Electronic Supplementary Information (ESI) for:

Mn(II) and Zn(II) interactions with peptide fragments from Parkinson's disease genes

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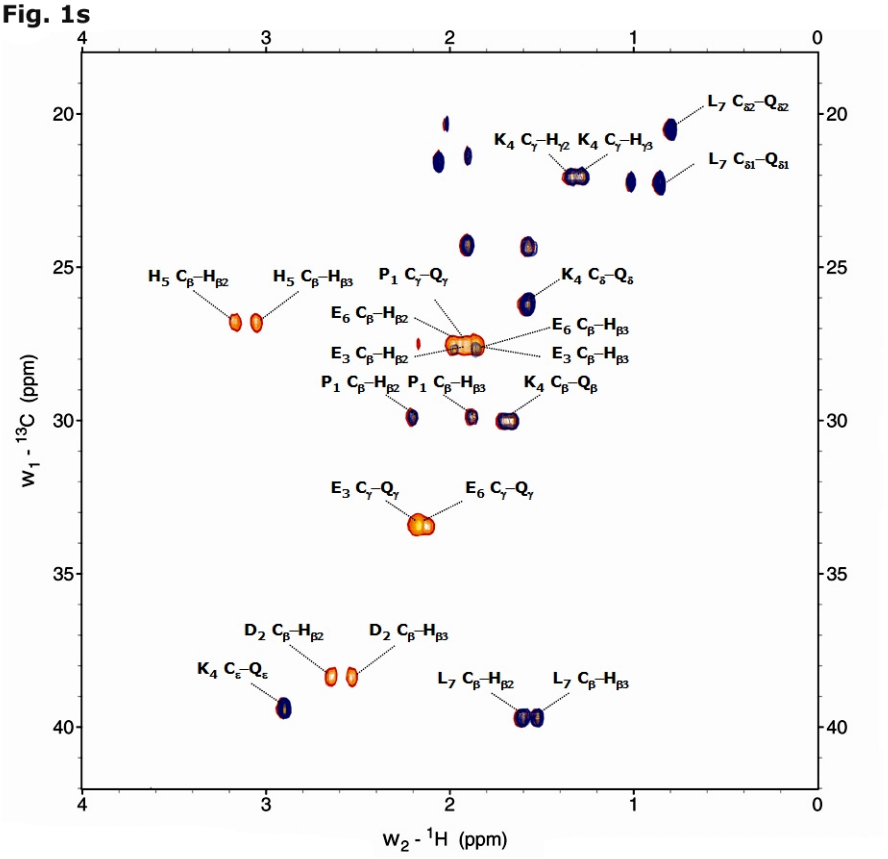
Fig. 1s



Mn(II): Ac-$P_1D_2E_3K_4H_5E_6L_7$-Am

Fig. 2s a

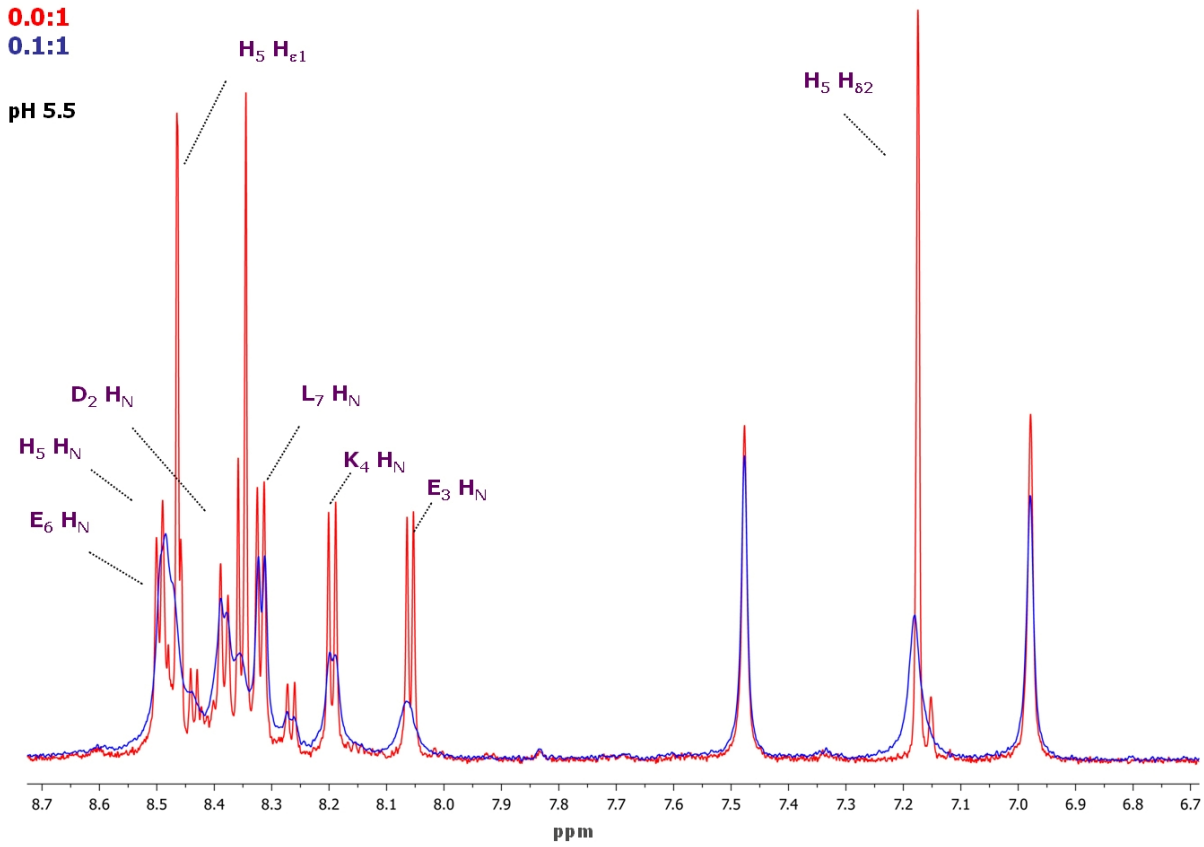
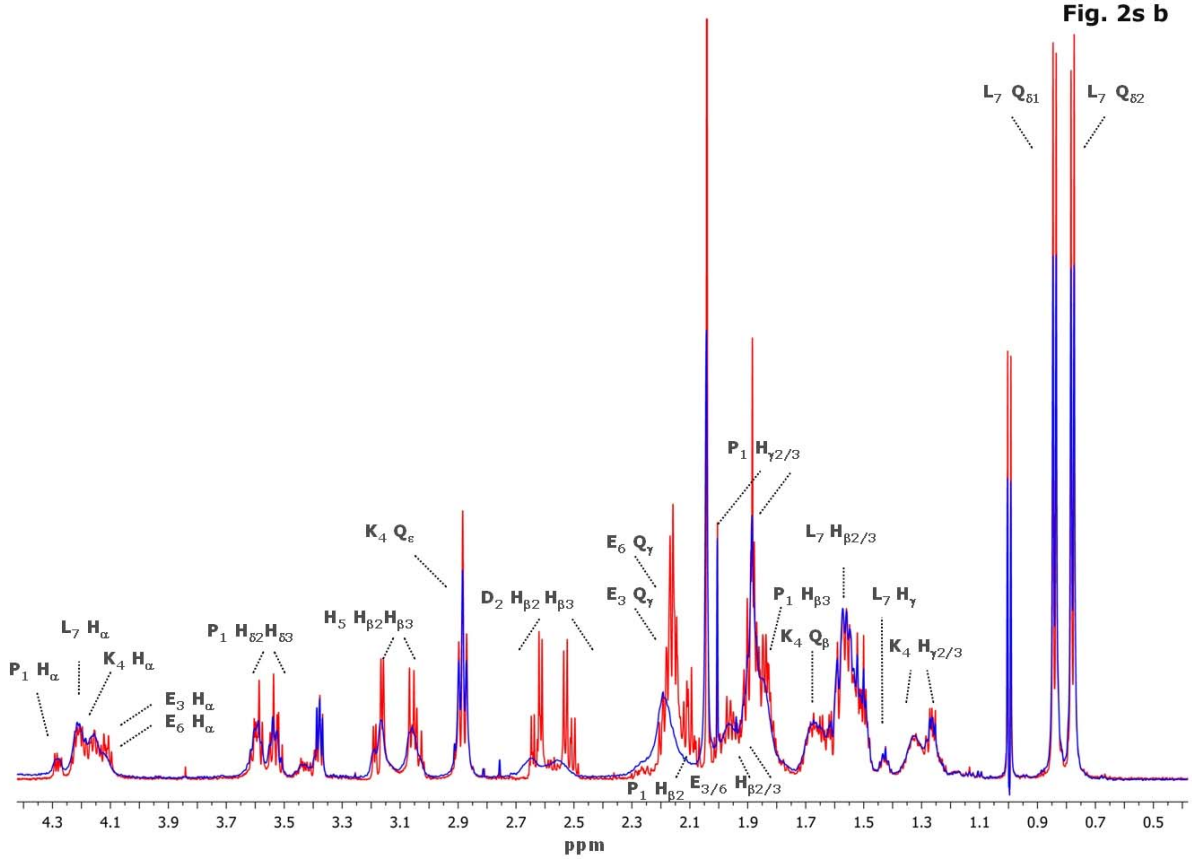


Fig. 2s b



Mn(II): Ac-$P_1D_2E_3K_4H_5E_6L_7$-Am

Fig. 3s a

0.0:1
0.1:1

pH 6.8

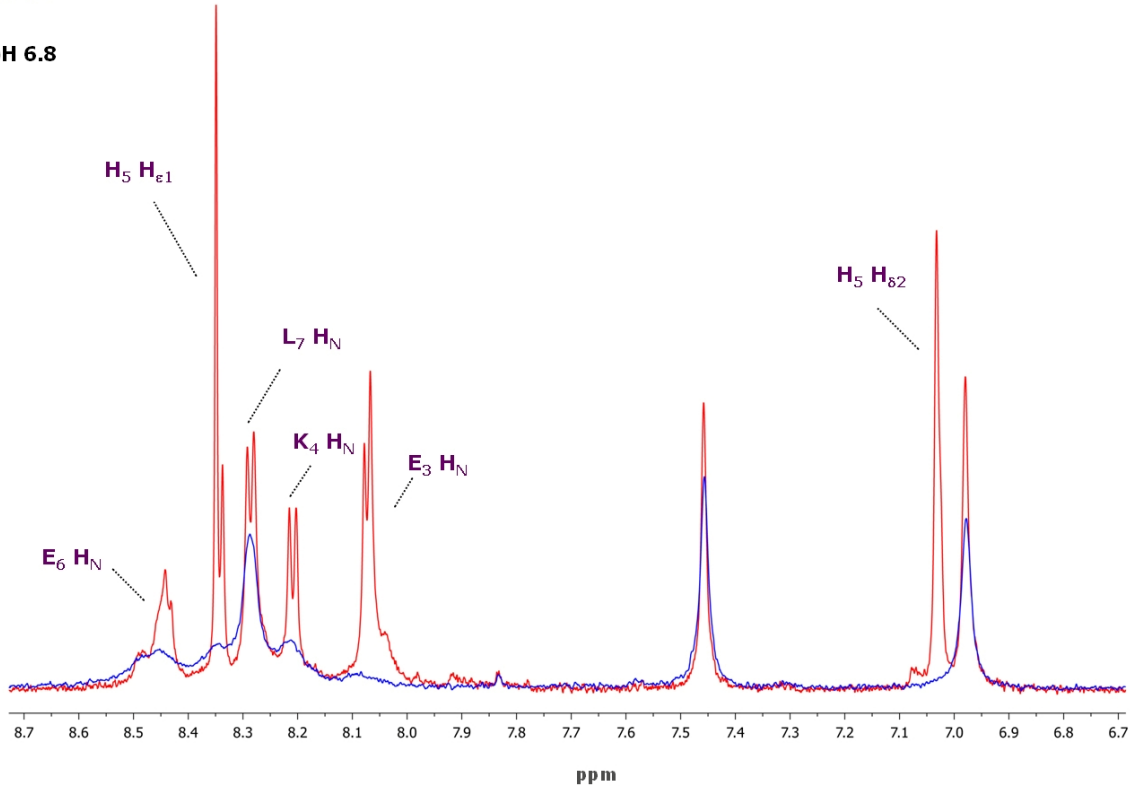
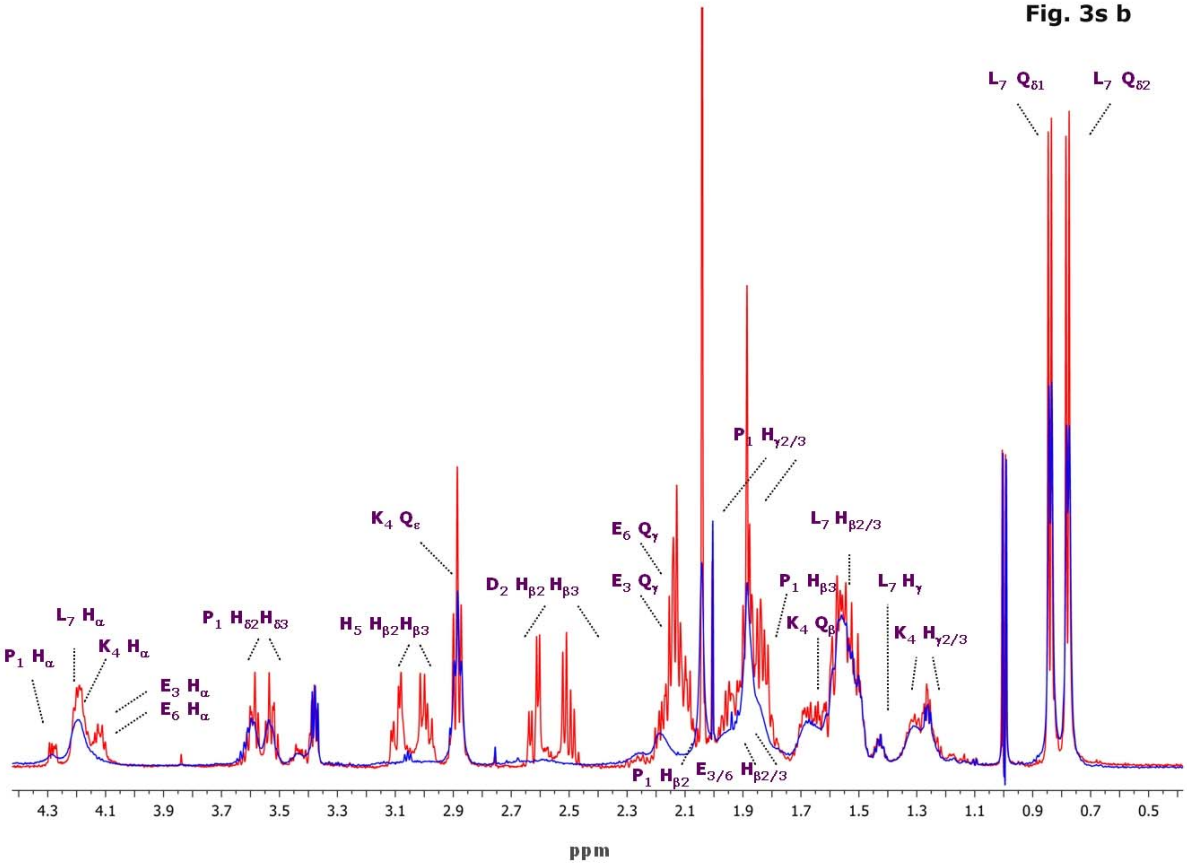


Fig. 3s b



Zn(II): Ac-$P_1D_2E_3K_4H_5E_6L_7$-Am

Fig. 4s

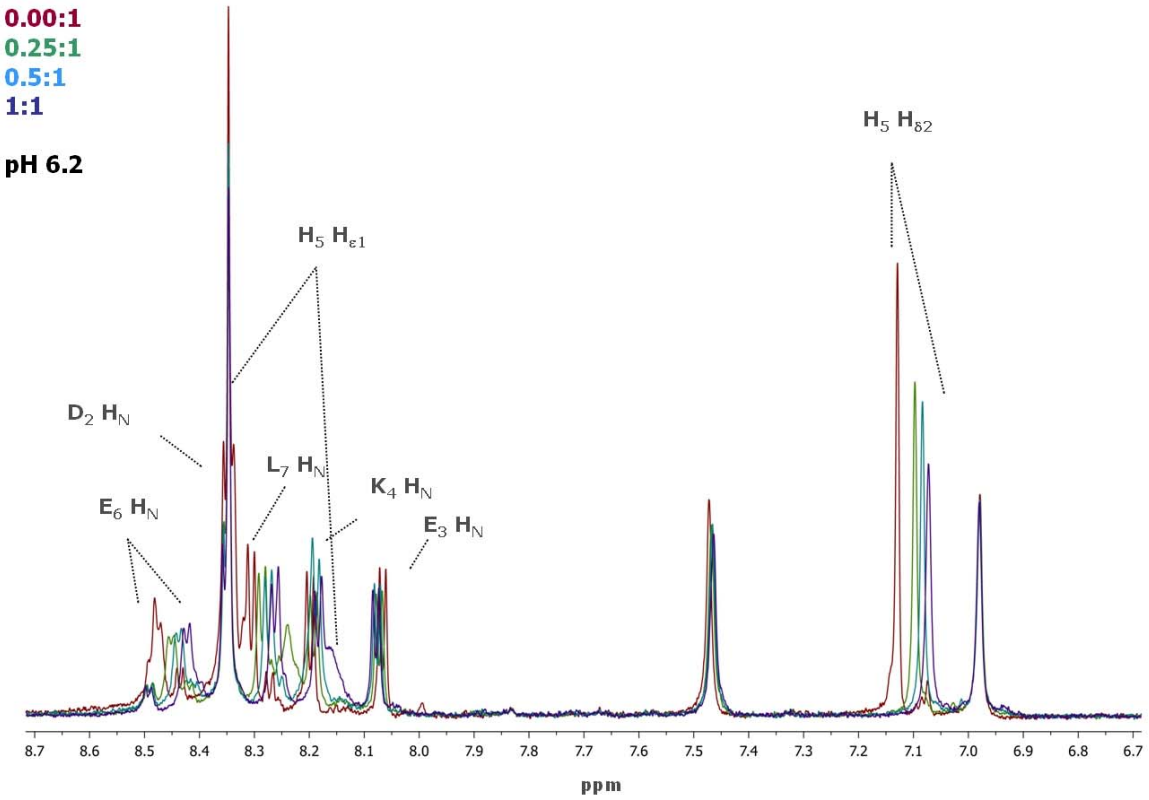


Fig. 5s

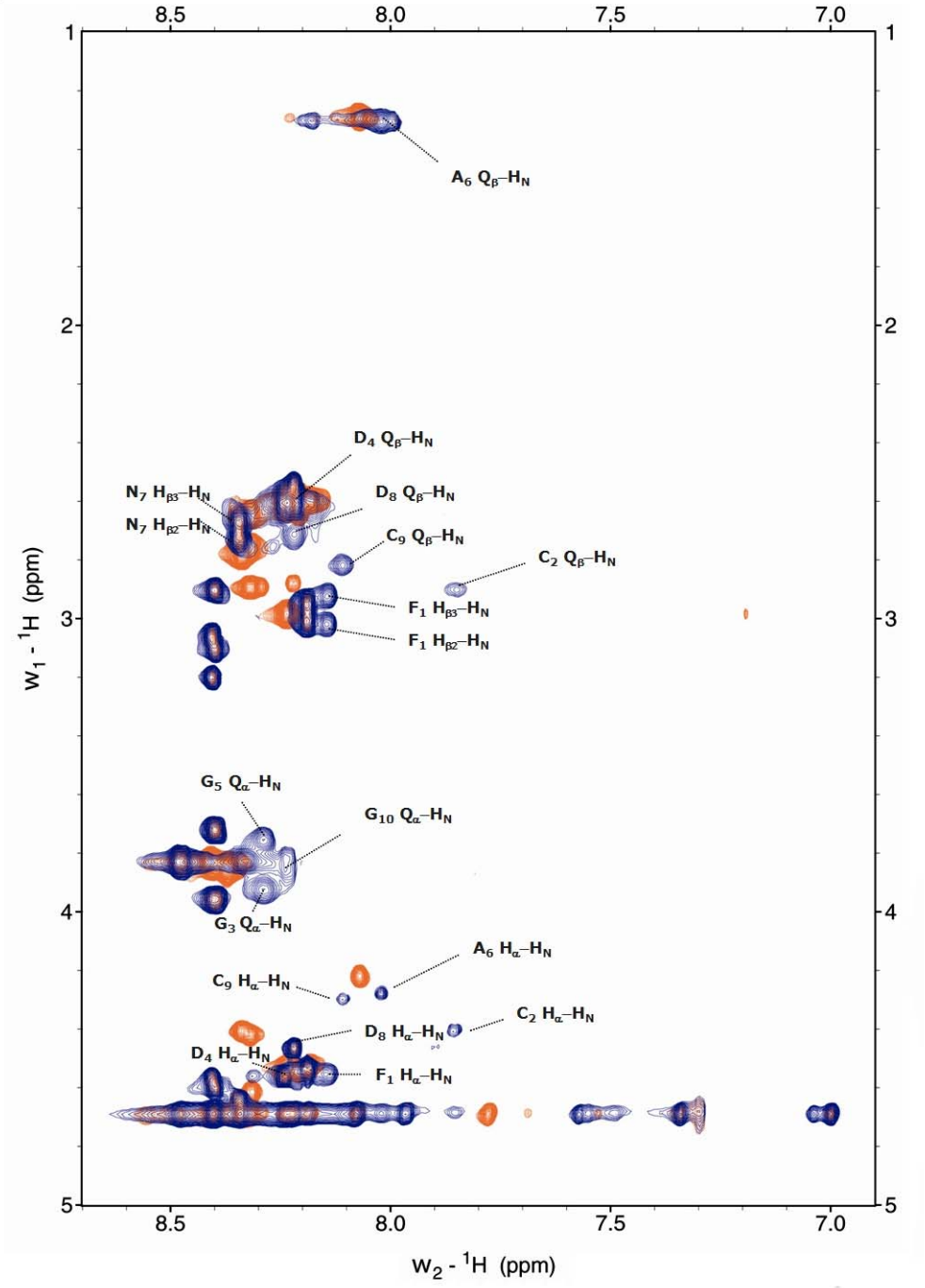


Table 1s ^{1}H and ^{13}C resonance assignment of the free peptide1 Ac-$P_1D_2E_3K_4H_5E_6L_7$-Am and the Zn-bound peptide1 at pH 6.2. Chemical shift differences ($\Delta\delta=\delta_{holo}-\delta_{apo}$) are also reported.

Residue-Proton	Free Ac-PDEHHEL-Am δ chemical shift (ppm)	Ac-PDEHHEL-Am:Zn 1:1 δ chemical shift (ppm)	Δδ
P1-Hα	4.294	4.302	**0.008**
P1-Hβ2	2.202	2.202	**0.000**
P1-Hβ3	1.885	1.892	**0.007**
P1-Qγ	1.896	1.899	**0.003**
P1-Hδ2	3.604	3.605	**0.000**
P1-Hδ3	3.545	3.546	**0.001**
D2-HN	8.353	8.362	**0.009**
D2-Hα	4.530	4.545	**0.015**
D2-Hβ2	2.630	2.642	**0.012**
D2-Hβ3	2.520	2.548	**0.028**
E3-HN	8.071	8.091	**0.020**
E3-Hα	4.126	4.150	**0.024**
E3-Hβ2	1.901	1.932	**0.031**
E3-Hβ3	1.848	1.849	**0.001**
E3-Qγ	2.153	2.170	**0.017**
K4-HN	8.211	8.199	**-0.012**
K4-Hα	4.179	4.178	**-0.001**
K4-Qβ	1.661	1.669	**0.008**
K4-Hγ2	1.329	1.285	**-0.044**
K4-Hγ3	1.279	1.283	**0.004**
K4-Qδ	1.573	1.573	**0.000**
K4-Qε	2.897	2.897	**0.000**
K4-Hz	7.438	7.438	**0.000**
H5-HN	8.352	8.347	**-0.005**
H5-Hα	4.588	4.582	**-0.006**
H5-Hβ2	3.152	3.149	**-0.003**
H5-Hβ3	3.041	3.023	**-0.018**
H5-Hδ2	7.129	7.079	**-0.050**
H5-He1	8.326	8.159	**-0.167**
E6-HN	8.490	8.428	**-0.062**
E6-Hα	4.221	4.218	**-0.003**
E6-Hβ2	1.969	1.975	**0.006**
E6-Hβ3	1.853	1.859	**0.006**
E6-Qγ	2.159	2.160	**0.001**
L7-HN	8.317	8.269	**-0.048**
L7-Hα	4.214	4.214	**0.000**
L7-Hβ2	1.593	1.597	**0.004**
L7-Hβ3	1.522	1.525	**0.003**
L7-Hγ	1.569	1.572	**0.003**
L7-Qδ1	0.852	0.851	**-0.001**
L7-Qδ2	0.789	0.789	**0.000**

Residue-Carbon	Free Ac-PDEHHEL-Am δ chemical shift (ppm)	Ac-PDEHHEL-Am:Zn 1:1 δ chemical shift (ppm)	Δδ
P1-Cα	60.460	60.409	**-0.051**
P1-Cβ	29.904	29.913	**0.009**
P1-Cγ	24.327	24.299	**-0.028**
P1-Cδ	48.704	48.737	**0.033**
D2-Cα	51.325	51.288	**-0.037**
D2-Cβ	38.348	38.222	**-0.126**
E3-Cα	53.976	53.978	**0.002**
E3-Cβ	27.560	27.454	**-0.106**
E3-Cγ	33.449	33.314	**-0.135**
K4-Cα	53.455	53.669	**0.214**
K4-Cβ	30.014	29.955	**-0.059**
K4-Cγ	22.034	21.976	**-0.058**
K4-Cδ	26.244	26.234	**-0.010**
K4-Cε	39.403	39.397	**-0.006**
H5-Cα	52.822	53.111	**0.289**
H5-Cβ	26.821	26.843	**0.022**
H5-Cδ2	117.368	Disappeared	
H5-Cε1	134.172	135.200	**1.028**
E6-Cα	53.872	53.851	**-0.021**
E6-Cβ	27.595	27.444	**-0.151**
E6-Cγ	33.443	33.313	**-0.130**
L7-Cα	52.393	52.452	**0.059**
L7-Cβ	39.710	39.717	**0.007**
L7-Cγ	24.349	24.343	**-0.006**
L7-Cδ1	22.260	22.284	**0.024**
L7-Cδ2	20.517	20.513	**-0.004**

Table 2s ^{1}H and ^{13}C resonance assignment of the free peptide 2 Ac-$F_1C_2G_3D_4G_5A_6N_7D_8C_9G_{10}$-Am and the Zn-bound peptide2 at pH 6.3. Chemical shift differences ($\Delta\delta=\delta_{holo}-\delta_{apo}$) are also reported

Residue-Proton	Free Ac-FCGDGANDCG-Am δ chemical shift (ppm)	Ac-FCGDGANDCG-Am:Zn 1:1 δ chemical shift (ppm)	Δδ
F1-HN	8.234	8.144	**-0.090**
F1-Hα	4.531	4.550	**0.019**
F1-Hβ2	2.990	3.015	**0.025**
F1-Hβ3	2.990	2.949	**-0.041**
F1-Hδ1	7.202	7.195	**-0.007**
F1-Hδ2	7.202	7.196	**-0.006**
F1-Hε1	7.290	7.289	**-0.001**
F1-Hε2	7.291	7.290	**-0.001**
F1-Hz	7.247	7.247	**0.000**
C2-HN	8.319	7.851	**-0.468**
C2-Hα	4.430	4.385	**-0.045**
C2-Qβ	2.898	2.906	**0.008**
G3-HN	8.374	8.289	**-0.085**
G3-Qα	3.849	3.918	**0.069**
D4-HN	8.207	8.238	**0.031**
D4-Hα	4.545	4.564	**0.019**
D4-Qβ	2.620	2.610	**-0.010**
G5-HN	8.371	8.328	**-0.043**
G5-Qα	3.853	3.829	**-0.024**
A6-HN	8.070	8.021	**-0.049**
A6-Hα	4.229	4.277	**0.048**
A6-Qβ	1.295	1.308	**0.013**
N7-HN	8.318	8.343	**0.025**
N7-Hα	4.620	4.648	**0.028**
N7-Hβ2	2.754	2.730	**-0.024**
N7-Hβ3	2.657	2.678	**0.021**
N7-Nδ21	7.529	7.572	**0.043**
N7-Nδ22	6.805	6.814	**0.009**
D8-HN	8.201	8.219	**0.018**
D8-Hα	4.545	4.470	**-0.075**
D8-Qβ	2.613	2.722	**0.109**
C9-HN	8.340	8.109	**-0.231**
C9-Hα	4.413	4.311	**-0.102**
C9-Qβ	2.791	2.825	**0.034**
G10-HN	8.406	8.240	**-0.166**
G10-Qα	3.836	3.838	**0.002**

Residue-Carbon	Free Ac-FCGDGANDCG-Am δ chemical shift (ppm)	Ac-FCGDGANDCG-Am:Zn 1:1 δ chemical shift (ppm)	Δδ
F1-Cα	55.349	55.211	**-0.138**
F1-Cβ	37.045	37.165	**0.120**
F1-Cδ	129.284	129.290	**0.006**
F1-Cε	128.825	128.758	**-0.067**
F1-Cz	127.245	127.224	**-0.021**
C2-Cα	56.161	56.771	**0.610**
C2-Cβ	25.053	26.881	**1.828**
G3-Cα	42.638	42.906	**0.268**
D4-Cα	51.723	51.622	**-0.101**
D4-Cβ	38.349	38.171	**-0.178**
G5-Cα	42.689	42.697	**0.008**
A6-Cα	50.008	49.780	**-0.228**
A6-Cβ	16.540	16.720	**0.180**
N7-Cβ	36.375	36.679	**0.304**
D8-Cα	51.730	51.880	**0.150**
D8-Cβ	38.376	38.230	**-0.146**
C9-Cα	55.600	56.770	**1.170**
C9-Cβ	25.323	26.734	**1.411**
G10-Cα	42.566	42.655	**0.089**