

Supplementary Information

Coupling Reaction between CO₂ and Cyclohexene Oxide: Selective Control from Cyclic Carbonate to Polycarbonate by Ligand Design of Salen/Salalen Titanium Complexes

Yong Wang,^{a,b} Yusheng Qin,^{*a} Xianhong Wang,^{a} and Fosong Wang^a**

^a Key Laboratory of Polymer Ecomaterials, Changchun Institute of Applied Chemistry, Chinese Academy of Sciences, Changchun 130022, People's Republic of China.

^b University of Chinese Academy of Sciences, Beijing 100039, People's Republic of China.

*Corresponding author at: Key Laboratory of Polymer Ecomaterials, Changchun Institute of Applied Chemistry, Chinese Academy of Sciences, Changchun 130022, People's Republic of China. Fax: +86 0431 85262252; Tel: +86 0431 85262252, E-mail addresses: ysqin@ciac.jl.cn.

**Corresponding author at: Key Laboratory of Polymer Ecomaterials, Changchun Institute of Applied Chemistry, Chinese Academy of Sciences, Changchun 130022, People's Republic of China. Fax: +86 0431 85689095; Tel: +86 0431 85262250, E-mail addresses: xhwang@ciac.jl.cn.

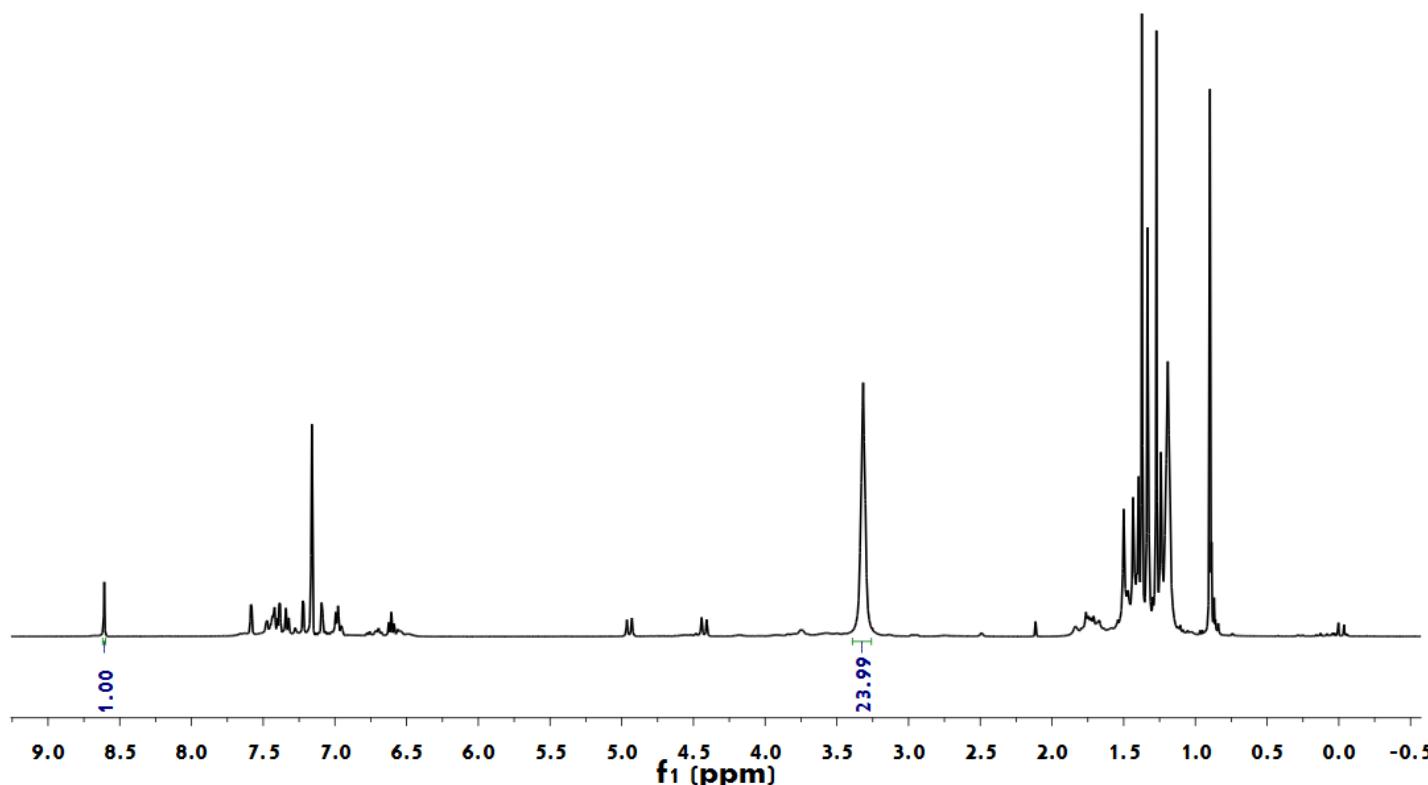


Fig. S1 ^1H NMR spectrum of the lithium salt of salalen (C_6D_6), the integral area of 1.00 stands for one H on the ligand (- $\text{CH}=\text{N}-$), thus the peak at 3.32ppm with an integral area of 23.99 stands for 24 H corresponding to hydrogen on THF(- $\text{O}-\text{CH}_2-$) corresponding to 6 THF.

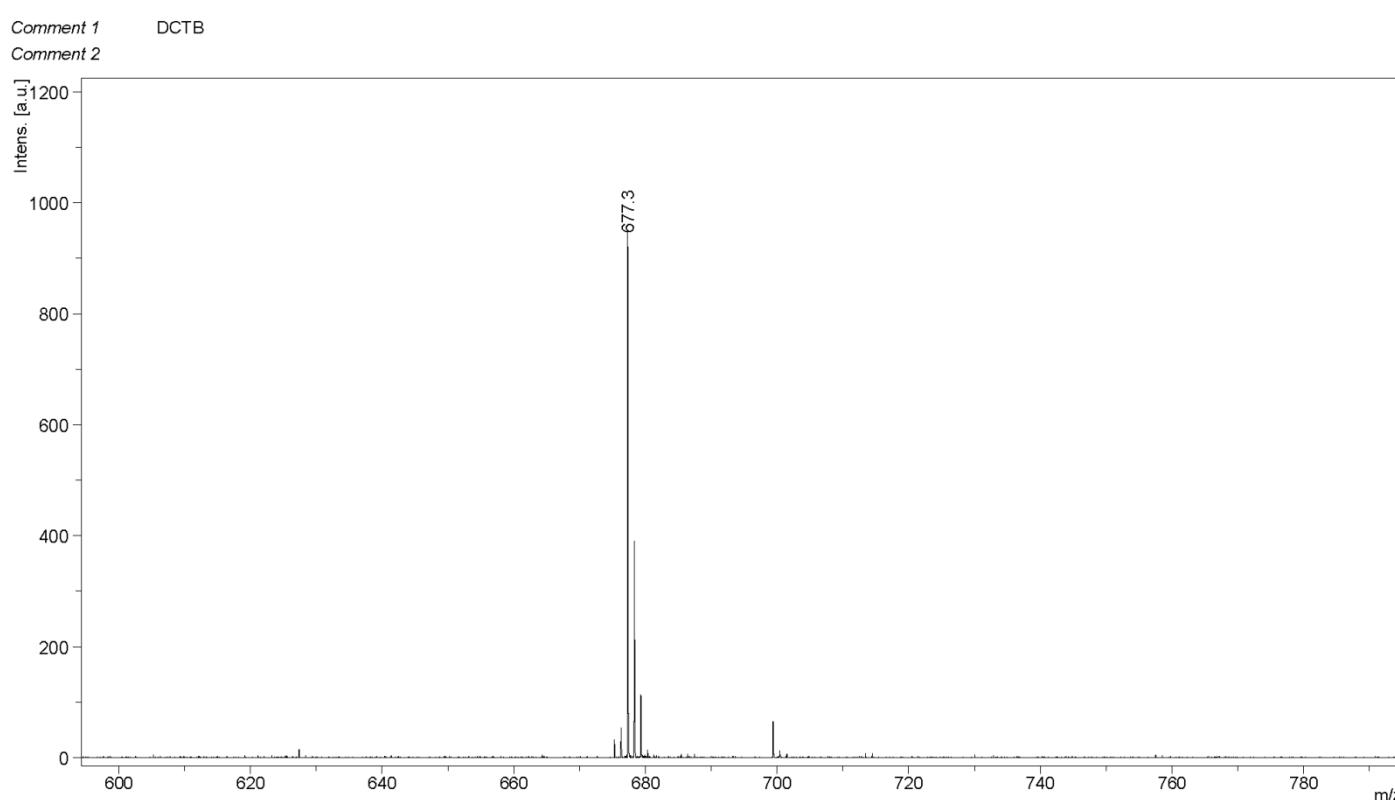


Fig. S2 MALDI-TOF-MS of complex **2**, DCTB, (2-[(2E)-3- (4-tert-butylphenyl)-2-Methylprop-2-enylidene] malononitrile) as matrix, m/z 677.3 $^+$ is corresponding to $[(\text{Salalen})\text{Ti}(\text{THF})\text{Cl}-\text{Cl}+\text{H}_2\text{O}]^+$.

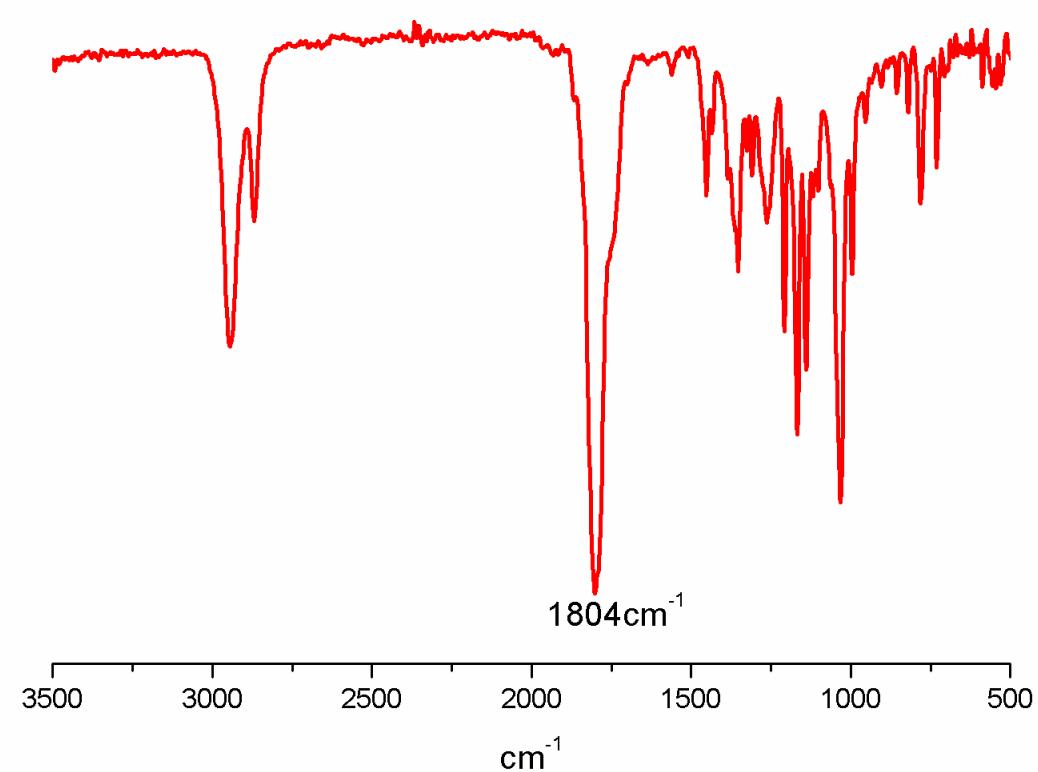


Fig. S3 FTIR spectrum of *cis*-CHC, peak at 1804 cm⁻¹ stands for the carbonyl stretching frequency.

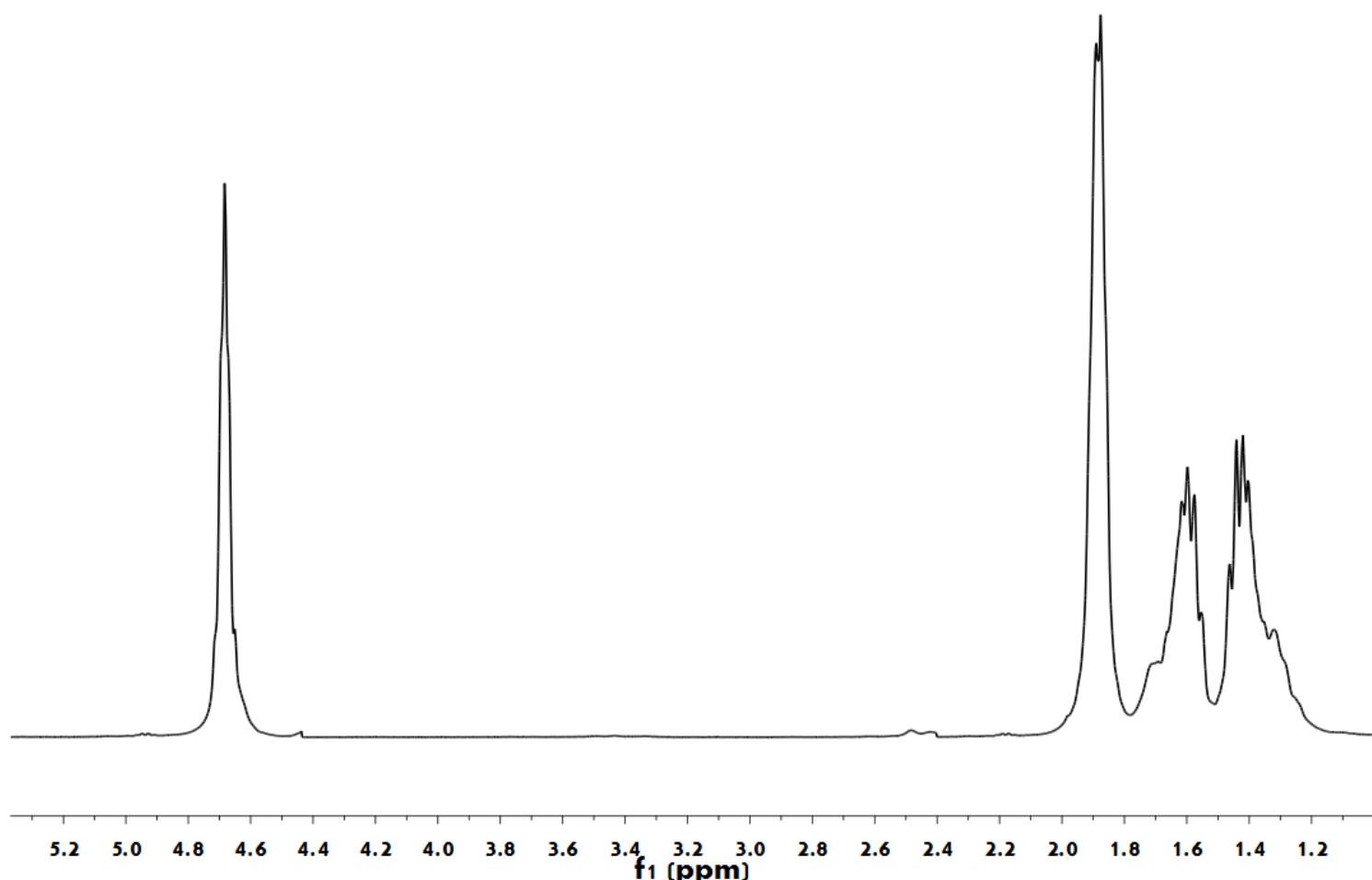


Fig. S4 ¹H NMR spectrum of *cis*-CHC (CDCl₃).

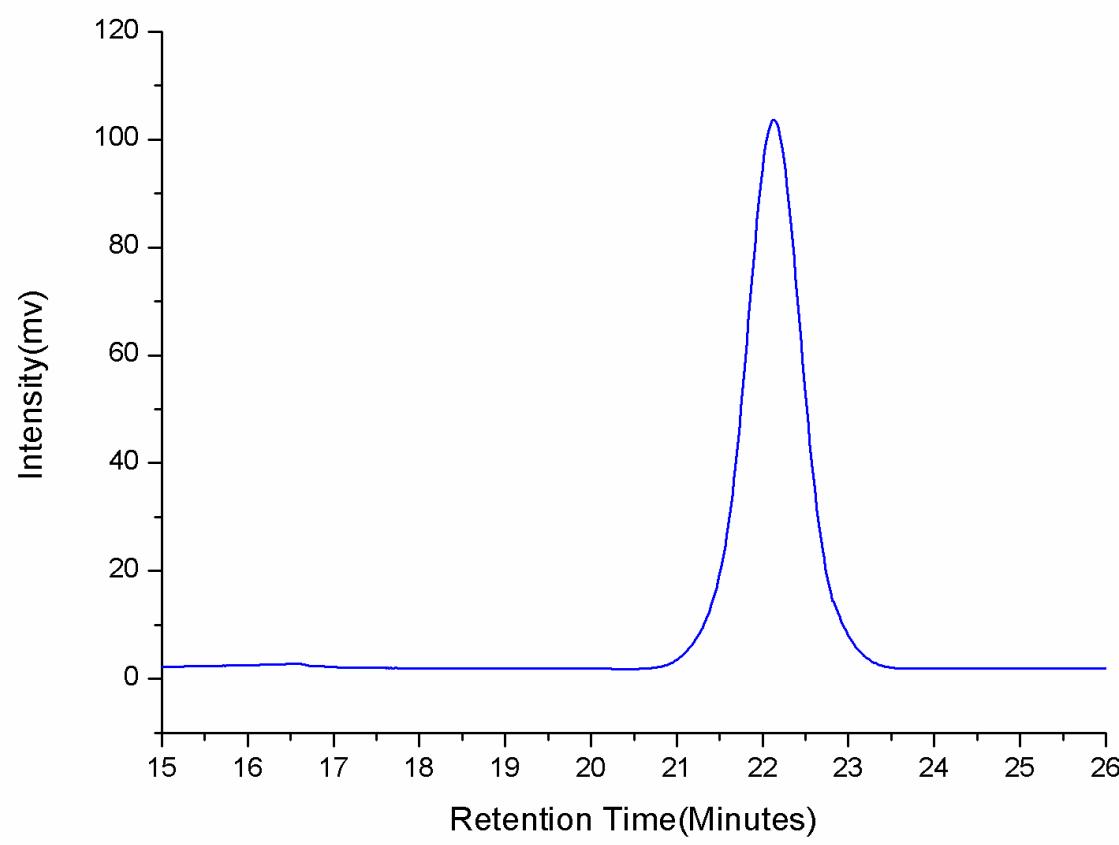


Fig. S4 GPC traces for PCHC produced using complex **2**, (Table 2 entry 11, Mn : 6000, Mw/Mn = 1.11) (CH_2Cl_2 eluent).

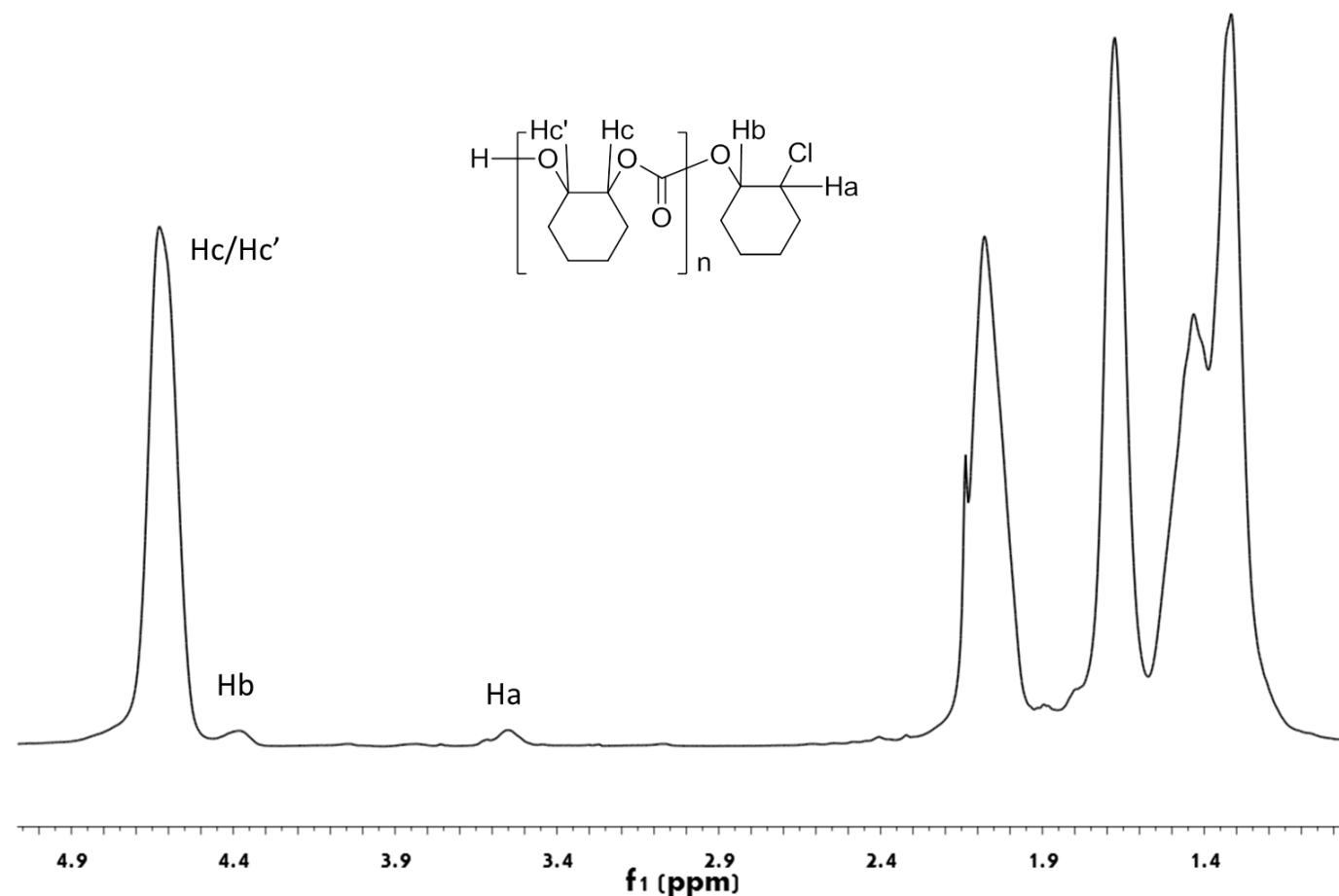


Fig. S5 ^1H NMR spectrum of the PCHC (Table 2, entry 11) (CDCl_3).

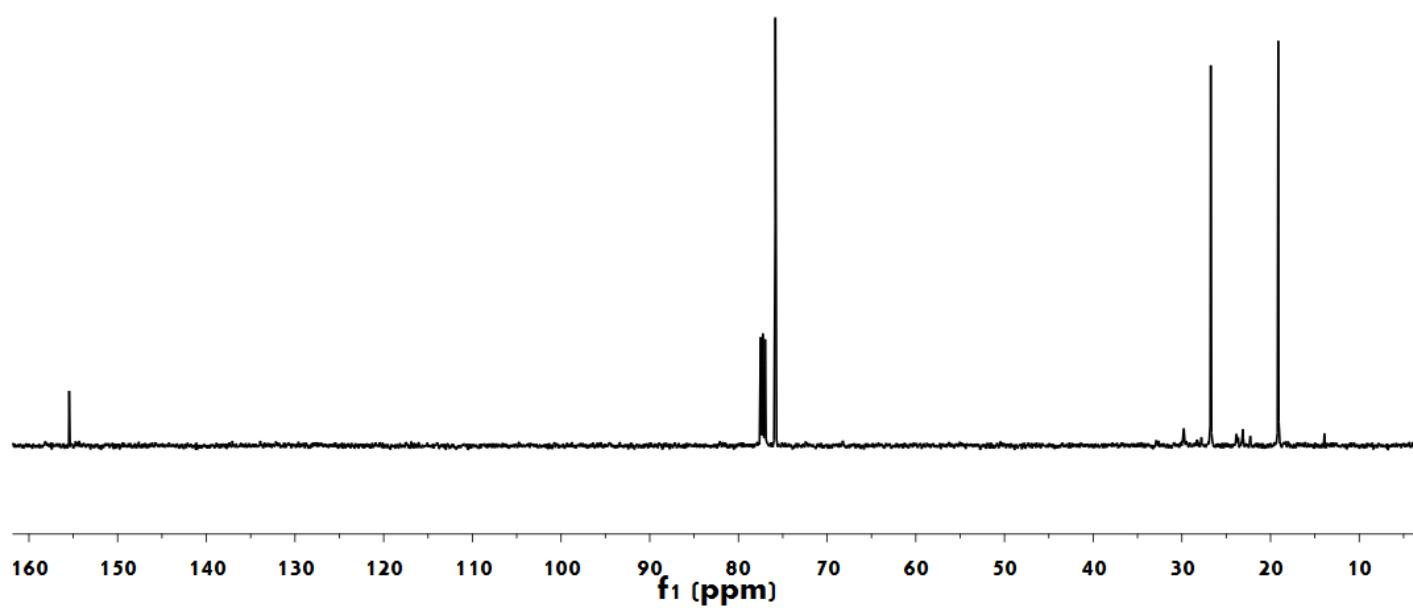


Fig. S7 ^{13}C NMR spectrum of *cis*-CHC (CDCl_3).

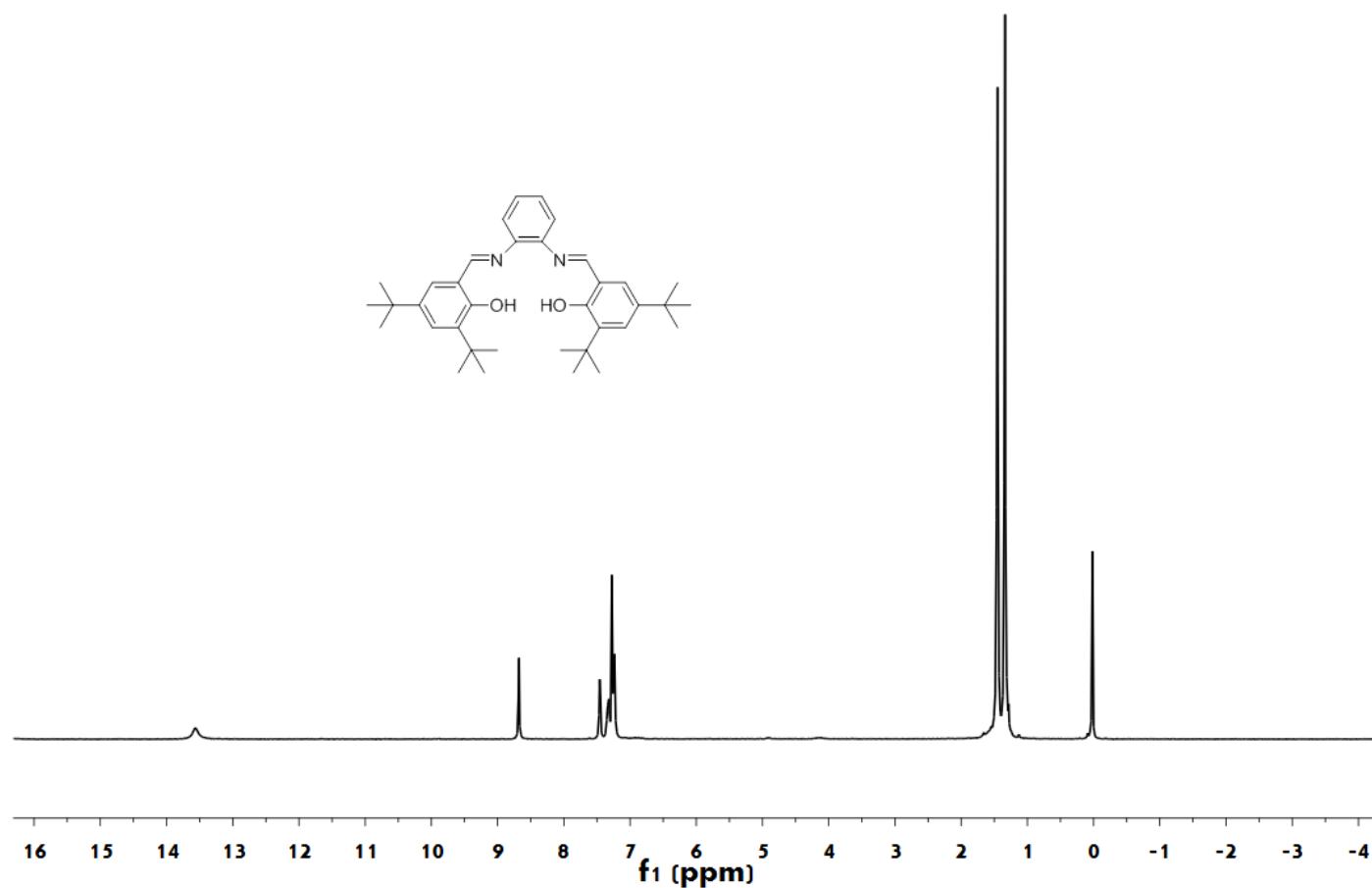


Fig. S8 ^1H NMR spectrum of salen ligand (CDCl_3)

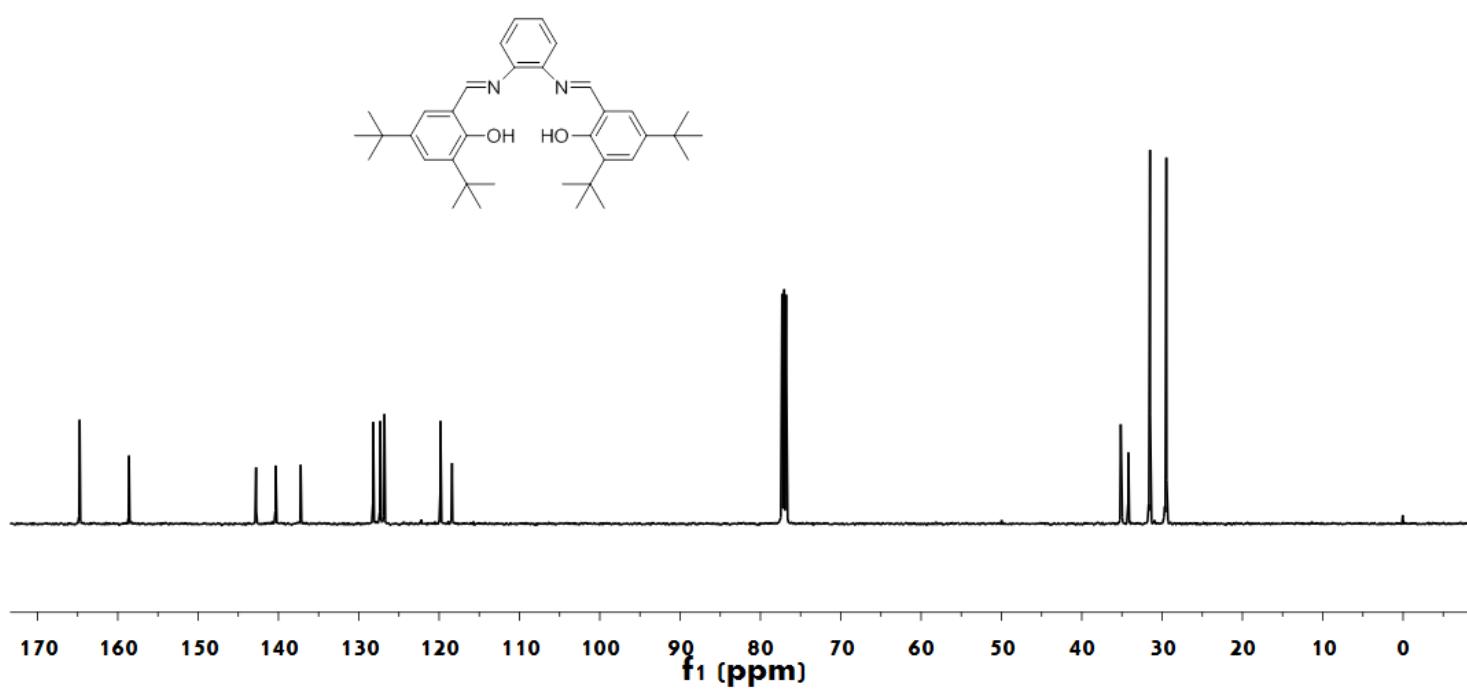


Fig. S9 ^{13}C NMR spectrum of salen ligand(CDCl_3)

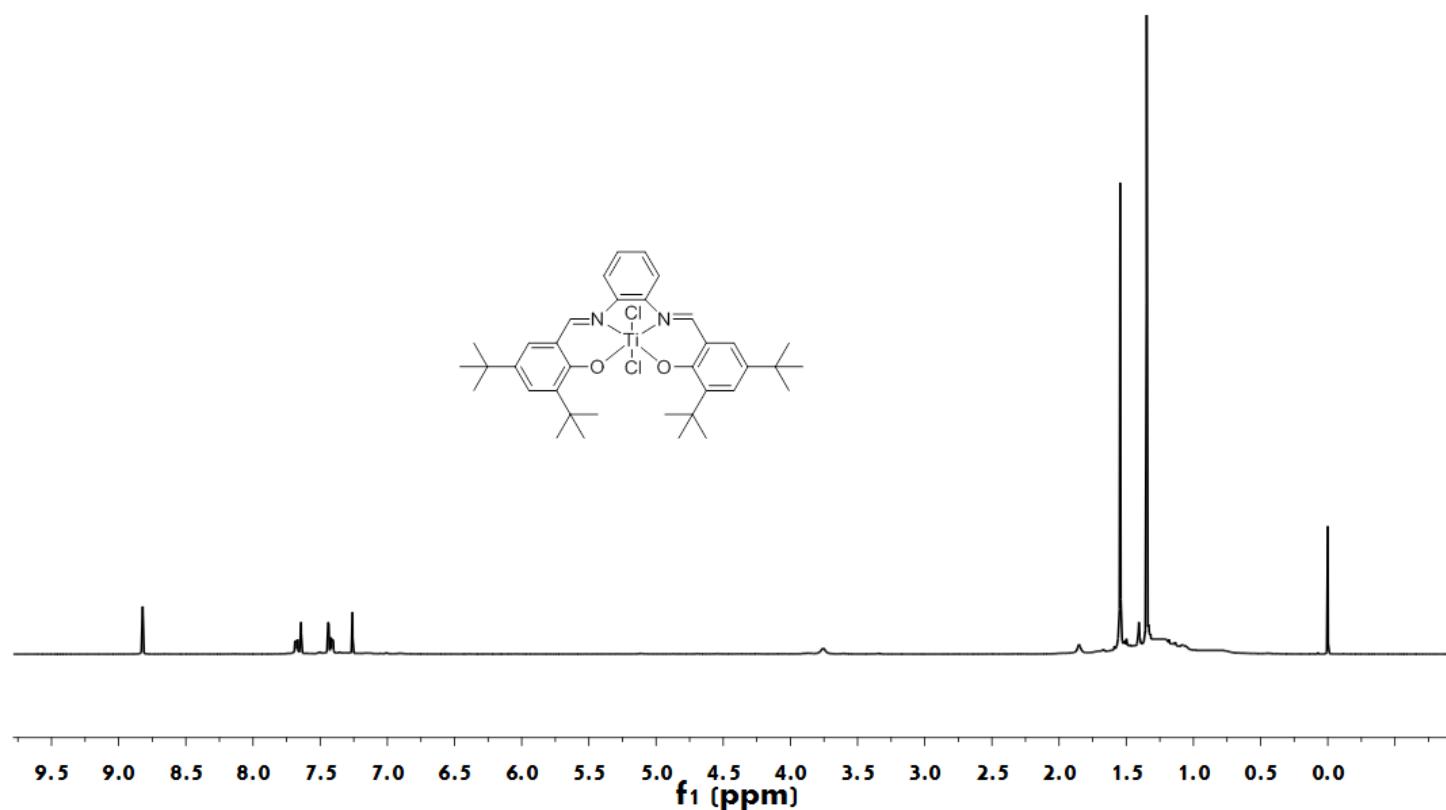


Fig. S10 ^1H NMR spectrum of (Salen)Ti(IV)Cl₂(CDCl_3)

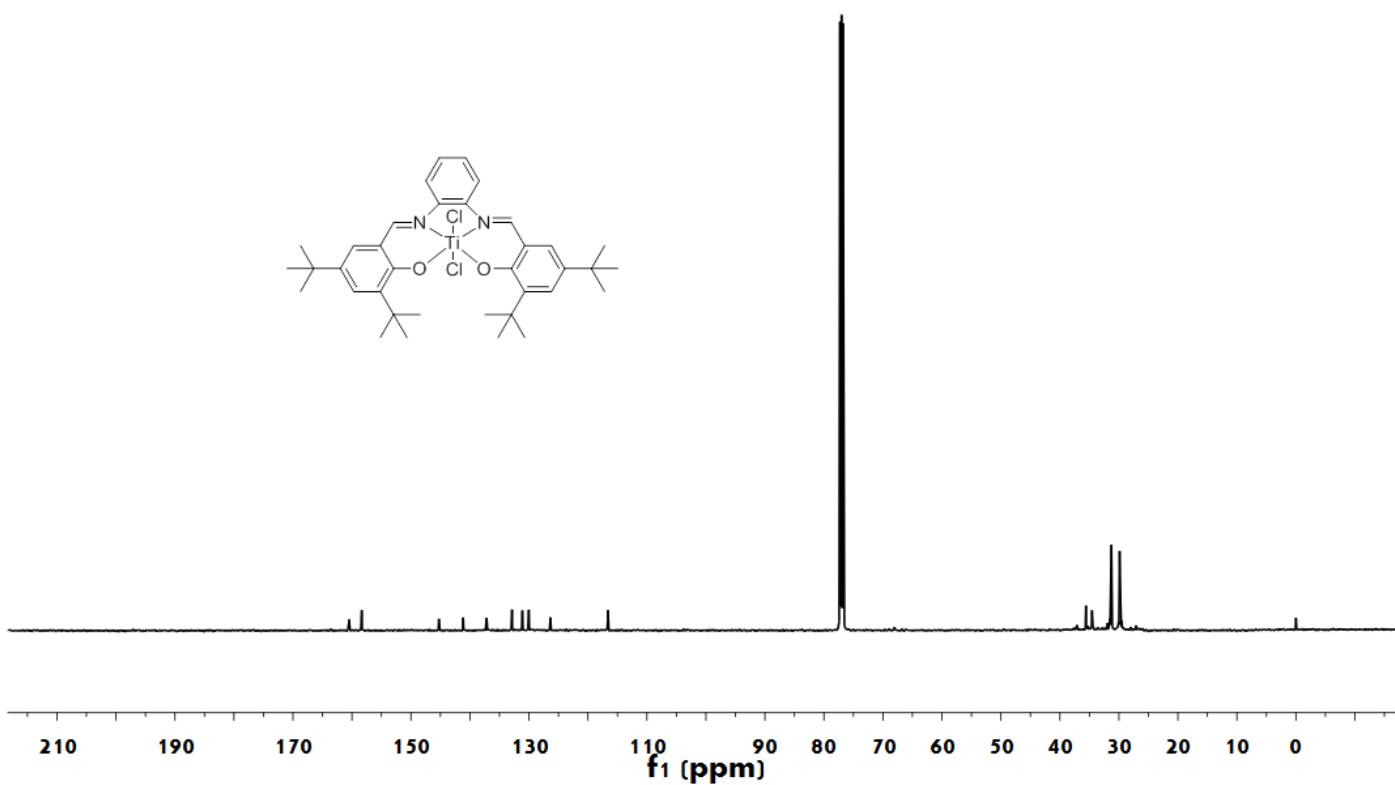


Fig. S11 ^{13}C NMR spectrum of $(\text{Salen})\text{Ti}(\text{IV})\text{Cl}_2(\text{CDCl}_3)$

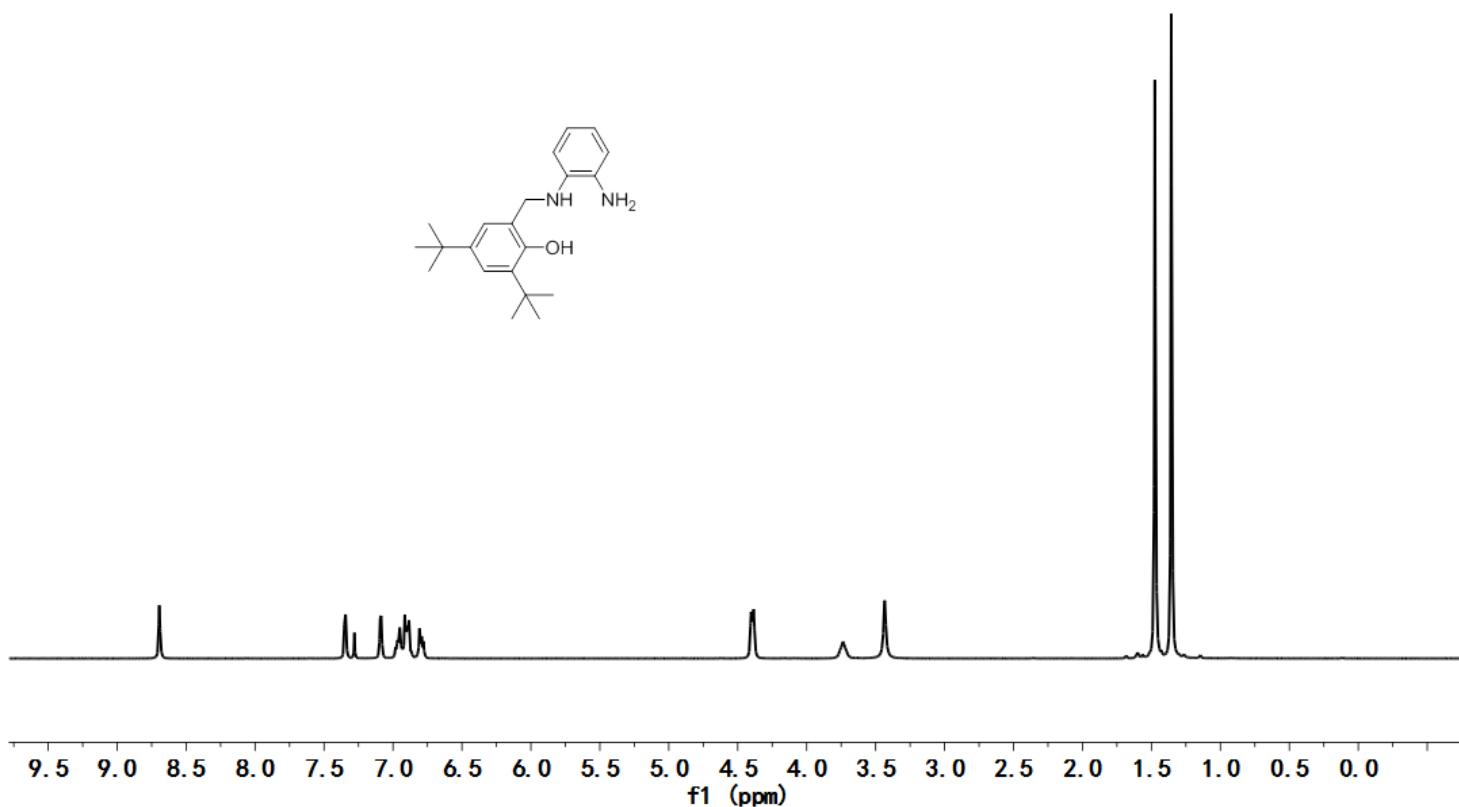


Fig. S12 ^1H NMR spectrum of compound **b** (CDCl_3)

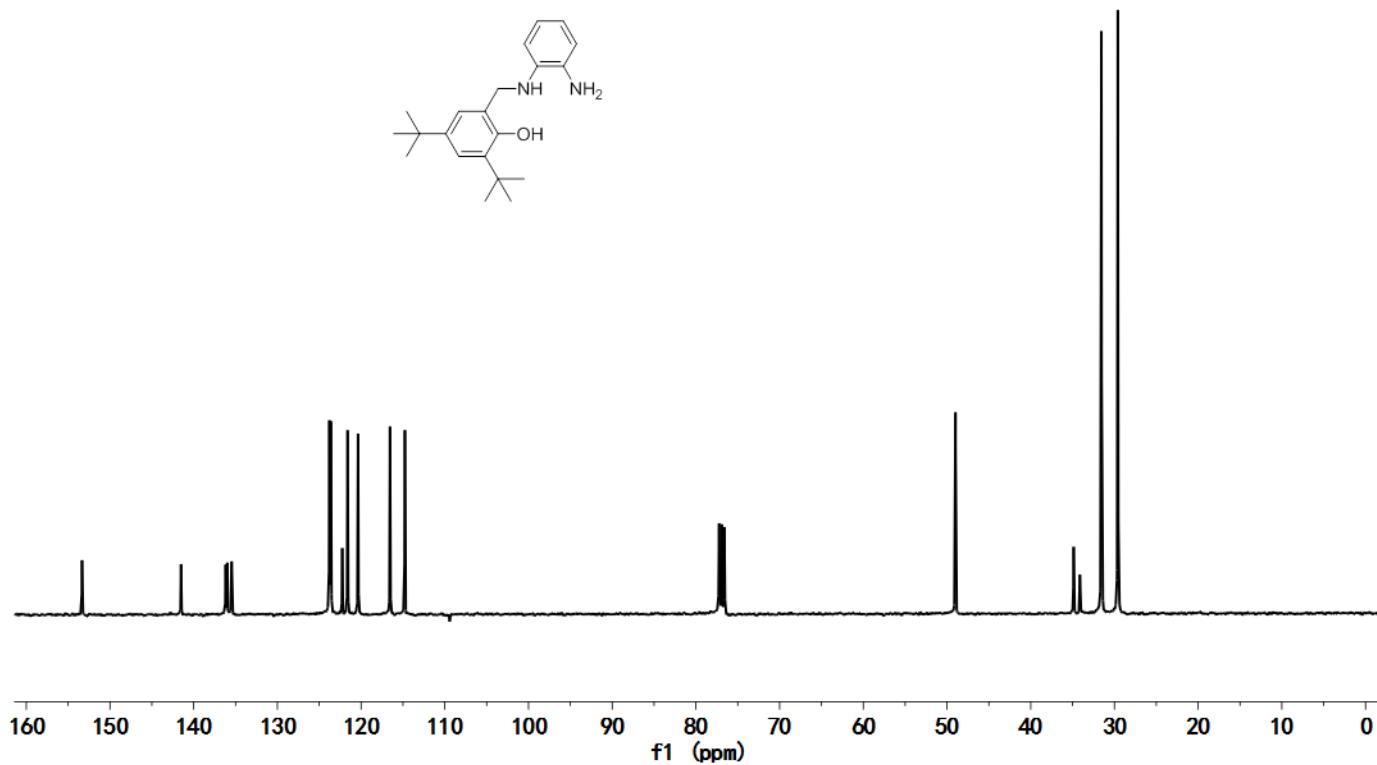


Fig. S13 ^{13}C NMR spectrum of compound **b** (CDCl_3)

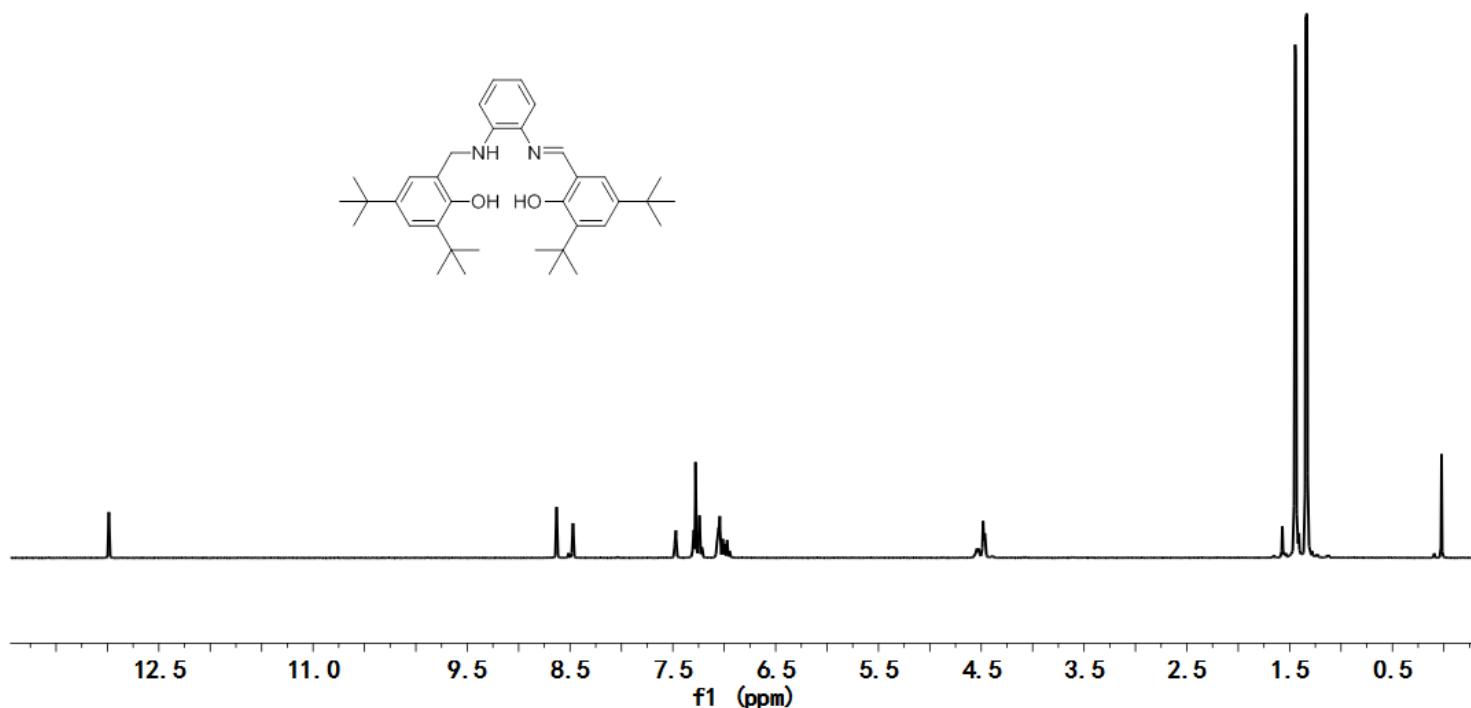


Fig. S14 ^1H NMR spectrum of salalen ligand (CDCl_3)

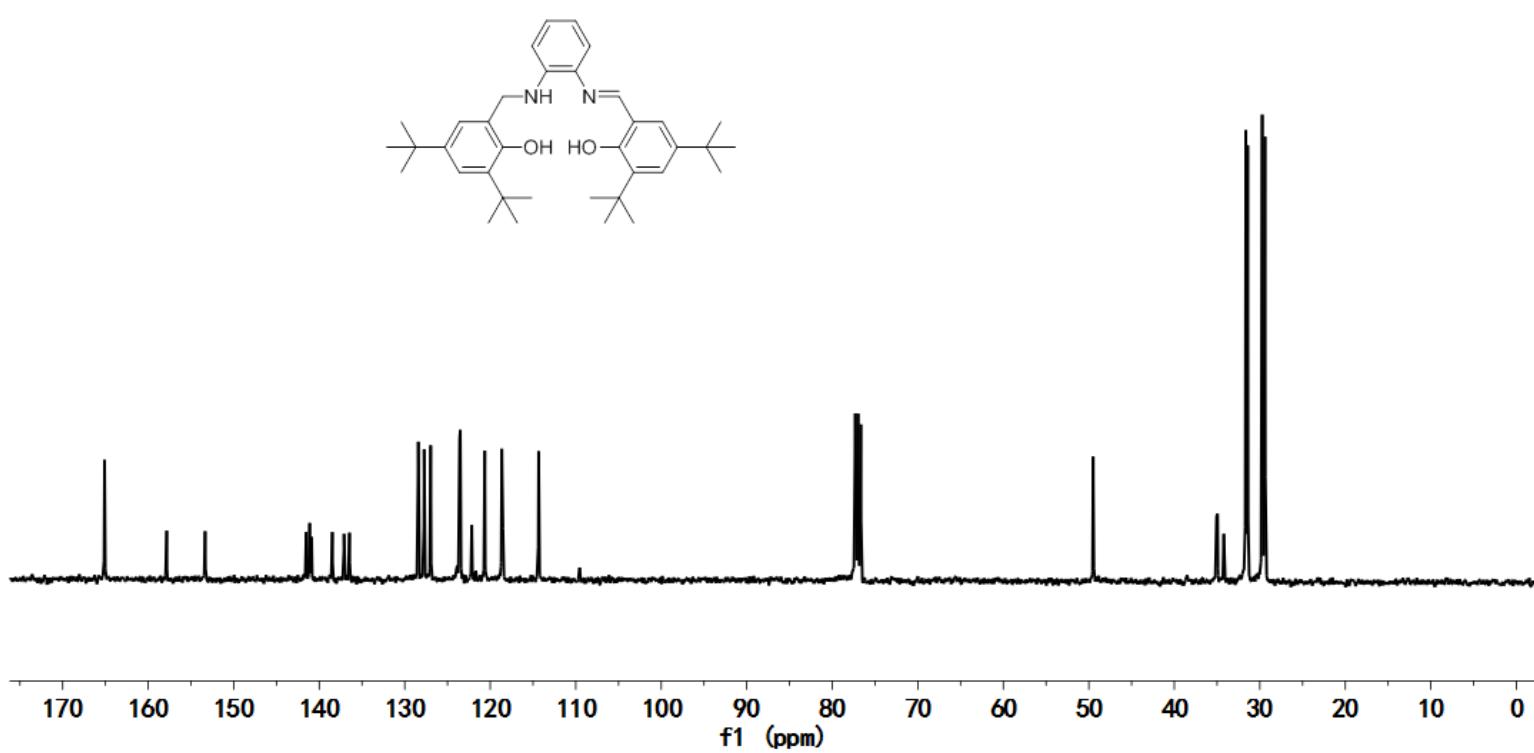


Fig. S15 ^{13}C NMR spectrum of salalen ligand (CDCl_3)

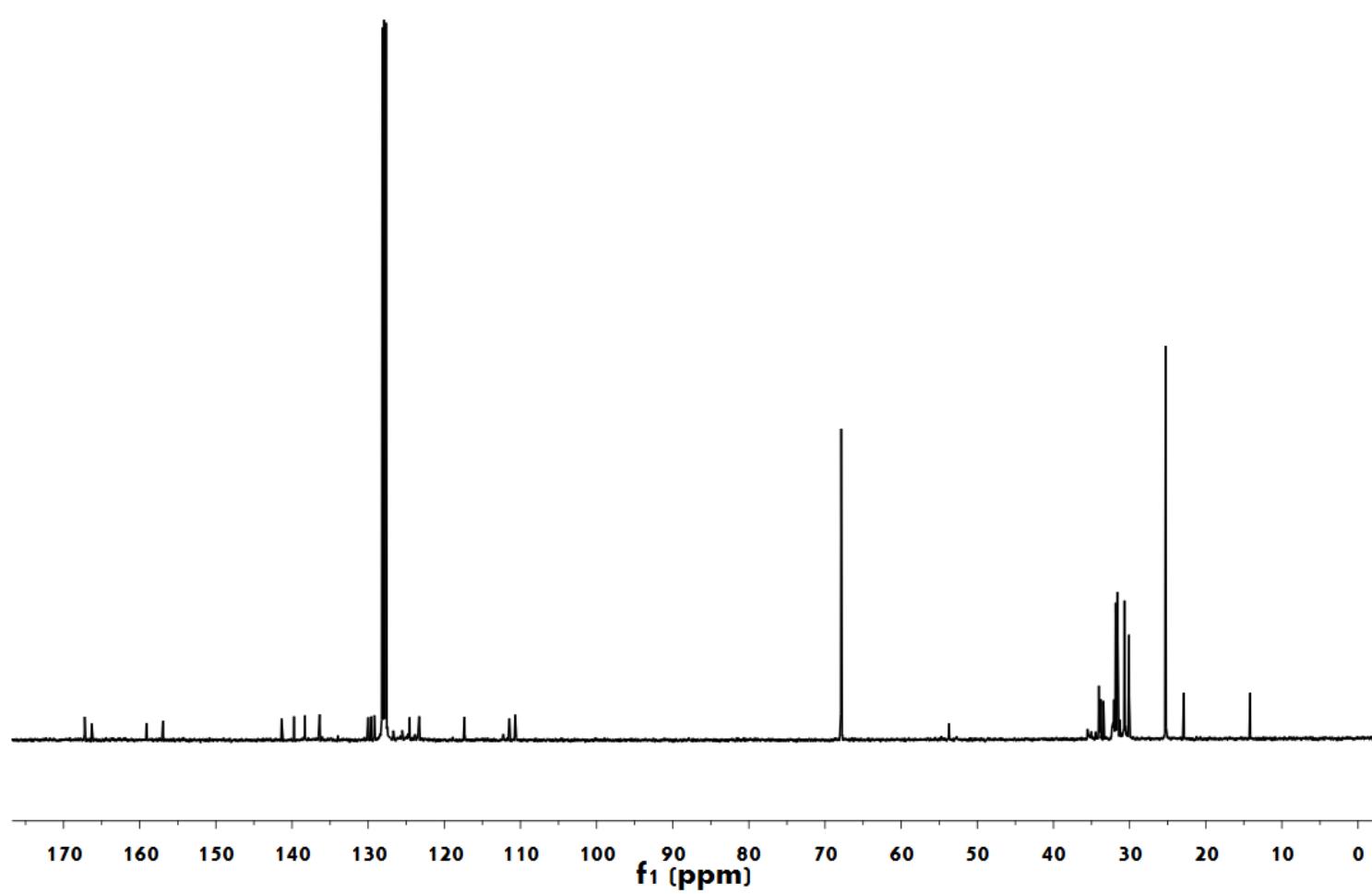


Fig. S16 ^{13}C NMR spectrum of the lithium salt of salalen (C_6D_6).