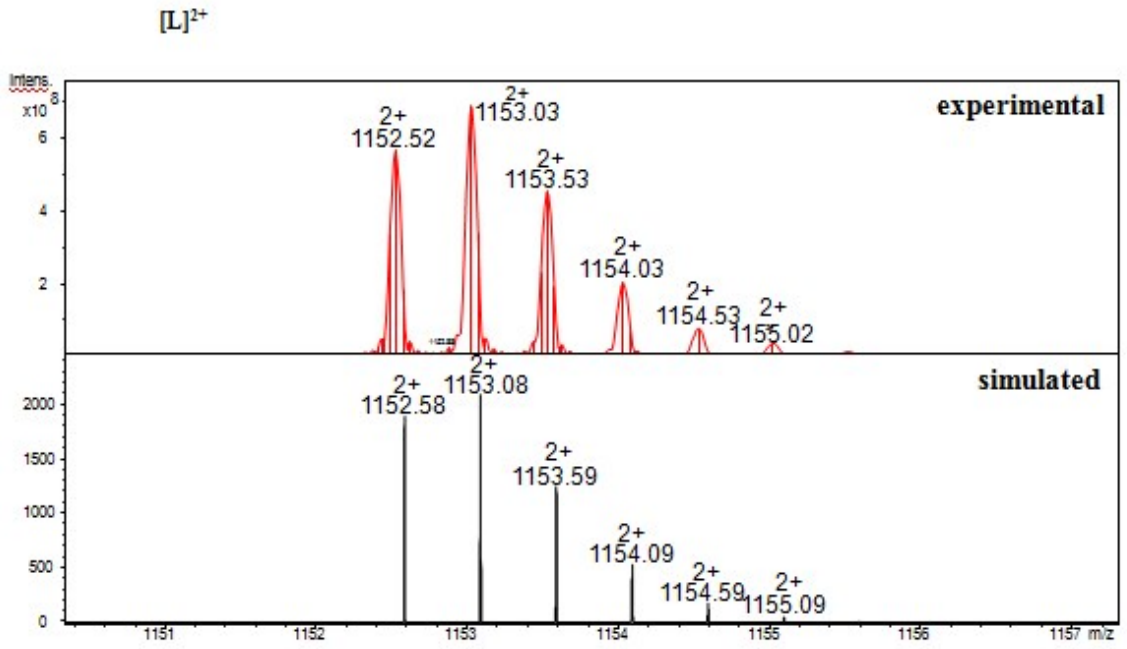

Figure S1. The fragment of the ESI-MS spectrum showing the isotope distribution of the peak at m/z = 1153.03 and simulation, corresponding to the free ligand (L1) Ac-$_{101}$DHHLAHIVVDAIAHASEDRR$_{120}$.

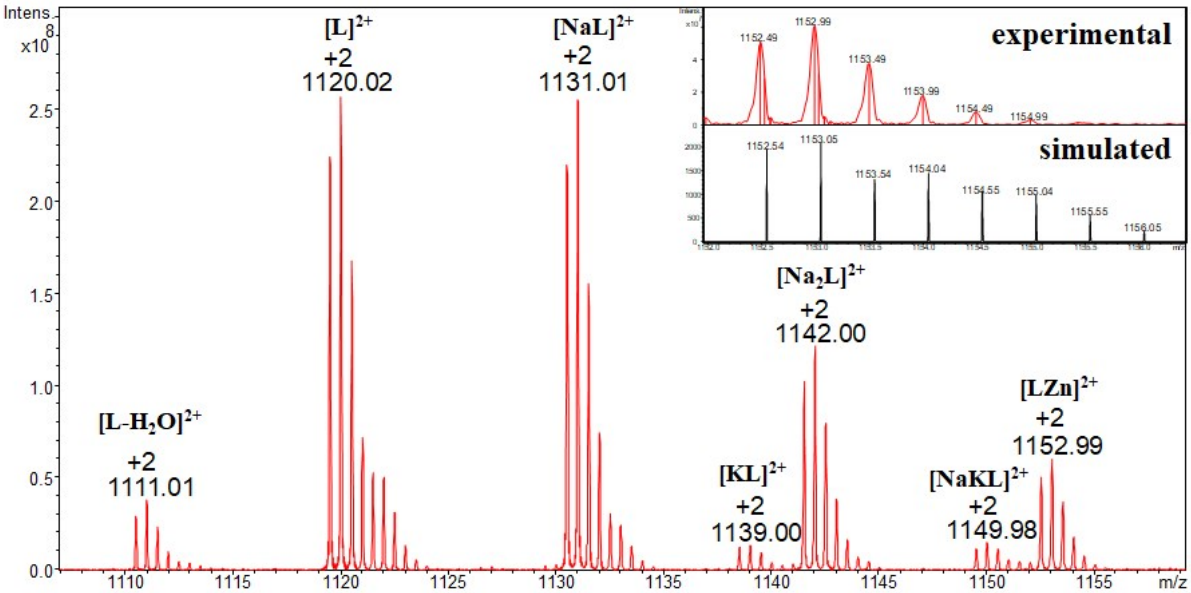

Figure S2. ESI-MS spectrum of a metal-ligand system composed of Ac-$_{101}$DHALAHIVVDAIAHASEDRR$_{120}$ peptide (L2) and zinc(II) ions in the m/z 1105-1160 range at pH 7 [M:L = 1:1.5]. The simulated and experimental isotopic distribution spectra of the peak at m/z = 1152.99 are presented in the upper right corner.

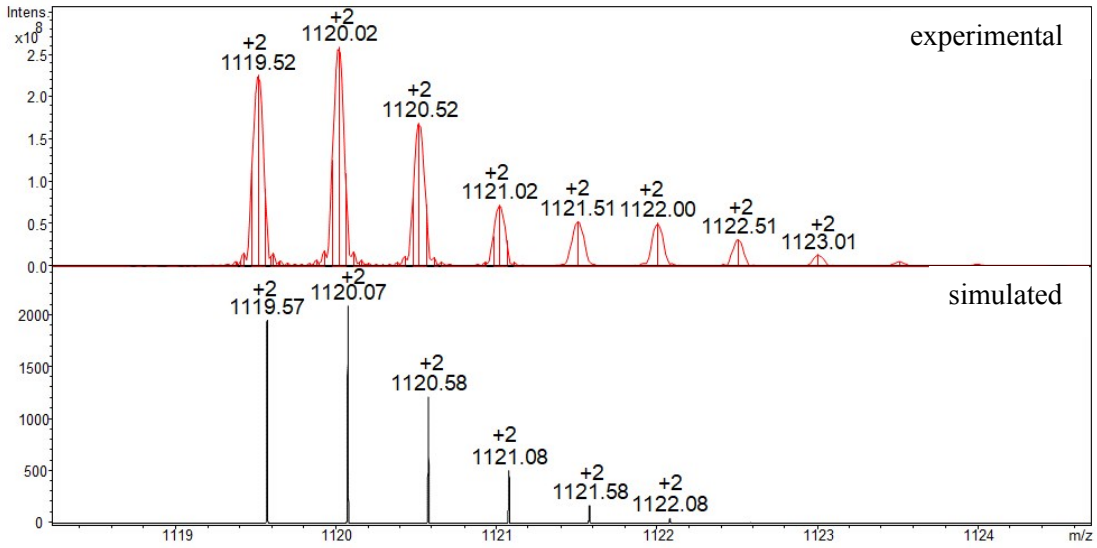

Figure S3. The fragment of the ESI-MS spectrum showing the isotope distribution of the peak at m/z = 1120.02 and simulation, corresponding to the free ligand (L2) Ac-$_{101}$DHALAHIVVDAIAHASEDRR$_{120}$.

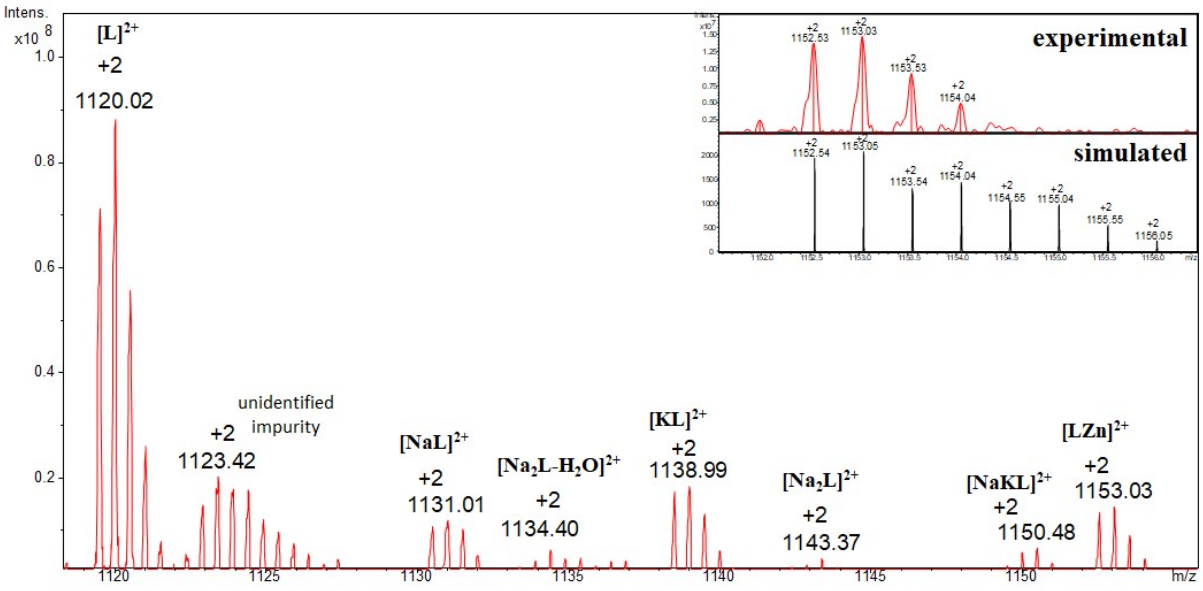

Figure S4. ESI-MS spectrum of a metal-ligand system composed of Ac-$_{101}$DHHLAHIVVDAIAAASEDRR$_{120}$ peptide (L3) and zinc(II) ions in the m/z 1120-1160 range at pH 7 [M:L = 1:1.5]. The simulated and experimental isotopic distribution spectra of the peak at m/z = 1153.03 are presented in the right corner.

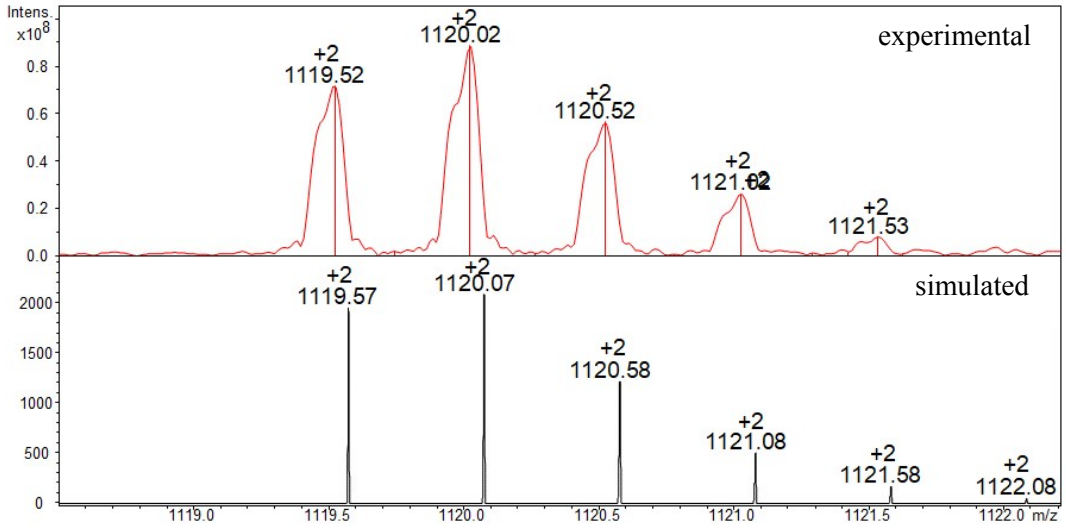

Figure S5. The fragment of the ESI-MS spectrum showing the isotope distribution of the peak at m/z = 1120.02 and simulation, corresponding to the free ligand (L3) Ac-$_{101}$DHHLAHIVVDAIAAASEDRR$_{120}$.

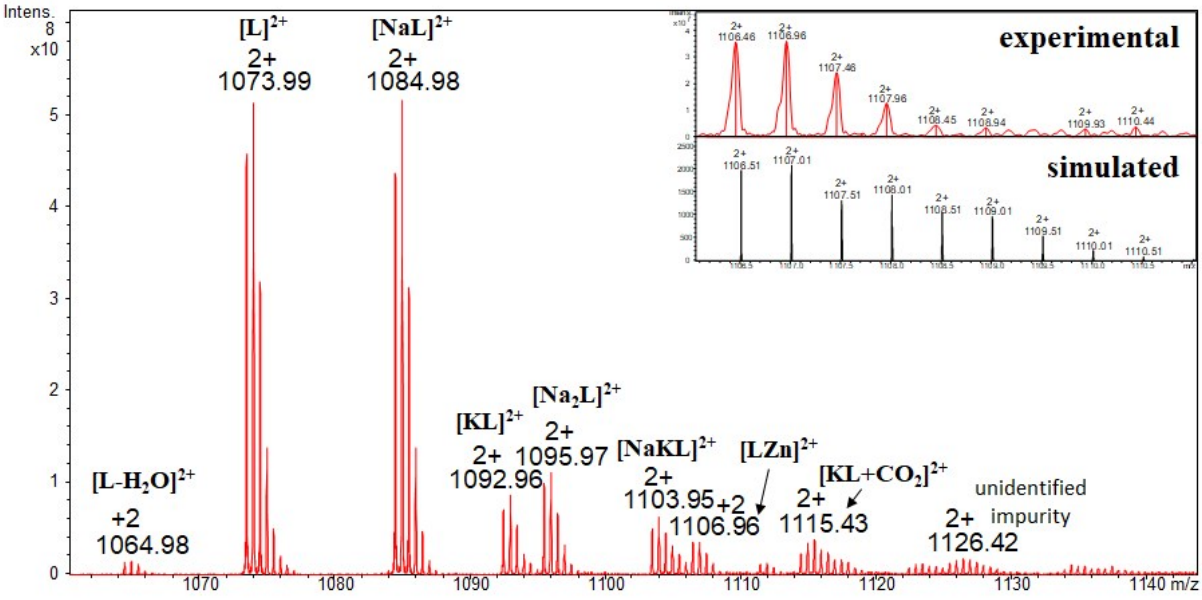

Figure S6. ESI-MS spectrum of a metal-ligand system composed of Ac-$_{116}$DHHLAHIVLDAVAHAGEDAI$_{135}$ peptide (L4) and zinc(II) ions in the m/z 1055-1405 range at pH 7 [M:L = 1:1.5]. The simulated and experimental isotopic distribution spectra of the peak at m/z = 1106.96 are presented in the right corner.

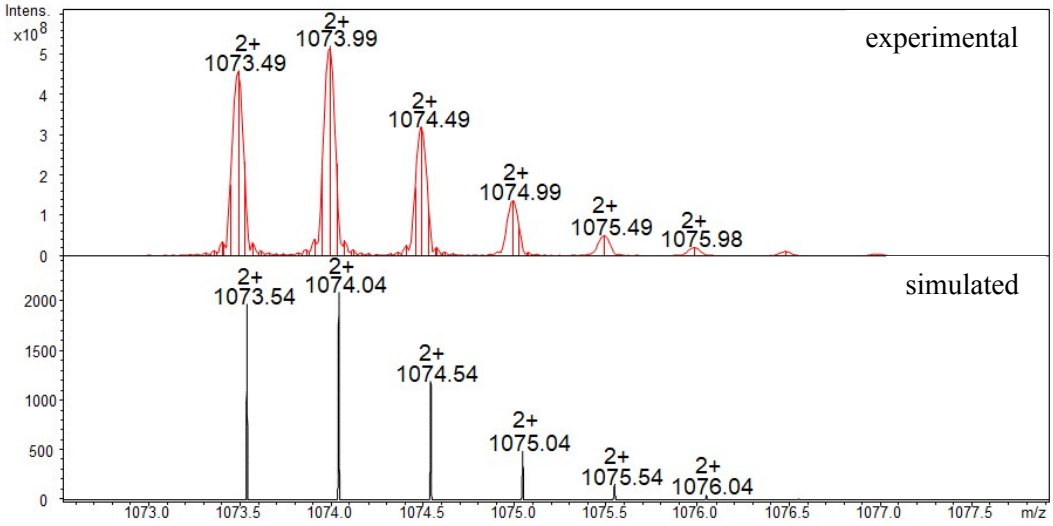

Figure S7. The fragment of the ESI-MS spectrum showing the isotope distribution of the peak at m/z = 1073.99 and simulation, corresponding to the free ligand (L4) Ac-$_{116}$DHHLAHIVLDAVAHAGEDAI$_{135}$.