

Supporting information

Aluminum complexes based on pyridine substituted alcohols: synthesis, structure, catalytic application in ROP

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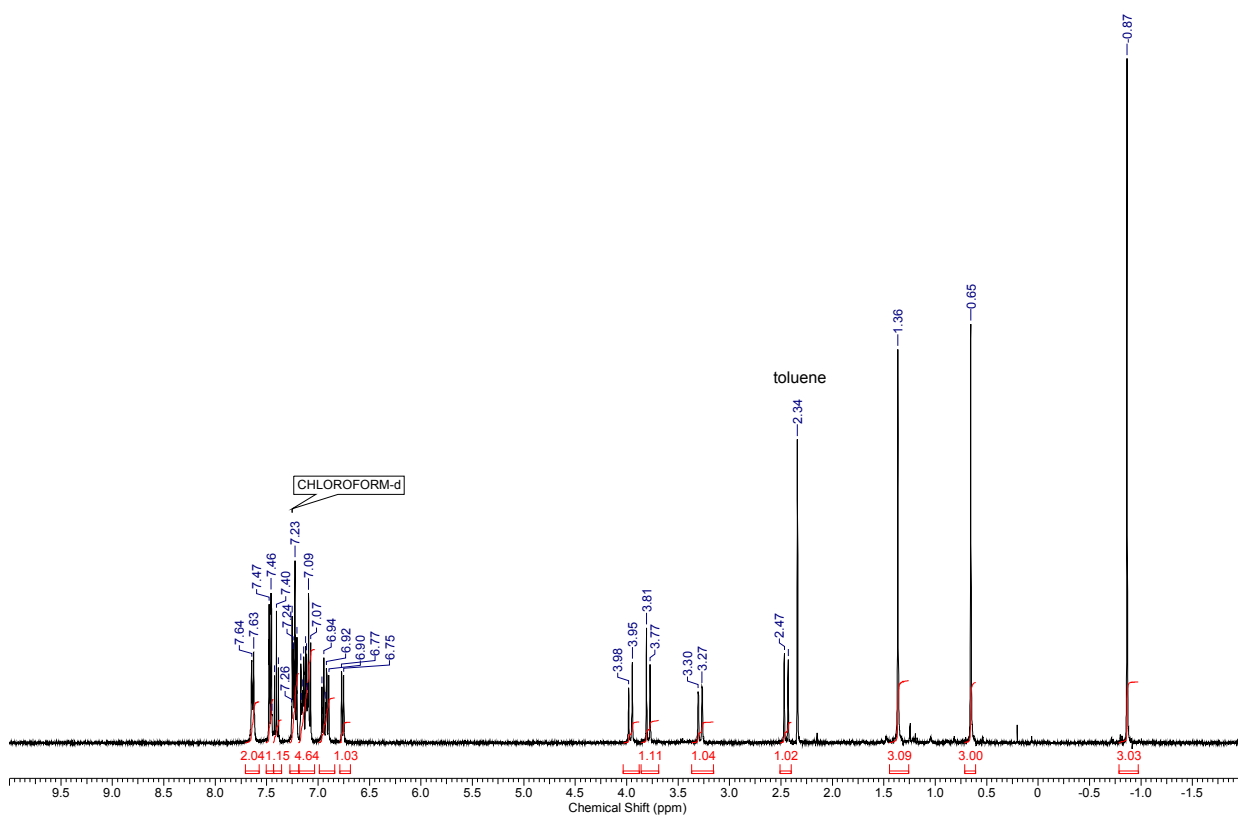


Fig. S1 ¹H NMR spectrum for **3a** (CDCl₃, rt).

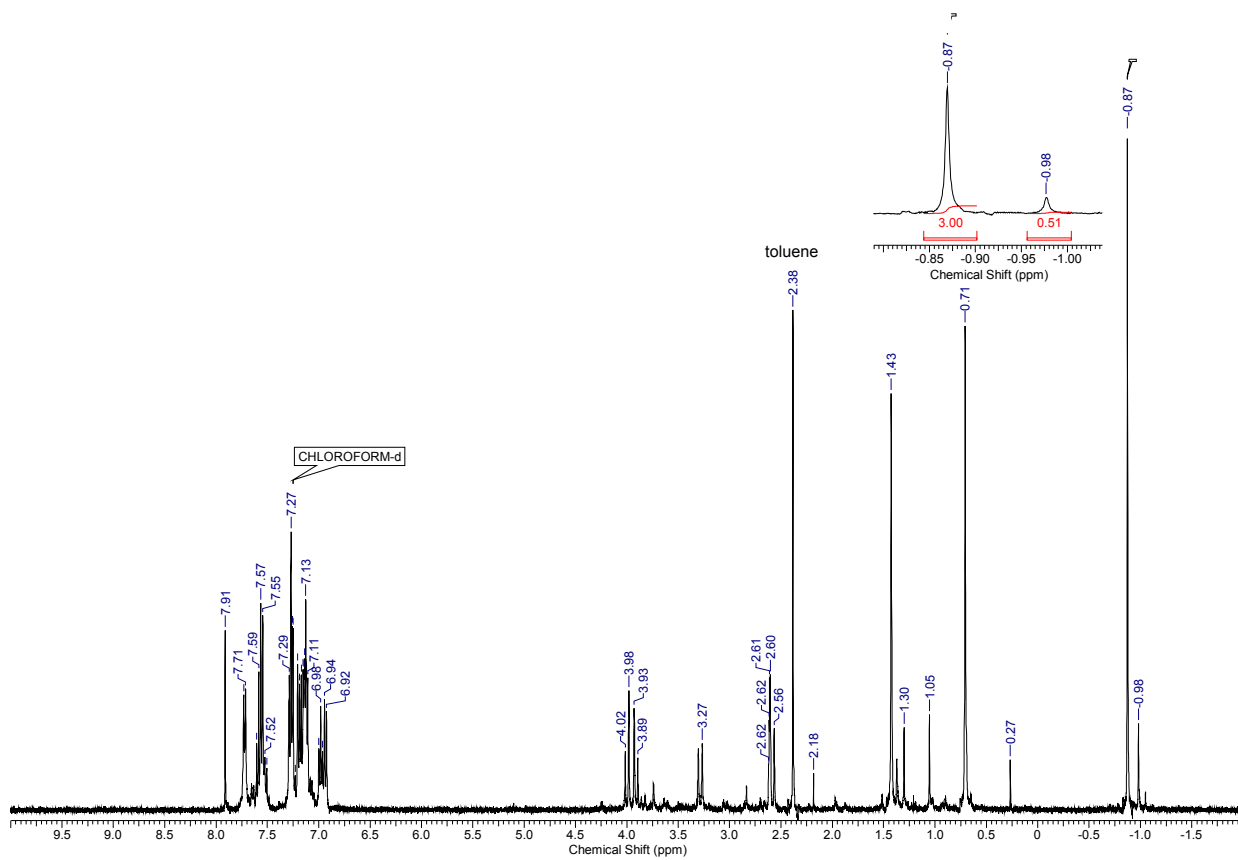


Fig. S2 ¹H NMR spectrum for **3a** (CDCl₃+ 20 % DMSO-d₆, rt).

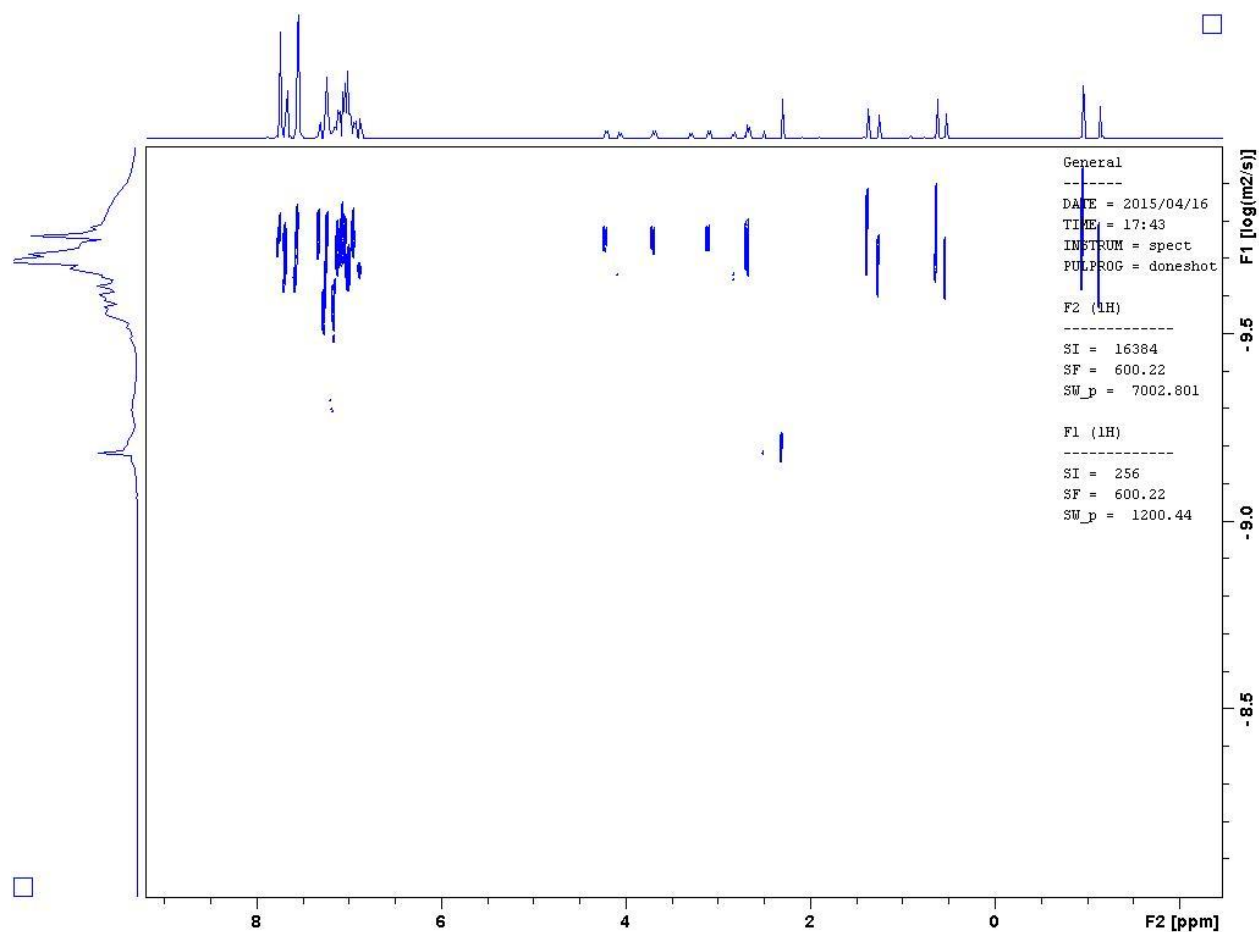


Fig. S3 DOSY NMR spectrum for **3a** (600 MHz, DMSO-d6, room temperature; the admixture of toluene is present).

The formula of MW calculation [*Angew. Chem., Int. Ed.* 2013, **52**, 3199 – 3202]

$$D = \frac{k_B T \left(\frac{3\alpha}{2} + \frac{1}{1+\alpha} \right)}{6\pi\eta_3 \sqrt{\frac{3MW}{4\pi\rho_{eff}N_A}}}, \text{ where}$$

$$\alpha = \sqrt[3]{\frac{MW_S}{MW}}$$

MW_S – molecular weight of the solvent

MW – molecular weight of the solute

ρ_{eff} - the effective density of a small molecule

η -viscosity

N_A - the Avogadro number

k_B - Boltzmann constant

D – diffusion coefficient

T - temperature

Using known calculation algorithm the molecular weights of two particles was established:

$M_1 = 820$ g/mol, $D = 1.74 \cdot 10^{-10}$ m²/s ($M_1(\text{theor}) = 774.9$), what corresponds to dimeric (**3a**)₂;

$M_2 = 497.1$ g/mol, $D = 2.19 \cdot 10^{-10}$ m²/s ($M_1(\text{theor}) = 465.6$), what corresponds to adduct of monomer with DMSO.

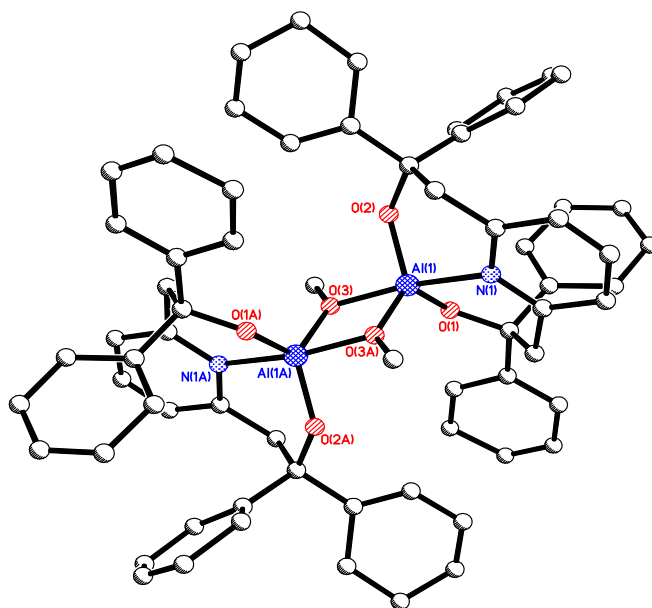


Fig. S4 Molecular structure of complex **2c**. Hydrogen atoms are omitted for clarity.

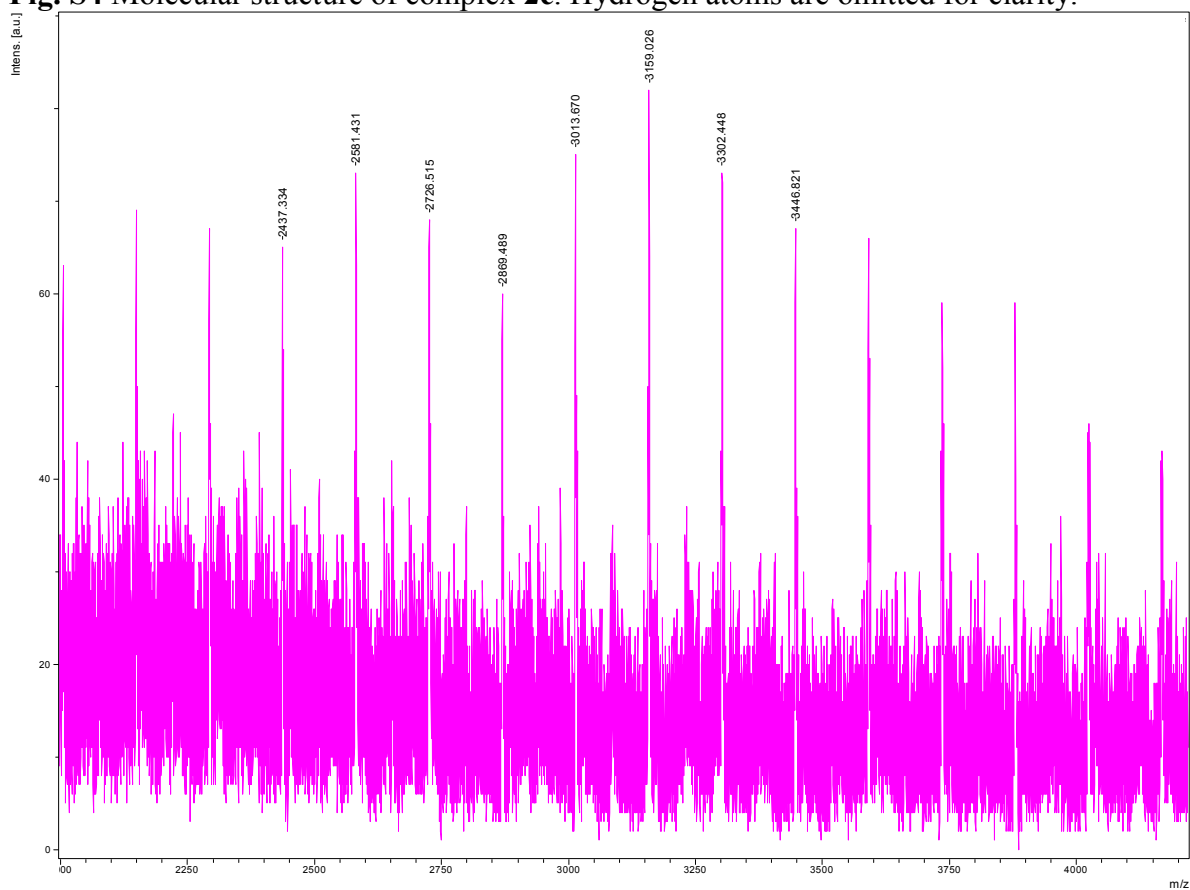


Fig. S5. MALDI-TOF mass spectrum of a PLA sample prepared with **2a** (Table 2, entry 1) (solvent THF, HABA matrix, 2,5-dihydroxybenzoic acid).

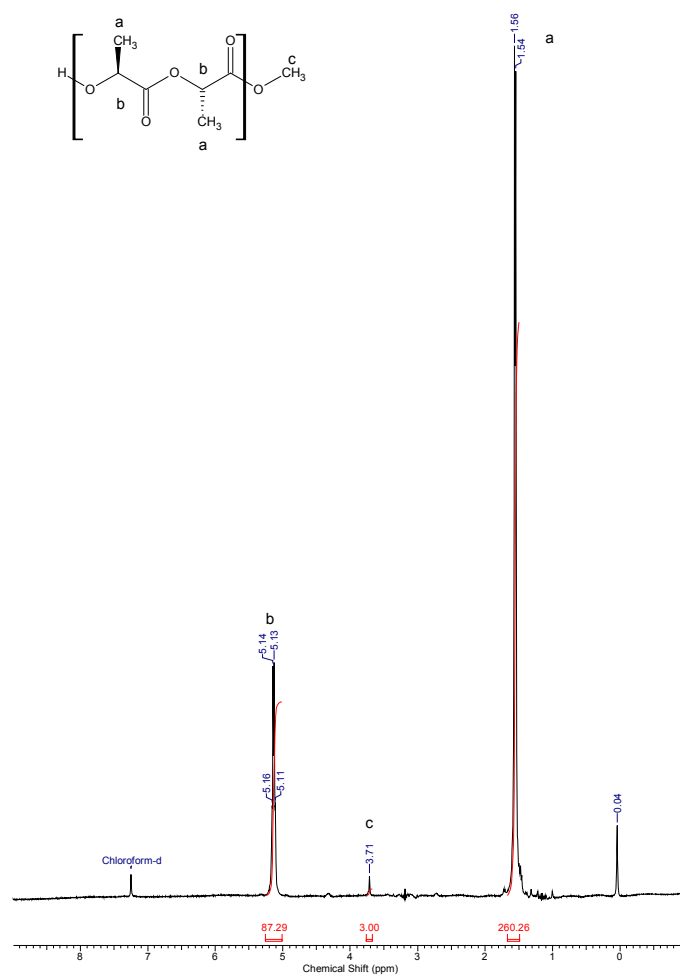


Fig. S7. ¹H NMR spectra (CDCl₃) for MeO-PLLA, prepared with **2c** (100 % conversion).

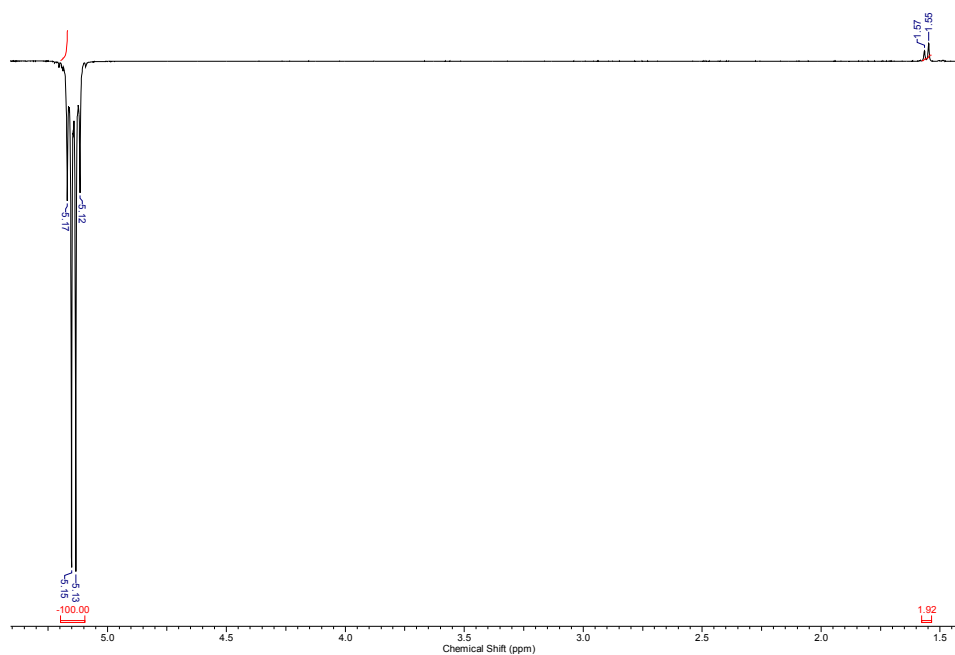


Fig. S8. Homodecoupled ¹H NMR spectra (CDCl₃) for BnO-PLLA.

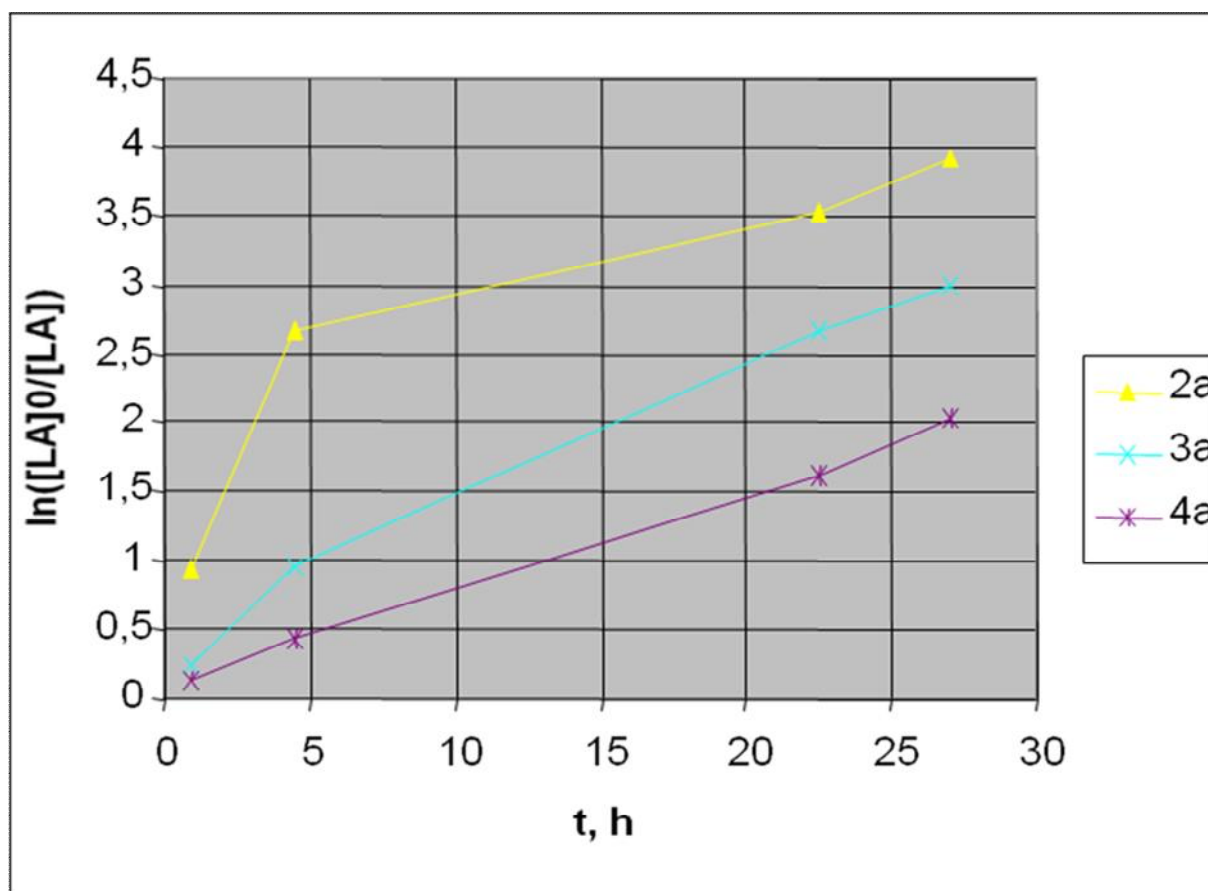


Fig. S9. $\ln([LA]_0/[LA])$ versus time plot for *L*-lactide polymerization with **2a-4a**.

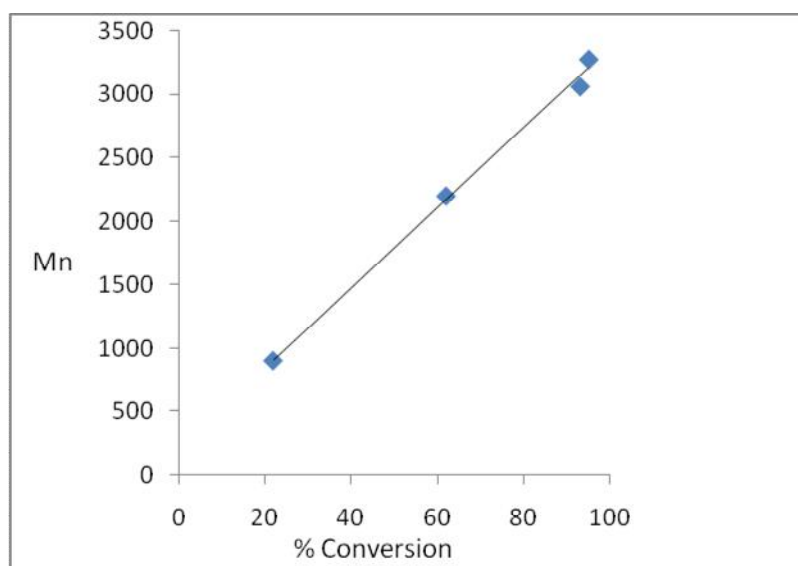


Fig. S10. M_n versus conversion plot for *L*-lactide polymerization with **3a**.

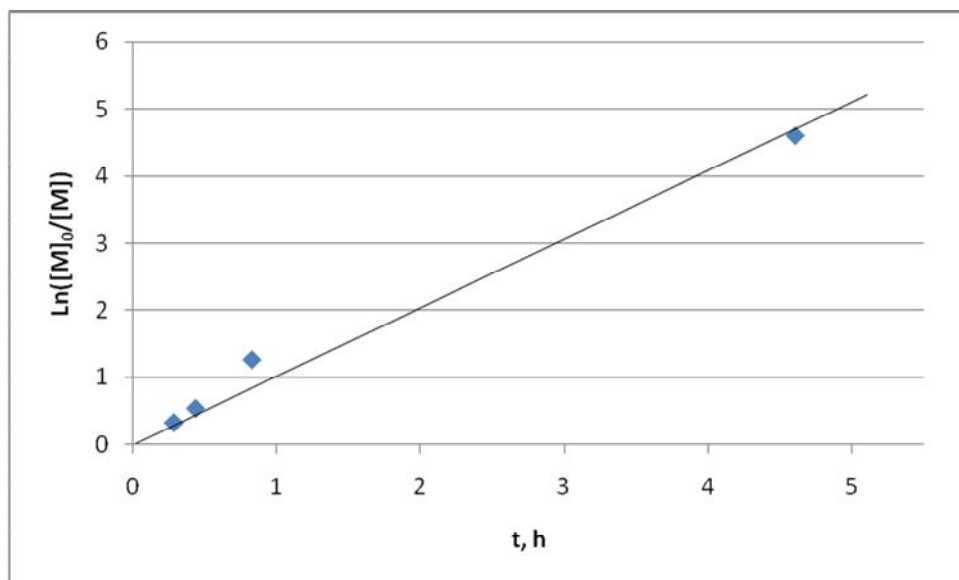


Fig. S11. $\text{Ln}([M]_0/[M])$ vs. time plots for the polymerization of *L*-lactide in the presence of catalytic complex **4a** (100:1:1) at 80 °C; $[\text{LA}]/[\text{initiator}] = 100$.

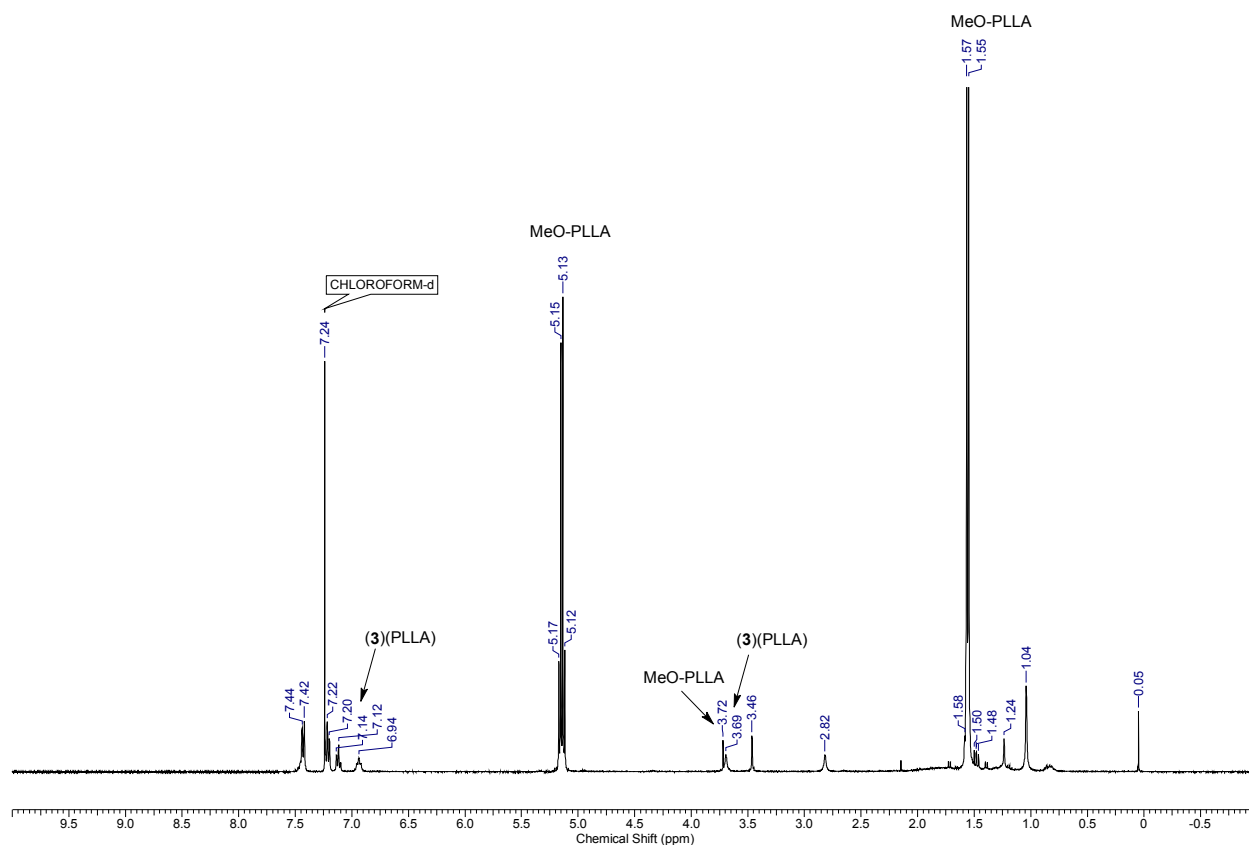


Fig. S12. ^1H NMR spectrum (CDCl_3 , rt) for PLLA (the sample contains the polymer, $[(3)(\text{PLLA})]$, with ligand fragment).

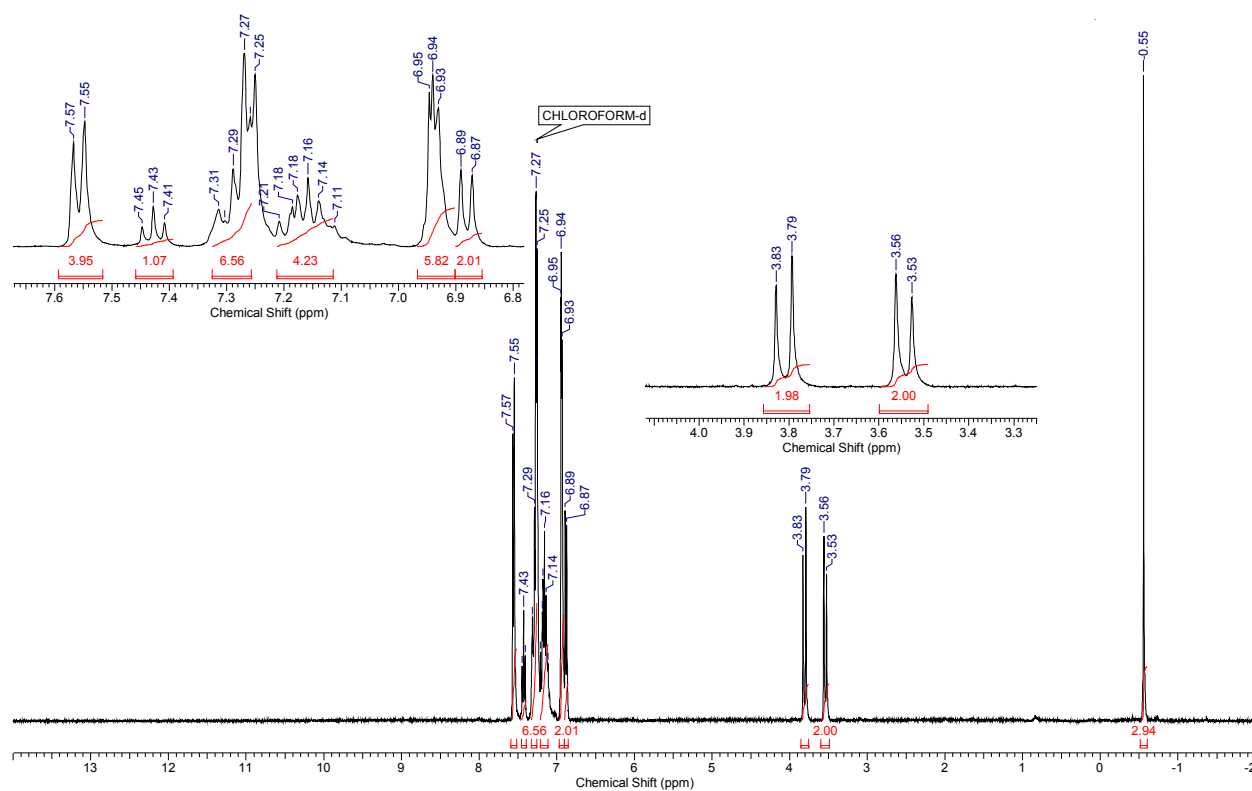


Figure S13. ¹H NMR spectrum (CDCl₃, rt) of complex 2a.

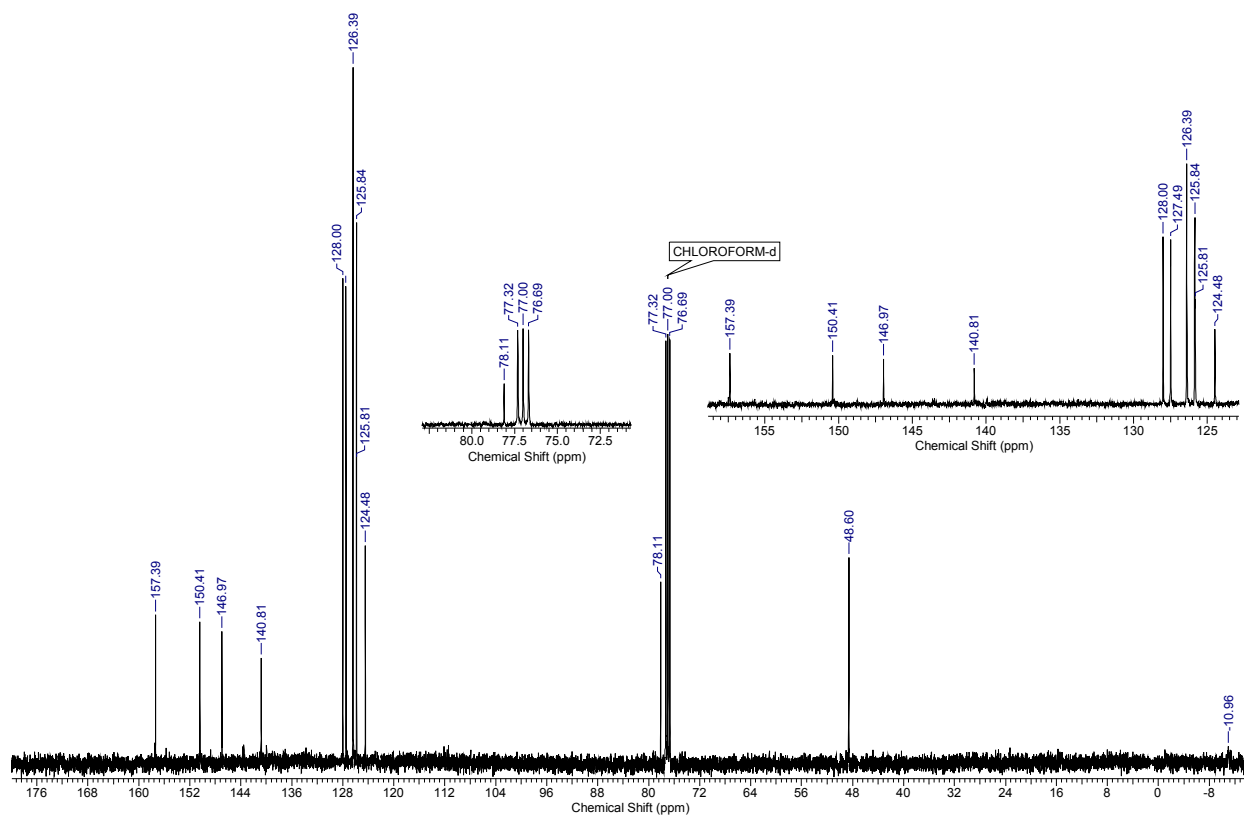


Figure S14. ¹³C NMR spectrum (CDCl₃, rt) of complex 2a.

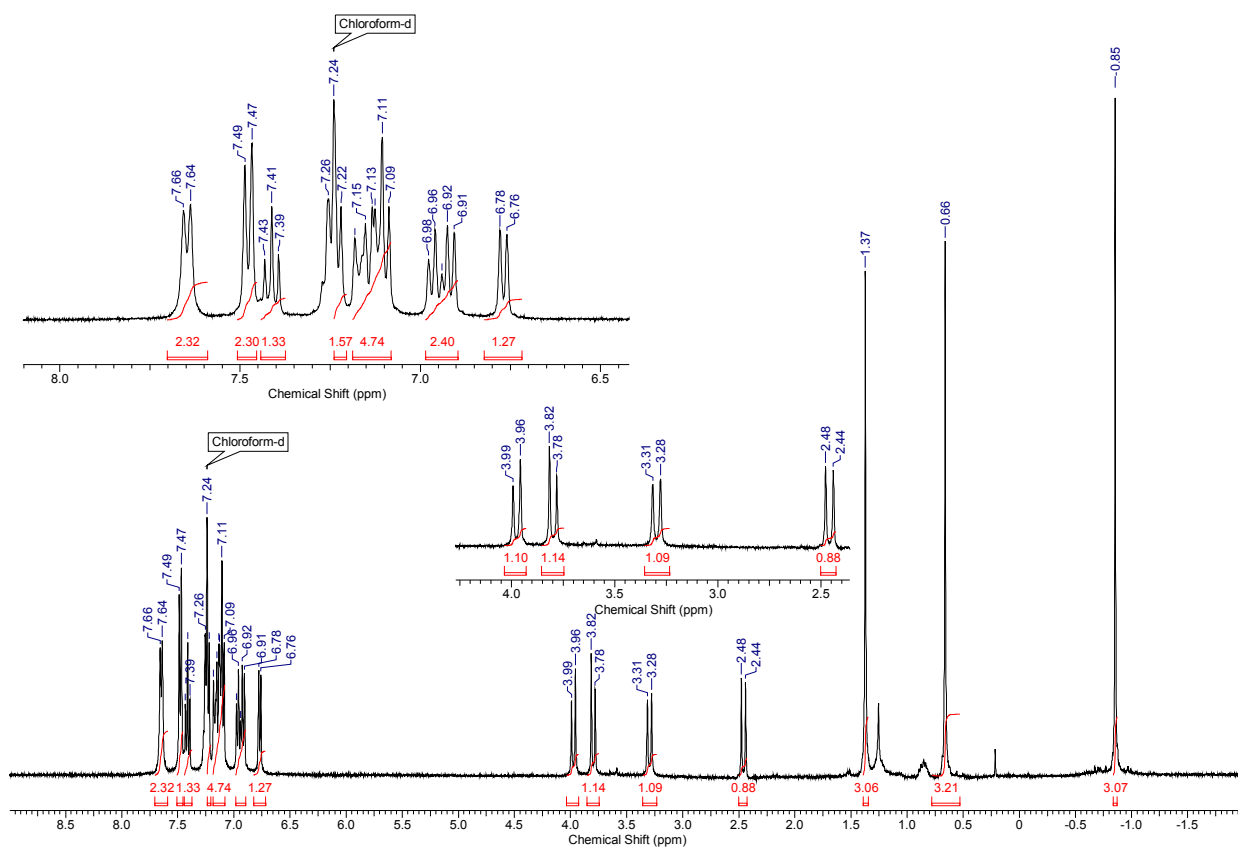


Figure S15. ¹H NMR spectrum (CDCl₃, rt) of complex 3a.

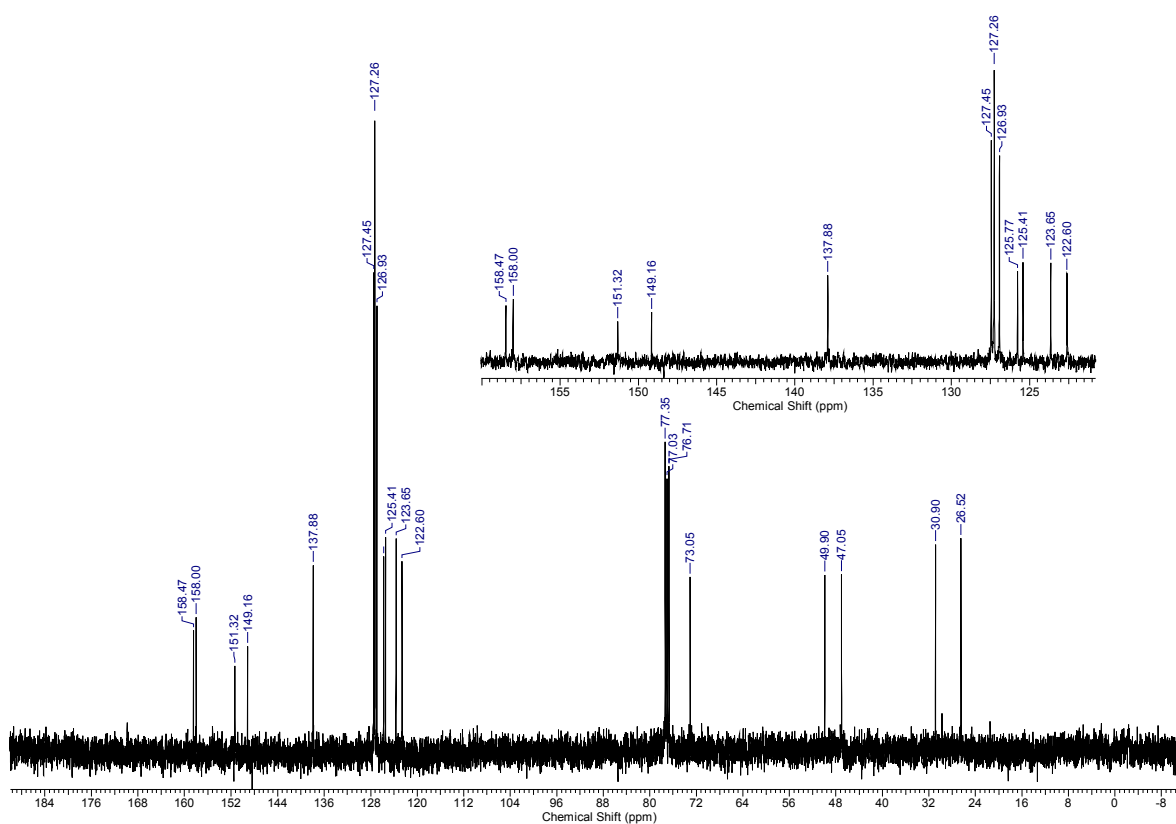


Figure S16. ¹³C NMR spectrum (CDCl₃, rt) of complex 3a.

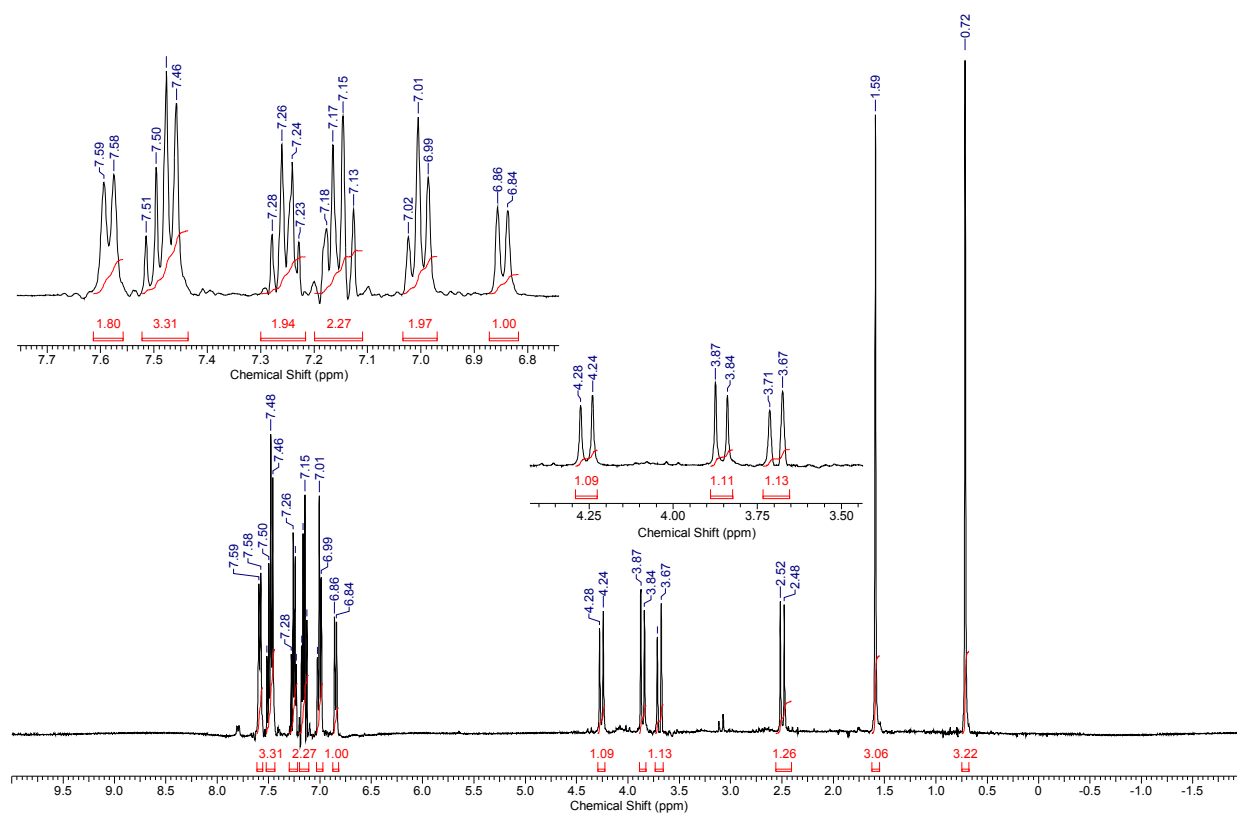


Figure S19. ^{13}C NMR spectrum (CDCl_3 , rt) of complex **3b**.

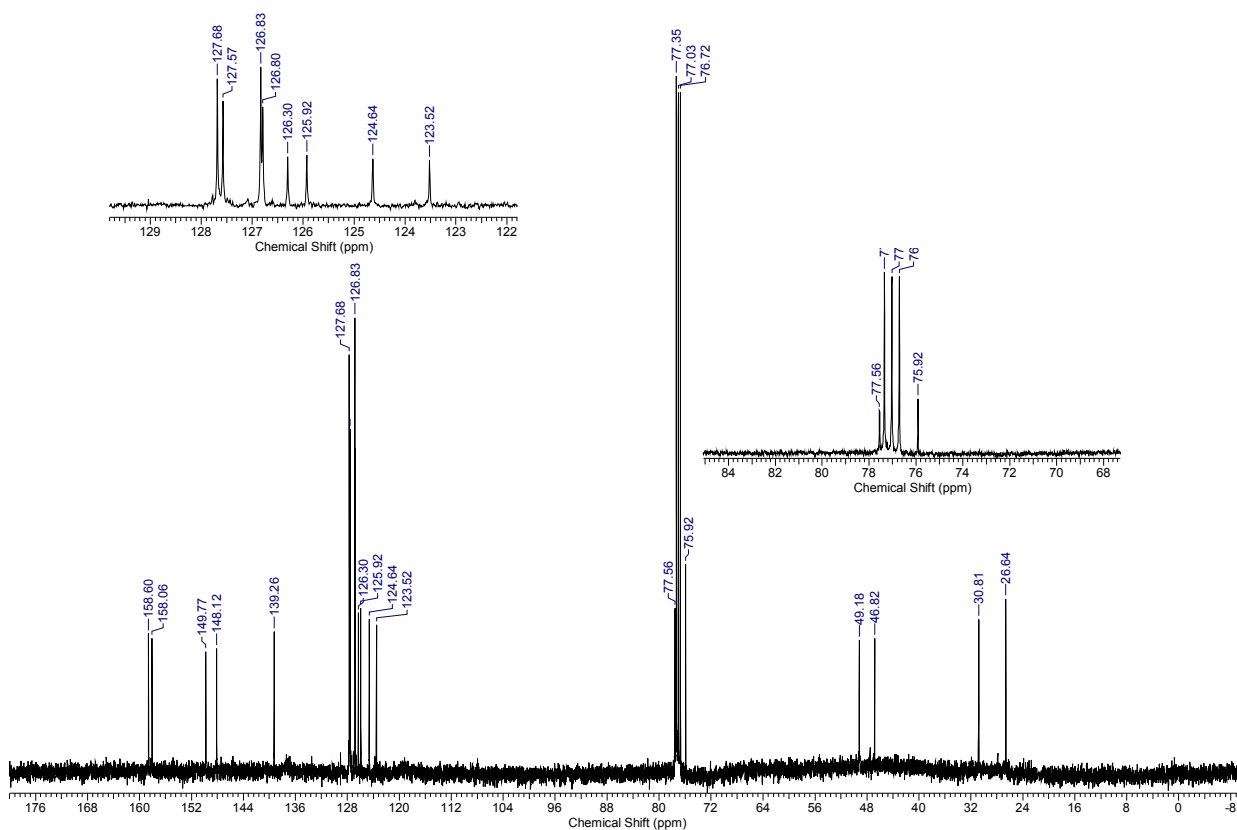


Figure S20. ^{13}C NMR spectrum (CDCl_3 , rt) of complex **3b**.

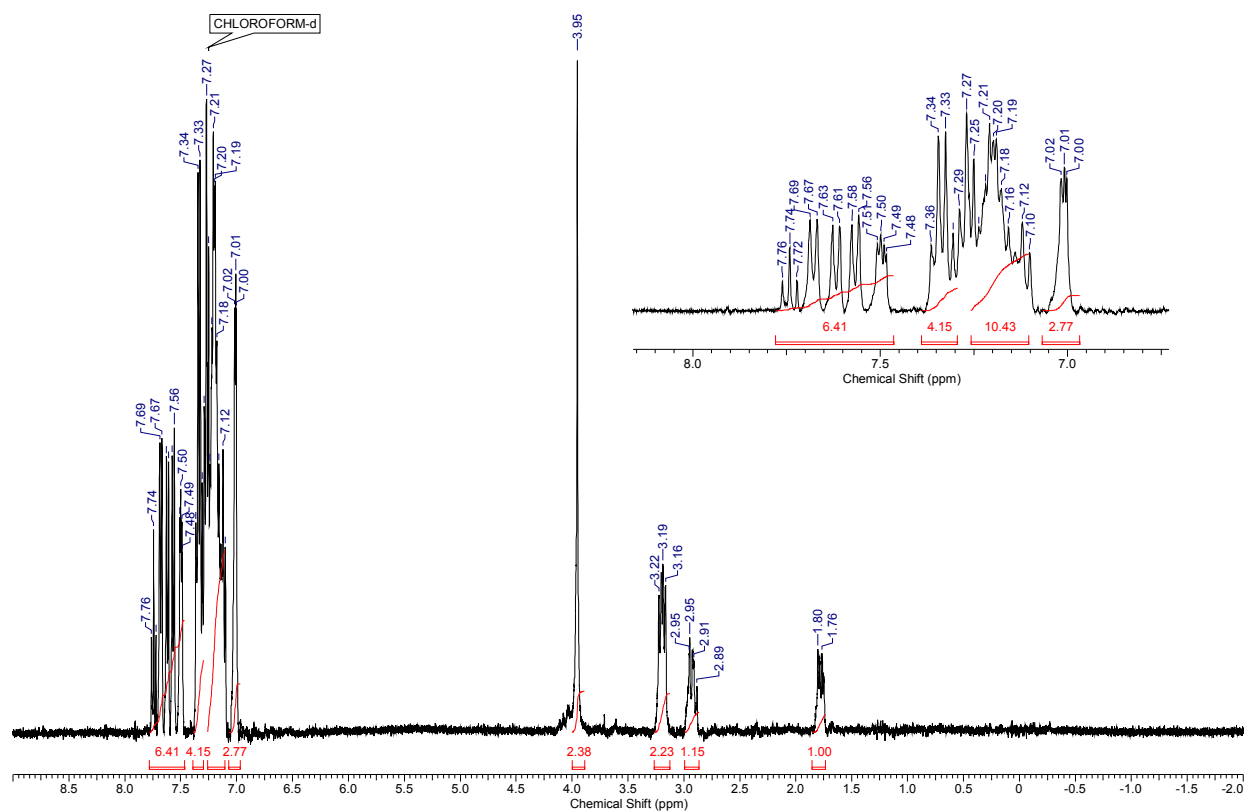


Figure S21. ¹H NMR spectrum (CDCl₃, rt) of complex **4b**.

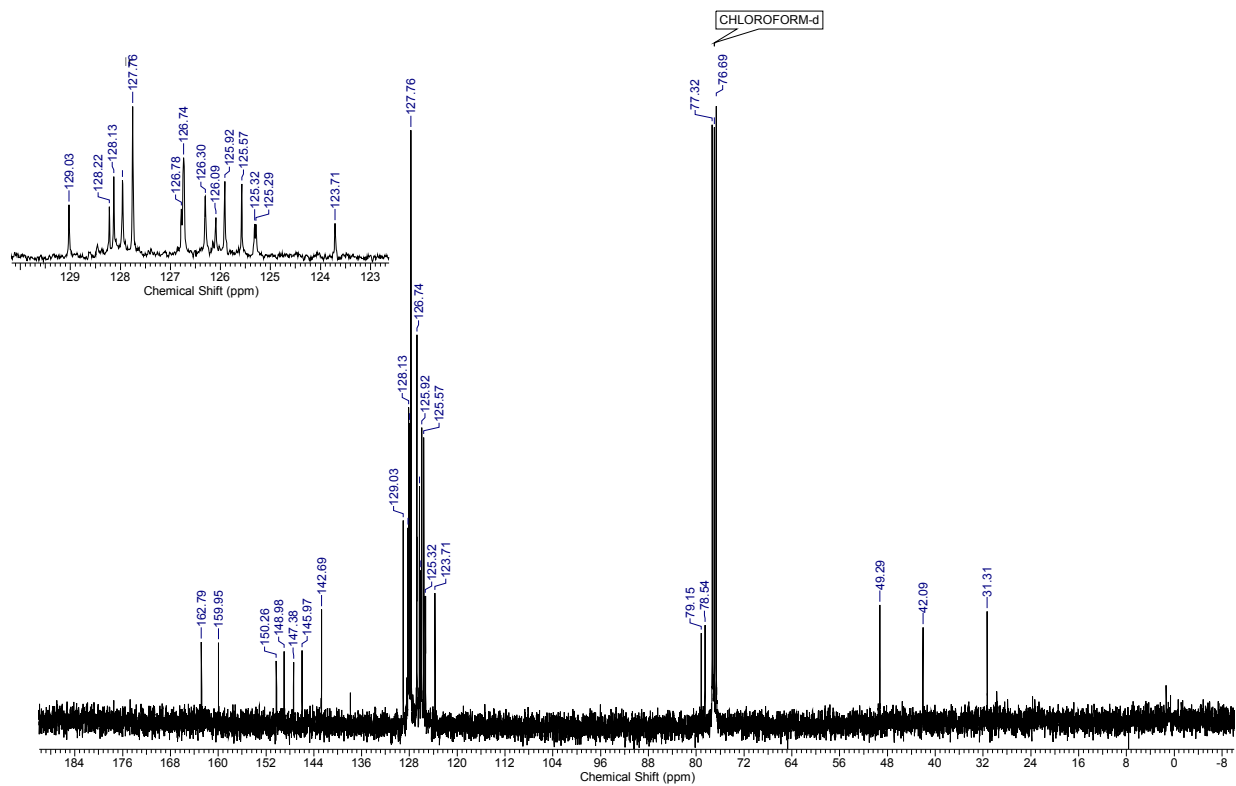


Figure S22. ¹³C NMR spectrum (CDCl₃, rt) of complex **4b**.

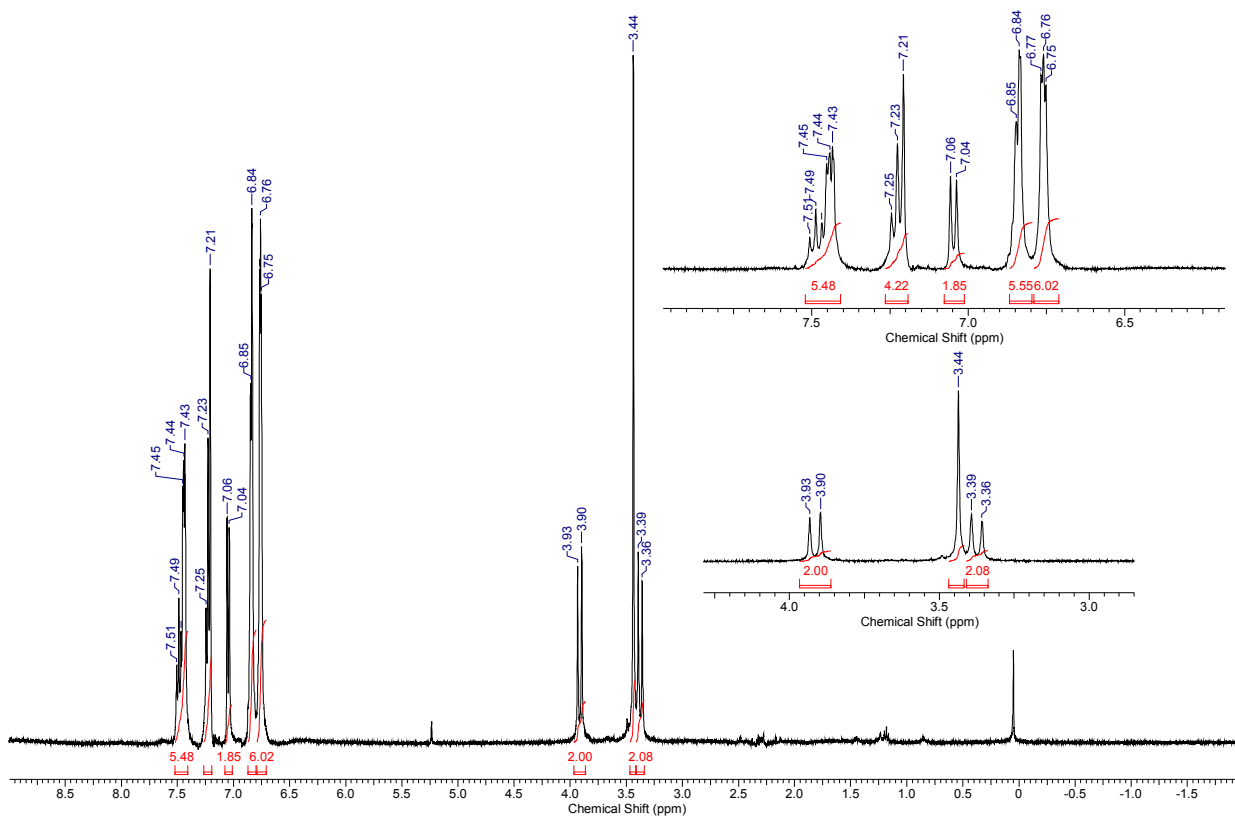


Figure S23. ¹H NMR spectrum (CDCl₃, rt) of complex **2c**.

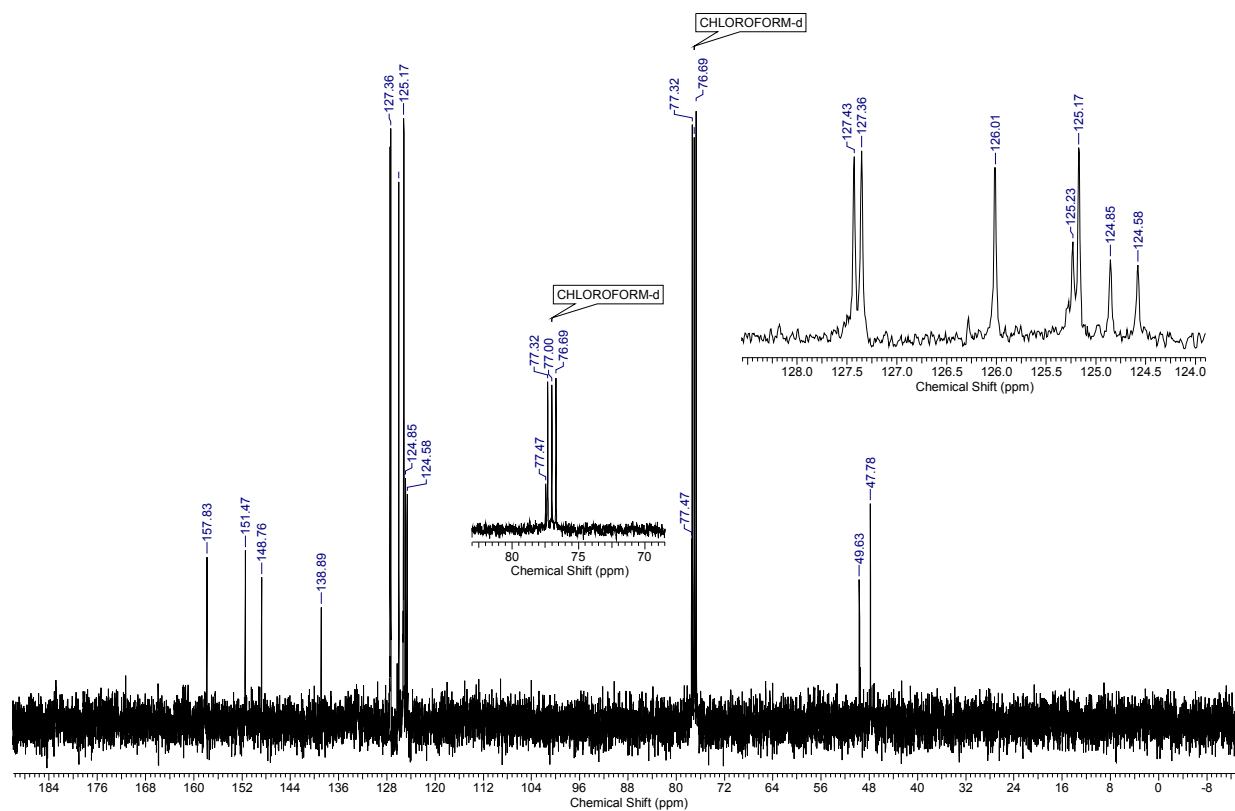


Figure S24. ¹³C NMR spectrum (CDCl₃, rt) of complex **2c**.

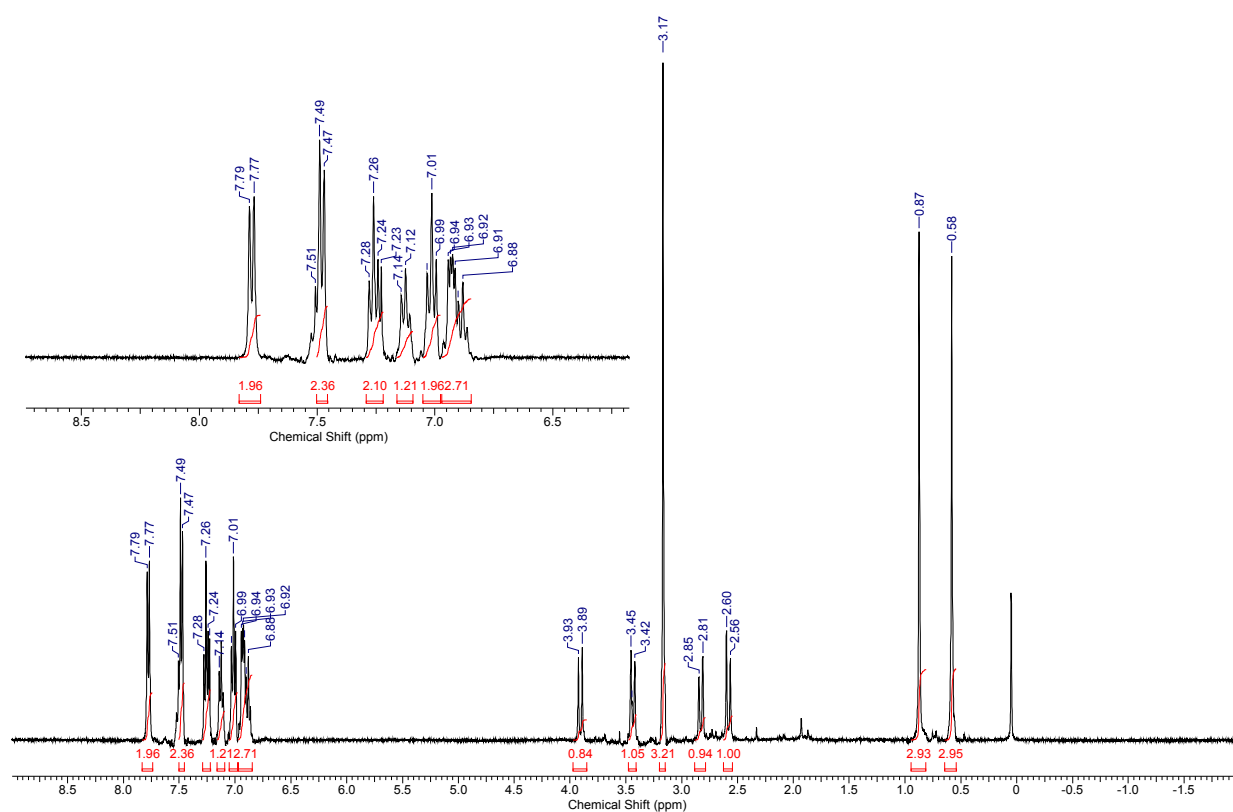


Figure S25. ¹H NMR spectrum (CDCl₃, rt) of complex **3c**.

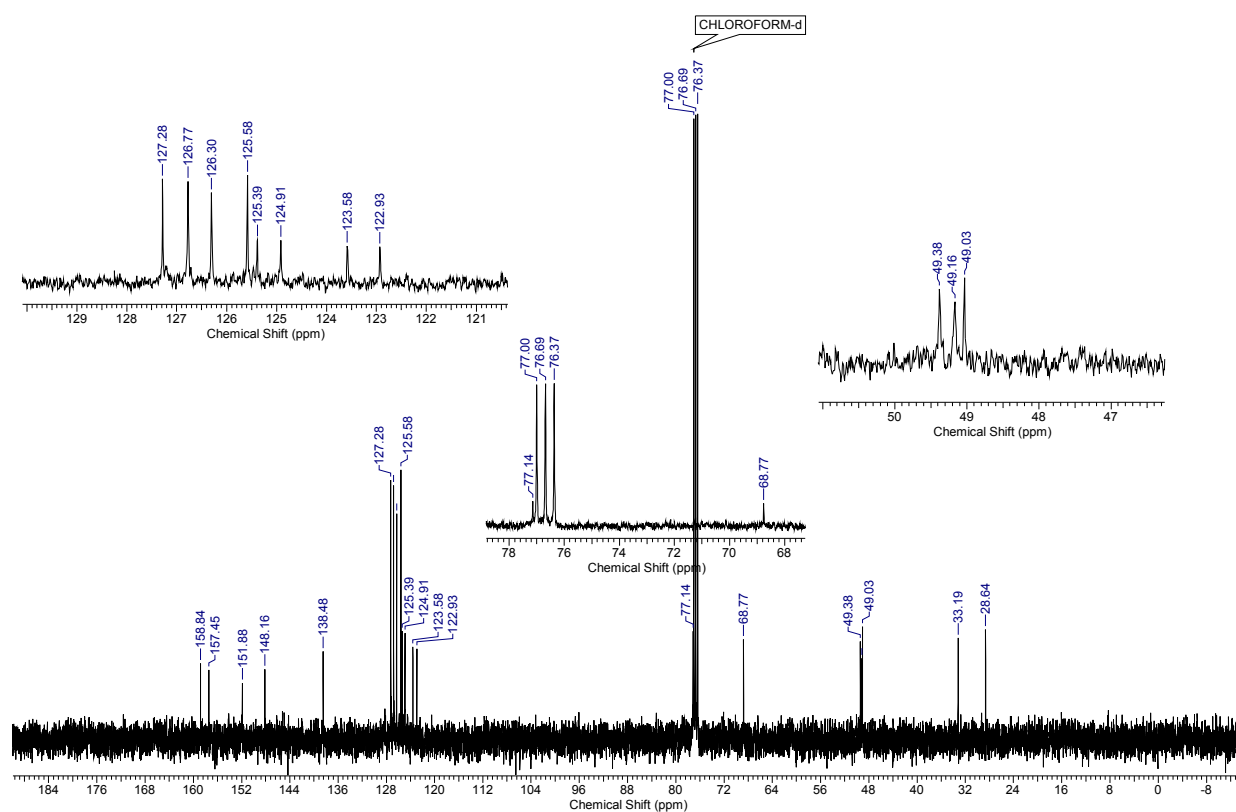


Figure S26. ¹³C NMR spectrum (CDCl₃, rt) of complex **3c**.

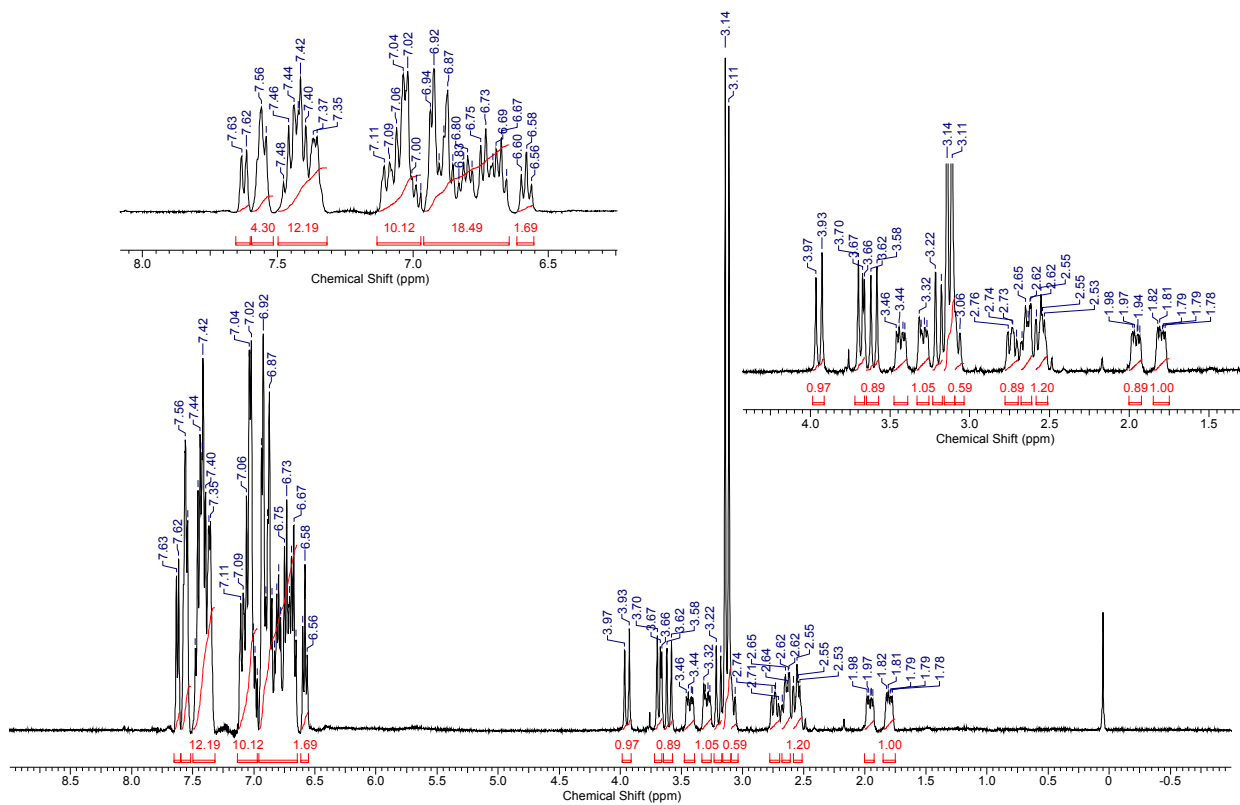


Figure S27. ^1H NMR spectrum (CDCl_3 , rt) of complex **4c**.

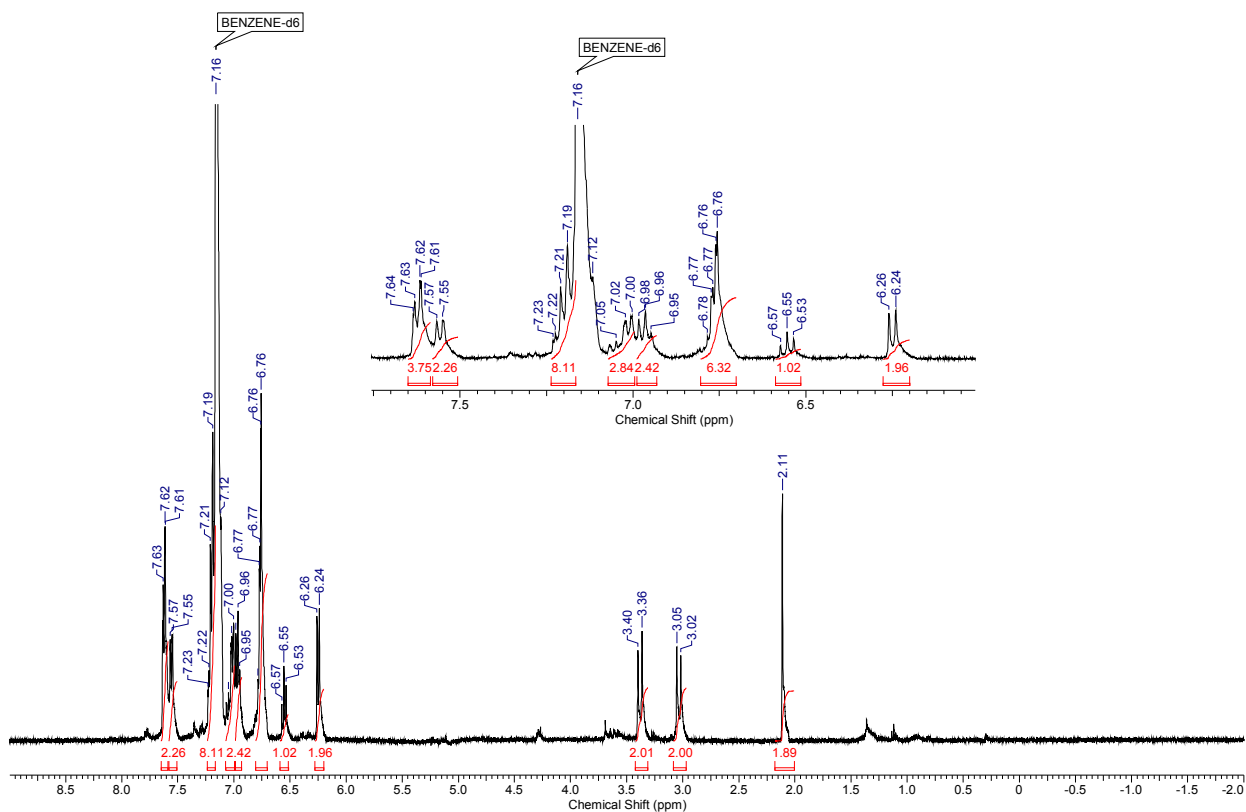


Figure S28. ^1H NMR spectrum (C_6D_6 , rt) of complex **2d**.

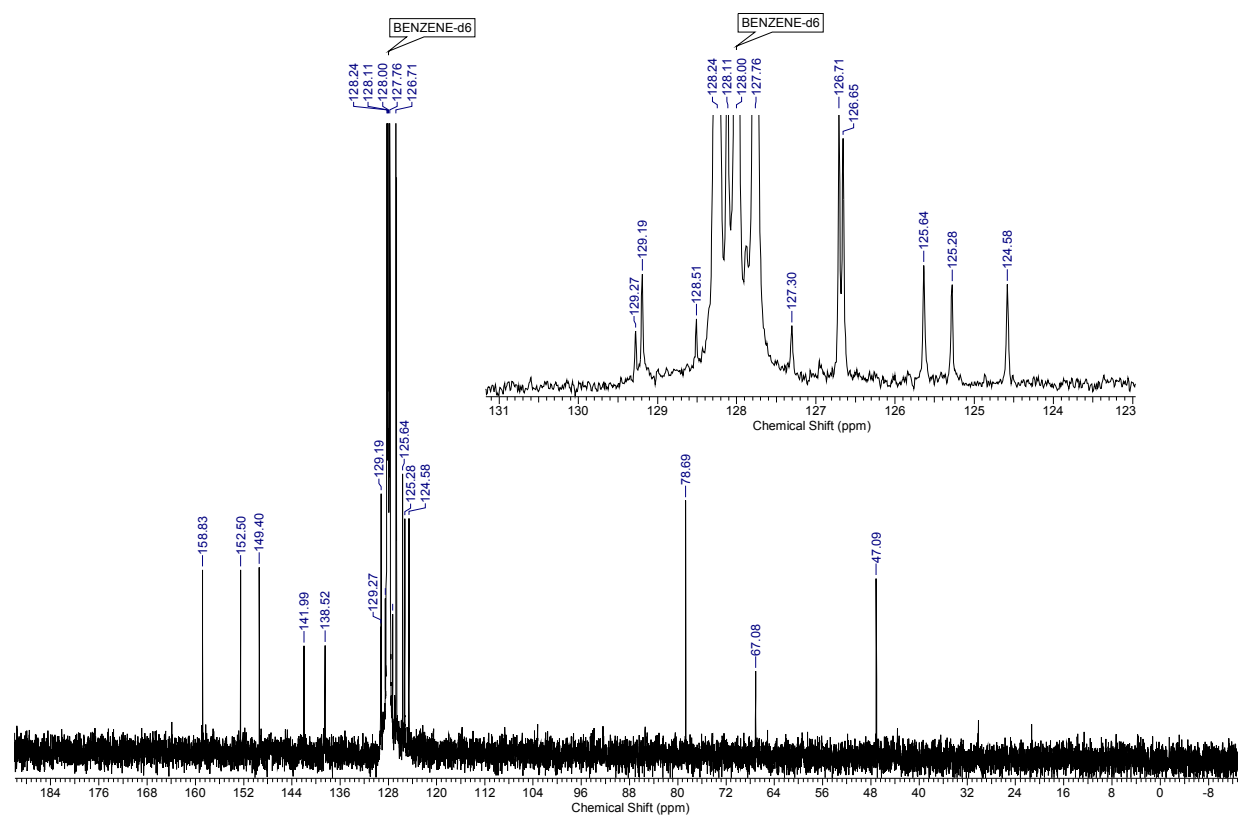


Figure S29. ^{13}C NMR spectrum (C_6D_6 , rt) of complex **2d**.