Electronic Supplementary Information

The hydrolytic stability of the human tubulin α 1A protein fragment – a potential reason for the role of metal ions in the development of neurodegenerative diseases

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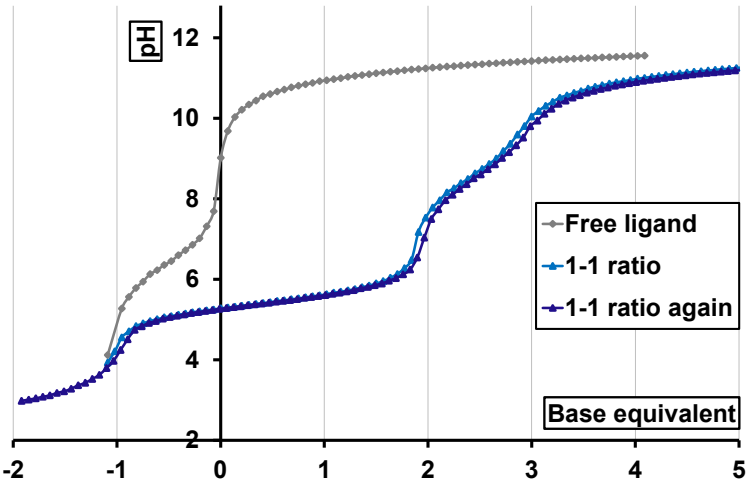

Figure S1. *Titration curves of the equimolar* ***Cu(II)****:Ac-L****TTH****TTL-NH$_2$ system and its repeated series after re-acidification signed with darker colour and '1-1 ratio again'*

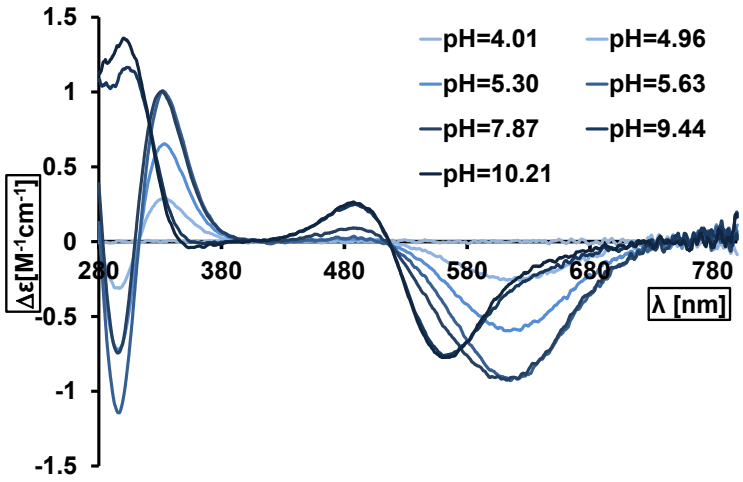

Figure S2. *pH dependent CD spectra of the equimolar* ***Cu(II)****:Ac-L****TTH****TTL-NH$_2$ system*

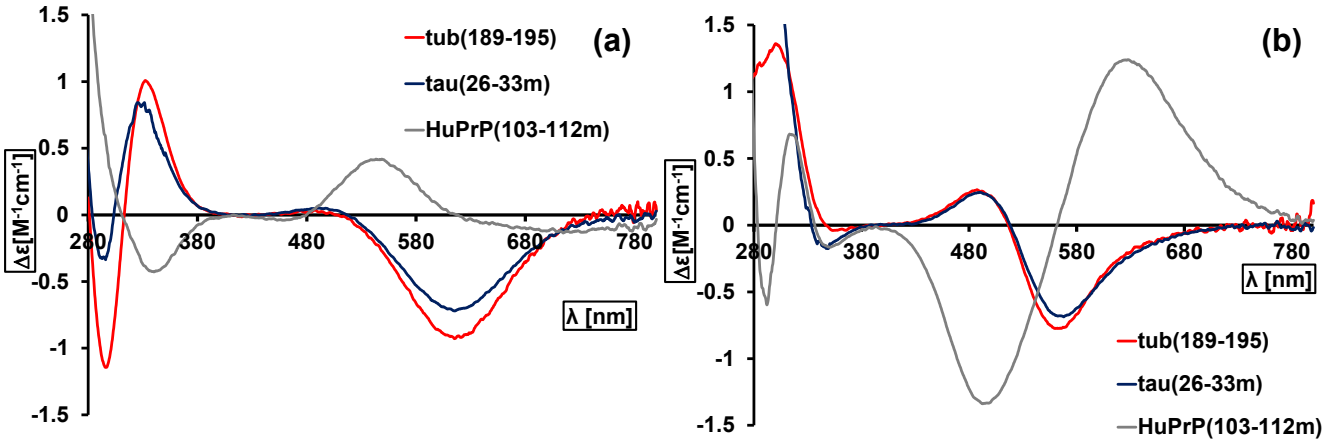

Figure S3. Comparison of the 3N **Cu(II)**-complexes (a) and 4N **Cu(II)**-complexes of tub(189-195) (red), tau(26-33m[1]) (blue) and HuPrP(103-112m) (grey) peptides (ref. 22 and 24) (The spectrum of complexes was recorded at the pH at which the complex is present in the highest amount.)

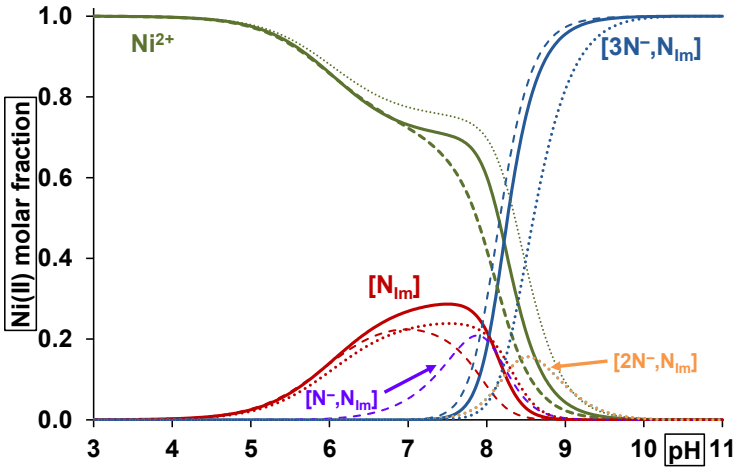

Figure S4. *The distribution curves of the complexes with different coordination mode in equimolar solution of* ***Ni(II)****-tub(189-195)(solid lines);* ***Ni(II)****-tau(26-33m) (dashed lines);* ***Ni(II)****- HuPrP(103-112m) (dotted lines) (c_L=c_M= 1mM)*

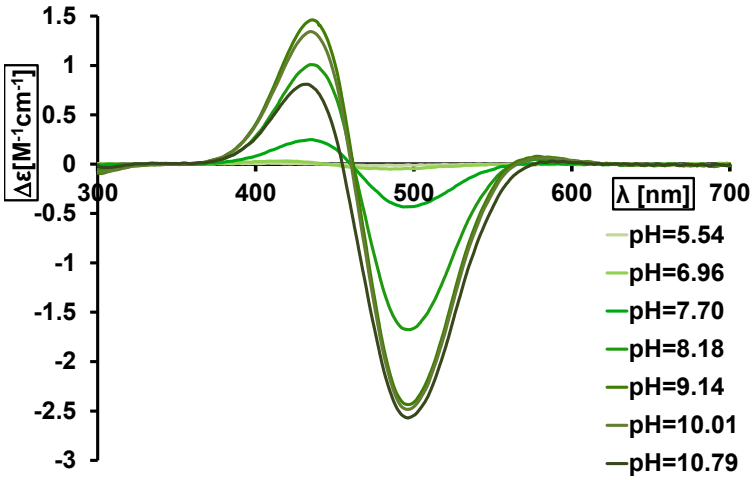

Figure S5. *pH dependent CD spectra of the equimolar* ***Ni(II)****:Ac-L****TTH****TTL-NH$_2$ system*

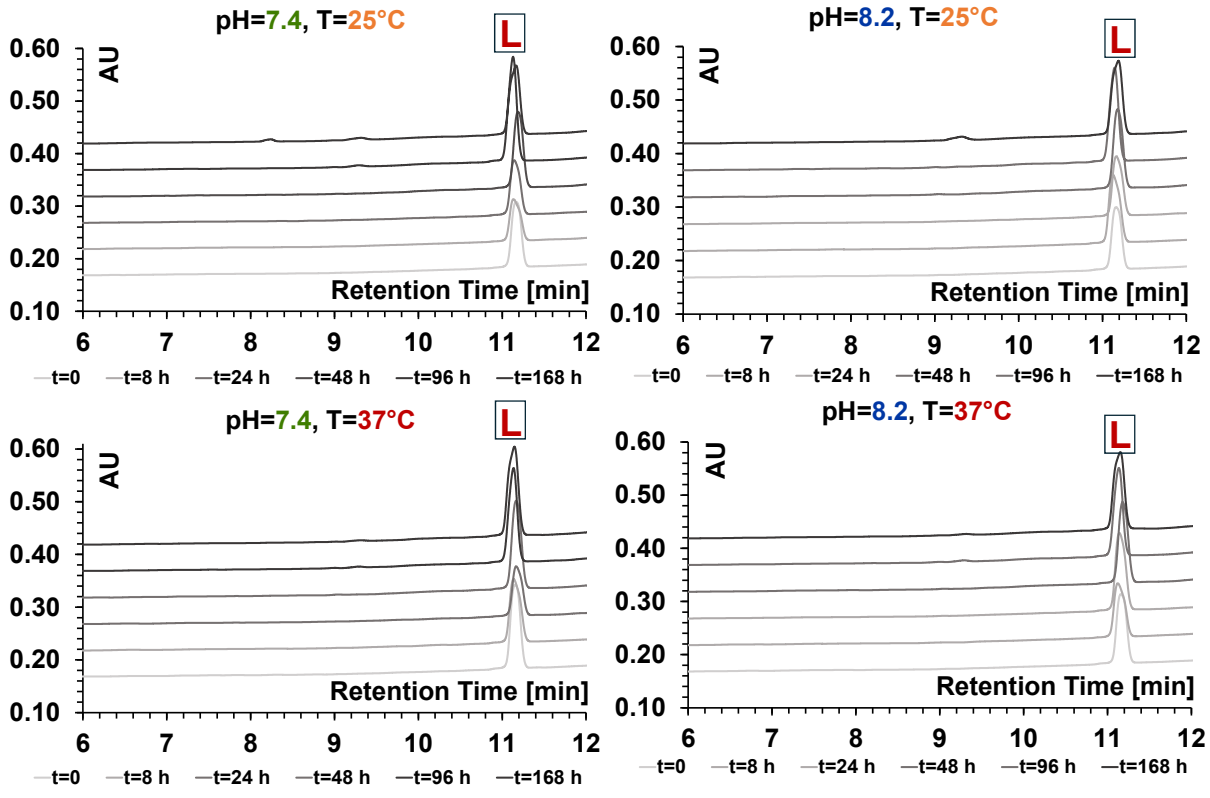

Figure S6. *Analysis of the HPLC chromatograms as a function of time for the control systems containing only the Ac-L****TTH****TTL-NH$_2$ protein fragment (****L****) at* ***25 °C*** *and* ***37 °C****, pH=****7.4*** *and* ***8.2*** *provided by 20 mM HEPES buffer.*

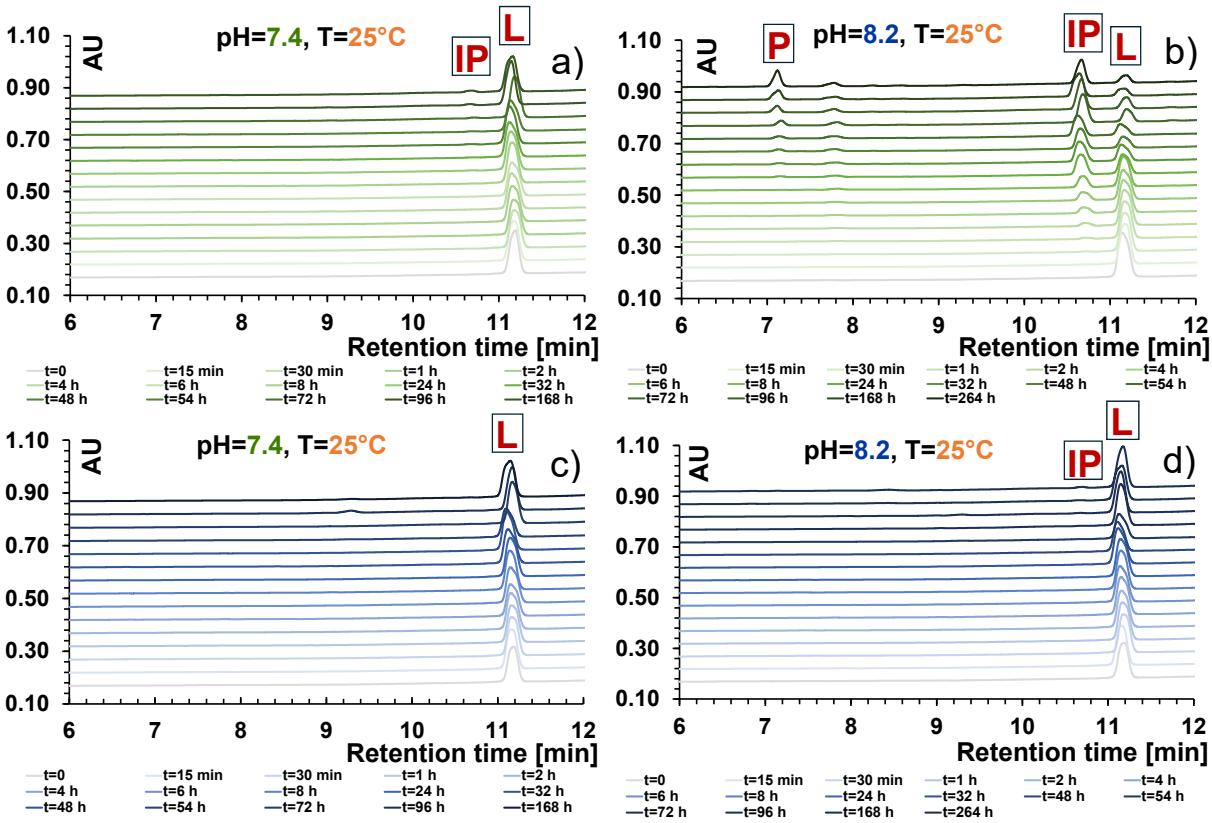

Figure S7. *Analysis of the HPLC chromatograms as a function of time for systems consisting of* ***Ni(II)****:Ac-L****TTH****TTL-NH_2 1:1 (****a*** *and* ***b****) or* ***Cu(II)****:Ac-L****TTH****TTL-NH_2 1:1 (****c*** *and* ***d****) at* ***25 °C****, pH=****7.4*** *and* ***8.2*** *provided by 20 mM HEPES buffer.*

Table S1. UV-Vis parameters (λmax [nm] (ε [M−1·cm−1]) of copper(II) complex of peptides completed with the calculated values (The spectral parameters of the complexes were determined at the pH where the complex is present in the highest amount.)

coordination mode	tub(189-195) Ac-L**TTH**TTL-NH_2	tau(26-33m)[22] Ac-KGGY**TMH**K-NH_2	Ac-TY**TEH**A-NH_2[23]	HuPrP(103-112m)[24] Ac-SKPKTNAK**H**A-NH_2	calculated l_{max} value*
N_{Im}	747(10)		690(36)	758(21)	760
$2N^-,N_{Im}$	591(79)	590(75)	567(122)	596(86)	583
$3N^-,N_{Im}$	562(91)	560(97)	556(142)	520(125)	522

* $l_{max} = 10^3/(0.294(C{=}O/H_2O) + 0.346(COO^-) + 0.460(NH_2) + 0.494(N{=}) + 0.434(N_{Im})$ (From ref. 25)

Table S2. Measured and calculated m/z values for the protein fragment (**L**), the intermediate product (**IP**) and the product (**P**)

Species	Retention time [min]	Composition	*m/z* (Measured)	*m/z* (Calculated)
Ac-L**TTH**TTL-NH_2 (**L**)	11.188	$C_{36}H_{62}N_{10}O_{12}$	827.4621	827.4621
Ac-L**TTH**TTL-NH_2 (**IP**)	10.684	$C_{36}H_{62}N_{10}O_{12}$	827.4619	827.4621
[**TTH**TTL-NH_2+H] (**P**)	7.097	$C_{28}H_{49}N_9O_{10}$	672.3673	672.3675

Table S3. The applied gradient program in case of the HPLC experiments

Retention time [min]	Solvent A	Solvent B
0	100	0
1	100	0
13	70	30
14	40	60
15	100	0
18	100	0