

Supplementary Material for

The Active Site of a Zinc-Dependent Metalloproteinase Influences the Computed pK_a of Ligands
Coordinated to the Catalytic Zinc Ion

Table S.1 Cartesian coordinates of the protonated and unprotonated structures used to calculate pK_a in this work.

Glu-406 (protonated)

C1	-2.9873175961	-1.8550550710	3.7474680187
O2	-3.8113837295	-0.8023436338	3.5243629293
O3	-3.3603115391	-2.8716937289	4.2923613447
H_pk	-4.6882797446	-1.0639911608	3.8642357778
N5	-1.4300000000	-4.2430000000	1.9020000000
C6	-2.1180000000	-3.1220000000	1.2400000000
C7	-2.0950000000	-3.1940000000	-0.2580000000
O8	-3.1140000000	-3.0540000000	-0.9940000000
C9	-1.5260000000	-1.7800000000	1.7000000000
C10	-1.6000000000	-1.6010000000	3.1940000000
H11	-0.6160000000	-4.0630000000	2.4540000000
H12	-3.1880000000	-3.1850000000	1.4360000000
H13	-0.4780000000	-1.7250000000	1.4060000000
H14	-2.0760000000	-0.9610000000	1.2360000000
H15	-0.9170000000	-2.2990000000	3.6780000000
H16	-1.3180000000	-0.5800000000	3.4520000000
H17	-2.0660000000	-4.7000000000	2.5390000000
C18	-0.7330000000	-3.4540000000	-0.8860000000
H19	-0.8360000000	-3.4870000000	-1.9990000000
H20	-0.0280000000	-2.6330000000	-0.6000000000
H21	-0.3340000000	-4.4330000000	-0.5190000000

Glu-406 (unprotonated)

C1	-3.0521663022	-1.9068167680	3.7213513168
O2	-3.9047919743	-1.0922999995	3.3029120172
O3	-3.1925875432	-2.9330954985	4.3961994635
X_pk	-4.7634000000	-1.4102000000	3.7914000000
N5	-1.4300000000	-4.2430000000	1.9020000000
C6	-2.1180000000	-3.1220000000	1.2400000000
C7	-2.0950000000	-3.1940000000	-0.2580000000
O8	-3.1140000000	-3.0540000000	-0.9940000000
C9	-1.5260000000	-1.7800000000	1.7000000000
C10	-1.6000000000	-1.6010000000	3.1940000000
H11	-0.6160000000	-4.0630000000	2.4540000000
H12	-3.1880000000	-3.1850000000	1.4360000000
H13	-0.4780000000	-1.7250000000	1.4060000000
H14	-2.0760000000	-0.9610000000	1.2360000000
H15	-0.9170000000	-2.2990000000	3.6780000000
H16	-1.3180000000	-0.5800000000	3.4520000000
H17	-2.0660000000	-4.7000000000	2.5390000000
C18	-0.7330000000	-3.4540000000	-0.8860000000
H19	-0.8360000000	-3.4870000000	-1.9990000000
H20	-0.0280000000	-2.6330000000	-0.6000000000
H21	-0.3340000000	-4.4330000000	-0.5190000000

Glu-406 + Zn(Imd)₃ + H₂O (protonated)

O1	-5.7103616765	-3.1996710397	5.4943293798
H2	-4.7840826590	-3.1364538698	5.8317829342
C3	-2.9809000000	-1.8801000000	4.0525000000
O4	-4.0299000000	-1.8831000000	3.3545000000
O5	-2.9649000000	-2.1011000000	5.2725000000
Zn6	-6.7139000000	-4.9121000000	4.9575000000
C7	-2.8199000000	-6.6191000000	4.6455000000
N8	-3.3609000000	-7.7291000000	5.1905000000
C9	-3.7979000000	-5.6361000000	4.5915000000
C10	-4.6259000000	-7.5341000000	5.5485000000
N11	-4.8399000000	-6.3181000000	5.1685000000
C12	-6.6339000000	-4.4541000000	0.6635000000
N13	-7.6239000000	-5.4221000000	0.7375000000
C14	-6.2259000000	-4.1361000000	1.9135000000
C15	-7.8949000000	-5.6911000000	2.0025000000
N16	-7.0539000000	-4.9161000000	2.6595000000
C17	-9.6079000000	-8.1011000000	5.4435000000
N18	-10.2949000000	-7.0691000000	6.0165000000
C19	-8.3259000000	-7.6601000000	5.1645000000
C20	-9.5539000000	-5.9761000000	6.0795000000
N21	-8.3909000000	-6.3841000000	5.5845000000
H22	-2.8555000000	-8.6181000000	5.3138000000
H23	-8.0800000000	-5.8654000000	-0.0726000000
H24	-11.2652000000	-7.1341000000	6.3559000000
H25	-3.7520000000	-4.6194000000	4.2040000000
H26	-5.3098000000	-8.2254000000	6.0387000000
H27	-5.4479000000	-3.4451000000	2.2345000000
H28	-8.6328000000	-6.3838000000	2.4046000000
H29	-7.4897000000	-8.2008000000	4.7236000000
H30	-9.8285000000	-4.9880000000	6.4458000000
H_pk	-3.8681788096	-1.5764995271	2.4440577254
H32	-1.7907000000	-6.5130000000	4.3058000000
H33	-6.2459000000	-4.0184000000	-0.2561000000
H34	-10.0001000000	-9.0967000000	5.2415000000
N35	-1.4300000000	-4.2430000000	1.9020000000
C36	-2.1180000000	-3.1220000000	1.2400000000
C37	-2.0950000000	-3.1940000000	-0.2580000000
O38	-3.1140000000	-3.0540000000	-0.9940000000
C39	-1.5260000000	-1.7800000000	1.7000000000
C40	-1.6000000000	-1.6010000000	3.1940000000
H41	-0.6160000000	-4.0630000000	2.4540000000
H42	-3.1880000000	-3.1850000000	1.4360000000
H43	-0.4780000000	-1.7250000000	1.4060000000
H44	-2.0760000000	-0.9610000000	1.2360000000
H45	-0.9170000000	-2.2990000000	3.6780000000
H46	-1.3180000000	-0.5800000000	3.4520000000
H47	-2.0660000000	-4.7000000000	2.5390000000
C48	-0.7330000000	-3.4540000000	-0.8860000000
H49	-0.8360000000	-3.4870000000	-1.9990000000
H50	-0.0280000000	-2.6330000000	-0.6000000000
H51	-0.3340000000	-4.4330000000	-0.5190000000
H52	-5.7890000000	-2.3950000000	4.9560000000

Glu-406 + Zn(Imd)₃ + H₂O (unprotonated)

O1	-5.6084152821	-3.2036526762	5.4755927148
H2	-4.5971721418	-3.0426277277	5.5565075521
C3	-2.9809000000	-1.8801000000	4.0525000000
O4	-4.0401644564	-1.9889044920	3.3426557885
O5	-2.9649000000	-2.1011000000	5.2725000000
Zn6	-6.7139000000	-4.9121000000	4.9575000000
C7	-2.8199000000	-6.6191000000	4.6455000000
N8	-3.3609000000	-7.7291000000	5.1905000000
C9	-3.7979000000	-5.6361000000	4.5915000000
C10	-4.6259000000	-7.5341000000	5.5485000000
N11	-4.8399000000	-6.3181000000	5.1685000000
C12	-6.6339000000	-4.4541000000	0.6635000000
N13	-7.6239000000	-5.4221000000	0.7375000000
C14	-6.2259000000	-4.1361000000	1.9135000000
C15	-7.8949000000	-5.6911000000	2.0025000000
N16	-7.0539000000	-4.9161000000	2.6595000000
C17	-9.6079000000	-8.1011000000	5.4435000000
N18	-10.2949000000	-7.0691000000	6.0165000000
C19	-8.3259000000	-7.6601000000	5.1645000000
C20	-9.5539000000	-5.9761000000	6.0795000000
N21	-8.3909000000	-6.3841000000	5.5845000000
H22	-2.8555000000	-8.6181000000	5.3138000000
H23	-8.0800000000	-5.8654000000	-0.0726000000
H24	-11.2652000000	-7.1341000000	6.3559000000
H25	-3.7520000000	-4.6194000000	4.2040000000
H26	-5.3098000000	-8.2254000000	6.0387000000
H27	-5.4479000000	-3.4451000000	2.2345000000
H28	-8.6328000000	-6.3838000000	2.4046000000
H29	-7.4897000000	-8.2008000000	4.7236000000
H30	-9.8285000000	-4.9880000000	6.4458000000
X_pk	-3.9053450261	-1.5208108745	2.4889597727
H32	-1.7907000000	-6.5130000000	4.3058000000
H33	-6.2459000000	-4.0184000000	-0.2561000000
H34	-10.0001000000	-9.0967000000	5.2415000000
N35	-1.4300000000	-4.2430000000	1.9020000000
C36	-2.1180000000	-3.1220000000	1.2400000000
C37	-2.0950000000	-3.1940000000	-0.2580000000
O38	-3.1140000000	-3.0540000000	-0.9940000000
C39	-1.5260000000	-1.7800000000	1.7000000000
C40	-1.6000000000	-1.6010000000	3.1940000000
H41	-0.6160000000	-4.0630000000	2.4540000000
H42	-3.1880000000	-3.1850000000	1.4360000000
H43	-0.4780000000	-1.7250000000	1.4060000000
H44	-2.0760000000	-0.9610000000	1.2360000000
H45	-0.9170000000	-2.2990000000	3.6780000000
H46	-1.3180000000	-0.5800000000	3.4520000000
H47	-2.0660000000	-4.7000000000	2.5390000000
C48	-0.7330000000	-3.4540000000	-0.8860000000
H49	-0.8360000000	-3.4870000000	-1.9990000000
H50	-0.0280000000	-2.6330000000	-0.6000000000
H51	-0.3340000000	-4.4330000000	-0.5190000000
H52	-5.7890000000	-2.3950000000	4.9560000000

Glu-406 + Zn(Imd)₃ + Acetohydroxamate (protonated)

N1	-1.3990000000	-4.4320000000	2.1730000000
C2	-2.0870000000	-3.3110000000	1.5120000000
C3	-2.0640000000	-3.3830000000	0.0130000000
O4	-3.0830000000	-3.2430000000	-0.7220000000
C5	-1.4950000000	-1.9690000000	1.9710000000
C6	-1.5690000000	-1.7900000000	3.4660000000
C7	-2.9200000000	-2.0230000000	4.0910000000
O8	-4.0550000000	-2.0260000000	3.3350000000
O9	-2.9040000000	-2.2440000000	5.3100000000
H10	-0.5850000000	-4.2520000000	2.7260000000
H11	-3.1440000000	-3.3460000000	1.8120000000
H12	-0.4370000000	-1.9210000000	1.6730000000
H13	-2.0400000000	-1.1490000000	1.4810000000
H14	-0.8670000000	-2.4980000000	3.9320000000
H15	-1.2500000000	-0.7650000000	3.7040000000
H16	-1.7430000000	-5.3660000000	2.0700000000
C17	-0.7460000000	-3.6381000000	-0.6584000000
H_pk	-4.7997359072	-2.4004474196	3.9280478377
C19	-2.8450000000	-6.7620000000	4.6270000000
N20	-3.3860000000	-7.8720000000	5.1720000000
C21	-4.6510000000	-7.6770000000	5.5290000000
N22	-4.8650000000	-6.4610000000	5.1490000000
C23	-3.8230000000	-5.7790000000	4.5720000000
H24	-1.8160000000	-6.6560000000	4.2880000000
H25	-3.7770000000	-4.7620000000	4.1850000000
H26	-5.3350000000	-8.3680000000	6.0200000000
H27	-2.8810000000	-8.7610000000	5.2950000000
C28	-6.6590000000	-4.5970000000	0.6440000000
N29	-7.6490000000	-5.5650000000	0.7190000000
C30	-7.9200000000	-5.8340000000	1.9830000000
N31	-7.0790000000	-5.0590000000	2.6400000000
C32	-6.2510000000	-4.2790000000	1.8940000000
H33	-6.2720000000	-4.1620000000	-0.2760000000
H34	-5.4730000000	-3.5880000000	2.2160000000
H35	-8.6580000000	-6.5270000000	2.3860000000
H36	-8.1050000000	-6.0080000000	-0.0920000000
C37	-9.6330000000	-8.2440000000	5.4250000000
N38	-10.3200000000	-7.2120000000	5.9970000000
C39	-9.5790000000	-6.1190000000	6.0610000000
N40	-8.4160000000	-6.5270000000	5.5660000000
C41	-8.3510000000	-7.8030000000	5.1460000000
H42	-10.0250000000	-9.2400000000	5.2230000000
H43	-7.5150000000	-8.3440000000	4.7050000000
H44	-9.8540000000	-5.1310000000	6.4270000000
H45	-11.2900000000	-7.2770000000	6.3370000000
C46	-6.1428976194	-2.7522551267	8.4326784933
C47	-6.3394808395	-3.2764207294	7.0389562367
N48	-5.5387087355	-2.8284078595	6.0832743042
O49	-5.7038226434	-3.3041899148	4.8037737196
O50	-7.2415721471	-4.1252017529	6.7592524189
H51	-5.9414633536	-3.5871822063	9.1113319728
H52	-0.8969861546	-3.6510289304	-1.7390686119
H53	-4.6316007563	-2.3690953979	6.2147332209
H54	-7.0653013880	-2.2670639079	8.7681506016
H55	-5.3224279483	-2.0316033154	8.4925392423

Zn56	-6.7390000000	-5.0550000000	4.9380000000
H57	-0.0379000000	-2.8330000000	-0.4128000000
H58	-0.3401000000	-4.6070000000	-0.3322000000

Glu-406 + Zn(Imd)₃ + Acetohydroxamate (unprotonated)

N1	-1.3990000000	-4.4320000000	2.1730000000
C2	-2.0870000000	-3.3110000000	1.5120000000
C3	-2.0640000000	-3.3830000000	0.0130000000
O4	-3.0830000000	-3.2430000000	-0.7220000000
C5	-1.4950000000	-1.9690000000	1.9710000000
C6	-1.5690000000	-1.7900000000	3.4660000000
C7	-2.9200000000	-2.0230000000	4.0910000000
O8	-4.0550000000	-2.0260000000	3.3350000000
O9	-2.9040000000	-2.2440000000	5.3100000000
H10	-0.5850000000	-4.2520000000	2.7260000000
H11	-3.1440000000	-3.3460000000	1.8120000000
H12	-0.4370000000	-1.9210000000	1.6730000000
H13	-2.0400000000	-1.1490000000	1.4810000000
H14	-0.8670000000	-2.4980000000	3.9320000000
H15	-1.2500000000	-0.7650000000	3.7040000000
H16	-1.7430000000	-5.3660000000	2.0700000000
C17	-0.7460000000	-3.6381000000	-0.6584000000
X_pk	-4.8150000000	-2.1890000000	3.8980000000
C19	-2.8450000000	-6.7620000000	4.6270000000
N20	-3.3860000000	-7.8720000000	5.1720000000
C21	-4.6510000000	-7.6770000000	5.5290000000
N22	-4.8650000000	-6.4610000000	5.1490000000
C23	-3.8230000000	-5.7790000000	4.5720000000
H24	-1.8160000000	-6.6560000000	4.2880000000
H25	-3.7770000000	-4.7620000000	4.1850000000
H26	-5.3350000000	-8.3680000000	6.0200000000
H27	-2.8810000000	-8.7610000000	5.2950000000
C28	-6.6590000000	-4.5970000000	0.6440000000
N29	-7.6490000000	-5.5650000000	0.7190000000
C30	-7.9200000000	-5.8340000000	1.9830000000
N31	-7.0790000000	-5.0590000000	2.6400000000
C32	-6.2510000000	-4.2790000000	1.8940000000
H33	-6.2720000000	-4.1620000000	-0.2760000000
H34	-5.4730000000	-3.5880000000	2.2160000000
H35	-8.6580000000	-6.5270000000	2.3860000000
H36	-8.1050000000	-6.0080000000	-0.0920000000
C37	-9.6330000000	-8.2440000000	5.4250000000
N38	-10.3200000000	-7.2120000000	5.9970000000
C39	-9.5790000000	-6.1190000000	6.0610000000
N40	-8.4160000000	-6.5270000000	5.5660000000
C41	-8.3510000000	-7.8030000000	5.1460000000
H42	-10.0250000000	-9.2400000000	5.2230000000
H43	-7.5150000000	-8.3440000000	4.7050000000
H44	-9.8540000000	-5.1310000000	6.4270000000
H45	-11.2900000000	-7.2770000000	6.3370000000
C46	-4.9373772745	-2.5698342912	7.7402383842
C47	-5.8066547812	-3.1862560115	6.6808305043
N48	-5.8822343763	-2.5815084698	5.5021237827
O49	-6.6655688225	-3.1442254208	4.5319547517
O50	-6.4726315931	-4.2601101478	6.8947019326

H51	-4.3964374716	-3.3645866950	8.2634552252
H52	-0.8950429031	-3.6528749286	-1.7404788238
H53	-5.1001247562	-2.0483372614	5.0883480125
H54	-5.5567773112	-2.0436039173	8.4777485881
H55	-4.2164440816	-1.8823916577	7.2931124444
Zn56	-6.7390000000	-5.0550000000	4.9380000000
H57	-0.0379000000	-2.8330000000	-0.4128000000
H58	-0.3401000000	-4.6070000000	-0.3322000000

Glu-406 + Zn(Imd)₃ + Acetate (protonated)

N1	-1.3990000000	-4.4320000000	2.1730000000
C2	-2.0870000000	-3.3110000000	1.5120000000
C3	-2.0640000000	-3.3830000000	0.0130000000
O4	-3.0830000000	-3.2430000000	-0.7220000000
C5	-1.4950000000	-1.9690000000	1.9710000000
C6	-1.5690000000	-1.7900000000	3.4660000000
C7	-2.9200000000	-2.0230000000	4.0910000000
O8	-4.0550000000	-2.0260000000	3.3350000000
O9	-2.9040000000	-2.2440000000	5.3100000000
H10	-0.5850000000	-4.2520000000	2.7260000000
H11	-3.1440000000	-3.3460000000	1.8120000000
H12	-0.4370000000	-1.9210000000	1.6730000000
H13	-2.0400000000	-1.1490000000	1.4810000000
H14	-0.8670000000	-2.4980000000	3.9320000000
H15	-1.2500000000	-0.7650000000	3.7040000000
H16	-1.7430000000	-5.3660000000	2.0700000000
C17	-0.7460000000	-3.6381000000	-0.6584000000
H_pk	-4.8220000000	-2.1030000000	3.9440000000
C19	-2.8450000000	-6.7620000000	4.6270000000
N20	-3.3860000000	-7.8720000000	5.1720000000
C21	-4.6510000000	-7.6770000000	5.5290000000
N22	-4.8650000000	-6.4610000000	5.1490000000
C23	-3.8230000000	-5.7790000000	4.5720000000
H24	-1.8160000000	-6.6560000000	4.2880000000
H25	-3.7770000000	-4.7620000000	4.1850000000
H26	-5.3350000000	-8.3680000000	6.0200000000
H27	-2.8810000000	-8.7610000000	5.2950000000
C28	-6.6590000000	-4.5970000000	0.6440000000
N29	-7.6490000000	-5.5650000000	0.7190000000
C30	-7.9200000000	-5.8340000000	1.9830000000
N31	-7.0790000000	-5.0590000000	2.6400000000
C32	-6.2510000000	-4.2790000000	1.8940000000
H33	-6.2720000000	-4.1620000000	-0.2760000000
H34	-5.4730000000	-3.5880000000	2.2160000000
H35	-8.6580000000	-6.5270000000	2.3860000000
H36	-8.1050000000	-6.0080000000	-0.0920000000
C37	-9.6330000000	-8.2440000000	5.4250000000
N38	-10.3200000000	-7.2120000000	5.9970000000
C39	-9.5790000000	-6.1190000000	6.0610000000
N40	-8.4160000000	-6.5270000000	5.5660000000
C41	-8.3510000000	-7.8030000000	5.1460000000
H42	-10.0250000000	-9.2400000000	5.2230000000
H43	-7.5150000000	-8.3440000000	4.7050000000
H44	-9.8540000000	-5.1310000000	6.4270000000
H45	-11.2900000000	-7.2770000000	6.3370000000

C46	-6.2072578233	-1.5286039290	6.6849075453
C47	-6.4719876263	-2.8353608007	5.9920890775
O48	-6.0098539468	-3.0337479055	4.8097022220
O49	-7.1250337704	-3.7687142842	6.5488902038
H50	-6.6520503867	-1.5151160855	7.6798982225
H51	-6.6077943090	-0.7037426365	6.0860194766
H52	-5.1219082119	-1.3924832240	6.7497492241
H53	-0.8976000000	-3.6617000000	-1.7477000000
Zn54	-6.7390000000	-5.0550000000	4.9380000000
H55	-0.0379000000	-2.8330000000	-0.4128000000
H56	-0.3401000000	-4.6070000000	-0.3322000000

Glu-406 + Zn(Imd)₃ + Acetate (unprotonated)

N1	-1.3990000000	-4.4320000000	2.1730000000
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C5	-1.4950000000	-1.9690000000	1.9710000000
C6	-1.5690000000	-1.7900000000	3.4660000000
C7	-2.9200000000	-2.0230000000	4.0910000000
O8	-4.0550000000	-2.0260000000	3.3350000000
O9	-2.9040000000	-2.2440000000	5.3100000000
H10	-0.5850000000	-4.2520000000	2.7260000000
H11	-3.1440000000	-3.3460000000	1.8120000000
H12	-0.4370000000	-1.9210000000	1.6730000000
H13	-2.0400000000	-1.1490000000	1.4810000000
H14	-0.8670000000	-2.4980000000	3.9320000000
H15	-1.2500000000	-0.7650000000	3.7040000000
H16	-1.7430000000	-5.3660000000	2.0700000000
C17	-0.7460000000	-3.6381000000	-0.6584000000
X_pk	-4.8220000000	-2.1030000000	3.9440000000
C19	-2.8450000000	-6.7620000000	4.6270000000
N20	-3.3860000000	-7.8720000000	5.1720000000
C21	-4.6510000000	-7.6770000000	5.5290000000
N22	-4.8650000000	-6.4610000000	5.1490000000
C23	-3.8230000000	-5.7790000000	4.5720000000
H24	-1.8160000000	-6.6560000000	4.2880000000
H25	-3.7770000000	-4.7620000000	4.1850000000
H26	-5.3350000000	-8.3680000000	6.0200000000
H27	-2.8810000000	-8.7610000000	5.2950000000
C28	-6.6590000000	-4.5970000000	0.6440000000
N29	-7.6490000000	-5.5650000000	0.7190000000
C30	-7.9200000000	-5.8340000000	1.9830000000
N31	-7.0790000000	-5.0590000000	2.6400000000
C32	-6.2510000000	-4.2790000000	1.8940000000
H33	-6.2720000000	-4.1620000000	-0.2760000000
H34	-5.4730000000	-3.5880000000	2.2160000000
H35	-8.6580000000	-6.5270000000	2.3860000000
H36	-8.1050000000	-6.0080000000	-0.0920000000
C37	-9.6330000000	-8.2440000000	5.4250000000
N38	-10.3200000000	-7.2120000000	5.9970000000
C39	-9.5790000000	-6.1190000000	6.0610000000
N40	-8.4160000000	-6.5270000000	5.5660000000
C41	-8.3510000000	-7.8030000000	5.1460000000
H42	-10.0250000000	-9.2400000000	5.2230000000

H43	-7.5150000000	-8.3440000000	4.7050000000
H44	-9.8540000000	-5.1310000000	6.4270000000
H45	-11.2900000000	-7.2770000000	6.3370000000
C46	-7.1378027005	-1.7463563576	7.0277769275
C47	-7.1104290426	-3.0558020041	6.2824681636
O48	-6.1096316364	-3.8308173145	6.4417111145
O49	-8.0391901470	-3.3742891212	5.4715676436
H50	-6.8175766227	-1.8929325812	8.0625899340
H51	-8.1264697839	-1.2853930068	6.9869407962
H52	-6.4044465321	-1.0860774315	6.5508798302
H53	-0.8976000000	-3.6617000000	-1.7477000000
Zn54	-6.7390000000	-5.0550000000	4.9380000000
H55	-0.0379000000	-2.8330000000	-0.4128000000
H56	-0.3401000000	-4.6070000000	-0.3322000000

Acetohydroxamic acid (protonated)

O1	-5.8398810707	-2.6928362935	4.5977678916
N2	-5.7882880783	-2.3136640060	5.9498774352
C3	-6.4928129959	-3.1124970864	6.8103742581
O4	-7.2911571546	-3.9340641810	6.3614913982
C5	-6.2717133161	-2.8579969729	8.2828862840
H6	-4.8566465807	-1.9937331952	6.1858627508
H7	-7.2364829737	-2.6446018973	8.7522123056
H8	-5.5905978376	-2.0234374207	8.4746467142
H_pk	-6.5169923680	-3.4096329558	4.6410332159
H10	-5.8718775352	-3.7656076181	8.7467101128

Acetohydroxamic acid (unprotonated)

O1	-5.9853467786	-2.6829310094	4.5031290312
N2	-5.8915067664	-2.4763693887	5.8119232512
C3	-6.4657670840	-3.1625406790	6.8176415797
O4	-7.2182476318	-4.1600172408	6.7259640980
C5	-6.1153147023	-2.6118538202	8.2101304666
H6	-5.3102503968	-1.6834020765	6.1146355662
H7	-7.0389071906	-2.3385680773	8.7418513073
H8	-5.4502911862	-1.7354406080	8.2089975425
X_pk	-5.6201273787	-2.2870681160	3.9313854186
H10	-5.6381086974	-3.4016080107	8.8092857139

Acetohydroxamic acid + Zn(Imd)₃ (protonated)

O1	-5.6144310404	-2.6568068104	4.5687236478
N2	-5.6982523660	-1.9934904339	5.7965719618
C3	-6.3894574049	-2.6153574646	6.7770781799
O4	-7.0438696772	-3.6509829356	6.5246253749
C5	-6.3614160801	-1.9885306101	8.1352164590
H6	-4.9350352337	-1.3435835796	5.9640796410
H7	-7.3899225566	-1.7740194410	8.4433477105
H8	-5.7784927821	-1.0649241937	8.1674519529
Zn12	-6.7139000000	-4.9121000000	4.9575000000
C13	-2.8199000000	-6.6191000000	4.6455000000
N14	-3.3609000000	-7.7291000000	5.1905000000
C15	-3.7979000000	-5.6361000000	4.5915000000
C16	-4.6259000000	-7.5341000000	5.5485000000
N17	-4.8399000000	-6.3181000000	5.1685000000
C18	-6.6339000000	-4.4541000000	0.6635000000

N19	-7.6239000000	-5.4221000000	0.7375000000
C20	-6.2259000000	-4.1361000000	1.9135000000
C21	-7.8949000000	-5.6911000000	2.0025000000
N22	-7.0539000000	-4.9161000000	2.6595000000
C23	-9.6079000000	-8.1011000000	5.4435000000
N24	-10.2949000000	-7.0691000000	6.0165000000
C25	-8.3259000000	-7.6601000000	5.1645000000
C26	-9.5539000000	-5.9761000000	6.0795000000
N27	-8.3909000000	-6.3841000000	5.5845000000
H28	-2.8555000000	-8.6181000000	5.3138000000
H29	-8.0800000000	-5.8654000000	-0.0726000000
H30	-11.2652000000	-7.1341000000	6.3559000000
H31	-3.7520000000	-4.6194000000	4.2040000000
H32	-5.3098000000	-8.2254000000	6.0387000000
H33	-5.4479000000	-3.4451000000	2.2345000000
H34	-8.6328000000	-6.3838000000	2.4046000000
H35	-7.4897000000	-8.2008000000	4.7236000000
H36	-9.8285000000	-4.9880000000	6.4458000000
H_pk	-6.1549980978	-2.1228876476	3.9528939931
H38	-5.9461934456	-2.7093424966	8.8478891028
H40	-1.7907000000	-6.5130000000	4.3058000000
H41	-6.2459000000	-4.0184000000	-0.2561000000
H42	-10.0001000000	-9.0967000000	5.2415000000

Acetohydroxamic acid + Zn(Imd)₃ (protonated)

O1	-5.4714392601	-3.2915226543	4.7794135108
N2	-5.9942257579	-2.2888641612	5.5287990336
C3	-7.1117558136	-2.4433785650	6.2213320678
O4	-7.7323916315	-3.5564004020	6.1757231378
C5	-7.6144919759	-1.2952171219	7.0489364912
H6	-5.4508869540	-1.4333255521	5.5539212897
H7	-8.6244094708	-1.0235530515	6.7245810797
H8	-6.9716523333	-0.4128351518	6.9757247098
Zn12	-6.7139000000	-4.9121000000	4.9575000000
C13	-2.8199000000	-6.6191000000	4.6455000000
N14	-3.3609000000	-7.7291000000	5.1905000000
C15	-3.7979000000	-5.6361000000	4.5915000000
C16	-4.6259000000	-7.5341000000	5.5485000000
N17	-4.8399000000	-6.3181000000	5.1685000000
C18	-6.6339000000	-4.4541000000	0.6635000000
N19	-7.6239000000	-5.4221000000	0.7375000000
C20	-6.2259000000	-4.1361000000	1.9135000000
C21	-7.8949000000	-5.6911000000	2.0025000000
N22	-7.0539000000	-4.9161000000	2.6595000000
C23	-9.6079000000	-8.1011000000	5.4435000000
N24	-10.2949000000	-7.0691000000	6.0165000000
C25	-8.3259000000	-7.6601000000	5.1645000000
C26	-9.5539000000	-5.9761000000	6.0795000000
N27	-8.3909000000	-6.3841000000	5.5845000000
H28	-2.8555000000	-8.6181000000	5.3138000000
H29	-8.0800000000	-5.8654000000	-0.0726000000
H30	-11.2652000000	-7.1341000000	6.3559000000
H31	-3.7520000000	-4.6194000000	4.2040000000
H32	-5.3098000000	-8.2254000000	6.0387000000
H33	-5.4479000000	-3.4451000000	2.2345000000
H34	-8.6328000000	-6.3838000000	2.4046000000

H35	-7.4897000000	-8.2008000000	4.7236000000
H36	-9.8285000000	-4.9880000000	6.4458000000
X_pk	-5.6198000000	-2.2873000000	3.9313000000
H38	-7.6749452659	-1.6014301817	8.0985607251
H40	-1.7907000000	-6.5130000000	4.3058000000
H41	-6.2459000000	-4.0184000000	-0.2561000000
H42	-10.0001000000	-9.0967000000	5.2415000000

Acetic acid (protonated)

C1	2.4188837096	0.0510765159	-0.3862564890
O2	2.7851315849	-0.6698281239	0.7053405461
O3	2.4166032641	1.2610372000	-0.3937620337
C4	2.0330534185	-0.8457697507	-1.5359739643
H_pk	3.0149460111	-0.0143196315	1.3902731757
H6	1.7431904723	-0.2341449166	-2.3908494643
H7	2.8750179708	-1.4916916388	-1.8061366324
H8	1.2025949808	-1.4960506119	-1.2418425789

Acetic acid (unprotonated)

C1	2.4492015774	0.0188873257	-0.2950173592
O2	2.7838455195	-0.6655331173	0.7058770502
O3	2.4022122384	1.2666952840	-0.4357932413
C4	2.0288689355	-0.8336731480	-1.5531774147
X_pk	2.9869314143	0.0359059654	1.2877996882
H6	1.7414746972	-0.2052089806	-2.4060217683
H7	2.8570531782	-1.4909779880	-1.8567674754
H8	1.1878626365	-1.4947436047	-1.2967453499

Acetic acid + Zn(Imd)₃ (protonated)

C1	-2.8450000000	-6.7620000000	4.6270000000
N2	-3.3860000000	-7.8720000000	5.1720000000
C3	-4.6510000000	-7.6770000000	5.5290000000
N4	-4.8650000000	-6.4610000000	5.1490000000
C5	-3.8230000000	-5.7790000000	4.5720000000
H6	-1.8160000000	-6.6560000000	4.2880000000
H7	-3.7770000000	-4.7620000000	4.1850000000
H8	-5.3350000000	-8.3680000000	6.0200000000
H9	-2.8810000000	-8.7610000000	5.2950000000
C10	-6.6590000000	-4.5970000000	0.6440000000
N11	-7.6490000000	-5.5650000000	0.7190000000
C12	-7.9200000000	-5.8340000000	1.9830000000
N13	-7.0790000000	-5.0590000000	2.6400000000
C14	-6.2510000000	-4.2790000000	1.8940000000
H15	-6.2720000000	-4.1620000000	-0.2760000000
H16	-5.4730000000	-3.5880000000	2.2160000000
H17	-8.6580000000	-6.5270000000	2.3860000000
H18	-8.1050000000	-6.0080000000	-0.0920000000
C19	-9.6330000000	-8.2440000000	5.4250000000
N20	-10.3200000000	-7.2120000000	5.9970000000
C21	-9.5790000000	-6.1190000000	6.0610000000
N22	-8.4160000000	-6.5270000000	5.5660000000
C23	-8.3510000000	-7.8030000000	5.1460000000
H24	-10.0250000000	-9.2400000000	5.2230000000
H25	-7.5150000000	-8.3440000000	4.7050000000
H26	-9.8540000000	-5.1310000000	6.4270000000
H27	-11.2900000000	-7.2770000000	6.3370000000

C28	-7.8848251669	-2.2127369828	7.1507107116
C29	-6.5594937952	-2.3483812118	6.4715236547
O30	-5.7079518544	-1.3967100142	6.7441219851
O31	-6.2451970903	-3.2810557687	5.6995454315
H32	-8.0155208057	-3.0487054235	7.8483546149
H33	-8.6834697238	-2.2543591477	6.4022665959
H34	-7.9487008803	-1.2749201085	7.7029733473
H_pk	-4.8542404068	-1.5402794467	6.2862683212
Zn36	-6.7390000000	-5.0550000000	4.9380000000

Acetic acid + Zn(Imd)₃ (unprotonated)

C1	-2.8450000000	-6.7620000000	4.6270000000
N2	-3.3860000000	-7.8720000000	5.1720000000
C3	-4.6510000000	-7.6770000000	5.5290000000
N4	-4.8650000000	-6.4610000000	5.1490000000
C5	-3.8230000000	-5.7790000000	4.5720000000
H6	-1.8160000000	-6.6560000000	4.2880000000
H7	-3.7770000000	-4.7620000000	4.1850000000
H8	-5.3350000000	-8.3680000000	6.0200000000
H9	-2.8810000000	-8.7610000000	5.2950000000
C10	-6.6590000000	-4.5970000000	0.6440000000
N11	-7.6490000000	-5.5650000000	0.7190000000
C12	-7.9200000000	-5.8340000000	1.9830000000
N13	-7.0790000000	-5.0590000000	2.6400000000
C14	-6.2510000000	-4.2790000000	1.8940000000
H15	-6.2720000000	-4.1620000000	-0.2760000000
H16	-5.4730000000	-3.5880000000	2.2160000000
H17	-8.6580000000	-6.5270000000	2.3860000000
H18	-8.1050000000	-6.0080000000	-0.0920000000
C19	-9.6330000000	-8.2440000000	5.4250000000
N20	-10.3200000000	-7.2120000000	5.9970000000
C21	-9.5790000000	-6.1190000000	6.0610000000
N22	-8.4160000000	-6.5270000000	5.5660000000
C23	-8.3510000000	-7.8030000000	5.1460000000
H24	-10.0250000000	-9.2400000000	5.2230000000
H25	-7.5150000000	-8.3440000000	4.7050000000
H26	-9.8540000000	-5.1310000000	6.4270000000
H27	-11.2900000000	-7.2770000000	6.3370000000
C28	-6.2813500920	-1.3324267967	6.1512922954
C29	-6.4221591457	-2.7551961504	5.6745102192
O30	-5.5759435505	-3.2617041634	4.8696403113
O31	-7.4101907728	-3.4616581707	6.0780530386
H32	-6.3349320972	-1.3046245123	7.2439827681
H33	-7.1215842300	-0.7402360227	5.7722788316
H34	-5.3429233978	-0.8956223595	5.8088056594
X_pk	-5.6110000000	-2.9170000000	5.9020000000
Zn36	-6.7390000000	-5.0550000000	4.9380000000