

## Supplementary Materials

# Chiral Selectors in Voltammetric Sensors Based on the Mixed Phenylalanine/Alanine Cu(II) and Zn(II) Complexes

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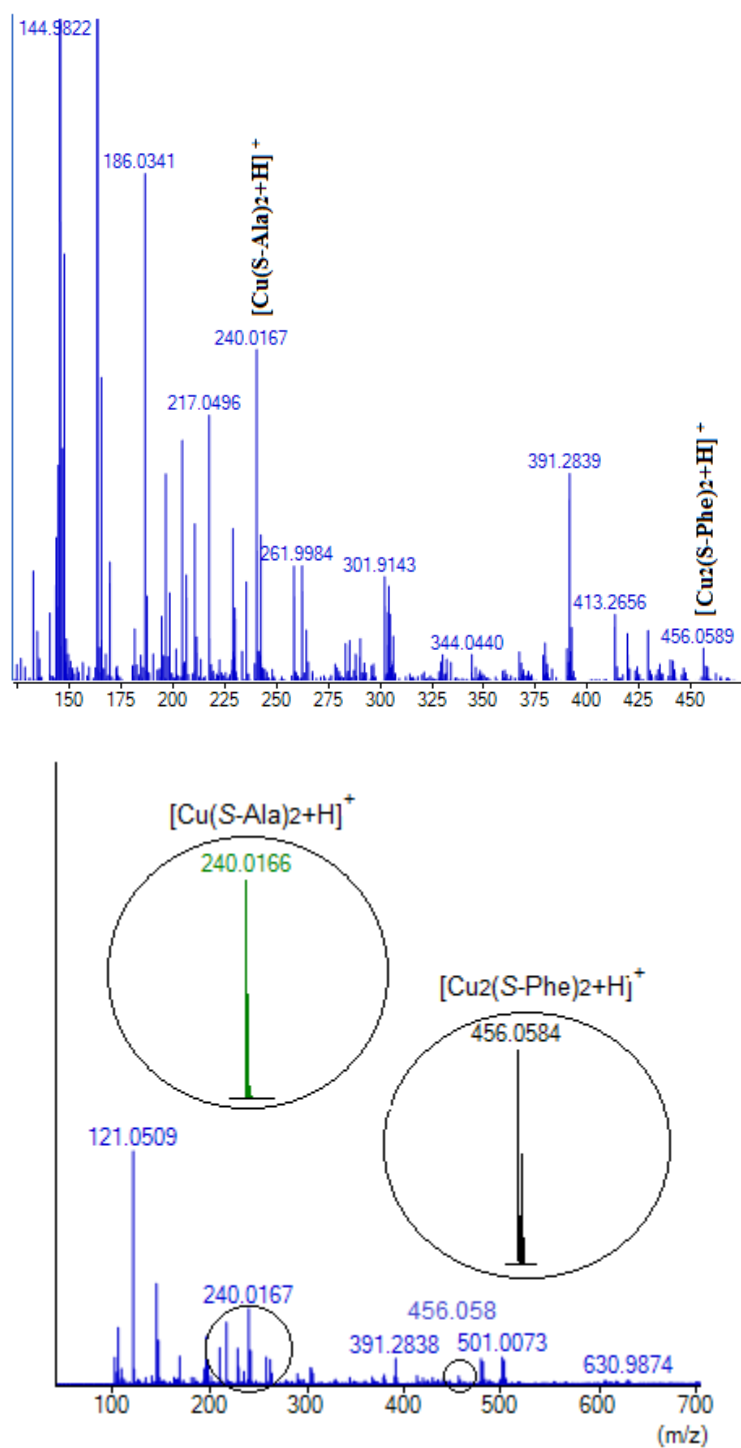
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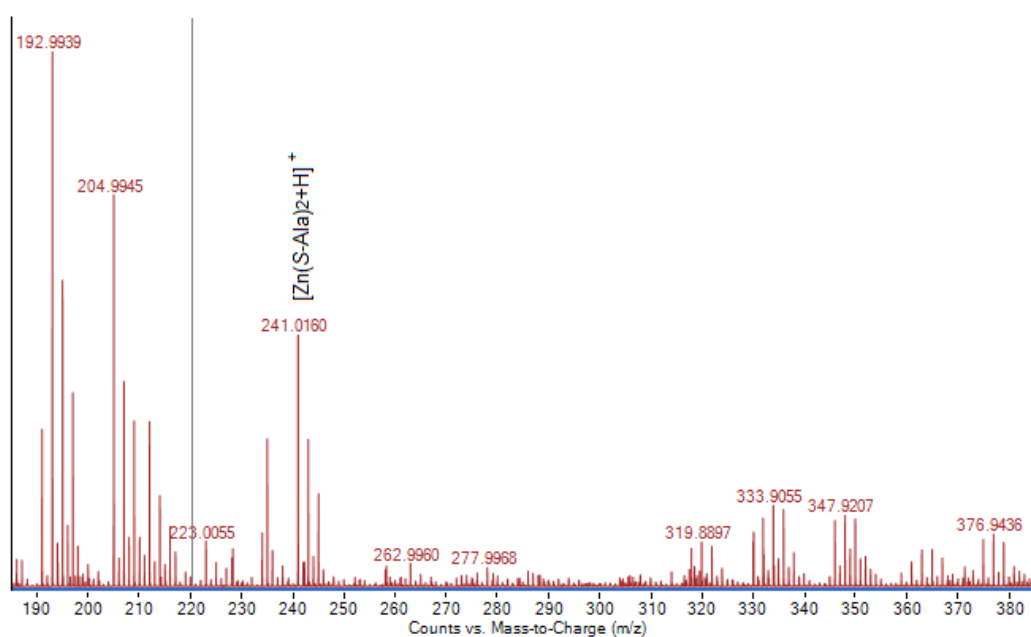
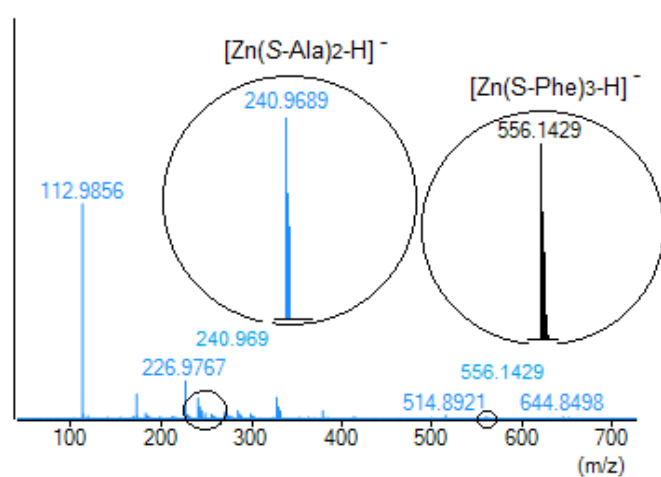
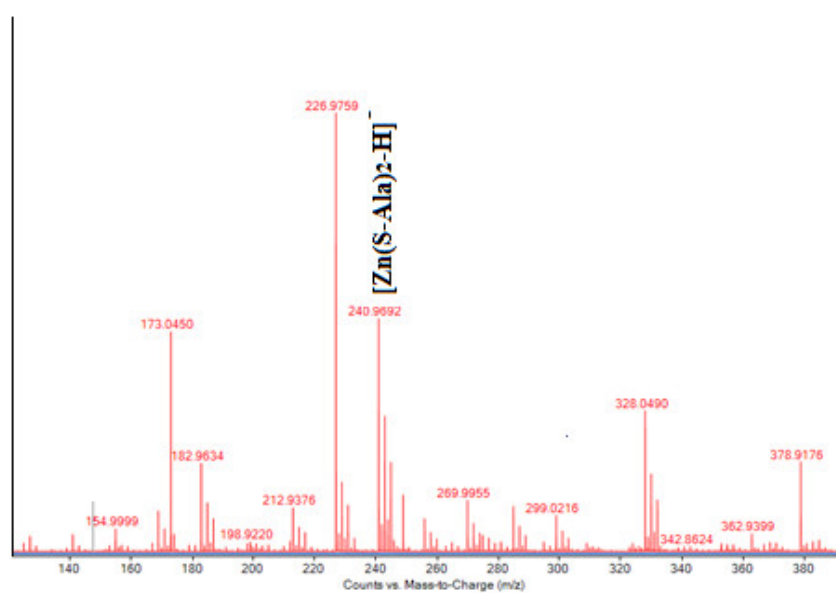


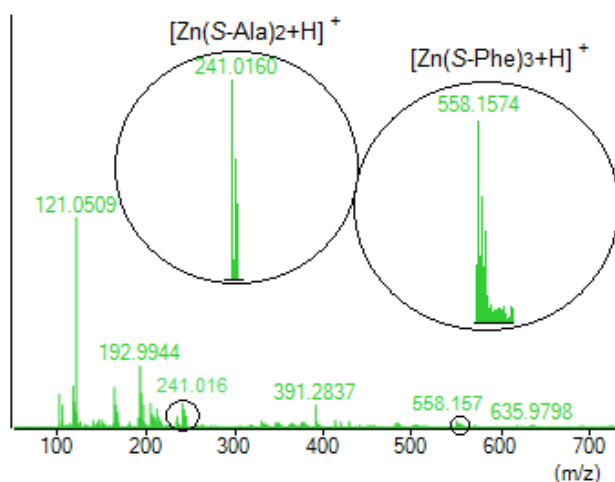
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## S-1 ESI-MS of the Composites of the Copper(II) and Zinc(II) Complexes



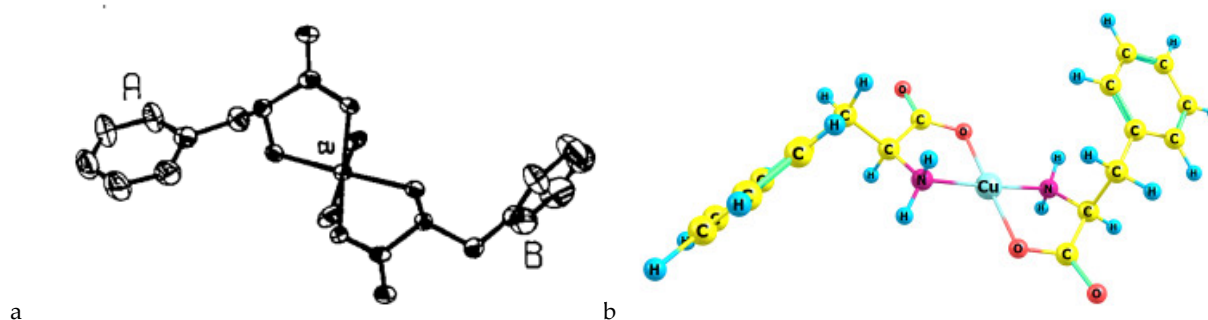
**Figure S1.** ESI-MS of the reaction mixture of composite  $[\text{Cu}(\text{S-Ala})_2] - [\text{Cu}(\text{S-Phe})_2]$  (1).





**Figure S2.** ESI-MS of the reaction mixture of composite  $[\text{Zn}(\text{S-Ala})_2(\text{H}_2\text{O})]$ - $[\text{Zn}(\text{S-Phe})_2(\text{H}_2\text{O})]$  (2).

## S-2 The structure of the Copper(II) and Zinc(II) Complexes



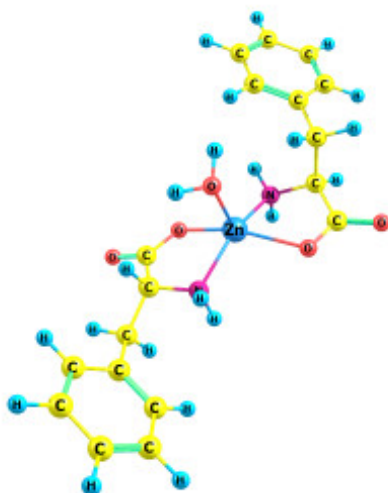
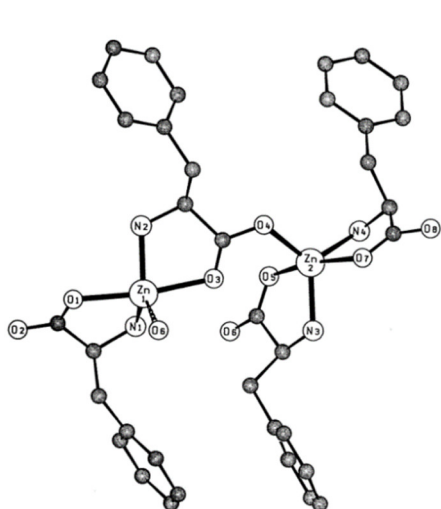
**Figure S3.** The structure of complex  $[\text{Cu}(\text{S-Phe})_2(\text{H}_2\text{O})]$  (1a) by X-Ray [34] (a), by DFT calculation (b).

### M06/6-311+G(d) (Solvent = Water)

#### Bis-*trans*- $[\text{Cu}(\text{S-Phe})_2]$ (1a) (*ta1-te1*)

0.316167000	6	3.322749000	-1.658098000	1.720306000	6	4.524912000	0.057100000
0.113881000	1	3.699612000	-2.592538000	2.483585000	1	3.756968000	-0.066776000
1.267044000	1	2.834274000	-1.914071000	1.920052000	6	5.559770000	0.963746000
0.631024000	6	2.274513000	-1.086043000	2.836192000	1	5.596935000	1.549301000
0.942779000	6	1.154939000	-2.079046000	0.952435000	6	6.543230000	1.120702000
1.099644000	8	1.423351000	-3.272190000	1.106386000	1	7.355109000	1.827975000
1.068289000	8	-0.023551000	-1.590624000	0.214580000	6	6.485375000	0.366636000
0.785932000	29	-0.190560000	0.344631000	0.975489000	1	7.254508000	0.481362000
0.505551000	8	-0.385141000	2.293889000	0.410096000	6	5.449817000	-0.536327000
0.443460000	6	-1.598955000	2.701276000	1.324459000	1	5.410774000	-1.128662000
0.243979000	8	-1.933223000	3.871690000	0.555894000	6	4.457108000	-0.704545000

1	-4.326332000	-3.263273000	7	1.696673000	0.177510000	-
1.383910000			0.137765000			
6	-5.959382000	-1.973368000	7	-2.123167000	0.482646000	-
0.841324000			1.306417000			
1	-6.694599000	-2.774769000	6	-2.673067000	1.624813000	-
0.831742000			0.559745000			
6	-6.343578000	-0.669669000	1	-3.552252000	2.040812000	-
0.544154000			1.067619000			
1	-7.381011000	-0.449407000	6	-3.056037000	1.194508000	
0.302131000			0.858785000			
6	-5.405831000	0.352820000	1	-2.146754000	0.874105000	
0.560193000			1.386587000			
1	-5.708586000	1.374299000	1	-3.441108000	2.079325000	
0.330662000			1.379766000			
1	-2.654547000	-0.370667000	6	-4.071978000	0.091103000	
1.129935000			0.874935000			
1	-2.174378000	0.661645000	6	-3.696425000	-1.219189000	
2.308393000			1.164735000			
1	1.654827000	0.163864000	1	-2.655569000	-1.433448000	
0.882868000			1.408904000			
1	2.286643000	0.969884000	6	-4.633767000	-2.246345000	
0.385470000			1.150505000			
1	2.745359000	-0.866909000	-1.600331000			



a b  
**Figure S4.** The structure of complex  $[\text{Zn}(\text{S-Phe})_2(\text{H}_2\text{O})]$  (**2a**) by X-Ray [35] (a), by DFT calculation (b).

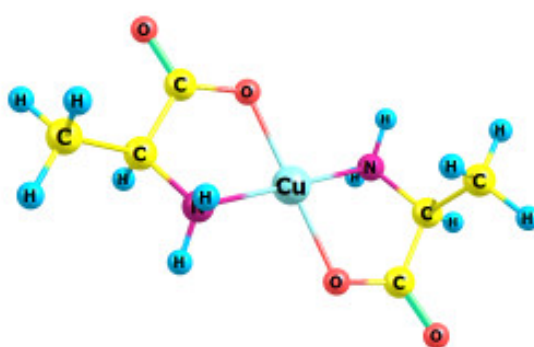
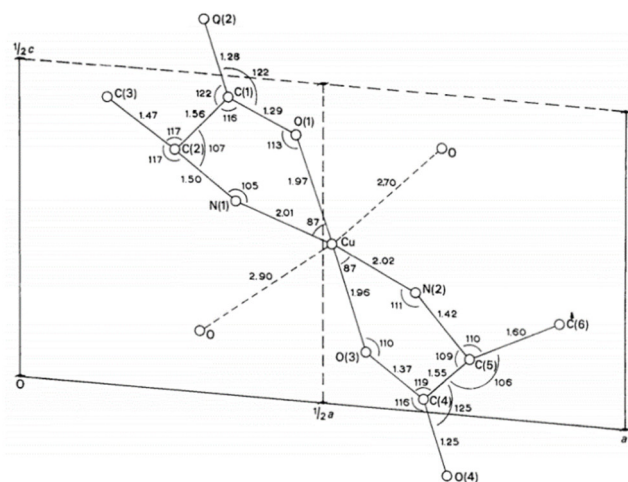
#### M06/6-311+G(d) (Solvent = Water)

##### Bis-*trans*- $[\text{Zn}(\text{S-Phe})_2(\text{H}_2\text{O})]$ (**2a**) (*ta1-te1*)

1	-7.53515	-2.12543	-0.26705	8	-0.38297	2.08299	0.17733
6	-6.7539	-0.15108	-0.62956	6	-1.50763	2.48114	-0.25159
1	-7.58757	0.14926	-1.26058	8	-1.8336	3.66901	-0.41436
6	-5.72012	0.73956	-0.37995	7	-1.93046	0.11083	-0.78056
1	-5.7441	1.73818	-0.81599	6	-2.56564	1.41455	-0.54644
1	-2.59768	-0.64992	-0.65364	1	-3.13586	1.73527	-1.4288
1	-1.61076	0.04809	-1.7457	6	-3.51355	1.33735	0.65391
6	3.91004	-1.57748	3.64343	1	-2.93634	1.0502	1.54398
1	3.30198	-2.41951	3.97349	1	-3.90399	2.34627	0.83259
6	4.5348	-0.76235	4.58076	6	-4.64499	0.37766	0.43274
1	4.41433	-0.96701	5.64248	6	-4.6303	-0.89949	0.99025
6	5.31033	0.31078	4.16284	1	-3.79873	-1.19294	1.63153
1	5.80033	0.94947	4.89433	6	-5.66294	-1.79669	0.73992
6	5.45953	0.56248	2.80292	1	-5.63521	-2.79035	1.18165
1	6.06832	1.39945	2.46748	6	-6.72623	-1.42529	-0.07138

8	0.17168	-2.08634	-0.07337
7	1.8584	-0.08471	0.47345
1	1.85213	-0.14279	1.49399
1	2.54211	0.63484	0.24681
1	1.7651	-1.6012	1.39742
30	-0.22875	-0.03962	0.42346
8	-0.77191	-0.27776	2.46001
1	-1.64762	-0.68218	2.51039
1	-0.16029	-0.90338	2.87002

6	4.83602	-0.25571	1.87121
1	4.95958	-0.05935	0.80601
6	4.05628	-1.33867	2.27908
6	3.37359	-2.20688	1.26343
1	4.08702	-2.50942	0.48931
1	3.0097	-3.1272	1.74212
6	2.25286	-1.51339	0.52887
6	1.25989	-2.68316	0.14395
8	1.60356	-3.85673	-0.07562



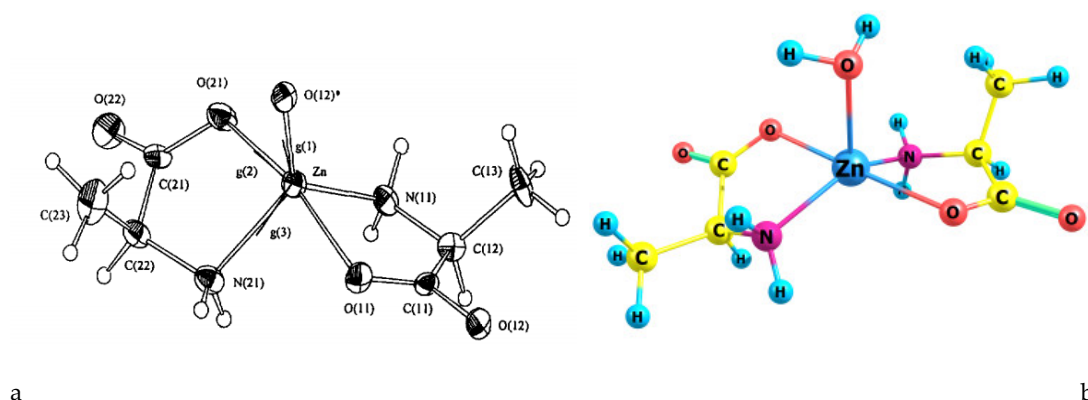
a b  
**Figure S5.** The structure of complex  $[\text{Cu}(\text{S-Ala})_2(\text{H}_2\text{O})]$  (**1b**) by X-Ray [33] (a), by DFT calculation (b).

#### M06/6-311+G(d) (Solvent = Water)

##### Bis-*trans*- $[\text{Cu}(\text{S-Ala})_2]$ (**1b**) (*ta-te*)

1	-1.12045	0.60907	1.46116
1	-2.49005	1.72386	1.35983
1	-1.0105	-0.3602	-1.18892
1	-0.44635	0.8409	-2.14882
1	2.86419	0.41045	1.6012
1	3.51032	1.42931	0.5001
1	4.23218	-0.21224	-0.89132
6	4.8808	-1.02872	0.98513
1	4.45644	-1.42594	1.91519
1	5.48923	-1.81242	0.52664
1	5.54134	-0.1934	1.23915
1	-2.60076	0.09931	0.58626

6	3.78873	-0.57153	0.04796
6	2.83653	-1.69109	-0.36691
8	3.26889	-2.83556	-0.52116
8	1.61719	-1.35324	-0.57815
29	1.21849	0.55597	-0.28044
8	0.75313	2.45545	0.07881
6	-0.49326	2.71878	-0.05608
8	-1.00543	3.81896	0.16591
7	3.00309	0.55185	0.5994
7	-0.56631	0.55843	-1.17699
6	-1.38307	1.548	-0.45771
1	-2.20513	1.91497	-1.08524
6	-1.95483	0.93206	0.82229



**Figure S6.** The structure of complex  $[\text{Zn}(\text{S-Ala})_2(\text{H}_2\text{O})]$  (**2b**) by X-Ray [36] (a), by DFT calculation (b).

#### M06/6-311+G(d) (Solvent = Water)

Bis-*trans*- $[\text{Zn}(\text{S-Ala})_2(\text{H}_2\text{O})]$  (**2b**) (*ta-te*)

6	3.89373	-0.35992	-0.53565	8	0.62968	2.38817	0.04443
6	3.11238	-1.67919	-0.54398	6	-0.55358	2.60018	-0.35706
8	3.69917	-2.70713	-0.92007	8	-1.08796	3.71739	-0.45998
8	1.88924	-1.63045	-0.20595	7	-0.56053	0.21876	-0.98751
7	3.21527	0.62342	0.32698	6	-1.41259	1.37753	-0.69137
1	3.49274	0.46676	1.29744	1	-2.04375	1.62969	-1.55421
1	3.52	1.56576	0.09193	6	-2.30985	1.0862	0.51408
1	3.81361	0.02076	-1.56443	1	-1.67408	0.88449	1.38664
30	1.15059	0.3196	0.22343	1	-2.8778	1.99823	0.73316
8	0.71417	0.06254	2.29651	1	-1.08261	-0.65306	-0.90339
1	-0.09154	-0.45207	2.43325	1	-0.23898	0.26433	-1.95313
1	1.43119	-0.44722	2.69653	6	5.35357	-0.52866	-0.17699
1	5.8632	0.44055	-0.19708	1	5.86507	-1.19109	-0.87974
1	-2.95749	0.24707	0.30715	1	5.46348	-0.94972	0.83011

## S-2 NMR spectra of the Composites of the Zinc(II) Complexes

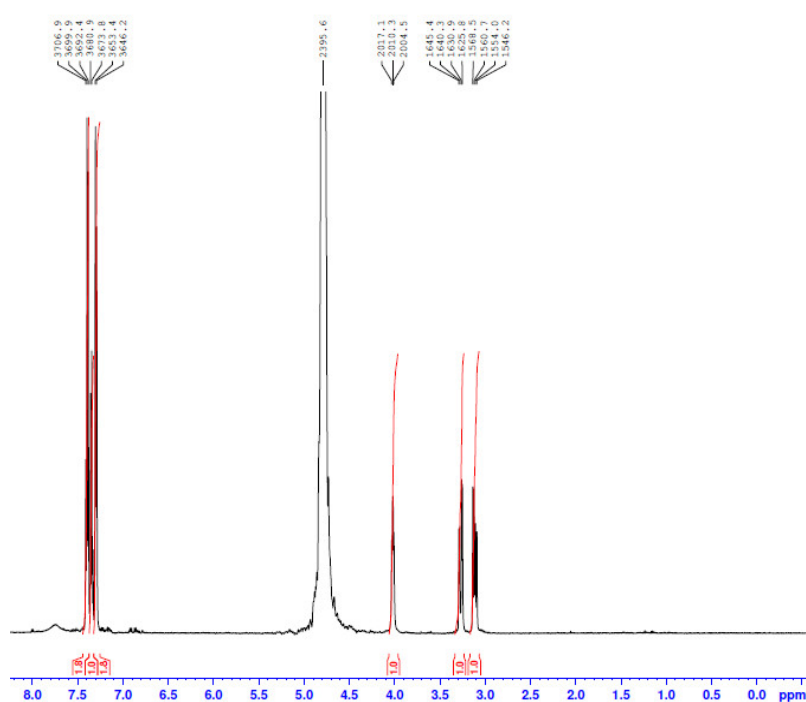


Figure S7. Complete  $^1\text{H}$  NMR spectrum of the *L*-Phenylalanine in  $\text{D}_2\text{O}$ , 500 MHz.

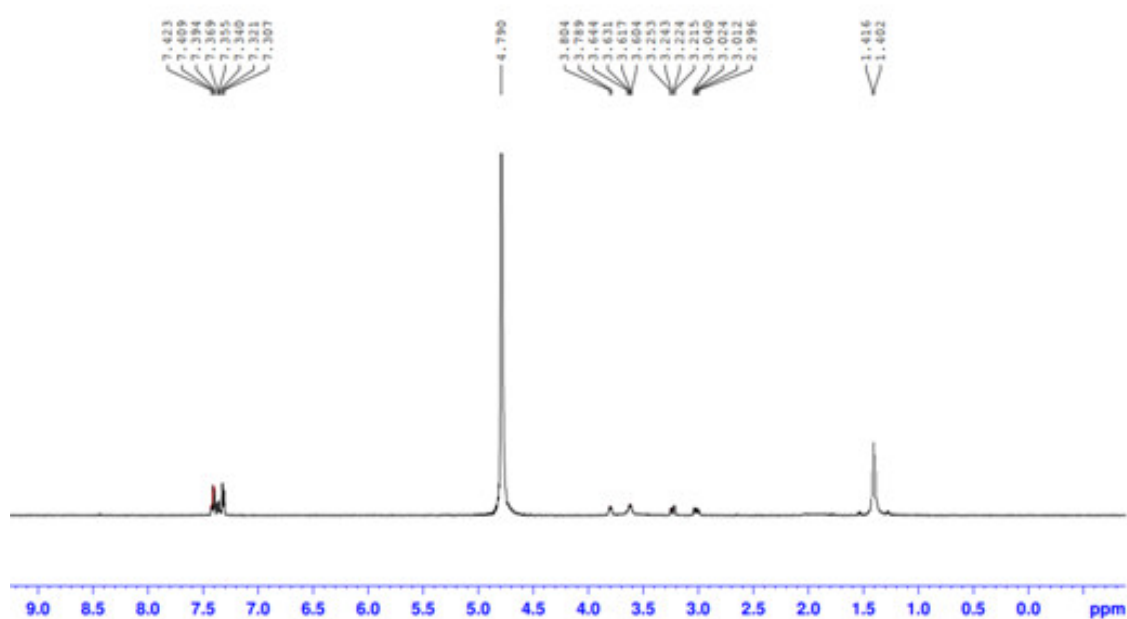


Figure S8. Complete  $^1\text{H}$  NMR spectrum of the composite  $[\text{Zn}(\text{S-Ala})_2(\text{H}_2\text{O})]\text{-}[\text{Zn}(\text{S-Phe})_2(\text{H}_2\text{O})]$  (2) in  $\text{D}_2\text{O}$ , 500 MHz.

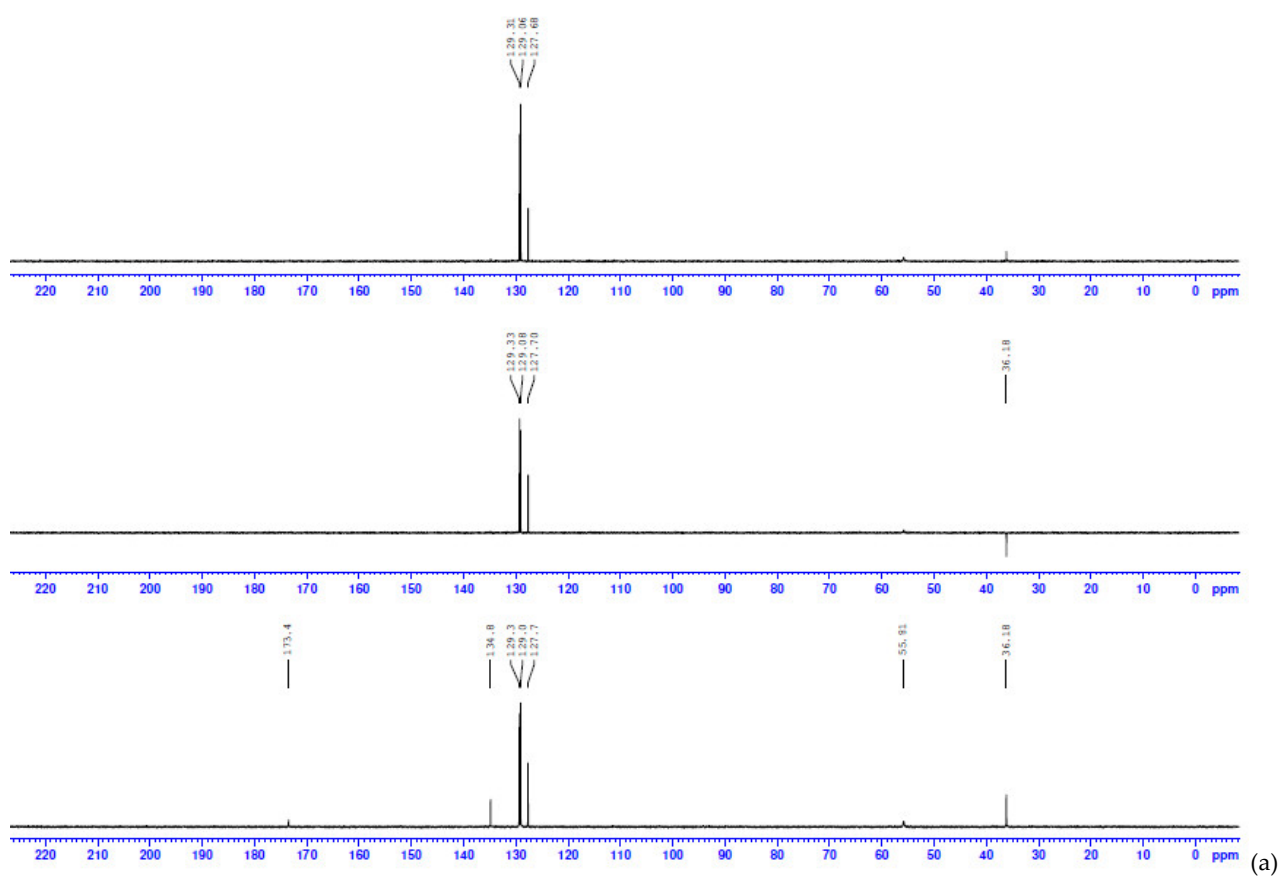


Figure S9.  $^{13}\text{C}$  NMR spectrum of the *L*-Phenylalanine in  $\text{D}_2\text{O}$ , 500 MHz.

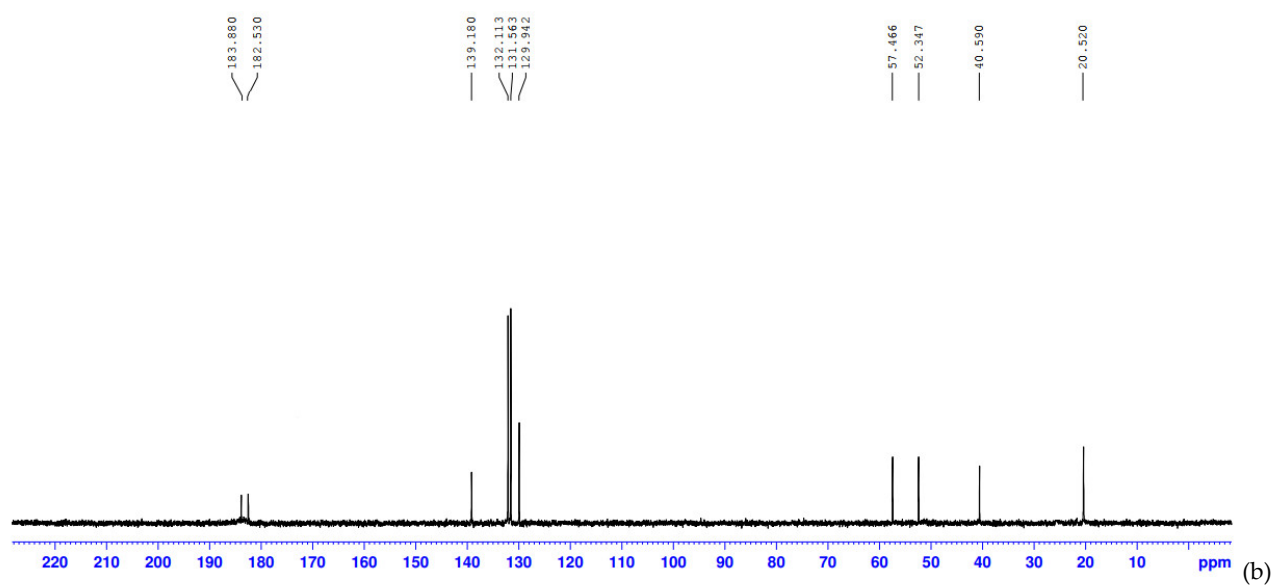


Figure S10.  $^{13}\text{C}$  NMR spectrum of the composite  $[\text{Zn}(\text{S-Ala})_2(\text{H}_2\text{O})]\text{-}[\text{Zn}(\text{S-Phe})_2(\text{H}_2\text{O})]$  (2) in  $\text{D}_2\text{O}$ , 500 MHz.