Supplementary Data

Copper(II)-binding induces a unique polyproline type II (PPII) helical structure within the ion-binding segment in the intrinsically disordered F-domain of ecdysteroid receptor from *Aedes aegypti*

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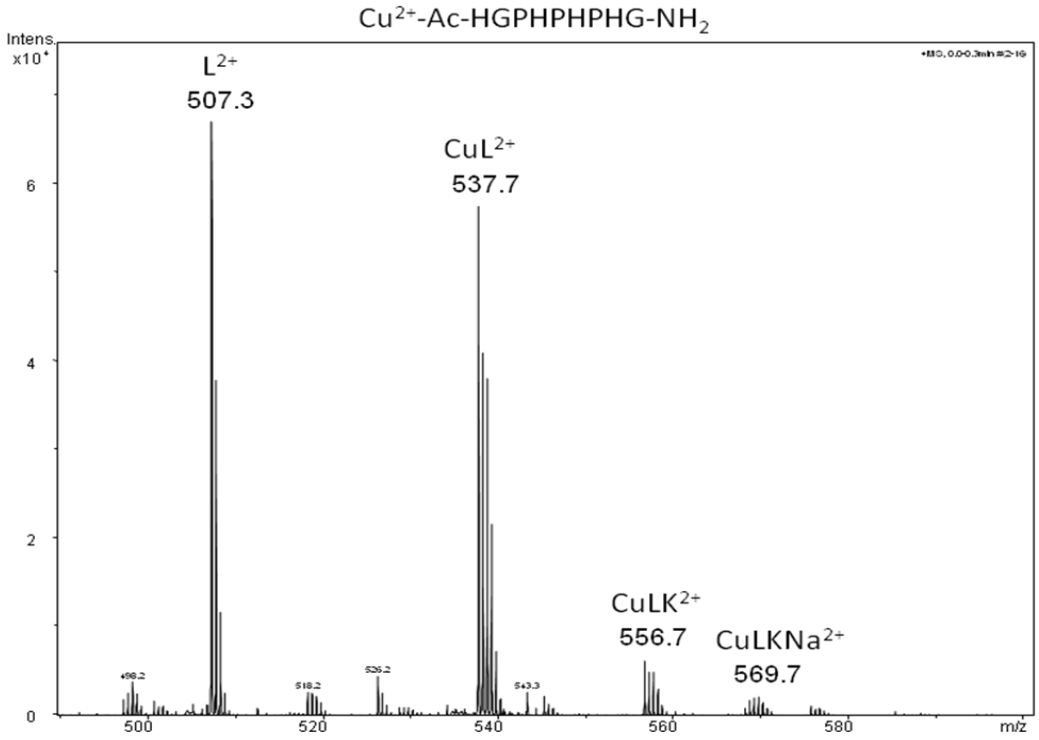
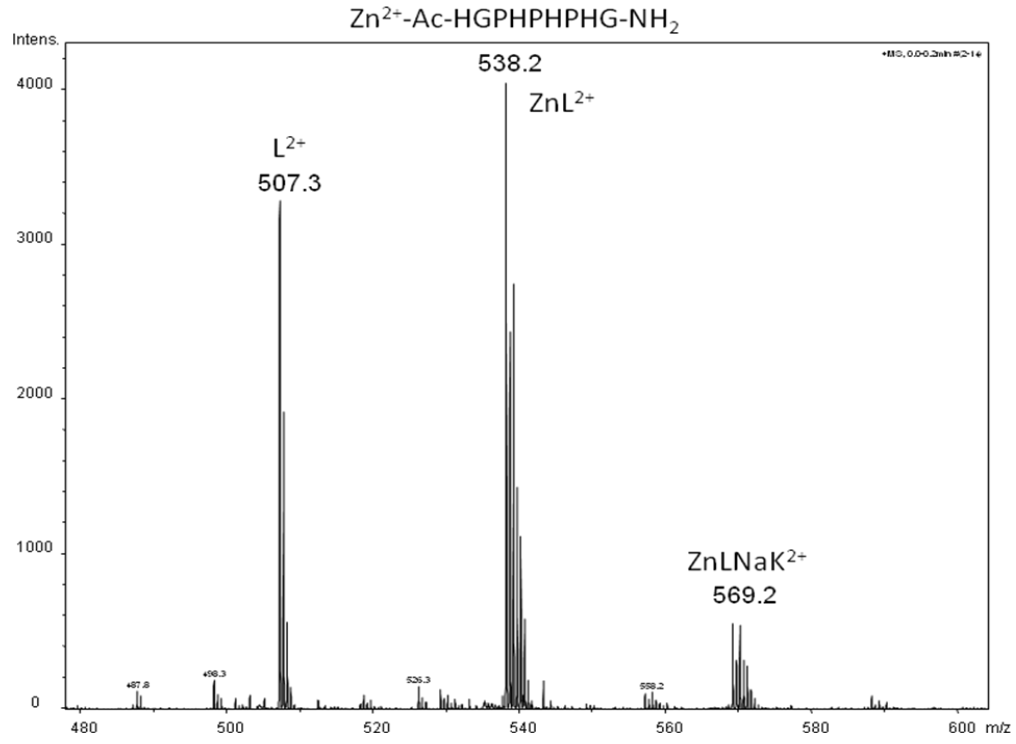
A)


Cu2+-Ac-HGPHPHPHG-NH2
Intens.
x10+
L2+
507.3
CuL2+
537.7
CuLK2+
556.7
CuLKNa2+
569.7
m/z

B)


Zn2+-Ac-HGPHPHPHG-NH2
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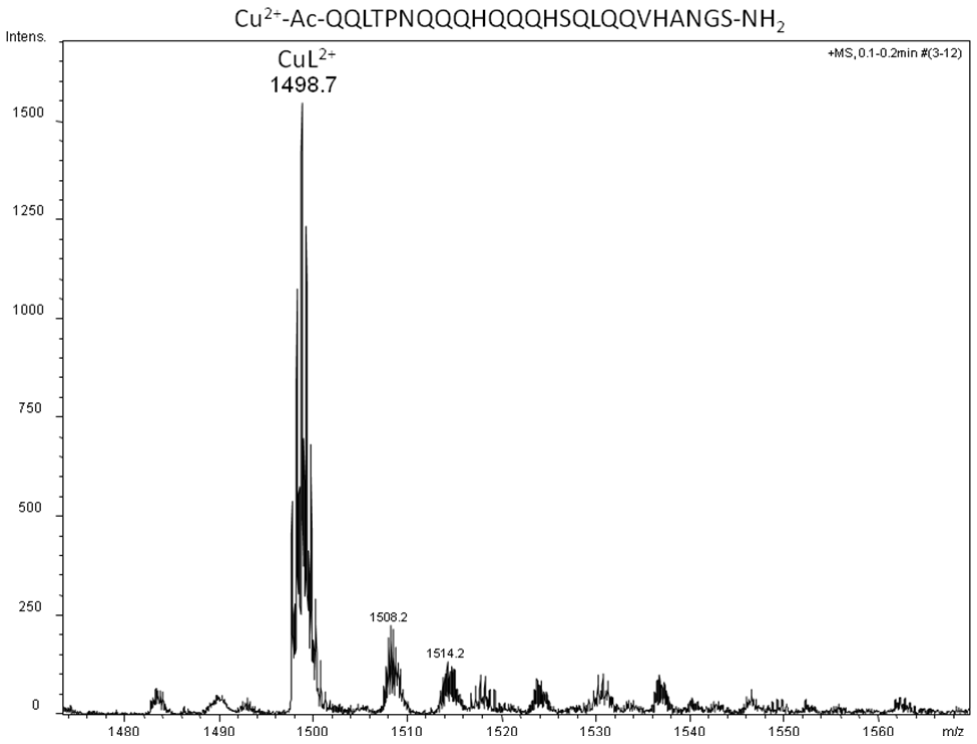
538.2
ZnL2+
L2+
507.3
ZnLNaK2+
569.2
m/z

C)



D)

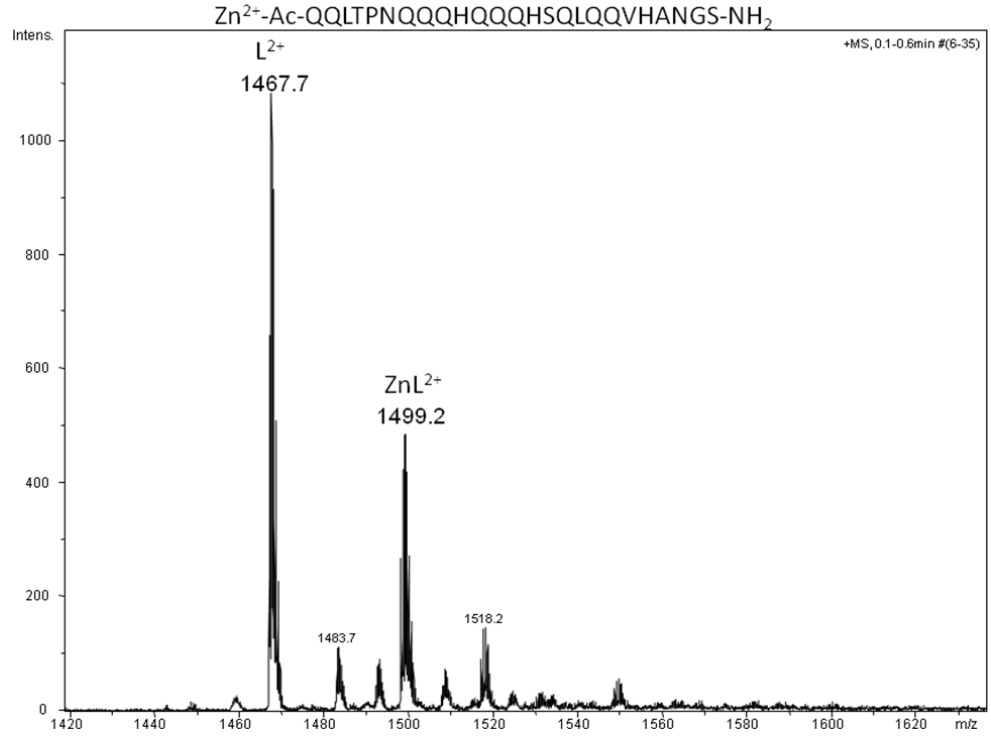
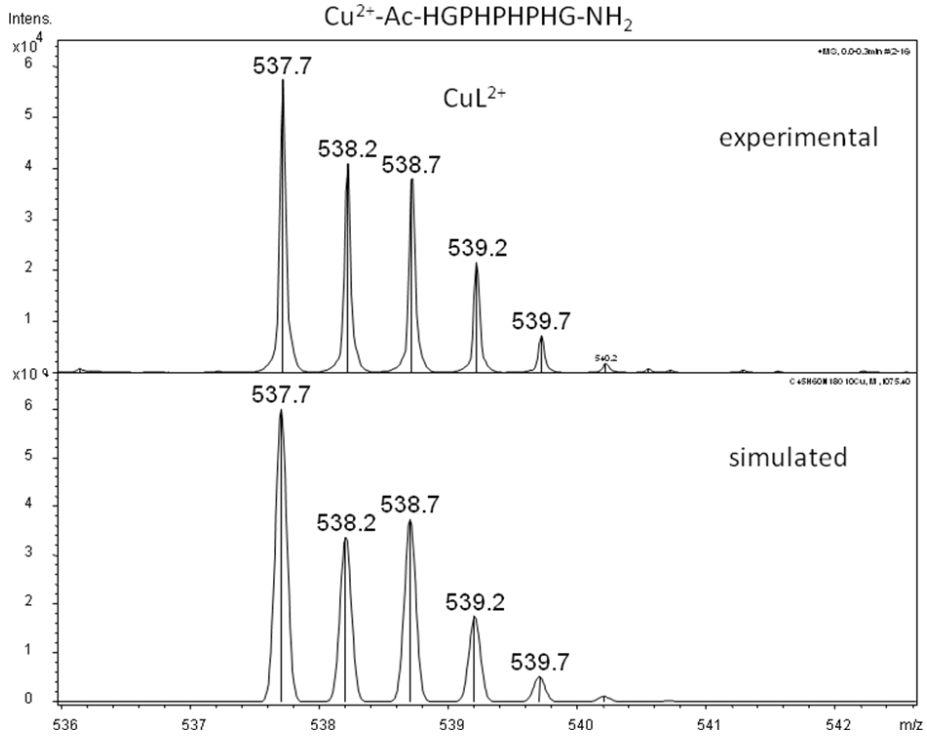
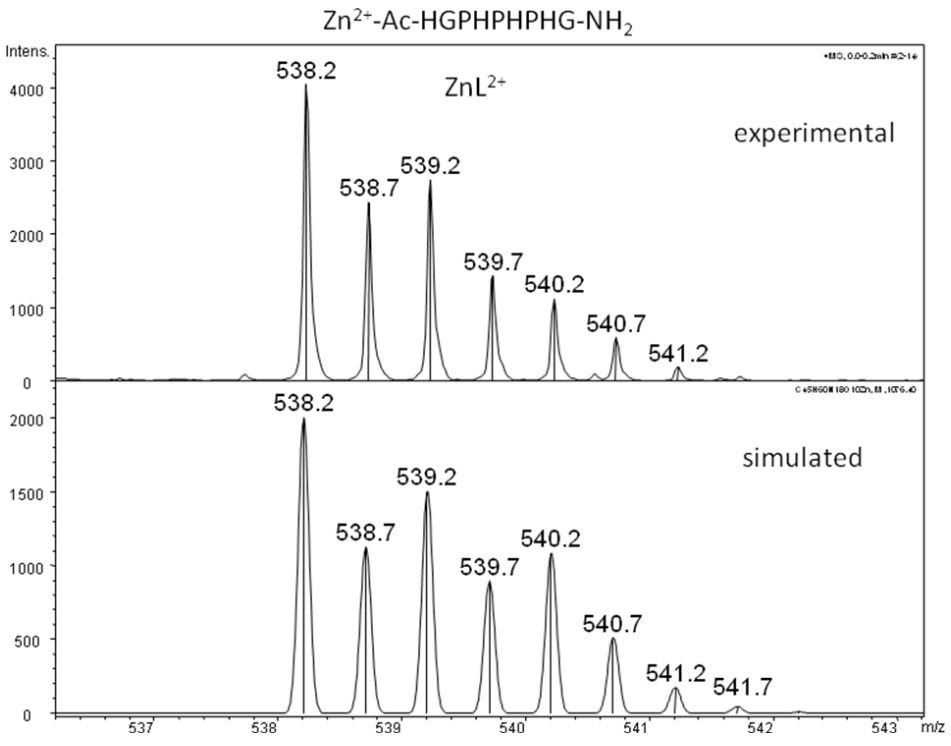


Figure S1. ESI-MS spectra of **A)** Cu^{2+}-Ac-HGPHPHPHG-NH_2, **B)** Zn^{2+}-Ac-HGPHPHPHG-NH_2, **C)** Cu^{2+}-Ac-QQLTPNQQQHQQQHSQLQQVHANGS-NH_2 and **D)** Zn^{2+}-Ac-QQLTPNQQQHQQQHSQLQQVHANGS-NH_2complexes, 1:1 metal/peptide ratio, $C_{peptide}$=0.1 mM. Samples prepared in a 1:1 MeOH/H2O mixture at pH 7.4 and measured in the positive ion mode.

A)


Cu2+-Ac-HGPHPHPHG-NH2
Intens.
x10 4
537.7
CuL2+
experimental
538.2
538.7
539.2
539.7
simulated
537.7
538.2
538.7
539.2
539.7
536
537
538
539
540
541
542
m/z

B)


Zn2+-Ac-HGPHPHPHG-NH2
Intens.
538.2
ZnL2+
experimental
538.7
539.2
539.7
540.2
540.7
541.2
simulated
538.2
539.2
538.7
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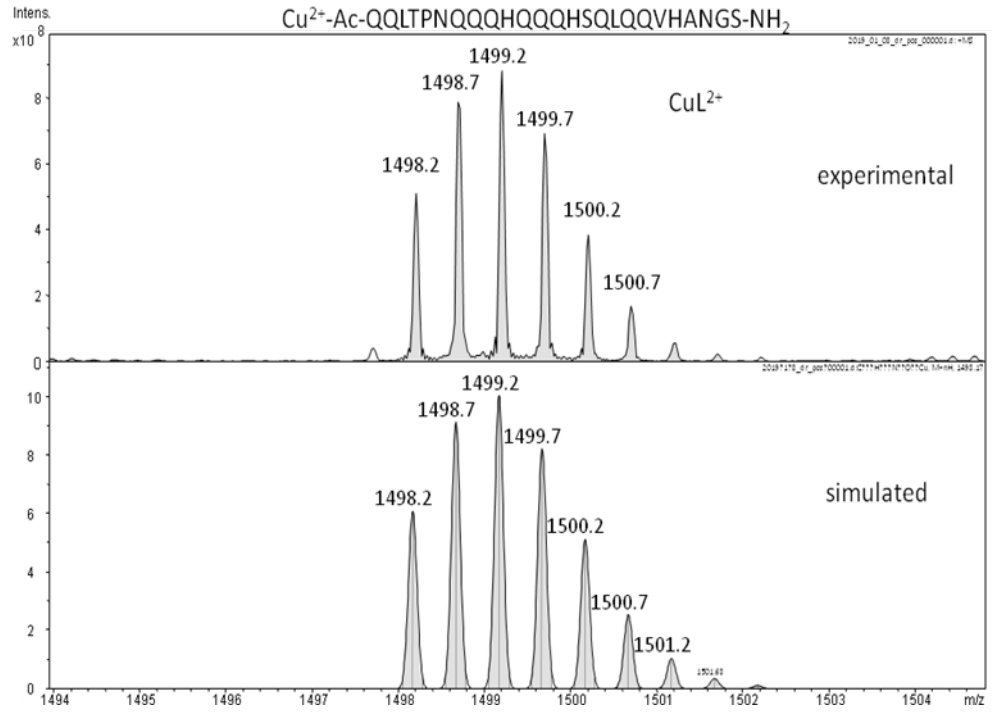
540
541
542
543
m/z

C)



D)

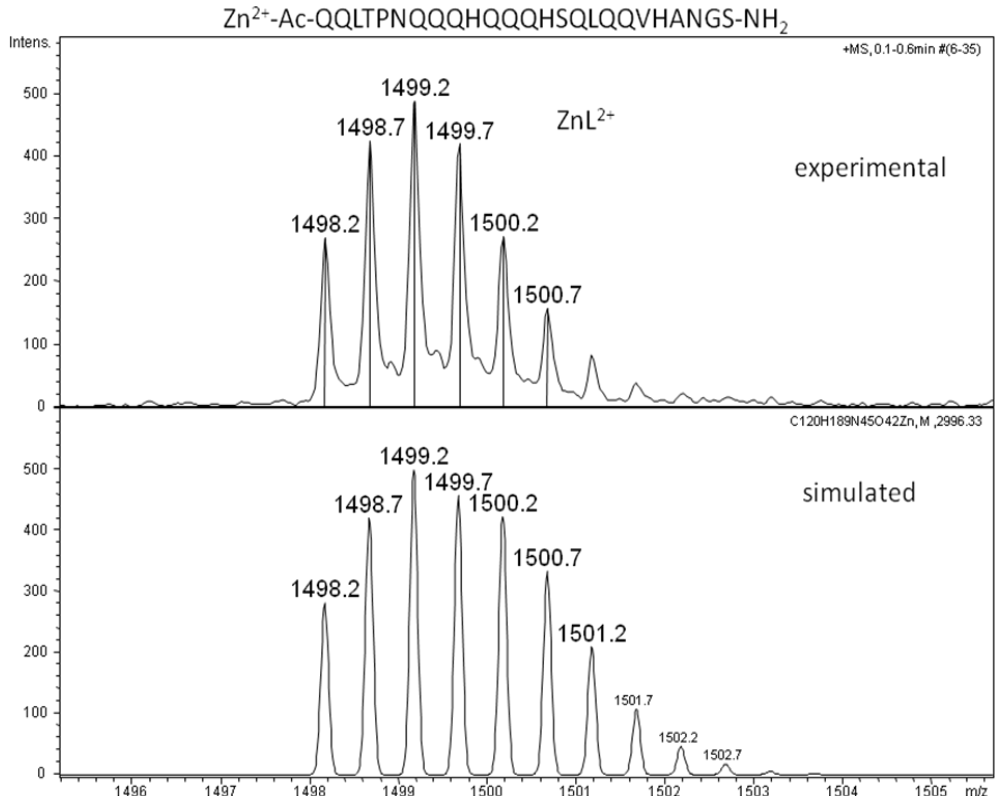


Figure S2. Comparison of $[MeL]^{2+}$ experimental and simulated signals of **A)** Cu^{2+}-Ac-HGPHPHPHG-NH_2, **B)** Zn^{2+}-Ac-HGPHPHPHG-NH_2, **C)** Cu^{2+}-Ac-QQLTPNQQQHQQQHSQLQQVHANGS-NH_2 and **D)** Zn^{2+}-Ac-QQLTPNQQQHQQQHSQLQQVHANGS-NH_2.

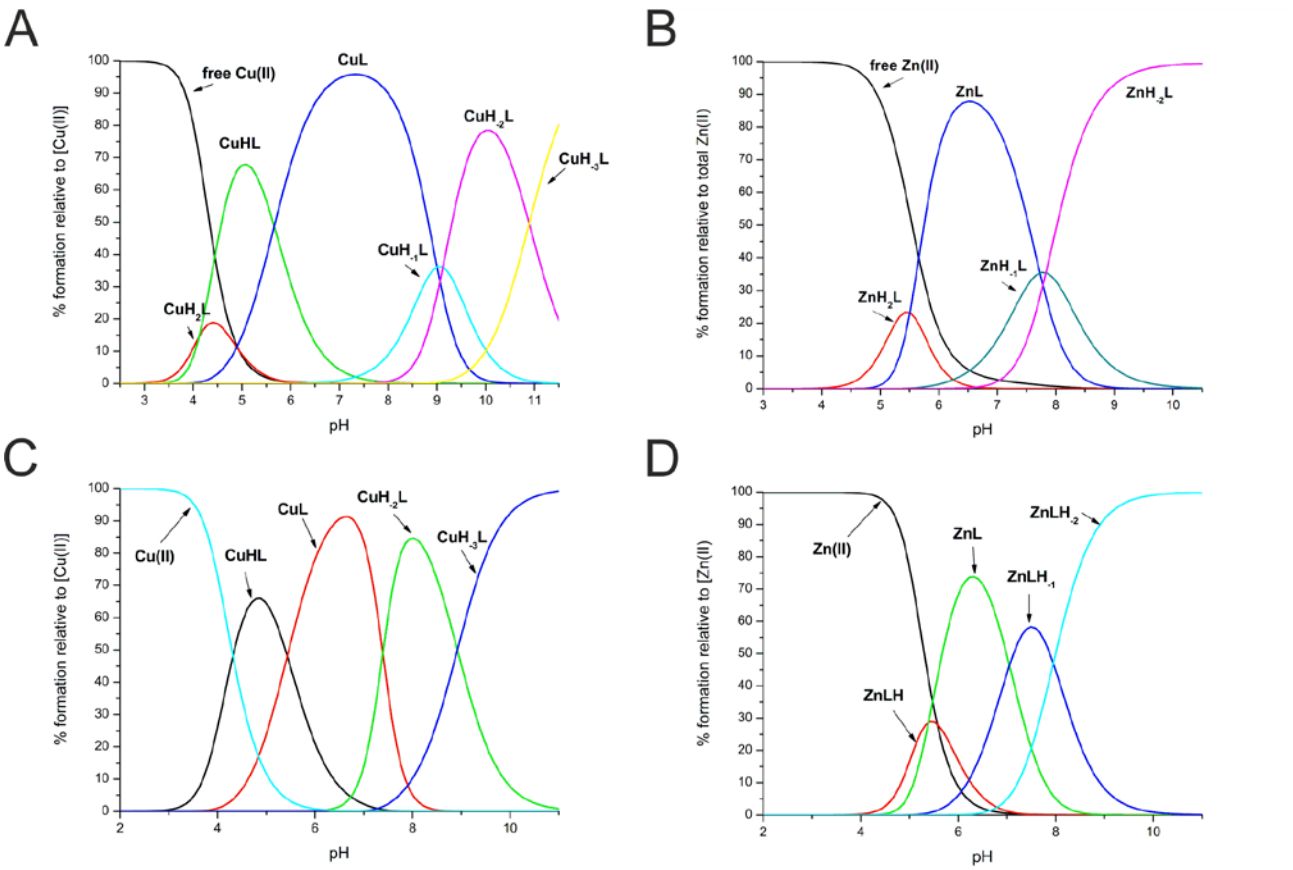


Figure S3. Species distribution of **A)** Cu^{2+}-Ac-HGPHPHPHG-NH_2, **B)** Zn^{2+}-Ac-HGPHPHPHG-NH_2, **C)** Cu^{2+}-Ac-QQLTPNQQQHQQQHSQLQQVHANGS-NH_2 and **D)** Zn^{2+}-Ac-QQLTPNQQQHQQQHSQLQQVHANGS-NH_2., complexes at 1:1 Me^{2+}/peptide ratio in DMSO/water (30:70) solution, T=298K, $C_{peptide}$=0.5 mM (for clarity, charges on the speciation plots were omitted).

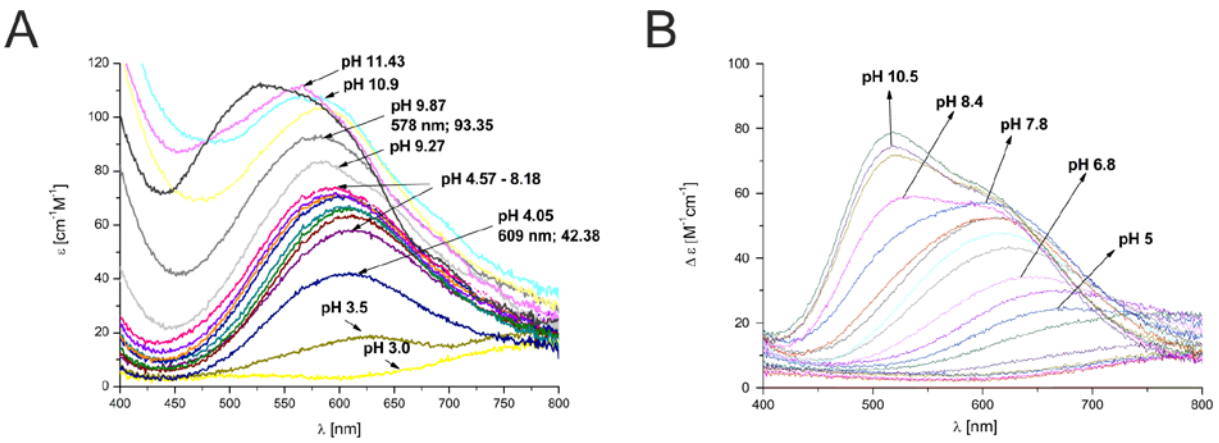


Figure S4. UV-Vis spectra of **A)** Cu^{2+}-Ac-HGPHPHPHG-NH_2 and **B)** Cu^{2+}-Ac-QQLTPNQQQHQQQHSQLQQ -VHANGS-NH_2.

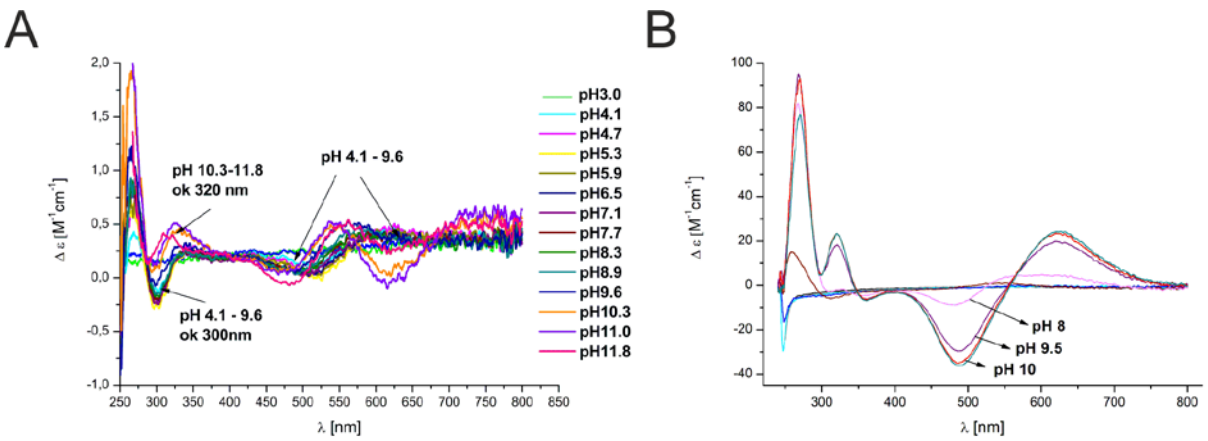


Figure S5. CD spectra of **A)** Cu^{2+}-Ac-HGPHPHPHG-NH_2 and **B)** Cu^{2+}-Ac-QQLTPNQQQHQQQHSQLQQVHANGS-NH_2.

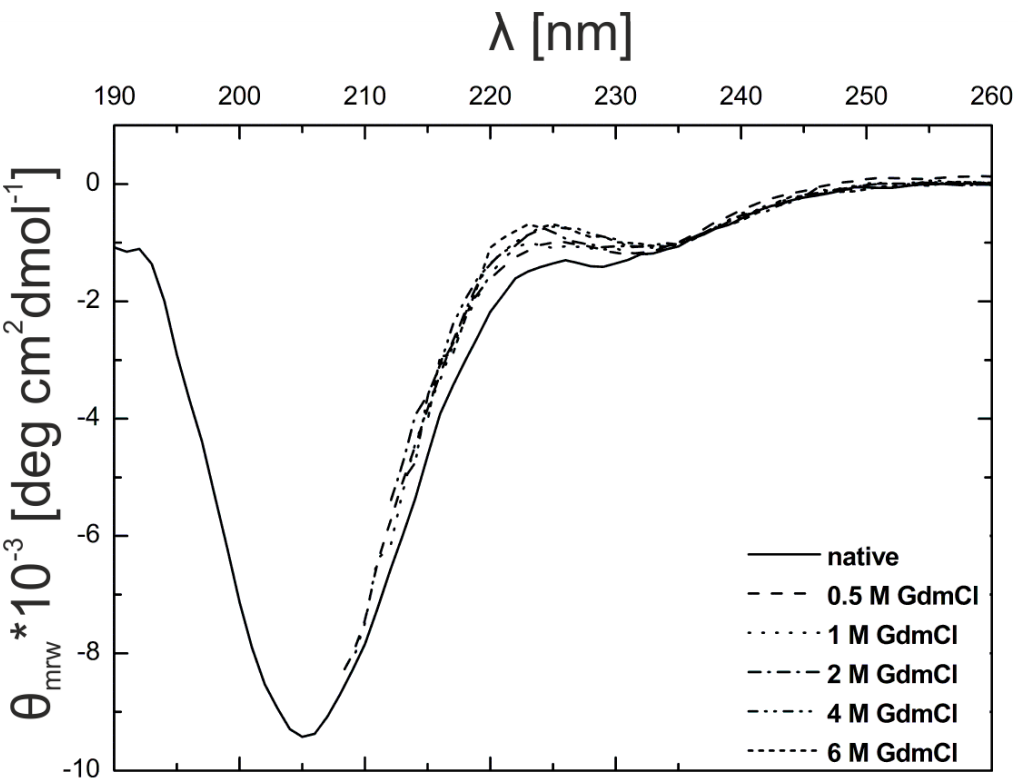


Figure S6. Far-UV CD spectra of Ac-HGPHPHPHG-NH_2 recorded in the presence of different GdmCl concentration.

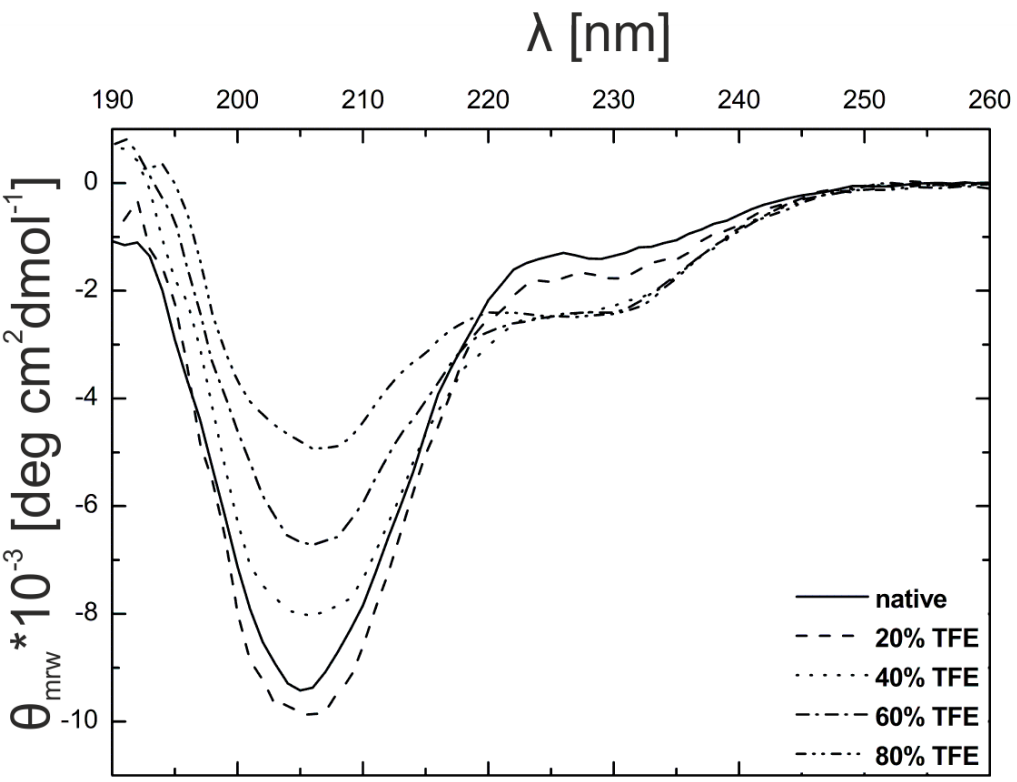


Figure S7. Far-UV CD spectra of Ac-HGPHPHPHG-NH_2 recorded in the presence of different TFE concentrations.

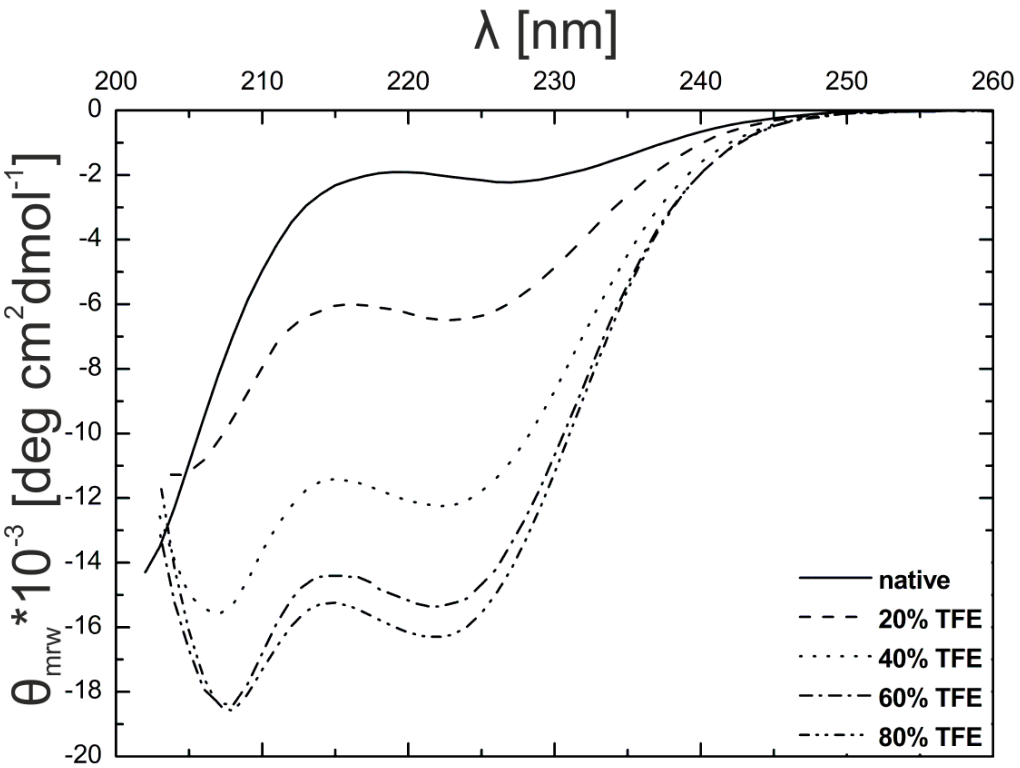


Figure S8. Far-UV CD spectra of Ac-QQLTPNQQQHQQQHSQLQQVHANGS-NH_2 recorded in the presence of different TFE concentration.

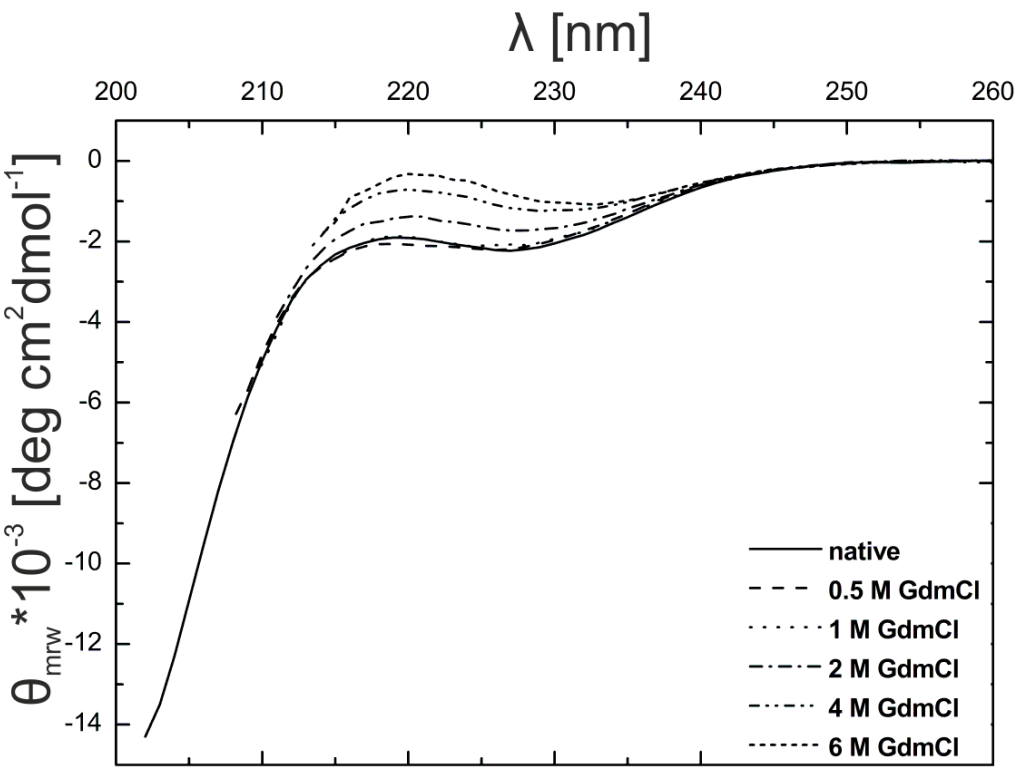


Figure S9. Far-UV CD spectra of Ac-QQLTPNQQQHQQQHSQLQQVHANGS-NH_2 recorded in the presence of different GdmCl concentrations.

Figure S10. The structures of the Ac-P_{10}-NH_2. The red tube follows the polyproline II helix backbone.

Table S1. The cation – peptide distance in Å.

	Ac-QQLTPNQQQHQQQHSQLQQVHANGS-NH_2		
Connection	$3NZn^{2+}$	$3NCu^{2+}$	$2NCu^{2+}$
His10	2.054	2.059	
His14	2.056	2.046	1.870
His21	2.048	2.030	1.854
	Ac-HGPHPHPHG-NH_2		
	$3NZn^{2+}$	$3NCu^{2+}$	2N
His8	2.312	1.856	-
His6	2.224	2.316	-
His4	2.250	1.873	-