Electronic Supplementary Material (ESI) for Materials Chemistry Frontiers.

Novel Chiral Aggregation Induced Emission Molecules: Self-Assembly, Circularly Polarized Luminescence and Copper (II) Ion Detection

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General information

Materials

$Pd(PPh_3)_2Cl_2$, PPh_3, CuI, benzophenone hydrazone and other chemicals and solvents were all purchased from Energy Chemical Company and used as received without further purification. Compounds5-ethynylsalicylaldehyde, 9-fluorenone hydrazine and (R)-methyl 2-(4-bromobenzamido)propanoate were prepared according to previous papers.[1]

Instruments and methods

^1H and ^{13}C NMR spectra were recorded on a VNMRS 400 (Varian, USA) NMR spectrometer. High resolution mass spectra (HR-MS) were recorded using a Thermo Finnigan MAT TSQ 7000 spectrometer (USA). UV spectra were recorded using a UV-2600 spectrometer (Shimadzu, Japan). CD spectra were recorded using a Chirascan spectrometer (Applied Photophysics, England). Fluorescence spectra were recorded using a F-7000 fluorescence spectrometer (Hitachi, Japan). The fluorescence quantum yield (Φ_f) in solution was measured by a relative method using fluorescein in 0.1 M NaOH (Φ_f = 95%) as a standard. CPL spectra were recorded using a CPL-200 instrument (JASCO, Japan) at room temperature. The surface morphologies and structures were characterized by scanning electron microscope (SEM, Hitachi FE-SEM S-4800 operated at 1 kV) and transmission electron microscope (TEM, JEOL JEM-2100F operated at 200 KV). Fluorescence images were captured using the fluorescence microscope DHG-9070A (Olympus, Japan). The theoretical ground-state geometry and electronic structure of molecules **1** and **2** were optimized using the density functional theory (DFT) with B3LYP hybrid functional at the basis set level of 6-31+G(d). All the theoretical calculations were performed using Gaussian 03 package.[2]

References

1. (a) F. Eißmann, and E. Weber, *J. Mol. Struct.*, 2011, **994**, 392-402; (b) Z. Wang, C. Gui, E. Zhao, J. Wang, X. Li, A. Qin, Z. Zhao, Z. Yu and B. Z. Tang, *ACS App. Mater. Interfaces*, 2016, **8**, 10193-10200; (c) J. Li, Y. Wu, F. Song, G. Wei, Y. Cheng and C. Zhu, *J. Mater. Chem.*, 2012, **22**, 478-482.
2. Gaussian 03, Revision E.01, M. J. Frisch et al., Gaussian, Inc., Wallingford CT, 2009.

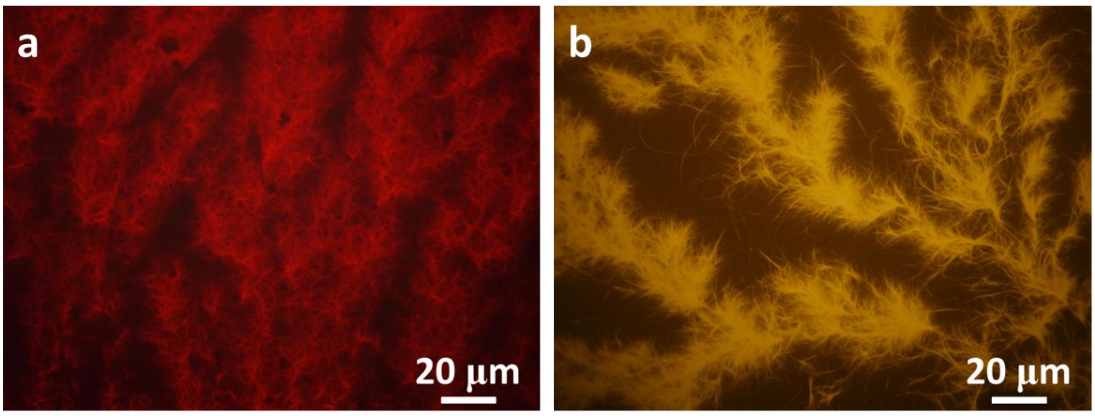

Figure S1. Fluorescence images of fluorescent fibers of (a) **1** and (b) **2** upon the evaporation of their THF solution. Solution concentration: 100 µM.

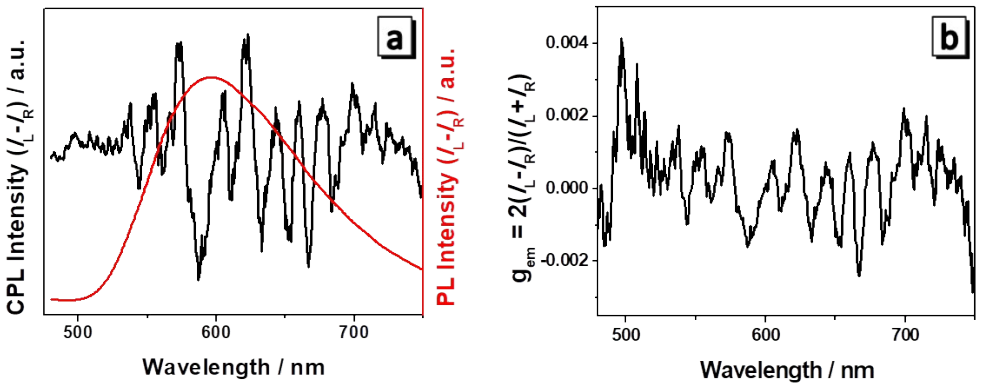

Figure S2. Plots of (a) CPL and PL and (b) CPL dissymmetry factor g_{em} of cast film of **2** formed by evaporation of its THF solution.

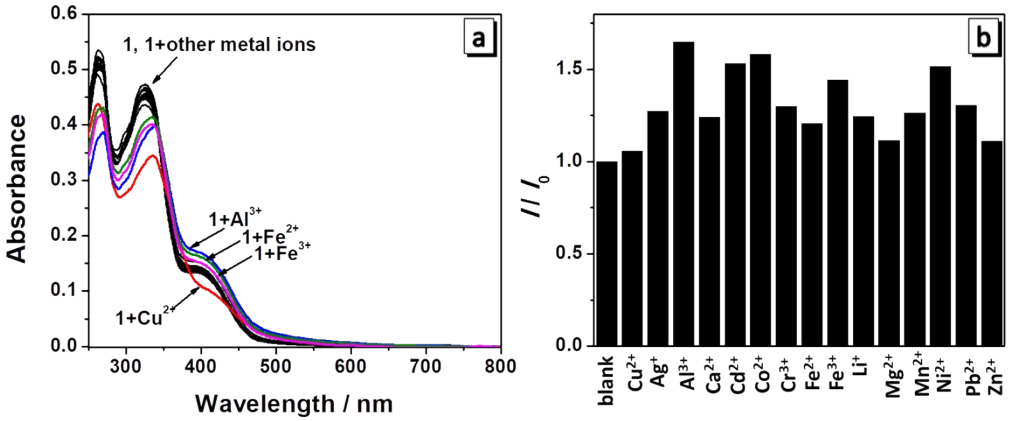

Figure S3. (a) Absorption spectra of **1** (10 μM) upon the addition of 1 equiv. of various metal cations in THF/H_2O (1/9, v/v); (b) Variation of the fluorescence intensity at 635 nm (λ_{ex} = 395 nm) of **1** (10 μM) in THF/H_2O (1/9, v/v) in absence and presence of 1 equiv. of various metal cations.

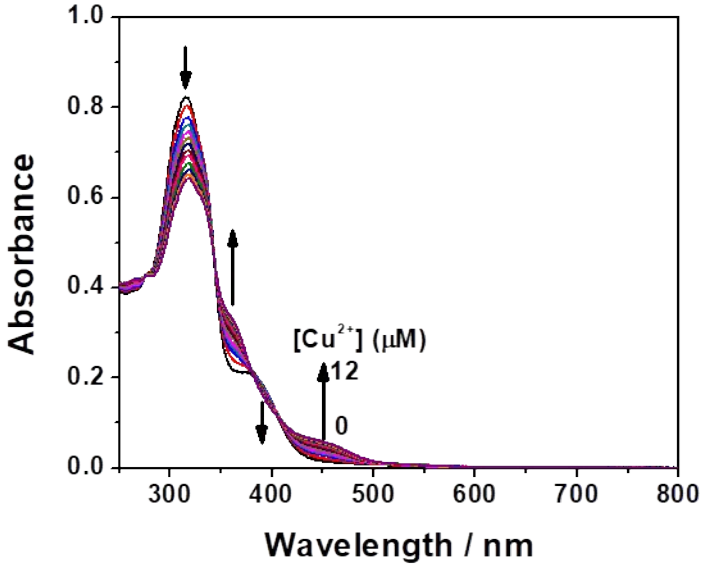

Figure S4. Absorption spectra of **2** (10 μM) upon the addition of 0-12 μM Cu^{2+} in THF/H_2O (1/9, v/v).

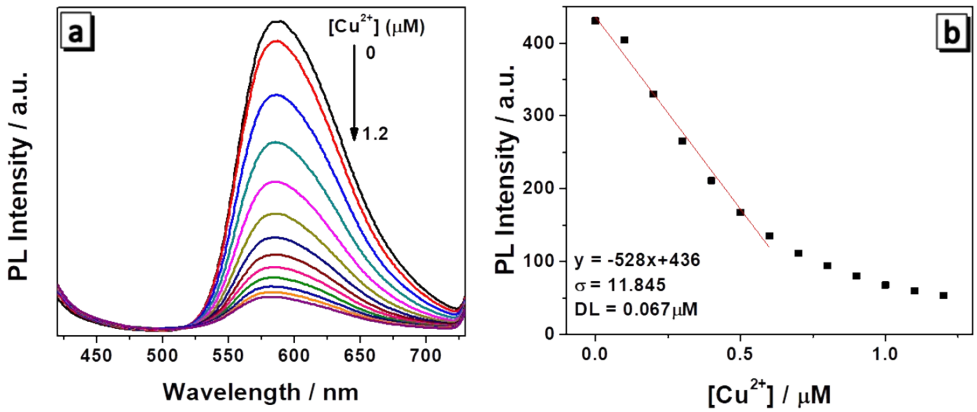

Figure S5. (a) Fluorescence spectra (λ_{ex} = 380 nm) of **2** (10 μM) upon the addition of 0-1.2 μM Cu^{2+} in THF/H_2O (1/9, v/v). (b) The plot of fluorescence intensity at 586 nm versus Cu^{2+} concentrations.

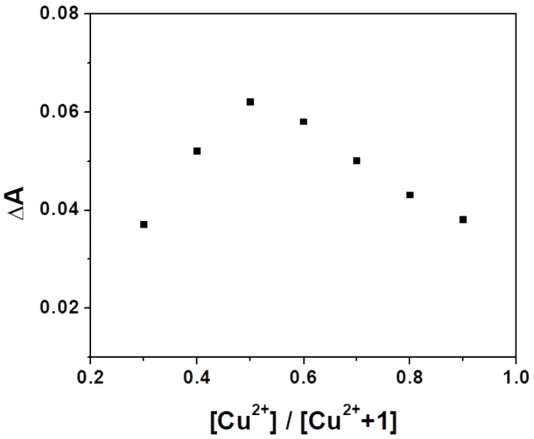

Figure S6. Job's plot of **2** with Cu^{2+} in THF/H_2O (1/9, v/v).

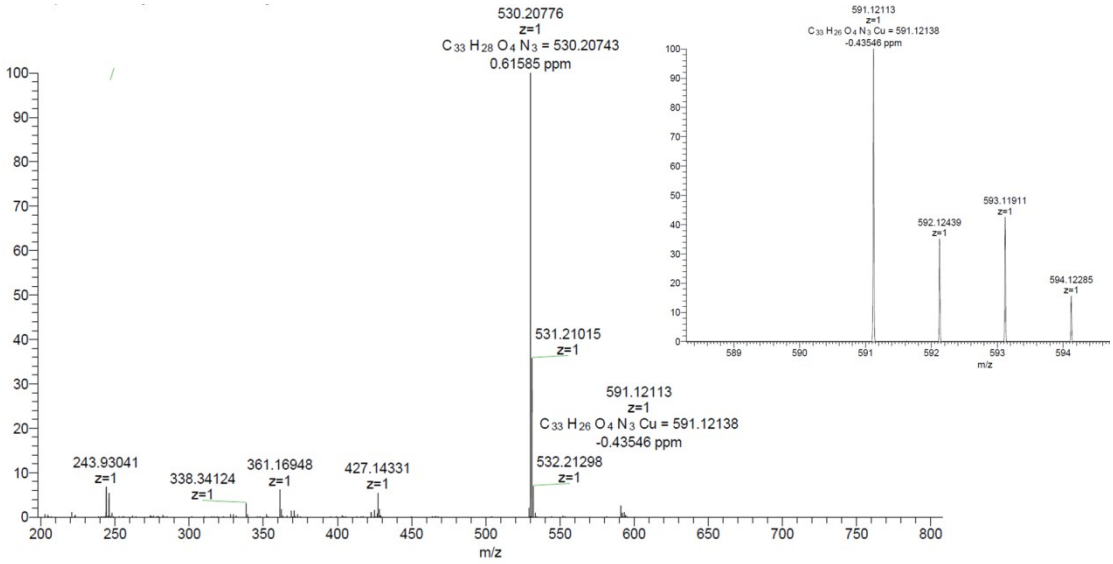

Figure S7. Mass spectrum of **2** in the presence of 1 equiv. of Cu^{2+} in THF/H_2O (1/9, v/v).

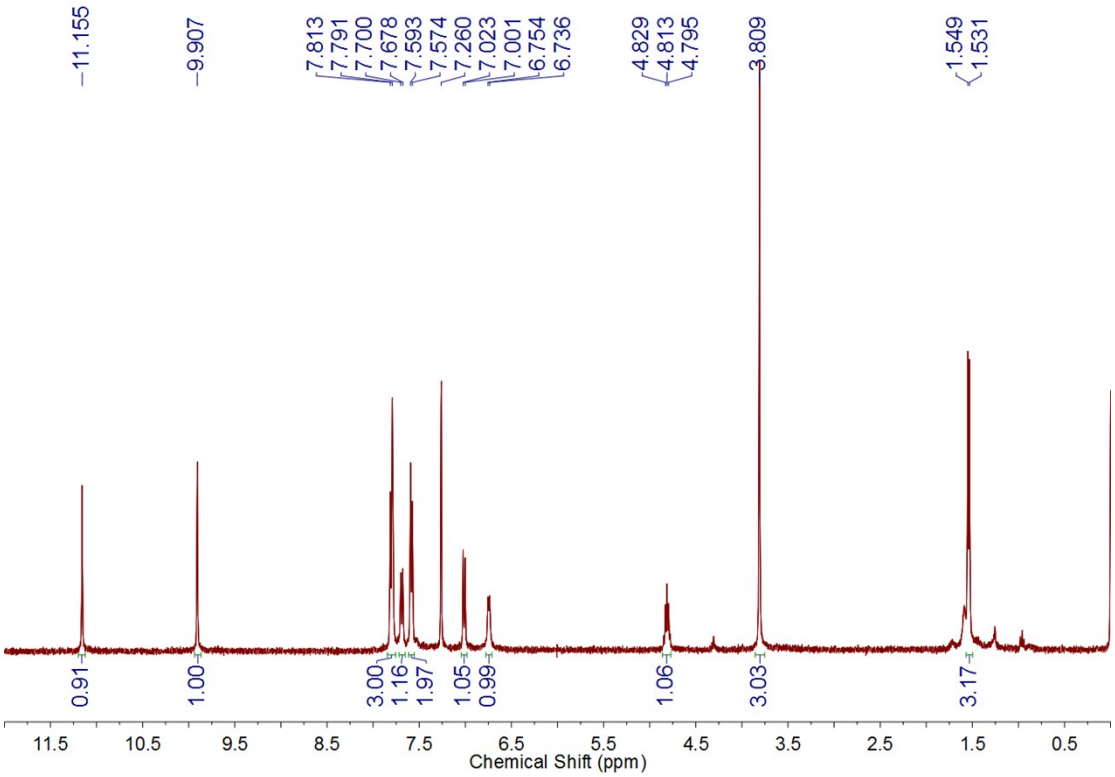

Figure S8. ^{1}H NMR of compound **3**.

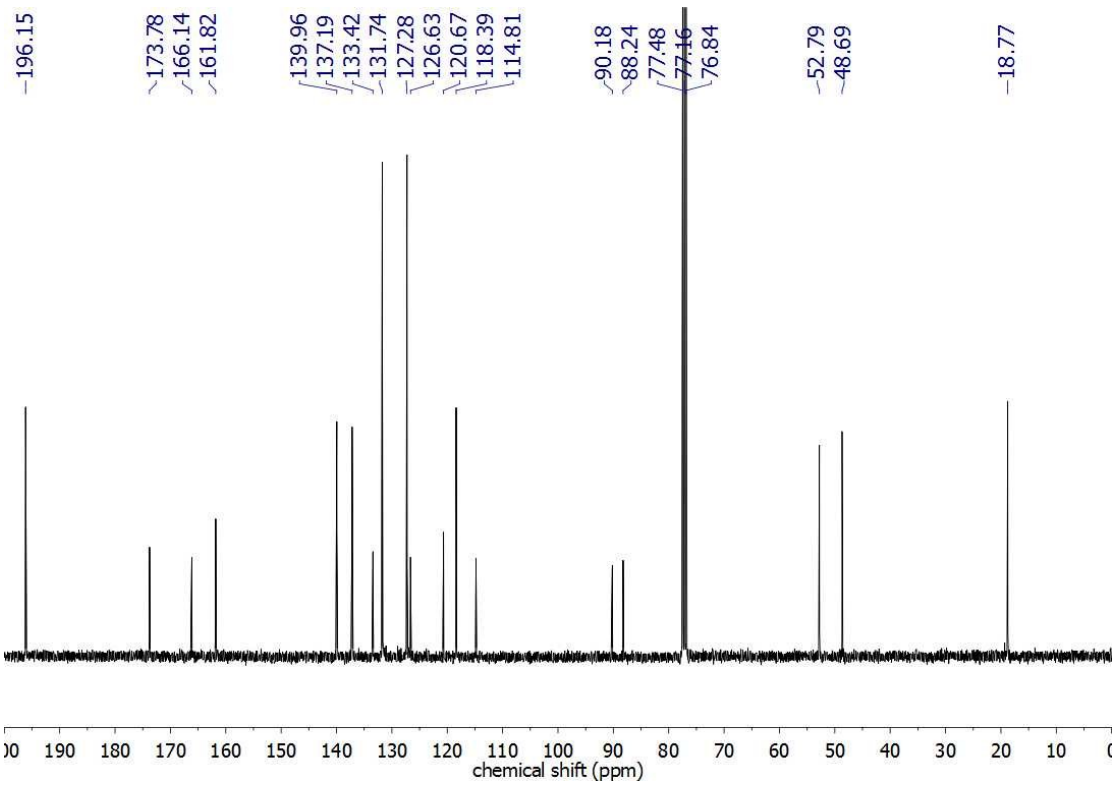

Figure S9. ^{13}C NMR of compound **3**.

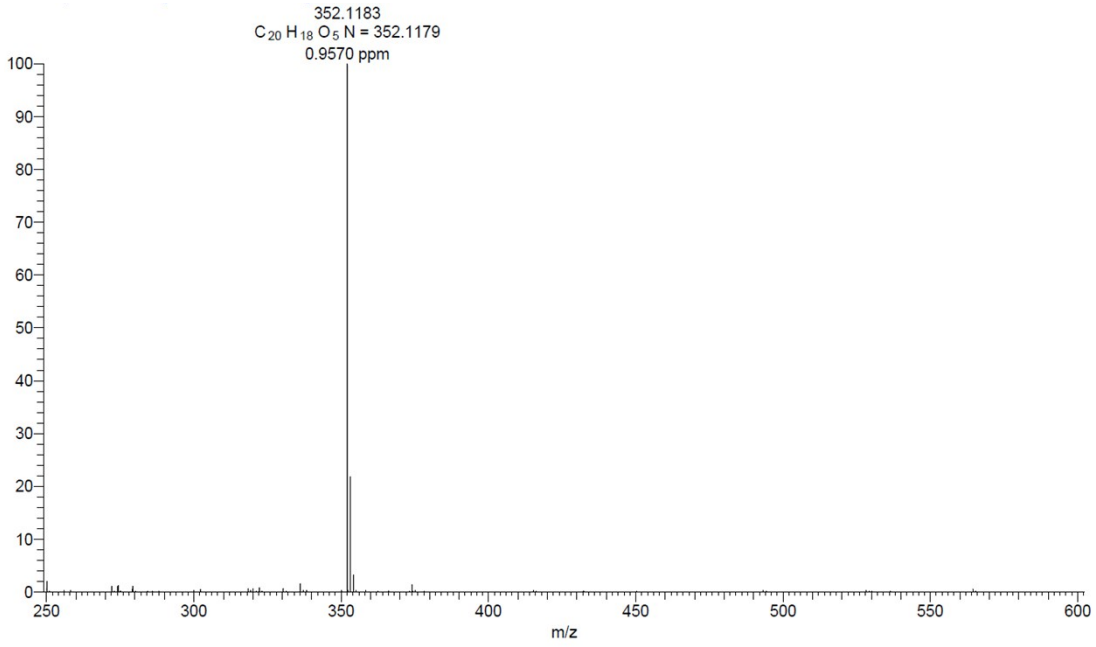

Figure S10. HRMS of compound **3**.

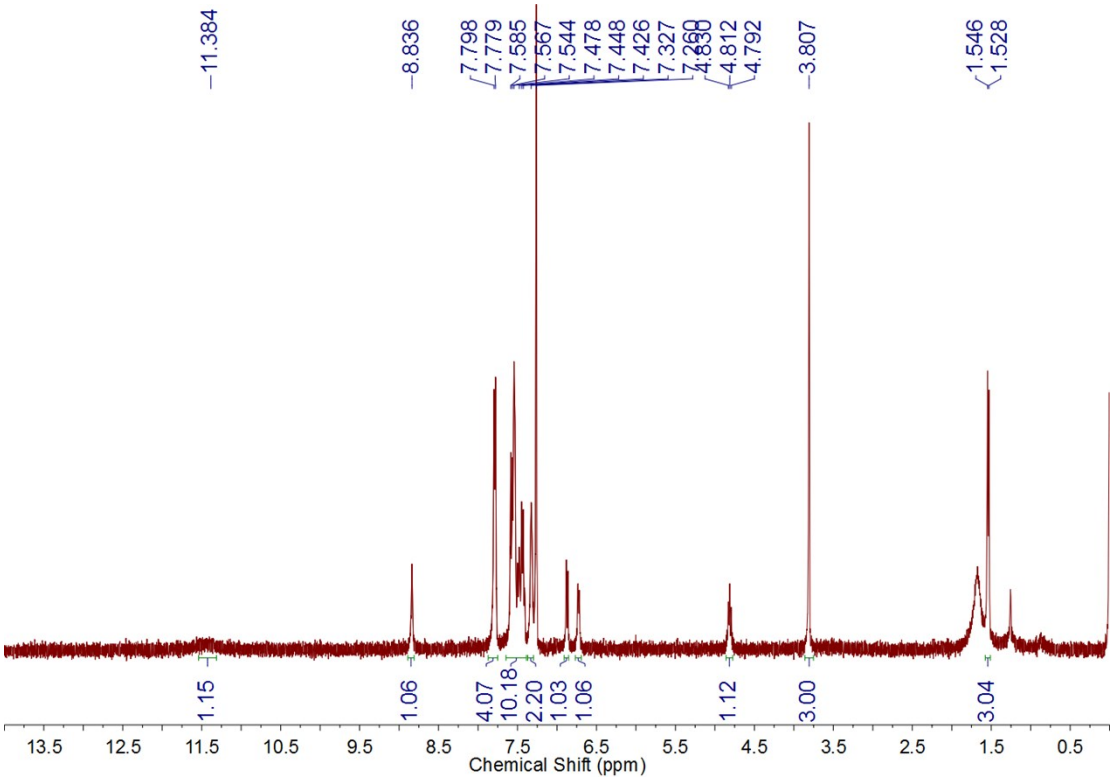

Figure S11. ^{1}H NMR of compound **2**.

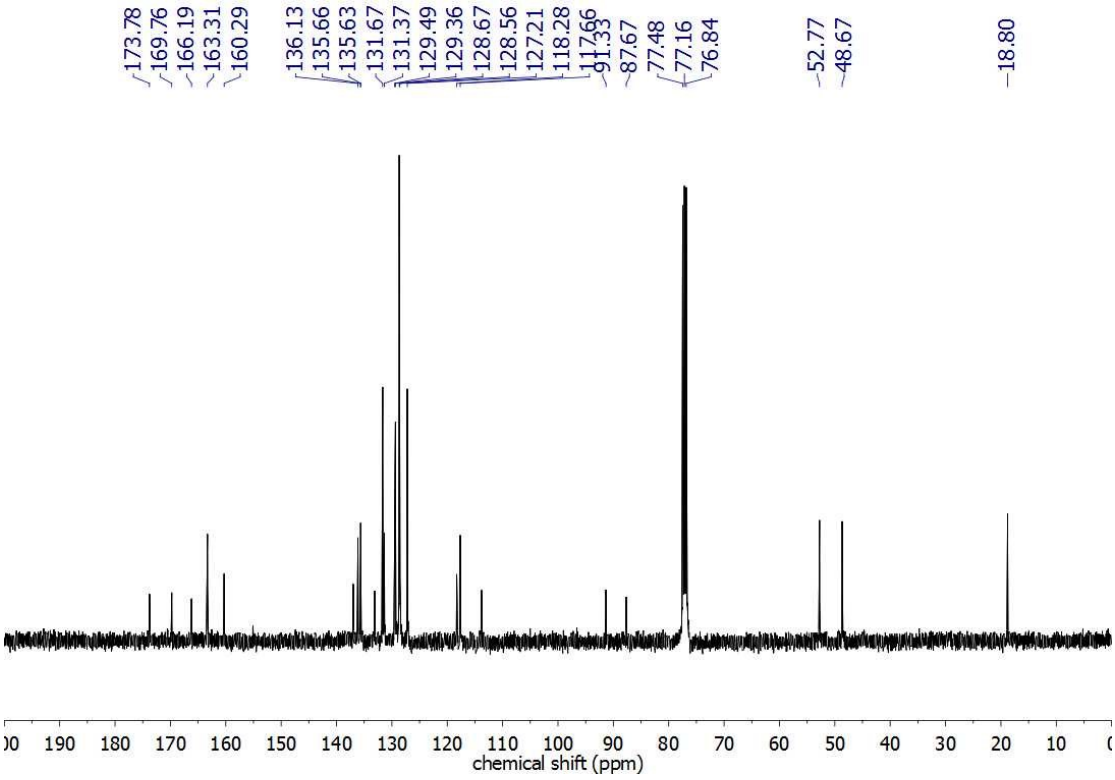

Figure S12. ^{13}C NMR of compound **2**.

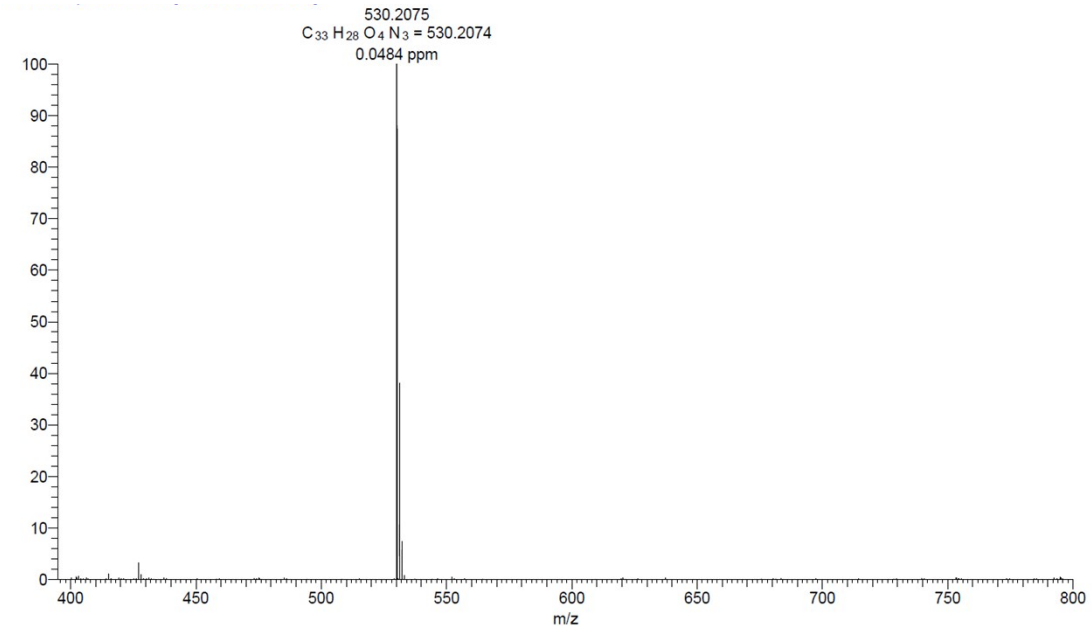

Figure S13. HRMS of compound **2**.

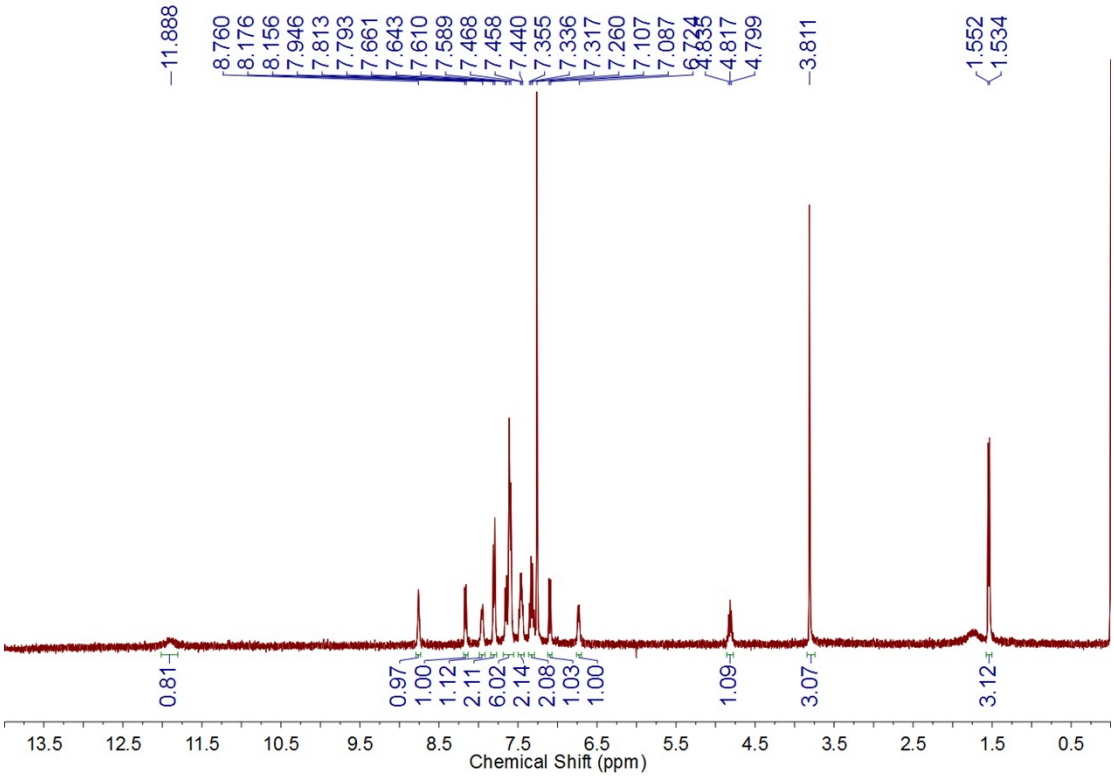

Figure S14. ^{1}H NMR of compound **1**.

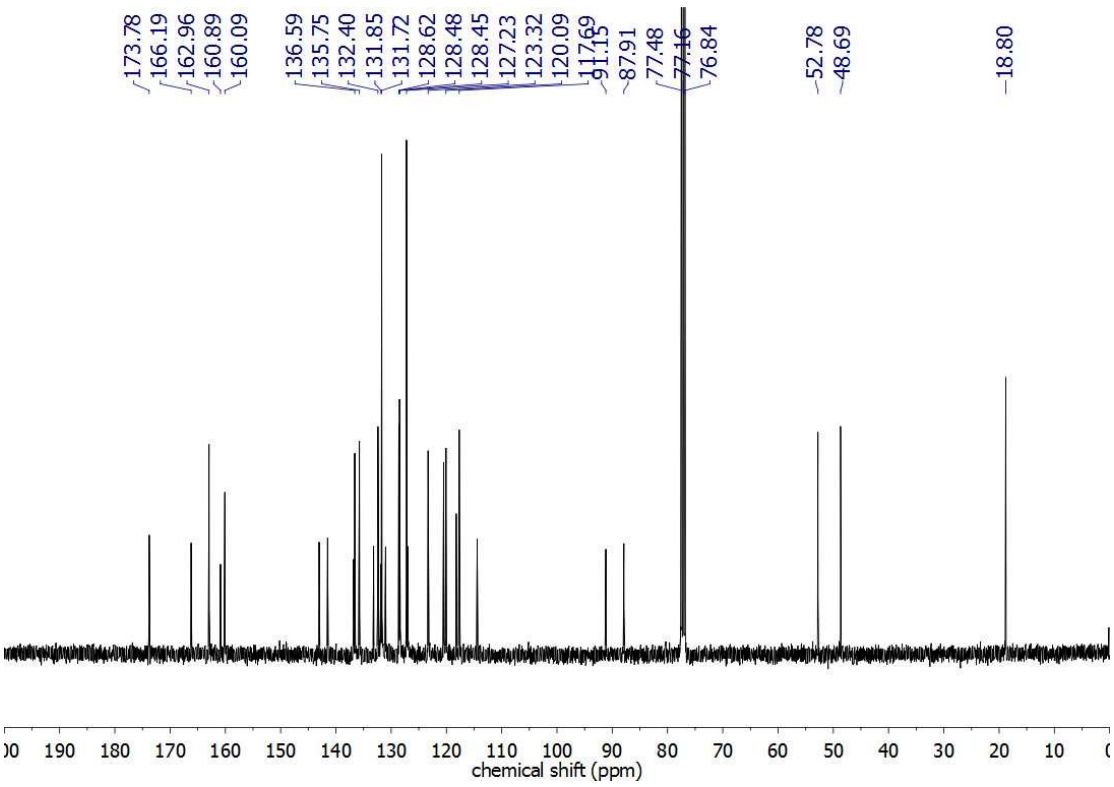

Figure S15. ^{13}C NMR of compound **1**.

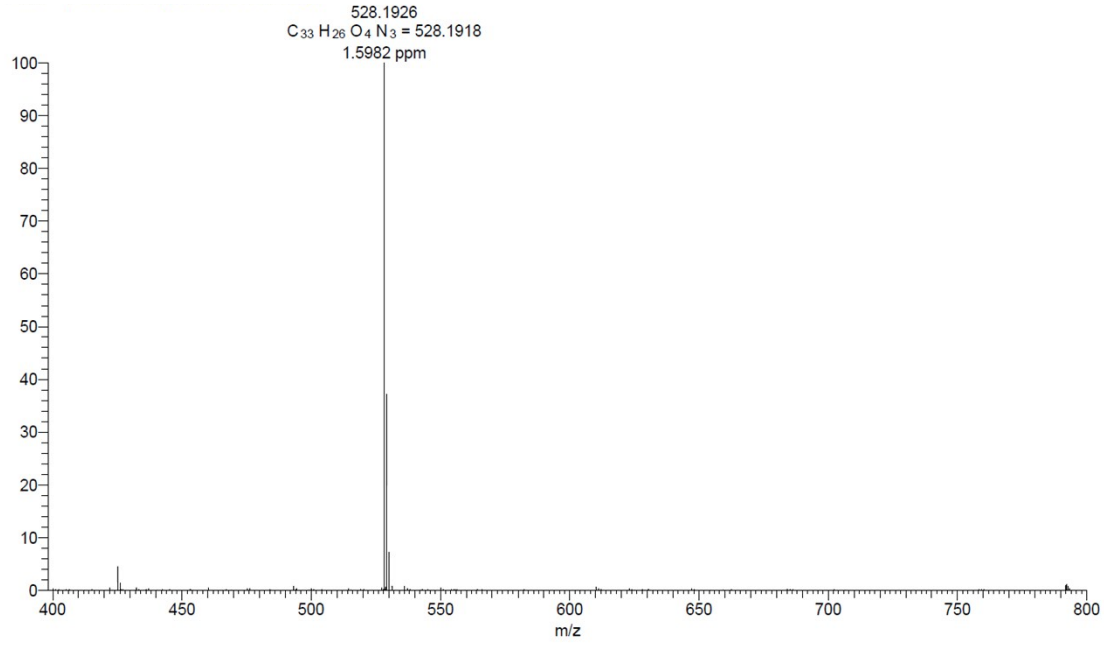

Figure S16. HRMS of compound **1**.