Electronic Supplementary Material (ESI) for Dalton Transactions.

Supplementary Information

Zinc(II) binding sites in Pra1, a zincophore from *Candida albicans*

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1    MNYLLFCLFFAFSVAAP---------V-TVTRFVDASPTGYDWRADWVKGFPIDSSCNAT   50   P87020   PRA1_CANAL
1    MAALL-RLAVLLPLAAPLVATLPTSPVPIAARATPHEPVFFSWDAGAVTSFPIHSSCNAT   59   D3W9Z7   D3W9Z7_ASPFM
     *  **  * . : :***          *  .:* .  .*. :.* *  *..***.******

51   QYNQLSTGLQEAQLLAEHARDHTLRFGSKSPFFRKYFGNDTASAEVVGHFENVVGADKSS   110  P87020   PRA1_CANAL
60   QRRQIEAGLNEAVELARHAKAHILRWGNESEIYRKYFGNRPT-MEAVGAYDVIVNGDKAN   118  D3W9Z7   D3W9Z7_ASPFM
     * .*:.:**:**  **.**: * **:*.:* ::****** :  *.** :: :* .**:.

111  ILFLCDDLDDKCKNDGWAGYWRGSNHSDQTIICDLSFVTRRYLSQLCSGGYTVSKSKTNI   170  P87020   PRA1_CANAL
119  VLFRCDNPDGNCALEGWGGHWRGANATSETVICDRSYTTRRWLVSMCSQGYTVAGSETNT   178  D3W9Z7   D3W9Z7_ASPFM
     :** **: * :*  :**.*:***:* :.:*:*** *:.***:* .:** ****: *:**

171  FWAGDLLHRFWHLKSIGQLVIEHYADTYEEVLELAQENSTYAVRNSNSLIYYALDVYAYD   230  P87020   PRA1_CANAL
179  FWASDLMHRLYHVPAVGQGWVDHFADGYDEVIALAKSNGTESTHDSEALQYFALEAYAFD   238  D3W9Z7   D3W9Z7_ASPFM
     ***.**:**::*: ::**  ::*:** *:**: **:.*.* :.::*::* *:**:.**:*

231  VTIPGEGCNGDGTSYKKSDFSSFEDSD-SGS-DSGASSTASSSHQHTDSNPSATTDANSH   288  P87020   PRA1_CANAL
239  IAAPGVGCAGESHGPDQGHDTGSASAPASTSTSSSSSASGSGATTTPTDSPSATIDVPPN   298  D3W9Z7   D3W9Z7_ASPFM
     :: ** ** *:. . .:.. :.  .:  * * .*.:*::.*.:     ..**** *.  .

289  CHTHADGEVHC-   299  P87020   PRA1_CANAL
299  CHTHEGGQLHCT   310  D3W9Z7   D3W9Z7_ASPFM
     ****  *::**
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Figure S1. The alignment of Pra1 and Aspf2 sequences (Uniprot accession numbers P87020 and D3W9Z7, respectively). The two zincophores share 43% of identity.

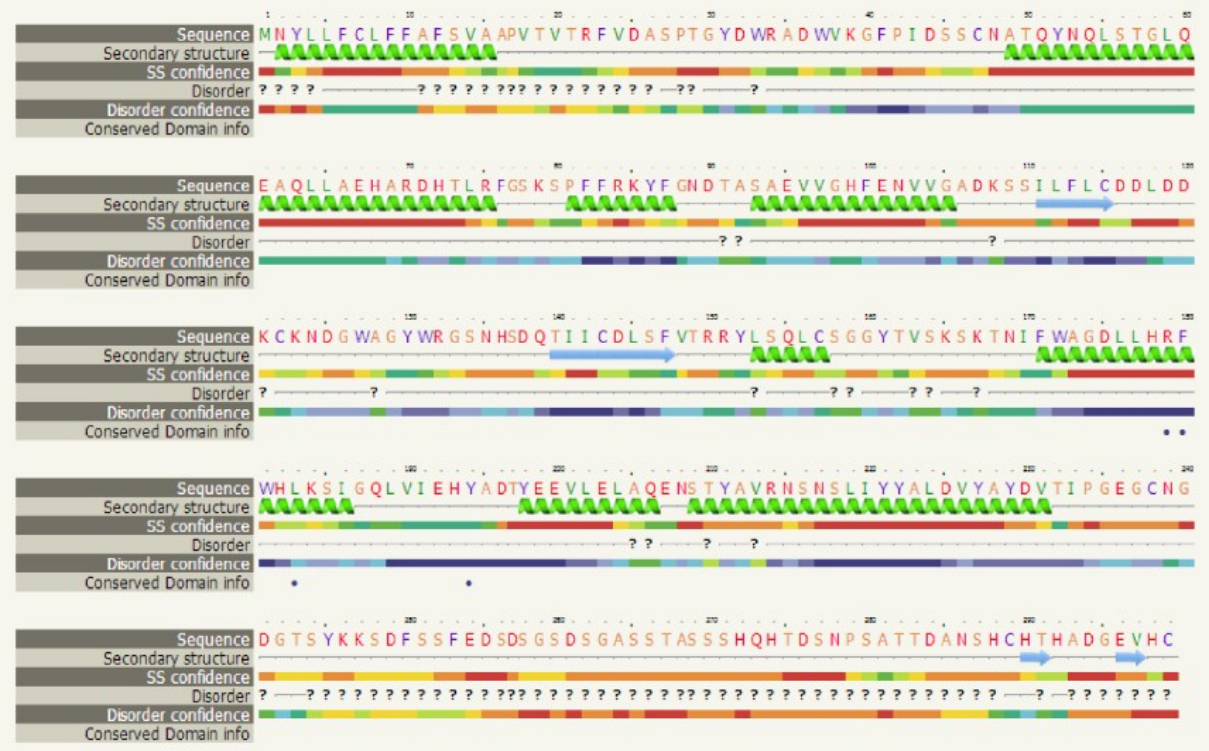

Figure S2. Probable secondary structure of Pra1 predicted by Phyre2.

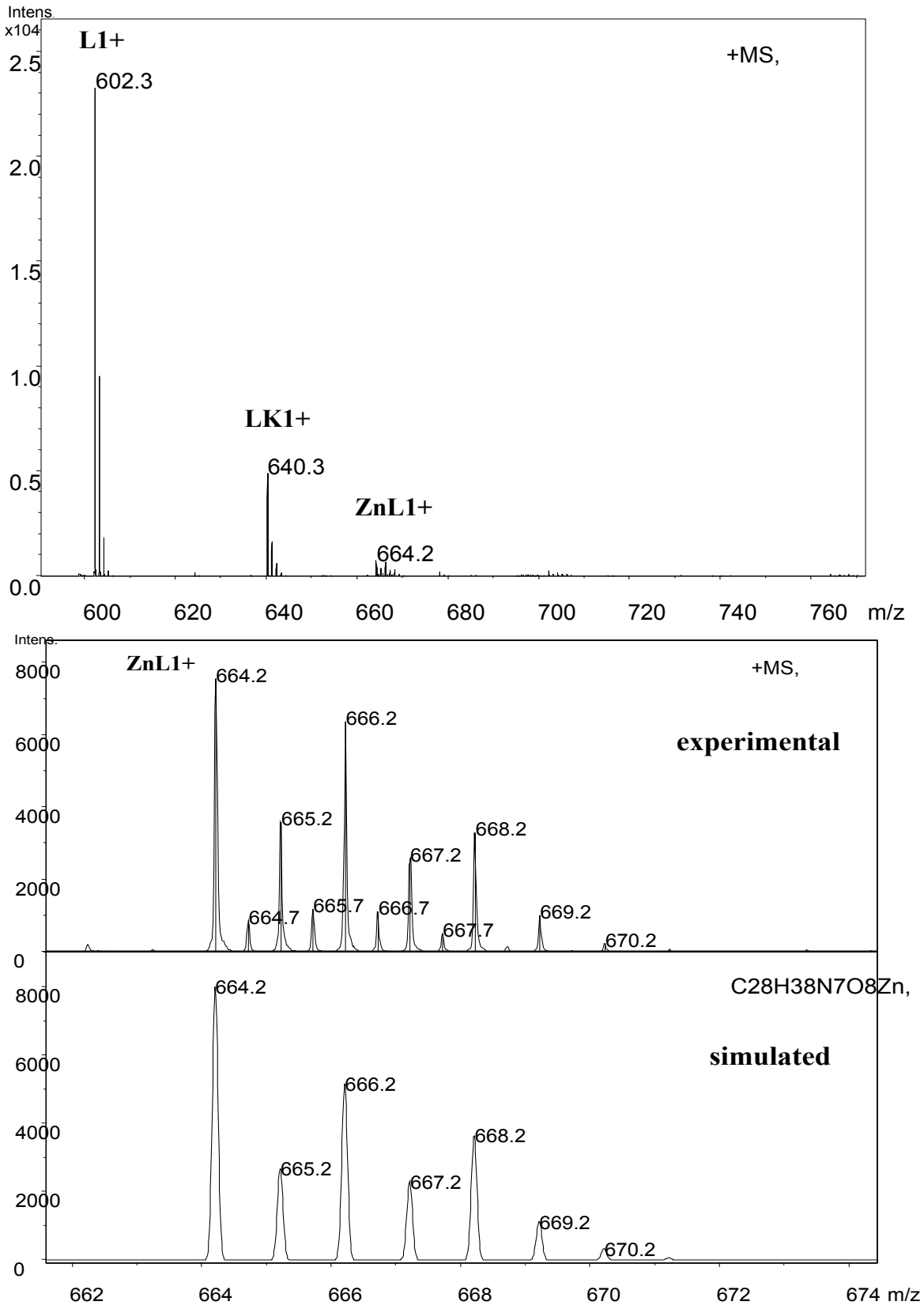

Figure S3. ESI-MS spectrum of Zn(II)-Ac-IEHY-NH_2 at pH 6.M/L molar ratio = 1:1.

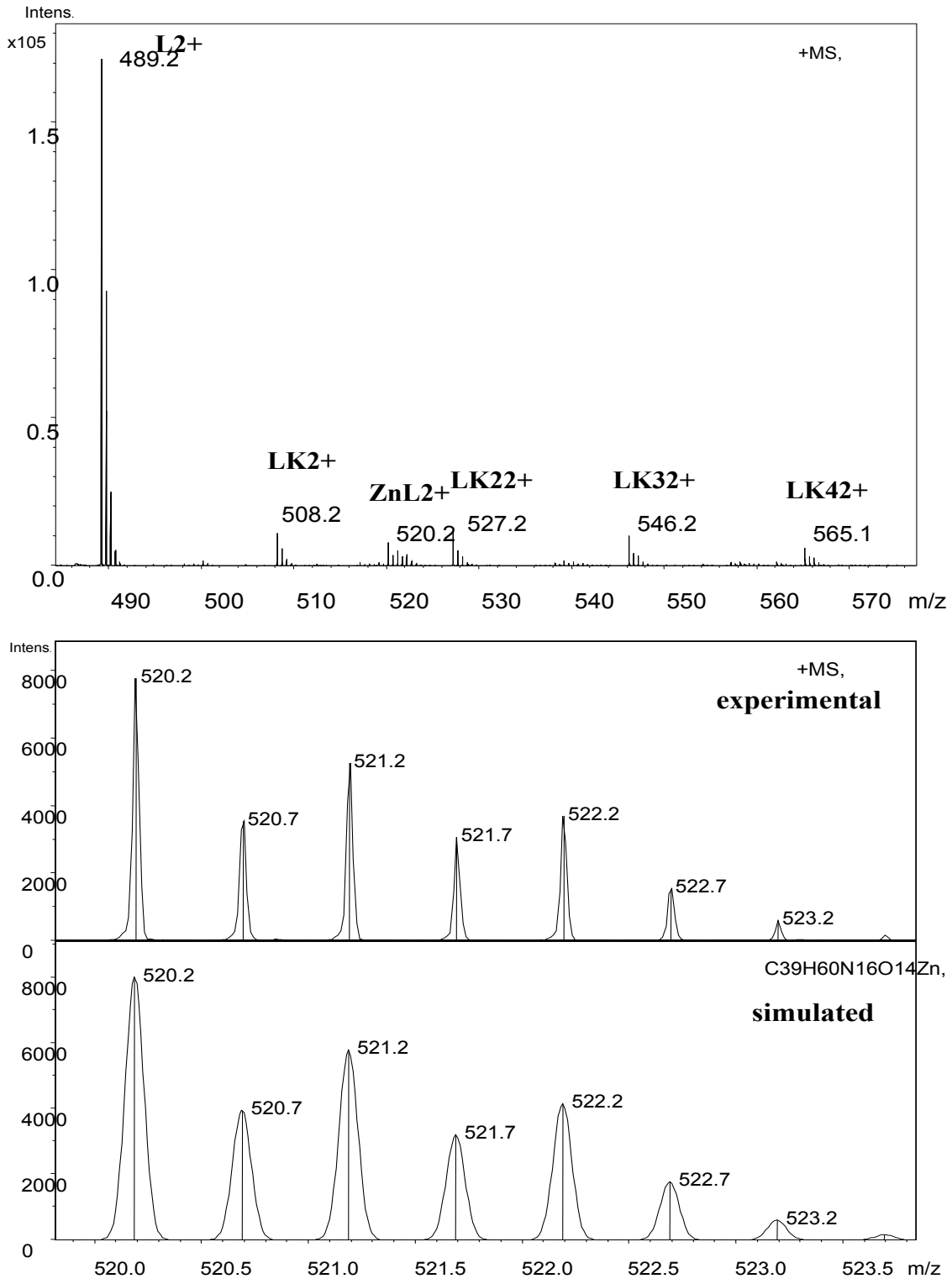

Figure S4. ESI-MS spectrum of Zn(II)-Ac-AEHARDH-NH_2at pH 6.M/L molar ratio = 1:1.

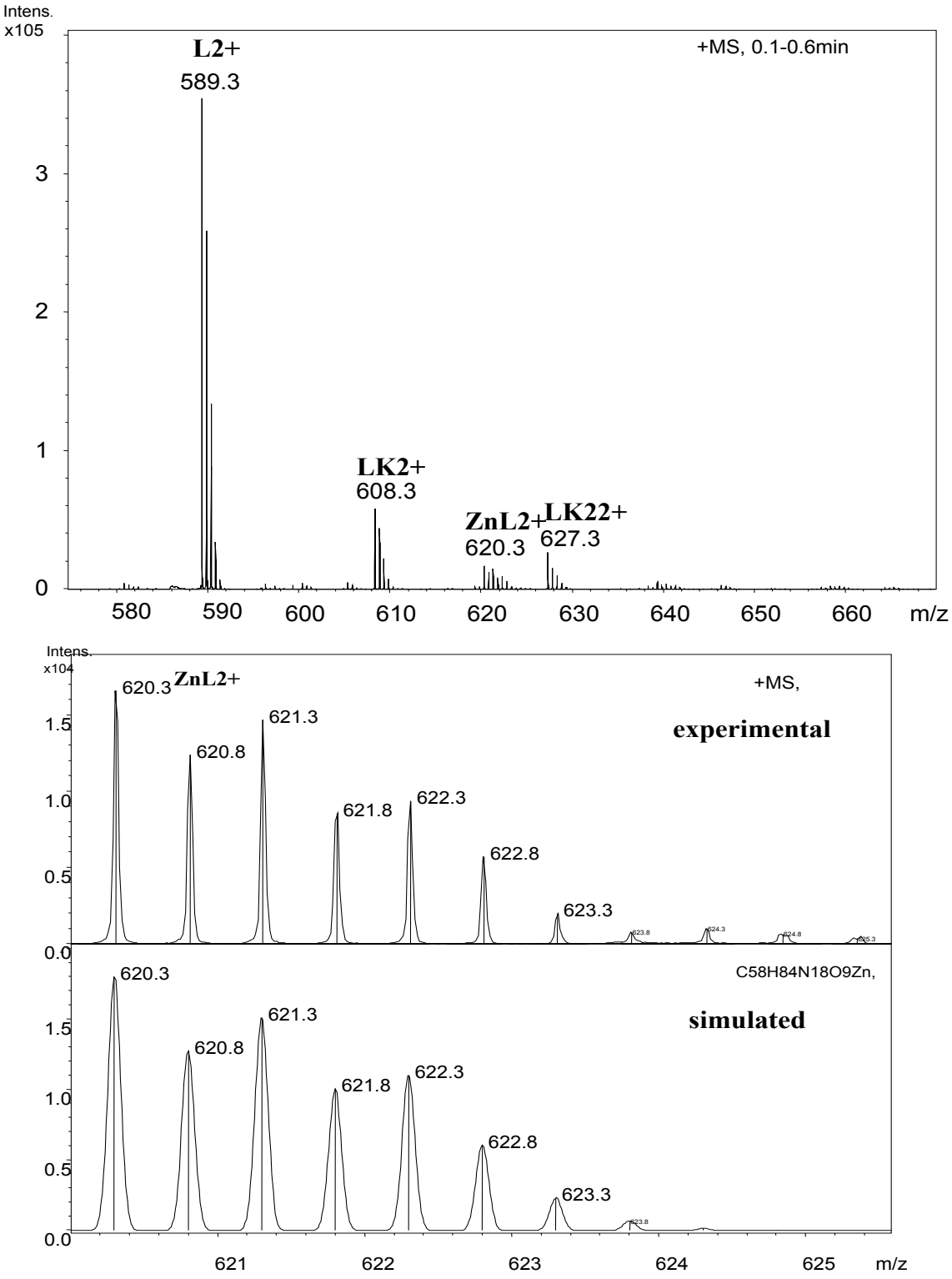

Figure S5. ESI-MS spectrum of Zn(II)-Ac-LHRFWHLK -NH_2at pH 6.M/L molar ratio = 1:1.

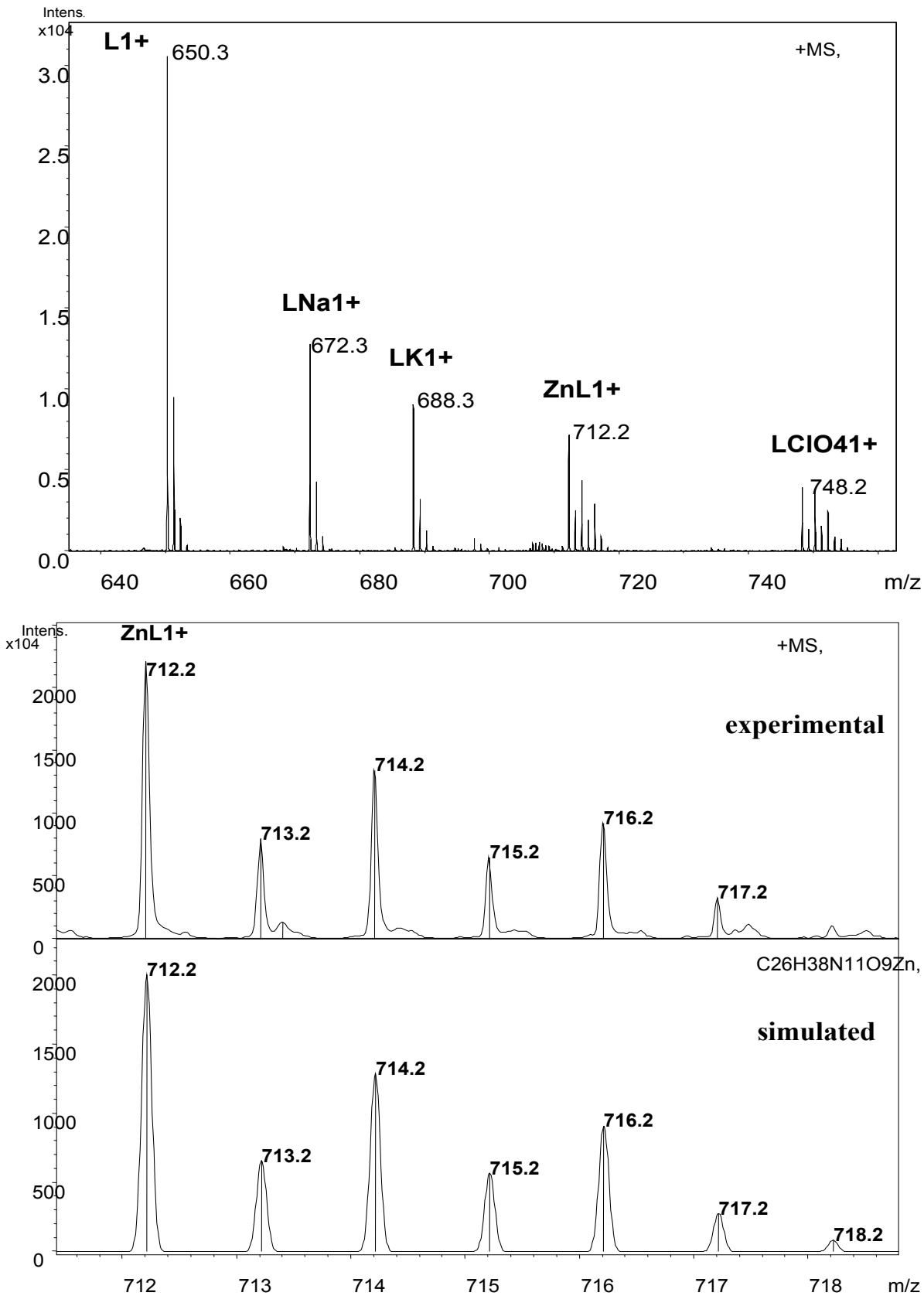

Figure S6. ESI-MS spectrum of Zn(II)-Ac-SHQHT-NH_2at pH 6.M/L molar ratio = 1:1.

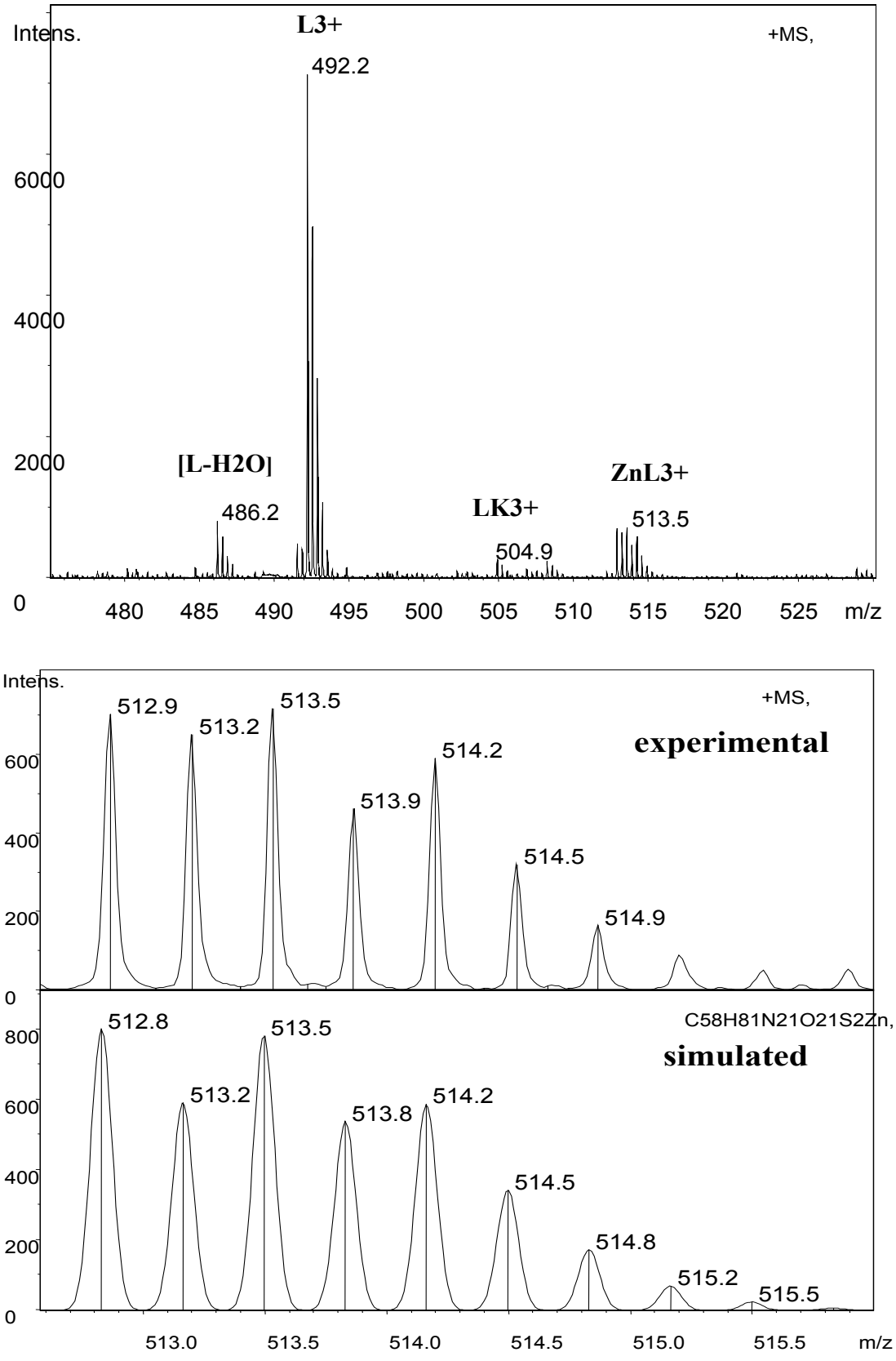

Figure S7. ESI-MS spectrum of Zn(II)-Ac-SHCHTHADGEVHC-COOH at pH 6.M/L molar ratio = 1:1.

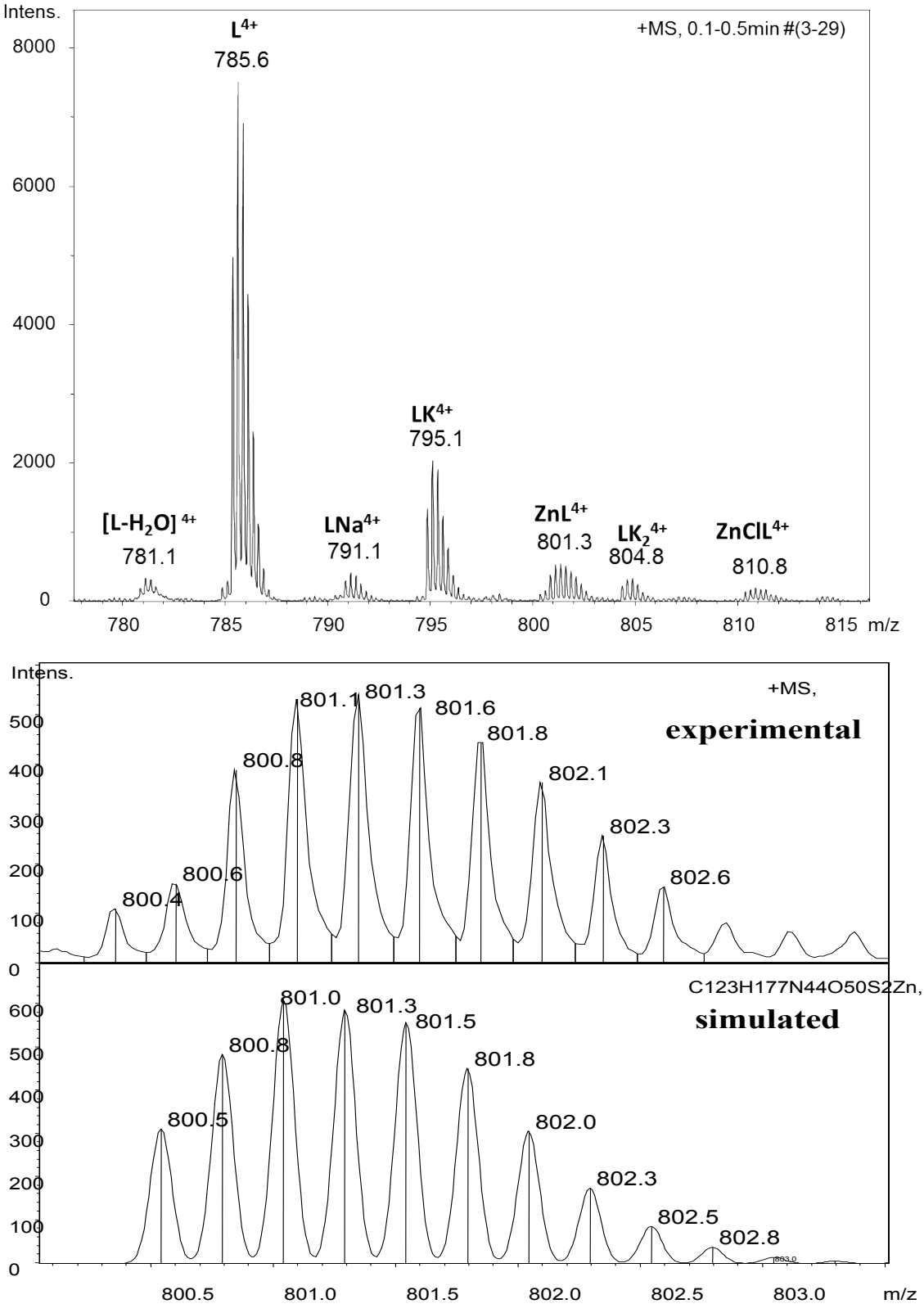

Figure S8. ESI-MS spectrum of Zn(II)-Ac-SHQHTDSNPSATTDANSHCHTHADGEVHC-COOH at pH 6. M/L molar ratio = 1:1.

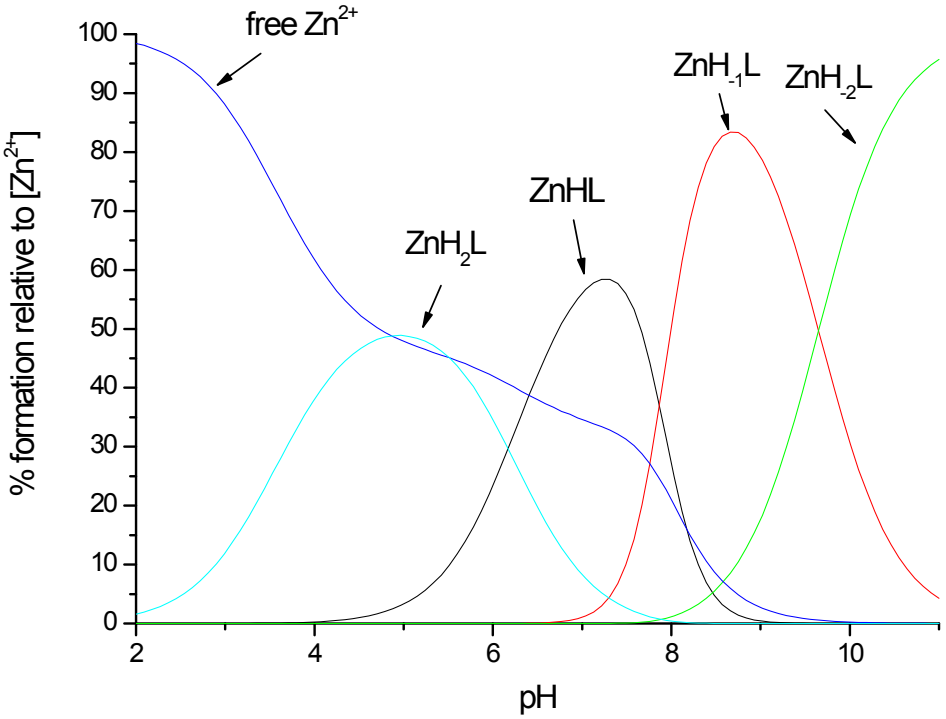

Figure S9. Distribution diagram for the formation Zn(II) complex with Ac-IEHY-NH_2at 25°C and I=0.1M.

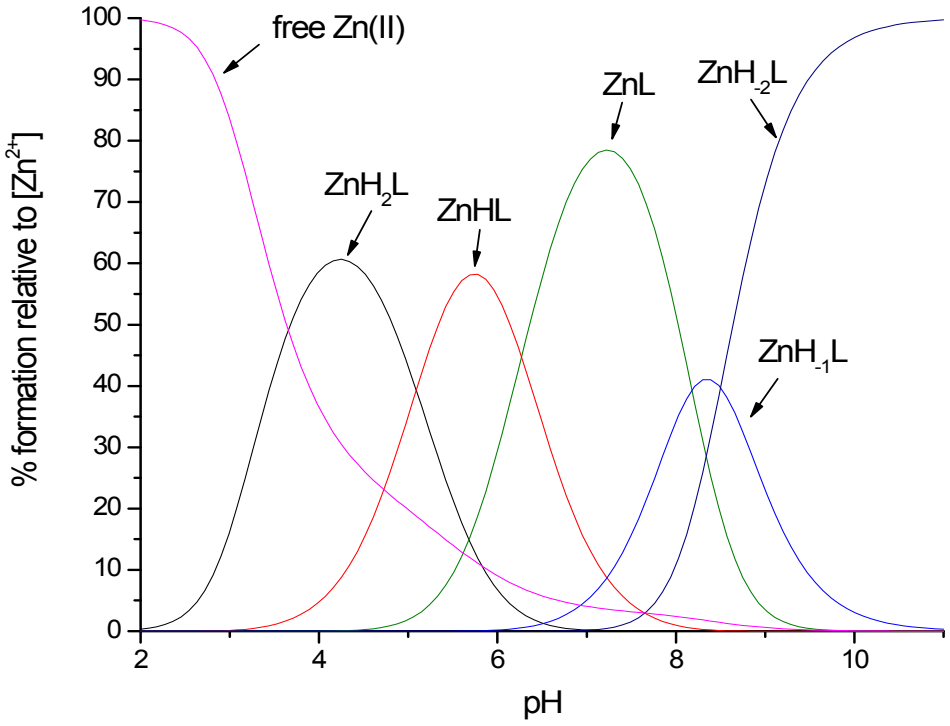

Figure S10. Distribution diagram for the formation Zn(II) complex with Ac-AEHARDH-NH_2 at 25°C and I=0.1M.

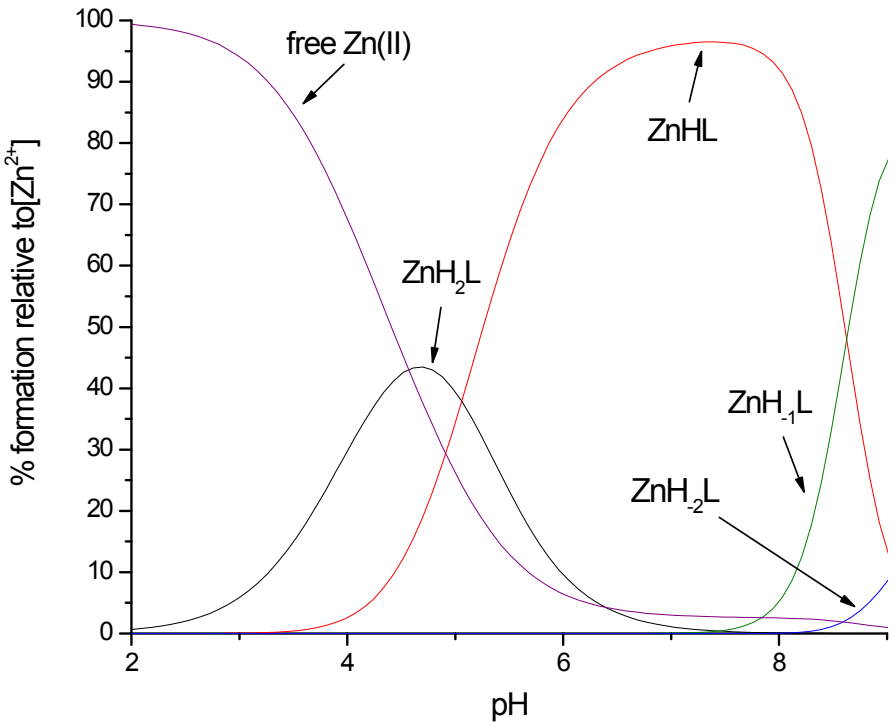

Figure S11. Distribution diagram for the formation Zn(II) complex with Ac-LHRFWHLK-NH_2at 25°C and I=0.1M.

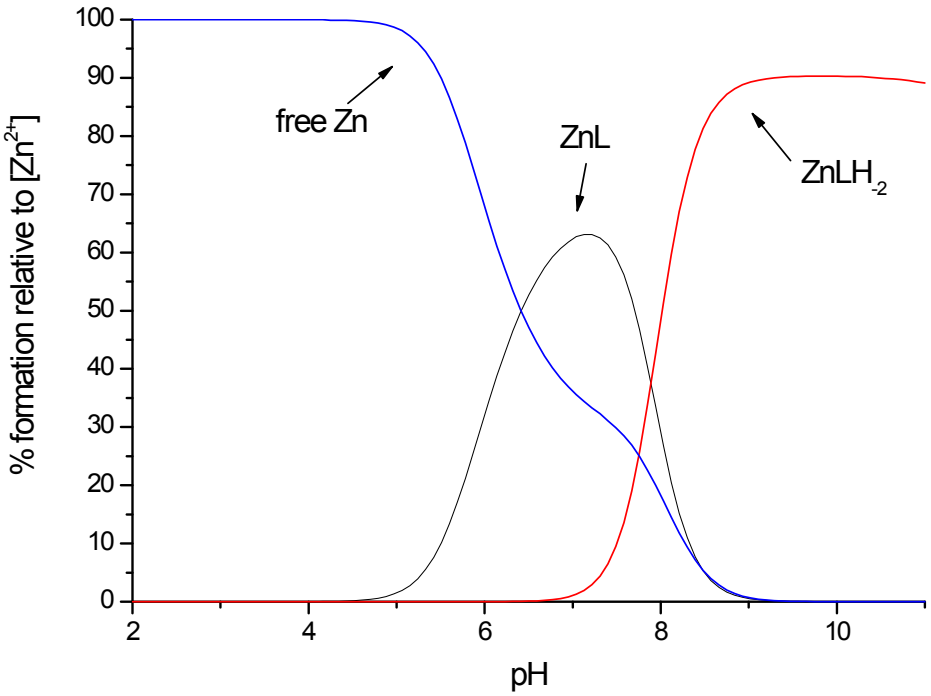

Figure S12. Distribution diagram for the formation Zn(II) complex with Ac-SHQHT-NH_2 at 25°C and I=0.1M.

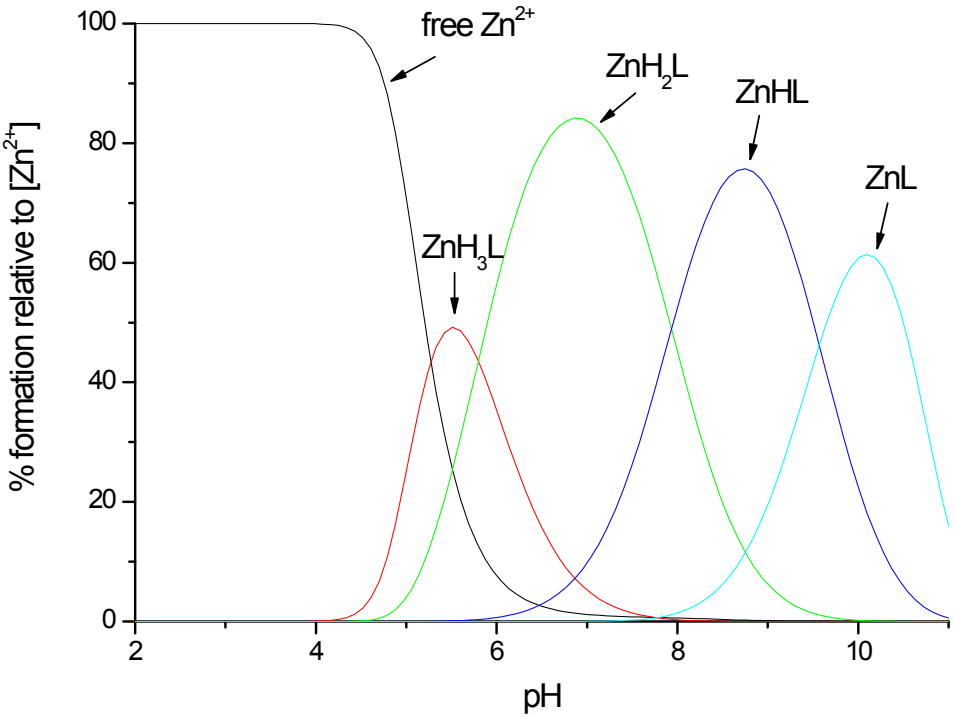

Figure S13. Distribution diagram for the formation Zn(II) complex with Ac-SHCHTHADGEVHC-COOH at 25°C and I=0.1M.

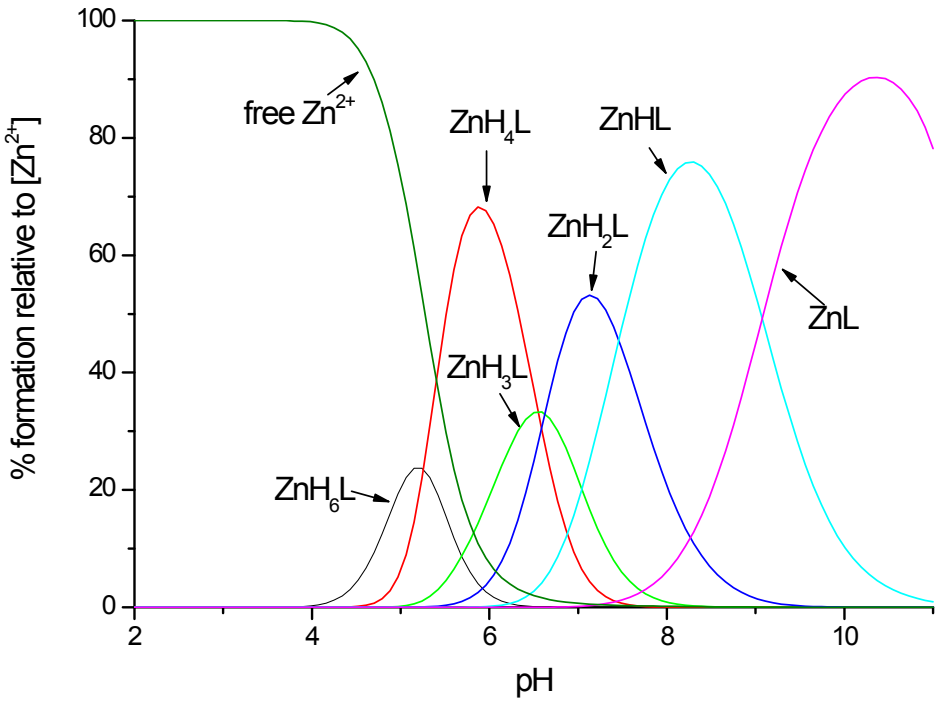

Figure S14. Distribution diagram for the formation Zn(II) complex with Ac-SHQHTDSNPSATTDANSH-CHTHADGEVHC-COOH at 25°C and I=0.1M.

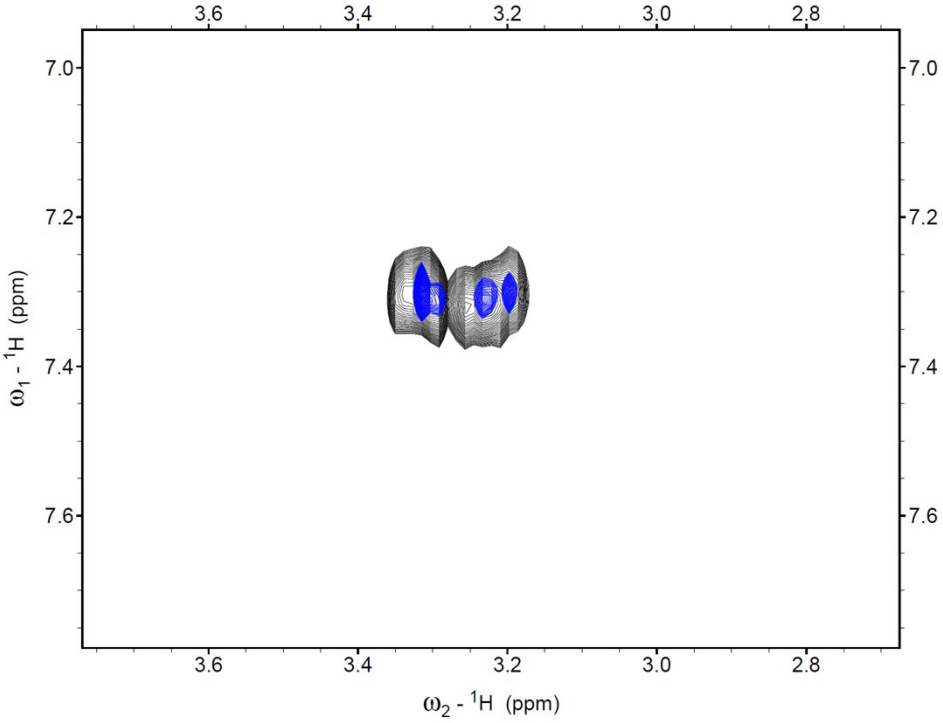

Figure S15. TOCSY spectra of 3 mMAc-SHQHTDSNPSATTDANSHCHTHADGEVHC-COOH, T=298 K, in the absence (black contours) and in presence (blue contours) of 1 Zn(II) equivalent, pH 5.

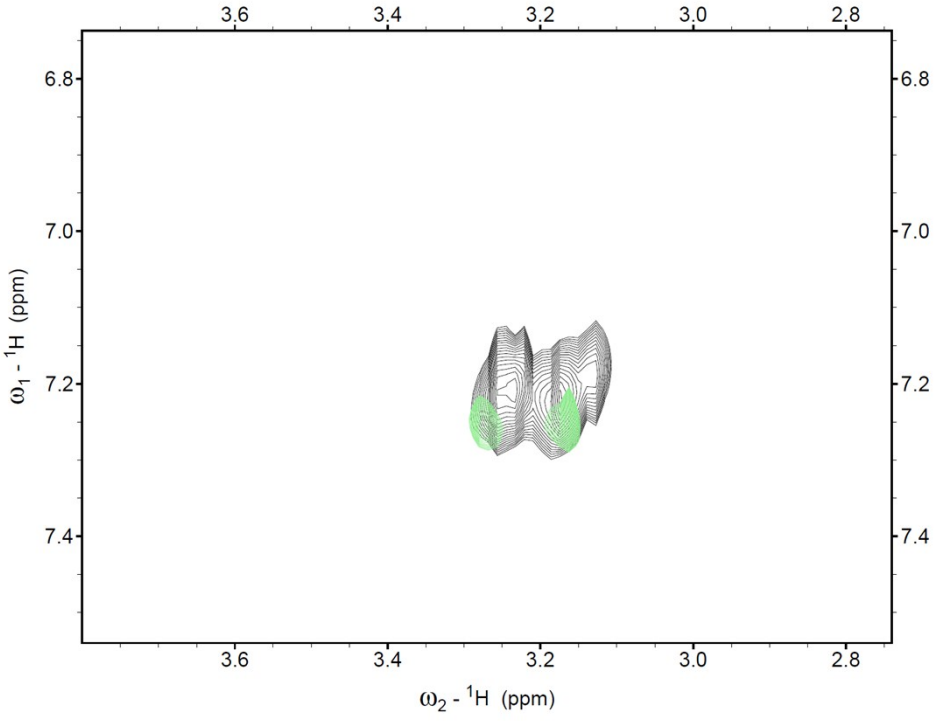

Figure S16. TOCSY spectra of 3 mMAc-SHQHTDSNPSATTDANSHCHTHADGEVHC-COOH, T=298 K, in the absence (black contours) and in presence (greencontours) of 1 Zn(II) equivalent, pH 6.

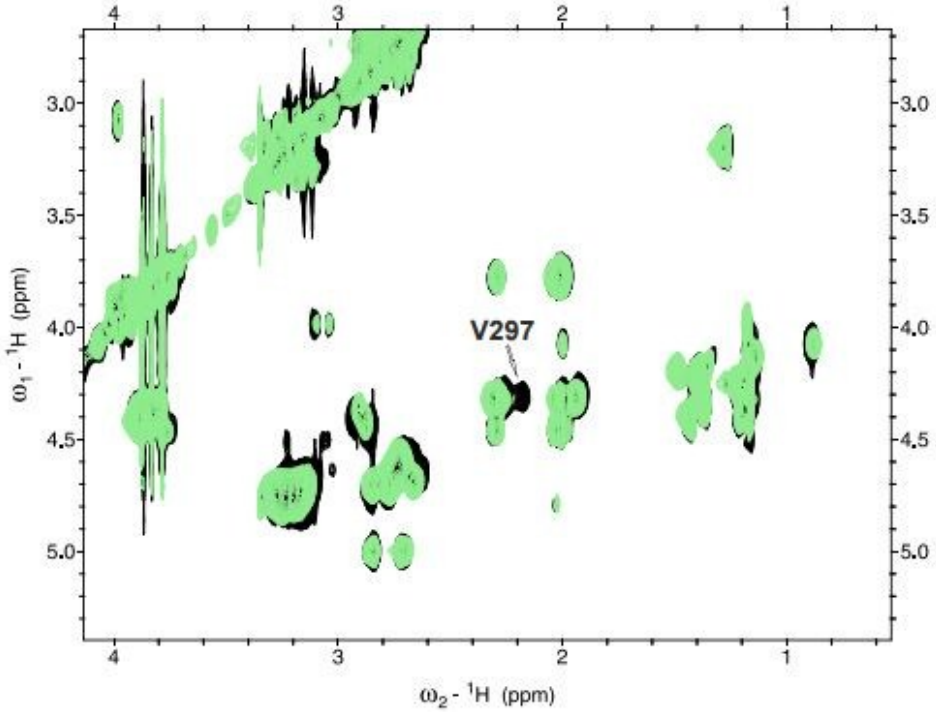

Figure S17. TOCSY spectra of 3 mMAc-SHQHTDSNPSATTDANSHCHTHADGEVHC-COOH, T=298 K, in the absence (black contours) and in presence (green contours) of 1 Zn(II) equivalent, pH 6.

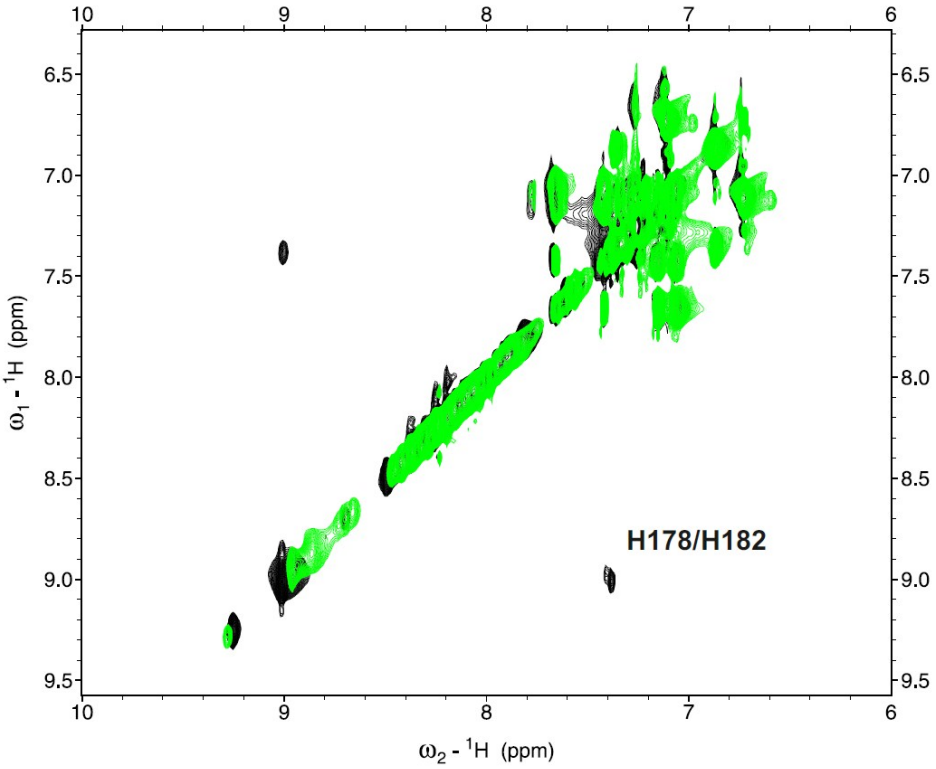

Figure S18. TOCSY spectra of 3 mMAc-LHRFWHLK-NH_2, T=298 K, in the absence (black contours) and in presence (bright green contours) of 1 Zn(II) equivalent, pH 3.5.