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Supplementary Information

The Metallacrowns as Templates for Spontaneous Self-Assembly of Polypeptides into a Tetra-Helical Bundle

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Table S1. The comparison of *m/z* values (experimental and calculated) for the most abundant monoisotopic peaks of metallacrowns formed by peptides: [ADK]-NHOH, [ADE]-NHOH, [AH]-NHOH, and [AH1]-NHOH.

peptide	z	experimental *m/z* value	calculated *m/z* value	elemental formula of complex
[ADK]-NHOH	5+	1453,0657	1453,0602	$C_{320}H_{603}N_{96}O_{72}Cu_5$
	6+	1211,0516	1211,0514	$C_{320}H_{604}N_{96}O_{72}Cu_5$
	7+	1038,1888	1038,1880	$C_{320}H_{605}N_{96}O_{72}Cu_5$
	8+	908,5416	908,5404	$C_{320}H_{606}N_{96}O_{72}Cu_5$
	9+	807,7036	807,7034	$C_{320}H_{607}N_{96}O_{72}Cu_5$
	10+	727,0339	727,0338	$C_{320}H_{608}N_{96}O_{72}Cu_5$
[ADE]-NHOH	4-	1819,7484	1819,7436	$C_{296}H_{482}N_{72}O_{120}Cu_5$
	5-	1455,5954	1455,5932	$C_{296}H_{474}N_{72}O_{120}Cu_5$
	6-	1212,8272	1212,8263	$C_{296}H_{473}N_{72}O_{120}Cu_5$
	7-	1039,4228	1039,4213	$C_{296}H_{472}N_{72}O_{120}Cu_5$
	8-	909,3745	909,3676	$C_{296}H_{471}N_{72}O_{120}Cu_5$
	9-	808,2188	808,2147	$C_{296}H_{470}N_{72}O_{120}Cu_5$
[AH]-NHOH	4+	1797,9455	1797,9425	$C_{312}H_{546}N_{88}O_{84}Cu_5$
	5+	1438,5583	1438,5555	$C_{312}H_{547}N_{88}O_{84}Cu_5$
	6+	1198,9642	1198,9641	$C_{312}H_{548}N_{88}O_{84}Cu_5$
	7+	1027,8257	1027,8274	$C_{312}H_{549}N_{88}O_{84}Cu_5$
	8+	899,4762	899,4749	$C_{312}H_{550}N_{88}O_{84}Cu_5$
	9+	799,6462	799,6452	$C_{312}H_{551}N_{88}O_{84}Cu_5$
[AH1]-NHOH	5+	1495,3863	1495,3852	$C_{312}H_{561}N_{88}O_{88}Cu_5$
	6+	1246,3218	1246,3222	$C_{312}H_{562}N_{88}O_{88}Cu_5$
	7+	1068,4200	1068,4201	$C_{312}H_{563}N_{88}O_{88}Cu_5$
	8+	934,9935	934,9935	$C_{312}H_{564}N_{88}O_{88}Cu_5$
	9+	831,2172	831,2172	$C_{312}H_{565}N_{88}O_{88}Cu_5$

Mass Spectrometry Experiments

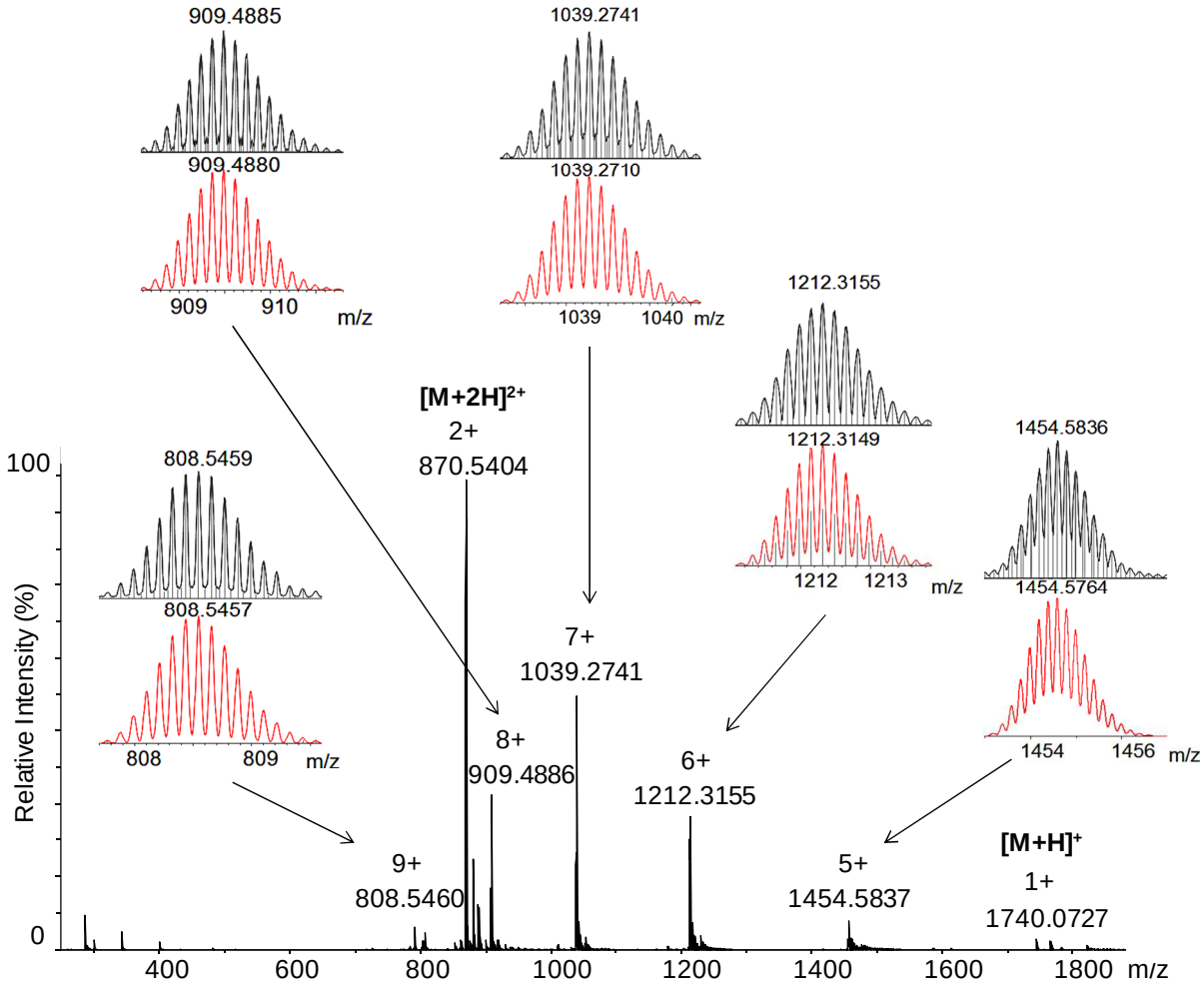

Fig. S1. MS spectrum of the solution containing peptide [AD]-NHOH and copper (II) ions. The spectrum was recorded on an FT-ICR-MS instrument in the positive ion mode. Red color corresponds to a simulated isotopic pattern ([AD]-NHOH:Cu^2 = 4:5) and black corresponds to the experimental data. M corresponds to [AD]-NHOH. For more details, see Table S1.

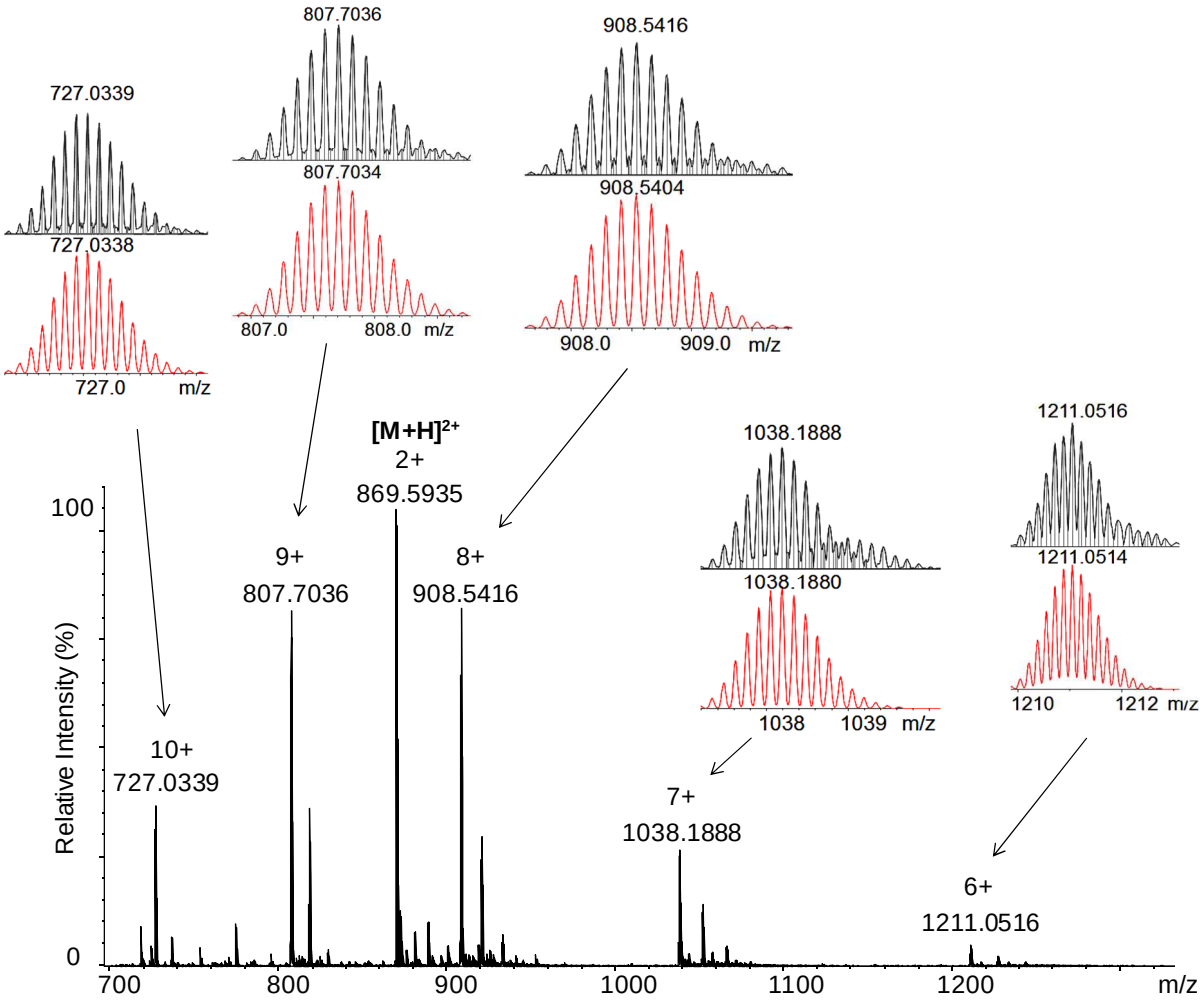

Fig. S 2. MS spectrum of the solution containing peptide [AHK]-NHOH and copper (II) ions. The spectrum was recorded on an FT-ICR-MS instrument in the positive ion mode. Red color corresponds to a simulated isotopic pattern ([ADK]-NHOH:Cu^{2+} = 4:5) and black corresponds to the experimental data. M corresponds to [ADK]-NHOH. For more details, see Table S1.

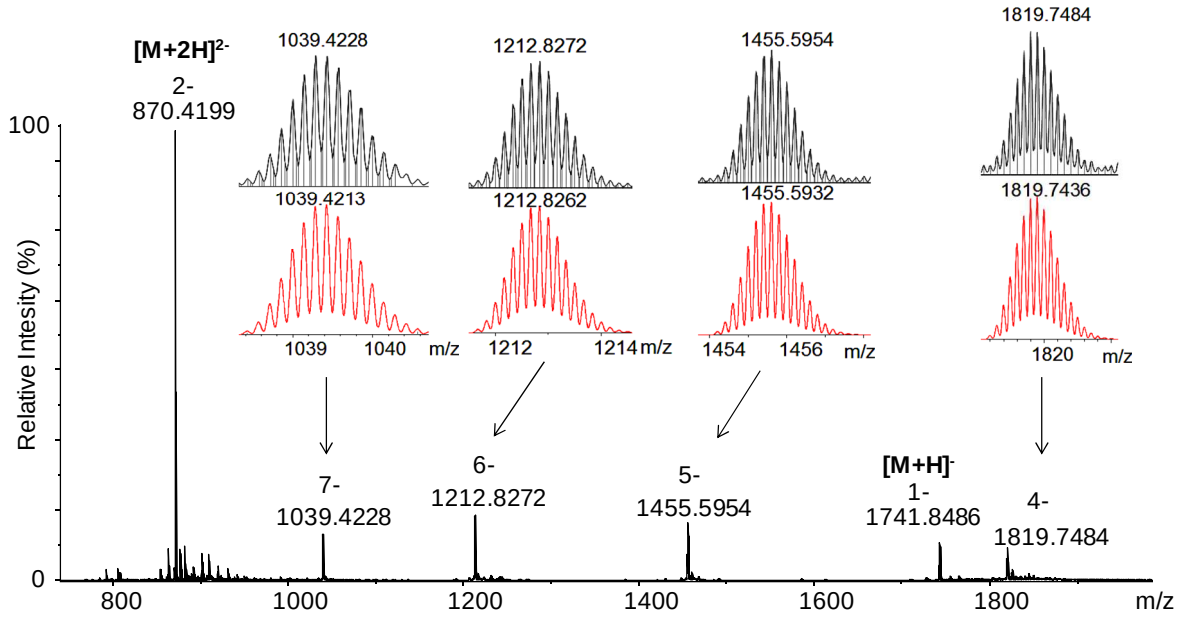

Fig. S3. MS spectrum of the solution containing peptide [ADE]-NHOH and copper (II) ions. The spectrum was recorded on a microTOF – MS instrument in the negative ion mode. Red color corresponds to a simulated isotopic pattern ([ADE]-NHOH:Cu^{2+} = 4:5) and black corresponds to the experimental data. M corresponds to [ADE]-NHOH. For more details, see Table S1.

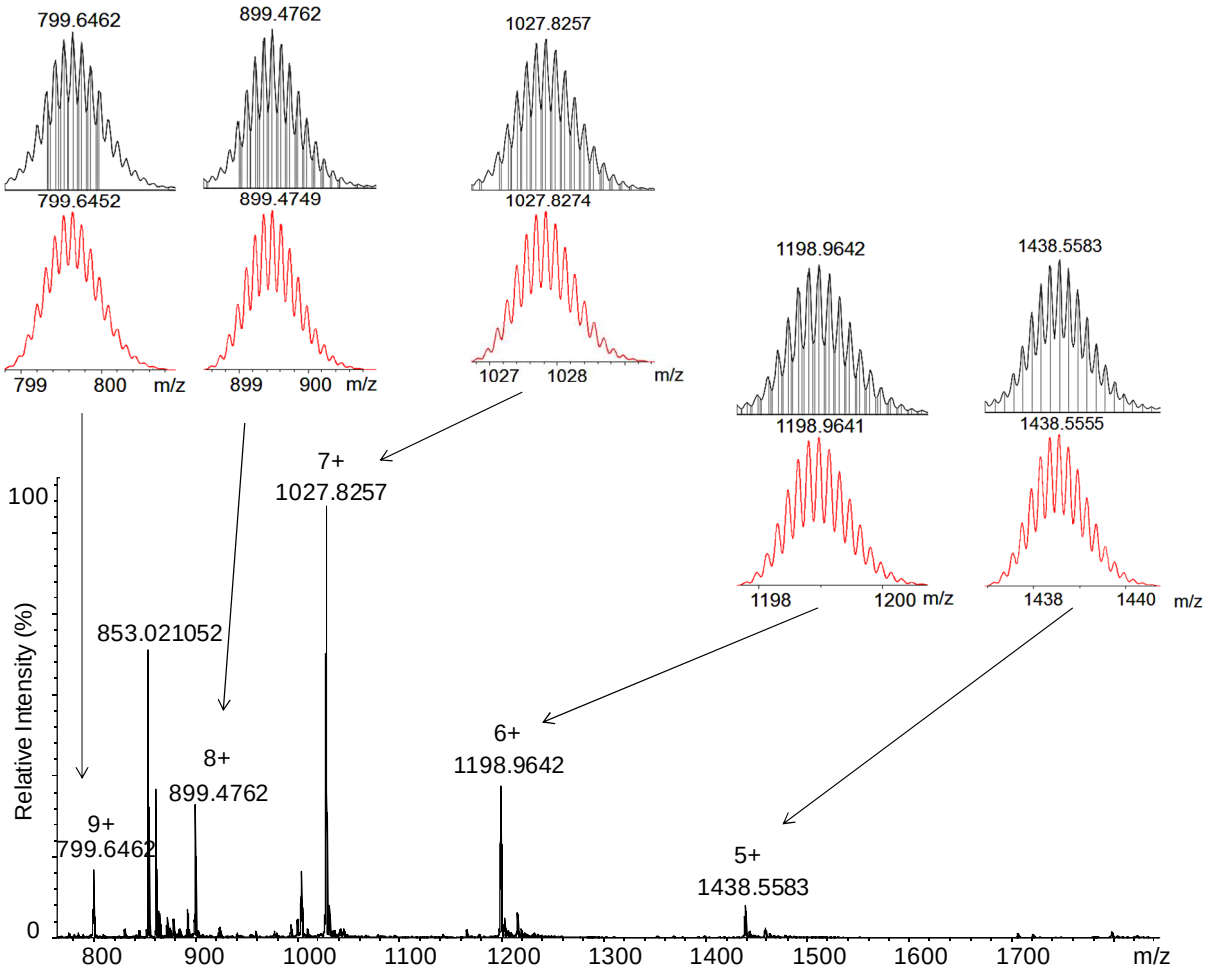

Fig. S4. MS spectrum of the solution containing peptide [AH]-NHOH and copper (II) ions. The spectrum was recorded on a microTOF – MS instrument in the positive ion mode. Red color correspond to a simulated isotopic pattern ([AH]-NHOH:Cu^{2+} = 4:5) and black corresponds to the experimental data. M corresponds to [AH]-NHOH. For more details, see Table S1.

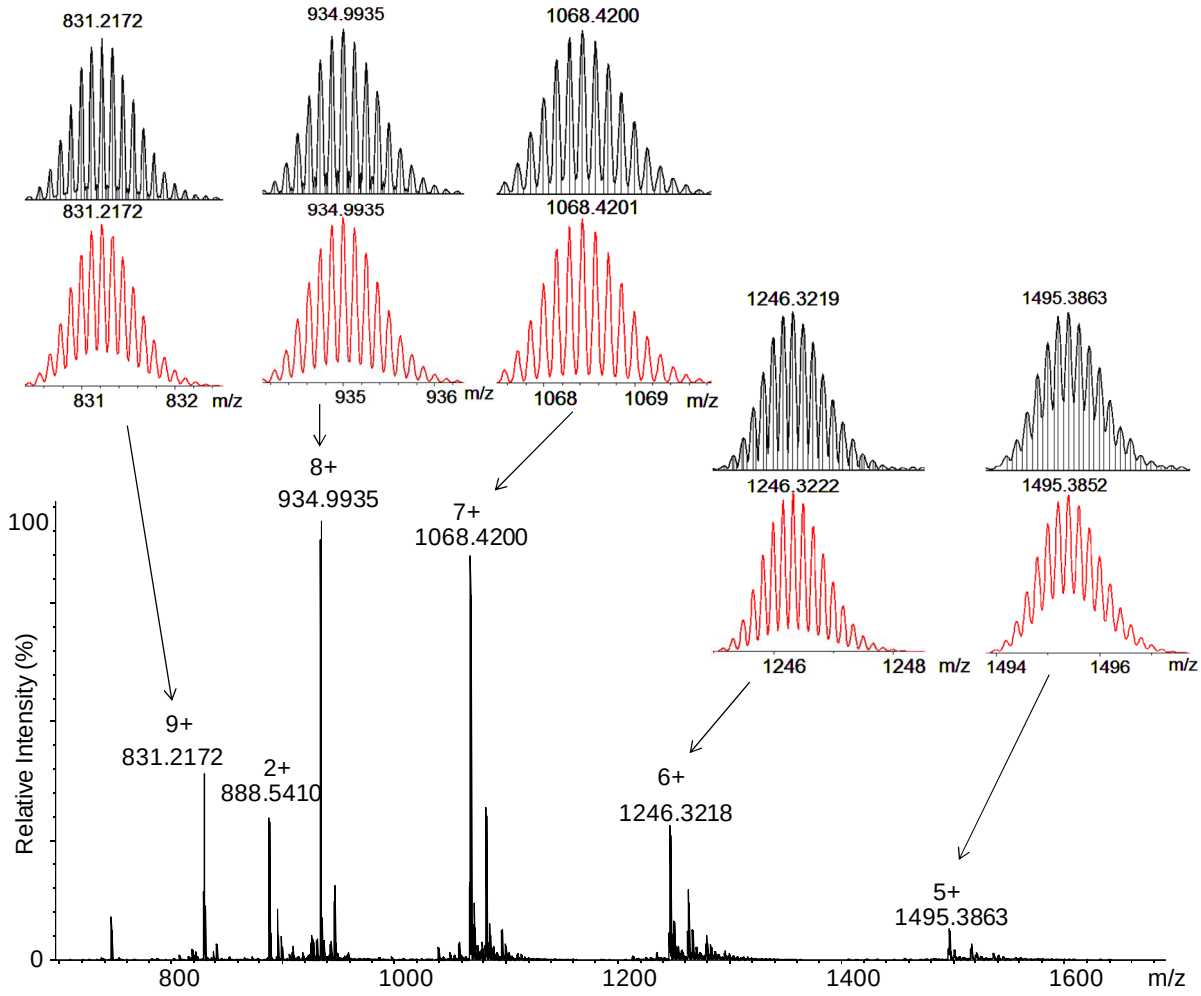

Fig. S5. MS spectra of the solution containing peptide [AH1]-NHOH and copper (II) ions. The spectrum was recorded on an FT-ICR-MS instrument in the positive ion mode. Red color corresponds to a simulated isotopic pattern ([AH1]-NHOH:Cu^{2+} = 4:5) and black corresponds to the experimental data. M corresponds to [AH1]-NHOH. For more details, see Table S1.

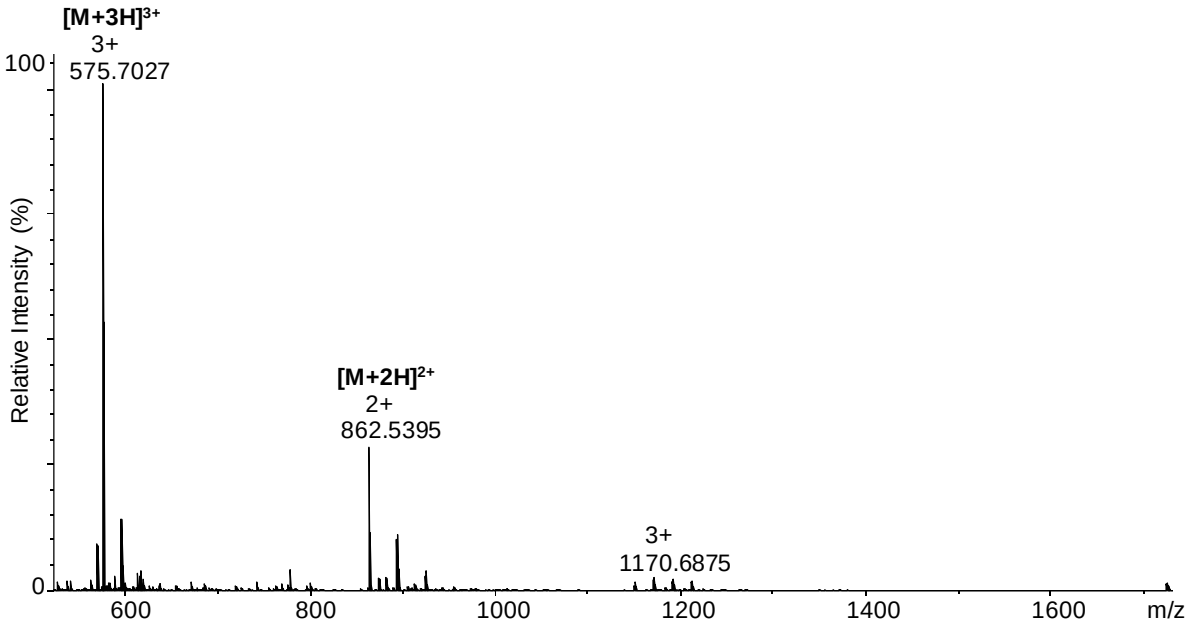

Fig. S6. MS spectrum of the complex of peptide [AH]-NH_2 and copper (II) ions. The spectrum was recorded on a microTOFQ-MS instrument in the positive ion mode. The signals $[M+3H]^{3+}$ and $[M+2H]^{2+}$ correspond to the ligand ([AH]-NH_2).

Circular Dichroism Experiments

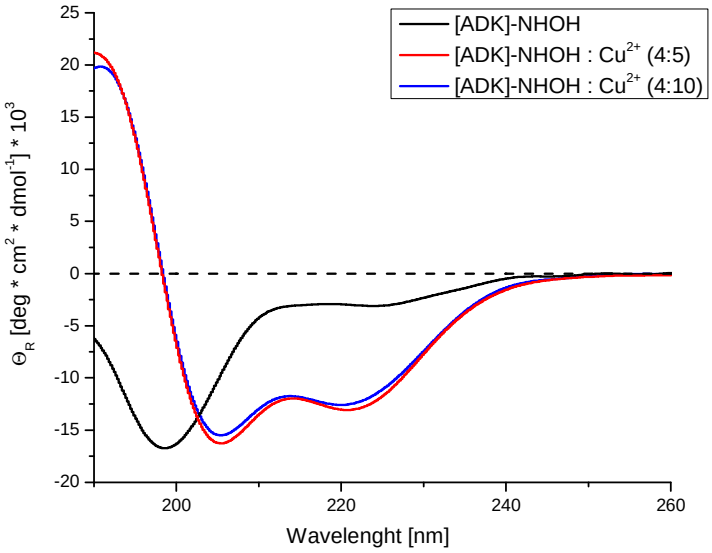

Fig. S7. The CD spectra of [ADK]-NHOH and [ADK]-NHOH/Cu^{2+}. Additional details are given in Materials and Methods.

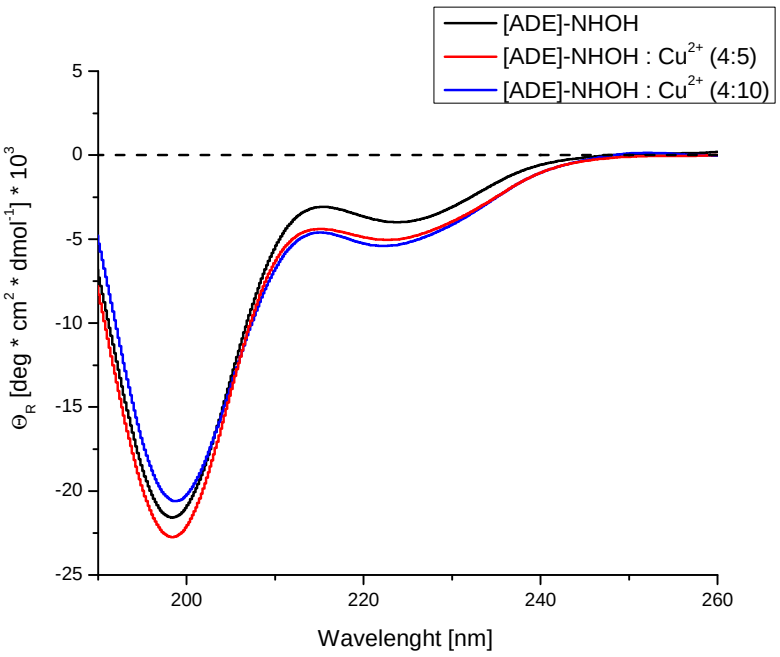

Fig. S8. The CD spectra of [ADE]-NHOH and [ADE]-NHOH/Cu^{2+}. Additional details are given in Materials and Methods.

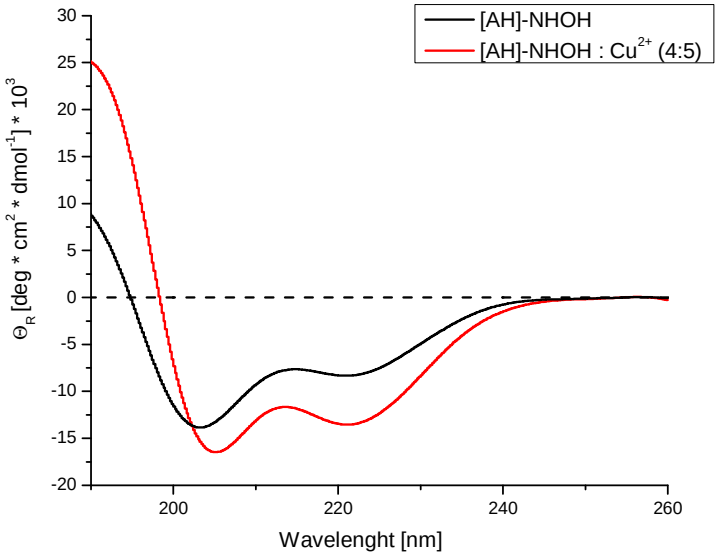

Fig. S9. The CD spectra of [AH]-NHOH and [AH]-NHOH/Cu^{2+}. Additional details are given in Materials and Methods.

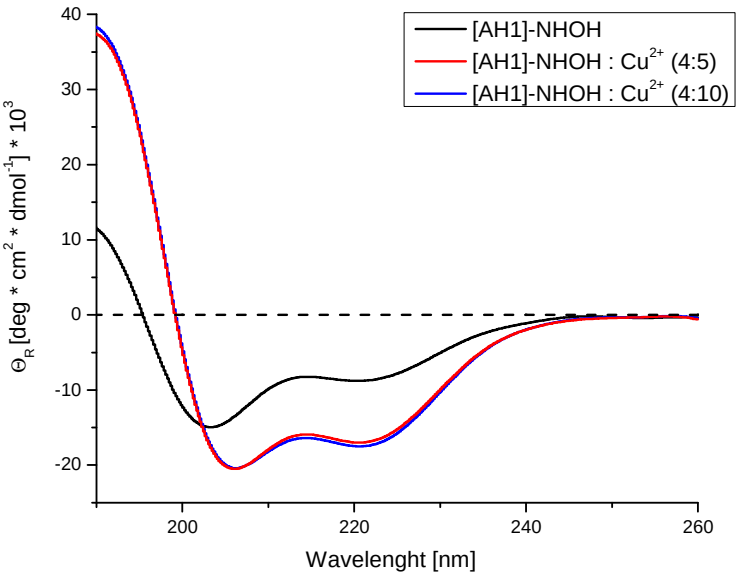

Fig. S10. The CD spectra of peptide [AH1]-NHOH and [AH1]/Cu^{2+}. Additional details are given in Materials and Methods.