

Electronic Supporting Information

**Zinc complexes bearing BIAN ligands as efficient catalysts for the formation of cyclic carbonates from CO<sub>2</sub> and epoxides.**

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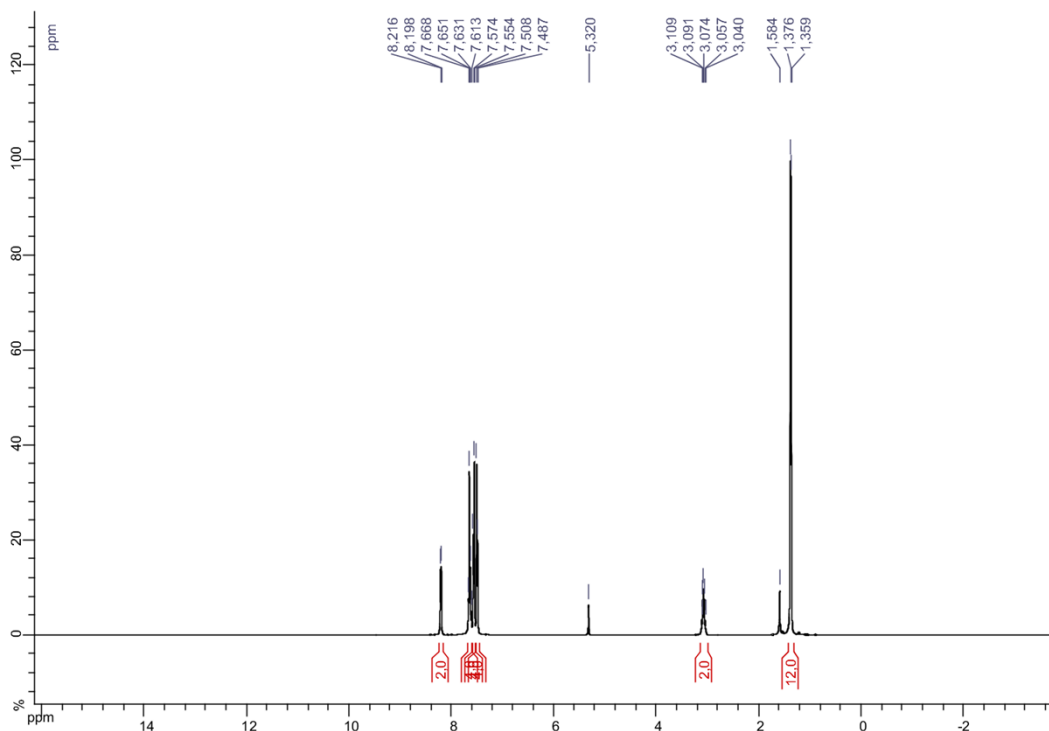


Figure S1.  $^1\text{H}$ -NMR spectra of complex **1** in  $\text{CD}_2\text{Cl}_2$ .

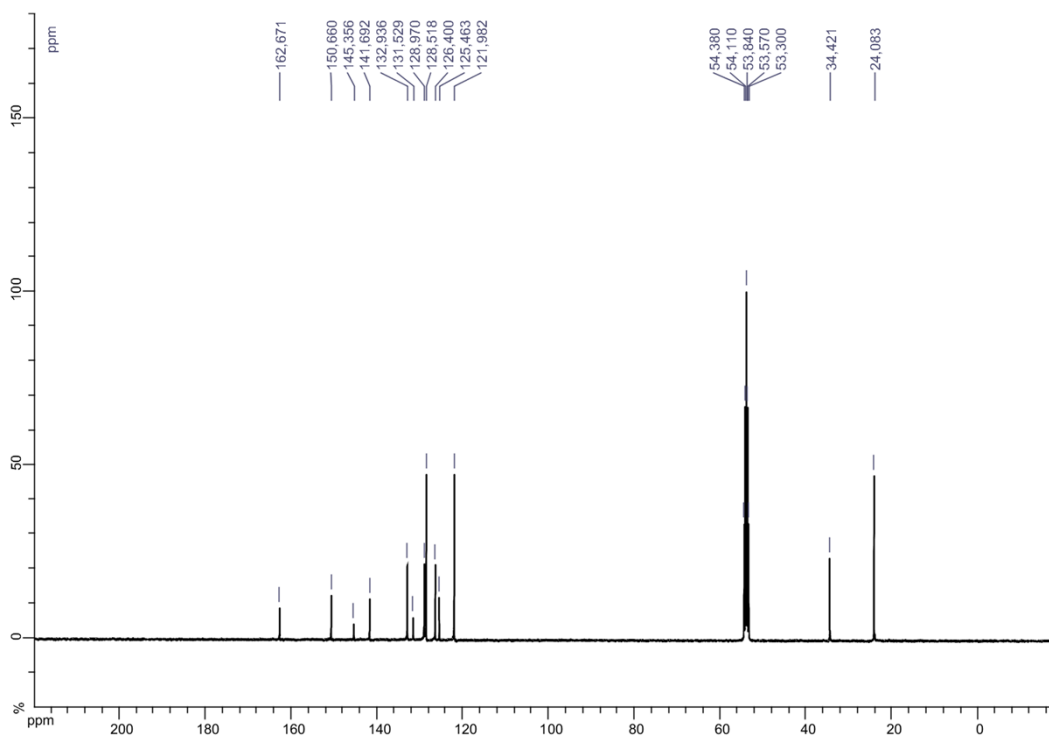


Figure S2.  $^{13}\text{C}$ -NMR spectra of complex **1** in  $\text{CD}_2\text{Cl}_2$ .

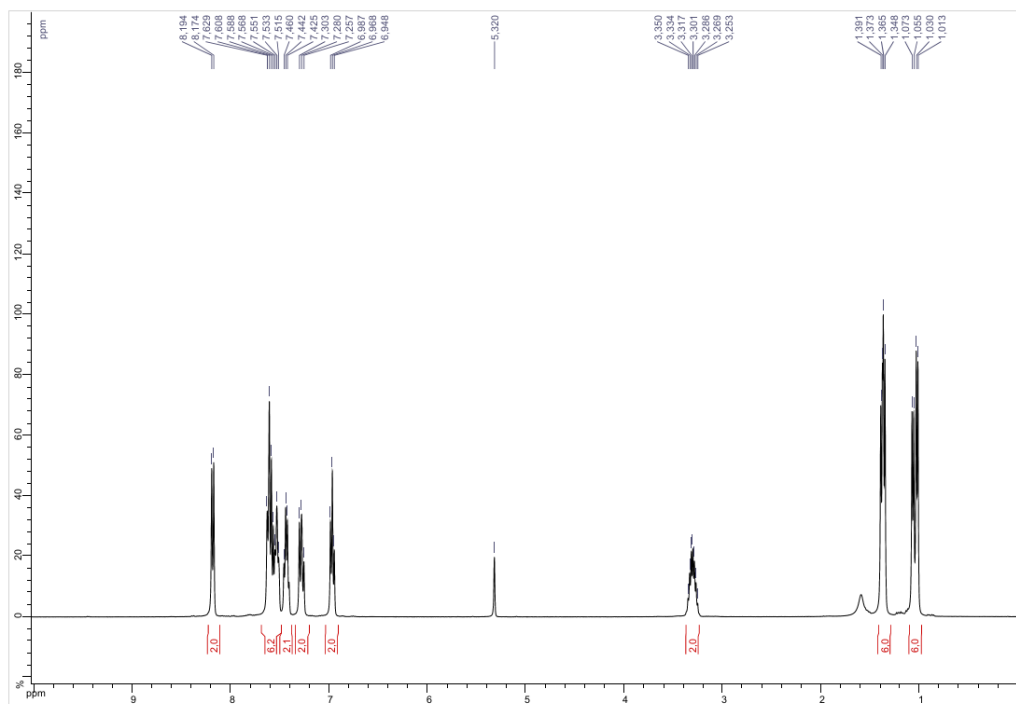


Figure S3.  $^1\text{H}$ -NMR spectra of complex **2** in  $\text{CD}_2\text{Cl}_2$ .

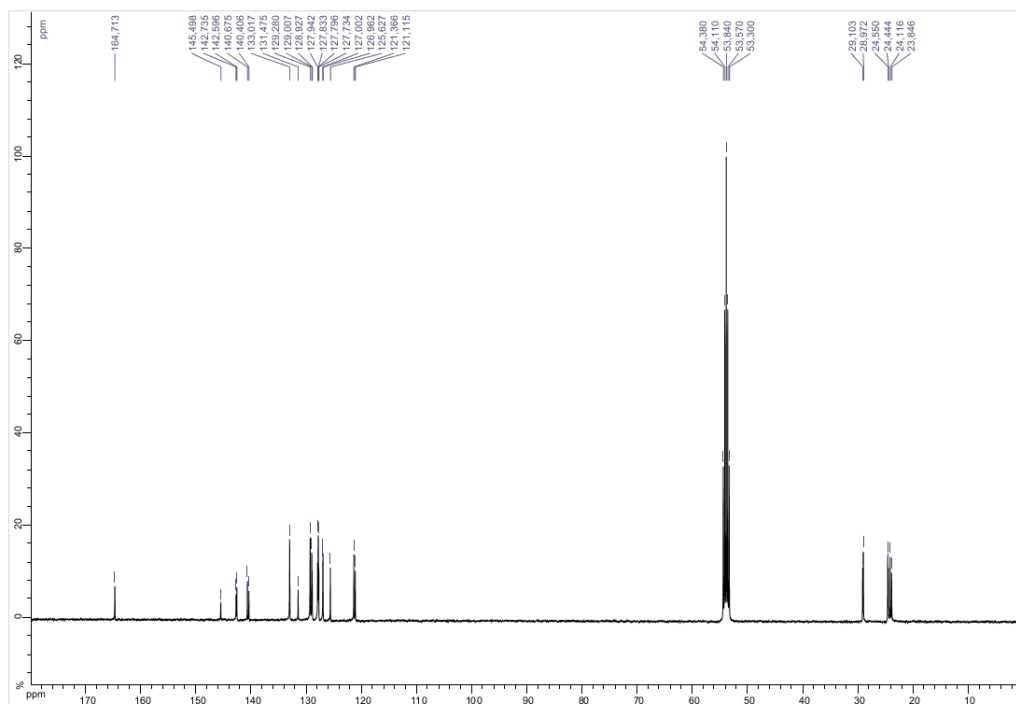


Figure S4.  $^{13}\text{C}$ -NMR spectra of complex **2** in  $\text{CD}_2\text{Cl}_2$ .

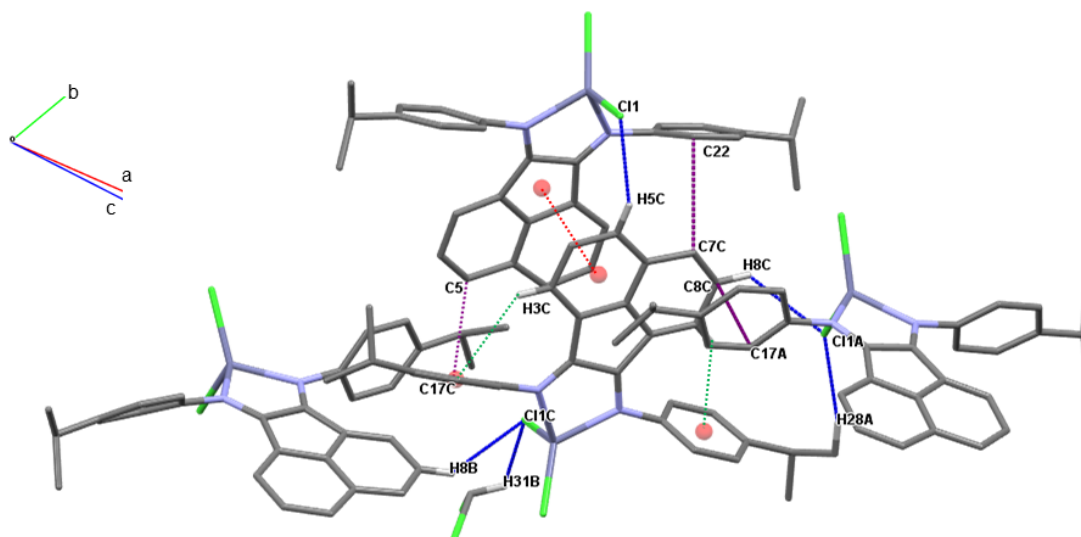


Figure S5. View of the 3D arrangement in the crystal structure of complex **1**. Donor and acceptor atoms are identified. Blue, green, red and purple dashed lines represent C–H...Cl, C–H... $\pi_{Cg}$ ,  $\pi_{Cg}$ ... $\pi_{Cg}$  and  $\pi$ ... $\pi$  interactions, respectively.

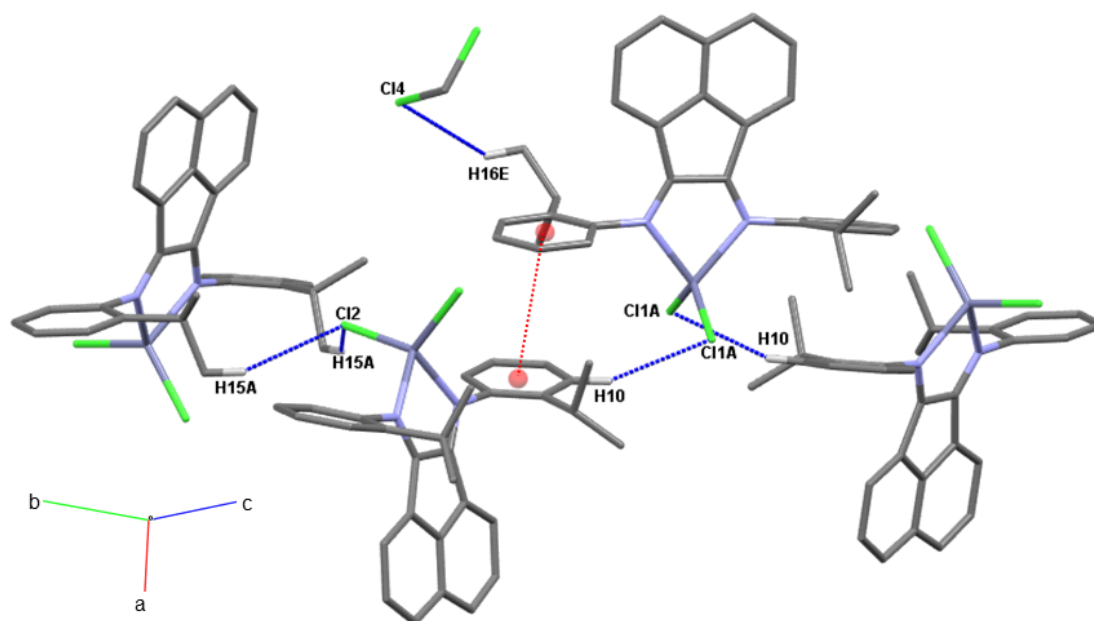


Figure S6. View of the 3D arrangement in the crystal structure of complex **2**. Donor and acceptor atoms are identified. Blue and red dashed lines represent C–H...Cl and  $\pi_{Cg}$ ... $\pi_{Cg}$  interactions, respectively.

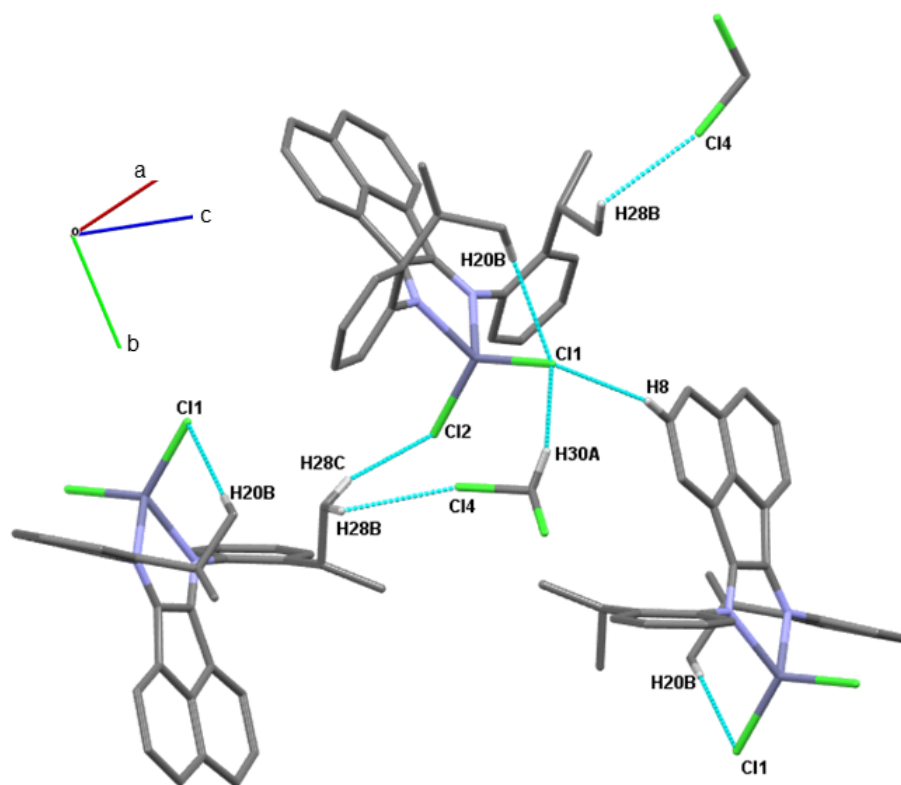


Figure S7. View of the 3D arrangement in the crystal structure of complex **2A**, generated by C–H...Cl interactions (light blue dashed lines). Donor and acceptor atoms are identified.

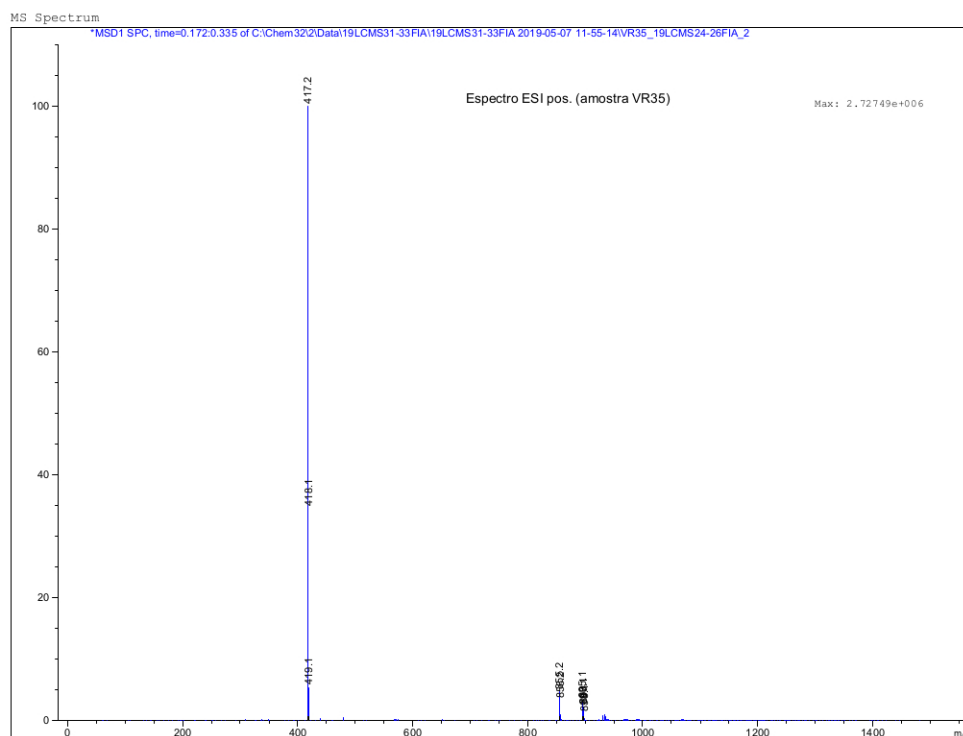


Figure S8. Mass spectrum of complex 1.

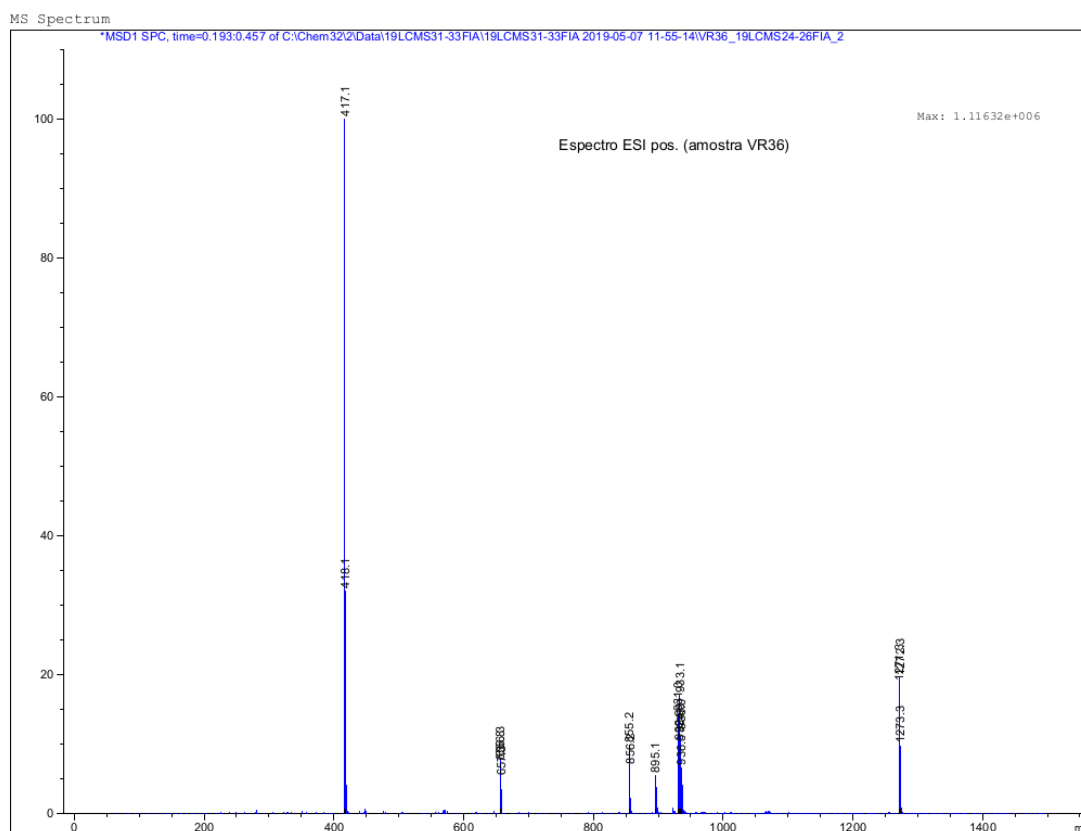


Figure S9. Mass spectrum of complex 2.

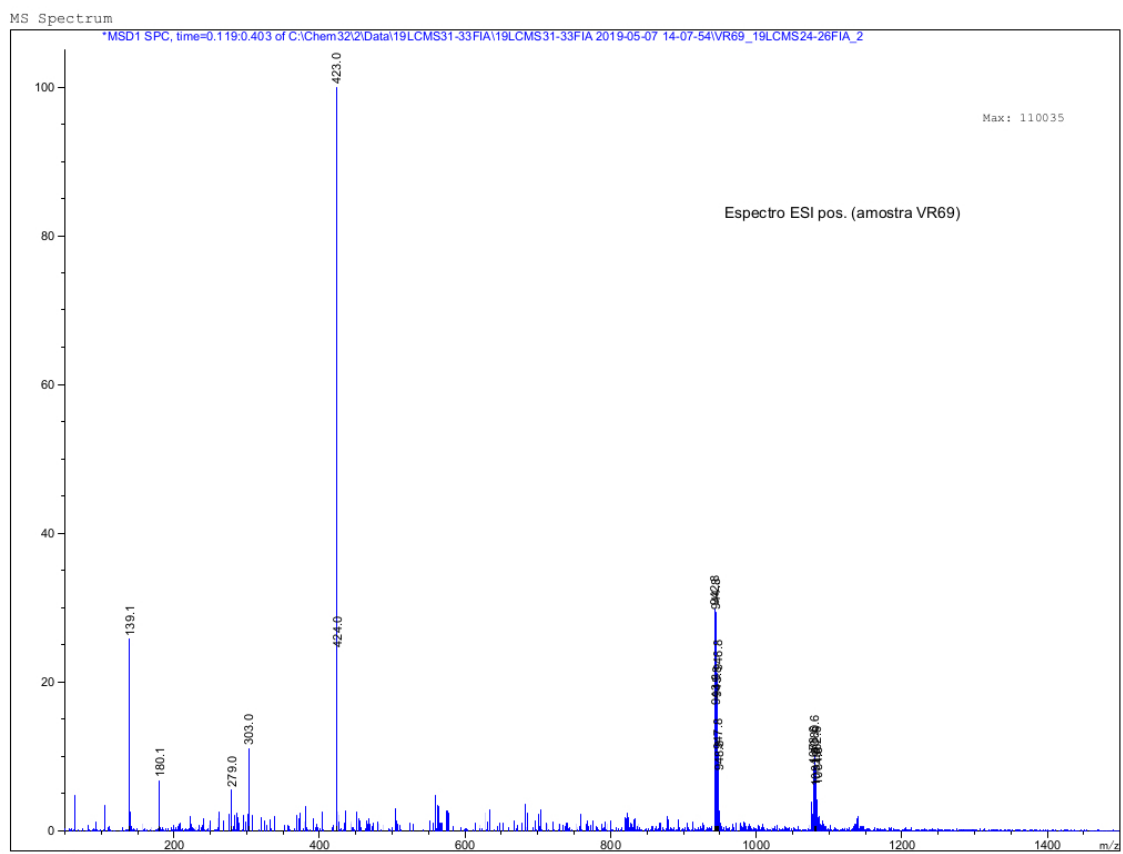


Figure S10 Mass spectrum of complex 3.

Catalysis NMR: General conditions 0.5 ml of epoxide, 0.2% mol of both catalyst and co-catalyst (TBABr), 4 MPa and 333K

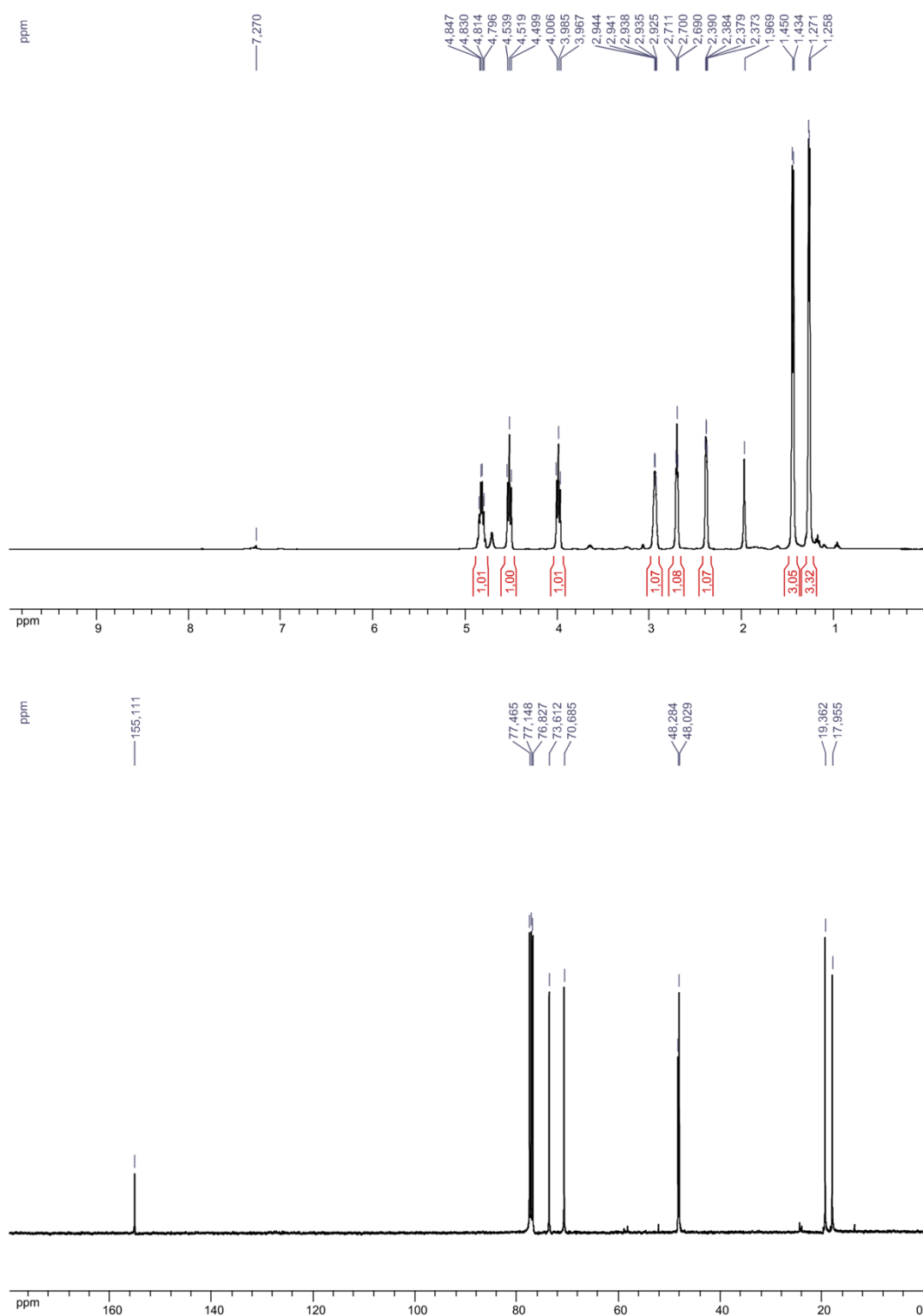


Figure S11: Crude  $^1\text{H}$ -NMR (top) and  $^{13}\text{C}$ -NMR (bottom) spectra of entry 1-Table 2. Epoxide = propylene oxide; Cat = **1**, **3h**.



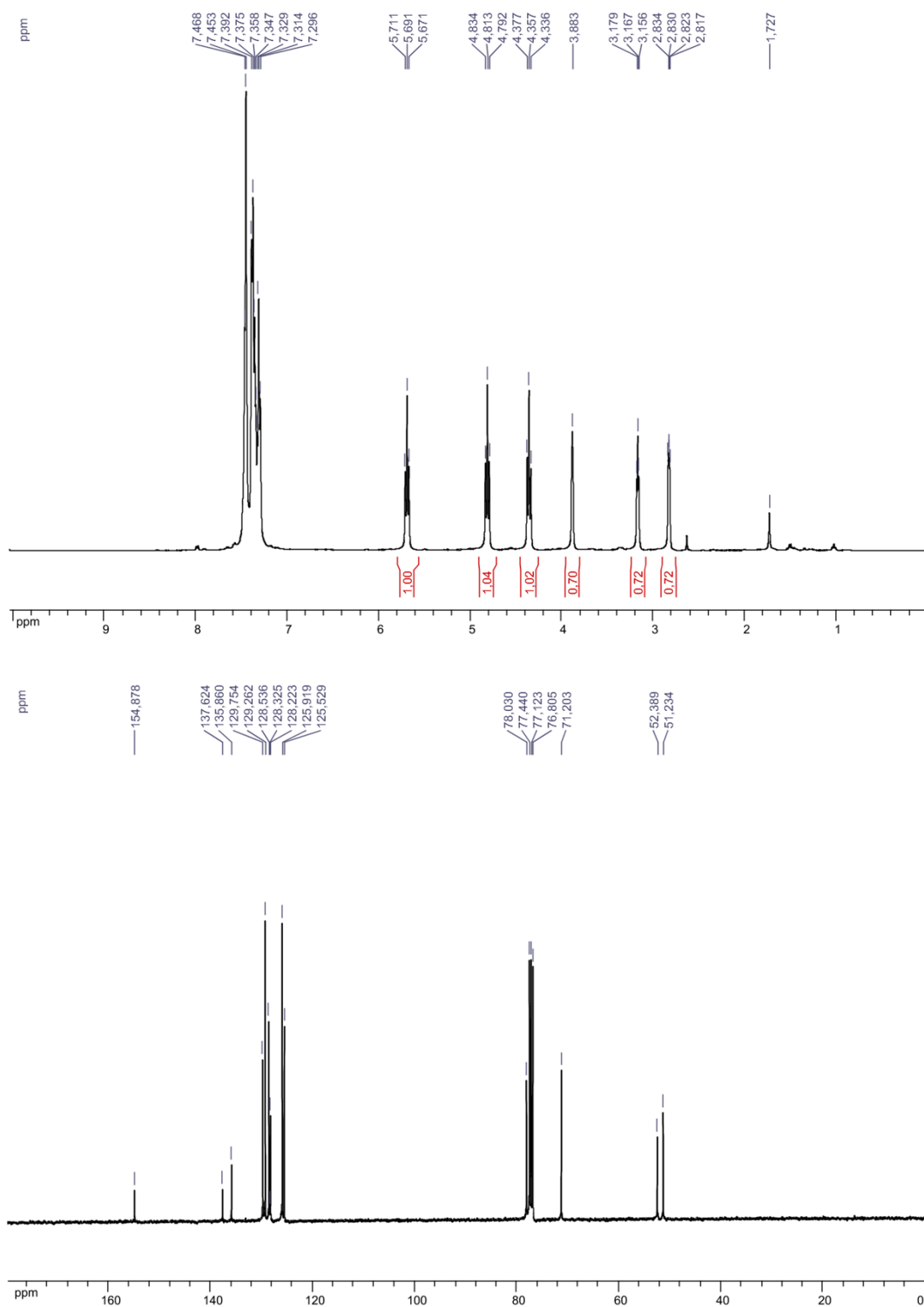


Figure S12: Crude <sup>1</sup>H-NMR (top) and <sup>13</sup>C-NMR (bottom) spectra of entry 10-Table 2. Epoxide = styrene oxide; Cat = **3**; 18h.

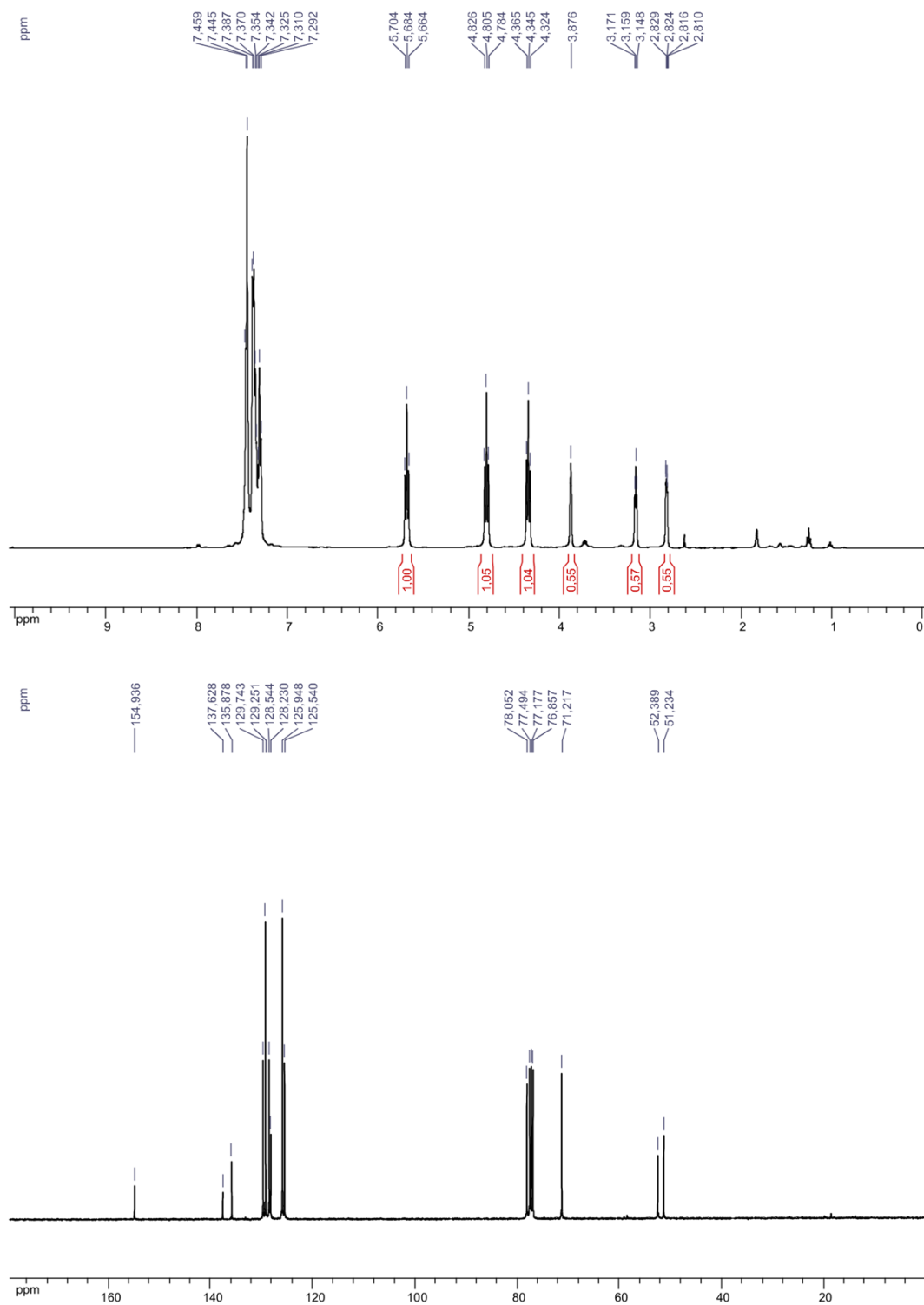


Figure S13: Crude  $^1\text{H-NMR}$  (top) and  $^{13}\text{C-NMR}$  (bottom) spectra of entry 11-Table 2. Epoxide = styrene oxide; Cat = **3**; 24h.

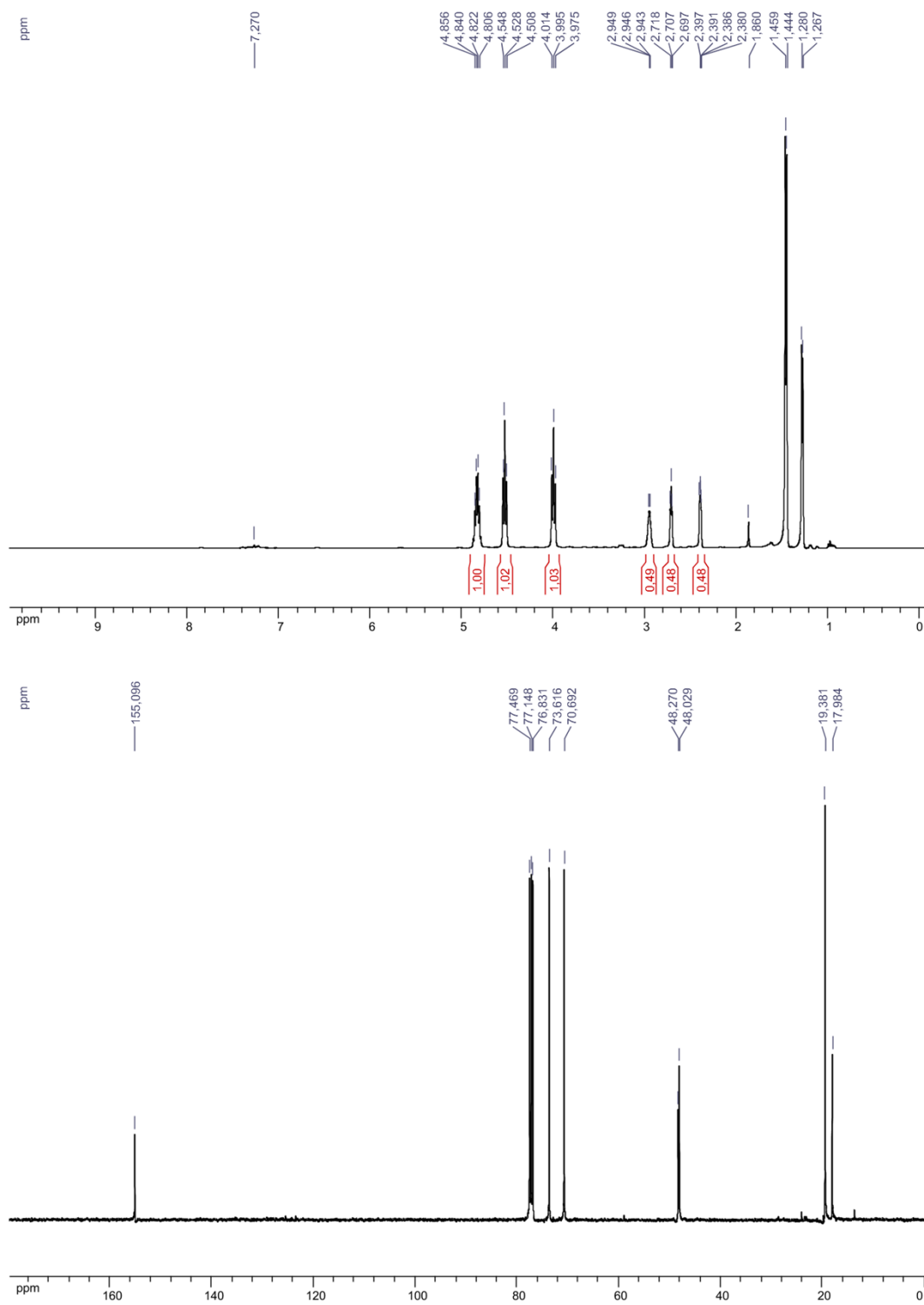


Figure S14: Crude  $^1\text{H}$ -NMR (top) and  $^{13}\text{C}$ -NMR (bottom) spectra of entry 13-Table 2. Epoxide = propylene oxide; Cat = **4**; 3h.

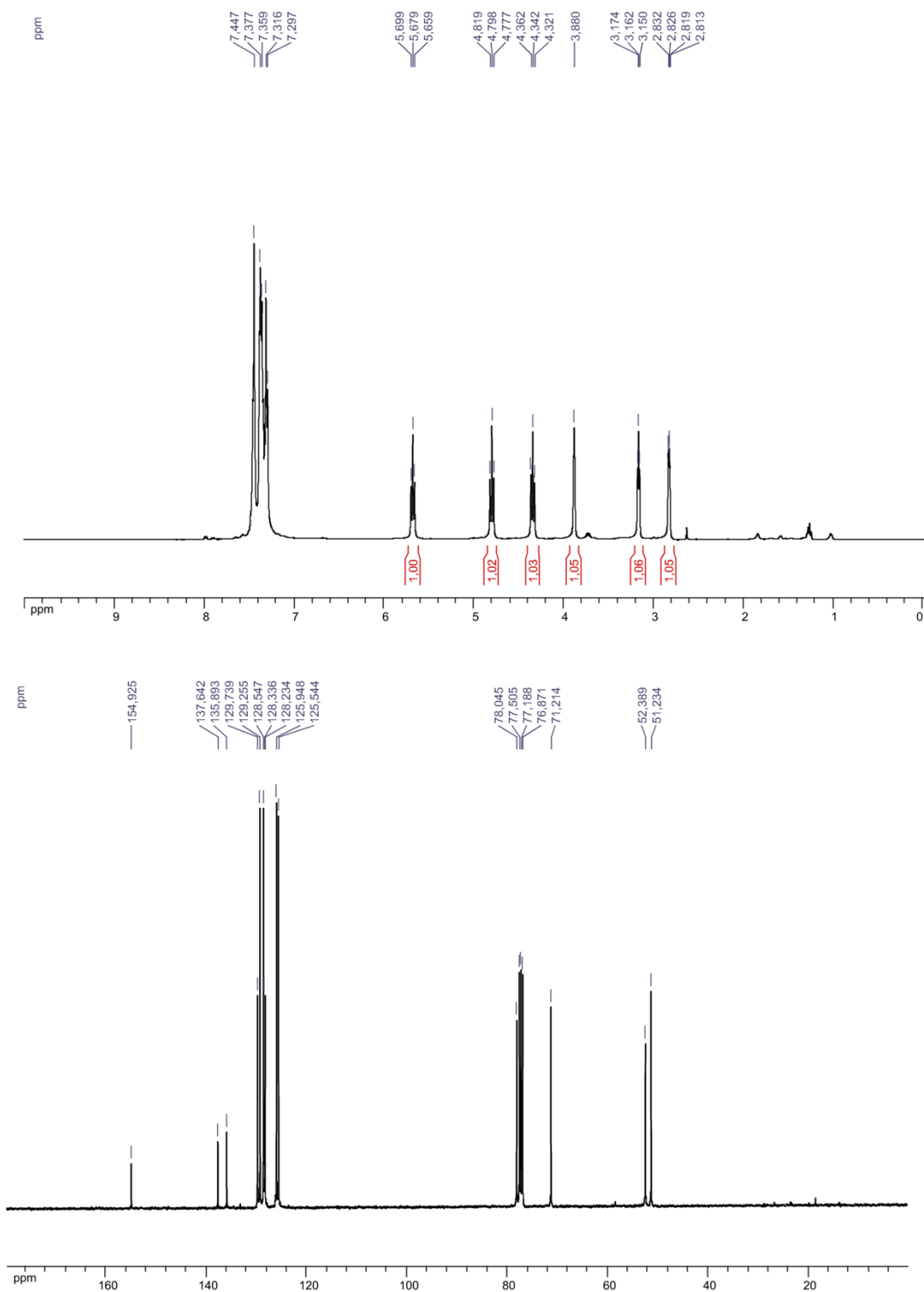


Figure S15: Crude  $^1\text{H-NMR}$  (top) and  $^{13}\text{C-NMR}$  (bottom) spectra of entry 14-Table 2. Epoxide = styrene oxide; Cat = **4**; 18h.

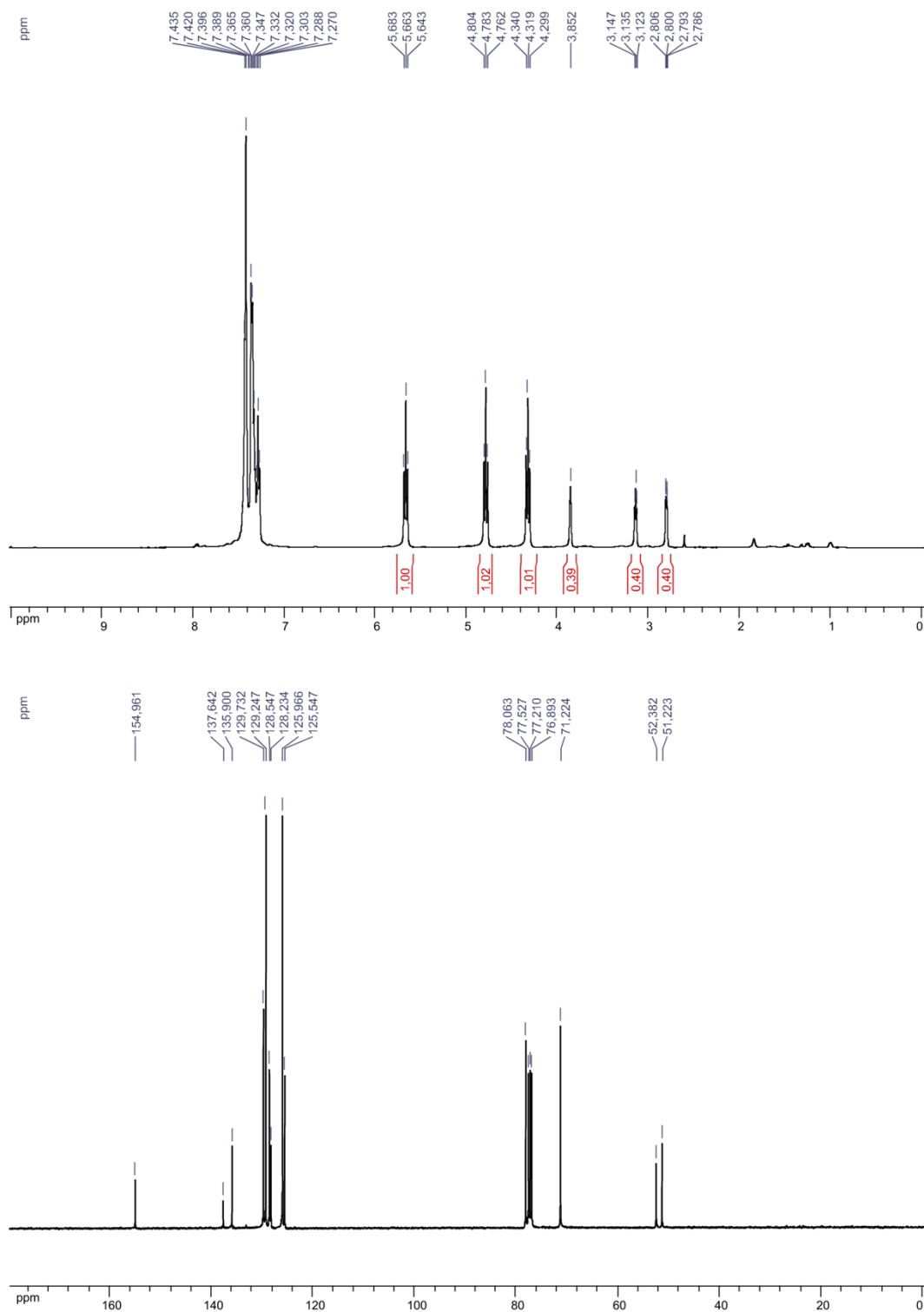


Figure S16: Crude <sup>1</sup>H-NMR (top) and <sup>13</sup>C-NMR (bottom) spectra of entry 15-Table 2. Epoxide = styrene oxide; Cat = **4**; 24h.

## RMN Kinetics:

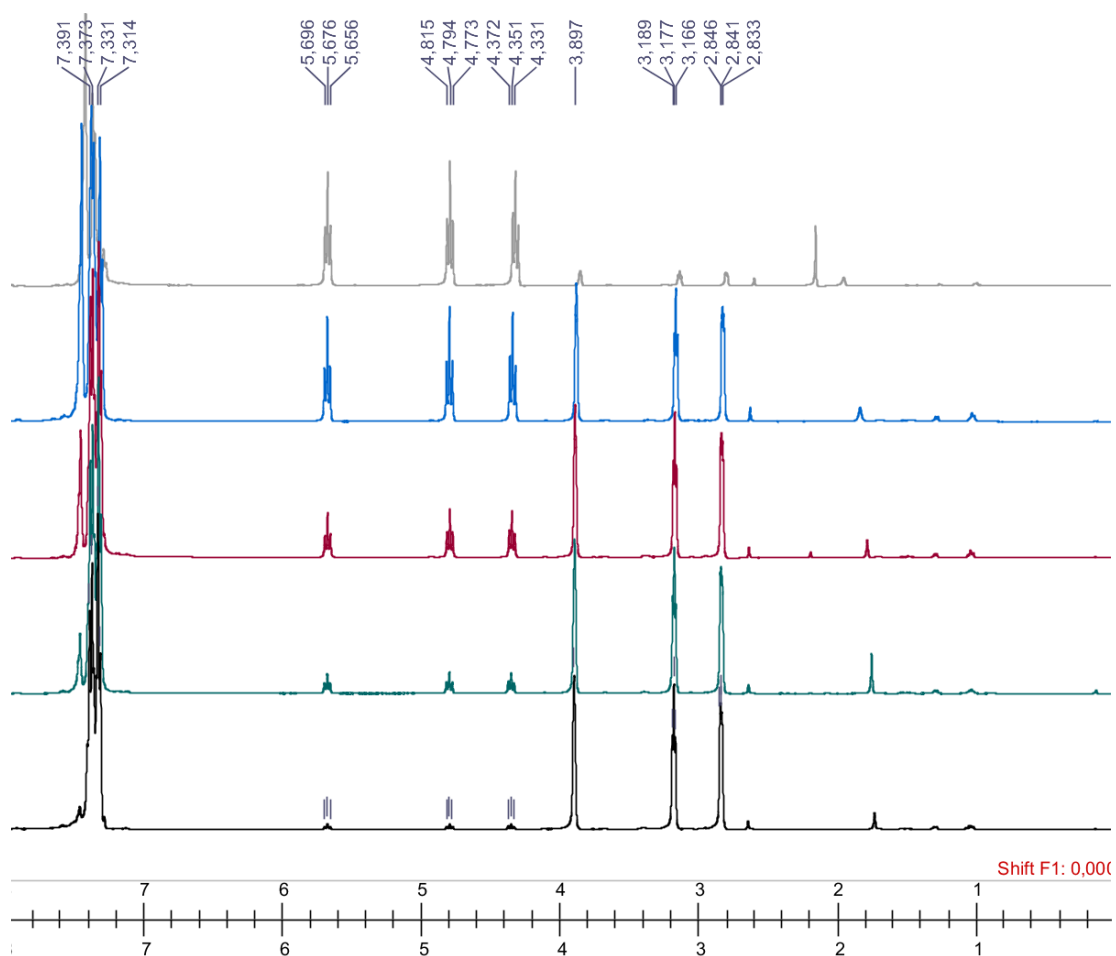


Figure S17: <sup>1</sup>H-NMR spectra of kinetic data for styrene oxide cycloaddition reaction with CO<sub>2</sub> to at 4 MPa, 333 K, and 0.2% mol of catalyst **4** and TBABr co-catalyst.

Bottom to top: 1h, 3h, 5h, 8h and 36h reaction time.

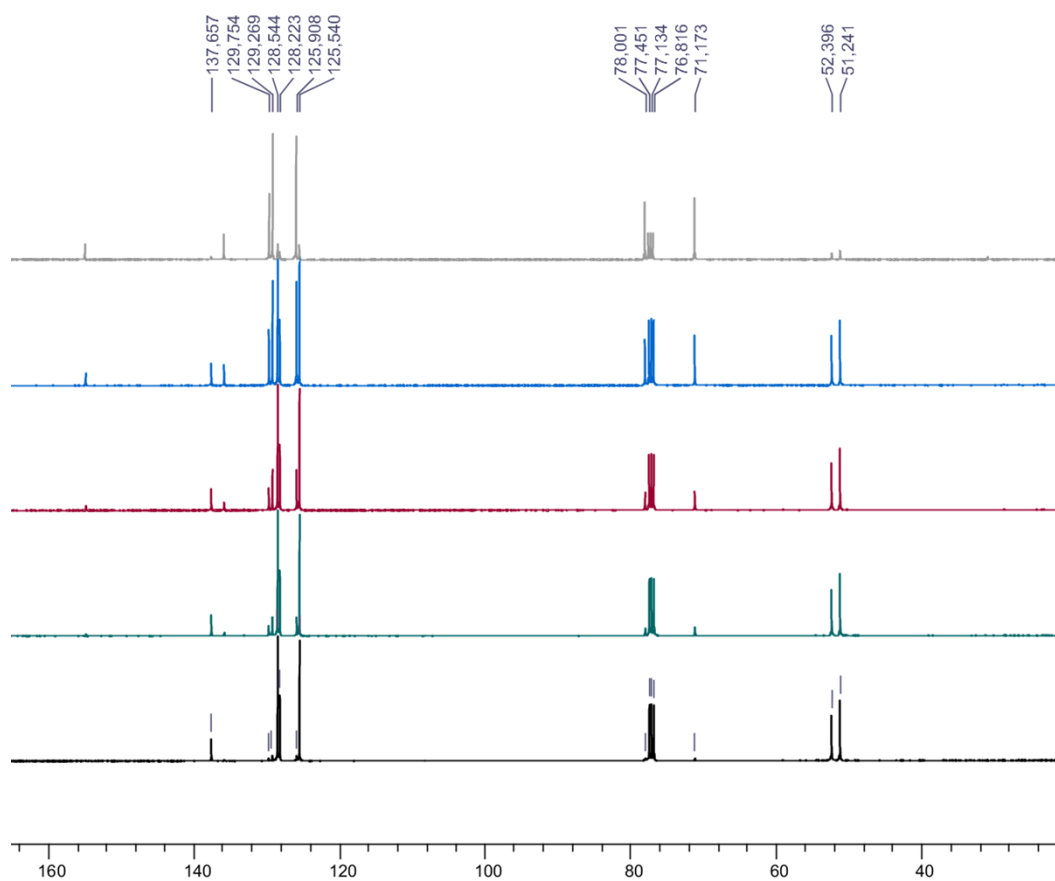


Figure 18:  $^{13}\text{C}$ -NMR spectra of kinetic data for styrene oxide cycloaddition reaction with  $\text{CO}_2$  to at 4 MPa, 333 K, and 0.2% mol of catalyst **4** and TBABr co-catalyst.

Bottom to top: 1h, 3h, 5h, 8h and 36h reaction time.

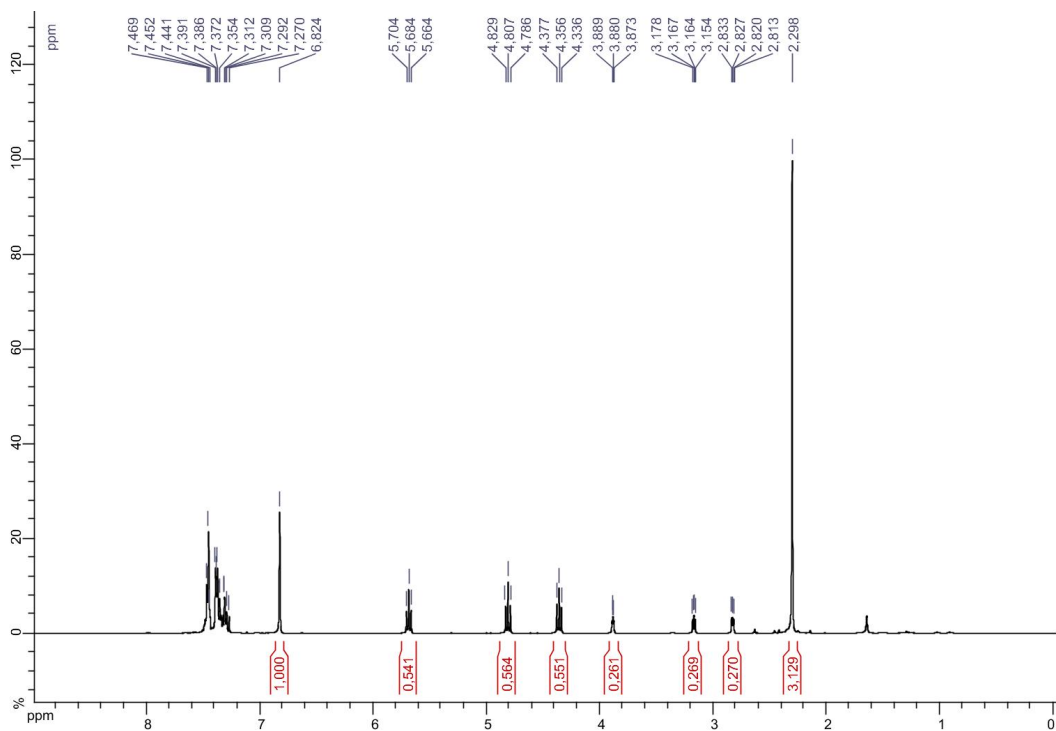


Figure 19: Crude <sup>1</sup>H-NMR spectrum of entry 11-Table 2 experiment using mesitylene as internal standard. Conversion 67%.



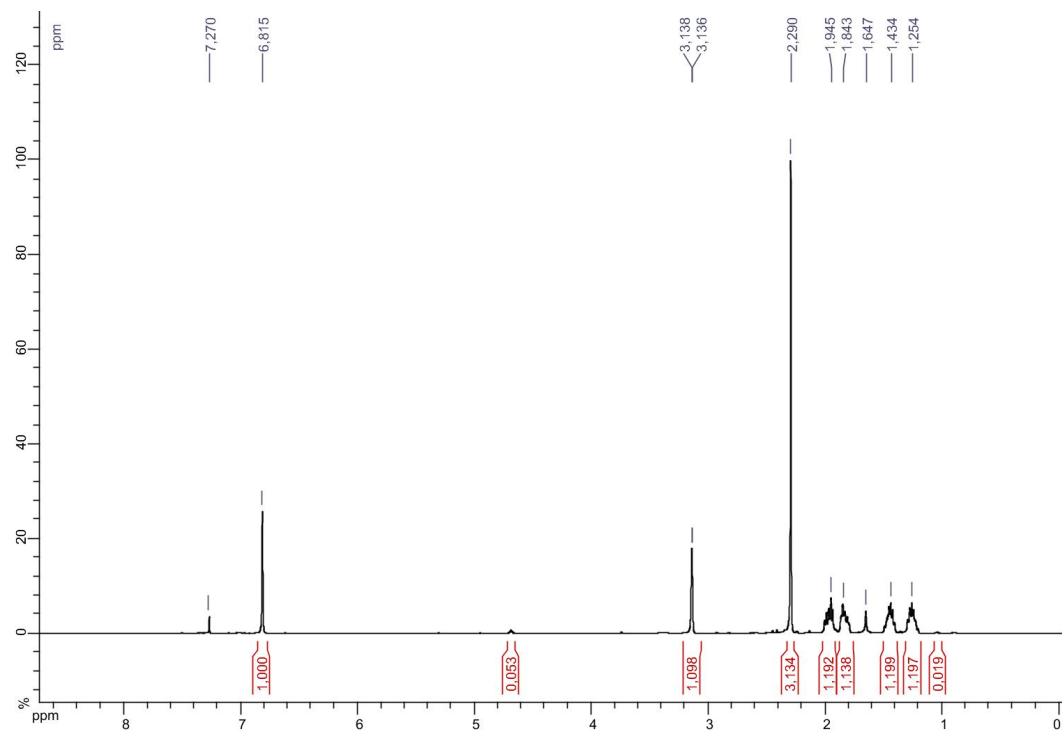


Figure 20: Crude <sup>1</sup>H-NMR spectrum of entry 4-Table 2 experiment using mesitylene as internal standard. Conversion 5%.