How Simple is Too Simple? Computational Perspective on Importance of Second-Shell Environment for Metal-Ion Selectivity

Supplementary Material

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Table S1: and values in kcal.mol^{-1} for

system: **CC**

model: ***TINY***

Single-point Structure with… optimized with…	**Mn^{2+}**	**Fe^{2+}**	**Co^{2+}**	**Ni^{2+}**	**Cu^{2+}**	**Zn^{2+}**	**Cd^{2+}**	**Hg^{2+}**	*AAD*
Mn^{2+}	-1.3	-2.2	-3.9	-7.1	-8.0	-1.0	0.0	-3.0	2.3
Fe^{2+}	-1.6	-0.9	-1.6	-10.1	-6.6	-0.8	0.0	-3.2	2.7
Co^{2+}	-2.3	0.0	-1.9	-6.4	-3.0	-0.9	-1.3	-5.6	1.7
Ni^{2+}	-1.7	-1.1	-3.3	-5.9	-6.1	-0.3	0.0	-3.4	2.0
Cu^{2+}	-1.9	-1.7	N/A	-4.6	-4.3	-0.9	0.0	-3.6	1.5
Zn^{2+}	-1.8	-2.2	-3.8	-7.6	-8.1	-0.9	0.0	-3.3	2.3
Cd^{2+}	-0.7	N/A	-3.8	-5.4	-7.4	-0.8	0.0	-3.3	2.2
Hg^{2+}	-1.0	-3.0	-0.9	-1.8	-4.8	-1.1	0.0	-3.2	1.3

Table S2 = Table 3: and values in kcal.mol^{-1} for

system: **CC**

model: ***SMALL***

Single-point Structure with… optimized with…	**Mn^{2+}**	**Fe^{2+}**	**Co^{2+}**	**Ni^{2+}**	**Cu^{2+}**	**Zn^{2+}**	**Cd^{2+}**	**Hg^{2+}**	*AAD*
Mn^{2+}	-0.5	-0.5	-1.7	-2.3	-2.4	-0.8	0.0	-0.8	0.8
Fe^{2+}	-0.6	-0.7	-1.6	-2.7	-2.9	-1.0	0.0	-0.9	0.8
Co^{2+}	-0.6	-0.2	-1.6	-2.8	-2.4	-0.9	0.0	-0.6	0.8
Ni^{2+}	-0.6	-0.3	-1.8	-3.1	-2.8	-0.9	0.0	-0.6	1.0
Cu^{2+}	-0.6	-0.7	N/A	-3.2	-2.4	-1.1	0.0	-0.9	0.9
Zn^{2+}	-0.6	-0.5	-2.0	-2.8	-3.1	-1.0	0.0	-0.9	1.0
Cd^{2+}	-0.5	N/A	-1.8	-2.3	-2.6	-0.6	0.0	-0.7	0.9
Hg^{2+}	-0.4	-1.1	-1.2	-1.9	-1.9	-0.6	0.0	-0.4	0.6

Table S3: and values in kcal.mol^{-1} for

system: **CC**

model: ***ALPHA***

Single-point Structure with… optimized with…	**Mn^{2+}**	**Fe^{2+}**	**Co^{2+}**	**Ni^{2+}**	**Cu^{2+}**	**Zn^{2+}**	**Cd^{2+}**	**Hg^{2+}**	*AAD*
Mn^{2+}	-0.4	0.0	-1.3	-1.9	-1.6	-0.8	-0.2	-0.7	0.5
Fe^{2+}	-0.3	0.0	-0.5	-2.1	-1.9	-0.8	0.0	-0.4	0.6
Co^{2+}	-0.7	0.0	-1.7	-2.5	-1.9	-1.2	-0.6	-0.9	0.6
Ni^{2+}	-0.7	0.0	-1.8	-2.7	-2.1	-1.2	-0.6	-0.8	0.7
Cu^{2+}	-0.3	0.0	N/A	-2.0	-1.6	-0.8	0.0	-0.5	0.6
Zn^{2+}	-0.4	0.0	-1.6	-2.2	-2.0	-0.9	-0.2	-0.7	0.7
Cd^{2+}	0.0	N/A	-0.9	-1.1	-1.1	-0.4	0.0	-0.4	0.4
Hg^{2+}	-0.3	-0.6	-0.8	-0.8	-0.9	-0.5	0.0	-0.2	0.2

Table S4: and values in kcal.mol^{-1} for

system: **CC**

model: ***FULL_AA***

Single-point Structure with… optimized with…	**Mn^{2+}**	**Fe^{2+}**	**Co^{2+}**	**Ni^{2+}**	**Cu^{2+}**	**Zn^{2+}**	**Cd^{2+}**	**Hg^{2+}**	*AAD*
Mn^{2+}	0.0	-0.1	-0.3	-0.5	-0.6	-0.1	-0.1	-0.4	0.2
Fe^{2+}	0.0	-0.1	-0.3	-0.5	-0.5	0.0	0.0	-0.2	0.2
Co^{2+}	0.0	-0.1	-0.2	-0.6	-0.6	-0.2	-0.1	-0.3	0.2
Ni^{2+}	0.0	-0.1	-0.2	-0.7	-0.7	-0.2	-0.2	-0.5	0.2
Cu^{2+}	0.0	0.0	N/A	-0.5	-0.4	0.0	0.0	-0.3	0.2
Zn^{2+}	-0.1	-0.2	-0.3	-0.6	-0.6	-0.1	0.0	-0.3	0.2
Cd^{2+}	0.0	N/A	-0.3	-0.4	-0.6	-0.2	-0.1	-0.4	0.2
Hg^{2+}	-0.1	-0.2	-0.2	-0.2	-0.4	-0.1	0.0	-0.4	0.1

Table S5: and values in kcal.mol^{-1} for

system: **MM**

model: ***TINY***

Single-point Structure with… optimized with…	**Mn^{2+}**	**Fe^{2+}**	**Co^{2+}**	**Ni^{2+}**	**Cu^{2+}**	**Zn^{2+}**	**Cd^{2+}**	**Hg^{2+}**	*AAD*
Mn^{2+}	-1.5	-3.9	-5.3	-10.0	-11.7	-2.3	0.0	-6.3	3.2
Fe^{2+}	-2.5	-4.9	-6.7	-11.3	-12.8	-2.8	0.0	-6.1	3.3
Co^{2+}	-3.0	N/A	-6.2	N/A	-11.9	-2.1	0.0	-6.2	3.2
Ni^{2+}	-3.1	-5.2	-5.9	-10.8	-12.3	-1.5	0.0	-5.9	3.1
Cu^{2+}	-1.2	N/A	-7.7	-10.3	N/A	0.0	-0.8	-8.4	4.1
Zn^{2+}	-2.6	N/A	-7.4	-11.4	-11.7	-2.8	0.0	-6.6	3.7
Cd^{2+}	0.0	N/A	-6.1	N/A	-11.0	-3.4	-2.0	-11.1	3.8
Hg^{2+}	0.0	N/A	-6.4	-9.7	-11.1	-5.3	-4.4	-14.4	3.8

Table S6: and values in kcal.mol^{-1} for

system: **MM**

model: ***SMALL***

Single-point Structure with… optimized with…	**Mn^{2+}**	**Fe^{2+}**	**Co^{2+}**	**Ni^{2+}**	**Cu^{2+}**	**Zn^{2+}**	**Cd^{2+}**	**Hg^{2+}**	*AAD*
Mn^{2+}	-0.7	-1.6	-1.7	-3.1	-3.1	-1.4	0.0	-2.0	0.8
Fe^{2+}	-1.0	-2.2	-2.3	-3.7	-3.5	-1.8	0.0	-1.8	0.9
Co^{2+}	-0.6	N/A	-1.8	N/A	-3.8	-1.1	0.0	-2.1	1.0
Ni^{2+}	-0.3	-1.2	-1.2	-2.7	-3.0	-0.8	0.0	-2.1	0.9
Cu^{2+}	-1.5	N/A	-6.7	-8.9	N/A	0.0	-0.7	-0.6	3.2
Zn^{2+}	-1.5	N/A	-3.2	-4.2	-4.7	-2.1	0.0	-1.5	1.4
Cd^{2+}	0.0	N/A	-1.8	N/A	-5.9	-0.8	0.0	-2.3	1.5
Hg^{2+}	0.0	N/A	-3.4	-6.9	-8.0	-0.9	0.0	-2.2	2.6

Table S7: and values in kcal.mol^{-1} for

system: **MM**

model: ***ALPHA***

Single-point Structure with… optimized with…	**Mn^{2+}**	**Fe^{2+}**	**Co^{2+}**	**Ni^{2+}**	**Cu^{2+}**	**Zn^{2+}**	**Cd^{2+}**	**Hg^{2+}**	*AAD*
Mn^{2+}	-1.0	-0.7	-0.7	-1.2	-2.1	-0.7	-0.6	0.0	0.4
Fe^{2+}	-0.9	-0.6	-0.6	-1.2	-1.9	-0.6	-0.6	0.0	0.4
Co^{2+}	-0.7	N/A	-0.3	N/A	-2.4	-0.4	-0.5	0.0	0.6
Ni^{2+}	-0.8	-0.6	-0.3	-0.7	-2.3	-0.5	-0.5	0.0	0.4
Cu^{2+}	-1.5	N/A	-4.6	-6.9	N/A	0.0	-2.4	-2.3	1.9
Zn^{2+}	-0.6	N/A	-0.5	-1.0	-1.8	-0.4	-0.4	0.0	0.4
Cd^{2+}	-0.2	N/A	0.0	N/A	-1.6	-0.5	-0.5	-0.7	0.4
Hg^{2+}	0.0	N/A	-1.4	-3.1	-3.3	-0.5	-0.3	-0.7	1.1

Table S8: and values in kcal.mol^{-1} for

system: **MM**

model: ***FULL_AA***

Single-point Structure with… optimized with…	**Mn^{2+}**	**Fe^{2+}**	**Co^{2+}**	**Ni^{2+}**	**Cu^{2+}**	**Zn^{2+}**	**Cd^{2+}**	**Hg^{2+}**	*AAD*
Mn^{2+}	-0.2	-0.1	0.0	-0.1	-0.3	-0.1	-0.1	0.0	0.1
Fe^{2+}	-0.2	-0.1	0.0	-0.2	-0.3	-0.1	-0.1	0.0	0.1
Co^{2+}	-0.3	N/A	0.0	N/A	-0.6	-0.2	-0.2	-0.2	0.1
Ni^{2+}	-0.3	-0.2	0.0	-0.2	-0.7	-0.3	-0.3	-0.2	0.1
Cu^{2+}	-1.7	N/A	-2.5	-3.1	N/A	0.0	-2.2	-1.8	0.7
Zn^{2+}	-0.1	N/A	-0.1	-0.1	-0.2	-0.1	-0.1	0.0	0.0
Cd^{2+}	-0.2	N/A	0.0	N/A	-0.4	-0.3	-0.3	-0.3	0.1
Hg^{2+}	0.0	N/A	-0.3	-1.0	-1.1	-0.1	0.0	-0.2	0.4

Table S9: and values in kcal.mol^{-1} for

system: **DHHD**

model: ***TINY***

Single-point Structure with… optimized with…	**Mn^{2+}**	**Fe^{2+}**	**Co^{2+}**	**Ni^{2+}**	**Cu^{2+}**	**Zn^{2+}**	**Cd^{2+}**	**Hg^{2+}**	*AAD*
Mn^{2+}	-1.1	-0.9	-0.5	-1.3	-0.7	0.0	-0.2	-0.3	0.4
Fe^{2+}	-0.9	-0.5	-0.3	-1.1	-1.2	0.0	-0.2	-0.4	0.4
Co^{2+}	-1.1	-1.3	-0.5	-1.3	-1.2	-0.1	0.0	0.0	0.5
Ni^{2+}	-1.2	0.0	-0.5	-1.3	-0.5	0.0	-0.1	-0.4	0.4
Cu^{2+}	-1.0	N/A	-0.4	-1.2	-0.4	0.0	-0.2	-0.1	0.4
Zn^{2+}	-0.9	-0.7	-0.2	-1.0	-1.1	0.0	-0.2	-0.4	0.4
Cd^{2+}	-0.9	-0.9	-2.9	-1.5	-0.7	0.0	-0.3	-0.4	0.6
Hg^{2+}	-0.9	-1.0	-0.9	-1.5	-0.5	0.0	-0.5	-0.5	0.3

Table S10: and values in kcal.mol^{-1} for

system: **DHHD**

model: ***SMALL***

Single-point Structure with… optimized with…	**Mn^{2+}**	**Fe^{2+}**	**Co^{2+}**	**Ni^{2+}**	**Cu^{2+}**	**Zn^{2+}**	**Cd^{2+}**	**Hg^{2+}**	*AAD*
Mn^{2+}	-0.8	-0.8	0.0	-0.7	-0.1	-0.1	-0.4	-0.5	0.3
Fe^{2+}	-0.9	-0.2	0.0	-1.1	-0.8	-0.2	-0.5	-0.6	0.3
Co^{2+}	-0.8	-0.7	0.0	-1.0	-0.7	-0.1	-0.1	-0.1	0.4
Ni^{2+}	-0.9	0.0	0.0	-0.8	0.0	0.0	-0.2	-0.3	0.3
Cu^{2+}	-0.9	N/A	-0.3	-1.0	0.0	-0.2	-0.5	-0.2	0.3
Zn^{2+}	-1.0	-0.6	0.0	-1.0	-0.7	-0.3	-0.6	-0.8	0.3
Cd^{2+}	-1.0	-0.8	-0.6	-1.1	0.0	-0.4	-0.8	-0.9	0.3
Hg^{2+}	-1.8	-1.6	-1.3	-1.6	0.0	-1.1	-1.8	-1.5	0.4

Table S11: and values in kcal.mol^{-1} for

system: **DHHD**

model: ***ALPHA***

Single-point Structure with… optimized with…	**Mn^{2+}**	**Fe^{2+}**	**Co^{2+}**	**Ni^{2+}**	**Cu^{2+}**	**Zn^{2+}**	**Cd^{2+}**	**Hg^{2+}**	*AAD*
Mn^{2+}	-0.8	-0.8	0.0	-0.7	-0.1	-0.3	-0.6	-0.7	0.3
Fe^{2+}	-0.9	-0.2	0.0	-1.0	-0.7	-0.4	-0.7	-0.8	0.3
Co^{2+}	-0.8	-0.6	0.0	-0.9	-0.6	-0.3	-0.4	-0.3	0.2
Ni^{2+}	-0.9	0.0	0.0	-0.9	-0.1	-0.3	-0.4	-0.4	0.3
Cu^{2+}	-0.9	N/A	-0.3	-1.0	0.0	-0.5	-0.7	-0.4	0.3
Zn^{2+}	-1.0	-0.5	0.0	-0.9	-0.6	-0.5	-0.8	-1.0	0.3
Cd^{2+}	-1.2	-0.9	-0.7	-1.1	0.0	-0.7	-1.1	-1.1	0.3
Hg^{2+}	-2.3	-1.9	-1.6	-1.8	0.0	-1.6	-2.4	-2.0	0.5

Table S12: and values in kcal.mol^{-1} for

system: **DHHD**

model: ***FULL_AA***

Single-point Structure with… optimized with…	**Mn^{2+}**	**Fe^{2+}**	**Co^{2+}**	**Ni^{2+}**	**Cu^{2+}**	**Zn^{2+}**	**Cd^{2+}**	**Hg^{2+}**	*AAD*
Mn^{2+}	-0.4	-0.3	0.0	-0.3	-0.2	0.0	-0.5	-0.7	0.2
Fe^{2+}	-0.6	N/A	0.0	-0.3	-0.3	-0.1	-0.6	-0.8	0.2
Co^{2+}	-0.5	-0.3	0.0	-0.3	-0.2	0.0	-0.2	-0.4	0.1
Ni^{2+}	-0.5	0.0	0.0	-0.2	0.0	0.0	-0.3	-0.6	0.2
Cu^{2+}	-0.3	N/A	-0.1	-0.3	-0.1	0.0	-0.2	-0.3	0.1
Zn^{2+}	-0.6	-0.9	0.0	-0.4	-0.3	-0.1	-0.5	-0.8	0.3
Cd^{2+}	-0.3	-0.3	-0.1	-0.3	-0.1	0.0	-0.4	-0.4	0.1
Hg^{2+}	-0.8	-0.9	-0.6	-0.8	0.0	-0.4	-1.0	-0.9	0.3

Table S13: and values in kcal.mol^{-1} for

system: **DNDO**

model: ***TINY***

Single-point Structure with… optimized with…	**Mn^{2+}**	**Fe^{2+}**	**Co^{2+}**	**Ni^{2+}**	**Cu^{2+}**	**Zn^{2+}**	**Cd^{2+}**	**Hg^{2+}**	*AAD*
Mn^{2+}	-0.7	-1.9	-0.9	-2.6	-3.2	-0.2	0.0	-2.8	1.1
Fe^{2+}	-0.7	-2.2	-0.9	-2.5	-3.6	-0.3	0.0	-3.2	1.2
Co^{2+}	-0.5	-1.0	-0.2	-1.7	-0.5	0.0	-0.3	-2.1	0.6
Ni^{2+}	-0.6	-1.1	0.0	-1.7	-0.9	N/A	-0.3	-2.2	0.6
Cu^{2+}	-0.5	-1.4	N/A	-2.3	-1.1	-0.2	0.0	-2.0	0.7
Zn^{2+}	-0.5	-1.1	N/A	-1.7	-0.5	0.0	-0.2	-2.0	0.6
Cd^{2+}	-0.7	-1.5	-1.6	-2.1	-2.1	-0.1	0.0	N/A	0.8
Hg^{2+}	-0.9	-1.7	N/A	-1.8	-2.2	N/A	0.0	-2.8	0.8

Table S14: and values in kcal.mol^{-1} for

system: **DNDO**

model: ***SMALL***

Single-point Structure with… optimized with…	**Mn^{2+}**	**Fe^{2+}**	**Co^{2+}**	**Ni^{2+}**	**Cu^{2+}**	**Zn^{2+}**	**Cd^{2+}**	**Hg^{2+}**	*AAD*
Mn^{2+}	-0.6	-1.5	-0.4	-2.4	-2.4	-0.2	0.0	-2.4	0.9
Fe^{2+}	-0.6	-1.9	-0.5	-2.4	-3.1	-0.4	0.0	-2.9	1.1
Co^{2+}	-0.6	-0.9	-0.1	-1.7	0.0	-0.2	-0.4	-2.0	0.6
Ni^{2+}	-0.7	-1.0	0.0	-1.8	-0.4	N/A	-0.5	-2.1	0.6
Cu^{2+}	-0.4	-1.2	N/A	-2.1	-0.3	-0.2	0.0	-1.7	0.7
Zn^{2+}	-0.6	-1.1	N/A	-1.7	0.0	-0.3	-0.4	-2.0	0.6
Cd^{2+}	-0.6	-1.2	-1.1	-1.4	-0.6	0.0	0.0	N/A	0.5
Hg^{2+}	-0.7	-1.3	N/A	-1.1	-0.4	N/A	0.0	-2.2	0.6

Table S15: and values in kcal.mol^{-1} for

system: **DNDO**

model: ***ALPHA***

Single-point Structure with… optimized with…	**Mn^{2+}**	**Fe^{2+}**	**Co^{2+}**	**Ni^{2+}**	**Cu^{2+}**	**Zn^{2+}**	**Cd^{2+}**	**Hg^{2+}**	*AAD*
Mn^{2+}	-0.1	-0.9	0.0	-2.1	-1.7	-0.5	0.0	-1.7	0.7
Fe^{2+}	-0.1	-1.2	-0.1	-2.2	-2.8	-0.6	0.0	-1.8	0.9
Co^{2+}	-0.6	-0.6	-0.3	-1.8	0.0	-0.6	-0.6	-1.5	0.4
Ni^{2+}	-0.5	-0.7	0.0	-1.6	-0.1	N/A	-0.6	-1.4	0.5
Cu^{2+}	-0.2	-0.7	N/A	-1.7	0.0	-0.4	-0.2	-1.3	0.5
Zn^{2+}	-0.8	-1.0	N/A	-1.9	0.0	-0.9	-0.9	-1.8	0.4
Cd^{2+}	-1.7	-1.7	-1.7	-1.8	0.0	-1.4	-1.6	N/A	0.4
Hg^{2+}	-1.9	-2.0	N/A	-1.5	0.0	N/A	-1.8	-3.2	0.7

Table S16: and values in kcal.mol^{-1} for

system: **DNDO**

model: ***FULL_AA***

Single-point Structure with… optimized with…	**Mn^{2+}**	**Fe^{2+}**	**Co^{2+}**	**Ni^{2+}**	**Cu^{2+}**	**Zn^{2+}**	**Cd^{2+}**	**Hg^{2+}**	*AAD*
Mn^{2+}	-0.2	-1.1	-0.4	-0.8	-1.5	-0.3	0.0	-0.9	0.4
Fe^{2+}	-0.1	-1.3	-0.5	-0.8	-2.0	-0.4	0.0	-1.2	0.5
Co^{2+}	-0.4	-0.7	-0.3	-0.7	0.0	-0.3	-0.5	-0.9	0.2
Ni^{2+}	-0.4	-0.8	0.0	-0.8	-0.3	N/A	-0.5	-0.9	0.3
Cu^{2+}	-0.1	-0.8	N/A	-0.9	0.0	-0.3	-0.2	-0.8	0.3
Zn^{2+}	-0.3	-0.8	N/A	-0.7	0.0	-0.3	-0.4	-0.9	0.2
Cd^{2+}	-0.3	-0.6	-0.1	0.0	-0.6	0.0	-0.3	N/A	0.2
Hg^{2+}	-0.8	-1.2	N/A	0.0	-0.8	N/A	-0.7	-1.4	0.3

Table S17: and values in kcal.mol^{-1} for

system: **CHCC**

model: ***TINY***

Single-point Structure with… optimized with…	**Mn^{2+}**	**Fe^{2+}**	**Co^{2+}**	**Ni^{2+}**	**Cu^{2+}**	**Zn^{2+}**	**Cd^{2+}**	**Hg^{2+}**	*AAD*
Mn^{2+}	-2.5	-7.3	-5.1	-6.9	-7.7	-1.5	0.0	-4.8	2.4
Fe^{2+}	-4.0	-7.1	-6.0	-7.1	-6.4	-1.8	0.0	-4.8	2.0
Co^{2+}	-3.6	-7.2	-5.6	-6.9	-6.4	-1.3	0.0	-4.9	2.1
Ni^{2+}	-4.7	-8.3	-7.5	-8.2	-7.7	-2.3	0.0	-5.7	2.4
Cu^{2+}	-4.7	-8.2	-7.8	-8.5	-7.5	-2.5	0.0	-5.1	2.4
Zn^{2+}	-3.4	-6.9	-5.9	-7.3	-5.9	-1.5	0.0	-4.7	2.1
Cd^{2+}	-1.4	-4.9	-4.2	-6.0	-6.1	-1.5	0.0	-5.4	2.1
Hg^{2+}	-0.5	-4.3	-4.7	-6.4	-7.1	-1.6	0.0	-6.2	2.4

Table S18: and values in kcal.mol^{-1} for

system: **CHCC**

model: ***SMALL***

Single-point Structure with… optimized with…	**Mn^{2+}**	**Fe^{2+}**	**Co^{2+}**	**Ni^{2+}**	**Cu^{2+}**	**Zn^{2+}**	**Cd^{2+}**	**Hg^{2+}**	*AAD*
Mn^{2+}	-1.7	-2.7	-2.1	-3.4	-2.1	-0.8	0.0	-2.5	0.8
Fe^{2+}	-2.5	-3.5	-3.0	-4.3	-2.9	-1.4	0.0	-2.9	0.9
Co^{2+}	-2.9	-3.8	-3.4	-4.7	-3.6	-1.7	0.0	-3.0	1.0
Ni^{2+}	-2.3	-3.5	-3.2	-4.4	-3.4	-1.3	0.0	-2.6	1.0
Cu^{2+}	-3.9	-4.9	-4.9	-6.5	-5.5	-2.9	0.0	-3.8	1.4
Zn^{2+}	-2.4	-3.3	-3.0	-4.5	-2.9	-1.5	0.0	-2.7	0.9
Cd^{2+}	-1.0	-2.1	-1.6	-2.9	-1.7	-0.5	0.0	-3.1	0.8
Hg^{2+}	-0.6	-2.0	-2.3	-3.2	-2.2	-0.6	0.0	-2.9	1.0

Table S19: and values in kcal.mol^{-1} for

system: **CHCC**

model: ***ALPHA***

Single-point Structure with… optimized with…	**Mn^{2+}**	**Fe^{2+}**	**Co^{2+}**	**Ni^{2+}**	**Cu^{2+}**	**Zn^{2+}**	**Cd^{2+}**	**Hg^{2+}**	*AAD*
Mn^{2+}	-1.4	-2.3	-2.0	-3.3	-2.5	-0.9	0.0	-1.8	0.8
Fe^{2+}	-1.8	-2.9	-2.5	-3.8	-2.9	-1.1	0.0	-1.7	0.9
Co^{2+}	-2.2	-3.2	-3.0	-4.4	-3.6	-1.4	0.0	-1.9	1.1
Ni^{2+}	-2.4	-3.6	-3.6	-4.8	-4.4	-1.8	0.0	-2.3	1.2
Cu^{2+}	-2.6	-3.7	-4.1	-5.6	-5.1	-2.1	0.0	-2.3	1.4
Zn^{2+}	-1.7	-2.7	-2.5	-4.0	-2.8	-1.2	0.0	-1.6	0.9
Cd^{2+}	-0.8	-1.8	-1.5	-2.8	-2.0	-0.6	0.0	-2.1	0.7
Hg^{2+}	-0.7	-1.8	-2.1	-3.0	-2.4	-0.7	0.0	-2.6	0.9

Table S20: and values in kcal.mol^{-1} for

system: **CHCC**

model: ***FULL_AA***

Single-point Structure with… optimized with…	**Mn^{2+}**	**Fe^{2+}**	**Co^{2+}**	**Ni^{2+}**	**Cu^{2+}**	**Zn^{2+}**	**Cd^{2+}**	**Hg^{2+}**	*AAD*
Mn^{2+}	-0.9	-1.2	-0.7	-1.1	0.0	-0.5	-0.7	-1.5	0.3
Fe^{2+}	-1.0	-1.2	-0.7	-1.0	0.0	-0.5	-0.7	-1.4	0.3
Co^{2+}	-1.0	-1.1	-0.7	-1.0	0.0	-0.4	-0.6	-1.3	0.3
Ni^{2+}	-0.7	-0.8	-0.4	-0.8	0.0	-0.2	-0.4	-1.2	0.3
Cu^{2+}	-0.5	-0.5	-0.3	-0.7	0.0	0.0	-0.2	-1.0	0.3
Zn^{2+}	-1.0	-1.2	-0.8	-1.1	0.0	-0.5	-0.7	-1.3	0.3
Cd^{2+}	-0.7	-1.1	-0.6	-1.1	0.0	-0.4	-0.6	-1.5	0.3
Hg^{2+}	-0.4	-0.9	-0.6	-1.0	0.0	-0.1	-0.3	-1.2	0.4

Table S21: and values in kcal.mol^{-1} for

system: **DDSOEE**

model: ***TINY***

Single-point Structure with… optimized with…	**Mn^{2+}**	**Fe^{2+}**	**Co^{2+}**	**Ni^{2+}**	**Cu^{2+}**	**Zn^{2+}**	**Cd^{2+}**	**Hg^{2+}**	*AAD*
Mn^{2+}	-1.3	-1.3	-0.6	-1.9	-1.9	0.0	-0.9	-3.8	0.8
Fe^{2+}	-1.3	-1.4	-0.4	-1.5	-1.6	0.0	-1.1	-3.5	0.7
Co^{2+}	-1.5	-1.3	0.0	-2.2	-2.2	-0.2	-1.2	-4.2	1.0
Ni^{2+}	-1.4	N/A	-0.7	-1.8	-1.8	0.0	-1.1	-4.2	0.9
Cu^{2+}	-1.7	-3.2	N/A	-1.5	-0.6	0.0	-1.4	-4.7	1.2
Zn^{2+}	-1.3	-1.3	-0.7	-1.9	-1.9	0.0	-1.0	-4.0	0.8
Cd^{2+}	-1.6	-2.0	-1.9	-2.8	-3.3	0.0	-0.7	-3.9	1.0
Hg^{2+}	-1.3	-1.8	-1.9	-2.8	-2.7	0.0	-0.1	-3.0	0.9

Table S22: and values in kcal.mol^{-1} for

system: **DDSOEE**

model: ***SMALL***

Single-point Structure with… optimized with…	**Mn^{2+}**	**Fe^{2+}**	**Co^{2+}**	**Ni^{2+}**	**Cu^{2+}**	**Zn^{2+}**	**Cd^{2+}**	**Hg^{2+}**	*AAD*
Mn^{2+}	-0.7	-0.5	-0.6	-1.6	-1.4	0.0	-0.5	-2.2	0.6
Fe^{2+}	-0.9	-0.4	-0.1	-1.2	-1.1	0.0	-0.7	-2.8	0.6
Co^{2+}	-0.5	-0.1	-1.5	-1.5	-1.7	0.0	-0.3	-2.0	0.7
Ni^{2+}	-0.6	N/A	-0.5	-1.3	-1.4	0.0	-0.4	-1.9	0.6
Cu^{2+}	-0.5	-1.0	N/A	-1.2	-1.2	0.0	-0.3	-2.5	0.6
Zn^{2+}	-0.7	-0.3	-0.6	-1.4	-1.4	0.0	-0.4	-2.1	0.6
Cd^{2+}	-0.9	-1.0	-1.4	-2.2	-1.8	0.0	-0.3	-2.4	0.7
Hg^{2+}	-0.8	-0.9	-1.5	-2.2	-1.4	-0.1	0.0	-2.0	0.7

Table S23: and values in kcal.mol^{-1} for

system: **DDSOEE**

model: ***ALPHA***

Single-point Structure with… optimized with…	**Mn^{2+}**	**Fe^{2+}**	**Co^{2+}**	**Ni^{2+}**	**Cu^{2+}**	**Zn^{2+}**	**Cd^{2+}**	**Hg^{2+}**	*AAD*
Mn^{2+}	-0.2	-0.2	0.0	-1.6	-1.7	-0.3	-0.2	-1.0	0.6
Fe^{2+}	-0.2	-0.2	0.0	-1.6	-1.9	-0.3	-0.2	-0.8	0.6
Co^{2+}	-0.4	-0.2	0.0	-1.7	-2.3	-0.5	-0.4	-1.0	0.7
Ni^{2+}	-0.2	N/A	0.0	-1.5	-1.8	-0.4	-0.3	-0.8	0.5
Cu^{2+}	0.0	-0.9	N/A	-1.2	-1.4	-0.1	0.0	-1.0	0.5
Zn^{2+}	-0.3	-0.2	0.0	-1.6	-2.0	-0.4	-0.3	-1.0	0.6
Cd^{2+}	-0.2	-0.5	-1.0	-1.9	-2.1	0.0	-0.1	-1.5	0.7
Hg^{2+}	-0.2	-0.5	-0.9	-1.7	-1.5	-0.1	0.0	-1.4	0.6

Table S24: and values in kcal.mol^{-1} for

system: **DDSOEE**

model: ***FULL_AA***

Single-point Structure with… optimized with…	**Mn^{2+}**	**Fe^{2+}**	**Co^{2+}**	**Ni^{2+}**	**Cu^{2+}**	**Zn^{2+}**	**Cd^{2+}**	**Hg^{2+}**	*AAD*
Mn^{2+}	-0.2	-0.2	0.0	-0.4	-0.2	0.0	-0.2	-0.5	0.1
Fe^{2+}	0.0	-0.5	-0.1	-0.4	-0.2	0.0	-0.1	-0.3	0.2
Co^{2+}	-0.2	-0.1	-0.1	-0.4	-0.5	0.0	-0.2	-0.4	0.2
Ni^{2+}	-0.2	N/A	-0.2	-0.4	-0.5	0.0	-0.1	-0.4	0.2
Cu^{2+}	-0.4	-0.5	N/A	-0.6	-0.3	0.0	-0.2	-0.7	0.2
Zn^{2+}	-0.2	-0.2	-0.1	-0.4	-0.4	0.0	-0.1	-0.4	0.1
Cd^{2+}	-0.1	-0.4	-0.4	-0.4	-0.7	0.0	-0.1	-0.6	0.2
Hg^{2+}	0.0	-0.3	-0.4	-0.3	-0.2	0.0	0.0	-0.5	0.2

Table S25: Number of hydrogen bonds to metal-ion binding atoms in Zn^{2+}-optimized structures. Only hydrogen bonds to atoms directly ligating the central metal ion are considered. See **Table 3**.

System / Model	CC	DHHD	DNDO	CHCC	DDSOEE
TINY	0	0	1	0	0
SMALL	0	0	1	0	0
ALFA	0	0	1	0	0
FULL_AA	1	1	4	3	4
FULL PEPTIDE	1	1	5	4	4

Table S26: and values in kcal.mol^{-1}. See **Table 3**.

system: **ester analogues based on Zn^{2+}-optimized structures of their peptide analogues**

model: ***TINY***

Single-point with… System	**Mn^{2+}**	**Fe^{2+}**	**Co^{2+}**	**Ni^{2+}**	**Cu^{2+}**	**Zn^{2+}**	**Cd^{2+}**	**Hg^{2+}**	*AAD*
CC	-1.56	-1.84	-2.64	-6.04	-6.41	-0.19	0.00	-3.15	1.85
DHHD	-1.25	-0.96	-0.59	-0.81	-1.08	0.00	-0.62	-1.07	0.42
DNDO	-0.97	-0.94	-0.42	-0.80	-1.43	0.00	-1.15	-3.07	0.20
CHCC	-2.36	-5.88	-4.79	-5.35	-5.13	-0.39	0.00	-3.40	0.17
DDSOEE	-1.97	-2.44	-1.26	-1.42	-1.23	0.00	-1.94	-5.14	0.22

Table S27: and values in kcal.mol^{-1}. See **Table 3**.

system: **ester analogues based on Zn^{2+}-optimized structures of their peptide analogues**

model: ***SMALL***

Single-point with… System	**Mn^{2+}**	**Fe^{2+}**	**Co^{2+}**	**Ni^{2+}**	**Cu^{2+}**	**Zn^{2+}**	**Cd^{2+}**	**Hg^{2+}**	*AAD*
CC	-0.37	-0.11	-0.78	-1.23	-1.40	-0.36	0.00	-0.76	0.42
DHHD	-1.02	-0.44	-0.06	-0.47	-0.36	0.00	-0.73	-1.15	0.20
DNDO	-0.82	-0.34	-0.09	-0.53	-0.55	0.00	-1.11	-2.69	0.17
CHCC	-1.33	-2.34	-1.86	-2.56	-2.17	-0.39	0.00	-1.36	0.22
DDSOEE	-1.35	-1.48	-1.16	-0.98	-0.82	0.00	-1.34	-3.24	0.23

Table S28: and values in kcal.mol^{-1}. See **Table 3**.

system: **ester analogues based on Zn^{2+}-optimized structures of their peptide analogues**

model: ***ALPHA***

Single-point with… / **System**	**Mn^{2+}**	**Fe^{2+}**	**Co^{2+}**	**Ni^{2+}**	**Cu^{2+}**	**Zn^{2+}**	**Cd^{2+}**	**Hg^{2+}**	*AAD*
CC	-0.59	0.00	-0.73	-1.00	-0.73	-0.63	-0.59	-0.91	0.20
DHHD	-0.98	-0.27	0.00	-0.35	-0.21	-0.15	-0.94	-1.28	0.17
DNDO	-0.48	-0.23	-0.04	-0.30	0.00	-0.08	-0.88	-1.86	0.22
CHCC	-0.61	-1.69	-1.36	N/A	-2.02	-0.09	0.00	-0.35	0.23
DDSOEE	-0.60	-1.00	-0.16	-0.77	-0.99	0.00	-0.86	-1.74	0.35

Table S29: and values in kcal.mol^{-1}. See **Table 3**.

system: **ester analogues based on Zn^{2+}-optimized structures of their peptide analogues**

model: ***FULL_AA***

Single-point with… / **System**	**Mn^{2+}**	**Fe^{2+}**	**Co^{2+}**	**Ni^{2+}**	**Cu^{2+}**	**Zn^{2+}**	**Cd^{2+}**	**Hg^{2+}**	*AAD*
CC	-0.05	0.00	-0.21	-0.42	-0.57	-0.12	-0.24	-0.47	0.17
DHHD	-0.63	-0.19	0.00	-0.38	-0.24	-0.15	-0.52	-0.80	0.22
DNDO	-0.11	0.00	-0.03	-0.17	-0.41	-0.05	-0.43	-0.88	0.23
CHCC	-0.53	-0.89	-0.78	-1.11	-1.40	-0.18	0.00	-0.72	0.35
DDSOEE	-0.42	N/A	-0.25	-0.42	0.00	-0.05	-0.40	-0.74	0.19

Table S30: and values in kcal.mol^{-1}. See **Table 4**.

system: **norvaline analogues of DNDO system peptide analogues based on Fe^{2+} optimized str.**

Single-point with… System	Mn^{2+}	Fe^{2+}	Co^{2+}	Ni^{2+}	Cu^{2+}	Zn^{2+}	Cd^{2+}	Hg^{2+}	*AAD*
TINY	-0.6	-1.3	-0.6	-2.3	-2.0	0.0	0.0	-2.6	0.9
SMALL	-0.5	-1.0	-0.1	-2.1	-1.5	0.0	0.0	-2.2	0.8
ALPHA	-0.2	-0.6	0.0	-2.2	-1.5	-0.5	-0.3	-1.4	0.6
FULL_AA	0.0	-0.4	-0.2	-0.5	-0.4	-0.1	0.0	-0.5	0.2

Table S31: and values in kcal.mol^{-1}. See **Table 4**.

system:**norvaline analogues of DNDO system peptide analogues based on Co^{2+} optimized str.**

Single-point with… System	Mn^{2+}	Fe^{2+}	Co^{2+}	Ni^{2+}	Cu^{2+}	Zn^{2+}	Cd^{2+}	Hg^{2+}	*AAD*
TINY	-0.5	-1.0	-0.2	-1.6	-1.6	0.0	-0.2	-2.0	0.7
SMALL	-0.5	-0.8	0.0	-1.6	-1.1	-0.1	-0.3	-1.9	0.5
ALPHA	-0.2	-0.3	0.0	-1.5	-0.9	-0.4	-0.3	-1.2	0.4
FULL_AA	0.0	-0.4	0.0	-0.4	-0.9	0.0	-0.1	-0.5	0.2

Table S32: and values in kcal.mol^{-1}. See **Table 5**.

system: **CCWW , Mn^{2+}-optimized**

Single-point with… System	Mn^{2+}	Fe^{2+}	Co^{2+}	Ni^{2+}	Cu^{2+}	Zn^{2+}	Cd^{2+}	Hg^{2+}	*AAD*
TINY	-1.1	N/A	-4.6	-3.9	-4.8	-1.1	0.0	-2.9	1.6
SMALL	-0.6	N/A	-1.5	-2.0	-2.6	-0.7	0.0	-0.9	0.7
ALPHA	-0.3	N/A	-1.5	-1.3	-2.7	-0.6	0.0	-0.4	0.7
FULL_AA	0.0	N/A	-0.2	0.0	-0.5	0.0	-0.1	-0.2	0.1

Table S33 and values in kcal.mol^{-1}. See **Table 5**

system: **based on Co^{2+}-optimized str. of DNDO; 2 water molecules removed**

system optimized

Single-point with… System	**Mn^{2+}**	**Fe^{2+}**	**Co^{2+}**	**Ni^{2+}**	**Cu^{2+}**	**Zn^{2+}**	**Cd^{2+}**	**Hg^{2+}**	*AAD*
TINY	-0.7	-0.7	-0.3	-2.5	-1.9	-0.8	0.0	-2.6	0.9
SMALL	-0.3	-0.6	0.0	-2.2	-0.6	-0.8	0.0	-2.1	0.7
ALPHA	0.0	-0.4	-0.2	-2.1	-0.1	-1.0	0.0	-0.6	0.5
FULL_AA	-0.2	0.0	-0.6	-1.3	-0.1	-0.9	-0.3	-0.6	0.4

Table S34 and values in kcal.mol^{-1}. See **Table 5**

system: **based on Co^{2+}-optimized str. of DNDO; 2 water molecules removed**

system NOT optimized

Single-point with… System	**Mn^{2+}**	**Fe^{2+}**	**Co^{2+}**	**Ni^{2+}**	**Cu^{2+}**	**Zn^{2+}**	**Cd^{2+}**	**Hg^{2+}**	*AAD*
TINY	-0.7	-1.7	-0.1	-1.3	-3.3	0.0	-0.3	-3.4	1.1
SMALL	-1.0	-1.7	0.0	-1.2	-2.8	-0.5	-0.8	-3.3	0.9
ALPHA	-1.1	-1.7	0.0	-0.8	-1.8	-1.0	-1.0	-1.6	0.4
FULL_AA	-0.6	-1.1	-0.1	0.0	-1.0	-0.6	-0.6	-1.0	0.3

Table S35 and values in kcal.mol^{-1}. See **Table 5**

system: **based on Hg^{2+}-optimized str. of DNDO; 2 water molecules removed**

system optimized

Single-point with… System	**Mn^{2+}**	**Fe^{2+}**	**Co^{2+}**	**Ni^{2+}**	**Cu^{2+}**	**Zn^{2+}**	**Cd^{2+}**	**Hg^{2+}**	*AAD*
TINY	-0.4	-1.1	-0.7	-1.9	-5.0	-0.1	0.0	-2.9	1.3
SMALL	-0.3	-0.7	-0.1	-0.9	-4.2	-0.2	0.0	-2.5	1.1
ALPHA	-0.8	-1.0	0.0	-0.6	-2.2	-0.8	-0.5	-1.4	0.4
FULL_AA	-0.7	-0.8	0.0	-0.5	-2.1	-0.8	-0.5	-1.0	0.4

Table S36 and values in kcal.mol^{-1}. See **Table 5**

system: **based on Hg^{2+}-optimized str. of DNDO; 2 water molecules removed**

system NOT optimized

Single-point with… System	**Mn^{2+}**	**Fe^{2+}**	**Co^{2+}**	**Ni^{2+}**	**Cu^{2+}**	**Zn^{2+}**	**Cd^{2+}**	**Hg^{2+}**	*AAD*
TINY	0.0	-1.0	-4.7	-8.7	-9.2	-0.6	0.0	-3.2	3.1
SMALL	0.0	-0.5	-3.3	-6.9	-7.0	-0.5	-0.1	-2.5	2.3
ALPHA	-0.4	0.0	-1.8	-4.1	-4.8	-0.1	-0.2	-0.7	1.5
FULL_AA	-0.2	0.0	-0.9	-2.4	-2.7	-0.2	-0.1	-0.2	0.9