

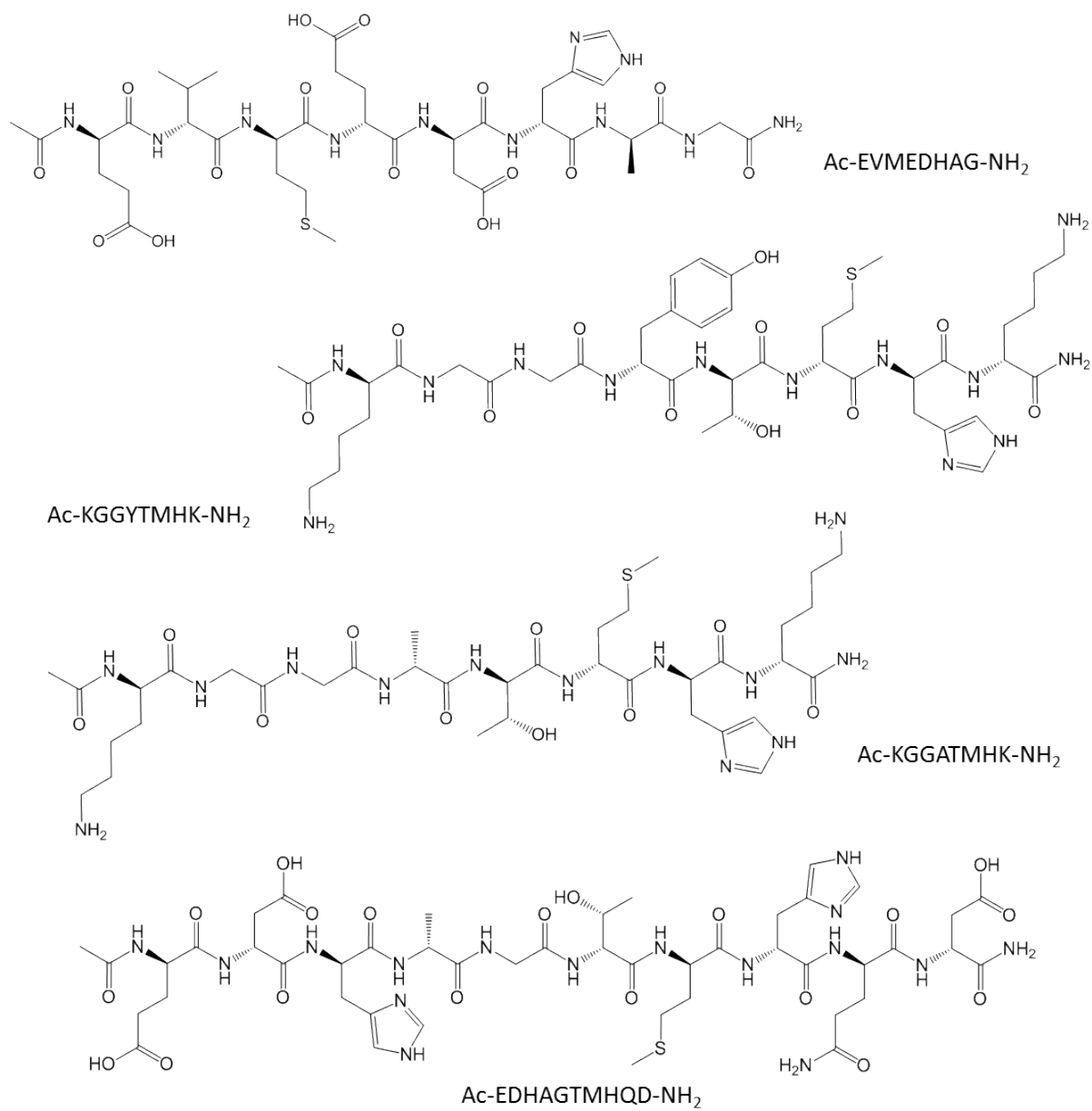
Electronic Supplementary Information

Thermodynamic and structural characterization of the nickel(II) and zinc(II) complexes of various peptide fragments of tau protein

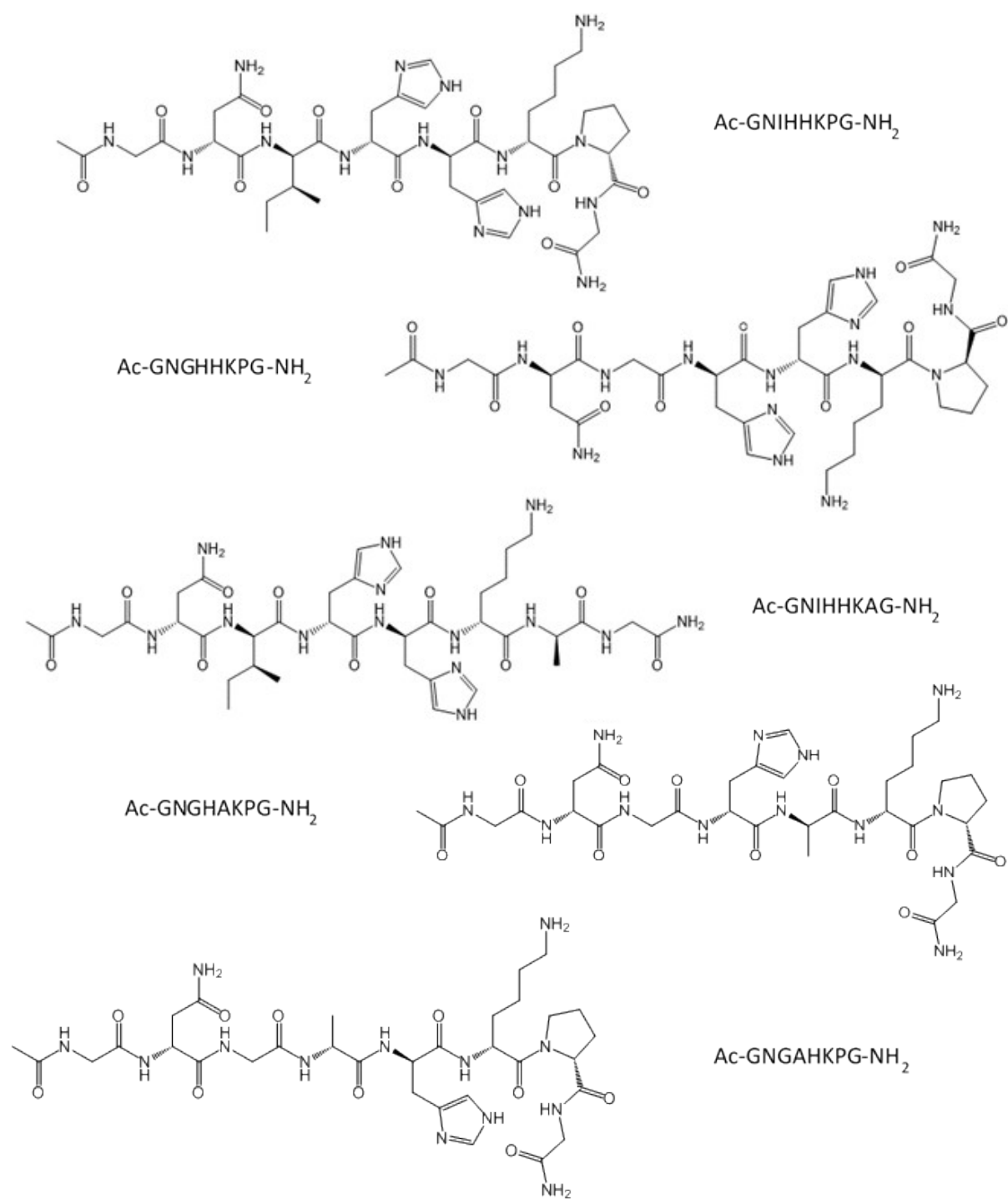
Bettina Diána Balogh, Györgyi Szunyog, Márton Lukács, Bence Szakács, Imre Sóvágó and Katalin Várnagy¹

Department of Inorganic and Analytical Chemistry, University of Debrecen, H-4032, Debrecen, Hungary

¹ Corresponding author (e-mail: varnagy.katalin@science.unideb.hu, tel: + 36 52 512 900, fax: + 36 52 518 660)



Scheme S1: Structural formulae of the studied peptides from the N-terminal domain of tau protein



Scheme S2: Structural formulae of the studied peptides from the R3 region of tau protein

Table S1: Deprotonation constants (pK) of the studied peptides (T = 298 K, I = 0.2 M KCl)

	Ac-EVMEDHAG-NH ₂ Tau(9-16)	Ac-KGGYTMHK-NH ₂ Tau(26-33) (Gln/Lys)	Ac-KGGATMHK-NH ₂ Tau(26-33) (Gln/Lys)(Tyr/Ala)	Ac-EDHAGTMHQD-NH ₂ Tau(12-16)(30-34)	Ac-GNIHHKPG-NH ₂ Tau(326-333)	Ac-GNGHHKPG-NH ₂	Ac-GNIHHKAG-NH ₂
pK(Im ₁)	6.70	6.22	6.18	6.27	5.81	5.86	6.07
pK(Im ₂)	–	–	–	7.12	6.71	6.69	6.64
pK(Asp ₁)	3.41	–	–	3.21	–	–	–
pK(Asp ₂)	–	–	–	3.85	–	–	–
pK(Glu ₁)	4.14	–	–	4.48	–	–	–
pK(Glu ₂)	4.68	–	–	–	–	–	–
pK(Lys ₁)	–	10.13	9.93	–	10.17	10.26	10.24
pK(Lys ₂)	–	10.71	10.77	–	–	–	–
pK(Tyr)	–	9.38	–	–	–	–	–

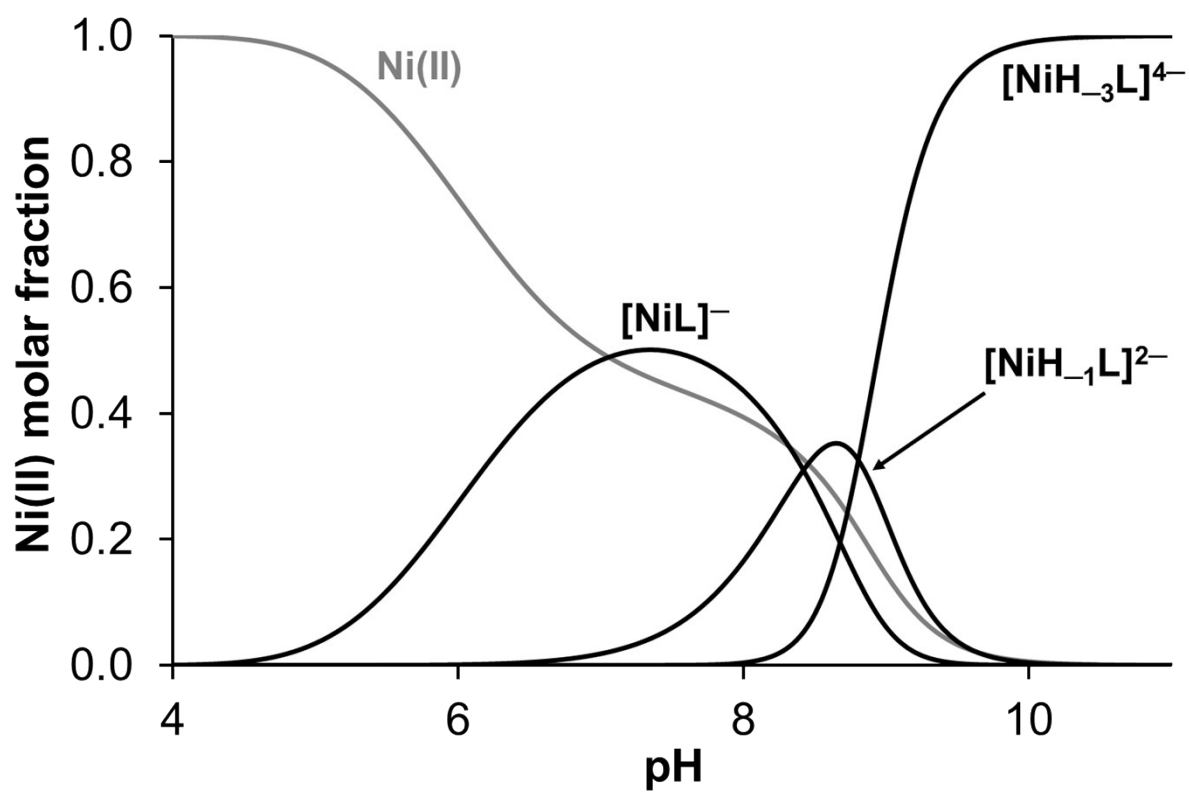


Figure S1: Concentration distribution curves of the major species formed in the nickel(II)-tau(9-16) system in equimolar concentration ($c(\text{L}) = 1 \text{ mM}$)

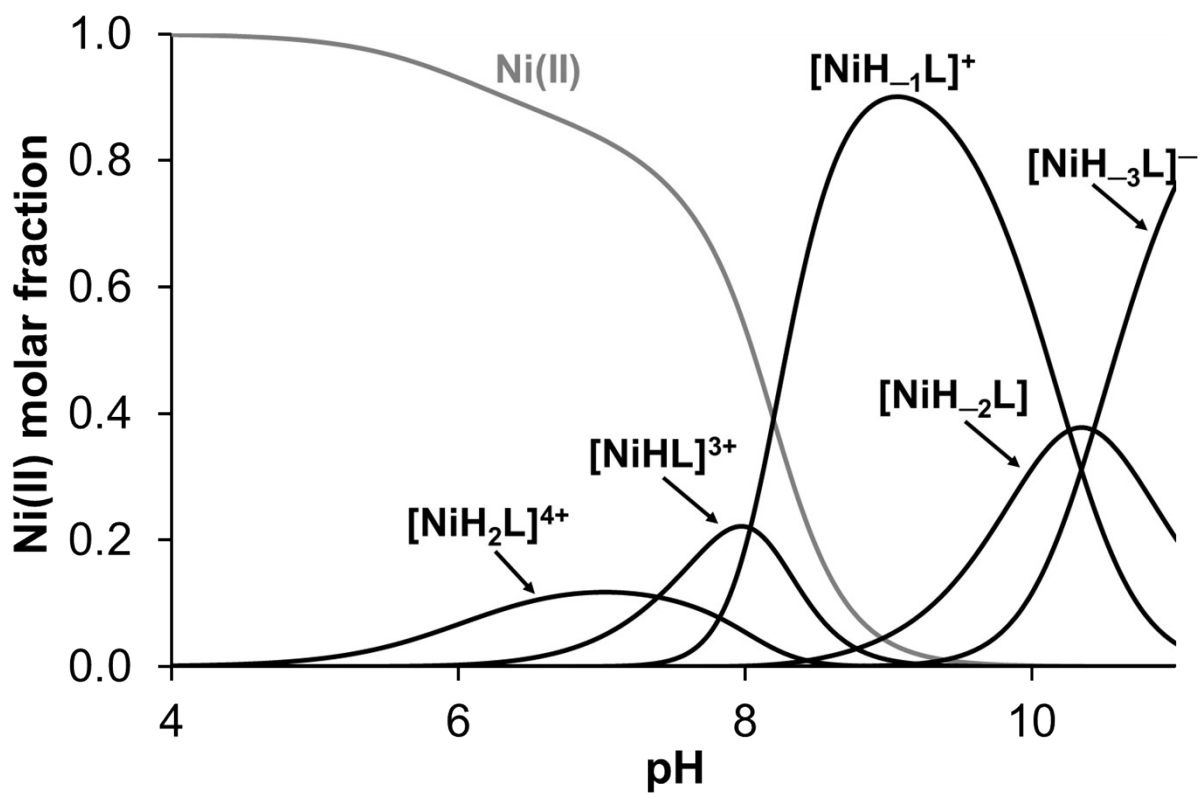


Figure S2: Concentration distribution curves of the major species formed in the nickel(II)-tau(26-33) (Gln/Lys)(Tyr/Ala) (Ac-KGGATM₁₀HK-NH₂) system in equimolar concentration ($c(\text{L}) = 1 \text{ mM}$)

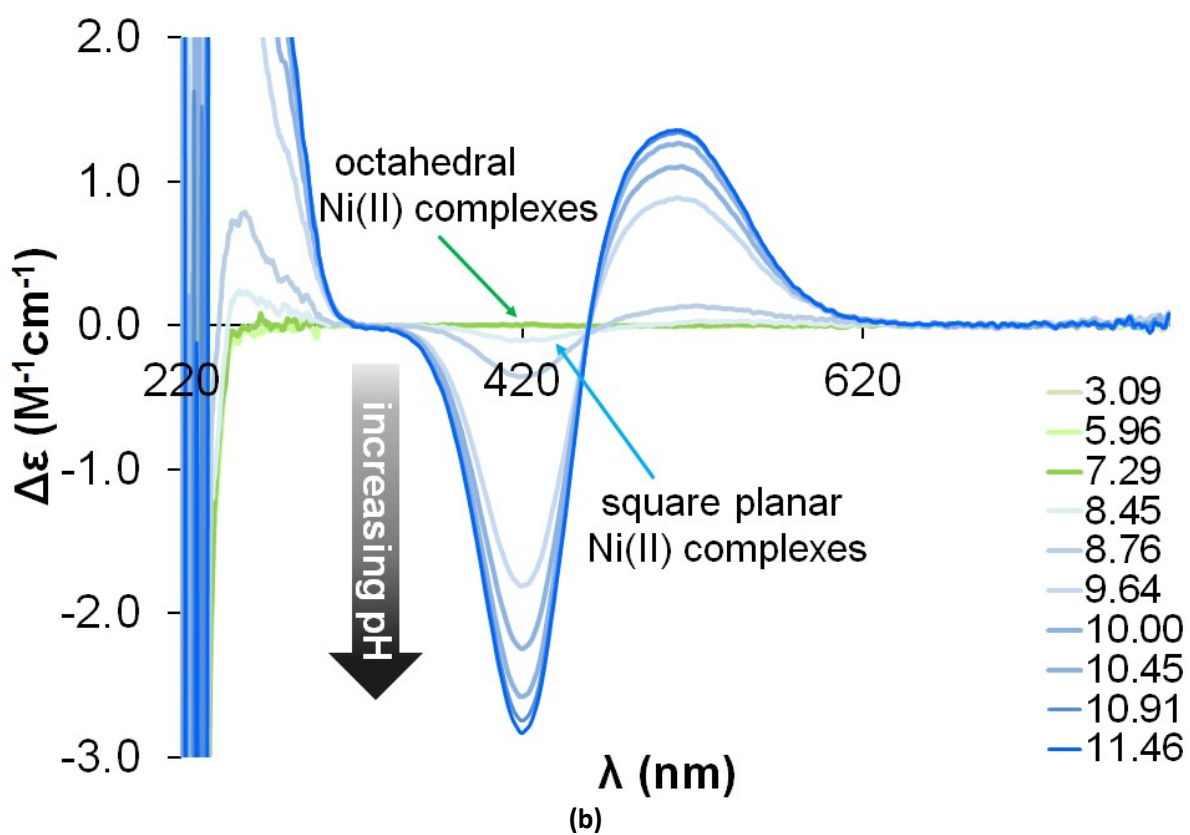
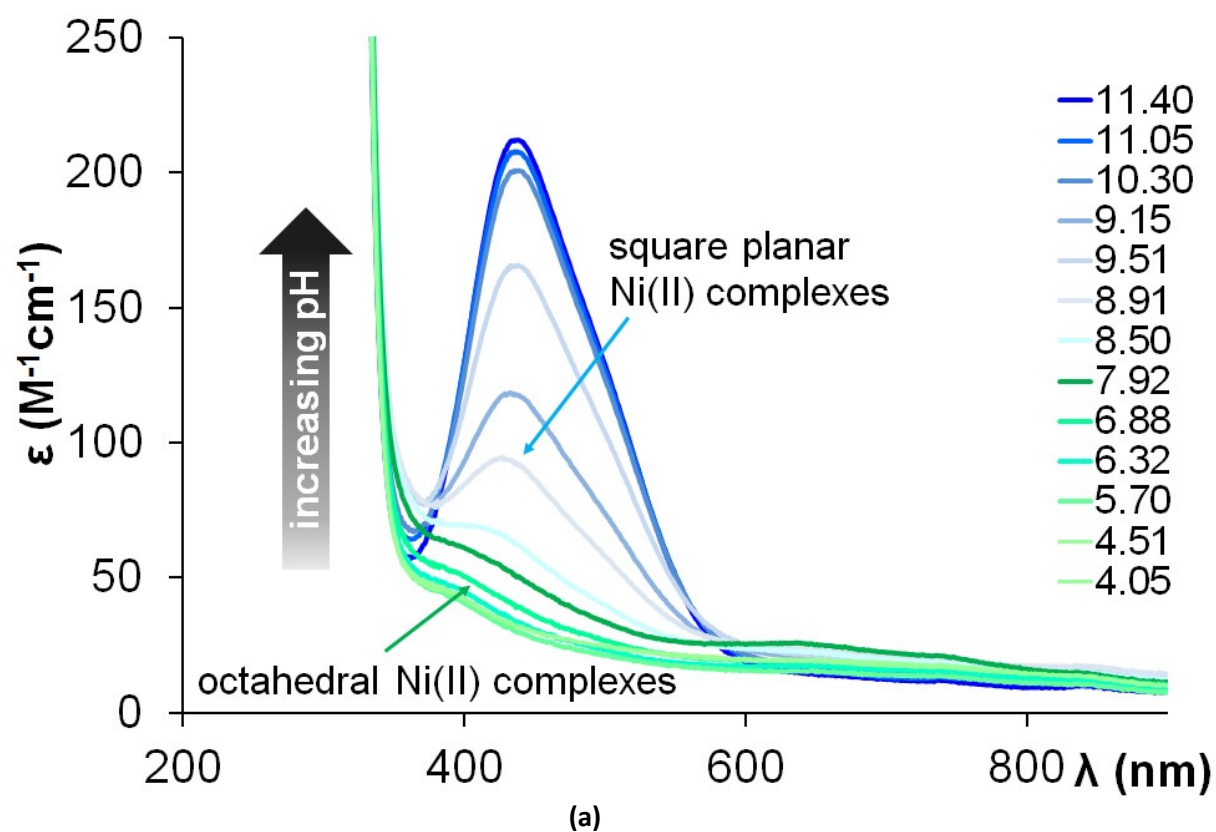


Figure S3: pH dependent absorption (a) and CD spectra (b) of the nickel(II)-Ac-EVMDHAG-NH₂ system in equimolar sample ($c(L) = 1.00$ mM)

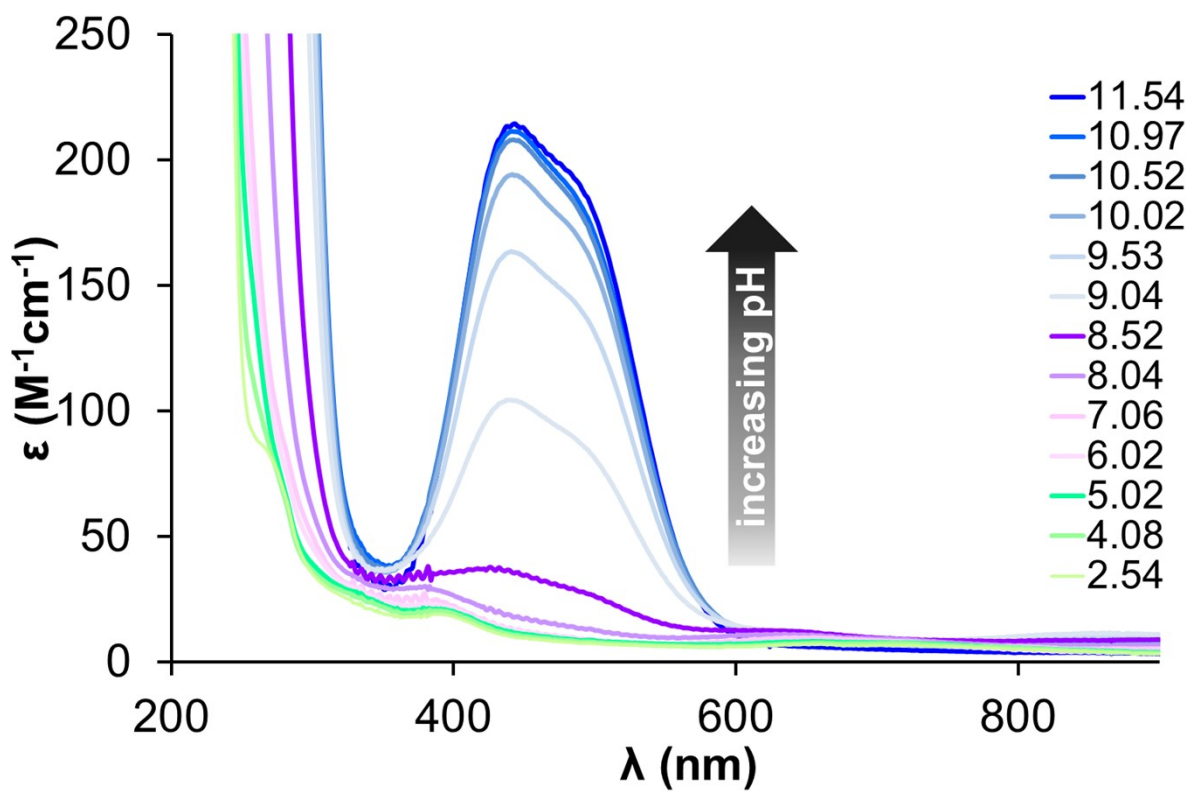


Figure S4: pH dependent absorption spectra of the nickel(II)-Ac-GNIHHKPG-NH₂ system in equimolar sample ($c(L) = 1.63$ mM)

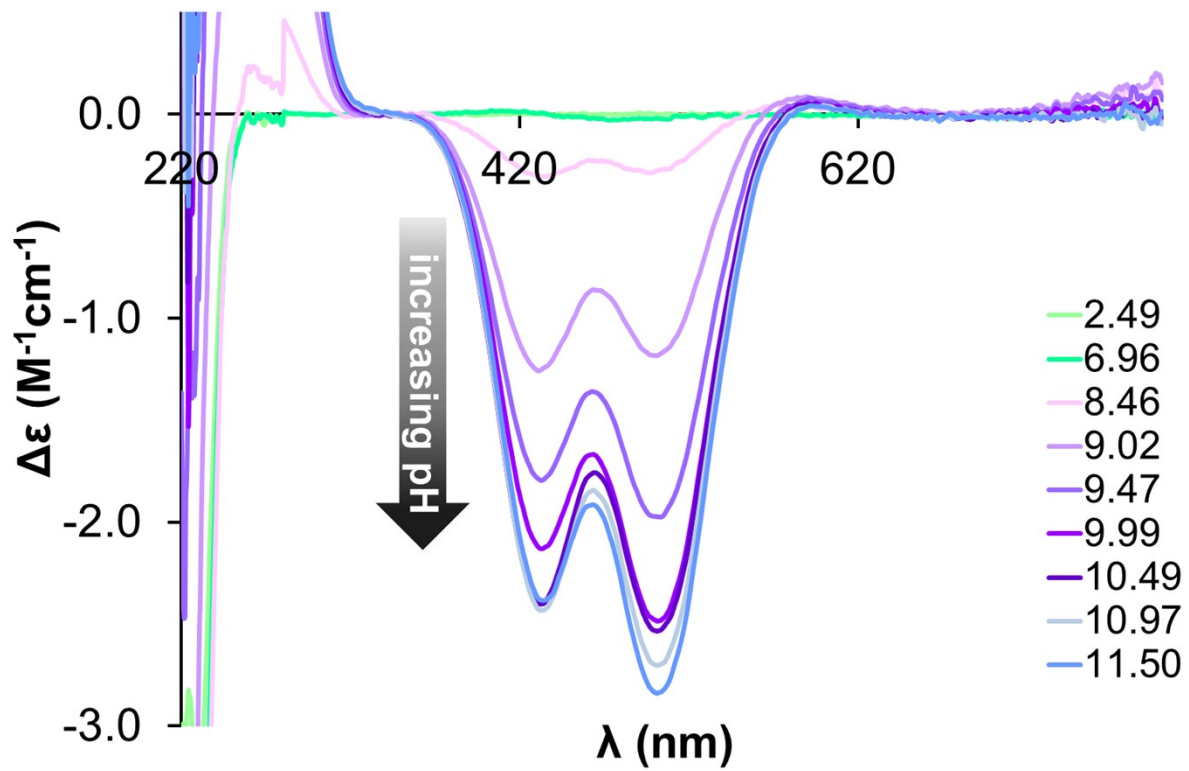


Figure S5: pH dependent CD spectra of the nickel(II)-Ac-GNIHHKPG-NH₂ system in equimolar system ($c(L) = 1.63$ mM)

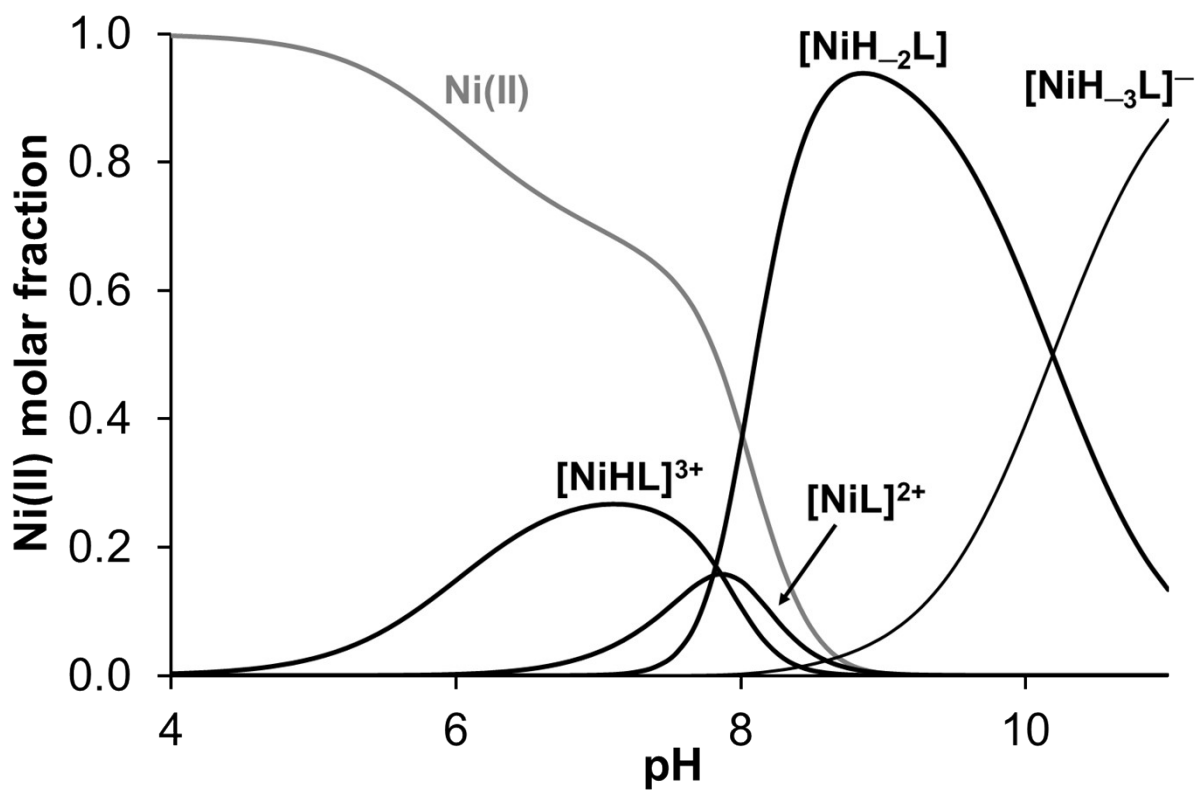


Figure S6: Metal ion speciation of the nickel(II)-Ac-GNGAHKPG-NH₂ system in equimolar sample ($c(L) = 2.033$ mM)

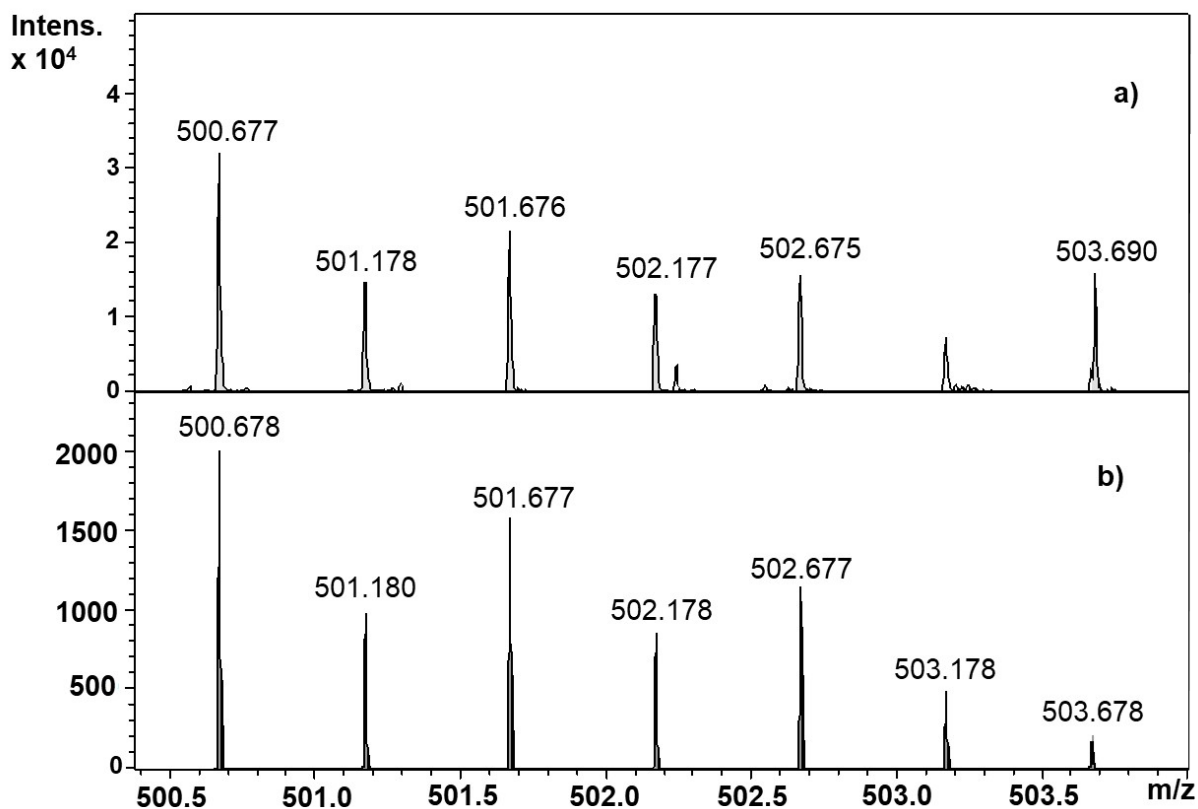


Figure S7: Enlargement of the a) measured ESI mass spectrum of the [ZnH₋₂L] species in the zinc(II):Ac-GNIHHKPG-NH₂ system at pH 10 (m/z = 500.677) and b) the simulated spectrum of the [ZnC₃₉H₅₉N₁₅O₁₀]K⁺H⁺ species (m/z = 500.678)