Supplementary Material

Enantioselectivity-evaluation of chiral copper(II) complex coordinated by novel chiral tetradentate ligand for free amino acids by mass spectrometry coupled with the isotopically labeled enantiomer method

Takashi Nakakoji1, Hirofumi Sato2,Hiroyuki Miyake1\*, Satoshi Shinoda1,Hiroshi Tsukube1,Hideya Kawasaki3,Ryuichi Arakawa3,Daisuke Ono2,Motohiro Shizuma2\*

1Department of Chemistry, Graduate School of Science, Osaka City University, Osaka, Japan

2Osaka Research Institute of Industrial Science and Technology, Osaka, Japan

3Faculty of Chemistry, Materials and Bioengineering, Kansai University, Suita, Japan

**\* Correspondence:**Hiroyuki Miyake  
miyake@sci.osaka-cu.ac.jp

Motohiro Shizuma  
shizuma@omtri.or.jp

Contents

**1 1H-NMR spectra of compounds** (Figures S1–S9)

**2 High resolution mass spectra of compounds** (Figures S10–S18)

**3 ESI mass spectra of the mass spectrometry/enantiomer-labeled (MS/EL) method of CuCl2/L3/*R*-Val/*S*-Val-*d8* and CuCl2/L8/ *R*-Val/*S*-Val-*d8* in water/methanol** (Figures S19–S26)

**4 ESI mass spectra of the MS/EL method of CuCl2/L/*R*-AA/S-AA-*dn* in water/ methanol** (Figures S27–S42)

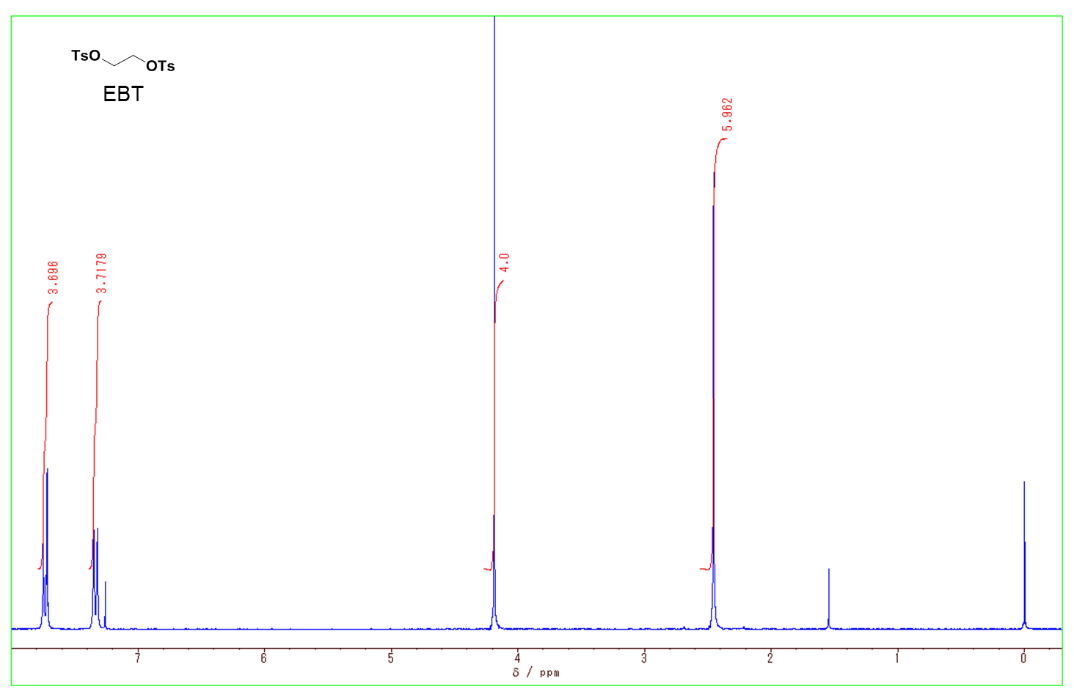
**5 Deuterated amino acids** (Table S1)

**6 DFT calculation of copper(II)-ligand complex [Cu(L)(MeOH)2]2+** (Figure S43)

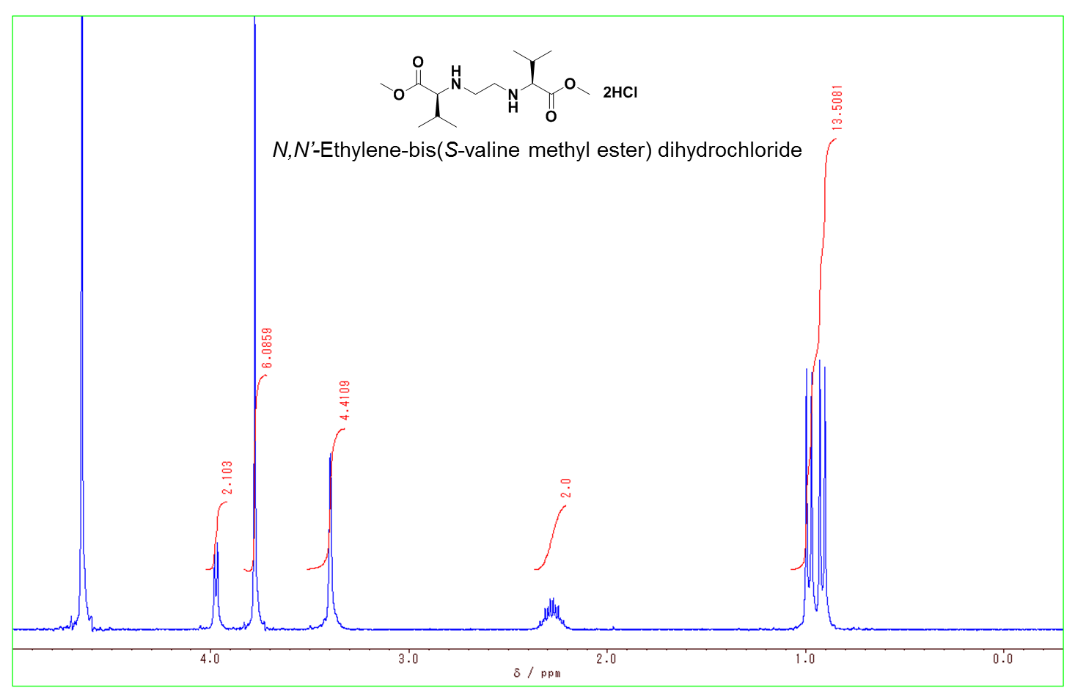
**7 Bond length of Cu-O, Cu-N, and Cu-(MeOH) of copper(II)-ligand complex [Cu(L)(MeOH)2]2+ by DFT** (Table S2)

**8 Coordinates of copper(II)-ligand complex [Cu(L)(MeOH)2]2+ by DFT (Tables S3-S4)**

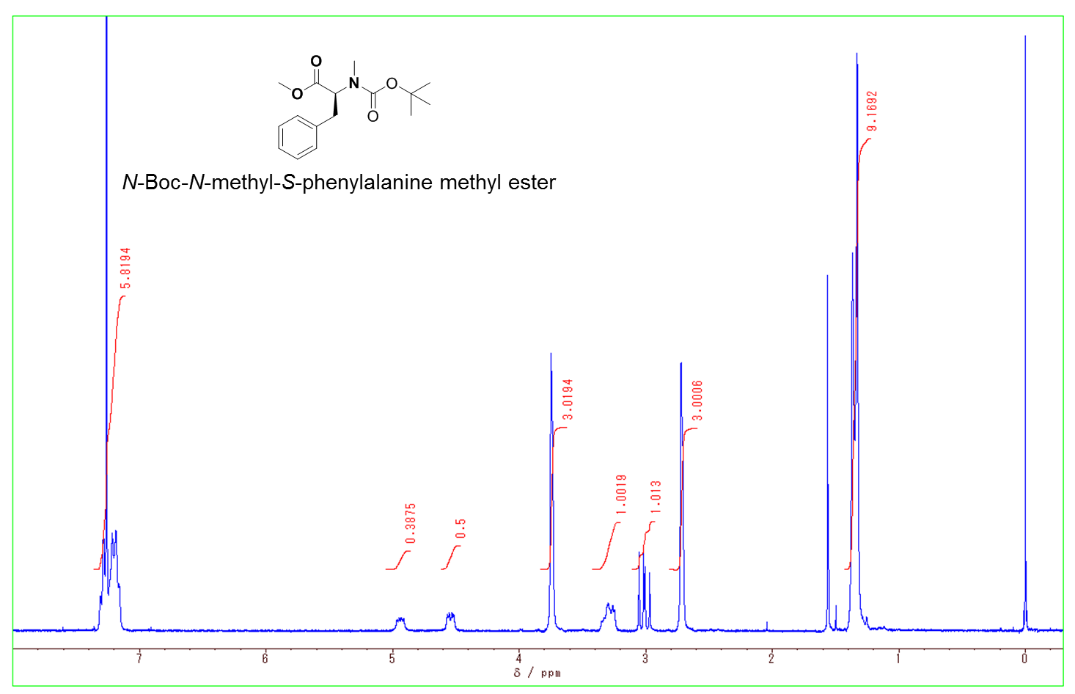
# 1H-NMR spectra of compounds



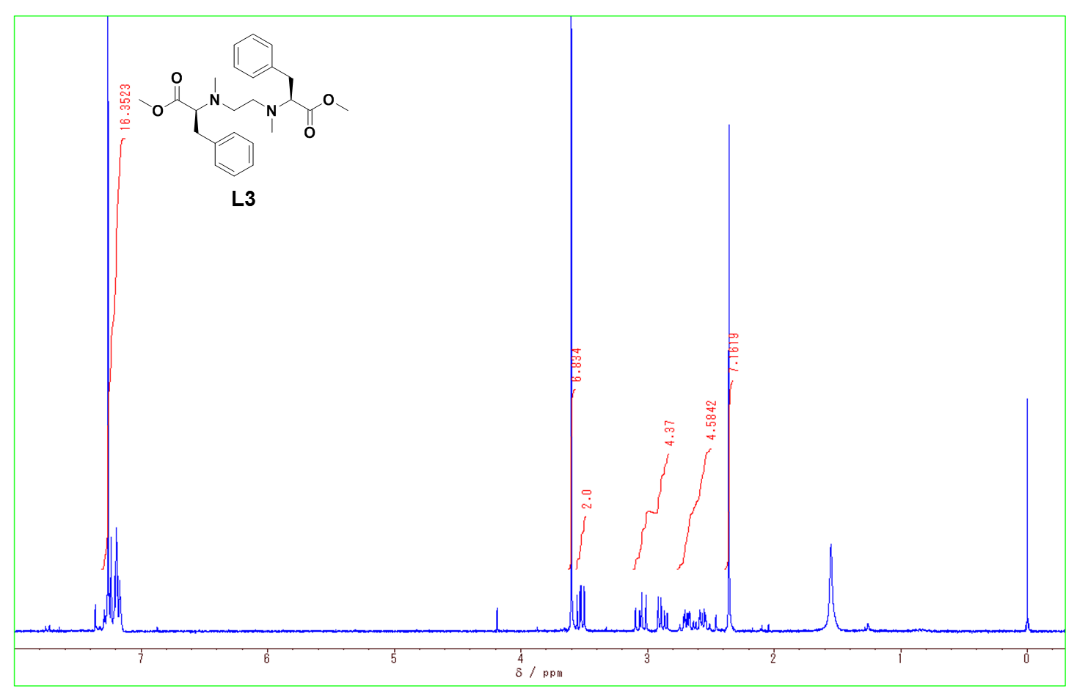
**Figure S1.** 1H NMR (270 MHz, CDCl3, 293 K) spectrum of ethylene bistsylate



**Figure S2.** 1H NMR (270 MHz, CDCl3, 293 K) spectrum of *N,N´-*ethylene-bis(*S*-valine methyl ester) dihydrochloride

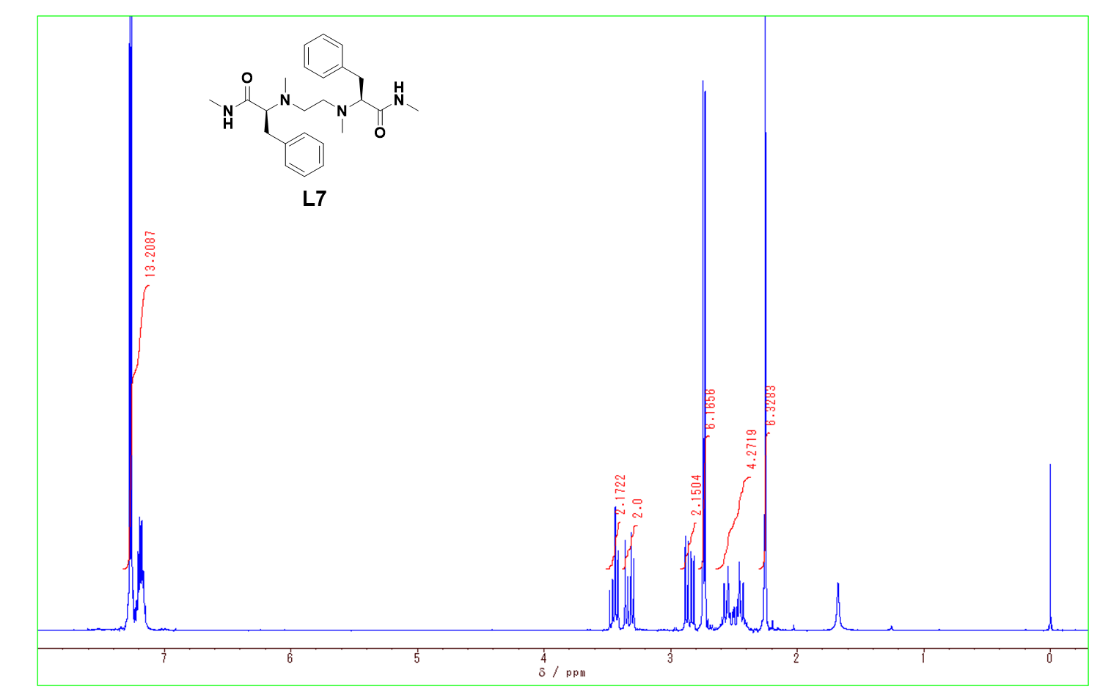


**Figure S3.** 1H NMR (270 MHz, CDCl3, 293 K) spectrum of *N*-Boc-*N*-methyl-*S*-phenylalanine methyl ester



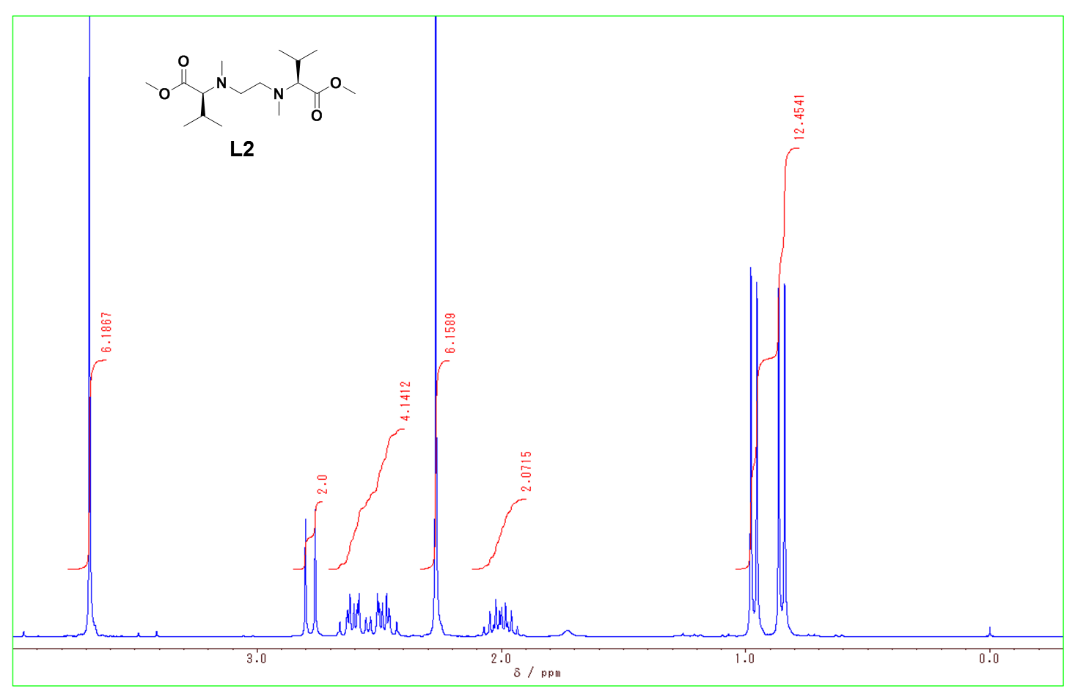
**L3**

**Figure S4.** 1H NMR (270 MHz, CDCl3, 293 K) spectrum of **L3**



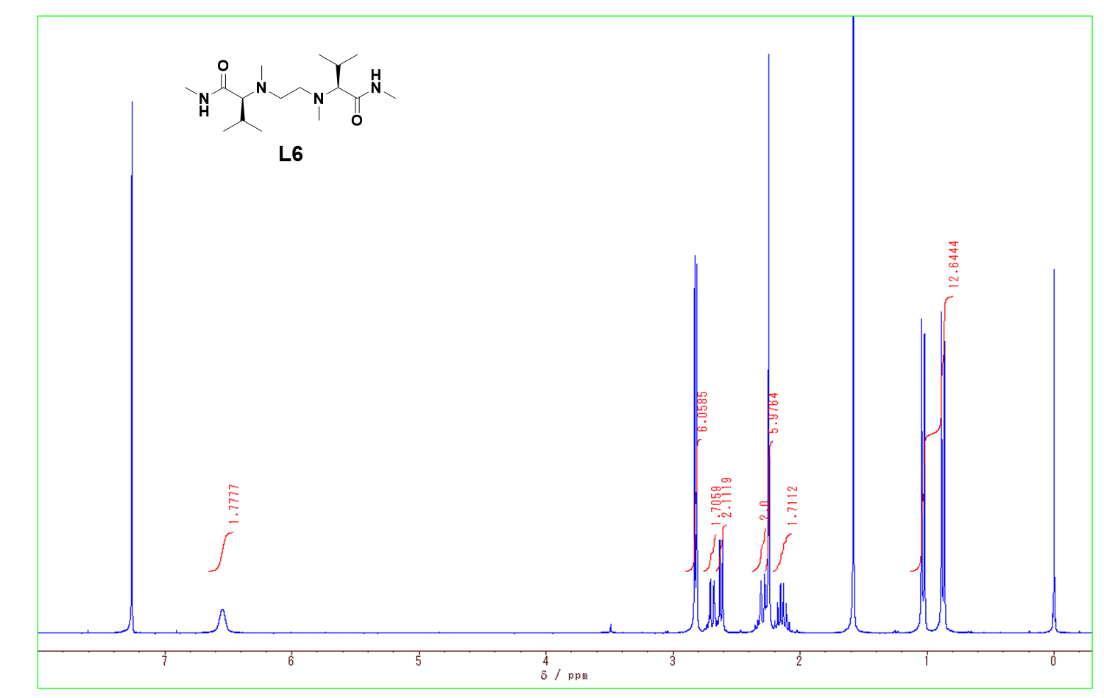
**L4**

**Figure S5.** 1H NMR (300 MHz, CDCl3, 293 K) spectrum of **L4**



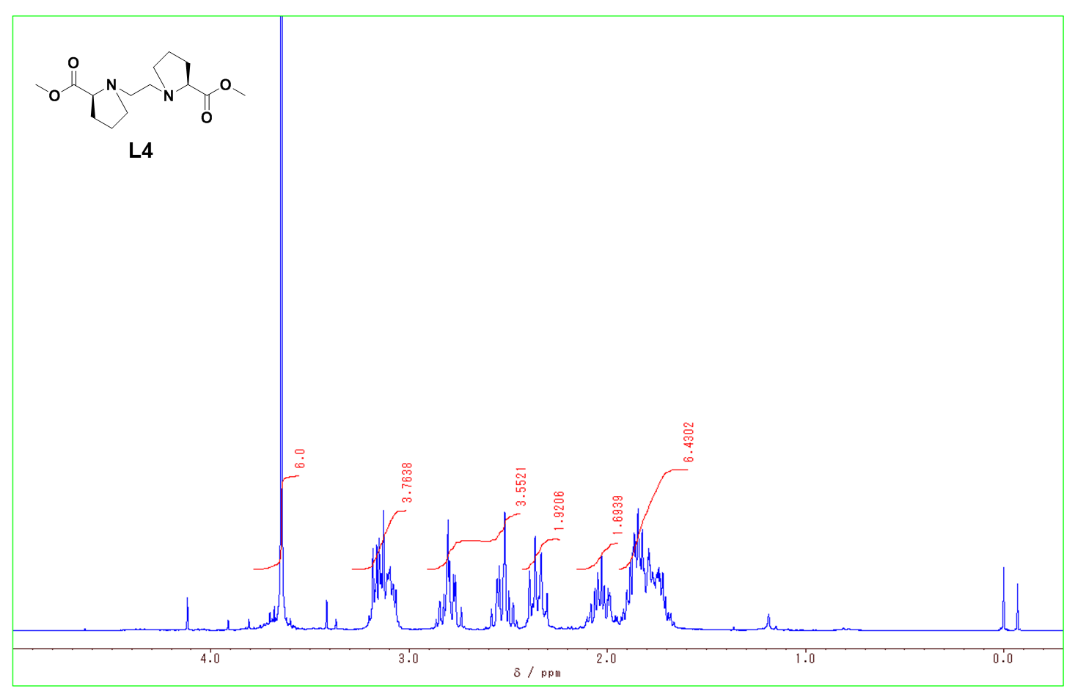
**L5**

**Figure S6.** 1H NMR (270 MHz, CDCl3, 293 K) spectrum of **L5**



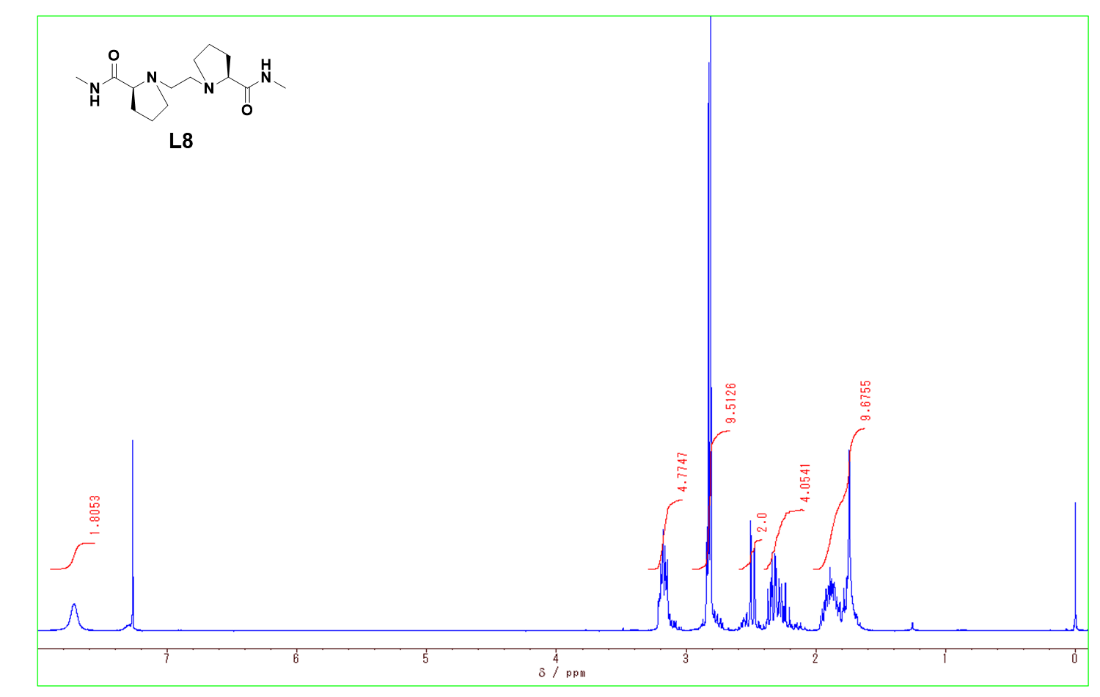
**L6**

**Figure S7.** 1H NMR (300 MHz, CDCl3, 293 K) spectrum of **L6**



**L7**

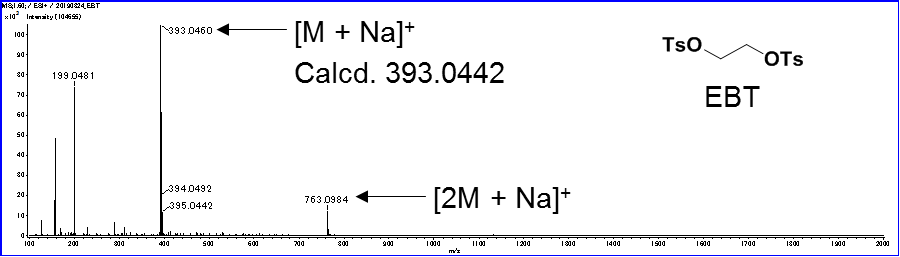
**Figure S8.** 1H NMR (300 MHz, CDCl3, 293 K) spectrum of **L7**



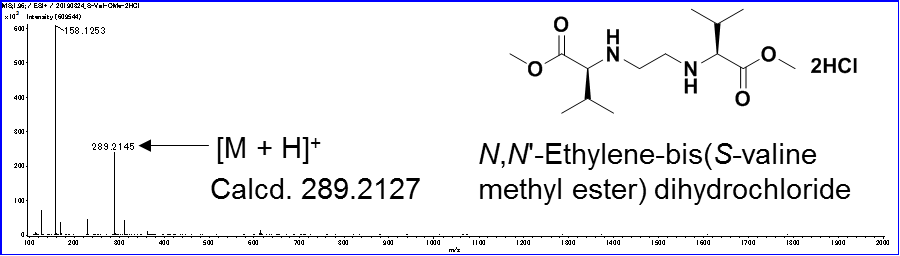
**L8**

**Figure S9.** 1H NMR (300 MHz, CDCl3, 293 K) spectrum of **L8**

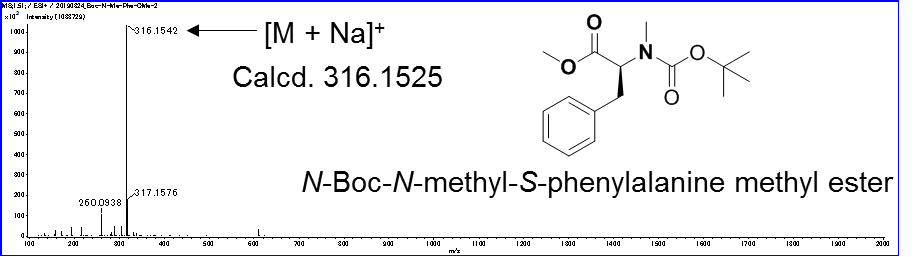
# High resolution mass spectra of compounds



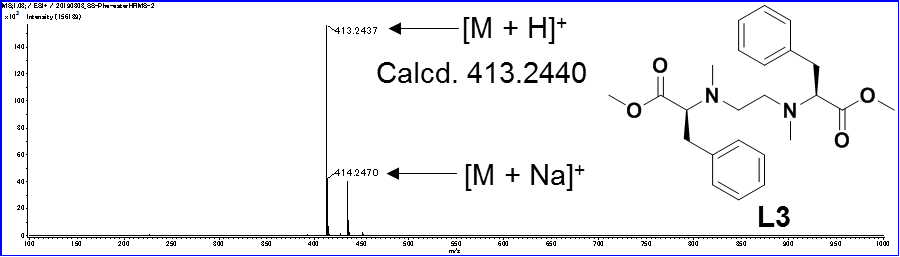
**Figure S10.** High resolution mass spectrum of ethylene bistsylate



**Figure S11.** High resolution mass spectrum of *N,N´-*ethylene-bis(*S*-valine methyl ester) dihydrochloride

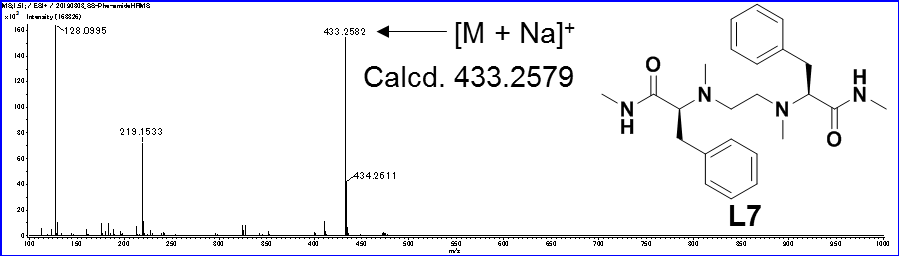


**Figure S12.** High resolution mass spectrum of *N*-Boc-*N*-methyl-*S*-phenylalanine methyl ester



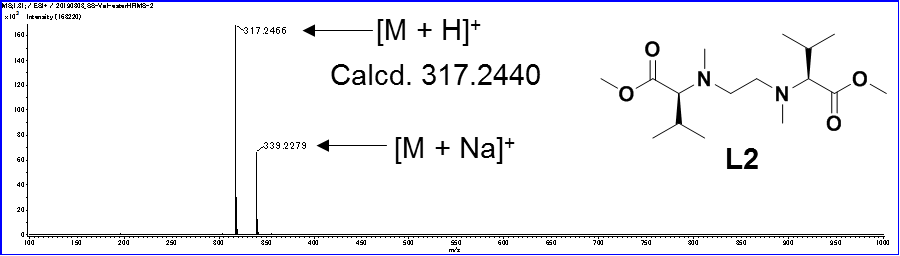
**L3**

**Figure S13.** High resolution mass spectrum of **L3**



**L4**

**Figure S14.** High resolution mass spectrum of **L4**



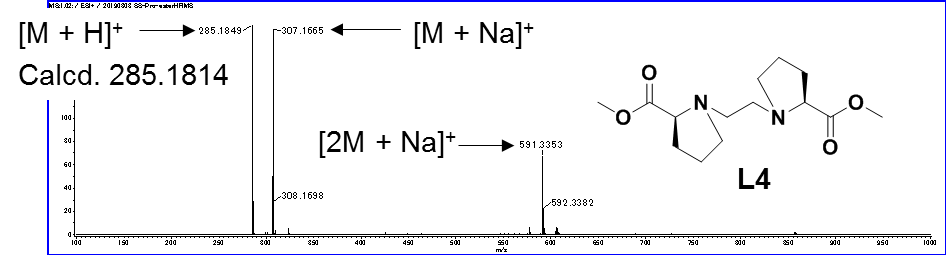
**L5**

**Figure S15.** High resolution mass spectrum of **L5**



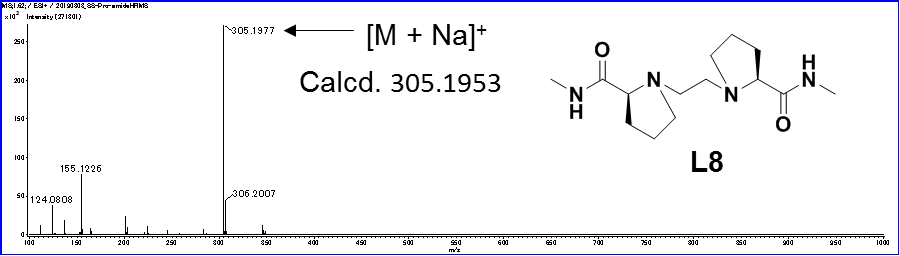
**L6**

**Figure S16.** High resolution mass spectrum of **L6**



**L7**

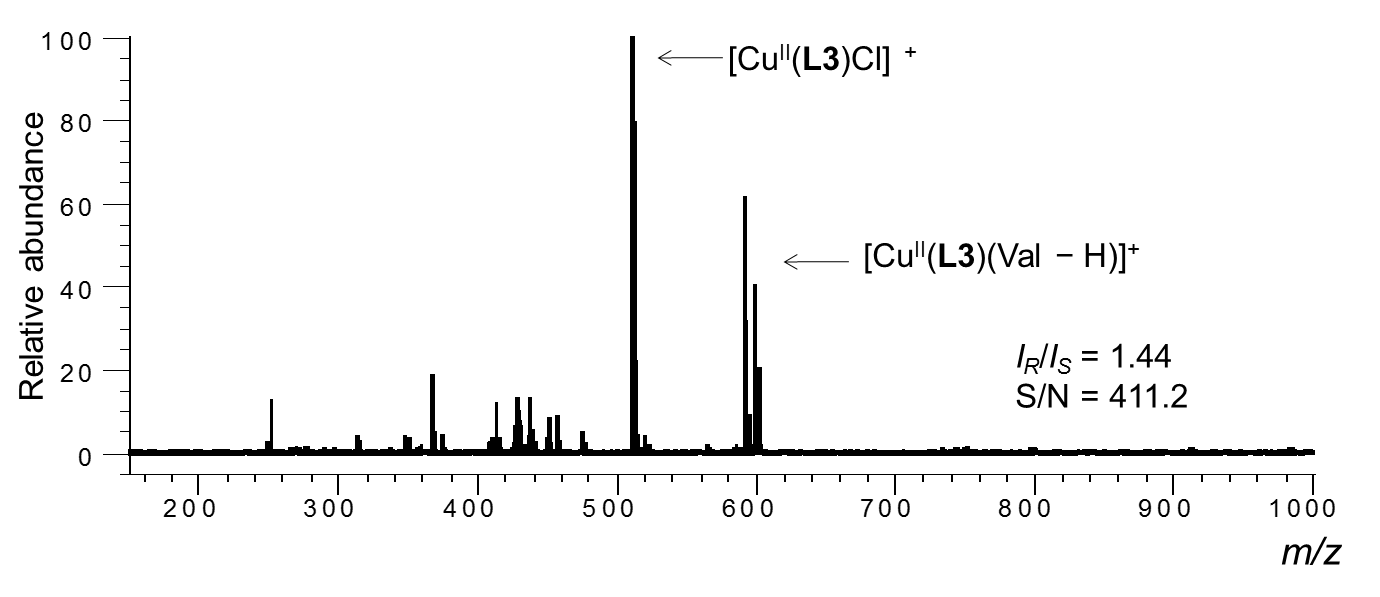
**Figure S17.** High resolution mass spectrum of **L7**



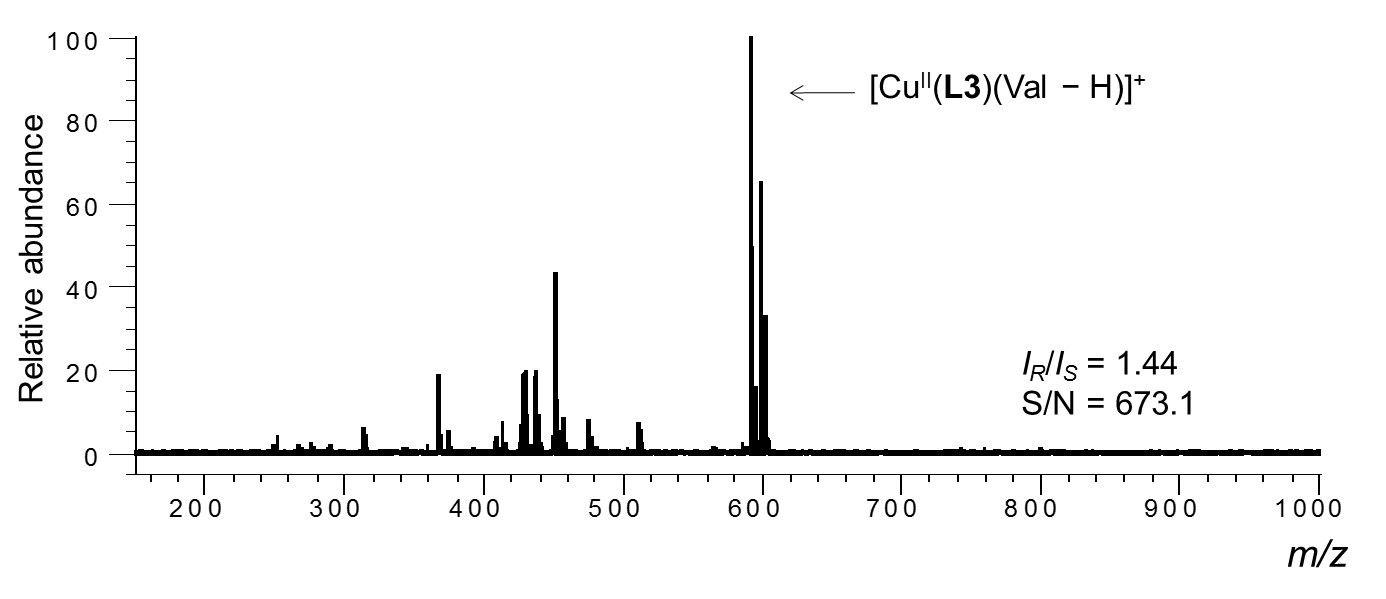
**L8**

**Figure S18.** High resolution mass spectrum of **L8**

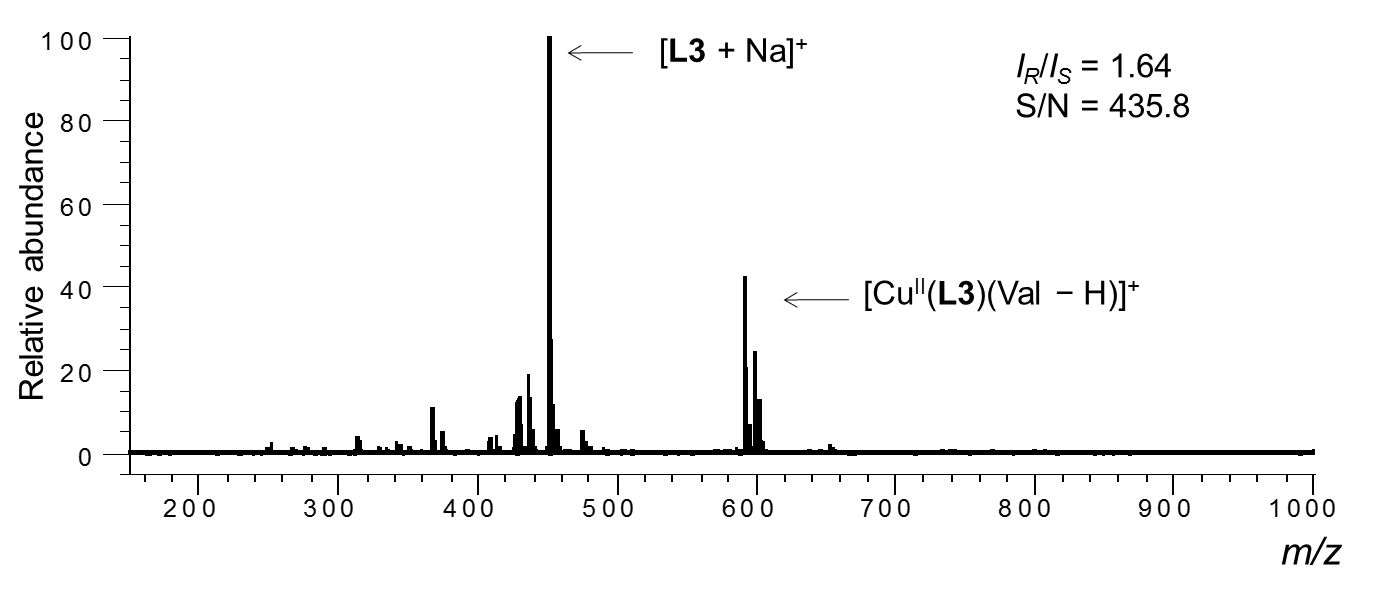
# ESI mass spectra of the MS/EL method of CuCl2/L3/*R*-Val/*S*-Val-*d8* and CuCl2/L8/ *R*-Val/*S*-Val-*d8* in water/methanol



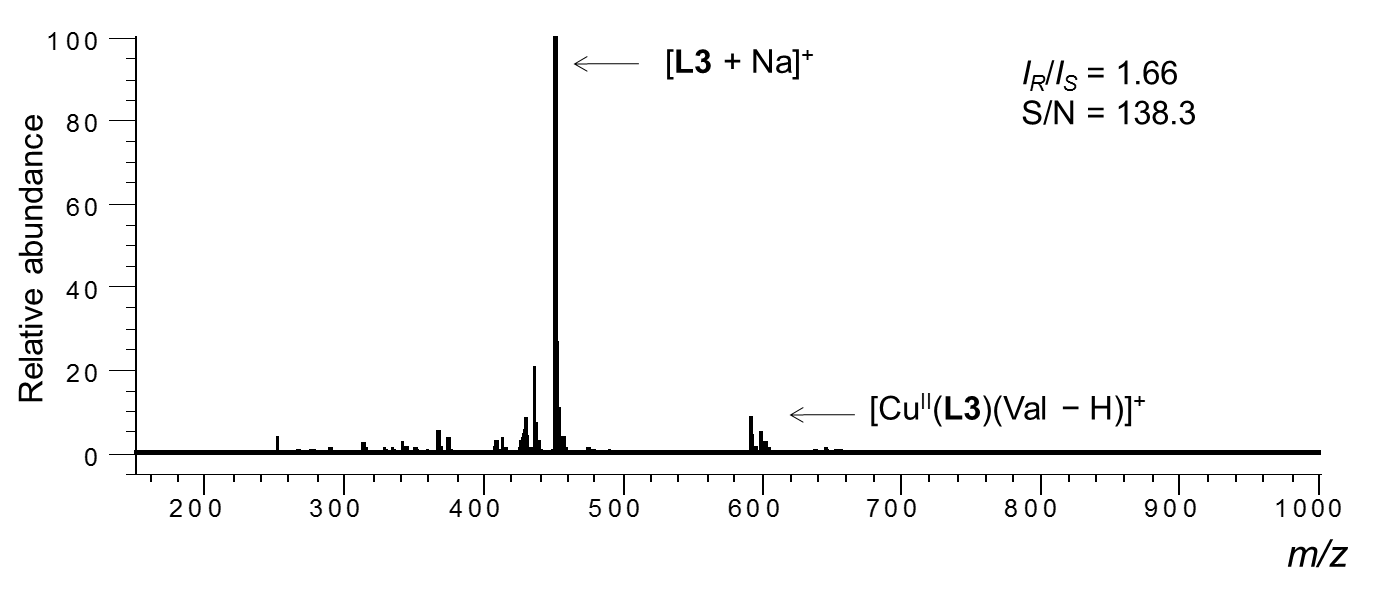
**Figure S19.** ESI mass spectra of a mixed solution of CuCl2/**L3**/*R*-Val/*S*-Val-*d*8 in water/methanol. The sample solution was prepared by mixing 1.00 mL of *in situ* prepared complex solution in methanol ([CuCl2]0 = 1.2 × 10−4 M and [**L3**]0 = 1.0 × 10−4 M) and a solution of an equimolar mixture of *R*-Val and *S*-Val-*d*8 ([*R*-Val]0 = *S*-Val-*d*8]0 = 5.0 × 10−4 M and [K2CO3]0 = 1.0 × 10−3 M) in water. The resulting mole ratio of each component [CuCl2]0/[**L3**]0/[*R*-Val]0/[*S*-Val-*d*8]0 (the amount of adding aqueous solution) = 1.2/1.0/0.25/0.25 (50 μL).



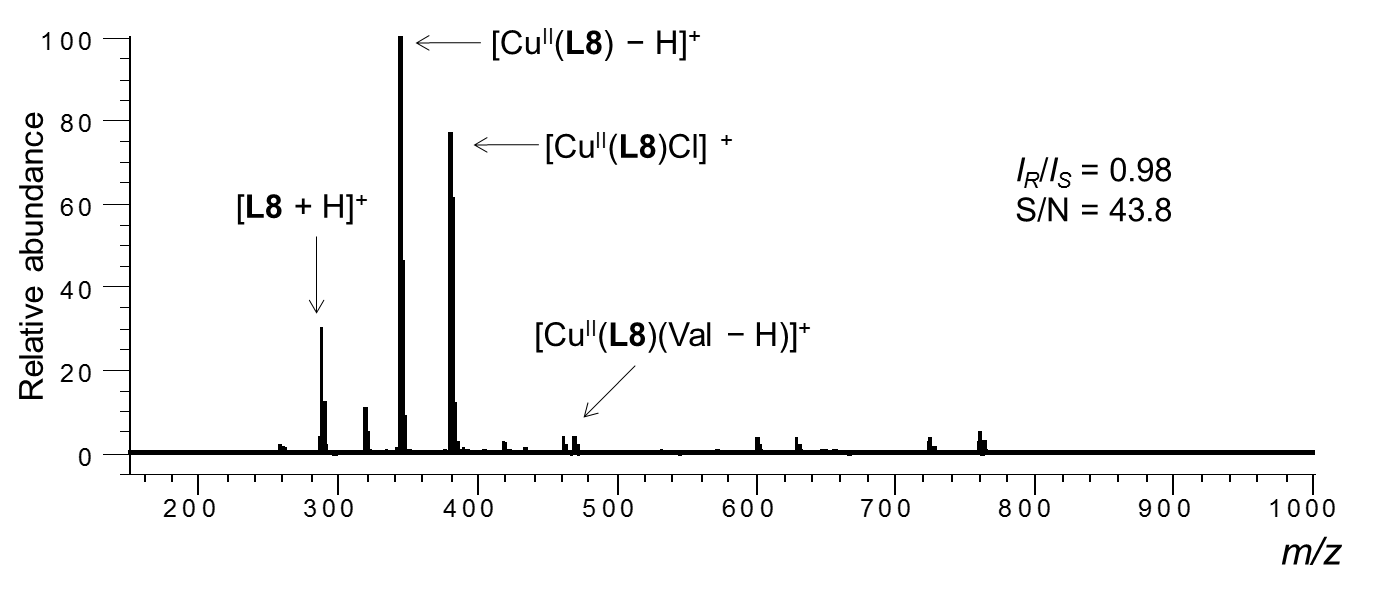
**Figure S20.** ESI mass spectra of a mixed solution of CuCl2/**L3**/*R*-Val/*S*-Val-*d*8 in water/methanol. The sample solution was prepared by mixing 1.00 mL of *in situ* prepared complex solution in methanol ([CuCl2]0 = 1.2 × 10−4 M and [**L3**]0 = 1.0 × 10−4 M) and a solution of an equimolar mixture of *R*-Val and *S*-Val-*d*8 ([*R*-Val]0 = *S*-Val-*d*8]0 = 5.0 × 10−4 M and [K2CO3]0 = 1.0 × 10−3 M) in water. The resulting mole ratio of each component [CuCl2]0/[**L3**]0/[*R*-Val]0/[*S*-Val-*d*8]0 (the amount of adding aqueous solution) = 1.2/1.0/0.5/0.5 (100 μL).



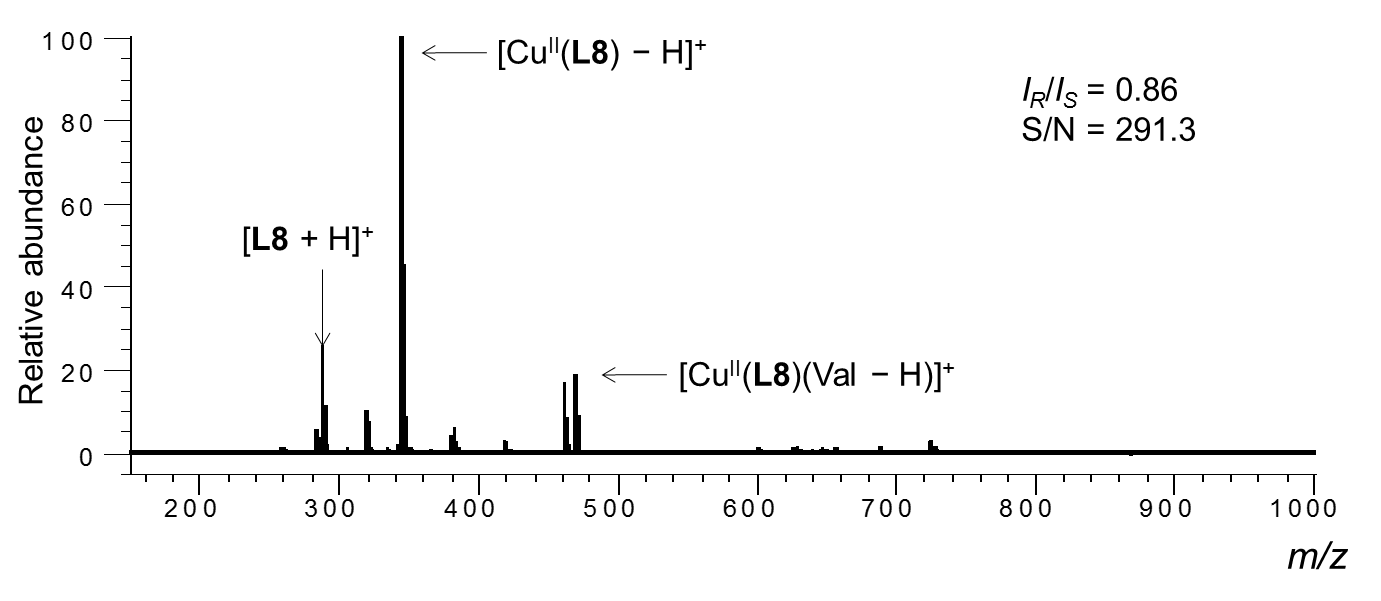
**Figure S21.** ESI mass spectra of a mixed solution of CuCl2/**L3**/*R*-Val/*S*-Val-*d*8 in water/methanol. The sample solution was prepared by mixing 1.00 mL of *in situ* prepared complex solution in methanol ([CuCl2]0 = 1.2 × 10−4 M and [**L3**]0 = 1.0 × 10−4 M) and a solution of an equimolar mixture of *R*-Val and *S*-Val-*d*8 ([*R*-Val]0 = *S*-Val-*d*8]0 = 5.0 × 10−4 M and [K2CO3]0 = 1.0 × 10−3 M) in water. The resulting mole ratio of each component [CuCl2]0/[**L3**]0/[*R*-Val]0/[*S*-Val-*d*8]0 (the amount of adding aqueous solution) = 1.2/1.0/0.75/0.75 (150 μL).



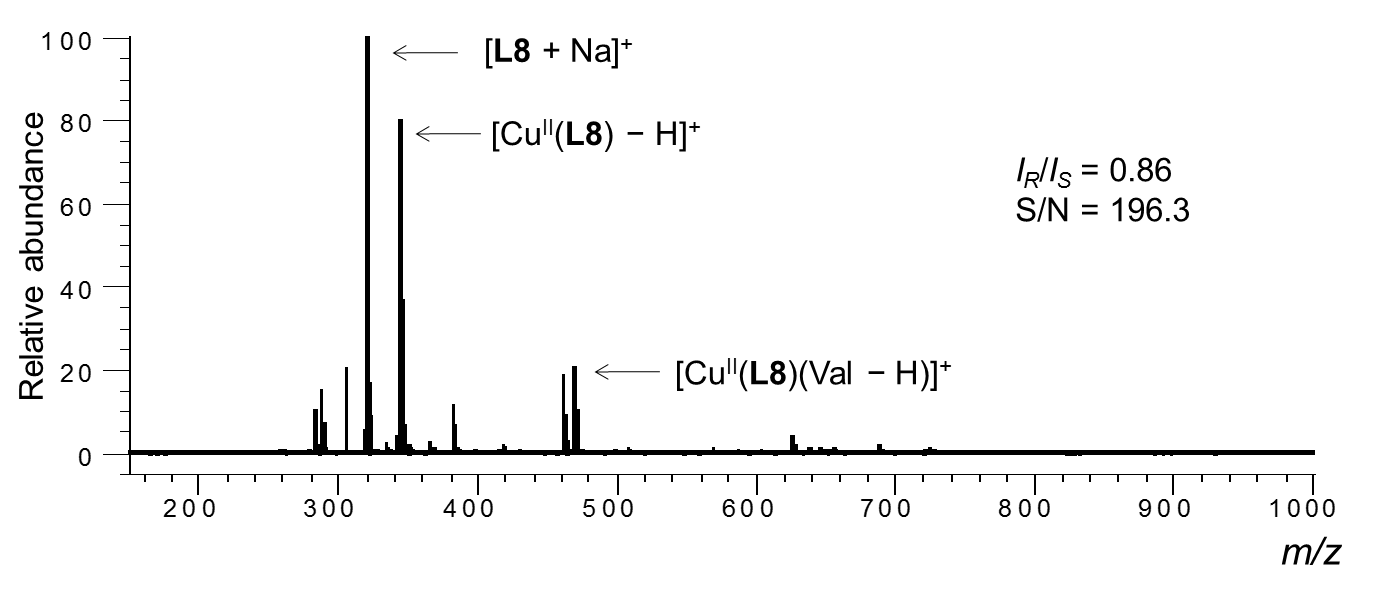
**Figure S22.** ESI mass spectra of a mixed solution of CuCl2/**L3**/*R*-Val/*S*-Val-*d*8 in water/methanol. The sample solution was prepared by mixing 1.00 mL of *in situ* prepared complex solution in methanol ([CuCl2]0 = 1.2 × 10−4 M and [**L3**]0 = 1.0 × 10−4 M) and a solution of an equimolar mixture of *R*-Val and *S*-Val-*d*8 ([*R*-Val]0 = *S*-Val-*d*8]0 = 5.0 × 10−4 M and [K2CO3]0 = 1.0 × 10−3 M) in water. The resulting mole ratio of each component [CuCl2]0/[**L3**]0/[*R*-Val]0/[*S*-Val-*d*8]0 (the amount of adding aqueous solution) = 1.2/1.0/1.0/1.0 (200 μL).



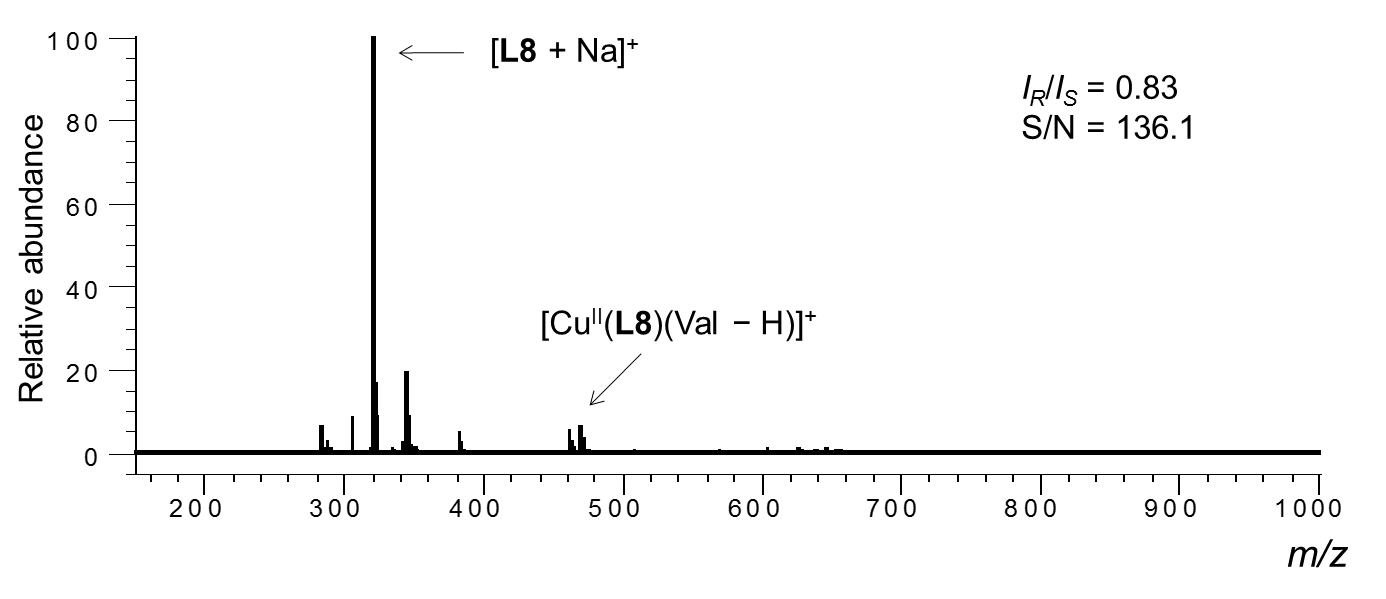
**Figure S23.** ESI mass spectra of a mixed solution of CuCl2/**L8**/*R*-Val/*S*-Val-*d*8 in water/methanol. The sample solution was prepared by mixing 1.00 mL of *in situ* prepared complex solution in methanol ([CuCl2]0 = 1.2 × 10−4 M and [**L8**]0 = 1.0 × 10−4 M) and a solution of an equimolar mixture of *R*-Val and *S*-Val-*d*8 ([*R*-Val]0 = *S*-Val-*d*8]0 = 5.0 × 10−4 M and [K2CO3]0 = 1.0 × 10−3 M) in water. The resulting mole ratio of each component [CuCl2]0/[**L8**]0/[*R*-Val]0/[*S*-Val-*d*8]0 (the amount of adding aqueous solution) = 1.2/1.0/0.25/0.25 (50 μL).



**Figure S24.** ESI mass spectra of a mixed solution of CuCl2/**L8**/*R*-Val/*S*-Val-*d*8 in water/methanol. The sample solution was prepared by mixing 1.00 mL of *in situ* prepared complex solution in methanol ([CuCl2]0 = 1.2 × 10−4 M and [**L8**]0 = 1.0 × 10−4 M) and a solution of an equimolar mixture of *R*-Val and *S*-Val-*d*8 ([*R*-Val]0 = *S*-Val-*d*8]0 = 5.0 × 10−4 M and [K2CO3]0 = 1.0 × 10−3 M) in water. The resulting mole ratio of each component [CuCl2]0/[**L8**]0/[*R*-Val]0/[*S*-Val-*d*8]0 (the amount of adding aqueous solution) = 1.2/1.0/0.5/0.5 (100 μL).

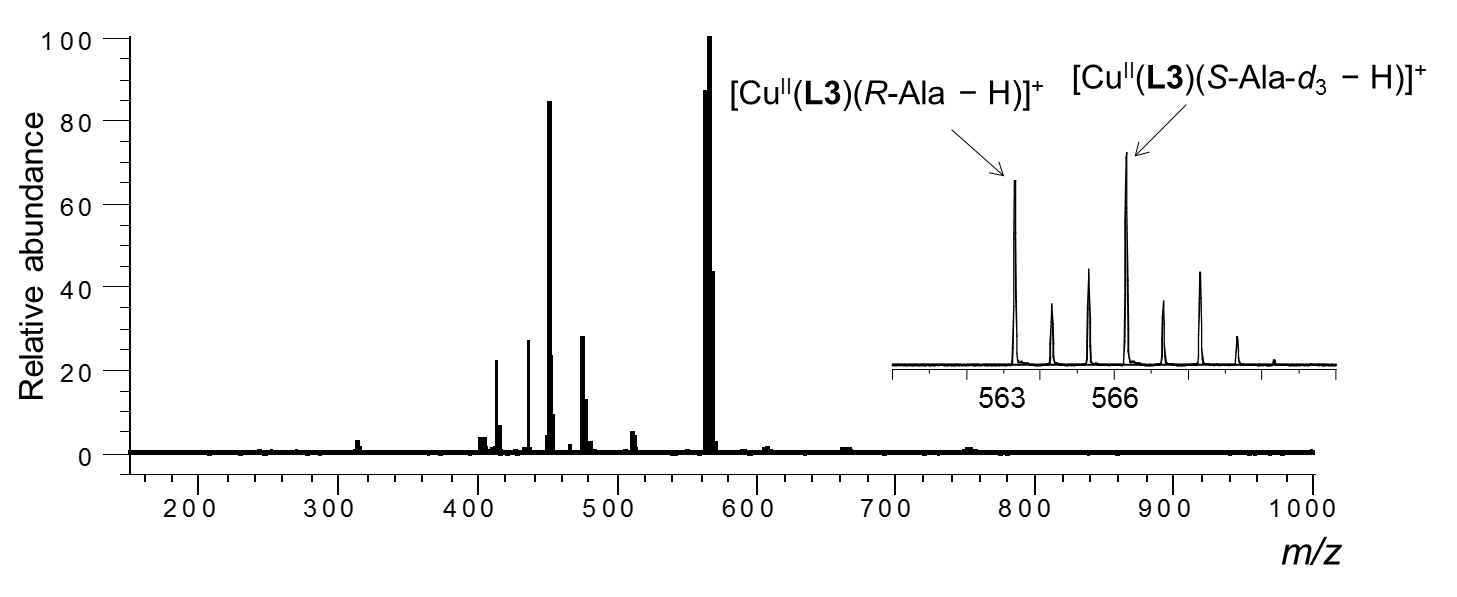


**Figure S25.** ESI mass spectra of a mixed solution of CuCl2/**L8**/*R*-Val/*S*-Val-*d*8 in water/methanol. The sample solution was prepared by mixing 1.00 mL of *in situ* prepared complex solution in methanol ([CuCl2]0 = 1.2 × 10−4 M and [**L8**]0 = 1.0 × 10−4 M) and a solution of an equimolar mixture of *R*-Val and *S*-Val-*d*8 ([*R*-Val]0 = *S*-Val-*d*8]0 = 5.0 × 10−4 M and [K2CO3]0 = 1.0 × 10−3 M) in water. The resulting mole ratio of each component [CuCl2]0/[**L8**]0/[*R*-Val]0/[*S*-Val-*d*8]0 (the amount of adding aqueous solution) = 1.2/1.0/0.75/0.75 (150 μL).

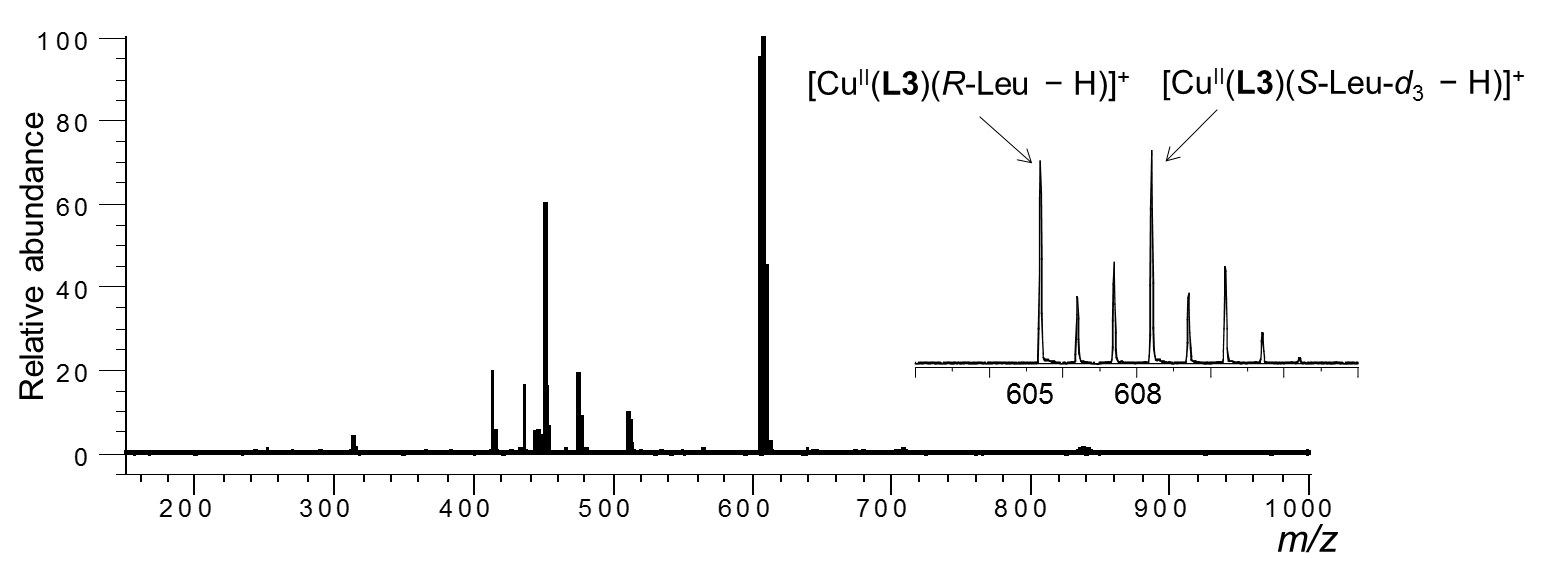


**Figure S26.** ESI mass spectra of a mixed solution of CuCl2/**L8**/*R*-Val/*S*-Val-*d*8 in water/methanol. The sample solution was prepared by mixing 1.00 mL of *in situ* prepared complex solution in methanol ([CuCl2]0 = 1.2 × 10−4 M and [**L8**]0 = 1.0 × 10−4 M) and a solution of an equimolar mixture of *R*-Val and *S*-Val-*d*8 ([*R*-Val]0 = *S*-Val-*d*8]0 = 5.0 × 10−4 M and [K2CO3]0 = 1.0 × 10−3 M) in water. The resulting mole ratio of each component [CuCl2]0/[**L8**]0/[*R*-Val]0/[*S*-Val-*d*8]0 (the amount of adding aqueous solution) = 1.2/1.0/1.0/1.0 (200 μL).

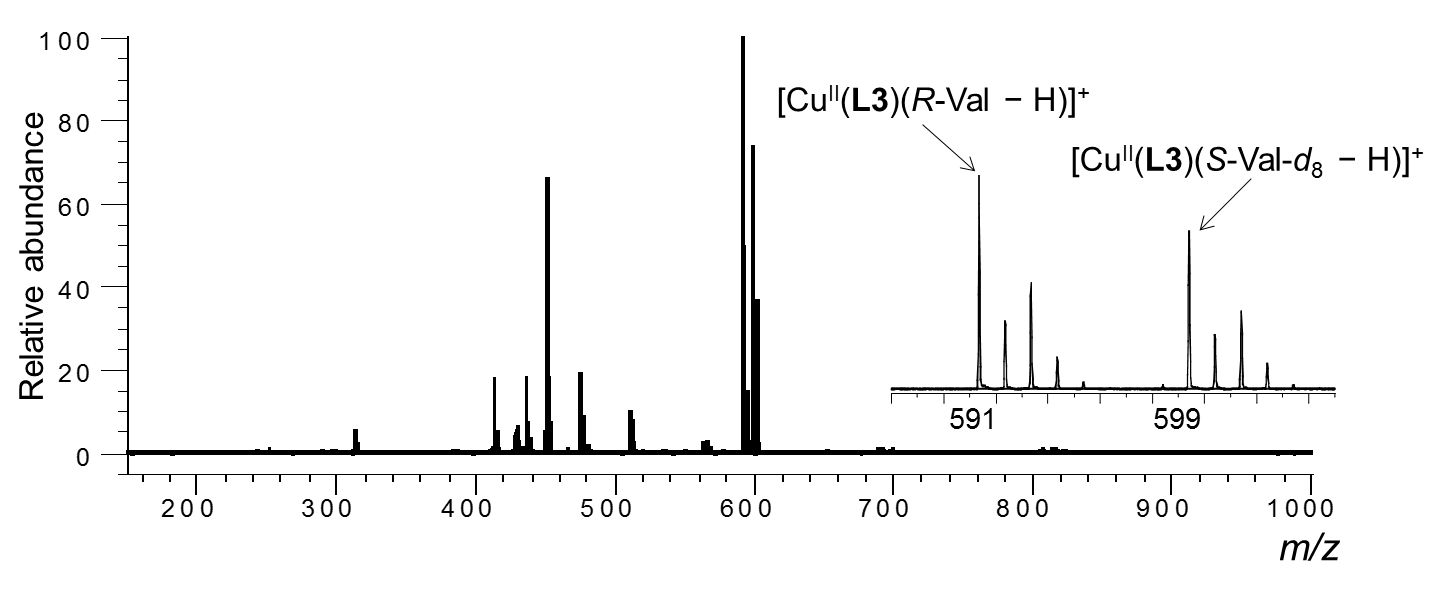
# ESI mass spectra of the MS/EL method of CuCl2/L/*R*-AA/S-AA-*dn* in water/ methanol



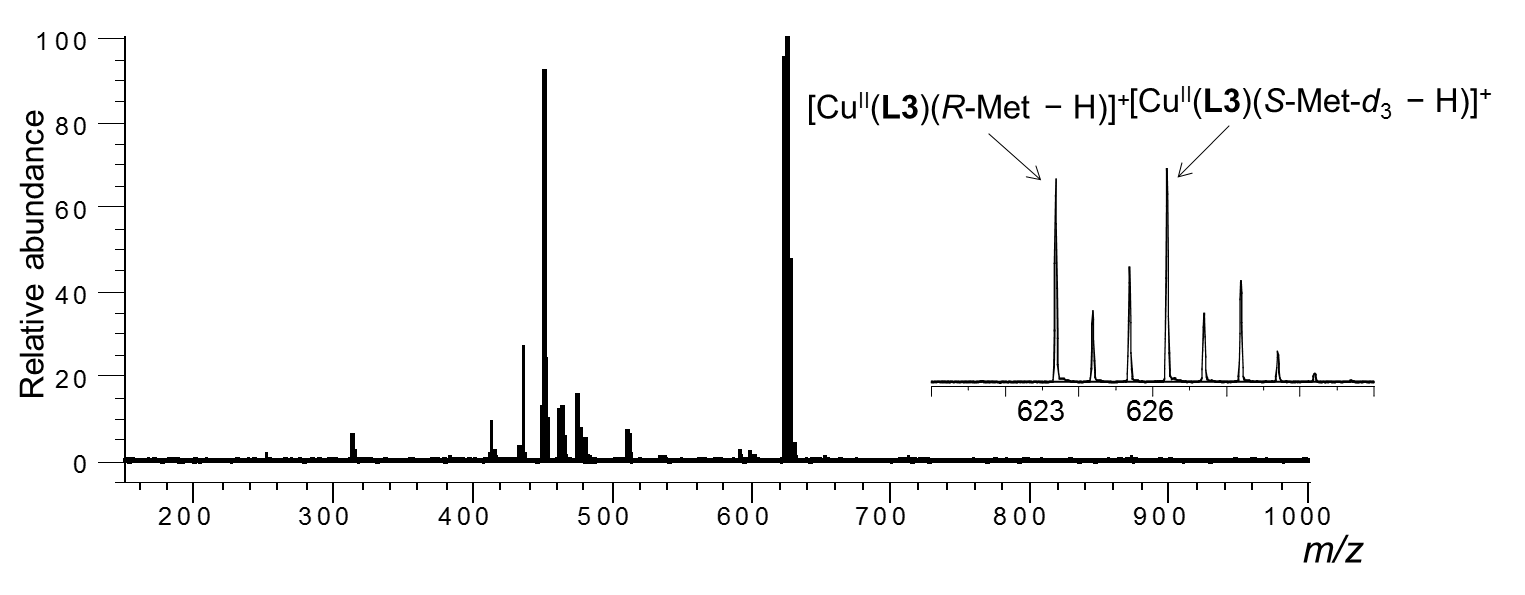
**Figure S27.** ESI mass spectra of the MS/EL method of CuCl2/**L**/*R*-AA/*S*-AA-*d*n- in water/methanol (1/10, v/v). [CuCl2]0 = 1.09 × 10−4 M, [**L**]0 = 9.09 × 10−5 M and [*R*-AA]0 = [*S*-AA-*d*n]0 = 4.55 × 10−5 M. [CuCl2]0/[**L**]0/[*R*-AA]0/[*S*-AA-*d*n]0 = 1.2/1.0/0.5/0.5. [K2CO3]0 = 9.09 × 10−5 M, **L** = **L3**, AA= *R*-Ala/*S*-Ala-*d*3.



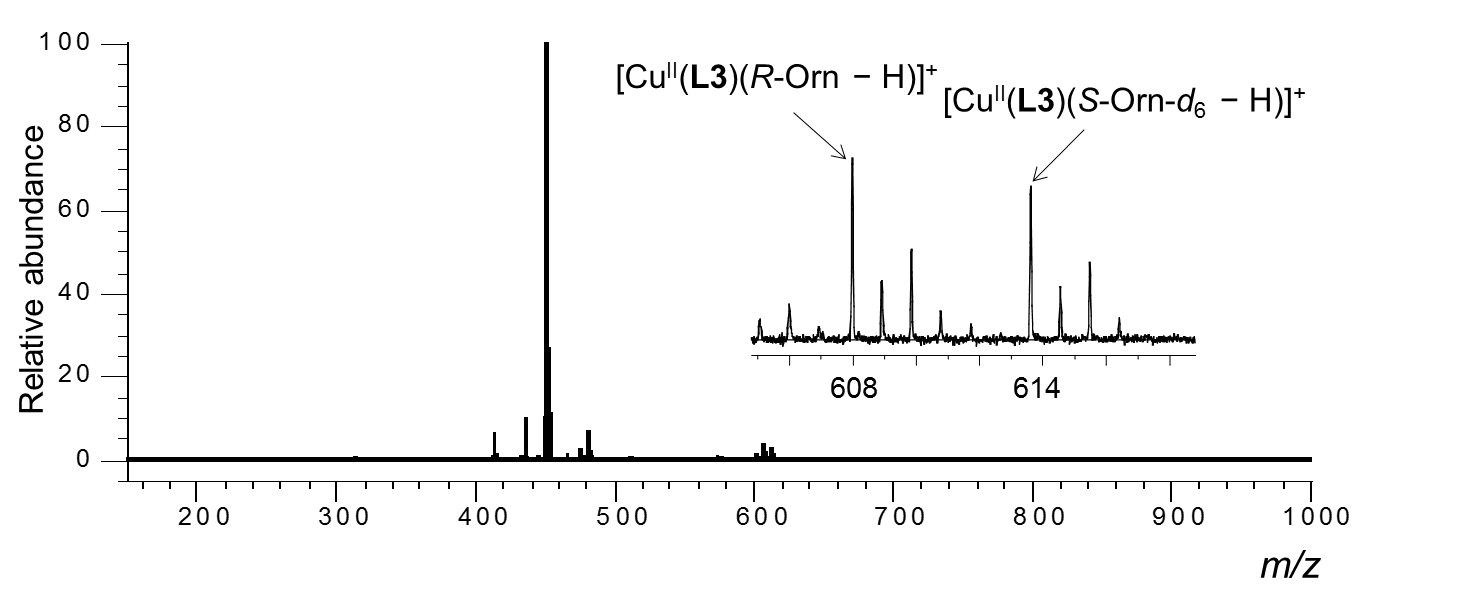
**Figure S28.** ESI mass spectra of the MS/EL method of CuCl2/**L**/*R*-AA/*S*-AA-*d*n- in water/methanol (1/10, v/v). [CuCl2]0 = 1.09 × 10−4 M, [**L**]0 = 9.09 × 10−5 M and [*R*-AA]0 = [*S*-AA-*d*n]0 = 4.55 × 10−5 M. [CuCl2]0/[**L**]0/[*R*-AA]0/[*S*-AA-*d*n]0 = 1.2/1.0/0.5/0.5. [K2CO3]0 = 9.09 × 10−5 M, **L** = **L3**, AA= *R*-Leu/*S*-Leu-*d*3.



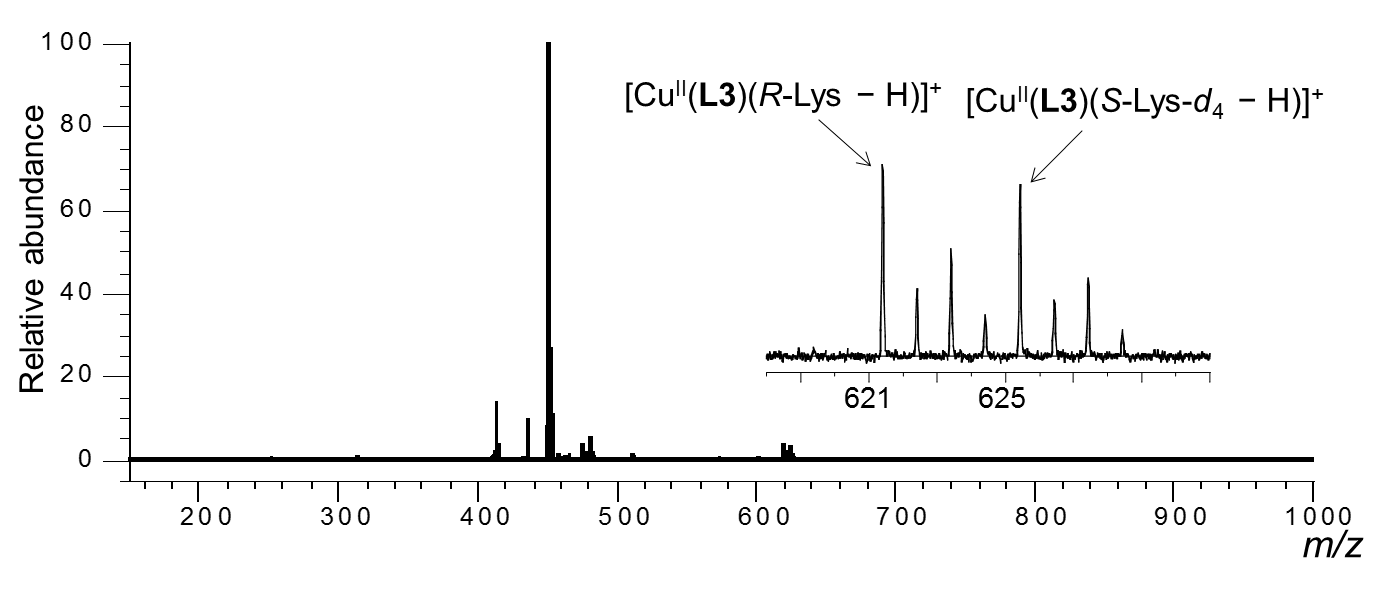
**Figure S29.** ESI mass spectra of the MS/EL method of CuCl2/**L**/*R*-AA/*S*-AA-*d*n- in water/methanol (1/10, v/v). [CuCl2]0 = 1.09 × 10−4 M, [**L**]0 = 9.09 × 10−5 M and [*R*-AA]0 = [*S*-AA-*d*n]0 = 4.55 × 10−5 M. [CuCl2]0/[**L**]0/[*R*-AA]0/[*S*-AA-*d*n]0 = 1.2/1.0/0.5/0.5. [K2CO3]0 = 9.09 × 10−5 M, **L** = **L3**, AA= *R*-Val/*S*-Val-*d*8.



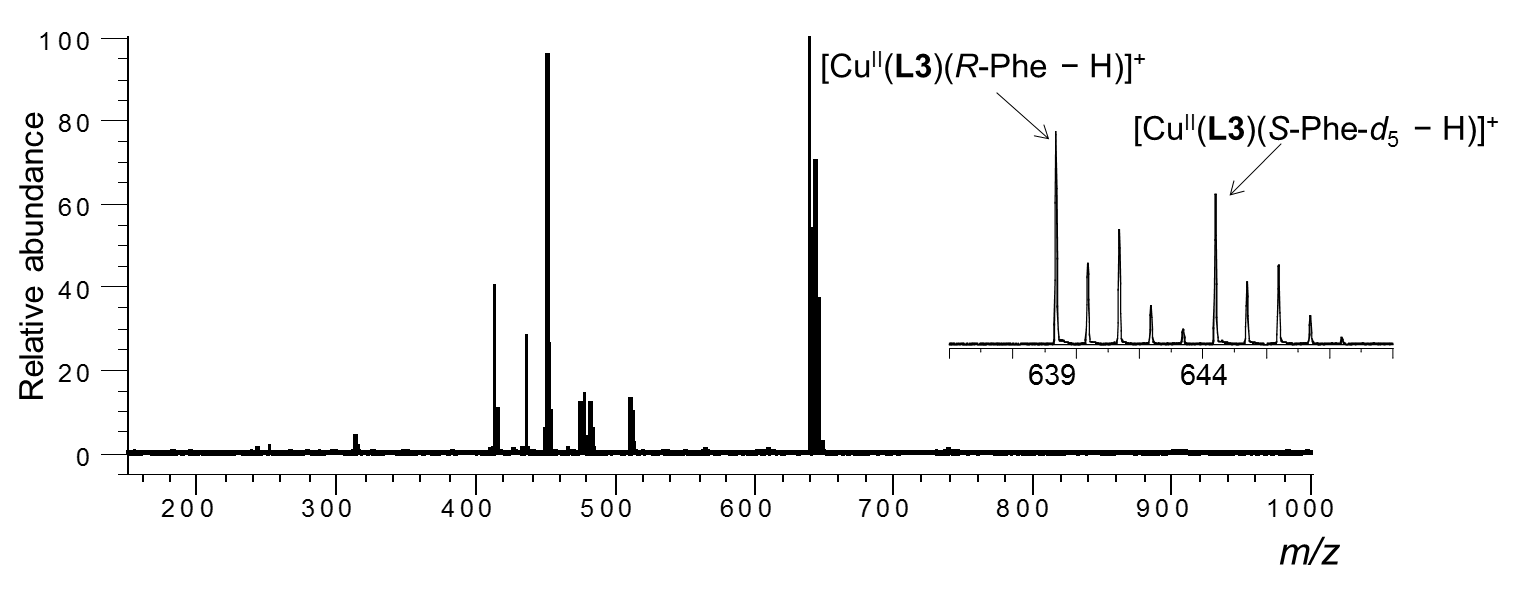
**Figure S30.** ESI mass spectra of the MS/EL method of CuCl2/**L**/*R*-AA/*S*-AA-*d*n- in water/methanol (1/10, v/v). [CuCl2]0 = 1.09 × 10−4 M, [**L**]0 = 9.09 × 10−5 M and [*R*-AA]0 = [*S*-AA-*d*n]0 = 4.55 × 10−5 M. [CuCl2]0/[**L**]0/[*R*-AA]0/[*S*-AA-*d*n]0 = 1.2/1.0/0.5/0.5. [K2CO3]0 = 9.09 × 10−5 M, **L** = **L3**, AA= *R*-Met/*S*-Met-*d*3.



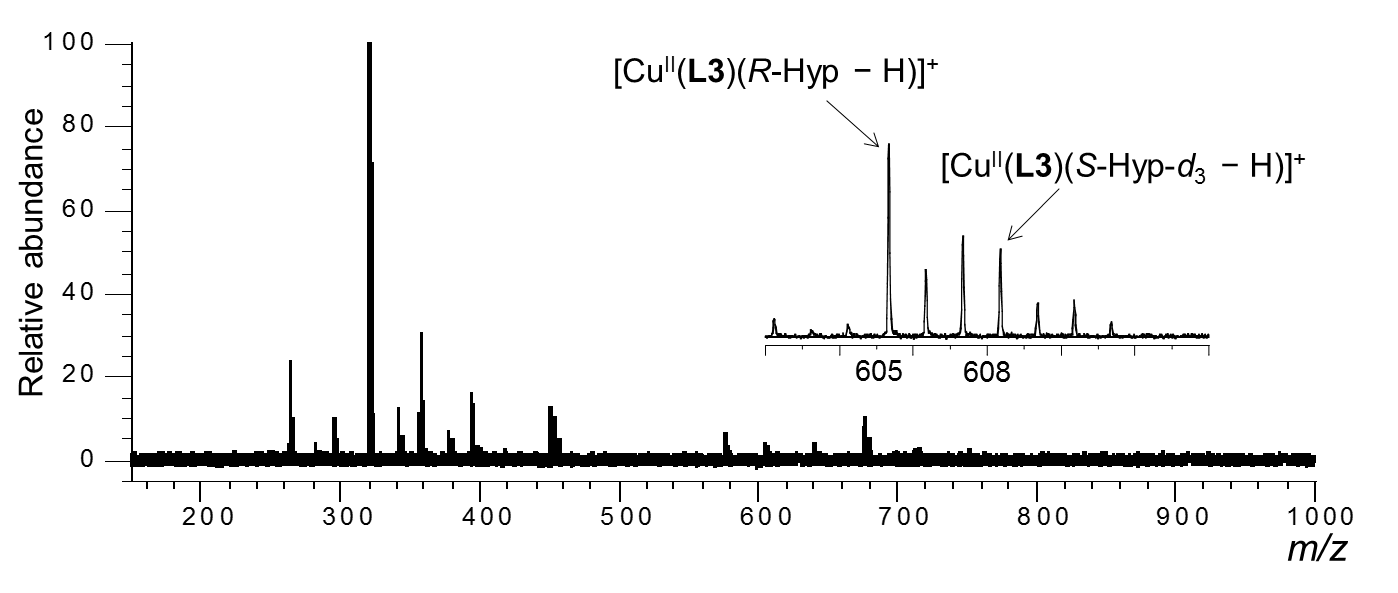
**Figure S31.** ESI mass spectra of the MS/EL method of CuCl2/**L**/*R*-AA/*S*-AA-*d*n- in water/methanol (1/10, v/v). [CuCl2]0 = 1.09 × 10−4 M, [**L**]0 = 9.09 × 10−5 M and [*R*-AA]0 = [*S*-AA-*d*n]0 = 4.55 × 10−5 M. [CuCl2]0/[**L**]0/[*R*-AA]0/[*S*-AA-*d*n]0 = 1.2/1.0/0.5/0.5. [K2CO3]0 = 9.09 × 10−5 M, **L** = **L3**, AA= *R*-Orn/*S*-Orn-*d*6.



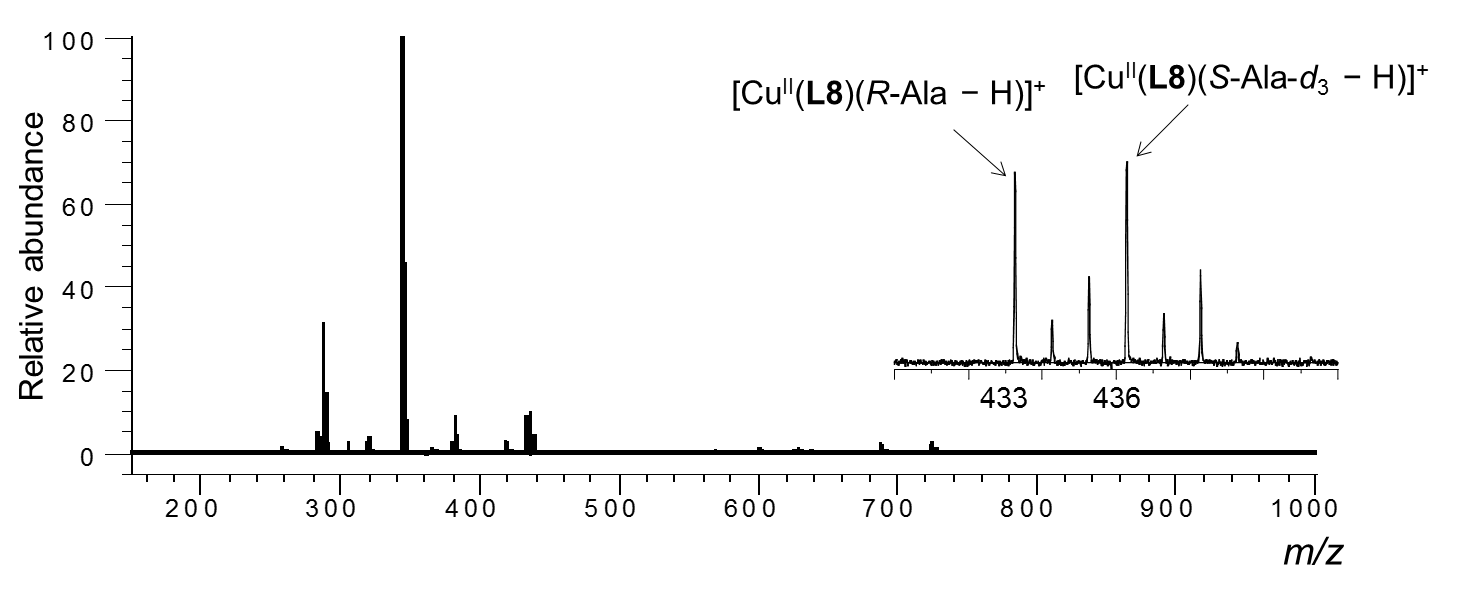
**Figure S32.** ESI mass spectra of the MS/EL method of CuCl2/**L**/*R*-AA/*S*-AA-*d*n- in water/methanol (1/10, v/v). [CuCl2]0 = 1.09 × 10−4 M, [**L**]0 = 9.09 × 10−5 M and [*R*-AA]0 = [*S*-AA-*d*n]0 = 4.55 × 10−5 M. [CuCl2]0/[**L**]0/[*R*-AA]0/[*S*-AA-*d*n]0 = 1.2/1.0/0.5/0.5. [K2CO3]0 = 9.09 × 10−5 M, **L** = **L3**, AA= *R*-Lys/*S*-Lys-*d*4.



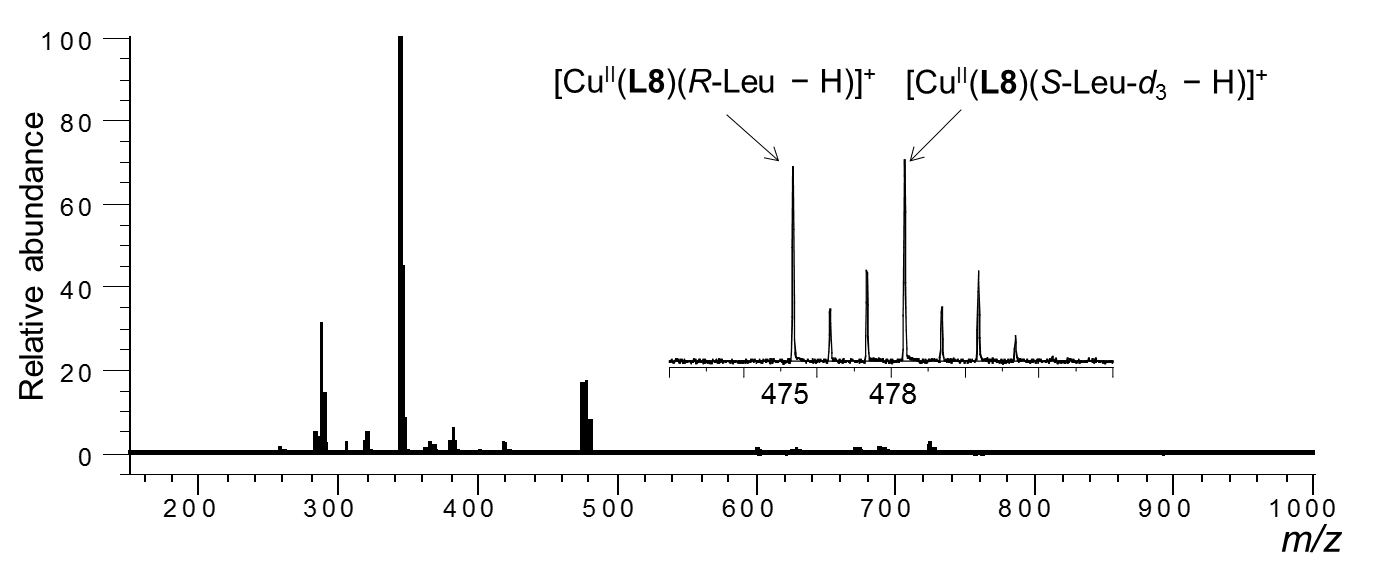
**Figure S33.** ESI mass spectra of the MS/EL method of CuCl2/**L**/*R*-AA/*S*-AA-*d*n- in water/methanol (1/10, v/v). [CuCl2]0 = 1.09 × 10−4 M, [**L**]0 = 9.09 × 10−5 M and [*R*-AA]0 = [*S*-AA-*d*n]0 = 4.55 × 10−5 M. [CuCl2]0/[**L**]0/[*R*-AA]0/[*S*-AA-*d*n]0 = 1.2/1.0/0.5/0.5. [K2CO3]0 = 9.09 × 10−5 M, **L** = **L3**, AA= *R*-Phe/*S*-Phe-*d*5.



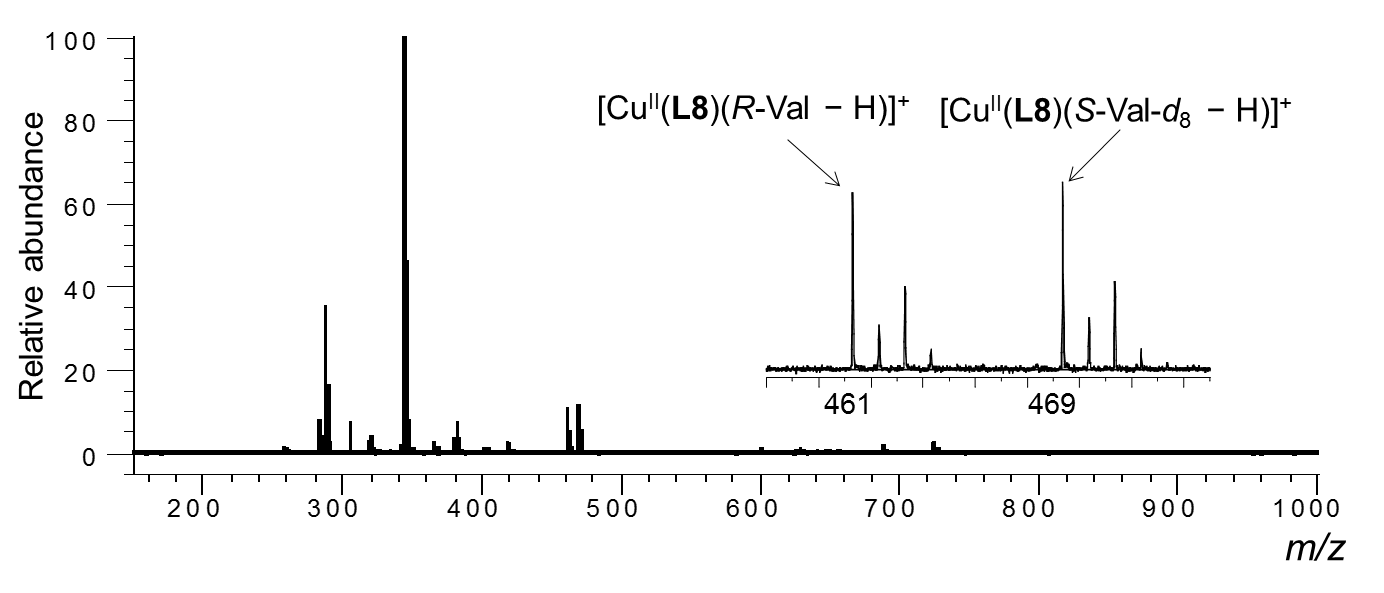
**Figure S34.** ESI mass spectra of the MS/EL method of CuCl2/**L**/*R*-AA/*S*-AA-*d*n- in water/methanol (1/10, v/v). [CuCl2]0 = 1.09 × 10−4 M, [**L**]0 = 9.09 × 10−5 M and [*R*-AA]0 = [*S*-AA-*d*n]0 = 4.55 × 10−5 M. [CuCl2]0/[**L**]0/[*R*-AA]0/[*S*-AA-*d*n]0 = 1.2/1.0/0.5/0.5. [K2CO3]0 = 9.09 × 10−5 M, **L** = **L3**, AA= *R*-Hyp/*S*-Hyp-*d*3.



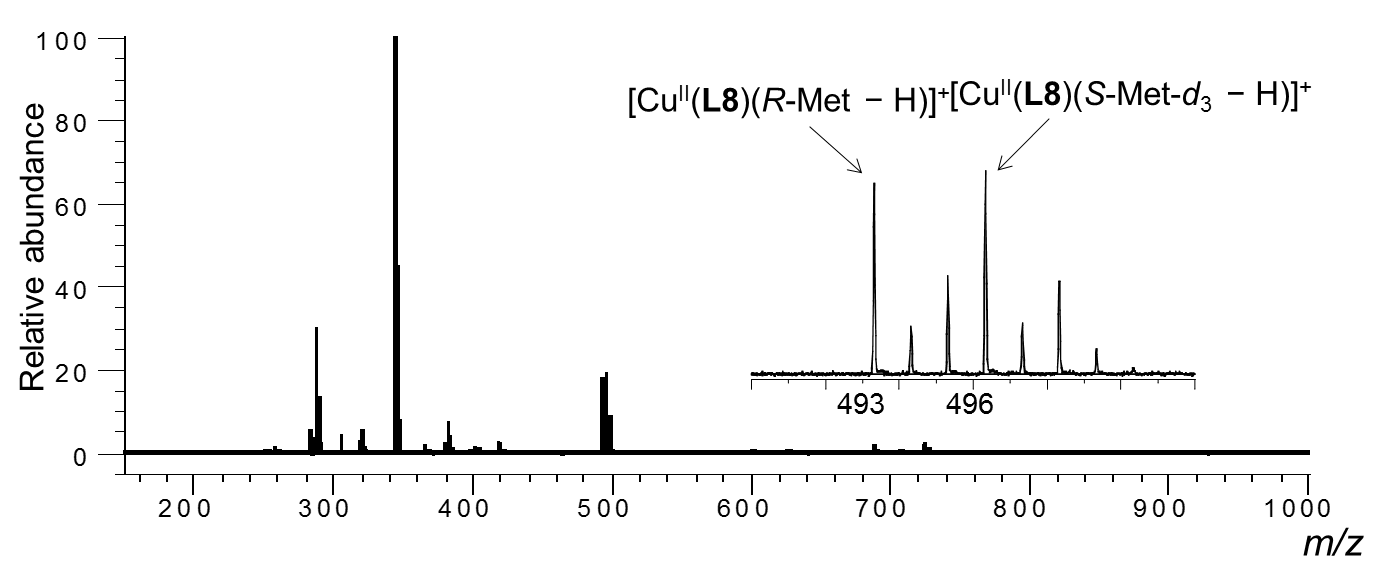
**Figure S35.** ESI mass spectra of the MS/EL method of CuCl2/**L**/*R*-AA/*S*-AA-*d*n- in water/methanol (1/10, v/v). [CuCl2]0 = 1.09 × 10−4 M, [**L**]0 = 9.09 × 10−5 M and [*R*-AA]0 = [*S*-AA-*d*n]0 = 4.55 × 10−5 M. [CuCl2]0/[**L**]0/[*R*-AA]0/[*S*-AA-*d*n]0 = 1.2/1.0/0.5/0.5. [K2CO3]0 = 9.09 × 10−5 M, **L** = **L8**, AA= *R*-Ala/*S*-Ala-*d*3.



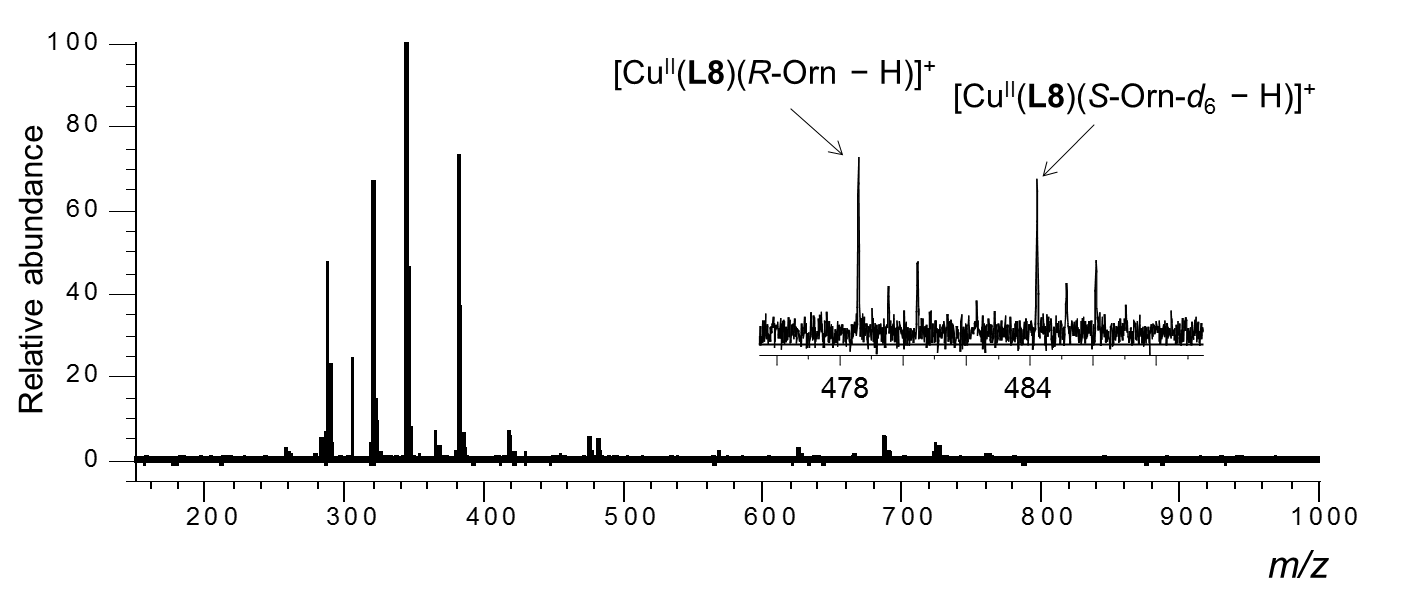
**Figure S36.** ESI mass spectra of the MS/EL method of CuCl2/**L**/*R*-AA/*S*-AA-*d*n- in water/methanol (1/10, v/v). [CuCl2]0 = 1.09 × 10−4 M, [**L**]0 = 9.09 × 10−5 M and [*R*-AA]0 = [*S*-AA-*d*n]0 = 4.55 × 10−5 M. [CuCl2]0/[**L**]0/[*R*-AA]0/[*S*-AA-*d*n]0 = 1.2/1.0/0.5/0.5. [K2CO3]0 = 9.09 × 10−5 M, **L** = **L8**, AA= *R*-Leu/*S*-Leu-*d*3.



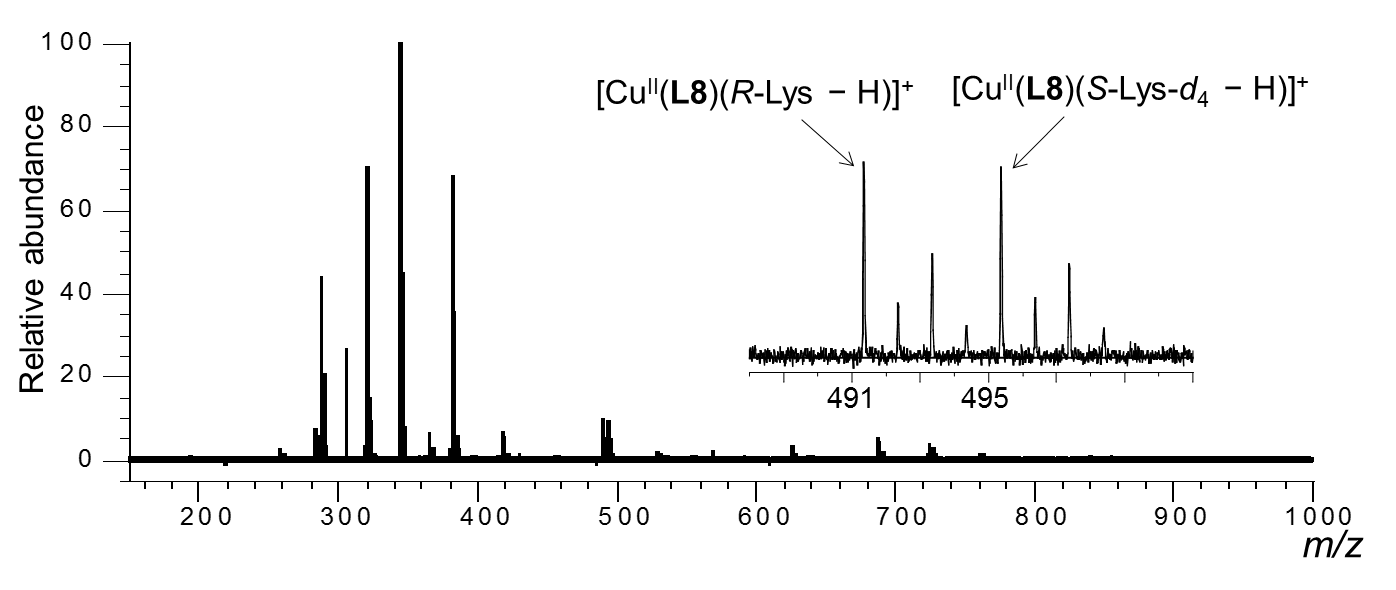
**Figure 37.** ESI mass spectra of the MS/EL method of CuCl2/**L**/*R*-AA/*S*-AA-*d*n- in water/methanol (1/10, v/v). [CuCl2]0 = 1.09 × 10−4 M, [**L**]0 = 9.09 × 10−5 M and [*R*-AA]0 = [*S*-AA-*d*n]0 = 4.55 × 10−5 M. [CuCl2]0/[**L**]0/[*R*-AA]0/[*S*-AA-*d*n]0 = 1.2/1.0/0.5/0.5. [K2CO3]0 = 9.09 × 10−5 M, **L** = **L8**, AA= *R*-Val/*S*-Val-*d*8.



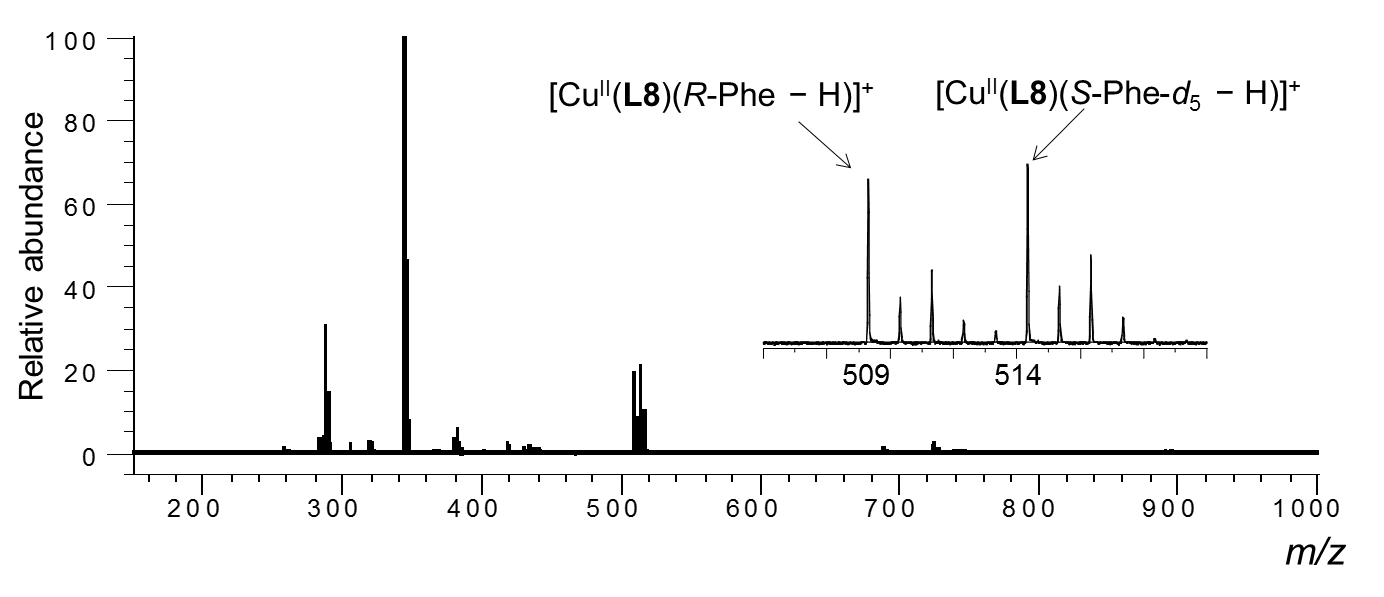
**Figure S38.** ESI mass spectra of the MS/EL method of CuCl2/**L**/*R*-AA/*S*-AA-*d*n- in water/methanol (1/10, v/v). [CuCl2]0 = 1.09 × 10−4 M, [**L**]0 = 9.09 × 10−5 M and [*R*-AA]0 = [*S*-AA-*d*n]0 = 4.55 × 10−5 M. [CuCl2]0/[**L**]0/[*R*-AA]0/[*S*-AA-*d*n]0 = 1.2/1.0/0.5/0.5. [K2CO3]0 = 9.09 × 10−5 M, **L** = **L8**, AA= *R*-Met/*S*-Met-*d*3.



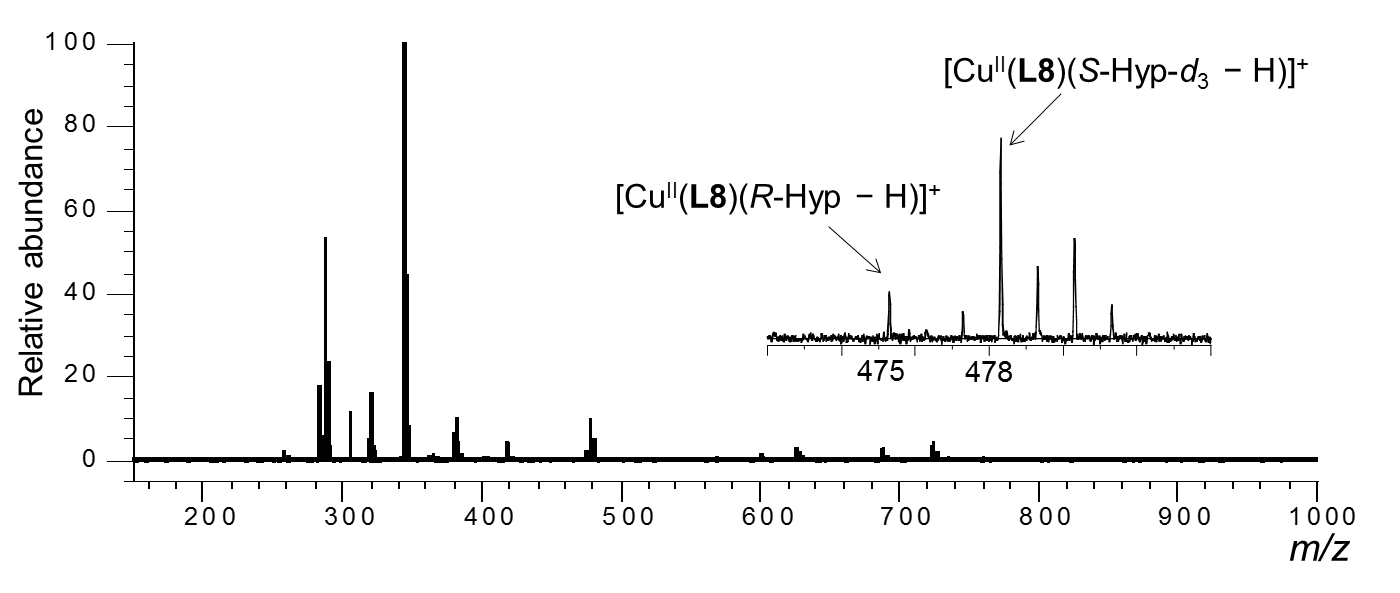
**Figure S39.** ESI mass spectra of the MS/EL method of CuCl2/**L**/*R*-AA/*S*-AA-*d*n- in water/methanol (1/10, v/v). [CuCl2]0 = 1.09 × 10−4 M, [**L**]0 = 9.09 × 10−5 M and [*R*-AA]0 = [*S*-AA-*d*n]0 = 4.55 × 10−5 M. [CuCl2]0/[**L**]0/[*R*-AA]0/[*S*-AA-*d*n]0 = 1.2/1.0/0.5/0.5. [K2CO3]0 = 9.09 × 10−5 M, **L** = **L8**, AA= *R*-Orn/*S*-Orn-*d*6.



**Figure S40.** ESI mass spectra of the MS/EL method of CuCl2/**L**/*R*-AA/*S*-AA-*d*n- in water/methanol (1/10, v/v). [CuCl2]0 = 1.09 × 10−4 M, [**L**]0 = 9.09 × 10−5 M and [*R*-AA]0 = [*S*-AA-*d*n]0 = 4.55 × 10−5 M. [CuCl2]0/[**L**]0/[*R*-AA]0/[*S*-AA-*d*n]0 = 1.2/1.0/0.5/0.5. [K2CO3]0 = 9.09 × 10−5 M, **L** = **L8**, AA= *R*-Lys/*S*-Lys-*d*4.



**Figure S41.** ESI mass spectra of the MS/EL method of CuCl2/**L**/*R*-AA/*S*-AA-*d*n- in water/methanol (1/10, v/v). [CuCl2]0 = 1.09 × 10−4 M, [**L**]0 = 9.09 × 10−5 M and [*R*-AA]0 = [*S*-AA-*d*n]0 = 4.55 × 10−5 M. [CuCl2]0/[**L**]0/[*R*-AA]0/[*S*-AA-*d*n]0 = 1.2/1.0/0.5/0.5. [K2CO3]0 = 9.09 × 10−5 M, **L** = **L8**, AA= *R*-Phe/*S*-Phe-*d*5.

.

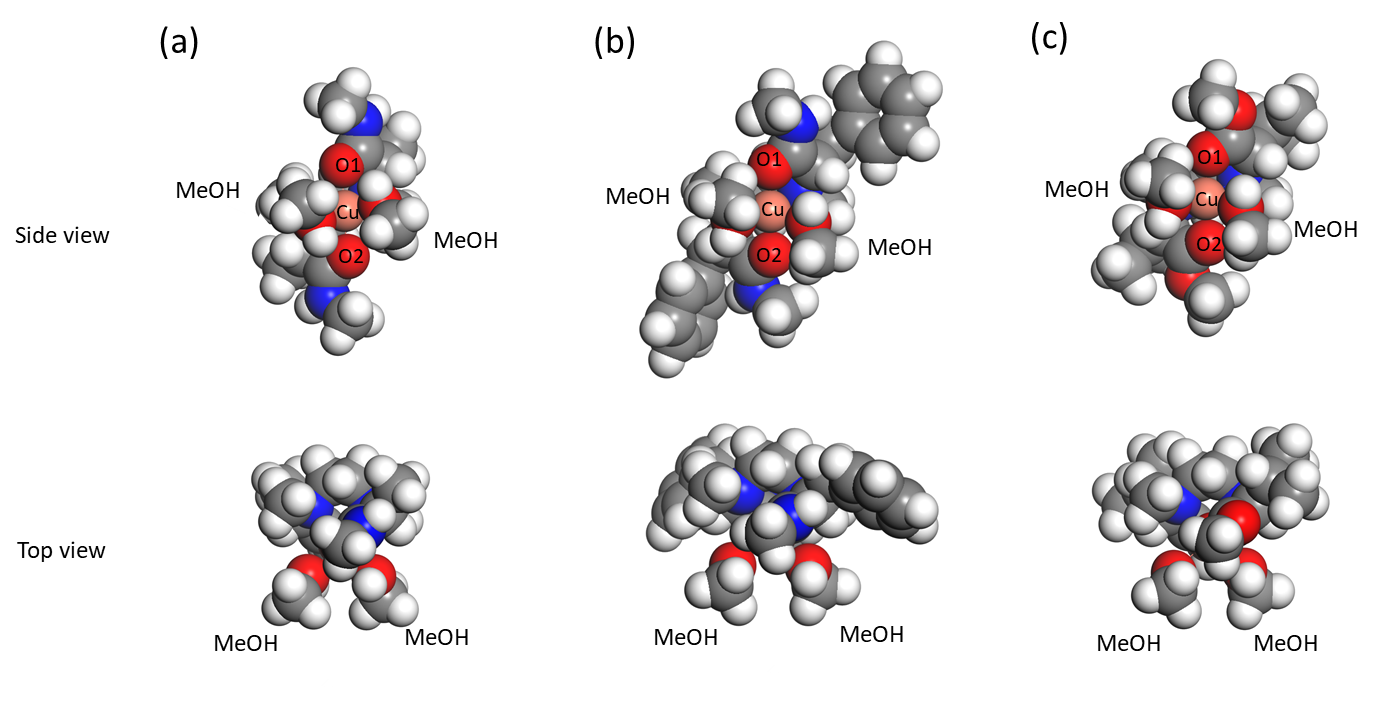
**Figure S42.** ESI mass spectra of the MS/EL method of CuCl2/**L**/*R*-AA/*S*-AA-*d*n- in water/methanol (1/10, v/v). [CuCl2]0 = 1.09 × 10−4 M, [**L**]0 = 9.09 × 10−5 M and [*R*-AA]0 = [*S*-AA-*d*n]0 = 4.55 × 10−5 M. [CuCl2]0/[**L**]0/[*R*-AA]0/[*S*-AA-*d*n]0 = 1.2/1.0/0.5/0.5. [K2CO3]0 = 9.09 × 10−5 M, **L** = **L8**, AA= *R*-Hyp/*S*-Hyp-*d*3.

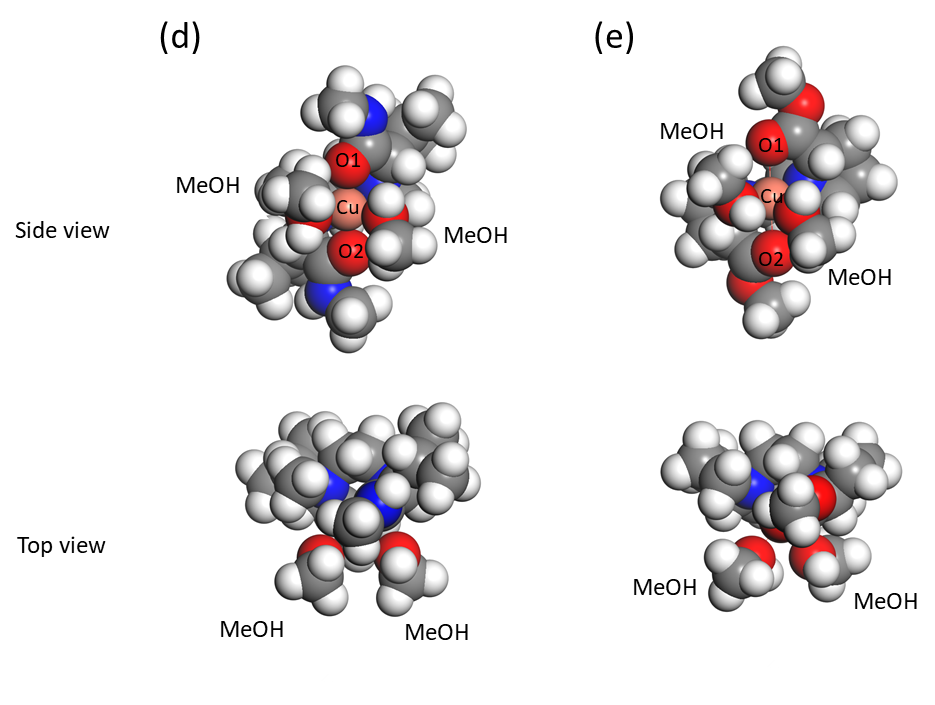
# Deuterated amino acids

**Table S1.** The structure and D contents of deuterated amino acids



# DFT calculation of copper(II)-ligand complex [Cu(L)(MeOH)2]2+





**Figure S43.** DFT calculation of the copper(II)-ligand complex [Cu(**L**)(MeOH)2]2+ in methanol. **L**: (a) **L2**, (b) **L4**, (c) **L5**, (d) **L6**, (e) **L7**.

# Bond length of Cu-O, Cu-N, and Cu-(MeOH) of copper(II)-ligand complex [Cu(L)(MeOH)2]2+ by DFT

**Table S2.** Bond length (Å) of Cu- Cu-O, Cu-N, and Cu-(MeOH) of copper(II)-ligand complex [Cu(**L**)(MeOH)2]2+ by DFT

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Complex ion | Cu-O1 | Cu-O2 | Cu-OMe1 | Cu-OMe2 | Cu-N1 | Cu-N2 |
| [Cu(**L1**)(MeOH)2]2+ | 2.15 | 2.15 | 2.22 | 2.22 | 2.28 | 2.27 |
| [Cu(**L2**)(MeOH)2]2+ | 2.13 | 2.13 | 2.28 | 2.28 | 2.28 | 2.29 |
| [Cu(**L3**)(MeOH)2]2+ | 2.14 | 2.13 | 2.24 | 2.26 | 2.32 | 2.34 |
| [Cu(**L4**)(MeOH)2]2+ | 2.10 | 2.08 | 2.25 | 2.31 | 2.39 | 2.31 |
| [Cu(**L5**)(MeOH)2]2+ | 2.08 | 2.09 | 2.25 | 2.22 | 2.31 | 2.50 |
| [Cu(**L6**)(MeOH)2]2+ | 2.03 | 2.04 | 2.31 | 2.25 | 2.32 | 2.47 |
| [Cu(**L7**)(MeOH)2]2+ | 2.51 | 2.55 | 2.15 | 2.22 | 2.15 | 2.14 |
| [Cu(**L8**)(MeOH)2]2+ | 2.51 | 2.44 | 2.19 | 2.22 | 2.18 | 2.14 |



**N2**

**OMe2**

**OMe1**

**N1**

**O2**

**O1**

# Coordinates of copper(II)-ligand complex [Cu(L)(MeOH)2]2+ by DFT

**Table S3.** Final Coordinates (Angstroms) of [CuII(**L1**)(MeOH)2]2+ complex calculated by DFT

ATOM X Y Z

1 O 1.230108 5.241101 26.225605

2 O -1.186360 3.690428 26.899695

3 H -0.597456 3.040821 26.492167

4 N -0.857349 6.938234 26.762265

5 O 1.278230 5.812985 24.069263

6 C 0.735559 5.828697 25.264595

7 C -0.068021 8.102401 27.235840

8 H -0.557073 9.038433 26.948140

9 H 0.903503 8.086407 26.746884

10 C -0.586523 6.587320 25.346190

11 C -2.302717 7.108494 27.020437

12 H -2.472766 7.271194 28.080966

13 H -2.832219 6.208597 26.716832

14 H -2.705929 7.965558 26.472725

15 C -2.380806 3.011511 27.343335

16 H -2.155271 2.329212 28.163956

17 H -2.817708 2.456105 26.512087

18 H -3.076335 3.774352 27.681235

19 C 2.498497 5.017613 23.909544

20 H 3.274156 5.413021 24.558345

21 H 2.764613 5.129567 22.865303

22 H 2.281890 3.981867 24.153149

23 C -0.688675 7.753788 24.364248

24 H -1.662892 8.231644 24.456440

25 H -0.594720 7.380708 23.346652

26 H 0.087145 8.498413 24.530775

27 O -1.241841 5.247100 29.736141

28 O 1.156754 3.661084 29.054411

29 H 0.555109 3.025327 29.464917

30 N 0.872088 6.915048 29.213472

31 O -1.289164 5.809201 31.895287

32 C -0.743031 5.823537 30.701797

33 C 0.108457 8.098318 28.744130

34 H 0.618404 9.022200 29.034592

35 H -0.862933 8.102258 29.233468

36 C 0.590844 6.562510 30.627339

37 C 2.321488 7.057301 28.960428

38 H 2.497664 7.224293 27.901560

39 H 2.830620 6.143829 29.258364

40 H 2.740863 7.901137 29.515873

41 C 2.333846 2.954836 28.605194

42 H 2.088676 2.276999 27.786526

43 H 2.762169 2.390904 29.434936

44 H 3.044313 3.701793 28.262894

45 C -2.519041 5.027053 32.049218

46 H -3.288887 5.433594 31.400463

47 H -2.785787 5.138367 33.093409

48 H -2.313381 3.989828 31.802402

49 C 0.709265 7.723155 31.614544

50 H 1.691743 8.184939 31.527484

51 H 0.605812 7.347548 32.630305

52 H -0.052860 8.481836 31.448427

53 Cu -0.001212 5.219669 27.984368

54 H 1.326656 5.800528 30.898903

55 H -1.336045 5.839338 25.073920

**Table S4.** Final Coordinates (Angstroms) of [CuII(**L2**)(MeOH)2]2+ complex calculated by DFT

ATOM X Y Z

1 O 1.197965 5.239458 26.216214

2 O -1.166049 3.678318 26.860022

3 H -0.522507 3.241932 26.285817

4 N -0.834500 7.008621 26.735277

5 N 1.466307 5.960645 24.095111

6 H 1.122859 6.567487 23.367301

7 C 0.797187 5.918964 25.243337

8 C -0.057108 8.172216 27.225590

9 H -0.538648 9.108718 26.927903

10 H 0.925030 8.157762 26.757452

11 C -0.546614 6.661781 25.319916

12 C -2.281953 7.185445 26.969081

13 H -2.467915 7.336717 28.028380

14 H -2.812793 6.294018 26.644081

15 H -2.667114 8.055122 26.428807

16 C -2.113890 2.691974 27.325681

17 H -1.632103 1.980035 27.997633

18 H -2.543092 2.160131 26.476766

19 H -2.893047 3.228348 27.858505

20 C 2.692973 5.216773 23.812090

21 H 3.563299 5.779624 24.152073

22 H 2.761050 5.073323 22.737094

23 H 2.669124 4.253542 24.312712

24 C -0.682058 7.832619 24.347922

25 H -1.658005 8.298537 24.467430

26 H -0.634407 7.481928 23.317436

27 H 0.085923 8.590245 24.494178

28 O -1.200455 5.261482 29.744549

29 O 1.102333 3.649867 29.104647

30 H 0.439465 3.249756 29.683601

31 N 0.855739 7.002262 29.230123

32 N -1.428043 5.932937 31.885724

33 H -1.072691 6.524214 32.620449

34 C -0.779645 5.917084 30.724895

35 C 0.087255 8.171725 28.740011

36 H 0.575617 9.104901 29.037403

37 H -0.894852 8.164493 29.208219

38 C 0.566182 6.656750 30.645130

39 C 2.304598 7.168979 28.997206

40 H 2.492539 7.321776 27.938450

41 H 2.828933 6.272924 29.320165

42 H 2.696151 8.034594 29.539628

43 C 1.988872 2.612174 28.630490

44 H 1.461128 1.922207 27.970512

45 H 2.404607 2.064451 29.476169

46 H 2.785464 3.106304 28.082547

47 C -2.645150 5.176132 32.175423

48 H -3.524633 5.742725 31.866217

49 H -2.690992 5.007852 33.247901

50 H -2.627327 4.225238 31.651686

51 C 0.705090 7.828229 31.616420

52 H 1.682451 8.290658 31.495809

53 H 0.657482 7.480176 32.647784

54 H -0.060439 8.587862 31.468642

55 Cu -0.003422 5.293080 27.979432

56 H 1.306660 5.900195 30.921291

57 H -1.288795 5.906516 25.044918

**Table S5.** Final Coordinates (Angstroms) of [CuII(**L3**)(MeOH)2]2+ complex calculated by DFT

ATOM X Y Z

1 O 1.015186 5.090006 26.294653

2 O -1.842080 3.723773 27.056156

3 N -1.032978 6.916750 26.650586

4 O 1.515601 6.031180 24.336132

5 C 0.721393 5.834590 25.358969

6 C -0.264682 8.059022 27.196667

7 H -0.728821 9.007970 26.912779

8 H 0.729314 8.052800 26.753268

9 C -0.634133 6.535105 25.276080

10 C -2.491385 7.101117 26.780680

11 H -2.995697 6.202313 26.434304

12 H -2.842937 7.964433 26.208000

13 H -2.745934 7.257963 27.825743

14 C -2.798796 2.930799 27.798462

15 H -2.379555 1.956016 28.048898

16 H -3.711158 2.804206 27.214434

17 H -3.019485 3.479187 28.707722

18 C 2.737019 5.236893 24.286721

19 H 3.216220 5.520635 23.357262

20 H 2.478473 4.182040 24.286485

21 H 3.367184 5.476270 25.138319

22 C -0.732161 7.656964 24.221898

23 H -0.038534 8.459984 24.466912

24 C -0.485644 7.215695 22.795573

25 H -1.738050 8.076660 24.296001

26 O -1.592155 5.248826 29.661158

27 O 0.884490 3.588723 29.085193

28 N 0.585925 6.850261 29.224222

29 O -1.733827 5.860275 31.799909

30 C -1.118953 5.820712 30.639445

31 C -0.148752 8.033706 28.718383

32 H 0.348100 8.960262 29.027116

33 H -1.142050 8.039289 29.164968

34 C 0.247594 6.495174 30.618712

35 C 2.043831 6.972173 29.036512

36 H 2.264886 7.142618 27.986878

37 H 2.524164 6.045706 29.344048

38 H 2.462856 7.804535 29.612389

39 C 2.007799 2.813380 28.611387

40 H 2.370005 3.299047 27.709516

41 H 1.697782 1.794539 28.376716

42 H 2.798883 2.797396 29.362140

43 C -3.003994 5.137803 31.878726

44 H -2.824148 4.082524 31.693215

45 H -3.698183 5.546142 31.149849

46 H -3.358486 5.306880 32.889533

47 C 0.390093 7.645462 31.650387

48 H -0.537349 8.212148 31.713765

49 C 0.823548 7.209689 33.026372

50 H 1.148015 8.327788 31.261772

51 Cu -0.327519 5.121010 27.944112

52 H 0.940244 5.696070 30.895468

53 H -1.322362 5.736248 24.989850

54 C 2.042055 6.543217 33.216637

55 C 2.476048 6.199639 34.494915

56 C 1.698374 6.519147 35.608593

57 C 0.484533 7.182281 35.430837

58 C 0.051379 7.521455 34.150511

59 C -1.042880 6.041467 22.274148

60 C -0.731991 5.624084 20.981046

61 C 0.116468 6.384681 20.177219

62 C 0.644179 7.577033 20.671425

63 C 0.342277 7.984287 21.969202

64 H 2.669345 6.302474 32.366901

65 H 3.422179 5.690067 34.623373

66 H 2.035549 6.259444 36.603805

67 H -0.123580 7.440258 36.287936

68 H -0.890025 8.039586 34.020423

69 H -1.706684 5.435116 22.876645

70 H -1.157268 4.704997 20.599214

71 H 0.356626 6.052788 19.175091

72 H 1.299144 8.179912 20.055826

73 H 0.780715 8.895544 22.356044

74 H 0.399652 3.066046 29.736551

75 H -1.539277 3.208113 26.297960

**Table S6.** Final Coordinates (Angstroms) of [CuII(**L4**)(MeOH)2]2+ complex calculated by DFT

ATOM X Y Z

1 O 0.895752 5.039247 26.355279

2 O -1.828285 3.598416 27.152931

3 N -1.086588 6.915778 26.621920

4 N 1.588037 5.882059 24.407574

5 C 0.687879 5.791881 25.376302

6 C -0.350225 8.067991 27.185816

7 H -0.840424 9.011403 26.919880

8 H 0.644022 8.098395 26.743739

9 C -0.655718 6.528743 25.259418

10 C -2.545774 7.071347 26.739132

11 H -3.031174 6.152794 26.417442

12 H -2.919655 7.912858 26.145615

13 H -2.803262 7.249240 27.780550

14 C -2.645634 2.705928 27.942022

15 H -2.131770 1.759391 28.117350

16 H -3.592690 2.522118 27.432799

17 H -2.826230 3.205201 28.888622

18 C 2.794120 5.063975 24.392781

19 H 3.387389 5.349996 23.529206

20 H 2.535353 4.007525 24.325311

21 H 3.373336 5.226361 25.299808

22 C -0.733634 7.674131 24.221944

23 H -0.052889 8.477317 24.501710

24 C -0.464508 7.290026 22.781493

25 H -1.741565 8.087145 24.290532

26 O -1.590389 5.223445 29.702322

27 O 0.993381 3.548409 29.031777

28 N 0.529365 6.850662 29.196232

29 N -1.777478 5.850418 31.854537

30 C -1.123626 5.820506 30.696922

31 C -0.239257 8.017431 28.707447

32 H 0.224215 8.953413 29.038253

33 H -1.234529 7.977501 29.146881

34 C 0.250140 6.509364 30.608853

35 C 1.975828 6.984369 28.939306

36 H 2.149021 7.088666 27.873068

37 H 2.485582 6.085765 29.278583

38 H 2.402400 7.859325 29.440367

39 C 1.952255 2.711519 28.346633

40 H 2.154058 3.182354 27.389748

41 H 1.543659 1.713418 28.189110

42 H 2.874441 2.644303 28.926984

43 C -3.057810 5.189167 32.081891

44 H -2.916324 4.164046 32.426983

45 H -3.621882 5.179559 31.154692

46 H -3.601574 5.750761 32.836993

47 C 0.447559 7.686003 31.602226

48 H -0.451788 8.300542 31.642815

49 C 0.866590 7.272197 32.992524

50 H 1.234839 8.324231 31.195219

51 Cu -0.376238 5.097081 27.995161

52 H 0.964674 5.723827 30.860313

53 H -1.351068 5.744183 24.951319

54 C 2.009719 6.482117 33.184633

55 C 2.423366 6.122999 34.463238

56 C 1.697364 6.546980 35.576825

57 C 0.565299 7.340101 35.401496

58 C 0.152628 7.700409 34.118049

59 C -1.015234 6.138239 22.201264

60 C -0.683964 5.774165 20.898530

61 C 0.178461 6.566171 20.140617

62 C 0.703461 7.733141 20.691595

63 C 0.382236 8.089292 22.001454

64 H 2.592568 6.153264 32.333528

65 H 3.309277 5.514606 34.591016

66 H 2.013903 6.267085 36.572560

67 H 0.001575 7.679632 36.260175

68 H -0.719338 8.331304 33.991082

69 H -1.686478 5.507783 22.769241

70 H -1.105876 4.874317 20.470547

71 H 0.428130 6.280843 19.127070

72 H 1.366244 8.362538 20.112360

73 H 0.814426 8.984558 22.431343

74 H 0.573406 3.029559 29.729401

75 H -1.546789 3.136660 26.352488

76 H -1.337732 6.287762 32.649939

77 H 1.412136 6.479356 23.614575

**Table S7.** Final Coordinates (Angstroms) of [CuII(**L5**)(MeOH)2]2+ complex calculated by DFT

ATOM X Y Z

1 O 1.117995 5.185168 26.329153

2 O -1.735851 3.669707 27.103378

3 N -0.926436 6.967067 26.663593

4 O 1.585610 5.987573 24.307867

5 C 0.809081 5.872670 25.352774

6 C -0.149186 8.092976 27.239511

7 H -0.598718 9.048105 26.951415

8 H 0.851616 8.072125 26.816161

9 C -0.536550 6.589021 25.273397

10 C -2.383808 7.182623 26.787462

11 H -2.912097 6.308875 26.413031

12 H -2.707537 8.071258 26.234450

13 H -2.644952 7.322595 27.833616

14 C -2.574753 2.817002 27.916210

15 H -2.081351 1.862979 28.104221

16 H -3.528570 2.649612 27.414541

17 H -2.738706 3.338741 28.852765

18 C 2.831362 5.228702 24.322308

19 H 3.325684 5.494507 23.396672

20 H 2.607230 4.167587 24.359321

21 H 3.427986 5.526699 25.178864

22 C -0.711830 7.654459 24.151404

23 C 0.282111 8.816086 24.120211

24 H -1.698893 8.088278 24.335443

25 O -1.400948 5.291200 29.631003

26 O 1.037008 3.623003 28.879632

27 N 0.716256 6.968871 29.322173

28 O -1.613498 5.764987 31.785545

29 C -0.962966 5.823546 30.651440

30 C -0.057853 8.092563 28.764501

31 H 0.393024 9.051612 29.038060

32 H -1.054072 8.081060 29.202618

33 C 0.373552 6.574230 30.704971

34 C 2.160052 7.009834 29.029339

35 H 2.321049 6.999279 27.954038

36 H 2.628718 6.124377 29.452136

37 H 2.641926 7.905213 29.432588

38 C 1.997668 2.714019 28.290765

39 H 2.295419 3.135658 27.336777

40 H 1.543385 1.735853 28.139950

41 H 2.865728 2.625611 28.944225

42 C -2.844682 4.983463 31.809104

43 H -2.597574 3.931926 31.693400

44 H -3.503660 5.319216 31.014478

45 H -3.276047 5.174749 32.784861

46 C 0.393458 7.653654 31.852516

47 H -0.588596 8.134071 31.867151

48 C 1.442639 8.751859 31.684563

49 Cu -0.249345 5.147955 27.910495

50 H 1.103274 5.803173 30.970482

51 H -1.233000 5.786746 25.007116

52 H 0.603638 3.170009 29.613880

53 H -1.486203 3.181992 26.307471

54 C 0.639793 6.980677 33.216858

55 C -0.785825 6.965856 22.775799

56 H 0.562452 7.727916 34.009564

57 H -0.065310 6.180353 33.430650

58 H 1.652896 6.567885 33.242918

59 H 2.452970 8.340632 31.669169

60 H 1.298100 9.359295 30.794241

61 H 1.377443 9.421314 32.543988

62 H 0.196164 9.469258 24.986896

63 H 0.072483 9.420937 23.235400

64 H 1.315650 8.478274 24.042989

65 H -1.143962 7.682148 22.034055

66 H -1.471646 6.114920 22.792053

67 H 0.194375 6.612683 22.454199

**Table S8.** Final Coordinates (Angstroms) of [CuII(**L6**)(MeOH)2]2+ complex calculated by DFT

ATOM X Y Z

1 O 1.132714 5.215996 26.361286

2 O -1.685044 3.677104 27.099452

3 N -0.915165 6.944979 26.692470

4 N 1.510217 5.738885 24.224586

5 C 0.779977 5.826773 25.323685

6 C -0.187030 8.098417 27.263188

7 H -0.676886 9.032076 26.969888

8 H 0.811665 8.116101 26.837004

9 C -0.534271 6.607027 25.294720

10 C -2.377134 7.068944 26.850324

11 H -2.847607 6.155640 26.493680

12 H -2.773776 7.925001 26.294535

13 H -2.618496 7.196756 27.903129

14 C -2.539896 2.842269 27.909518

15 H -2.060092 1.884410 28.115443

16 H -3.492244 2.676200 27.403189

17 H -2.705939 3.375217 28.839867

18 C 2.741313 4.960369 24.176698

19 H 3.231708 5.177258 23.231879

20 H 2.528699 3.892166 24.243026

21 H 3.382145 5.256360 25.006455

22 C -0.686515 7.756028 24.244184

23 C 0.392669 8.846120 24.202327

24 H -1.619294 8.243035 24.538593

25 O -1.258148 5.176186 29.648478

26 O 1.178420 3.628080 28.941677

27 N 0.726820 7.011257 29.339853

28 N -1.754199 5.831924 31.710269

29 C -0.936246 5.831470 30.668239

30 C -0.088568 8.104087 28.786479

31 H 0.325794 9.080366 29.055231

32 H -1.082257 8.050651 29.226481

33 C 0.402865 6.593929 30.720873

34 C 2.162546 7.090659 29.026006

35 H 2.311345 7.034653 27.950641

36 H 2.672665 6.245981 29.480406

37 H 2.613967 8.018938 29.383160

38 C 2.068216 2.701216 28.281075

39 H 2.350392 3.155329 27.336218

40 H 1.567254 1.750034 28.100019

41 H 2.956625 2.540772 28.894004

42 C -2.973098 5.032107 31.729478

43 H -2.733492 3.976087 31.604167

44 H -3.642038 5.340565 30.926131

45 H -3.457830 5.184667 32.689177

46 C 0.453956 7.643930 31.883001

47 H -0.531432 8.110761 31.955062

48 C 1.453985 8.788613 31.708125

49 Cu -0.142798 5.159993 27.956960

50 H 1.140572 5.823386 30.956116

51 H -1.267473 5.854755 24.991199

52 H 0.719948 3.167192 29.656010

53 H -1.415761 3.175756 26.319246

54 H -1.545259 6.392610 32.519763

55 H 1.253809 6.269326 23.409114

56 C 0.777875 6.939471 33.217907

57 C -0.928649 7.202807 22.824733

58 H 0.631448 7.635422 34.045606

59 H 0.175335 6.054003 33.415911

60 H 1.822918 6.621831 33.222945

61 H 2.481110 8.428588 31.639381

62 H 1.246480 9.412398 30.840940

63 H 1.394791 9.433103 32.587402

64 H 0.438775 9.440882 25.110950

65 H 0.161790 9.528715 23.382551

66 H 1.389765 8.444148 24.012441

67 H -1.490521 7.937244 22.246594

68 H -1.493492 6.268136 22.838031

69 H -0.002147 7.038255 22.269163

**Table S9.** Final Coordinates (Angstroms) of [CuII(**L7**)(MeOH)2]2+ complex calculated by DFT

ATOM X Y Z

1 O 0.233872 0.213637 -0.505720

2 O 3.640405 0.251073 0.328218

3 H 3.487999 1.203367 0.423172

4 N 1.414622 -2.226797 0.156131

5 O -0.583550 -0.744279 -2.376489

6 C 0.234700 -0.676036 -1.345868

7 C 0.146113 -2.706028 0.782208

8 H -0.076806 -3.731170 0.478644

9 H -0.679743 -2.079899 0.452113

10 C 1.243829 -1.800640 -1.263168

11 C 2.396787 -3.342188 0.031589

12 H 2.361084 -3.975343 0.912951

13 H 3.394417 -2.913529 -0.043037

14 C 5.016816 -0.029522 0.700623

15 H 5.177135 0.196031 1.756009

16 H 5.685750 0.566863 0.082516

17 H 5.187153 -1.085790 0.518179

18 C -1.573290 0.321491 -2.551418

19 H -1.122842 1.108351 -3.150582

20 H -1.887772 0.700798 -1.585551

21 H -2.393885 -0.147621 -3.082547

22 C 1.093250 -3.101939 -2.055406

23 H 1.395799 -2.970028 -3.091551

24 H 0.058592 -3.443576 -2.048194

25 O 3.188319 -1.632344 3.121284

26 O 1.810904 1.675165 1.853126

27 H 2.327088 1.986699 2.609739

28 N 0.469533 -1.233866 2.734855

29 O 2.772136 -2.326533 5.230890

30 C 2.453272 -1.740528 4.094698

31 C 0.273627 -2.649946 2.289029

32 H -0.617627 -3.084620 2.743884

33 H 1.126578 -3.243647 2.607823

34 C 1.075549 -1.127683 4.091412

35 C -0.844949 -0.569586 2.960612

36 H -1.536293 -0.805287 2.156805

37 H -0.676495 0.505463 2.967607

38 C 0.818017 2.678020 1.515477

39 H 1.316246 3.573624 1.145687

40 H 0.216269 2.915344 2.390891

41 H 0.196301 2.251105 0.736933

42 C 4.124794 -2.856649 5.385246

43 H 4.018419 -3.730676 6.018085

44 H 4.727974 -2.095111 5.873134

45 H 4.539202 -3.117532 4.417756

46 C -0.024447 -1.574059 5.062118

47 H 0.116257 -1.132212 6.046531

48 H -0.029030 -2.656920 5.179341

49 Cu 1.878111 -0.476818 1.317389

50 C -1.311159 -1.069240 4.351648

51 C 2.012981 -4.077570 -1.278787

52 H 2.910446 -4.319700 -1.846111

53 H 1.496263 -5.013697 -1.069306

54 H -2.036757 -1.875135 4.253329

55 H -1.788756 -0.259992 4.901672

56 H 1.262093 -0.060645 4.254323

57 H 2.188469 -1.331287 -1.553178

**Table S10.** Final Coordinates (Angstroms) of [CuII(**L8**)(MeOH)2]2+ complex calculated by DFT

ATOM X Y Z

1 O 0.215967 0.158645 -0.389633

2 O 3.376857 0.358747 0.072234

3 H 3.328929 1.286664 0.345256

4 N 1.474057 -2.232408 0.219898

5 N -0.596998 -0.737272 -2.311168

6 H -0.512743 -1.485116 -2.984833

7 C 0.242143 -0.716237 -1.277397

8 C 0.220956 -2.764452 0.826911

9 H 0.063073 -3.808367 0.546564

10 H -0.630347 -2.194835 0.461470

11 C 1.302743 -1.797846 -1.195169

12 C 2.503366 -3.302127 0.100249

13 H 2.478600 -3.948265 0.972636

14 H 3.482957 -2.830862 0.054263

15 C 4.769772 -0.014831 -0.006017

16 H 5.215671 -0.058030 0.987996

17 H 5.300403 0.708525 -0.622865

18 H 4.815927 -0.993343 -0.473794

19 C -1.626189 0.270291 -2.537115

20 H -1.453294 0.767245 -3.491572

21 H -1.592051 0.994817 -1.731736

22 H -2.605700 -0.207275 -2.560102

23 C 1.223479 -3.097595 -2.003918

24 H 1.532590 -2.948891 -3.036981

25 H 0.209616 -3.500951 -2.007439

26 O 3.132834 -1.339268 3.286880

27 O 2.032687 1.690052 2.052154

28 H 2.617185 1.864168 2.802246

29 N 0.393385 -1.235645 2.764191

30 N 2.683294 -2.324038 5.295081

31 H 1.968358 -2.498307 5.986367

32 C 2.350833 -1.611813 4.217499

33 C 0.301730 -2.666168 2.338308

34 H -0.570600 -3.153145 2.777247

35 H 1.184315 -3.196036 2.691190

36 C 0.937073 -1.072362 4.144939

37 C -0.966560 -0.645266 2.918296

38 H -1.608159 -0.953866 2.097911

39 H -0.868798 0.438696 2.887462

40 C 1.268260 2.876894 1.731624

41 H 1.940449 3.704856 1.510097

42 H 0.614026 3.137215 2.562190

43 H 0.677364 2.634992 0.854191

44 C 4.015477 -2.839248 5.572414

45 H 3.966604 -3.918153 5.715034

46 H 4.410417 -2.379418 6.478196

47 H 4.664436 -2.609542 4.733816

48 C -0.180934 -1.576022 5.066105

49 H -0.109550 -1.141335 6.062109

50 H -0.150528 -2.661483 5.166993

51 Cu 1.798755 -0.411809 1.372401

52 C -1.460239 -1.124195 4.308541

53 C 2.181640 -4.037968 -1.227319

54 H 3.098573 -4.222669 -1.785164

55 H 1.709735 -5.002051 -1.041807

56 H -2.167760 -1.947679 4.218255

57 H -1.963592 -0.310545 4.827873

58 H 1.045453 0.005629 4.294985

59 H 2.230335 -1.287905 -1.468580