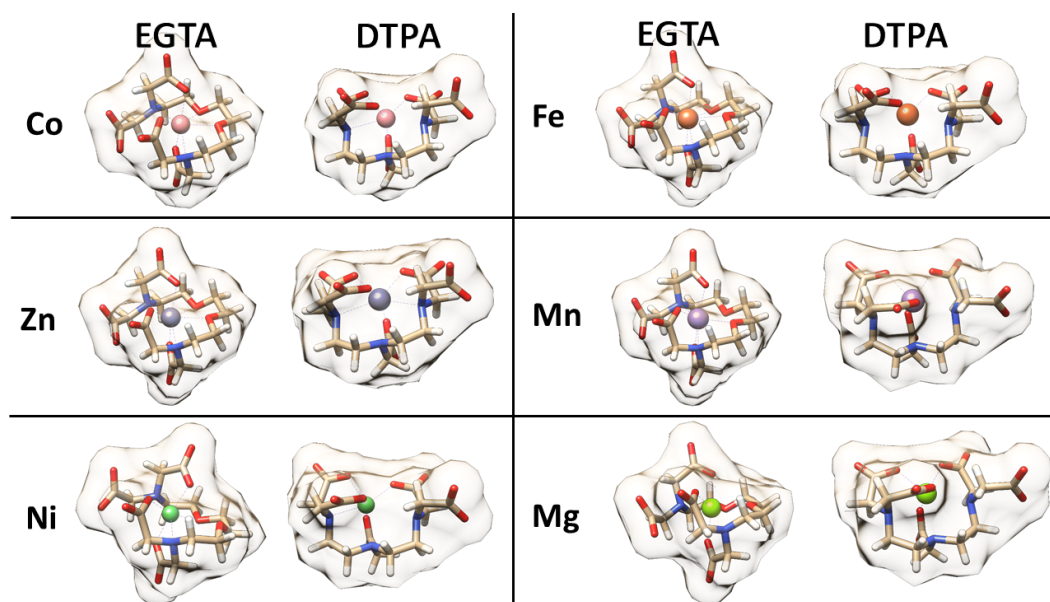


Figure S1. All divalent metals in this study coordinated by EGTA and DTPA, for use as a reference in determining metal binding affinities to HDAC8. Shaded areas surrounding each complex represent the solvent accessible surface area and highlight the solvent exclusion of these chelating complexes.

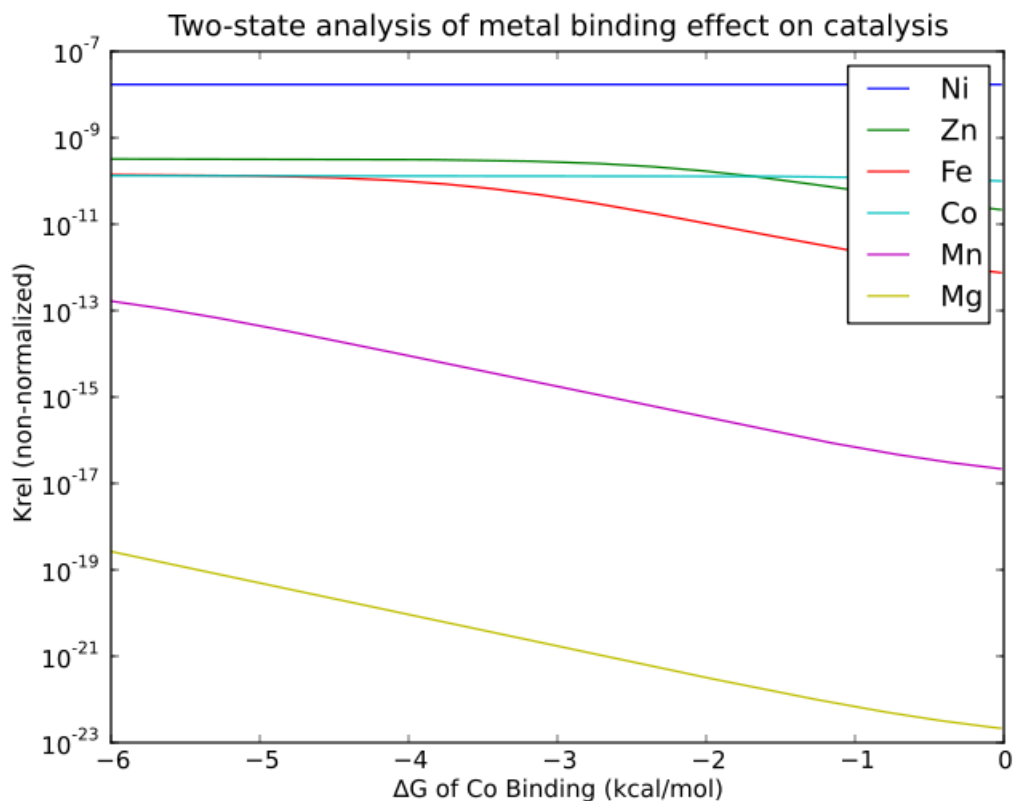


Figure S2. Catalytic model utilizing a two-state ensemble for $K_{binding}$ over a range of

possible binding affinities for Co. In this model, $K_{binding}(M) = \frac{e^{-(\Delta G_{Co} + \Delta \Delta G_M)/RT}}{1 + e^{-(\Delta G_{Co} + \Delta \Delta G_M)/RT}}$,

where ΔG_{Co} is the binding affinity of Co and $\Delta \Delta G_M$ is the binding affinity of metal M relative to Co.