Electronic Supplementary Material (ESI) for Dalton Transactions.

A novel polynobern-base chemosensor fluorescence sensing of Zn^{2+} and Cd^{2+} and subsequent pyrophosphate in absolute aqueous solution

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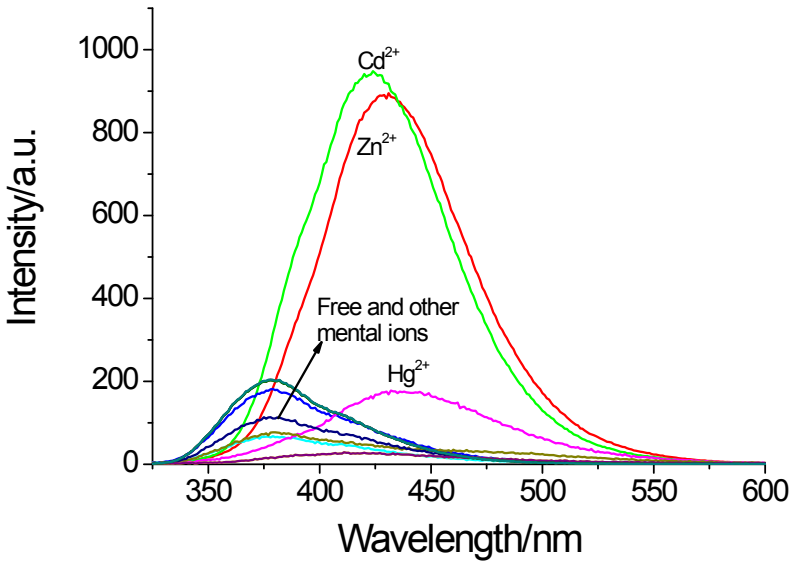

Figure S1. Emission spectra of **1** upon the addition of various metal ions (2 equiv) in CH_3CN solution

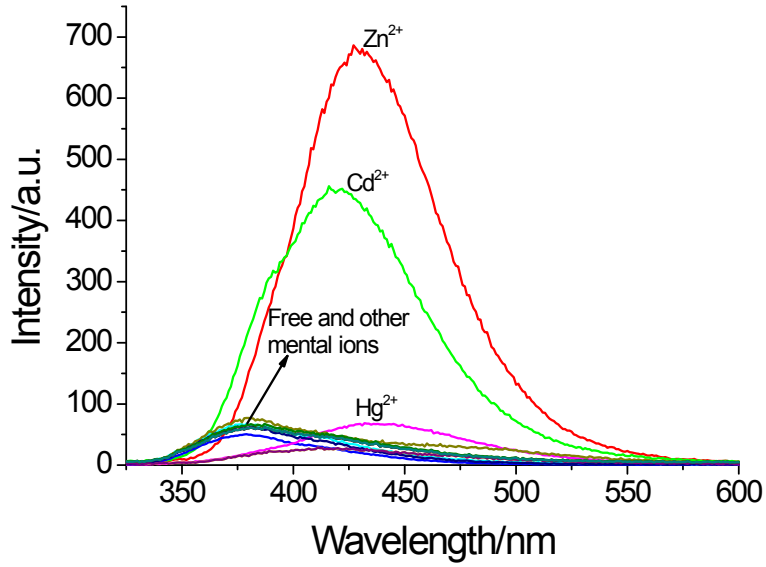

Figure S2 Emission spectra of **P1** upon the addition of various metal ions (2 equiv) in CH_3CN solution.

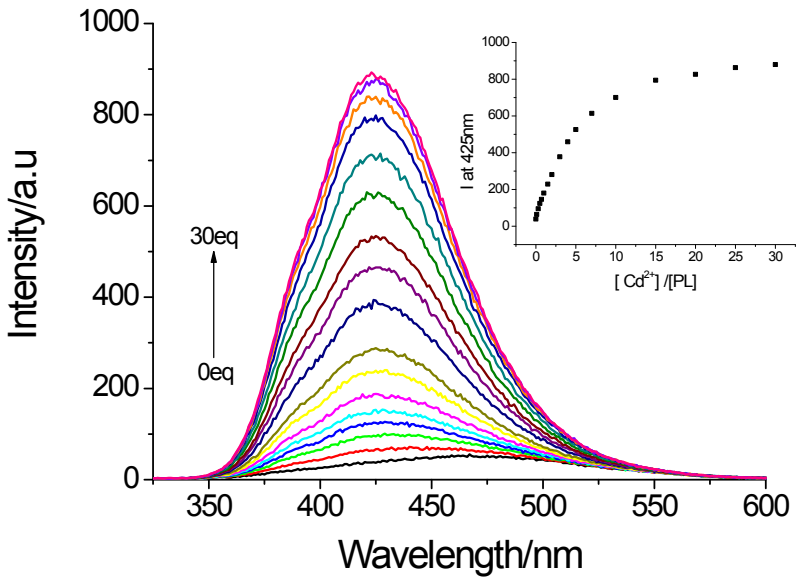

Figure S3. Emission titration of **P1** (20 mM) upon the addition of various Cd^{2+} ions in Tris-HCl solution (pH = 7.4). Inset: emission intensity at 425 nm upon titration with Cd^{2+}.

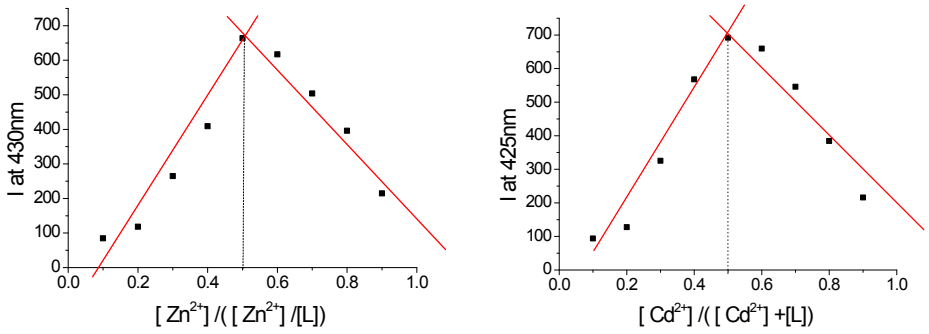

Figure S4. Job plots of **P1** with Zn^{2+} (left) and Cd^{2+} (right).

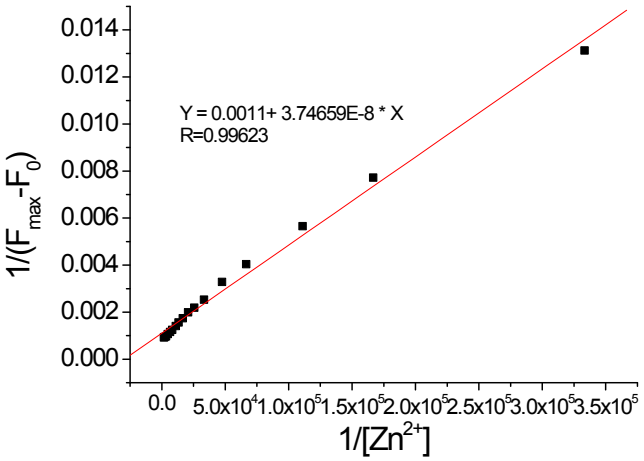

Figure S5. The calculated binding constants of **P1**-Zn^{2+}.

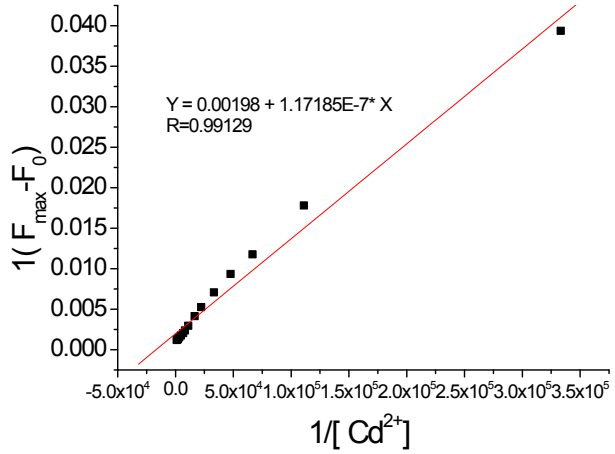

Figure S6. The calculated binding constants of **P1**-Cd^{2+}.

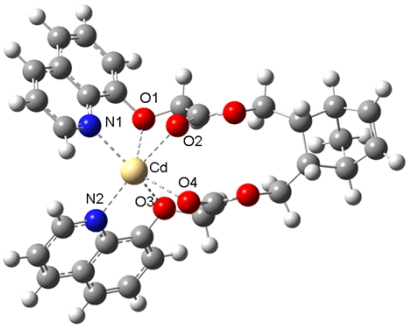

Figure S7. Optimized conformation of **1**-Cd^{2+} by DFT calculation. Selected distances (Å): Cd–N1, 2.320; Zn–N2, 2.328; Zn–O1, 2.478; Zn–O2, 2.366; Zn–O3, 2.512; Zn–O4, 2.324.

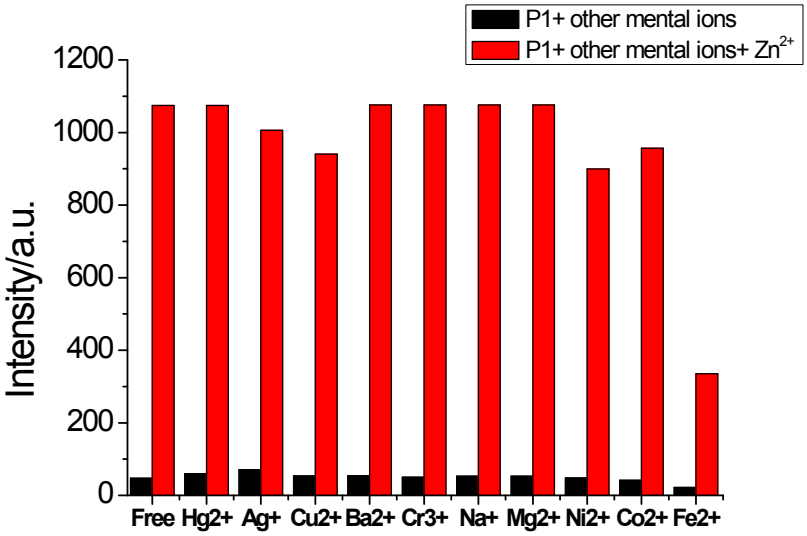

Figure S8. Competition experiments

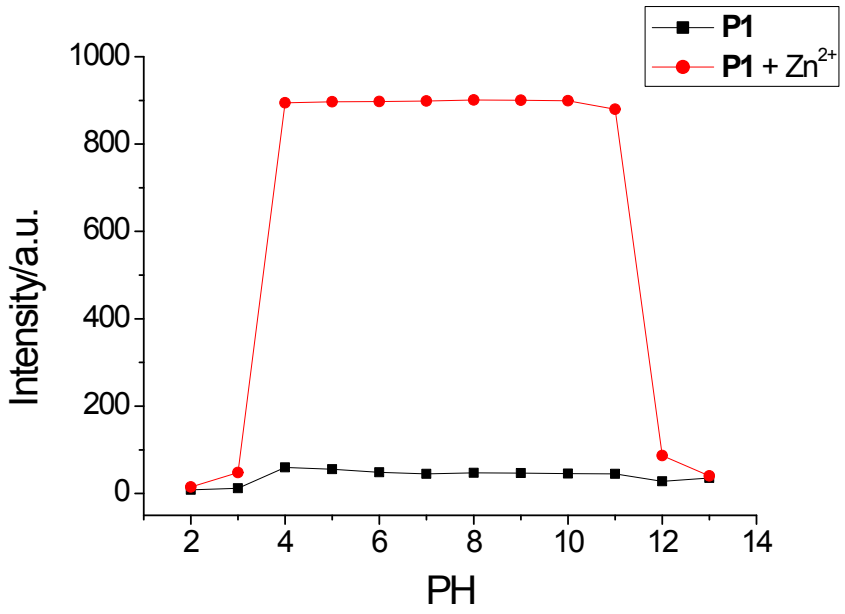

Figure S9. Fluorescence intensities of **P1** (20 μm) at 425 nm before and after the additional of Zn^{2+} (5 equiv) at various pH values in H_2O solution.

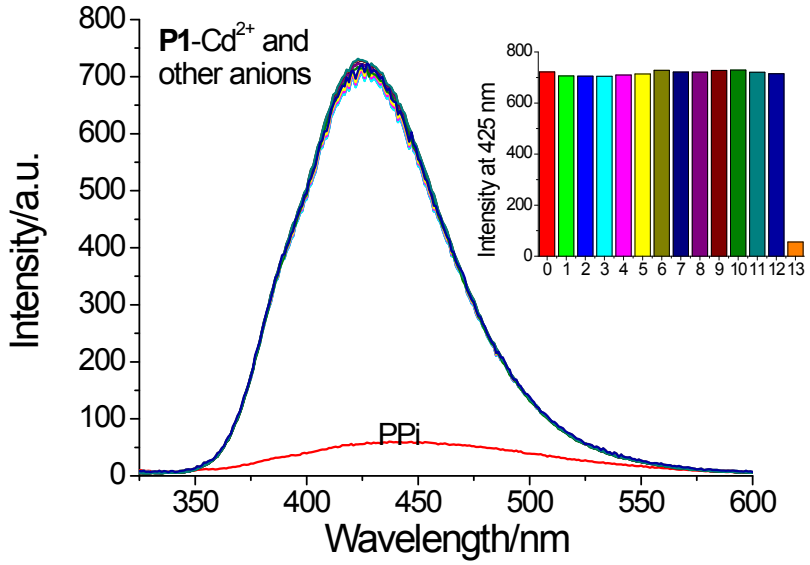

Figure S10. The emission spectra of **P1**-Cd^{2+} upon the addition of various anions (20 equiv) in aqueous solution. Inset shows the emission intensity at 425 nm upon the addition of various anions (0–**P1**-Cd^{2+}, 1–F^-, 2–Cl^-, 3–Br^-, 4–I^-, 5–NO_3^-, 6–CH_3COO^-, 7–CO_3^{2-}, 8–HSO_4^-, 9–Pi, 10–ATP, 11–AMP, 12–ADP, 13–PPi).

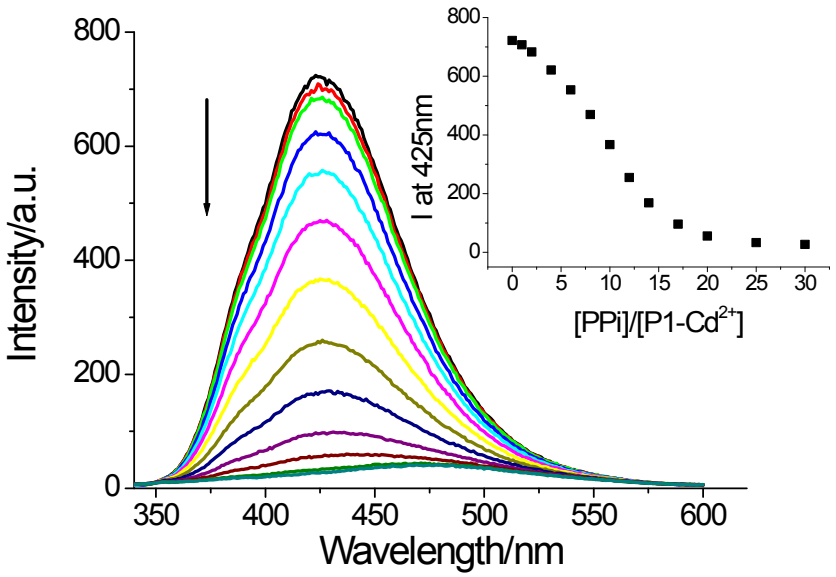

Figure S11. The emission titration of **P1**-Cd^{2+} upon the addition of PPi in 100% aqueous solution

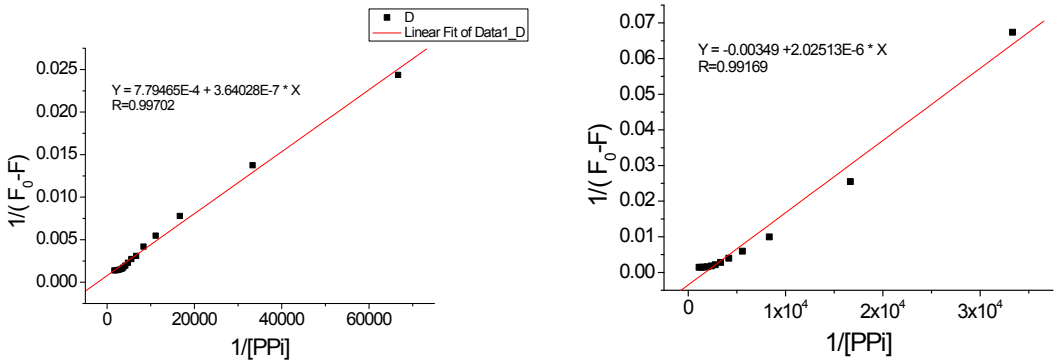

Figure S12. Benesi-Hildebrand plot of for evaluation of binding constants of PPi with **P1**-Zn^{2+} (left) and **P1**-Cd^{2+} (right) with the 1:1 binding stochiometry in aqueous (PH-7.4) solution.

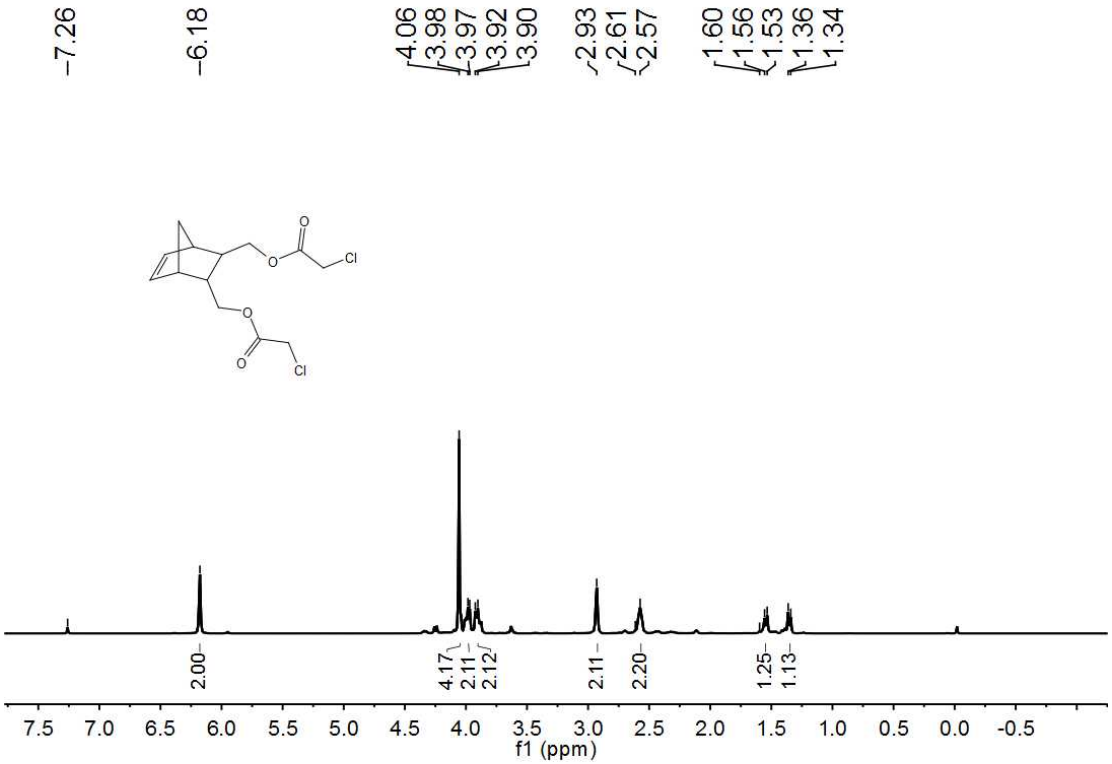

Figure S13. ^{1}H-NMR of **4** in $CDCl_3$ solution

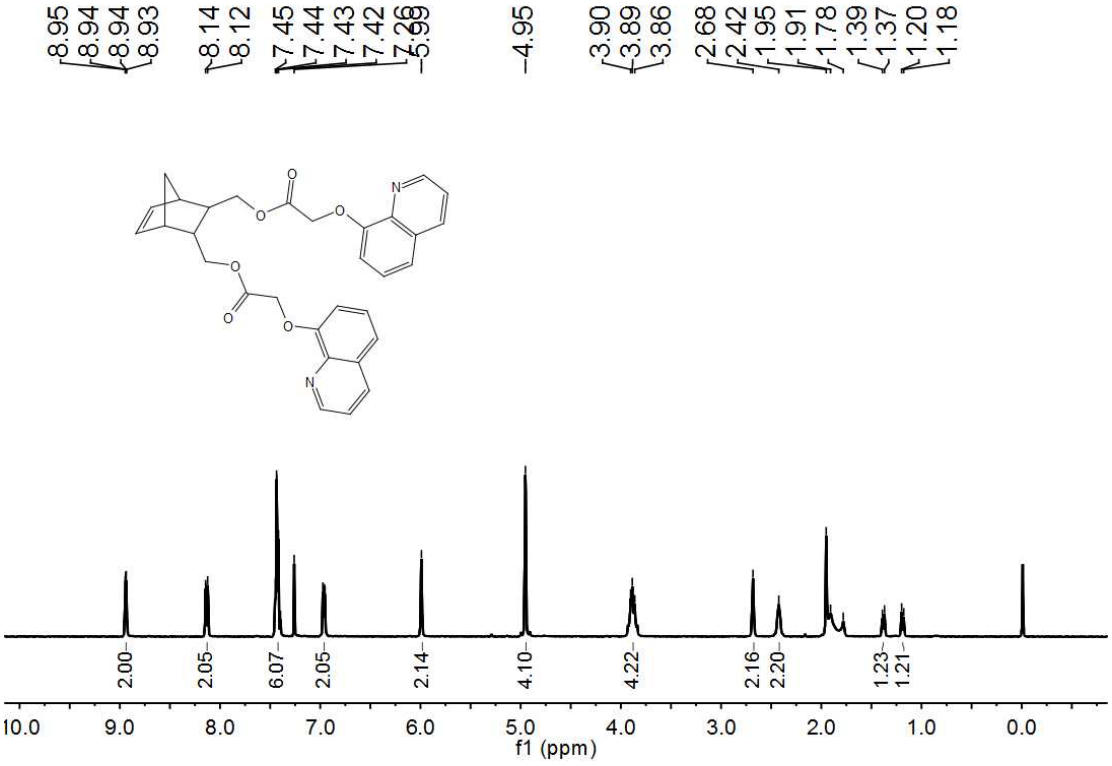

Figure S14. ^{1}H-NMR of **1** in $CDCl_3$ solution

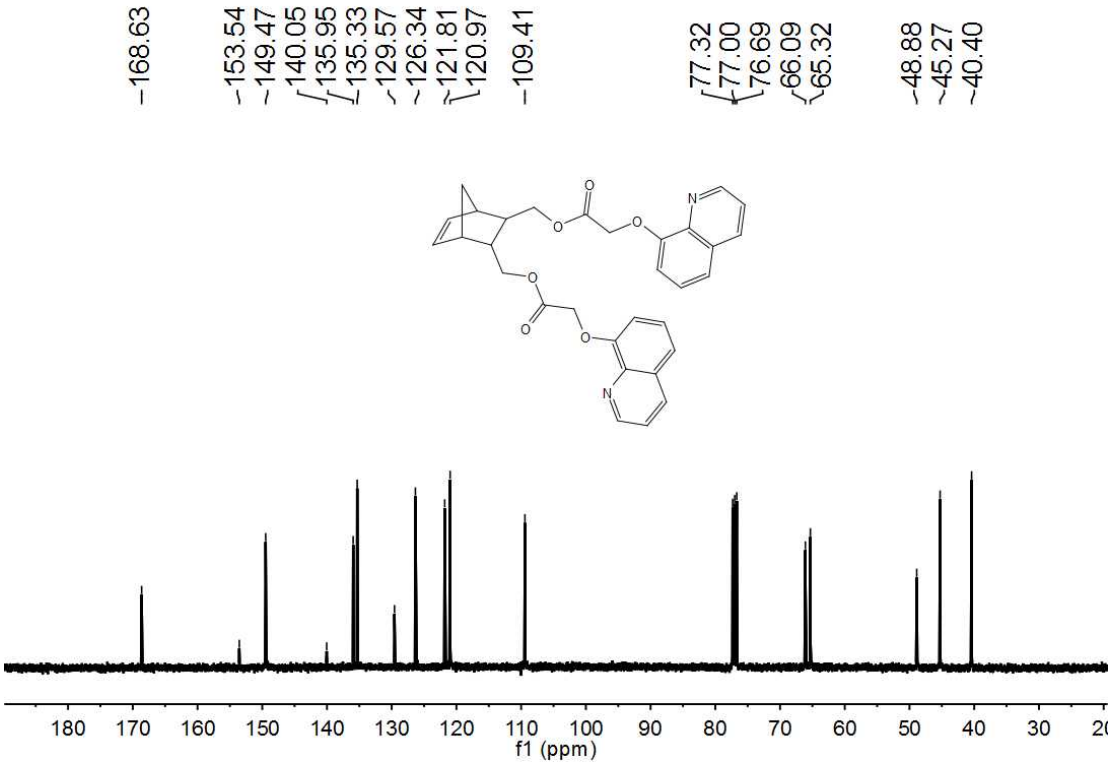

Figure S15. ^{13}C-NMR of **1** in $CDCl_3$ solution.

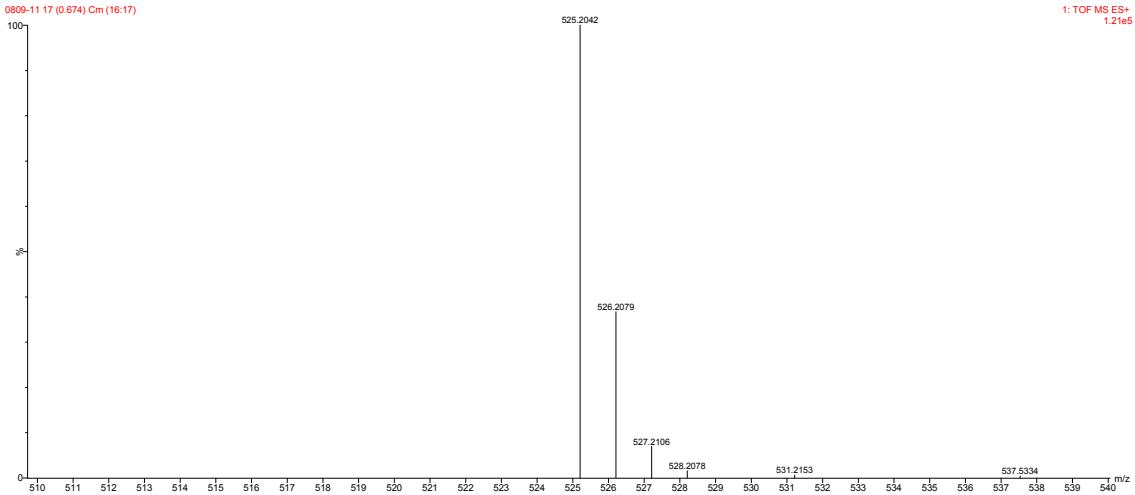

Figure S16. ESI-MS of **1**.

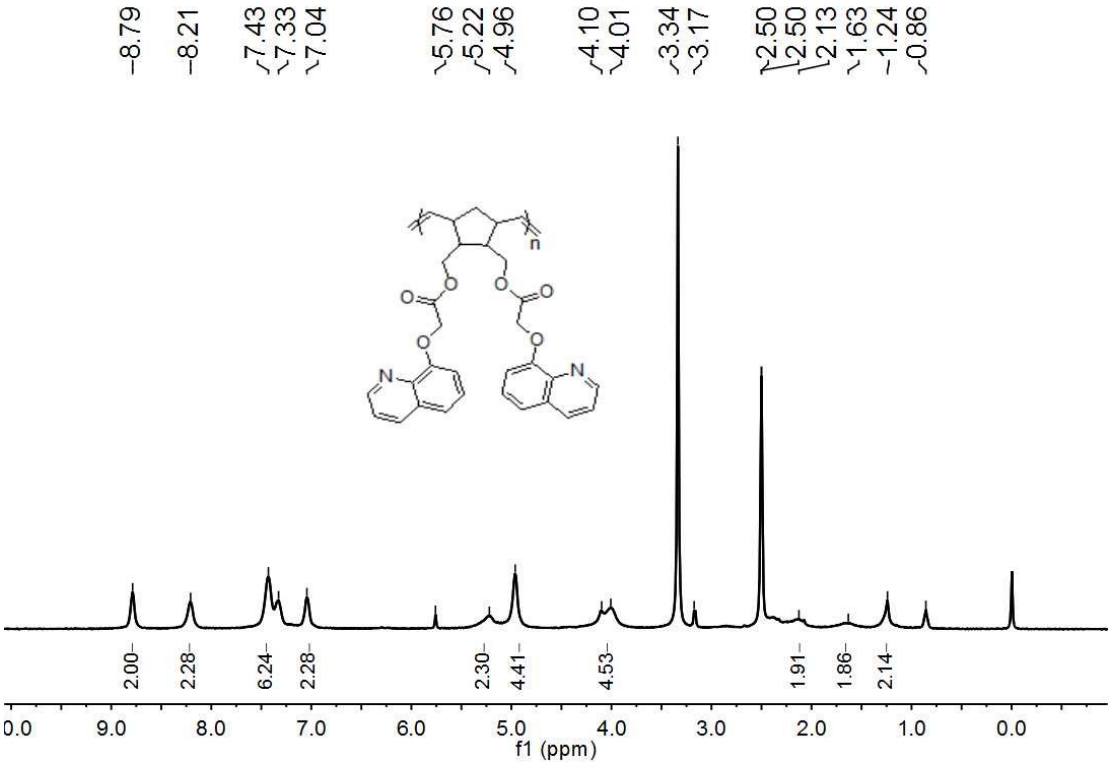

Figure S17. ^{1}H-NMR of **P1** in DMSO.