Supplementary Material (ESI) for Dalton Transactions

Preparation and characterization of alkoxy α-inserted dipyrrins and their metal complexes

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X-Ray Crystallographic Analysis. Single crystals of each compound suitable for X-ray diffraction structural determination were mounted on quartz capillaries or nylon loops by using Paratone oil and were cooled in a nitrogen stream on the diffractometer. Data were collected at 100 K on a Bruker AXS diffractometer using an area detector unless otherwise noted. Peak integrations were performed with the Siemens SAINT software package. Absorption corrections were applied using the program SADABS. Space group determinations were performed by the program XPREP. The structures were solved by direct methods and refined with the SHELXTL software package (Sheldrick, G. M. *SHELXTL vers. 5.1 Software Reference Manual*; Bruker AXS: Madison, WI, 1997). All hydrogen atoms were fixed at calculated positions with isotropic thermal parameters unless otherwise noted; all non-hydrogen atoms were refined anisotropically.

Structure of [α-OMe-4-cydpm]. Orange blocks of [α-OMe-4-cydpm] suitable for X-ray diffraction structural determination were grown by evaporation from a solution of the compound dissolved in CH_2Cl_2 and hexanes. No solvent molecules were found co-crystallized with the compound. The hydrogen atom on the nitrogen (H1N) was found in the difference map, and the position was refined.

Structure of [Zn(α-OMe-4-mecdpm)$_2$]. Orange rods of [Zn(α-OMe-4-mecdpm)$_2$] suitable for X-ray diffraction structural determination were grown by evaporation from a solution of the complex dissolved in $CHCl_3$, MeOH, and triethylamine. No solvent molecules were found co-crystallized with the complex.

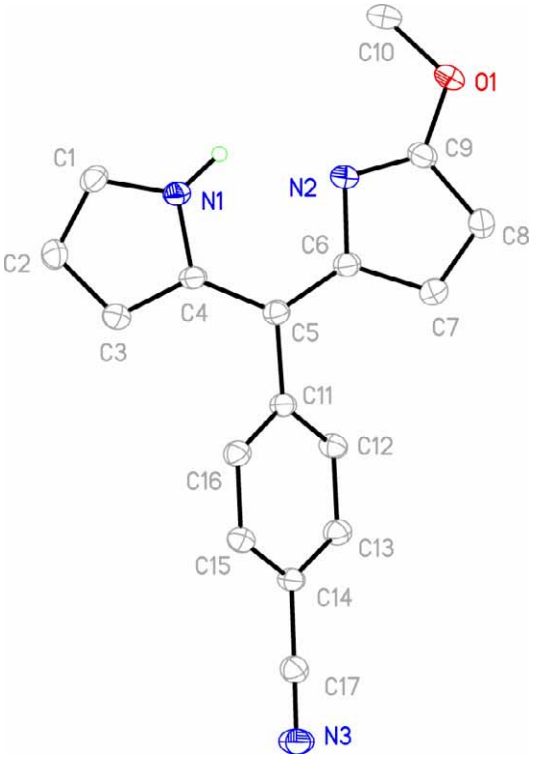

Figure S1. Structural diagram of α-OMe-4-cydpm with atom numbering schemes (ORTEP, 50% probability ellipsoids). Hydrogen atoms (except on N atom in dipyrrin) have been omitted for clarity.

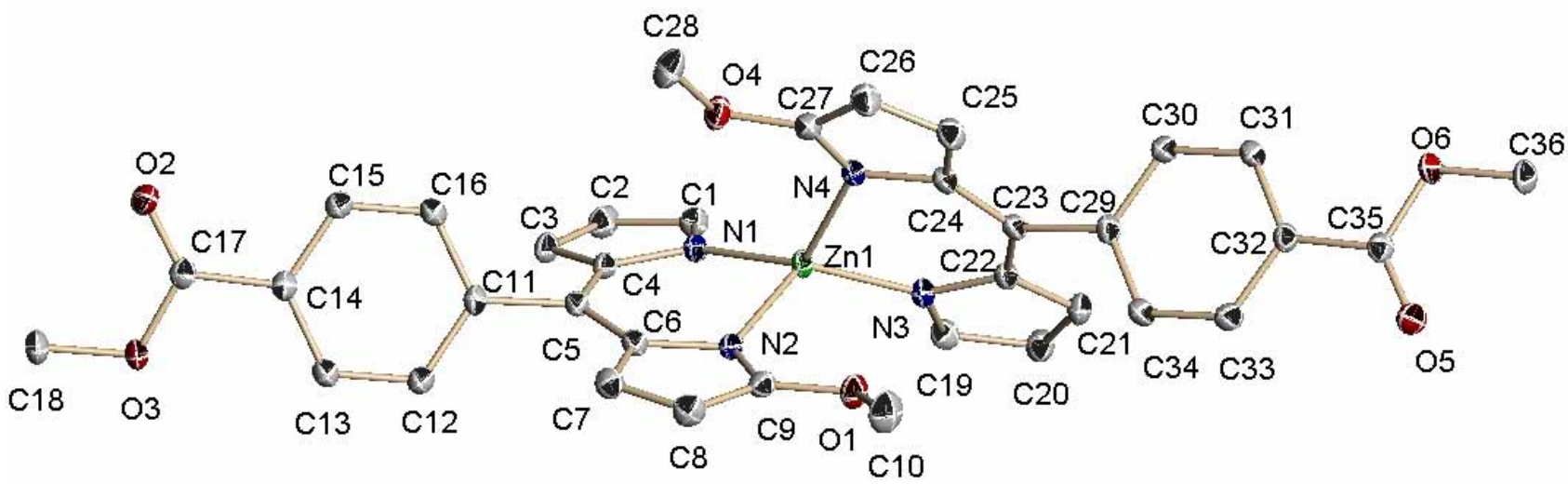

Figure S2. Structural diagram of Zn(α-OMe-4-mecdpm)$_2$ with atom numbering scheme (ORTEP, 50% probability ellipsoids). Hydrogen atoms have been omitted for clarity.

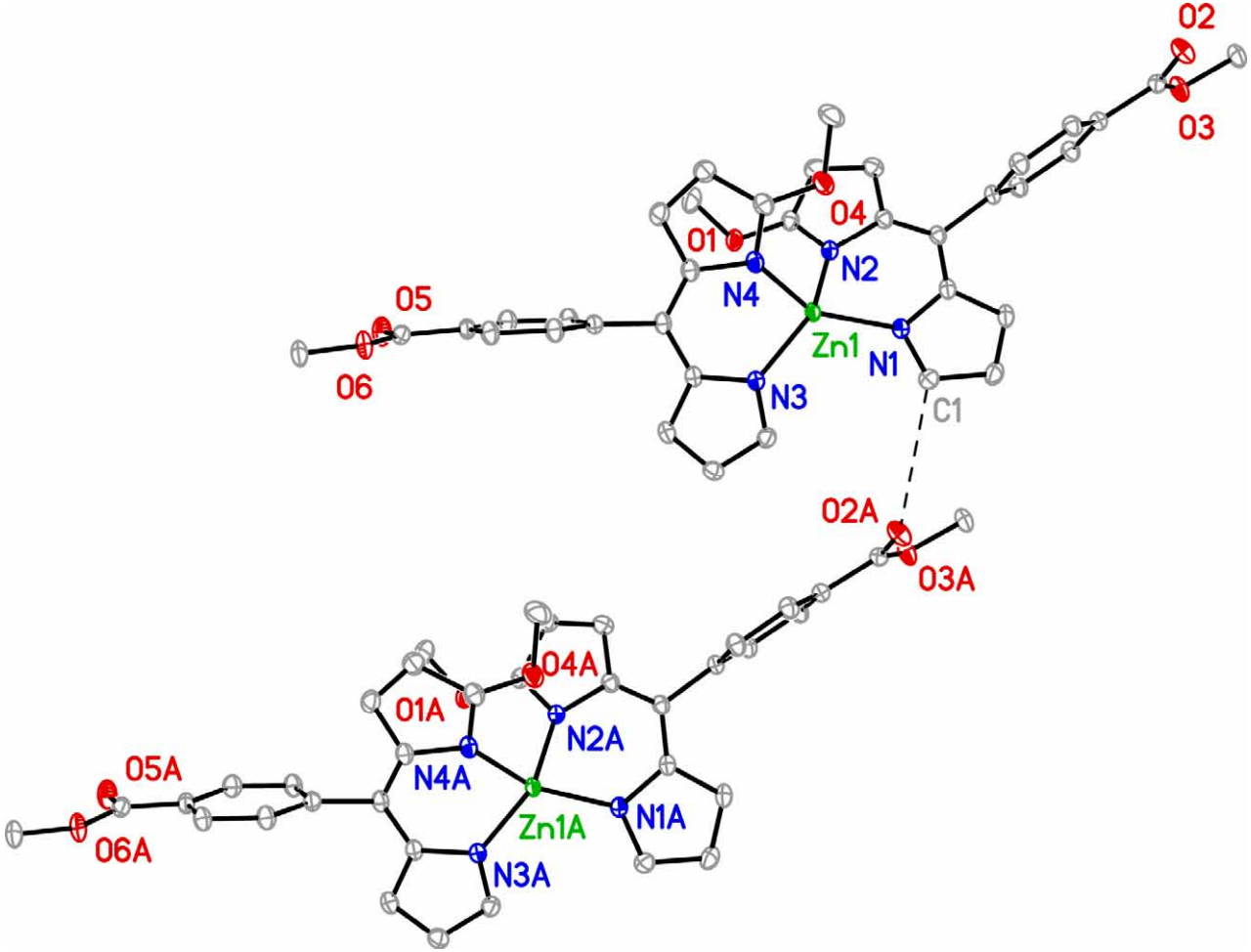

Figure S3. A drawing of the close contact between two [Zn(α-OMe-4-mecdpm)$_2$] complexes that may influence the geometry of the coordination sphere. Hydrogen atoms have been omitted for clarity.

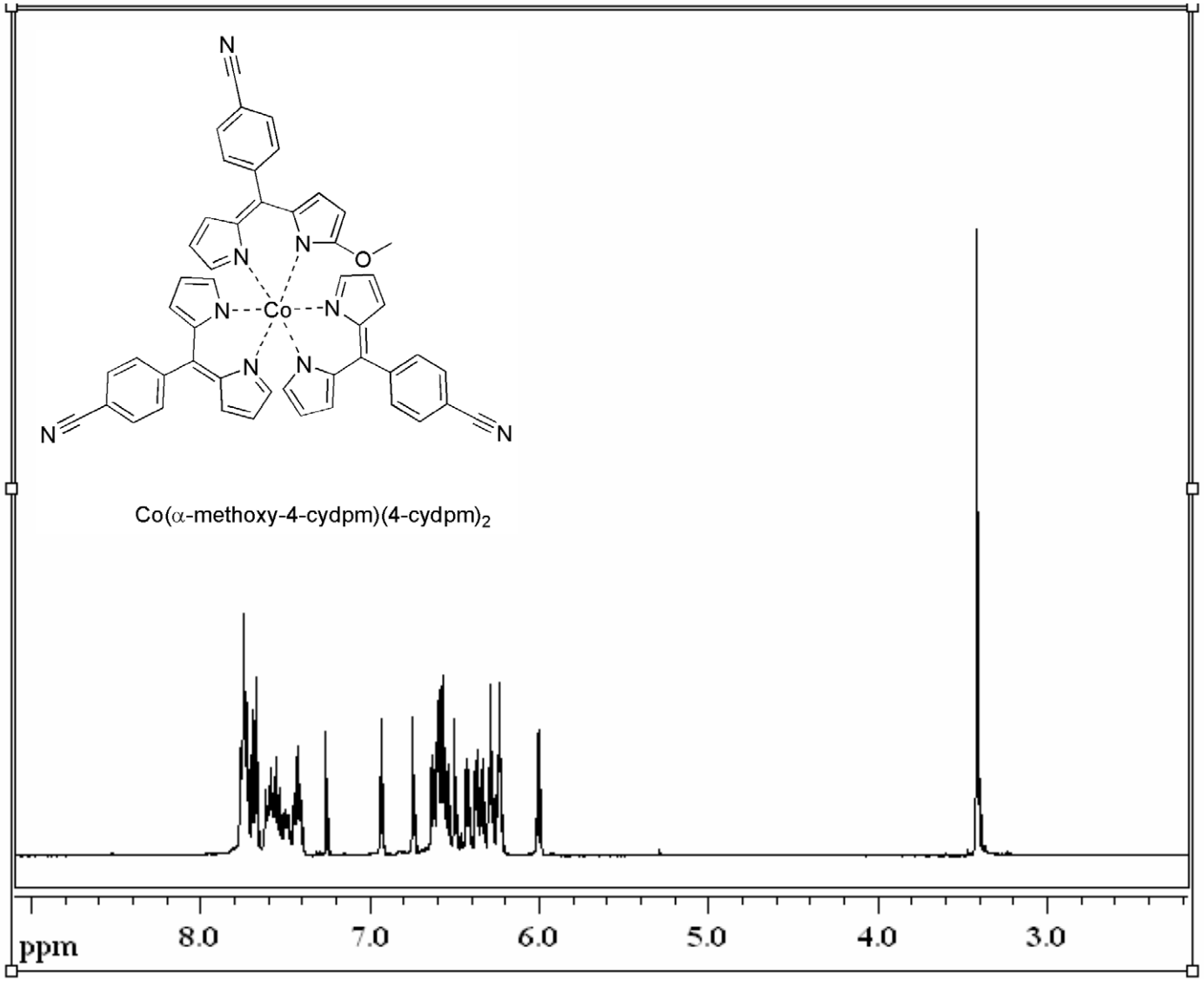

Figure S4. ^{1}H NMR of [Co(α-OMe-4-cydpm)(4-cydpm)$_2$] in $CDCl_3$.

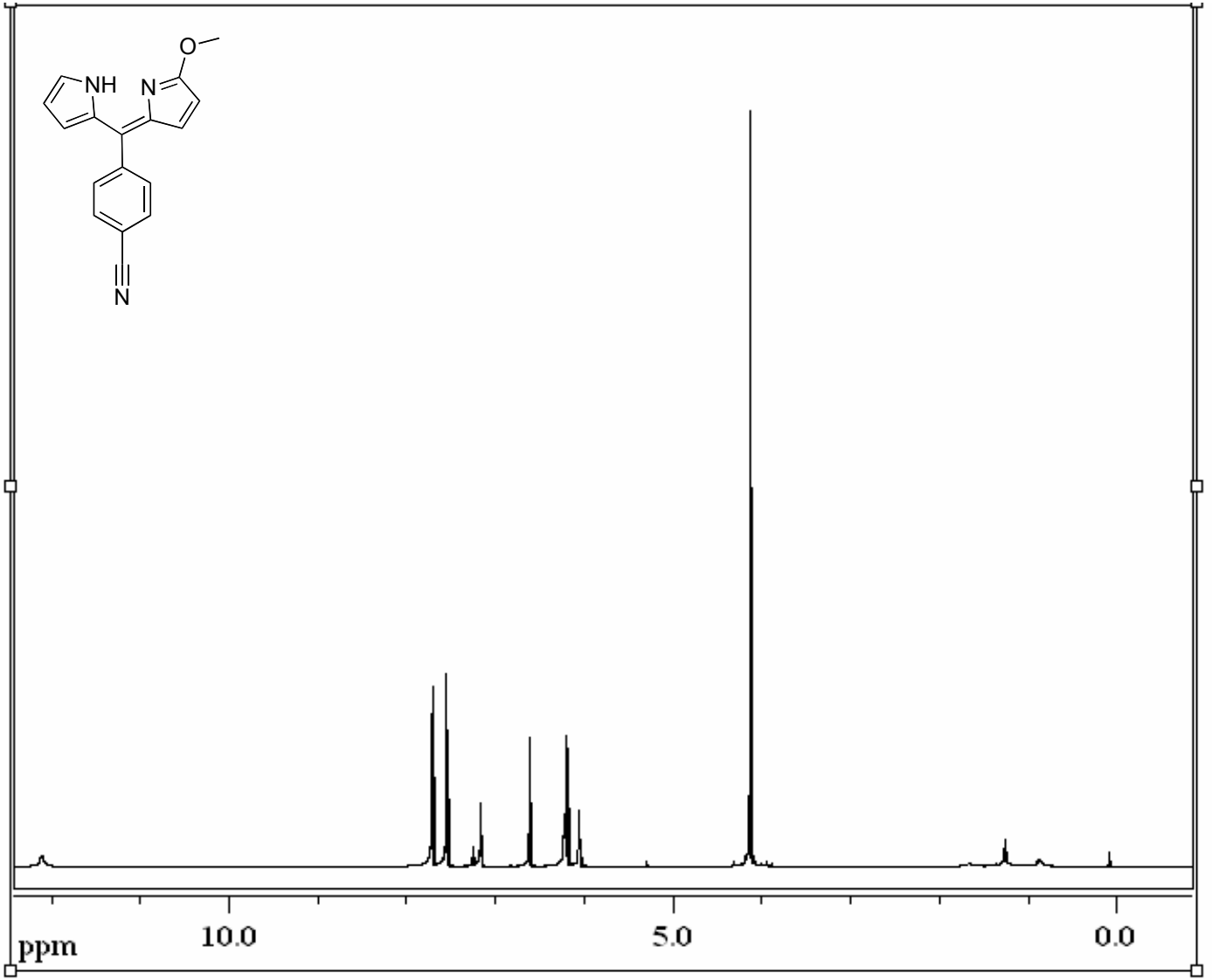

Figure S5. ^{1}H NMR of [α-OMe-4-cydpm] in $CDCl_3$.

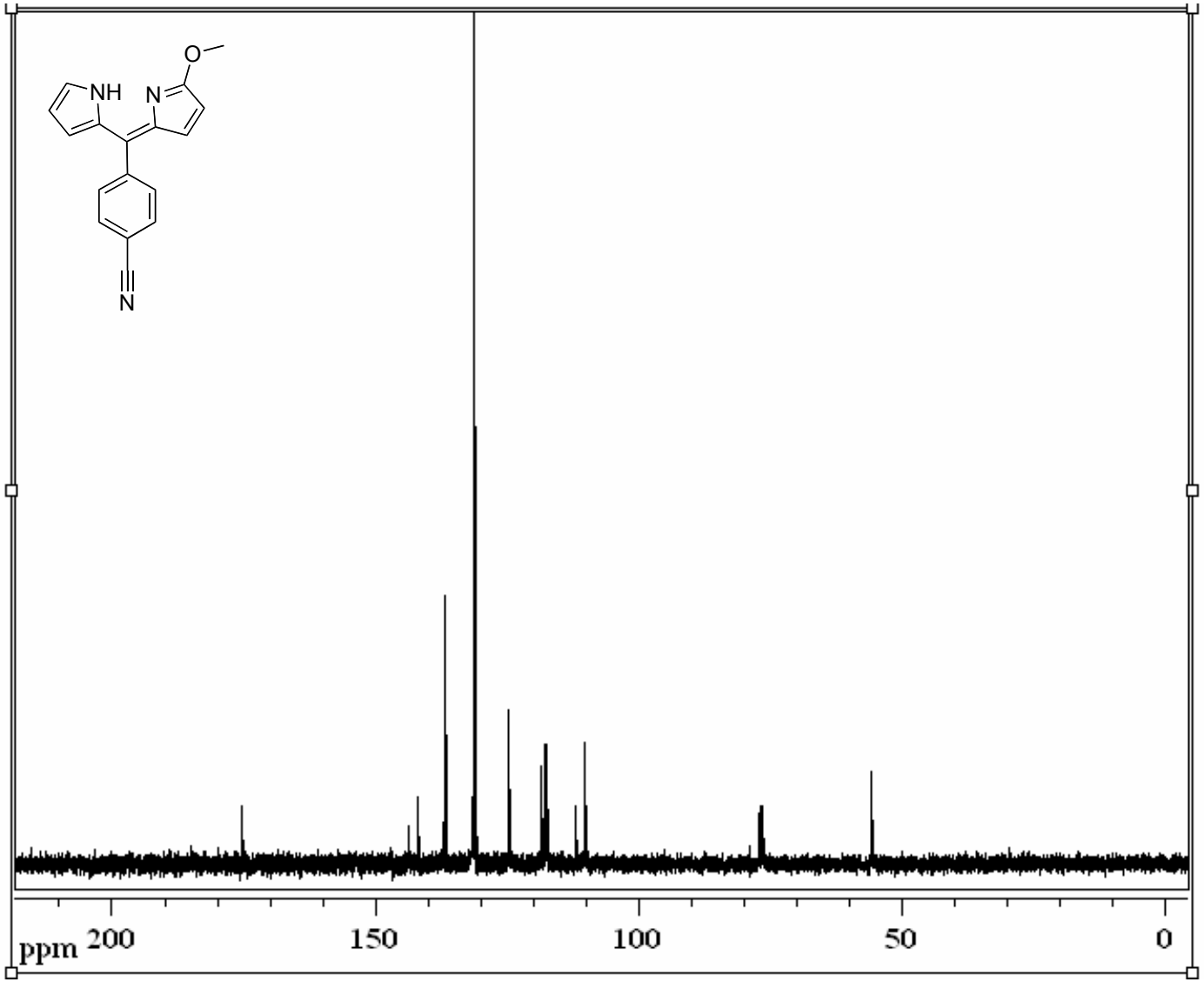

Figure S6. ^{13}C NMR of [α-OMe-4-cydpm] in $CDCl_3$.

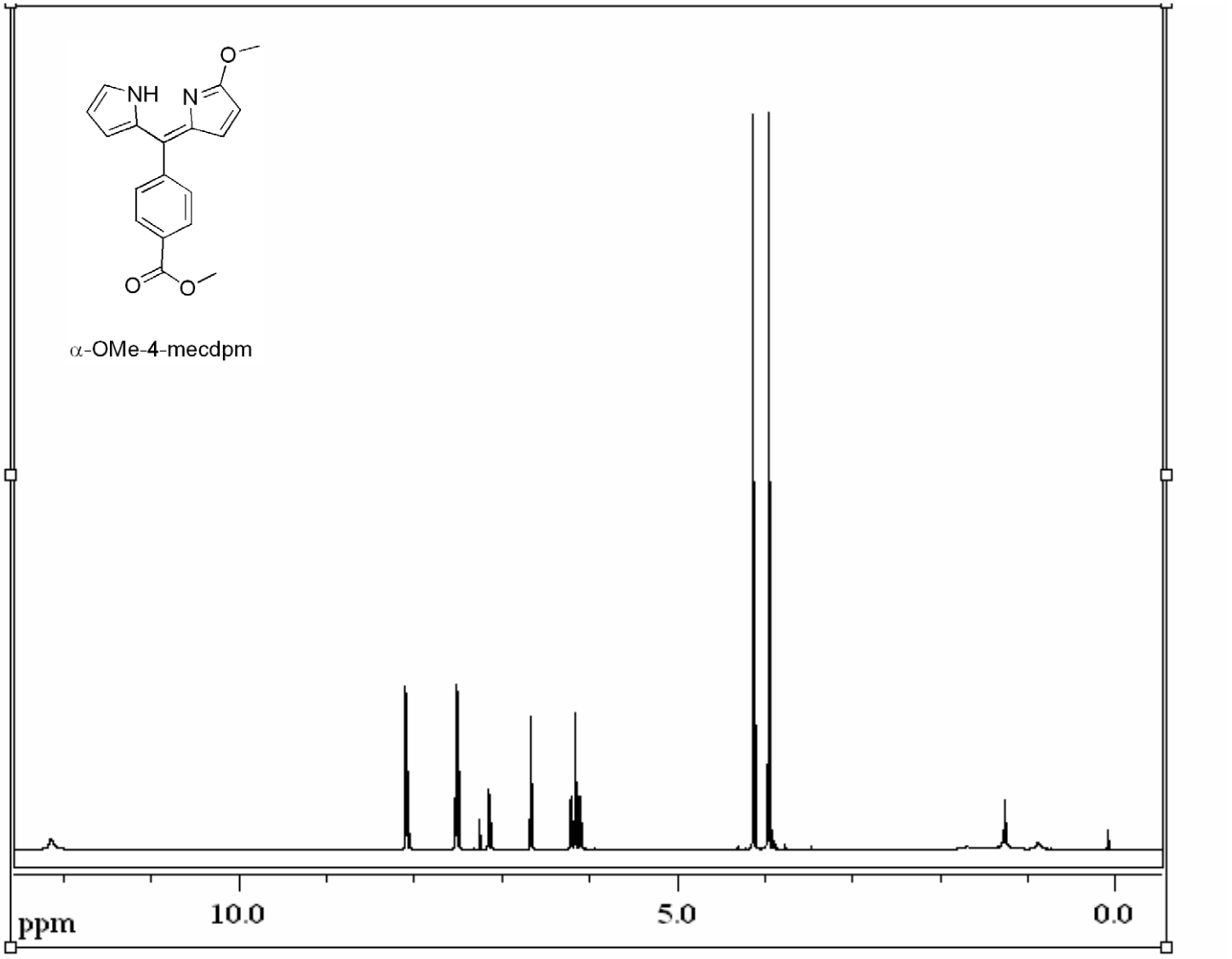

Figure S7 ^{1}H NMR of [α-OMe-4-mecdpm] in $CDCl_3$.

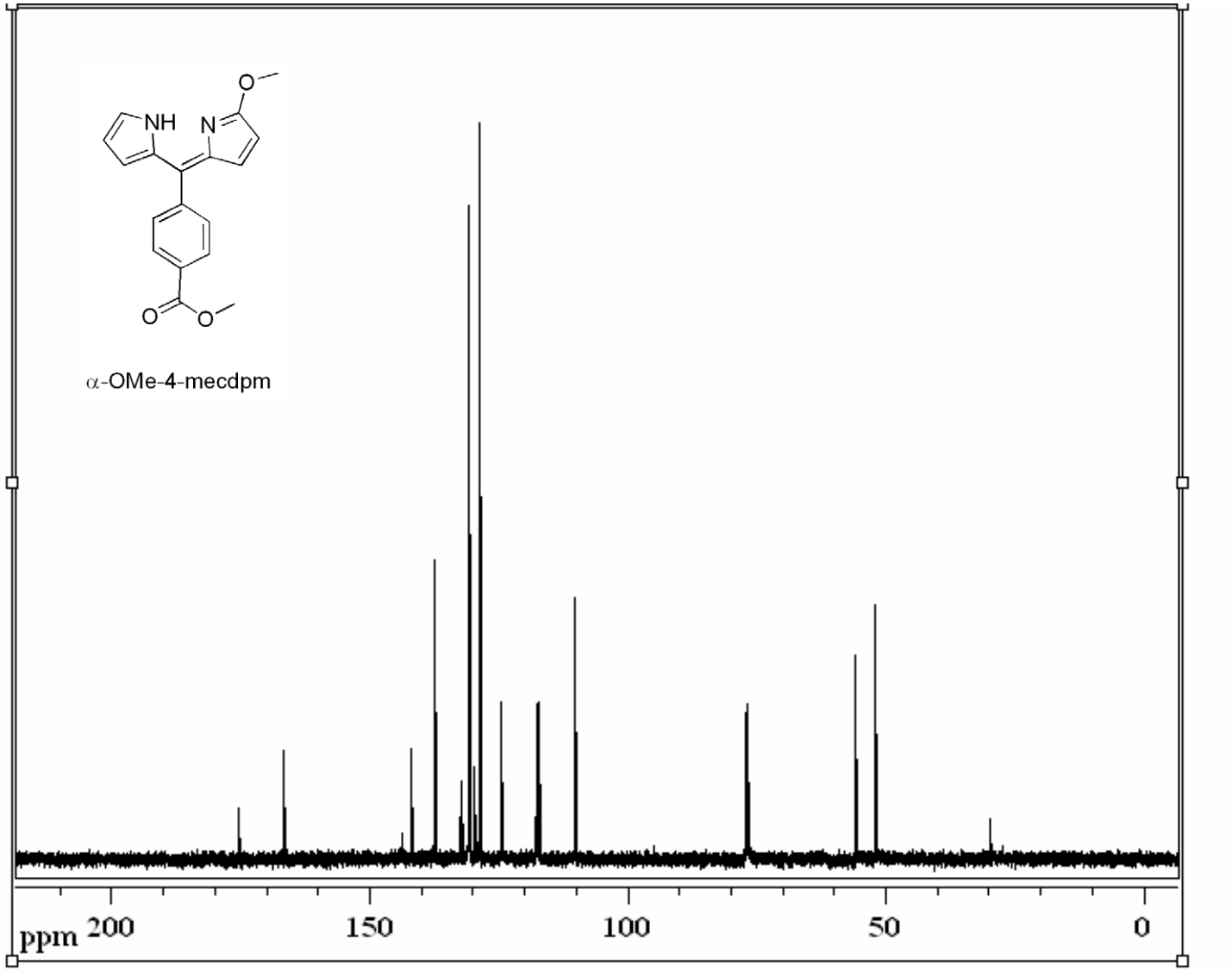

Figure S8. ^{13}C NMR of [α-OMe-4-mecdpm] in $CDCl_3$.

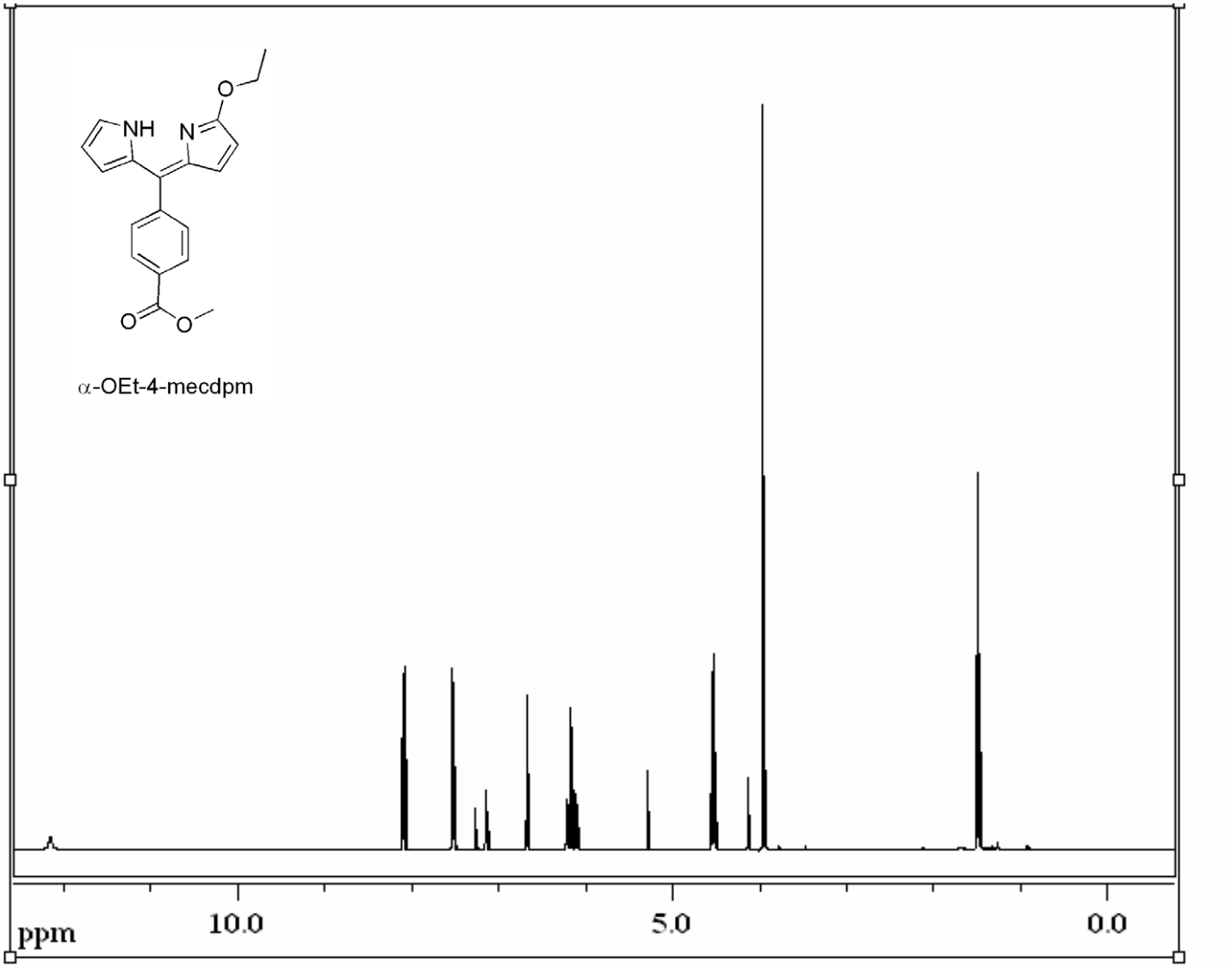

Figure S9. ^{1}H NMR of [α-OEt-4-mecdpm] in $CDCl_3$.

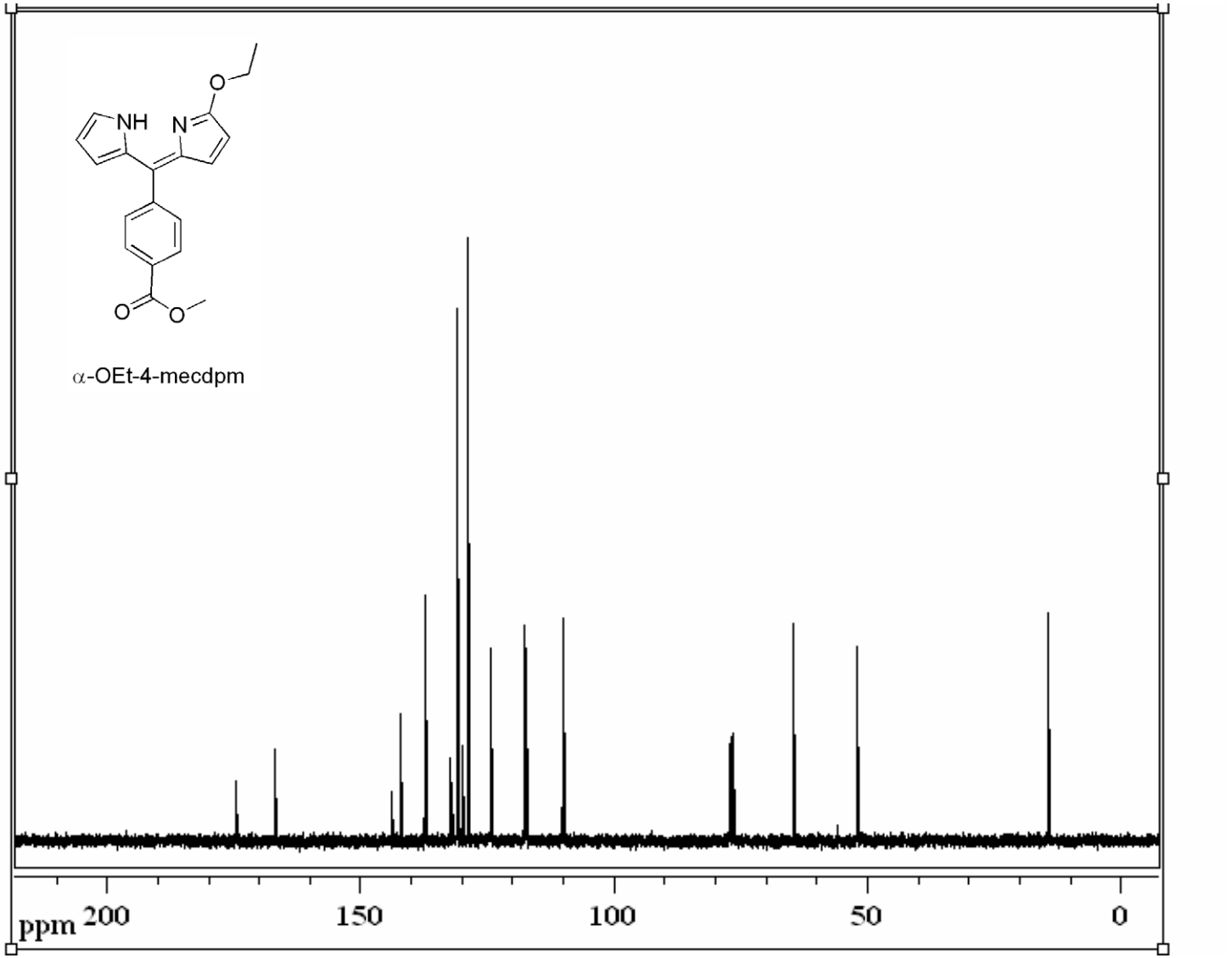

Figure S10. ^{13}C NMR of [α-OEt-4-mecdpm] in $CDCl_3$.

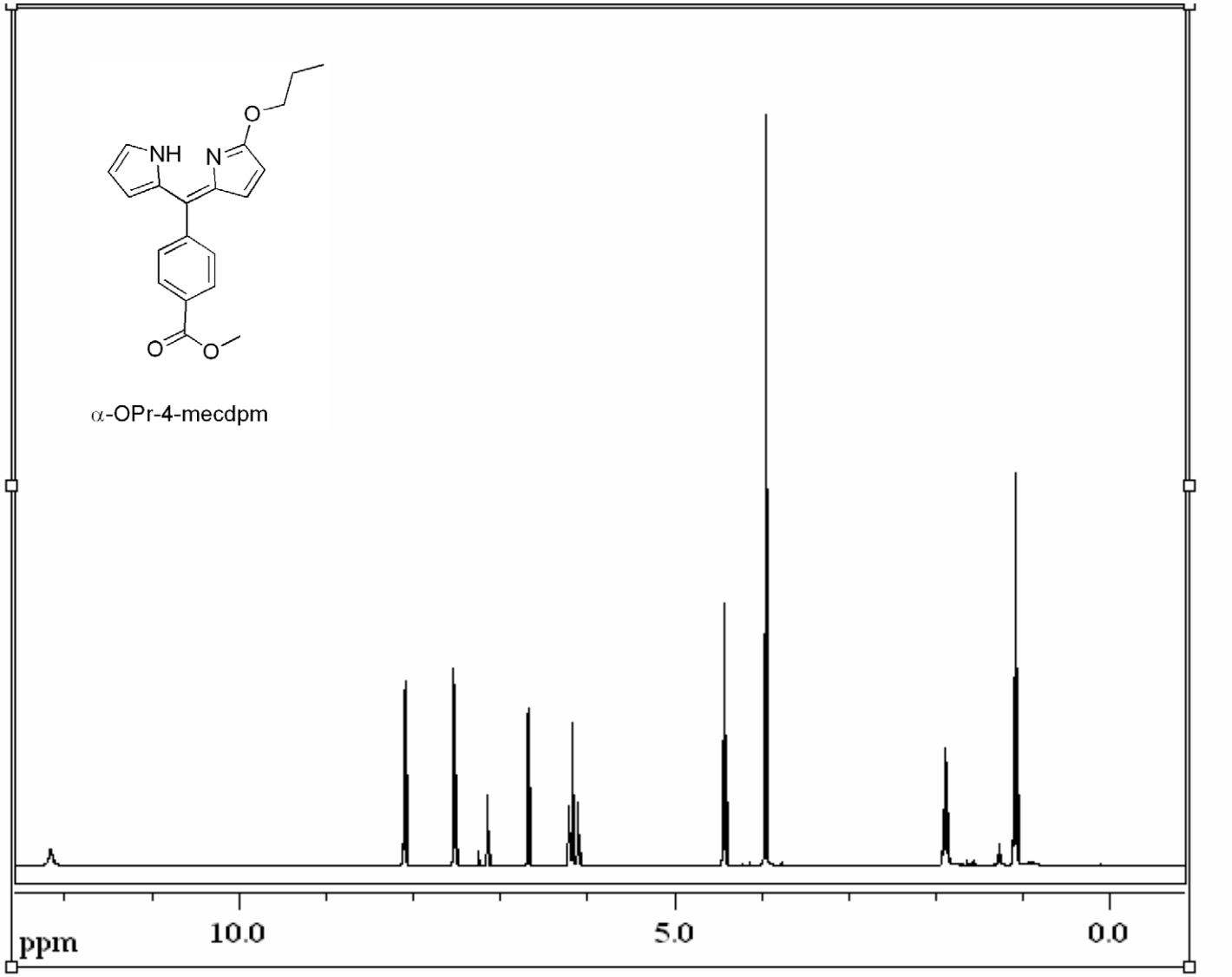

Figure S11. ^{1}H NMR of [α-OPr-4-mecdpm] in $CDCl_3$.

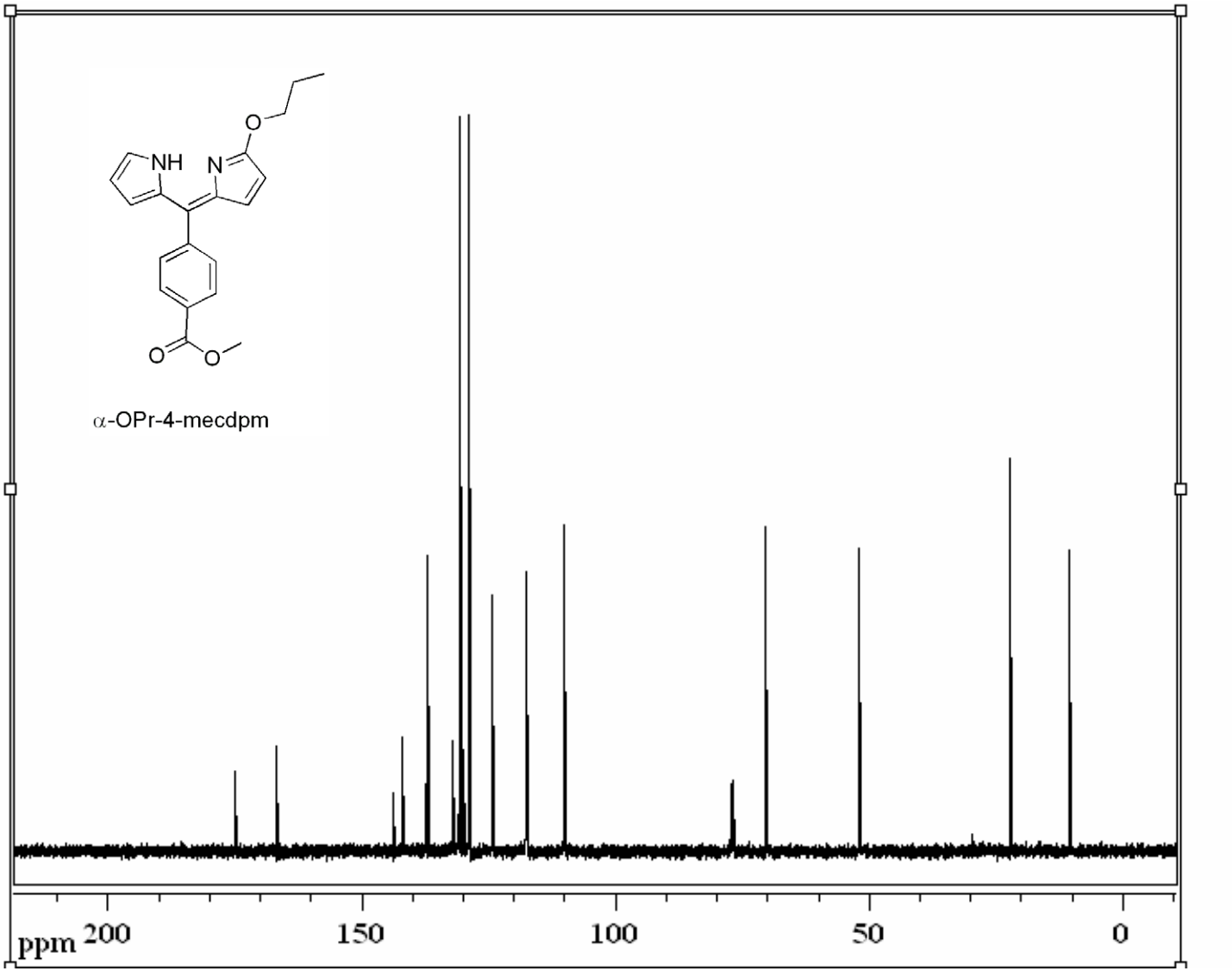

Figure S12. ^{13}C NMR of [α-OPr-4-mecdpm] in $CDCl_3$.

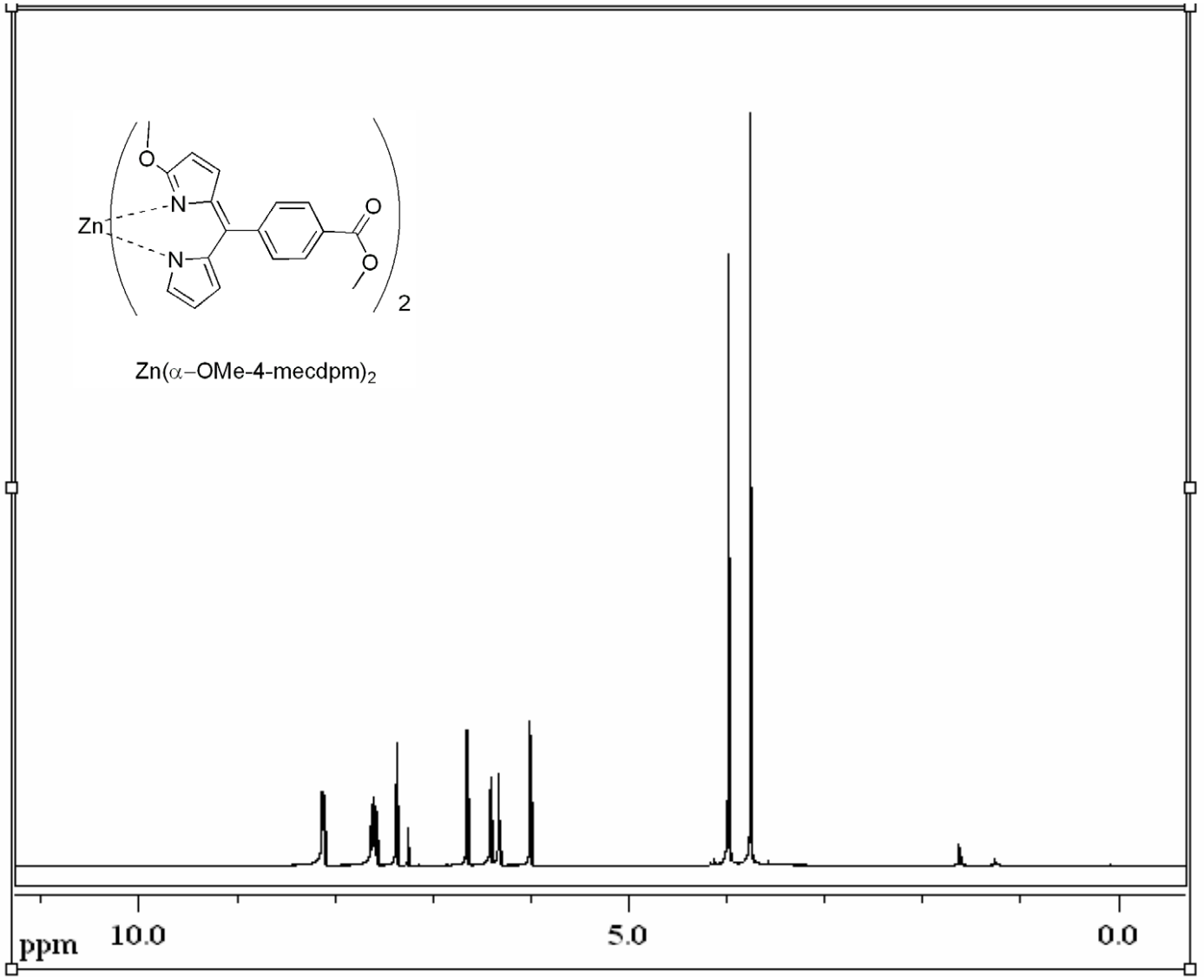

Figure S13. ^{1}H NMR of [Zn(α-OMe-4-mecdpm)$_2$] in $CDCl_3$.

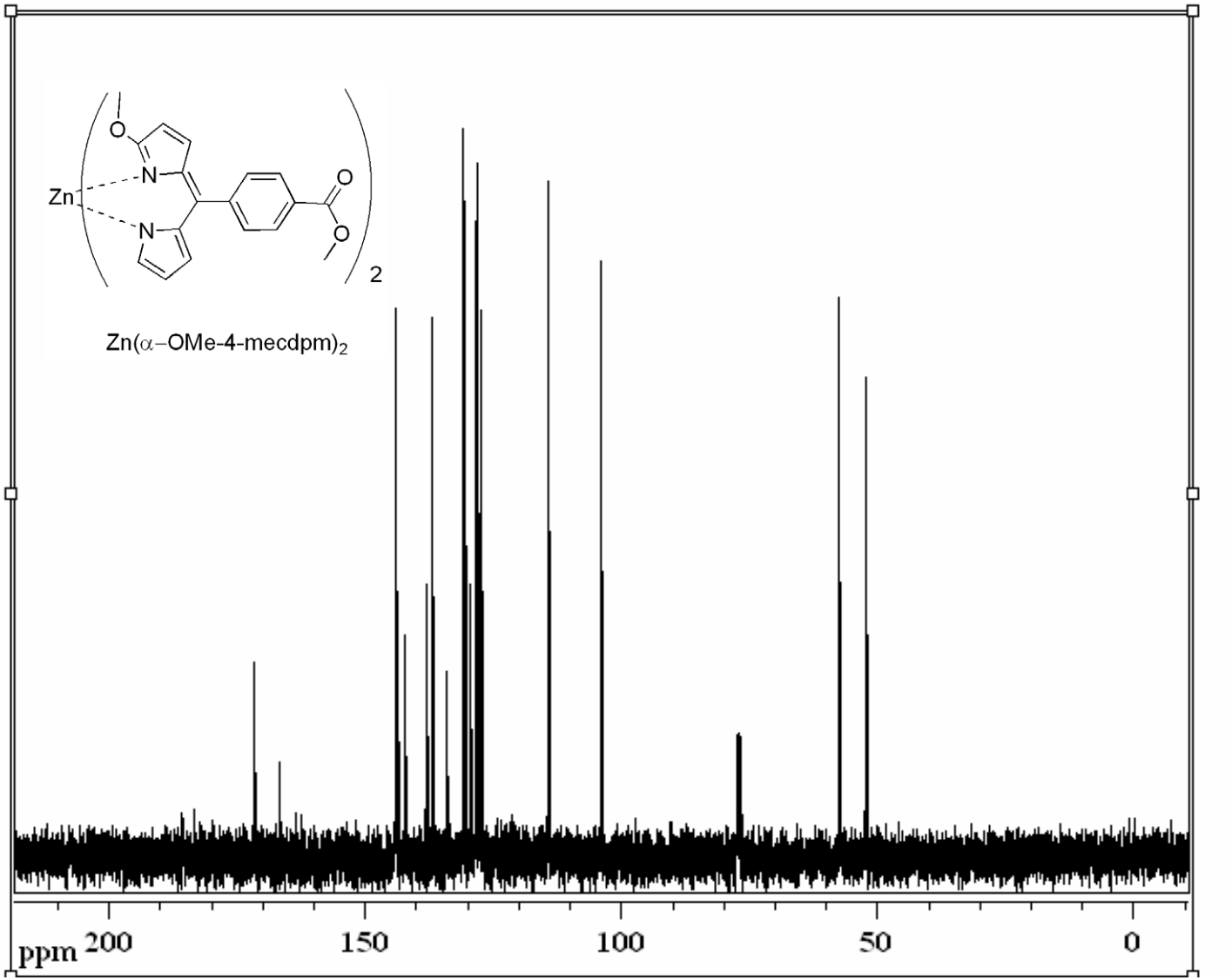

Figure S14. ^{13}C NMR of [Zn(α-OMe-4-mecdpm)$_2$] in $CDCl_3$.

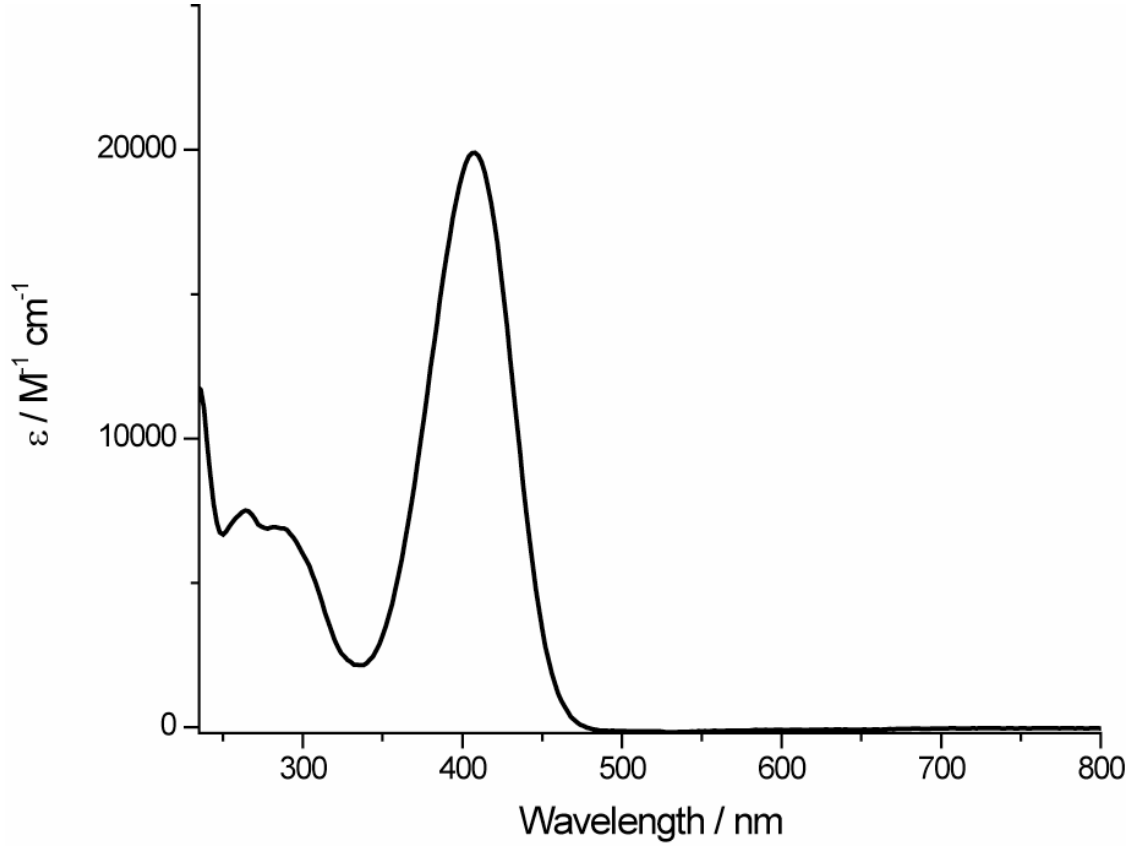

Figure S15. UV-Vis spectra of α-OMe-4-cydpm in CH_2Cl_2.