

Supplementary Materials

# New In Situ Catalysts Based on Nitro Functional Pyrazole Derivatives and Copper (II) Salts for Promoting Oxidation of Catechol to *o*-Quinone

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## 1. Characterization

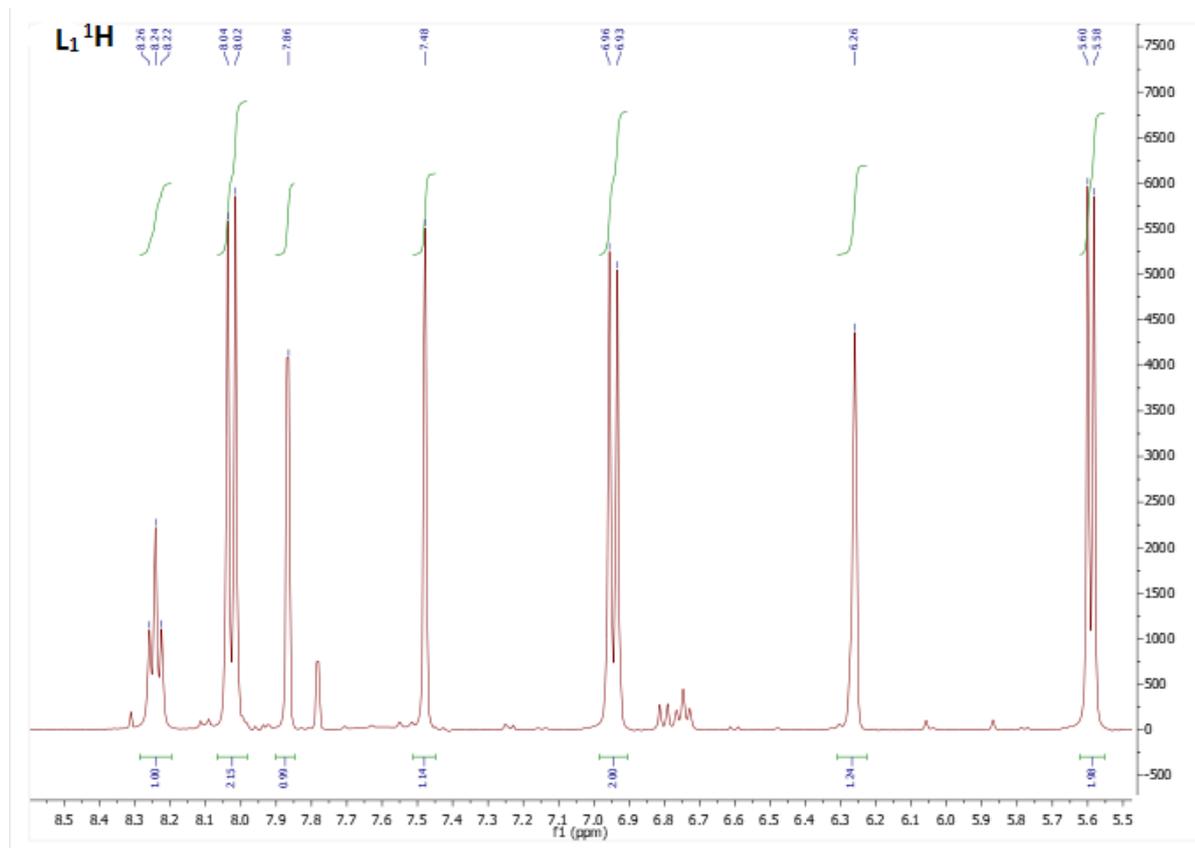


Figure S1. <sup>1</sup>H NMR spectrum of L1 in DMSO (400 MHz).

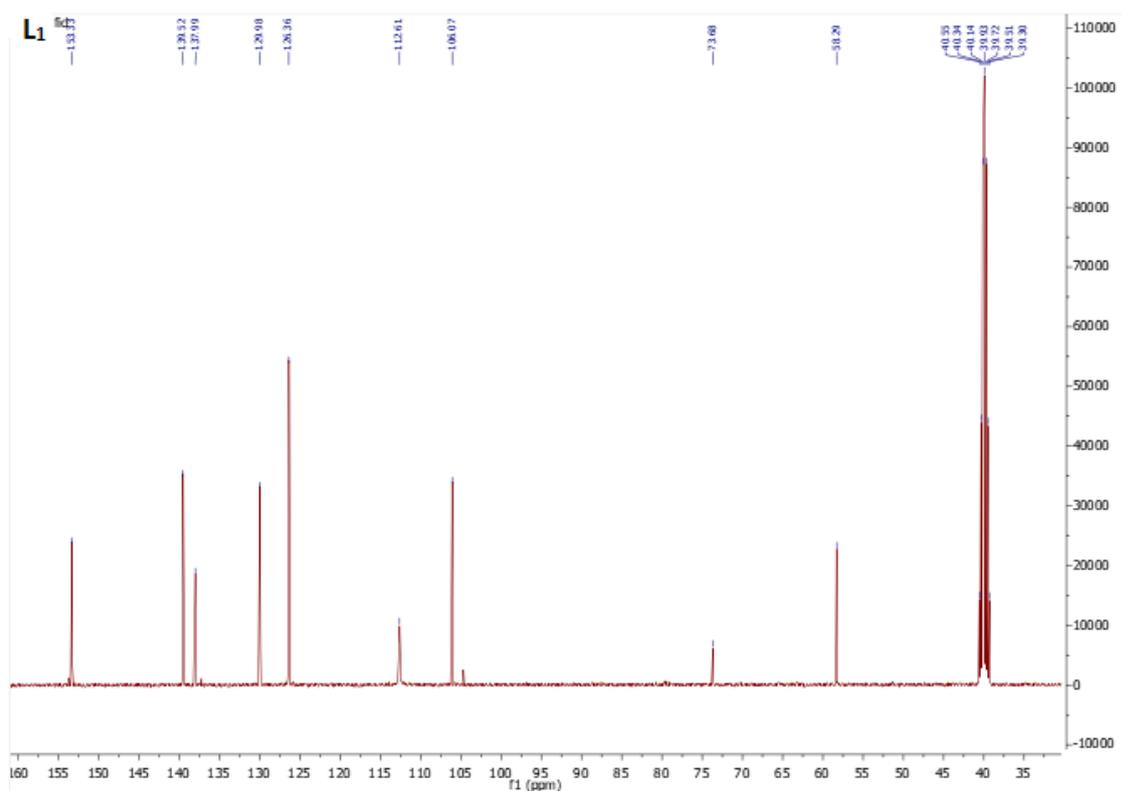


Figure S2. <sup>13</sup>C NMR spectrum of L<sub>1</sub> in DMSO (400 MHz).

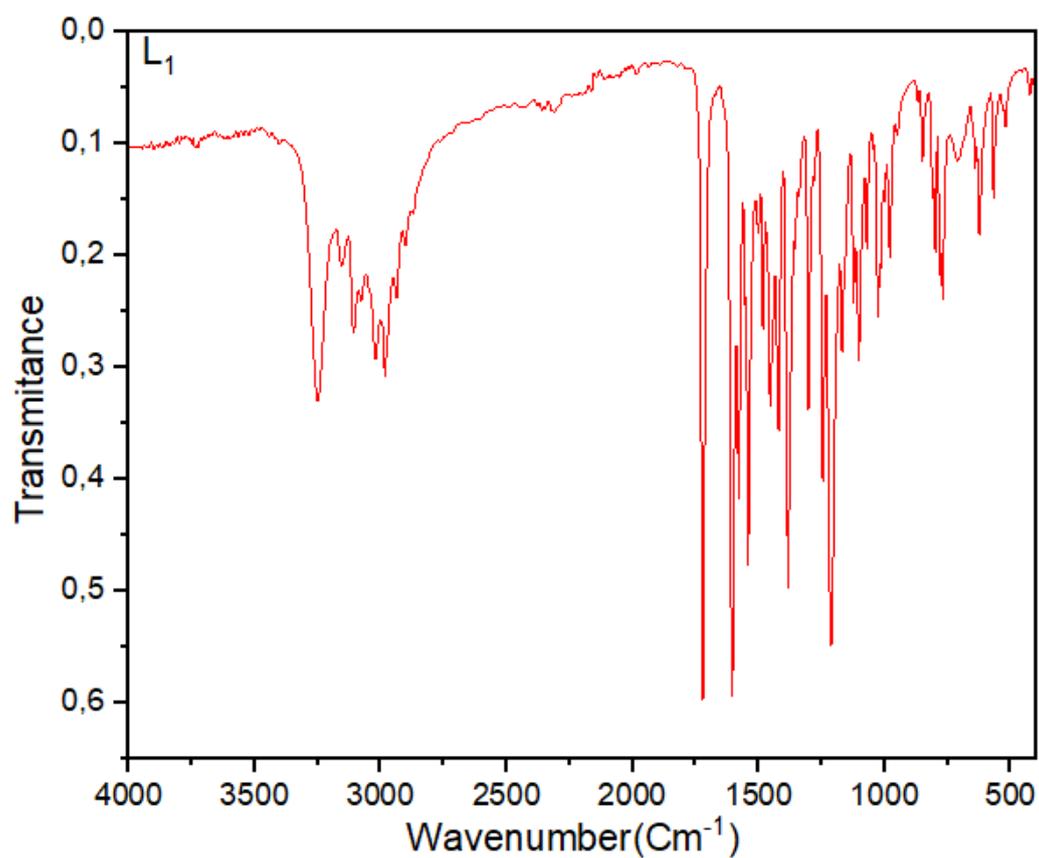


Figure S3. FT-IR spectrum of L<sub>1</sub>.

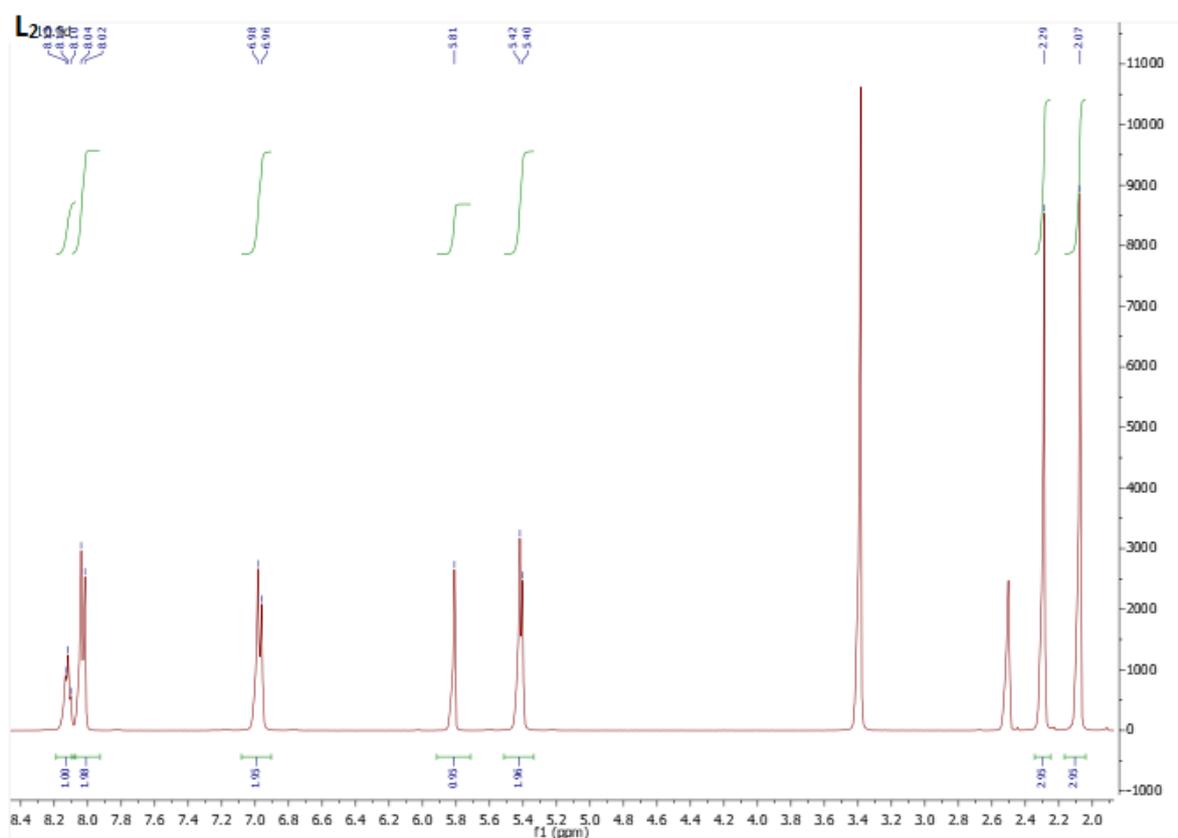


Figure S4.  $^1\text{H}$  NMR spectrum of L2 in DMSO (400 MHz).

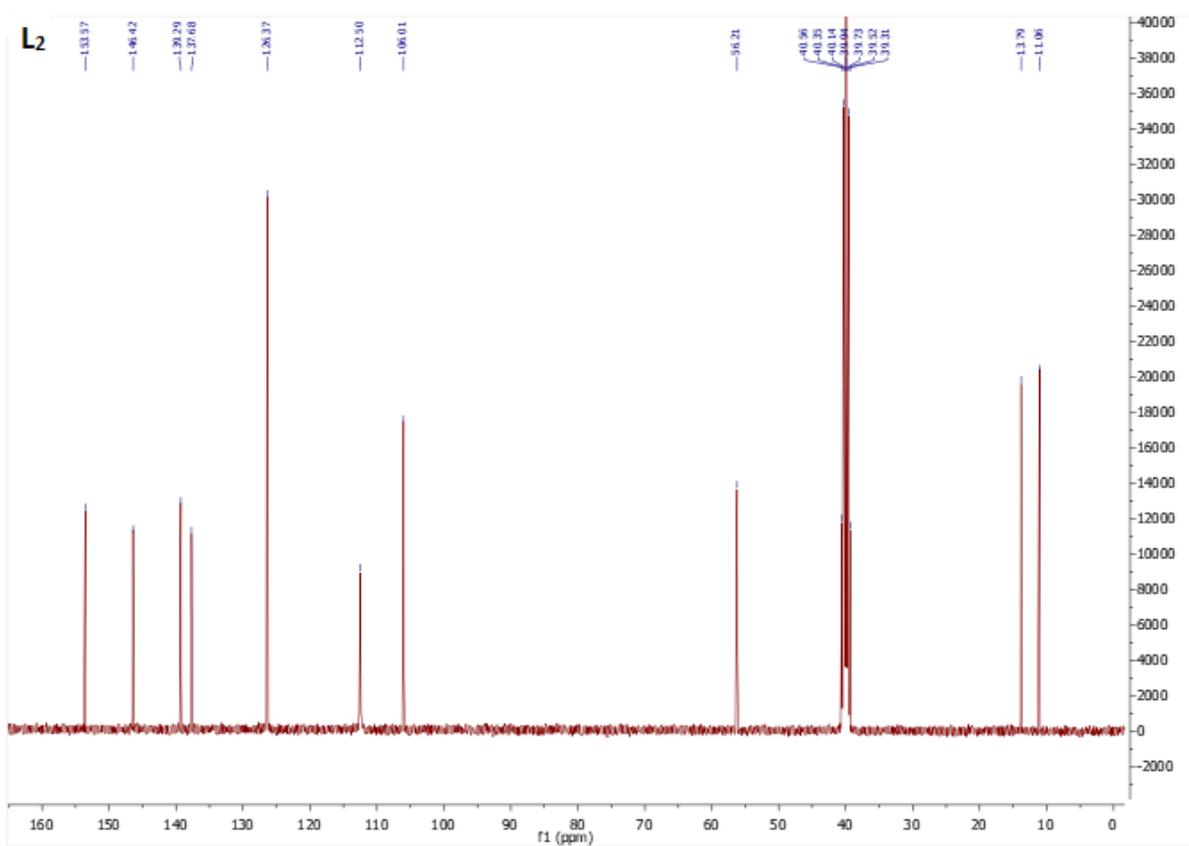


Figure S5.  $^{13}\text{C}$  NMR spectrum of L2 in DMSO (400 MHz).

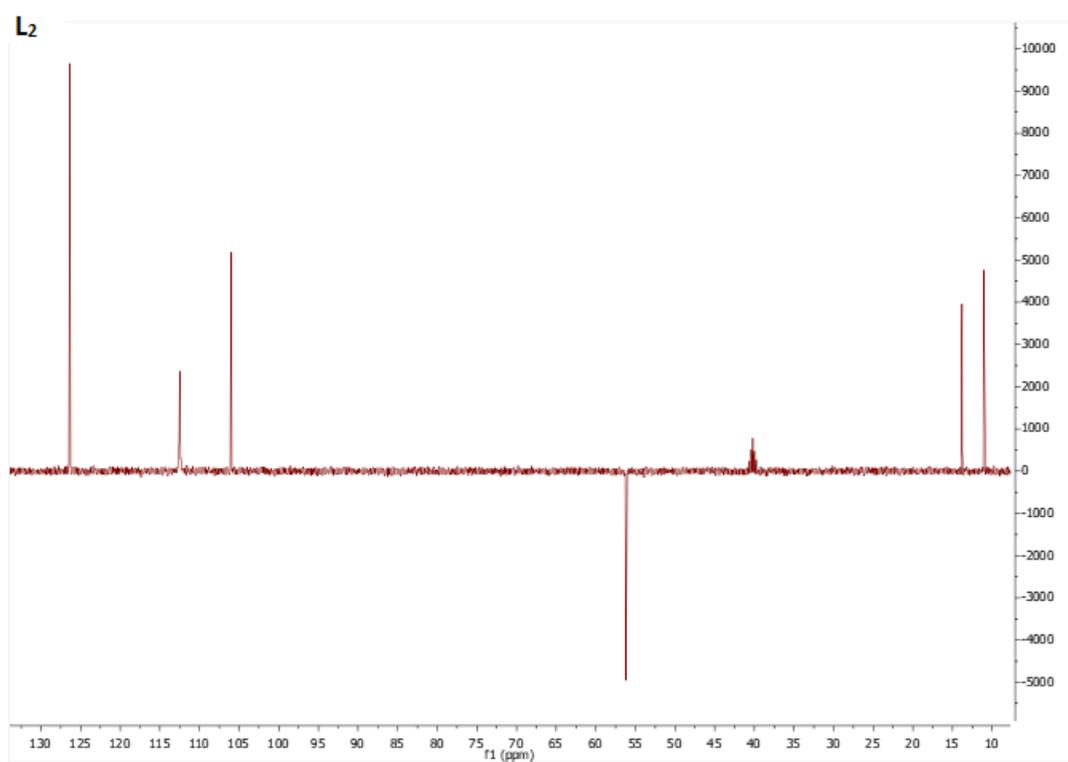


Figure S6. DEPT- 135 NMR spectrum of L<sub>2</sub> in DMSO (400 MHz).

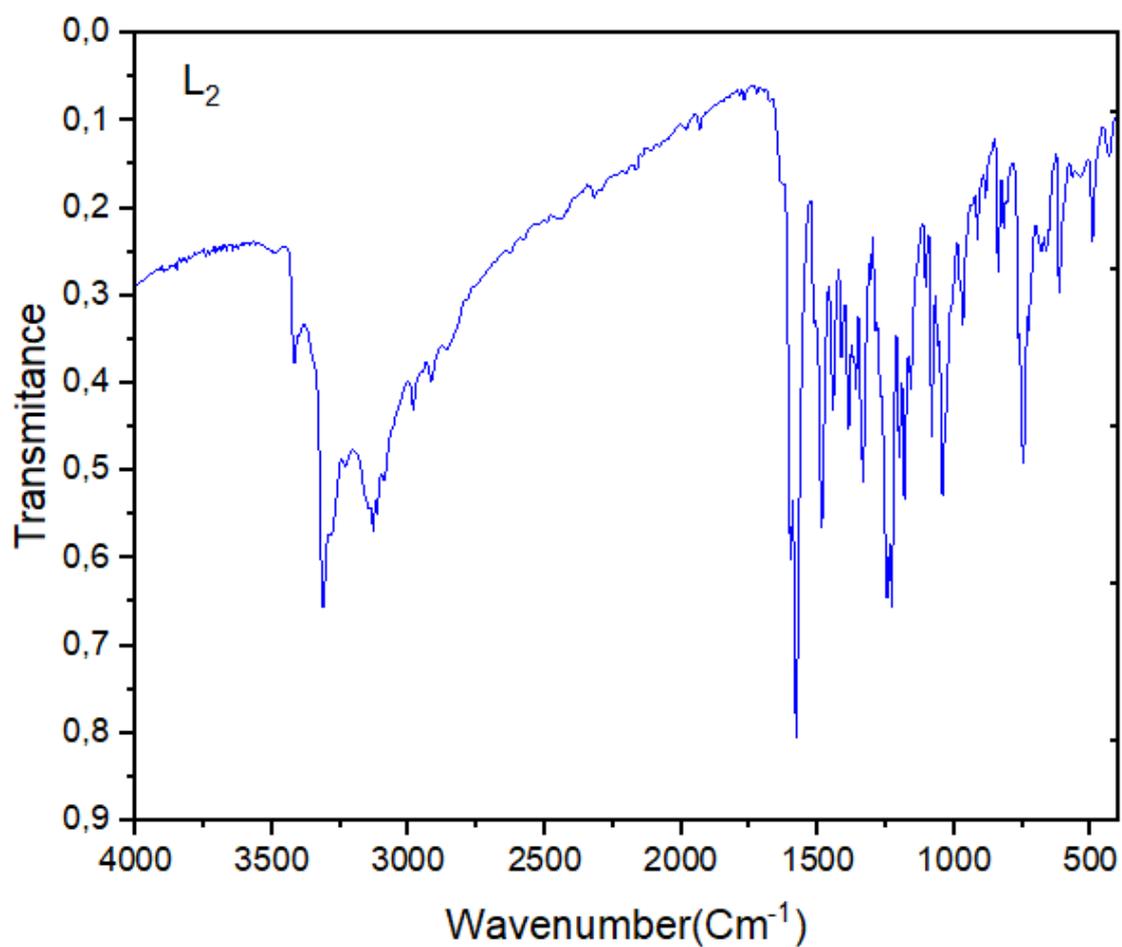


Figure S7. FT-IR spectrum of L<sub>2</sub>.

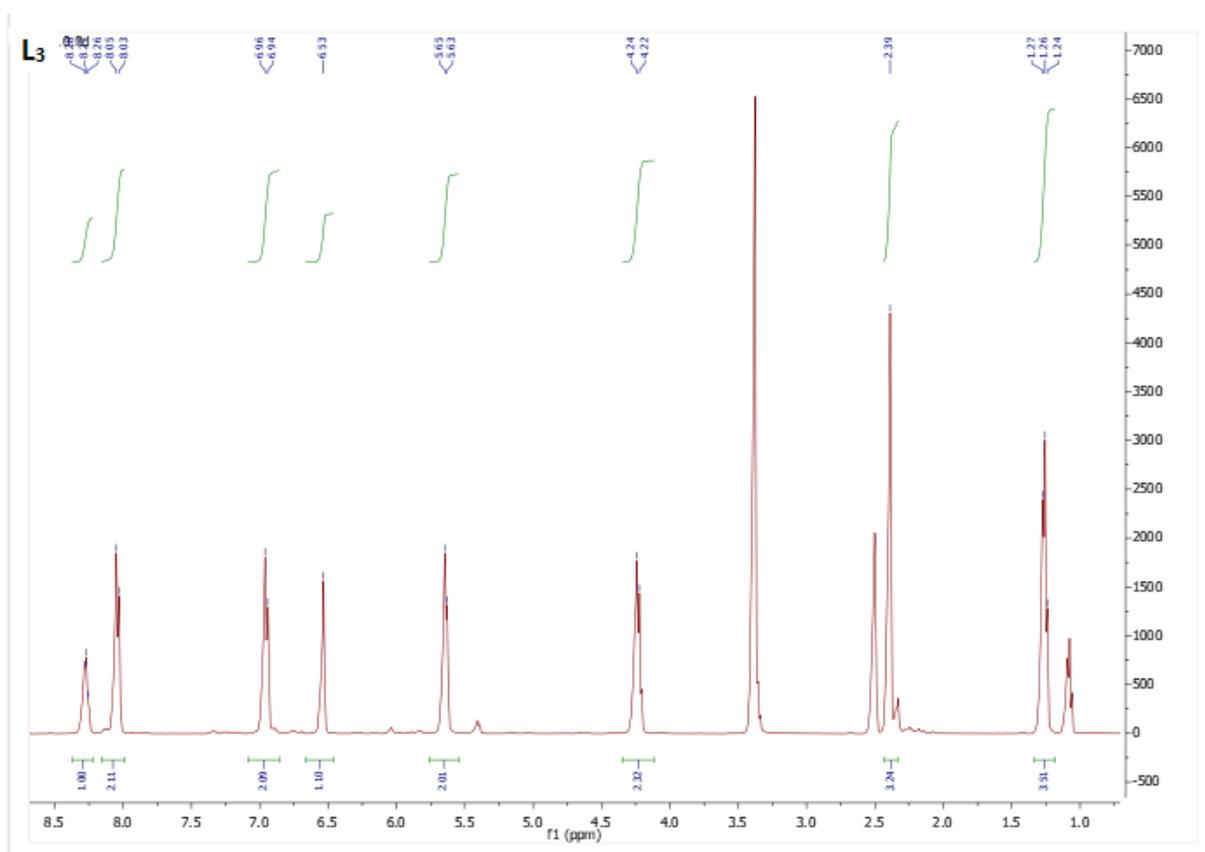


Figure S8.  $^1\text{H}$  NMR spectrum of L3 in DMSO (400 MHz).

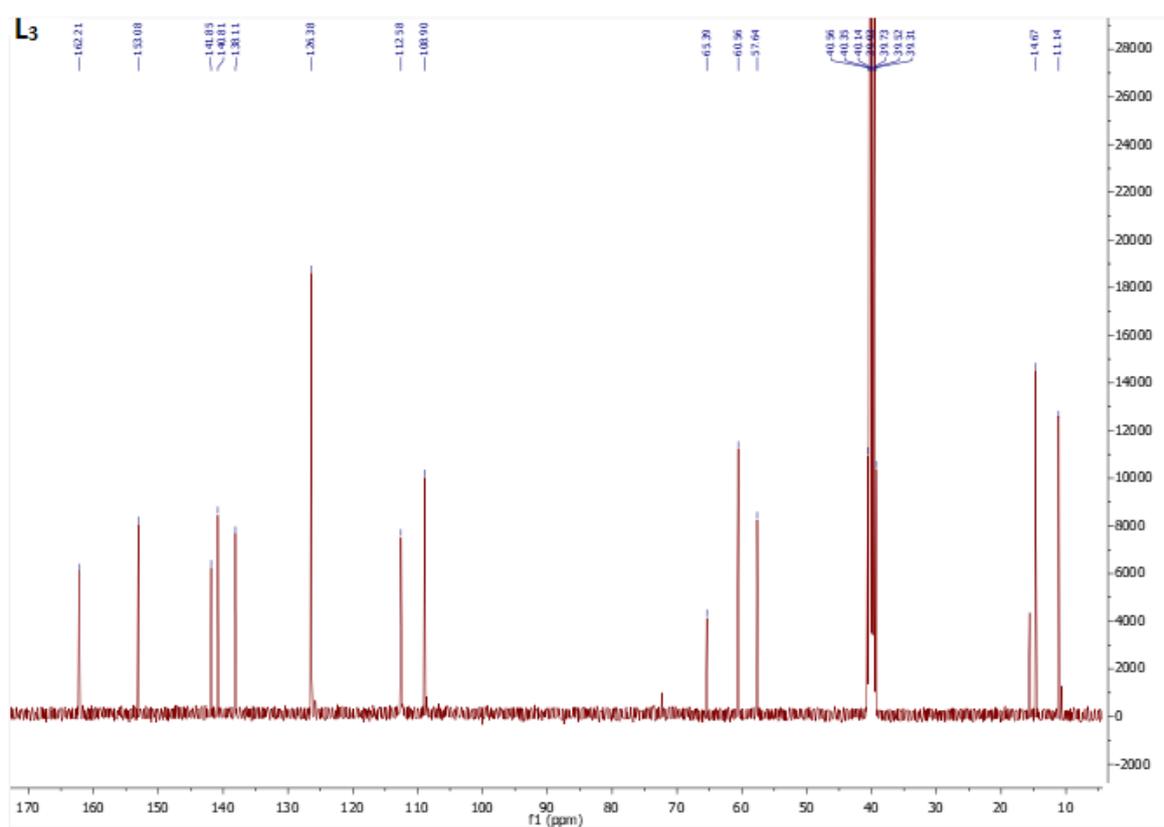


Figure S9.  $^{13}\text{C}$  NMR spectrum of L3 in DMSO (400 MHz).

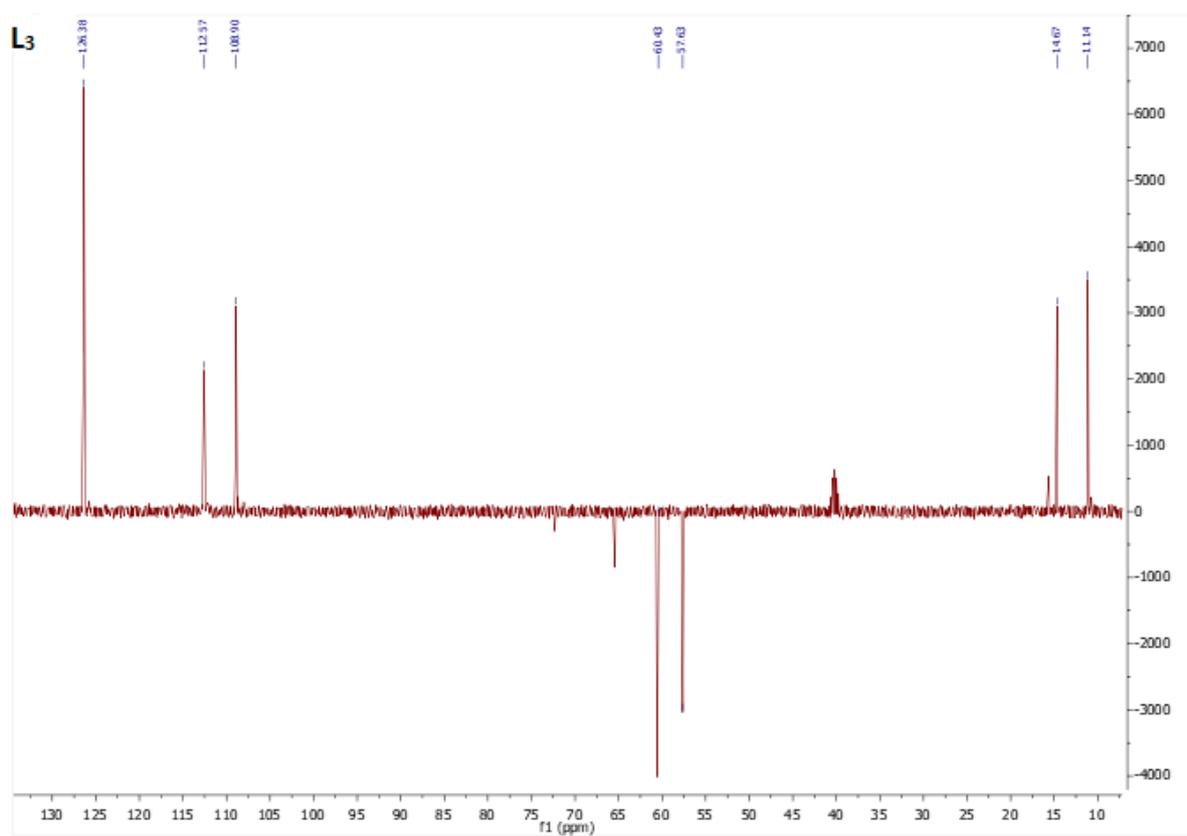


Figure S10. DEPT- 135 NMR spectrum of L<sub>3</sub> in DMSO (400 MHz).

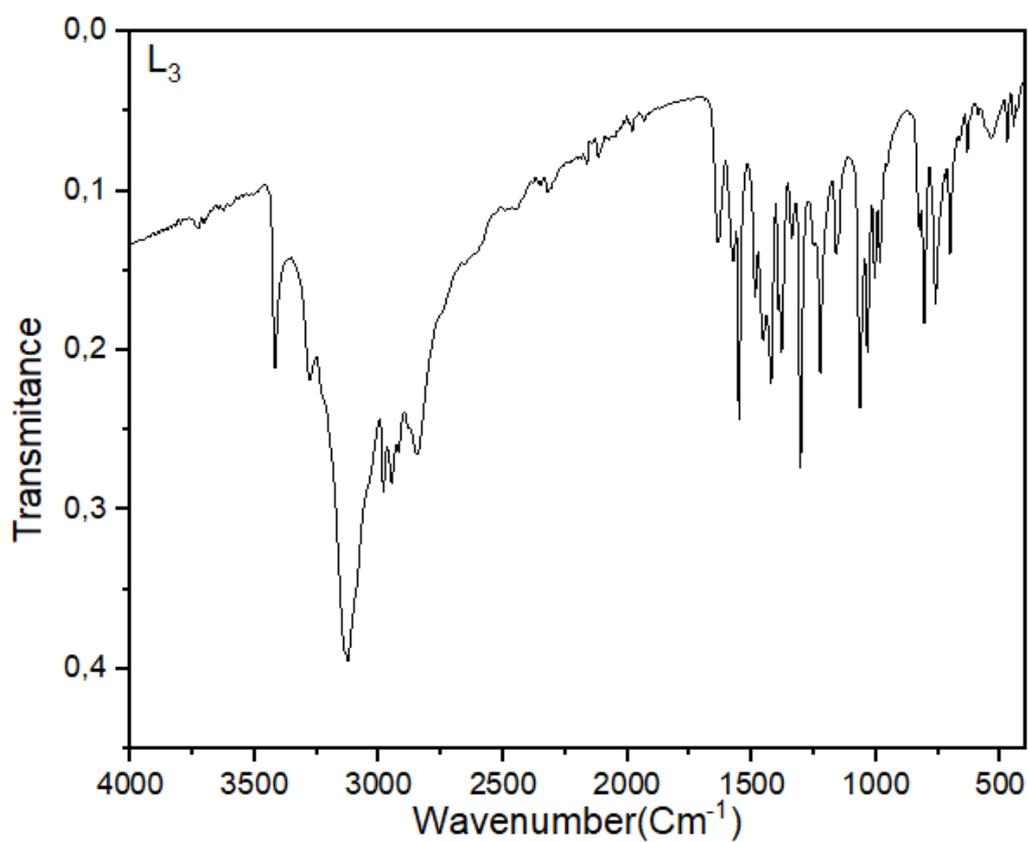


Figure S11. FT-IR spectrum of L<sub>3</sub>.

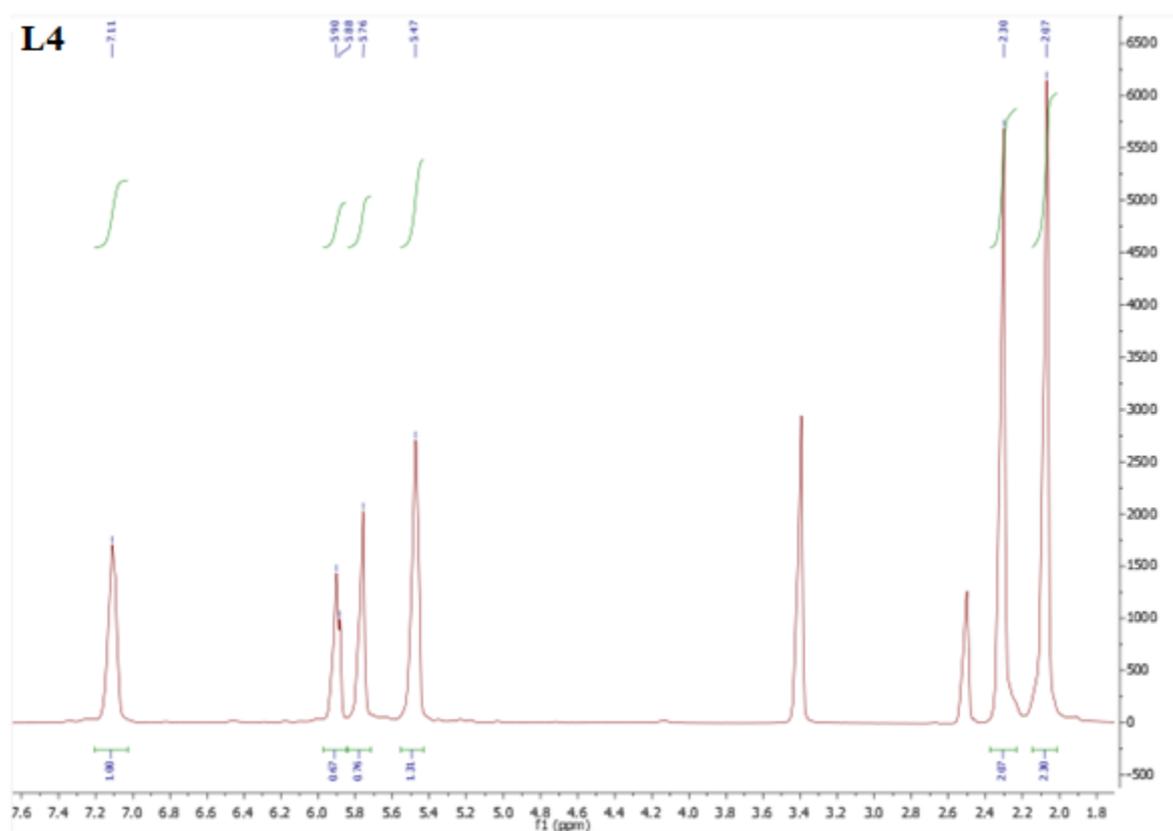


Figure S12.  $^1\text{H}$  NMR spectrum of L4 in DMSO (400 MHz).

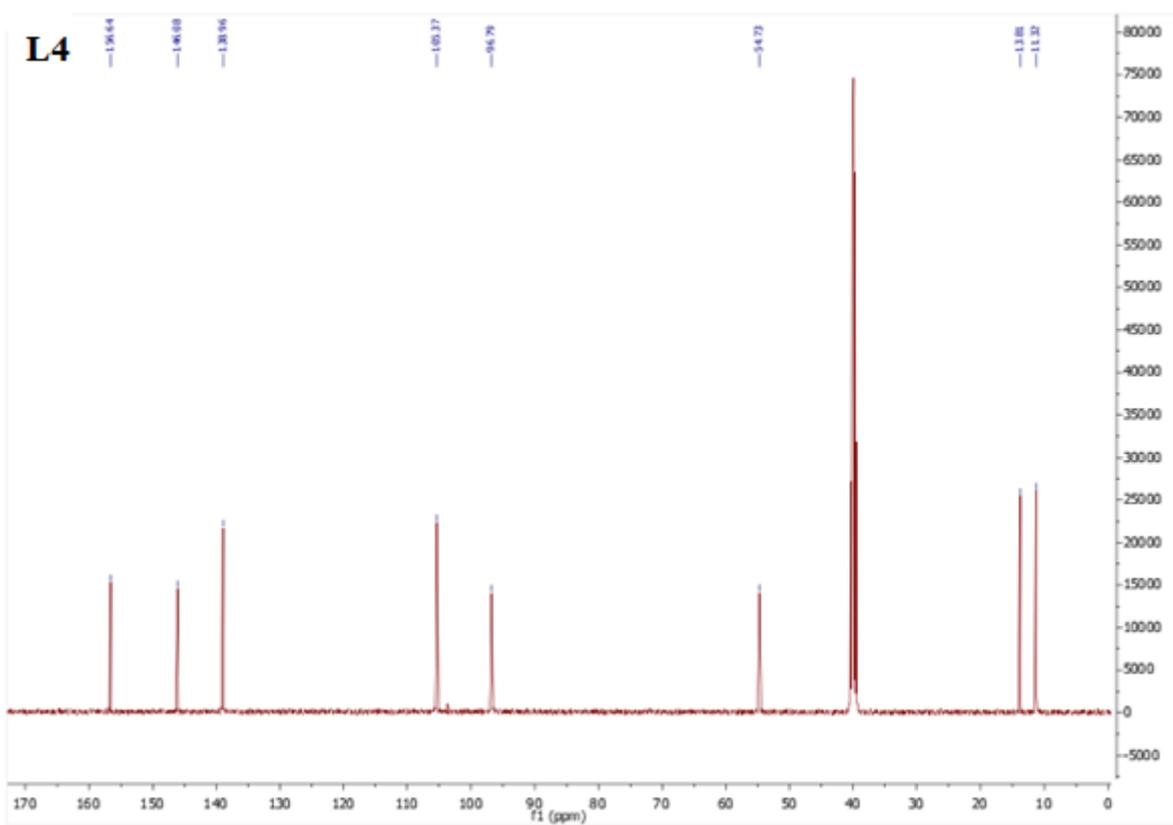


Figure S13.  $^{13}\text{C}$  NMR spectrum of L4 in DMSO (400 MHz).

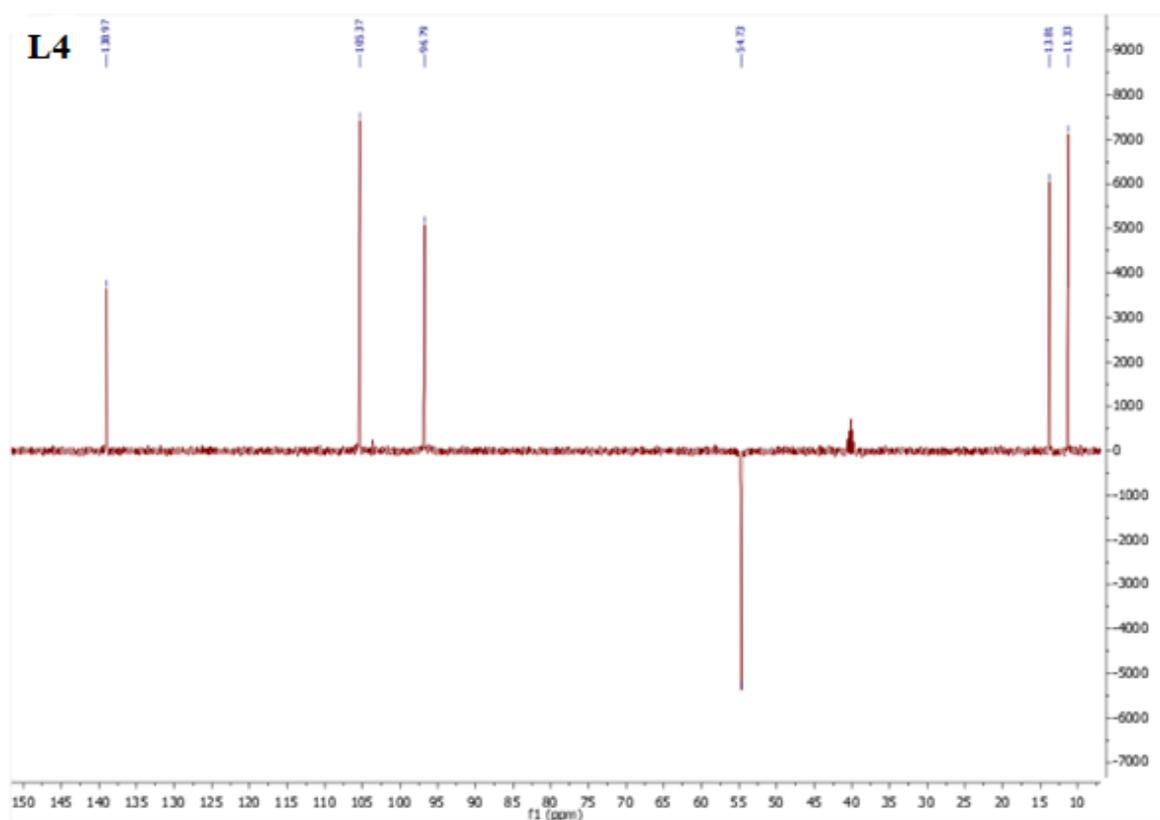


Figure S14.  $^{13}\text{C}$  NMR spectrum of L4 in DMSO (400 MHz).

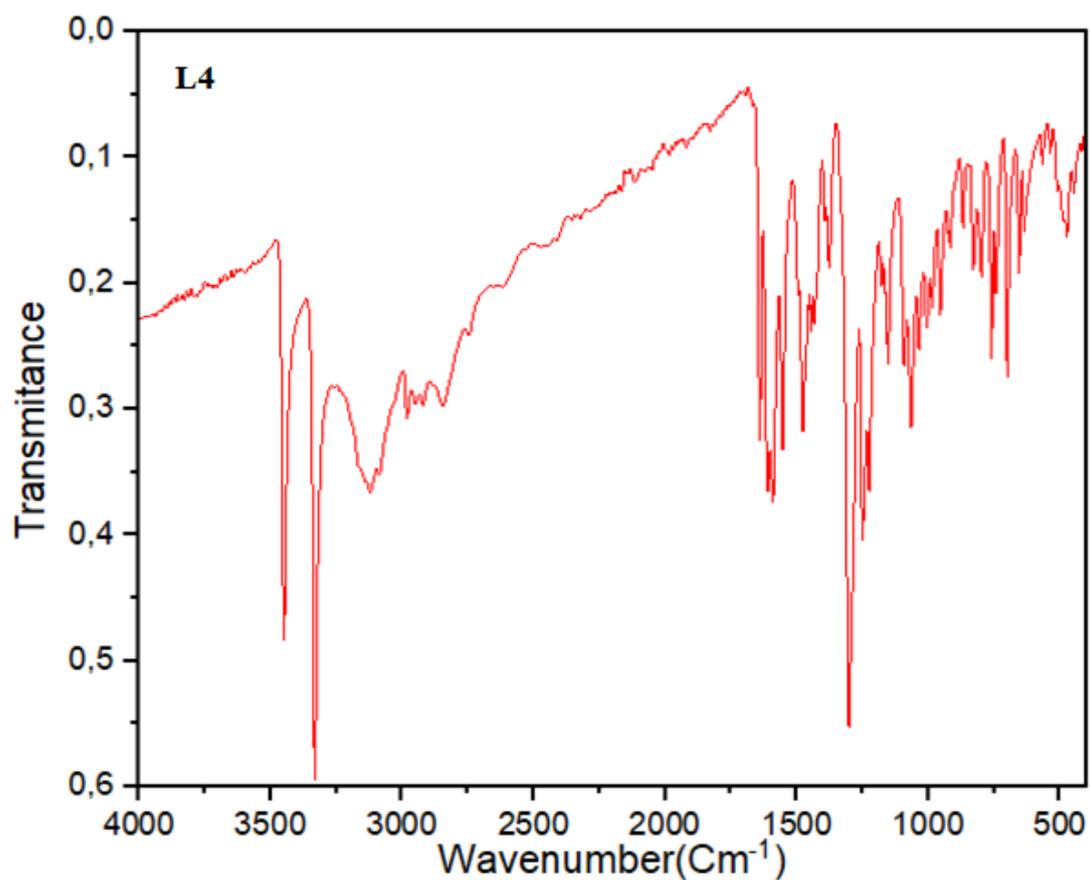


Figure S15. FT-IR spectrum of L4.

## 2. Effect of concentration

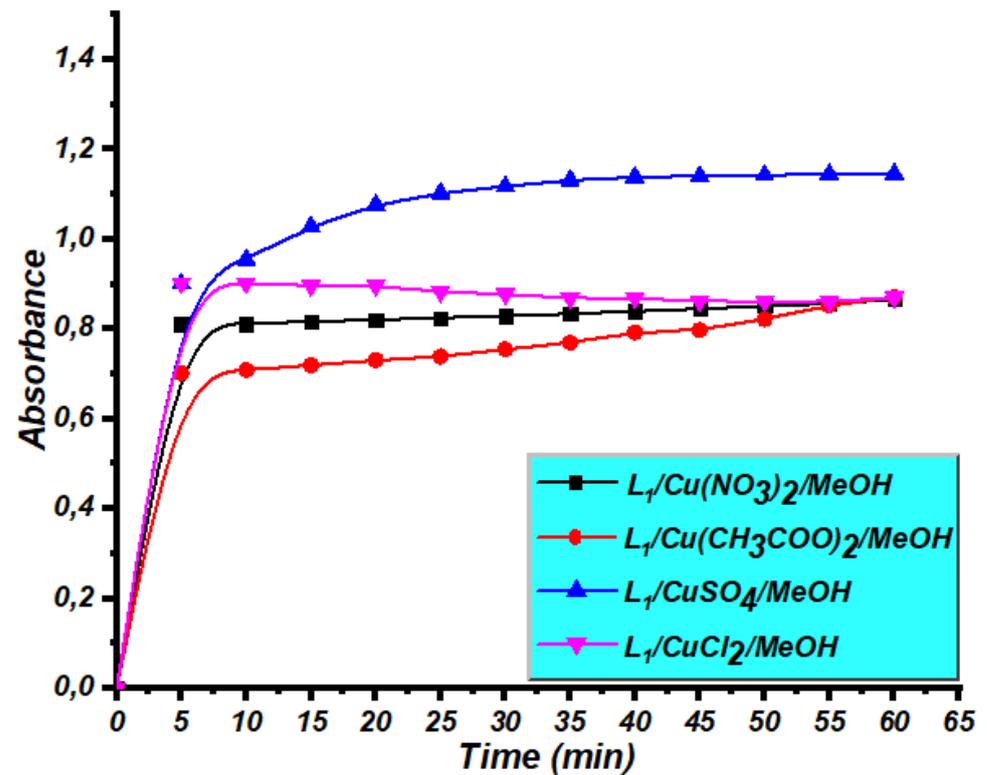


Figure S16. Absorbance evolution of *o*-quinone in presence of complexes formed by L<sub>1</sub> and different copper salts in MeOH.

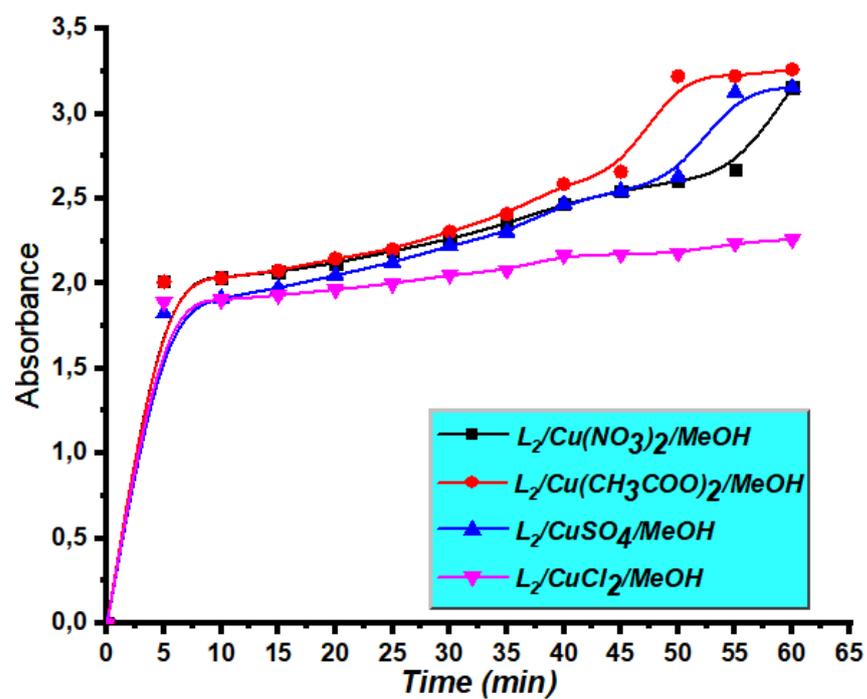


Figure S17. Absorbance evolution of *o*-quinone in presence of complexes formed by L<sub>2</sub> and different copper salts in MeOH.

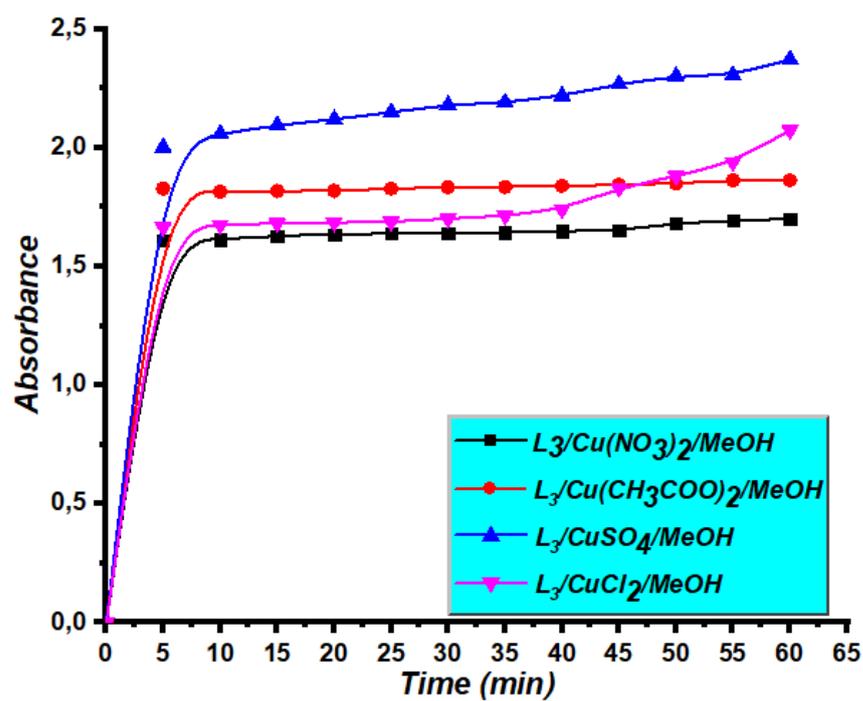


Figure S18. Absorbance evolution of *o*-quinone in presence of complexes formed by  $L_3$  and different copper salts in MeOH.

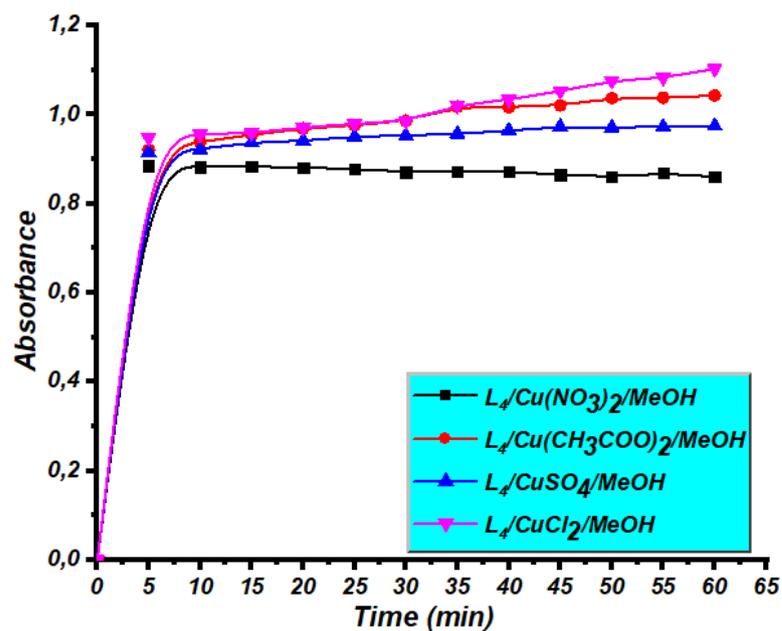


Figure S19. Absorbance evolution of *o*-quinone in presence of complexes formed by  $L_4$  and different copper salts in MeOH.

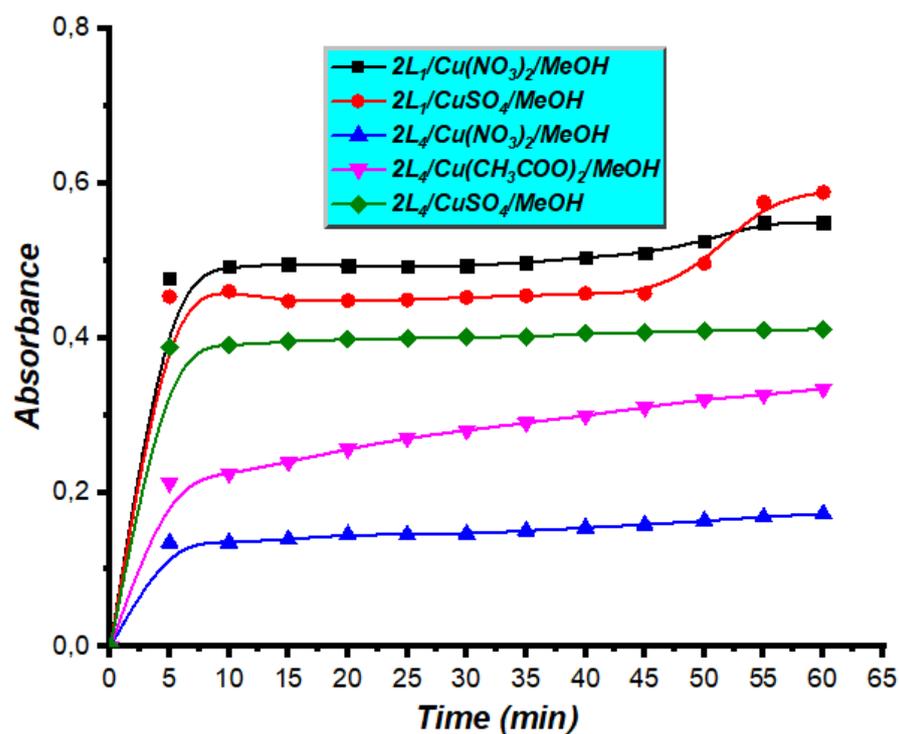


Figure S20. Absorbance evolution of *o*-quinone in presence of complexes formed by L<sub>1</sub> and L<sub>4</sub> with different copper salts in MeOH.

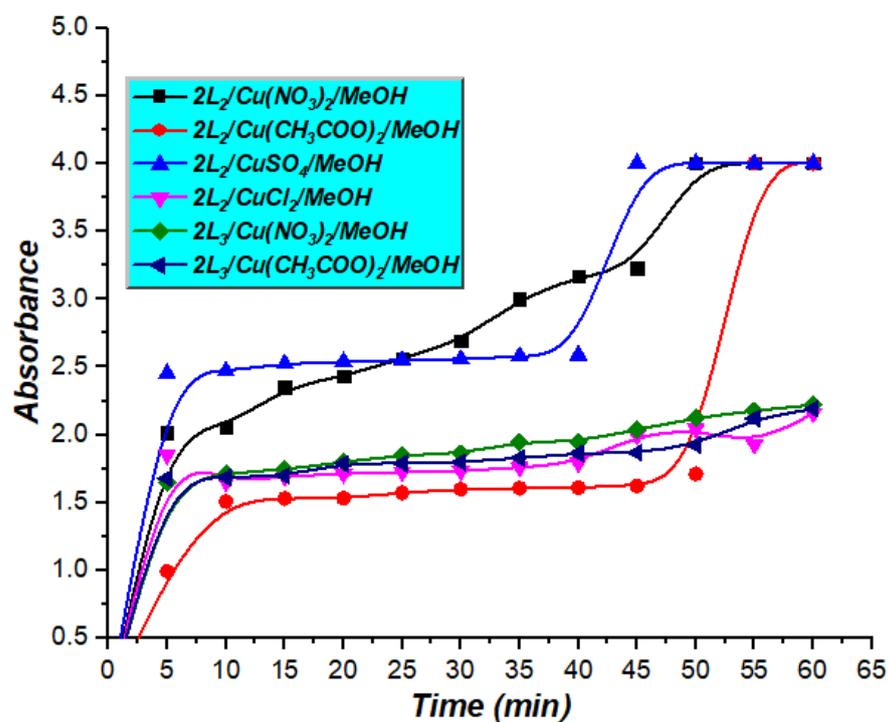


Figure S21. Absorbance evolution of *o*-quinone in presence of complexes formed by L<sub>2</sub> and L<sub>3</sub> with different copper salts in MeOH.

## 3. Solvent effect

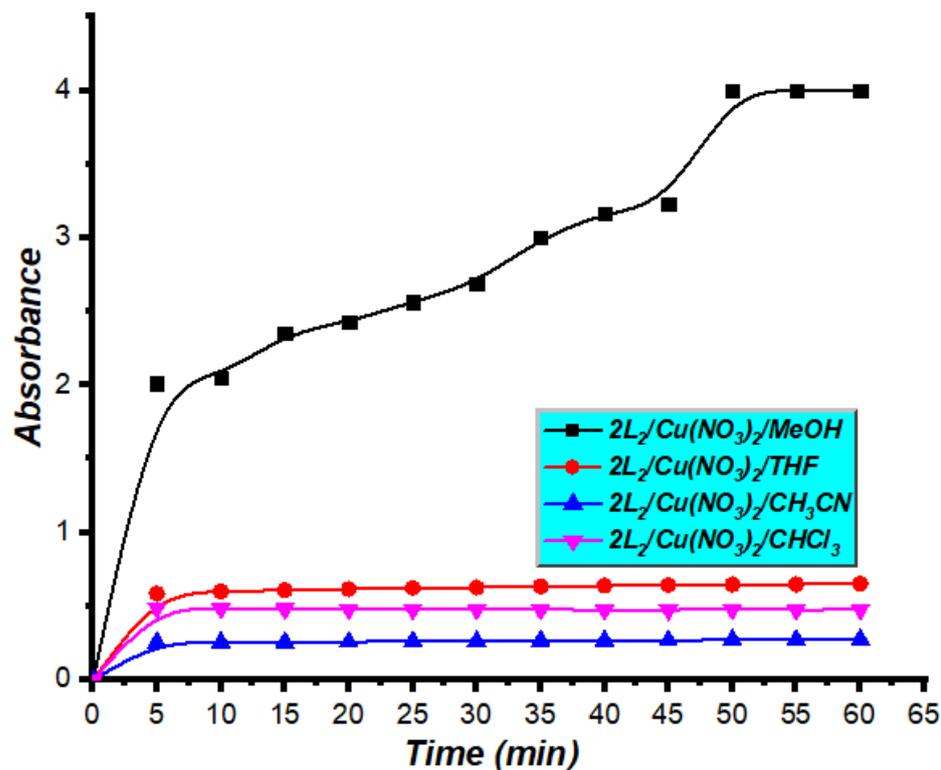


Figure S22. Absorbance evolution of *o*-quinone in presence of complexes formed by 2L<sub>2</sub>/Cu(NO<sub>3</sub>)<sub>2</sub> in different solvents.

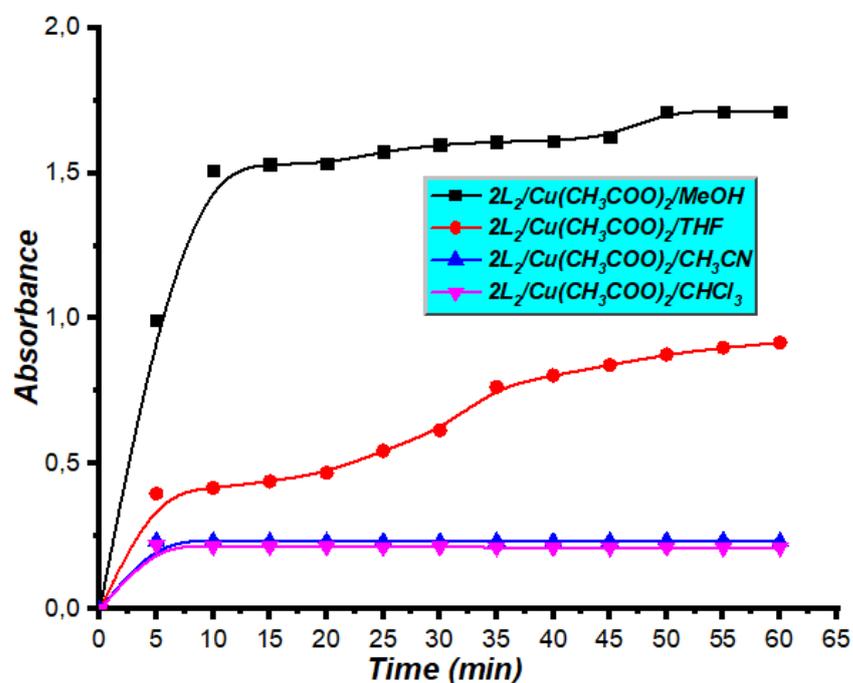


Figure S23. Absorbance evolution of *o*-quinone in presence of complexes formed by 2L<sub>2</sub>/Cu(CH<sub>3</sub>COO)<sub>2</sub> in different solvents.

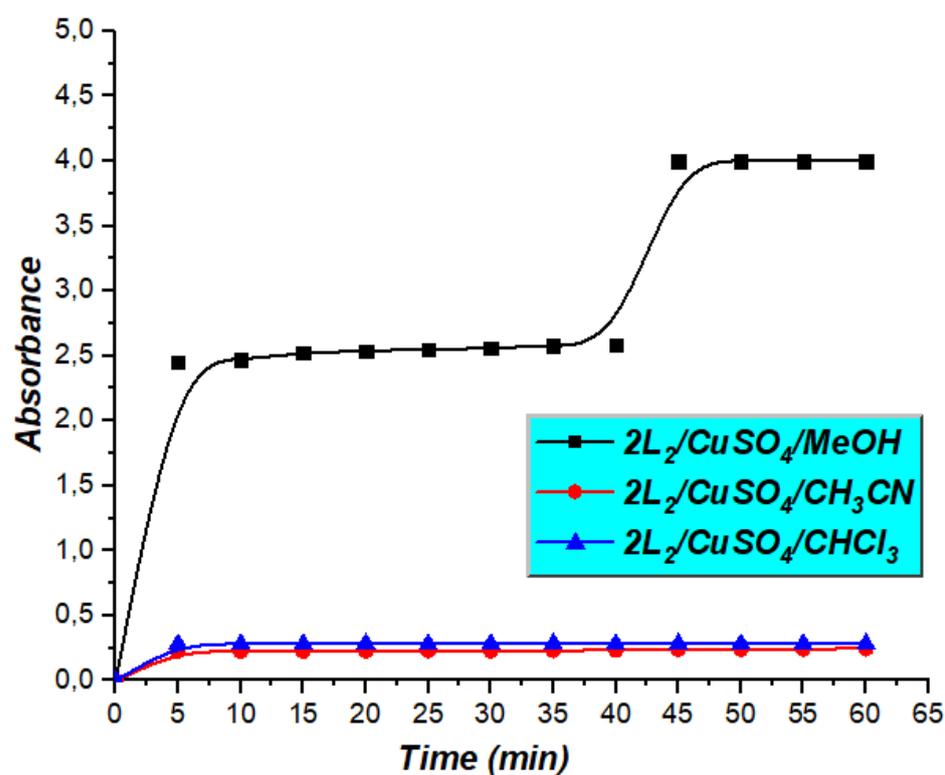


Figure S24. Absorbance evolution of *o*-quinone in presence of complexes formed by 2L<sub>2</sub>/CuCuSO<sub>4</sub> in different solvents.

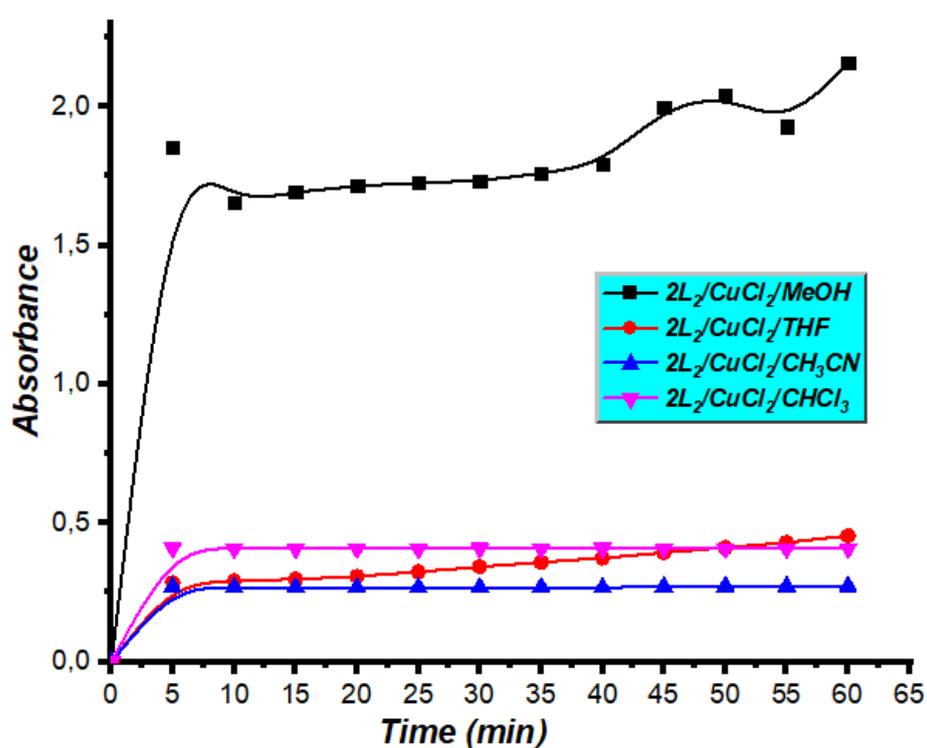
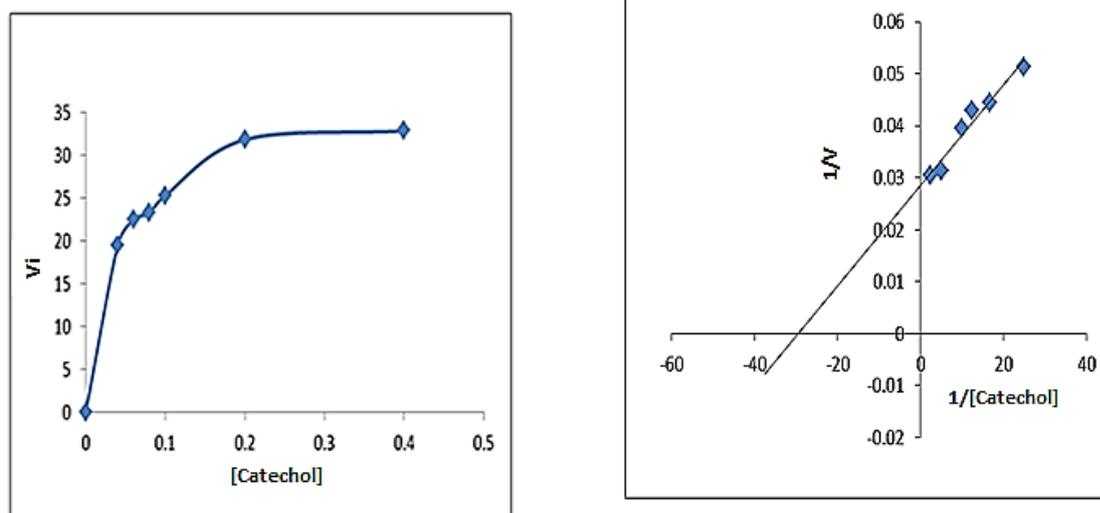
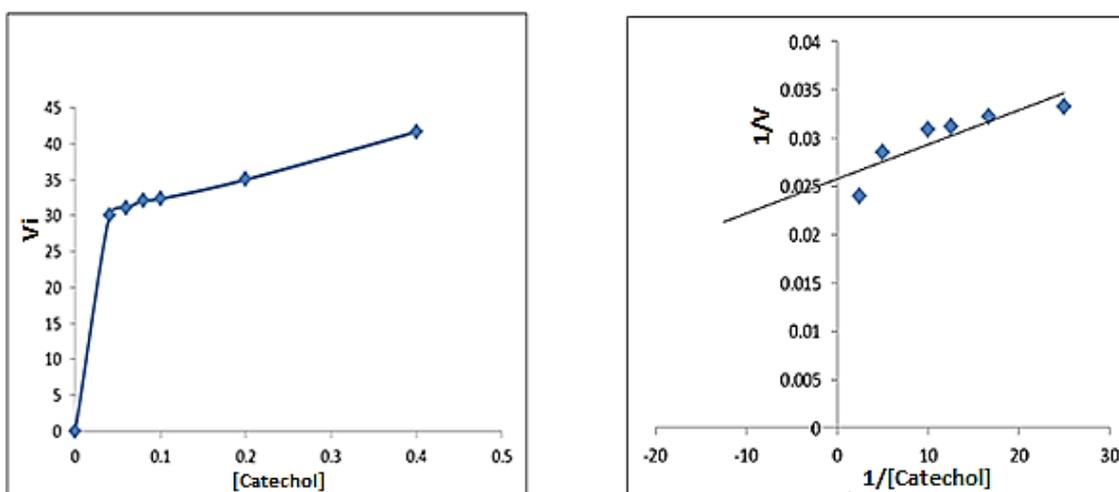
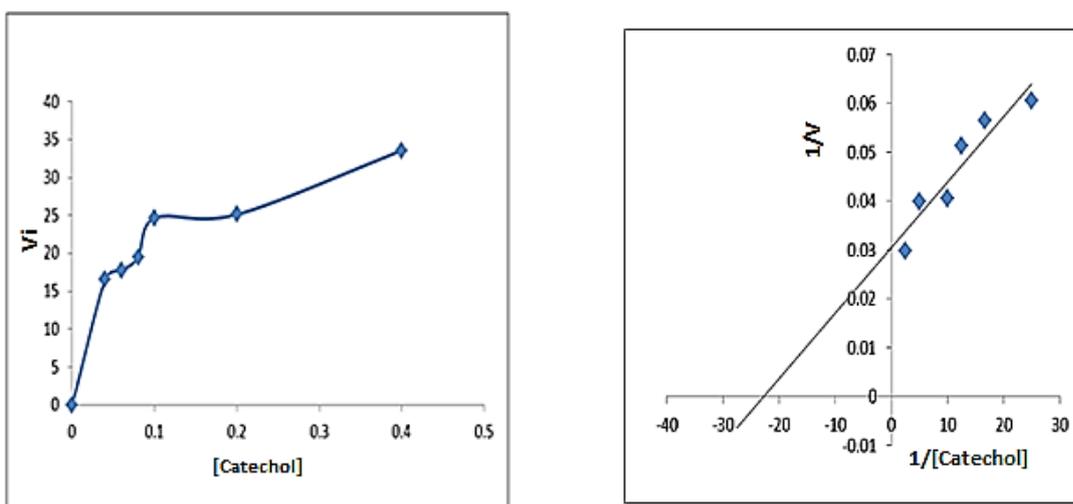


Figure S25. Absorbance evolution of *o*-quinone in presence of complexes formed by 2L<sub>2</sub>/CuCl<sub>2</sub> in different solvents.

## 4. Kinetic study

Figure S26. Reaction dependence on the concentration of catechol using  $2L_2/Cu(NO_3)_2$ .Figure S27. Reaction dependence on the concentration of catechol using  $2L_2/Cu(CH_3COO)_2$ .Figure S28. Reaction dependence on the concentration of catechol using  $2L_2/CuSO_4$ .