Electronic Supplementary Information

The influence of penicillamine/cysteine mutation on the metal complexes of peptides

Ágnes Grenács[a], Norbert Lihi[b], Imre Sóvágó[a], Katalin Várnagy[a]*

[a]*Department of Inorganic and Analytical Chemistry, University of Debrecen, H-4032, Debrecen, Hungary.*

[b]*MTA-DE Redox and Homogeneous Catalytic Reaction Mechanisms Research Group, University of Debrecen, H-4032, Debrecen, Hungary.*

* Corresponding author: Tel.: +3652 512900/22405 Fax.: +3652 518660 E-mail: varnagy.katalin@science.unideb.hu (K. Várnagy)

Figure S1
Concentration distribution of the various protonated forms of the peptide Pen-SSACS-NH_2. (c = 2 mM)

Figure S2
pH-dependent chemical shift values of the ^1H NMR spectra of the free Pen-SSACS-NH_2 peptide (black) and the nickel(II) containing system Ni(II):L=1:2 (grey) (c_L=0.005 M)

Figure S3
CD spectra of the nickel(II)-CSSA-Pen-S-NH_2 system at different pH values and 1:2 ratio. ($c_{Ni(II)}$ = 1 mM)

FigureS4
Sum of Ni(II)-Pen-SSACS-NH_2 and Ni(II)-CSSA-Pen-S-NH_2 complexes formed in the Ni(II) – Pen-SSACS-NH_2 – CSSA-Pen-S-NH_2 system at 1:2:2 ratio in the function of pH ($c_{Ni(II)}$ = 2.0 mM)

Figure S5
Concentration distribution of the species formed in the cadmium(II)-PenSSACS-NH_2 system at 1:1 ratio ($c_{Cd(II)}$ = 2 mM) and molar absorptivities measured at λ = 230 nm ($c_{Cd(II)}$ = 0.15 mM).

Figure S6
Concentration distribution of the species formed in the cadmium(II)-PenSSACS-NH_2 system at 1:2 ratio ($c_{Cd(II)}$ = 1 mM) and molar absorptivities measured at λ = 230 nm ($c_{Cd(II)}$ = 0.15 mM).

Figure S7
Concentration distribution of the species formed in the zinc(II)-CSSA-Pen-S-NH_2 system at 1:2 ratio ($c_{Zn(II)}$ = 1 mM).

Figure S8
Concentration distribution of the species formed in the cadmium(II)-CSSA-Pen-S-NH_2 system at 1:2 ratio ($c_{Cd(II)}$ = 1 mM).

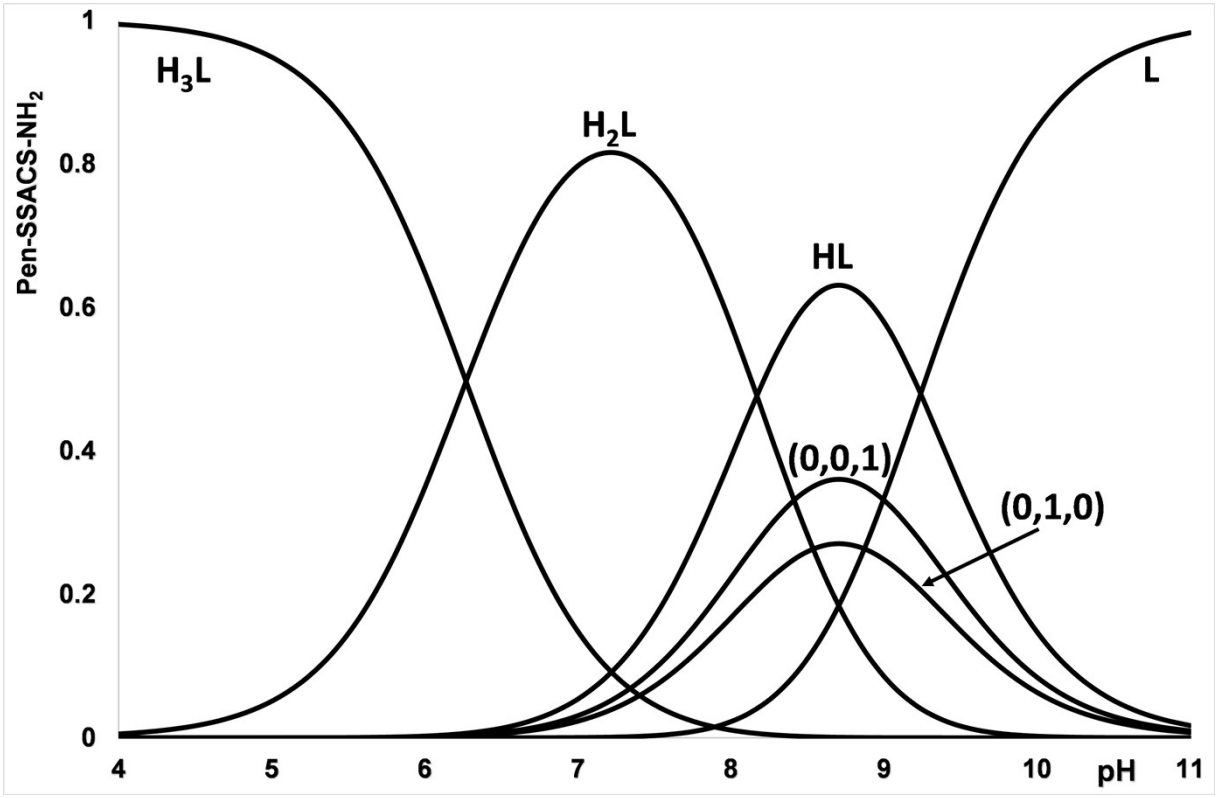
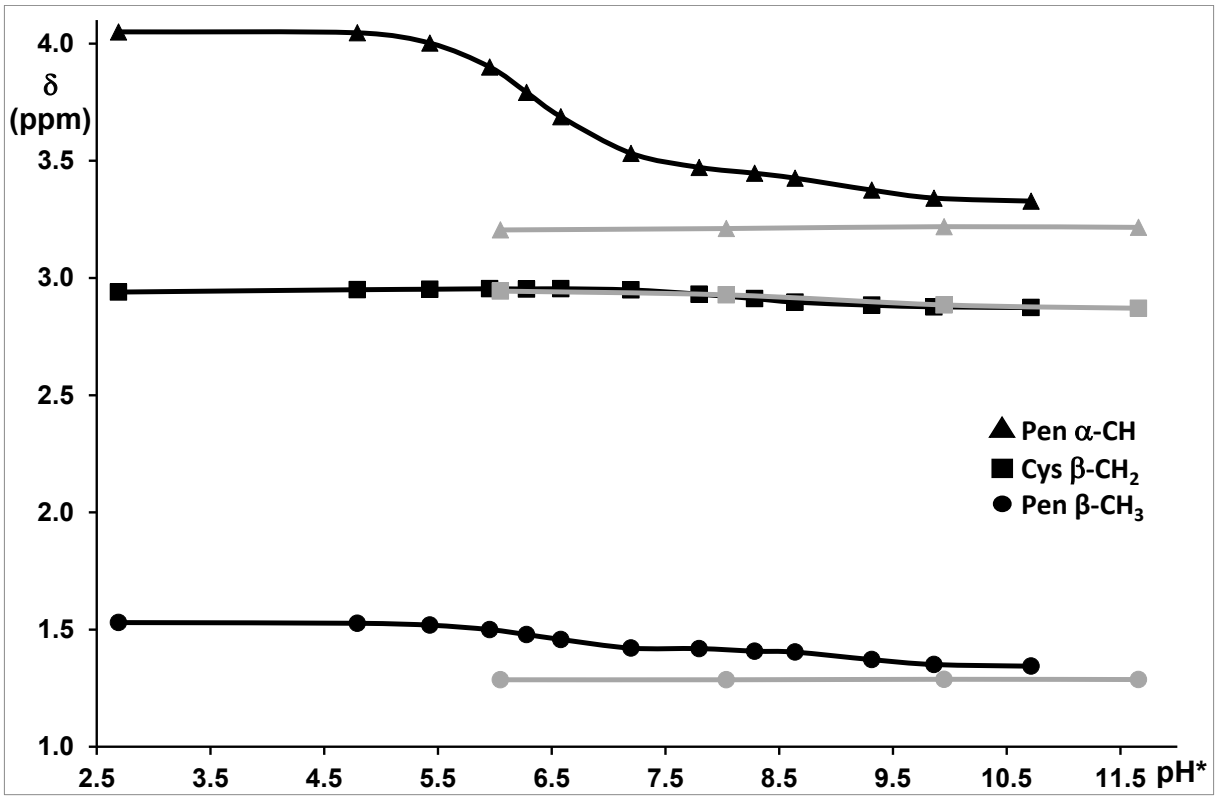


Figure S1


4.0
δ
(ppm)
3.5
3.0
2.5
2.0
1.5
1.0
2.5
3.5
4.5
5.5
6.5
7.5
8.5
9.5
10.5
11.5
pH*
Pen α-CH
Cys β-CH2
Pen β-CH3
Figure S2

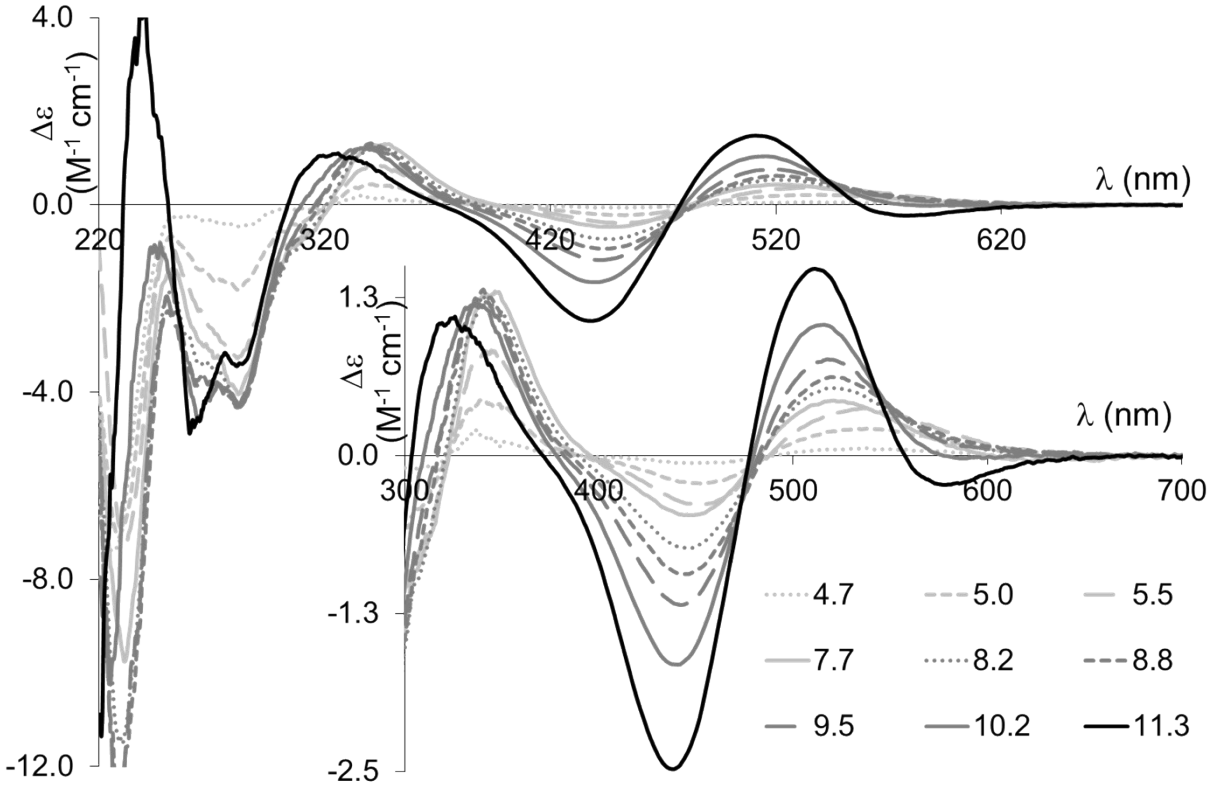

4.0
0.0
-4.0
-8.0
-12.0
Δε (M-1 cm-1)
220
320
420
520
620
λ (nm)
1.3
-1.3
-2.5
300
400
500
600
700
4.7
5.0
5.5
7.7
8.2
8.8
9.5
10.2
11.3

Figure S3

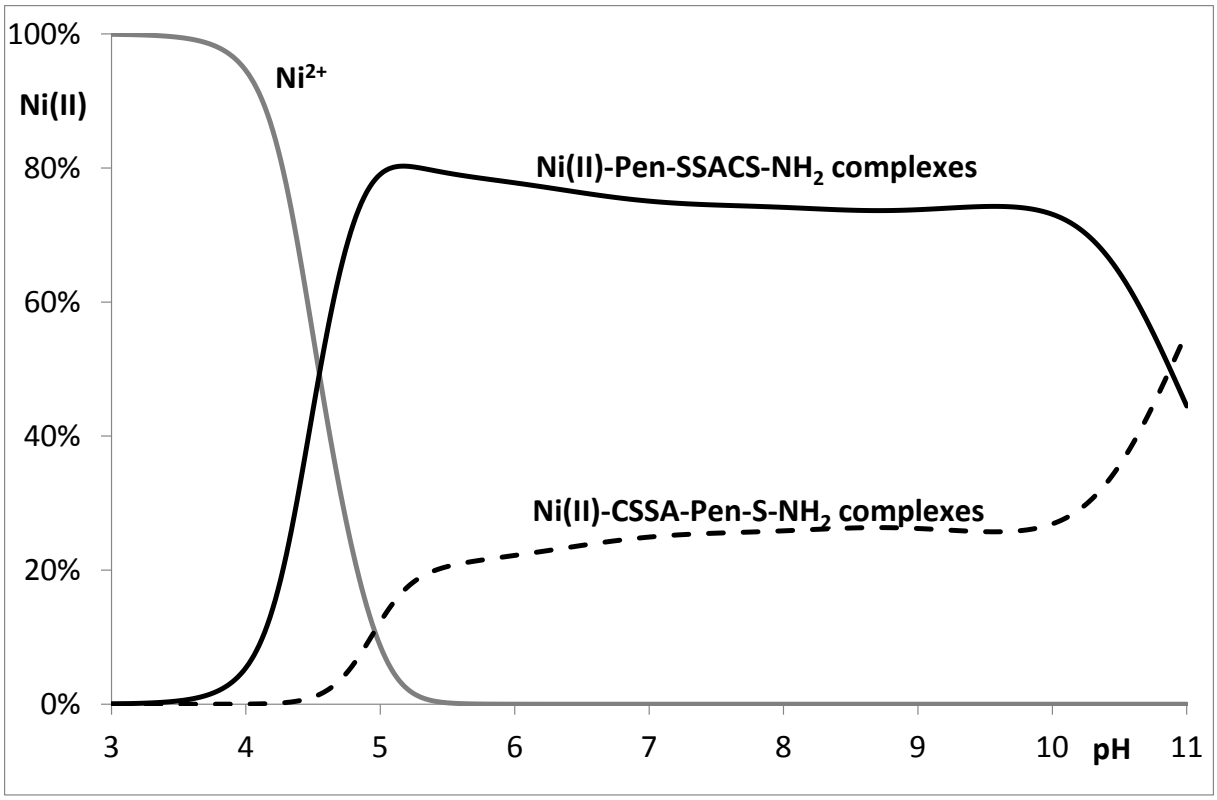
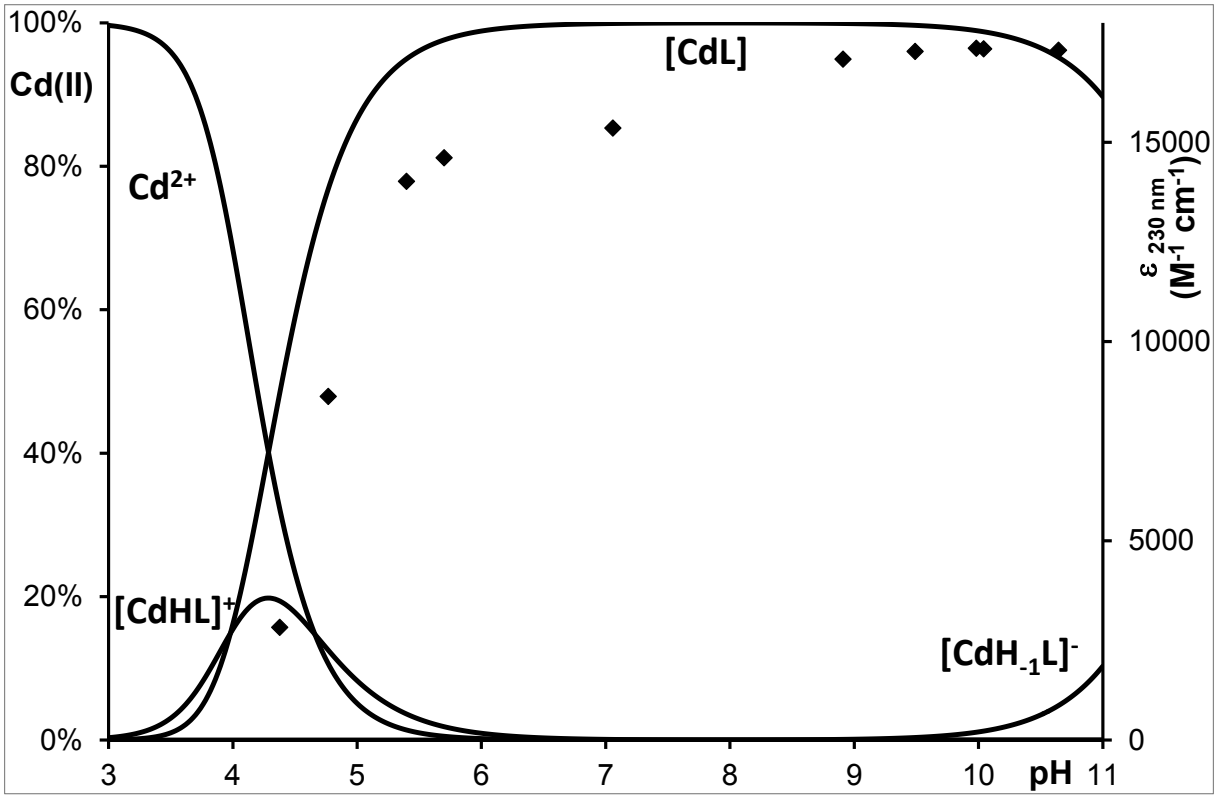
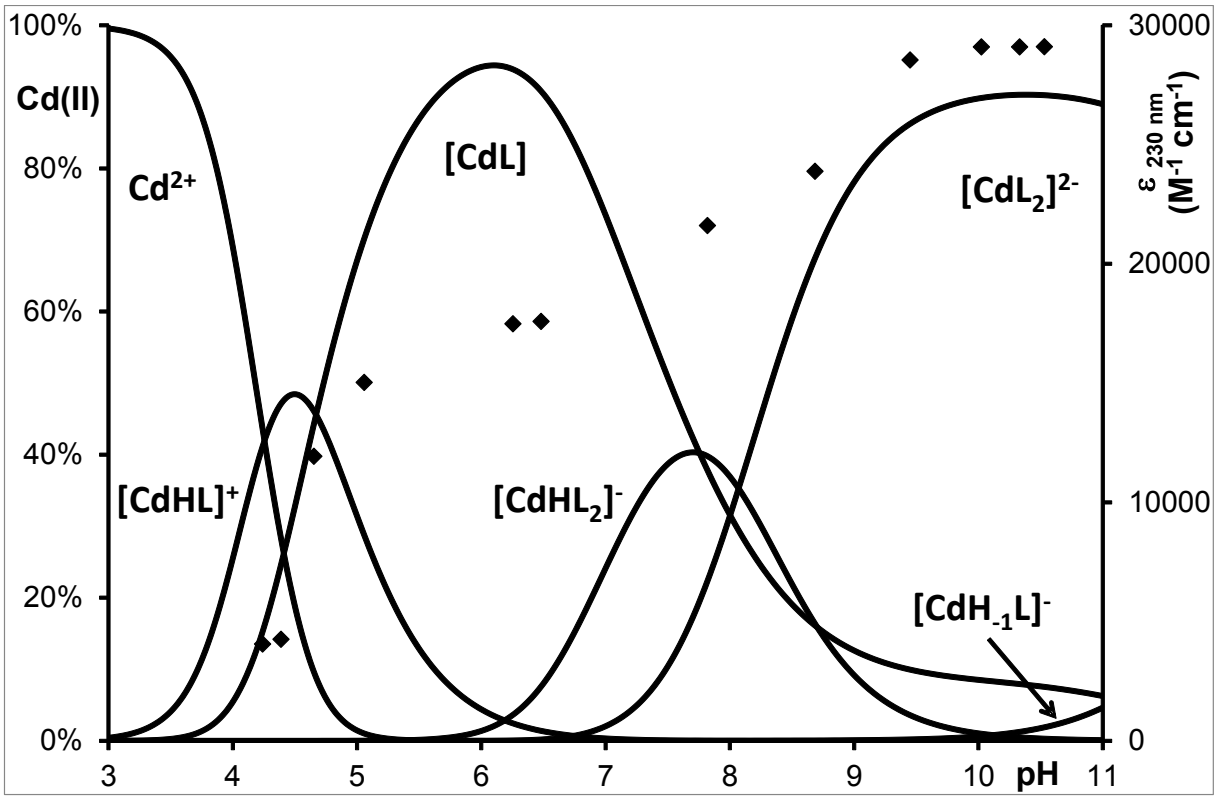
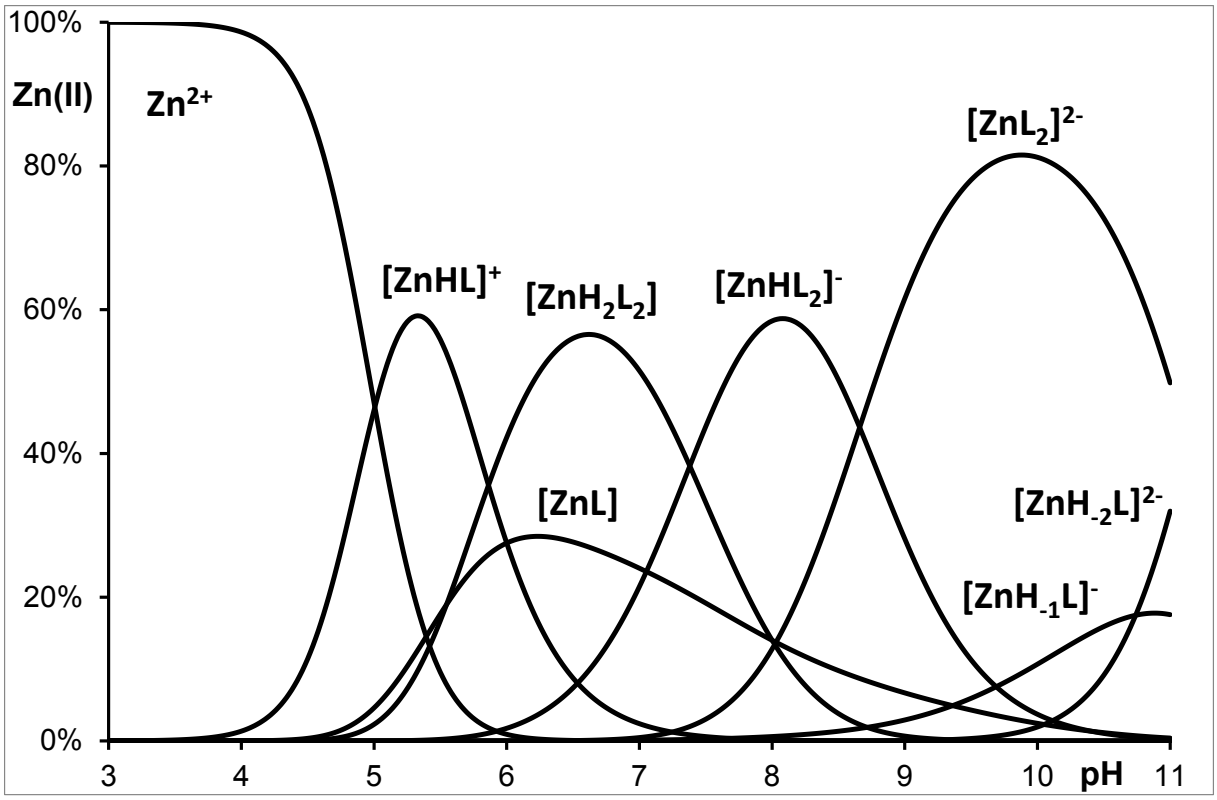
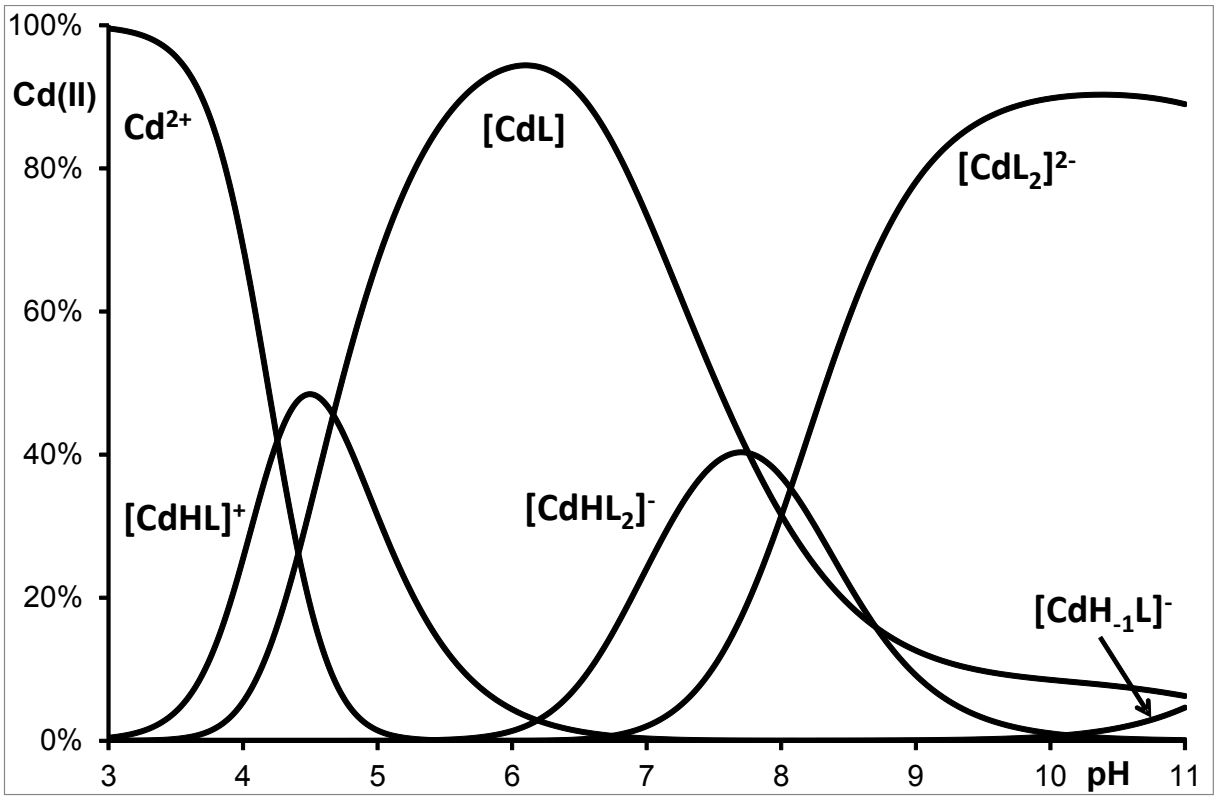

100%
Ni(II)
80%
60%
40%
20%
0%
Ni2+
Ni(II)-Pen-SSACS-NH2 complexes
Ni(II)-CSSA-Pen-S-NH2 complexes
3
4
5
6
7
8
9
10
pH
11

Figure S4


100%
Cd(II)
80%
60%
40%
20%
0%
Cd2+
[CdL]
[CdHL]+
[CdH-1L]-
15000
10000
5000
0
ε 230 nm (M-1 cm-1)
3
4
5
6
7
8
9
10
pH
11
Figure S5


100%
80%
60%
40%
20%
0%
Cd(II)
Cd2+
[CdL]
[CdL2]2-
[CdHL]+
[CdHL2]-
[CdH-1L]-
30000
20000
10000
0
ε 230 nm (M-1 cm-1)
3
4
5
6
7
8
9
10
11
pH
Figure S6


100%
Zn(II)
80%
60%
40%
20%
0%
Zn2+
[ZnHL]+
[ZnH2L2]
[ZnHL2]-
[ZnL2]2-
[ZnL]
[ZnH-2L]2-
[ZnH-1L]-
3
4
5
6
7
8
9
10
pH
11
Figure S7


100%
Cd(II)
80%
60%
40%
20%
0%
Cd2+
[CdL]
[CdL2]2-
[CdHL]+
[CdHL2]-
[CdH-1L]-
3
4
5
6
7
8
9
10
pH
11
Figure S8