

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

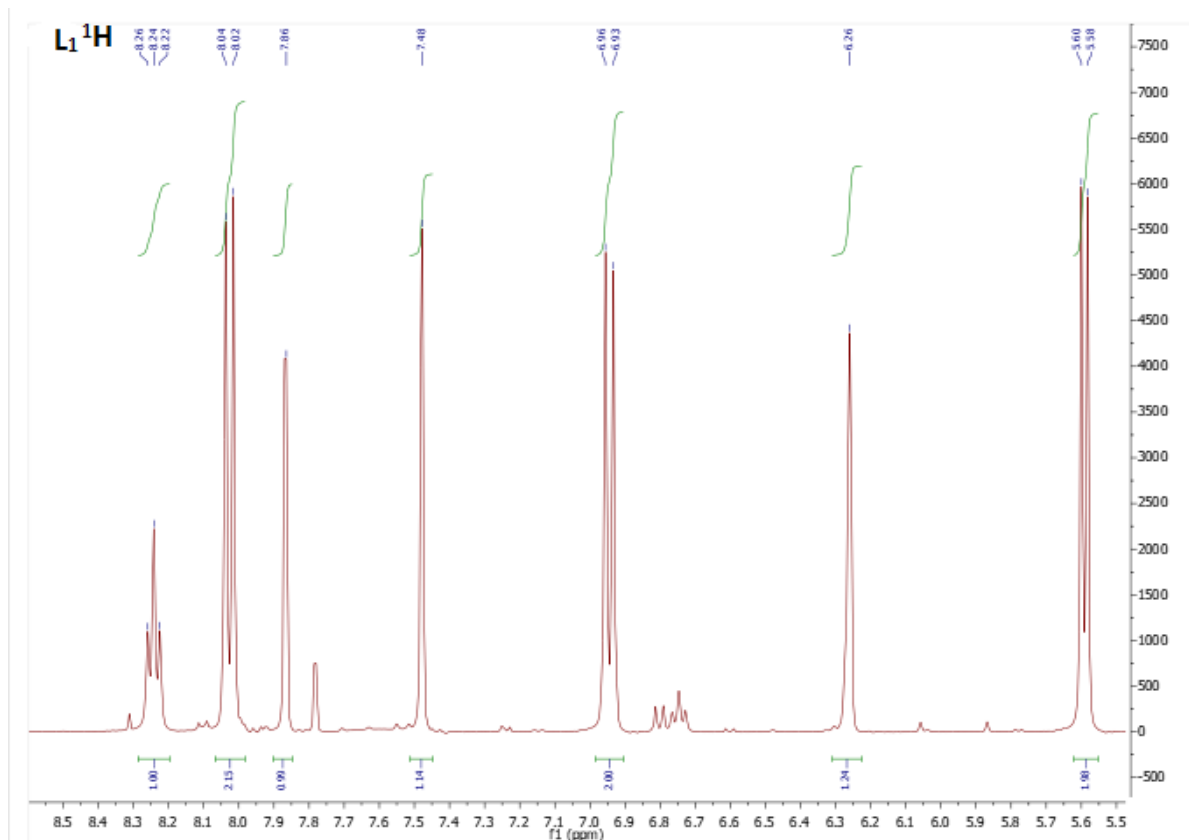


Figure S1. ¹H NMR spectrum of L1 in DMSO (400 MHz).

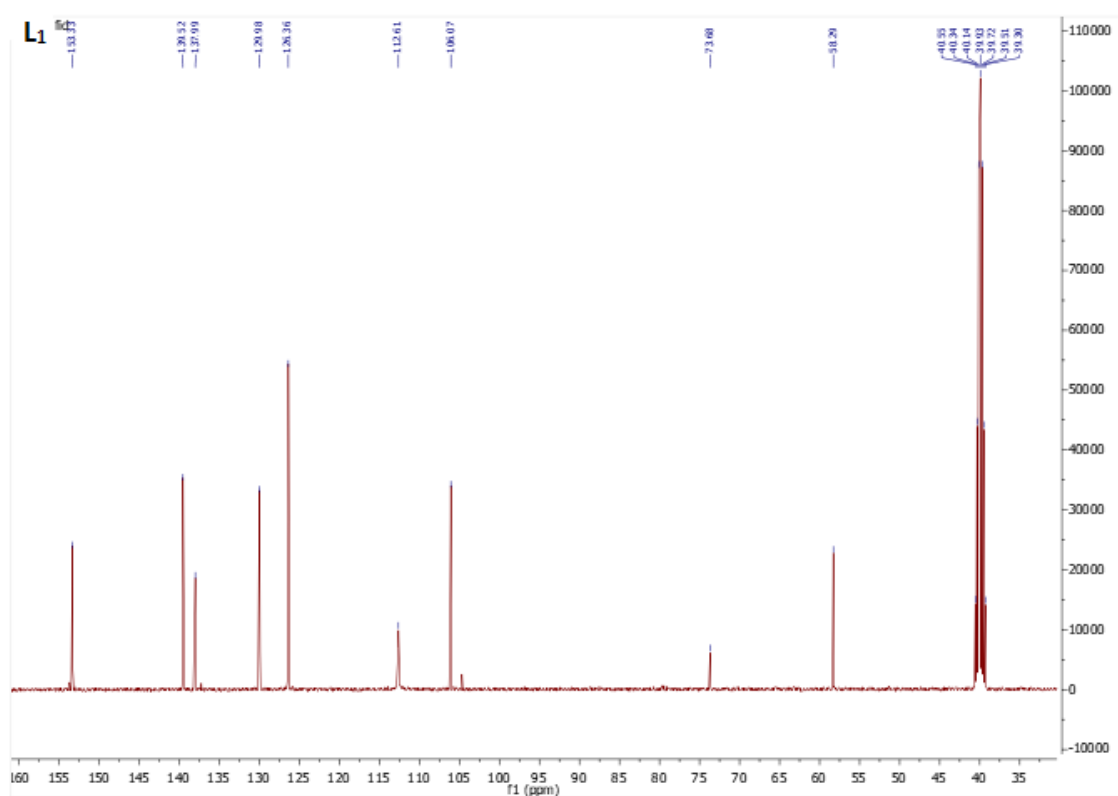


Figure S2. ¹³C NMR spectrum of **L1** in DMSO (400 MHz).

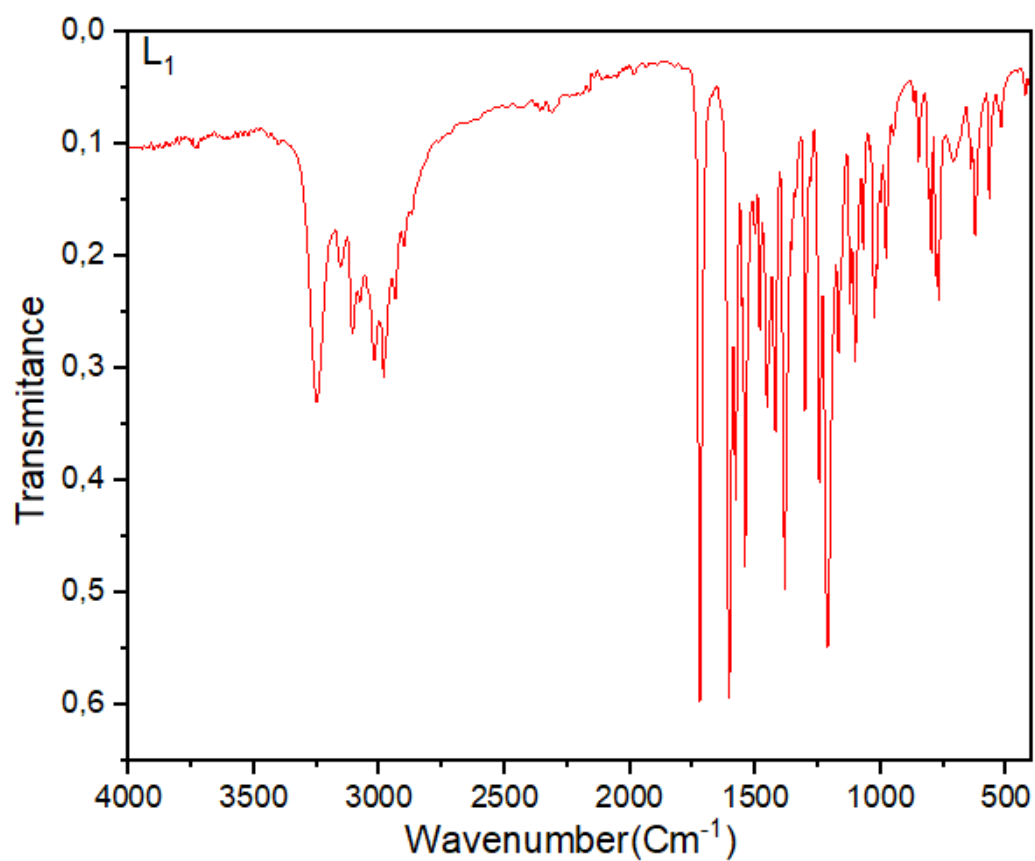


Figure S3. FT-IR spectrum of **L1**.

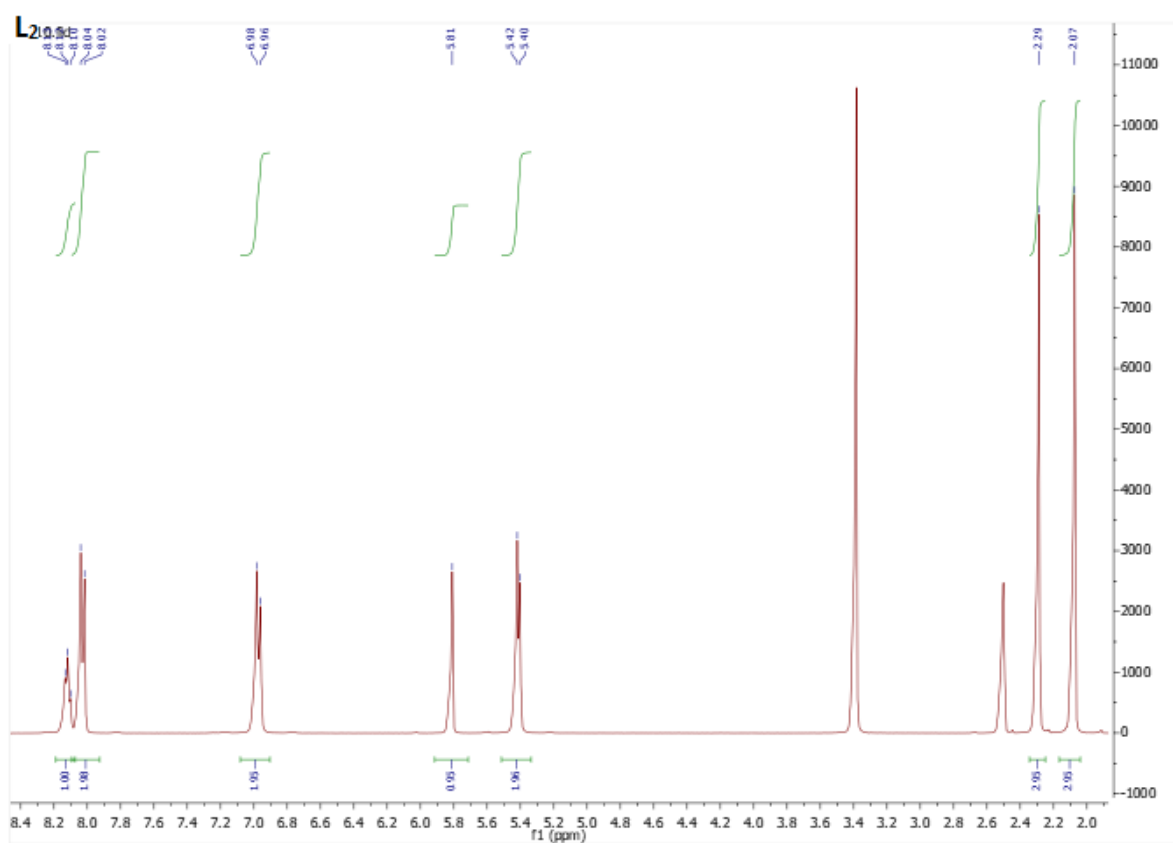


Figure S4. ^1H NMR spectrum of L_2 in DMSO (400 MHz).

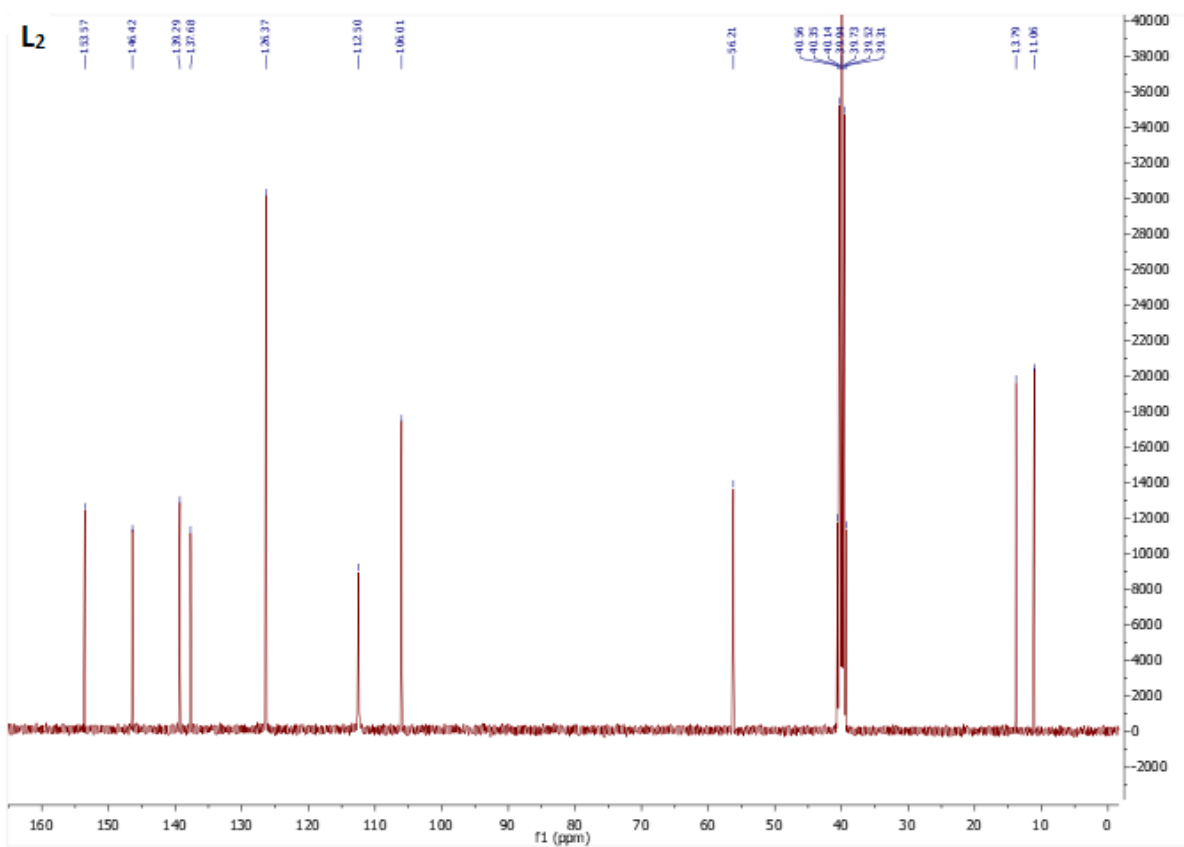


Figure S5. ^{13}C NMR spectrum of L_2 in DMSO (400 MHz).

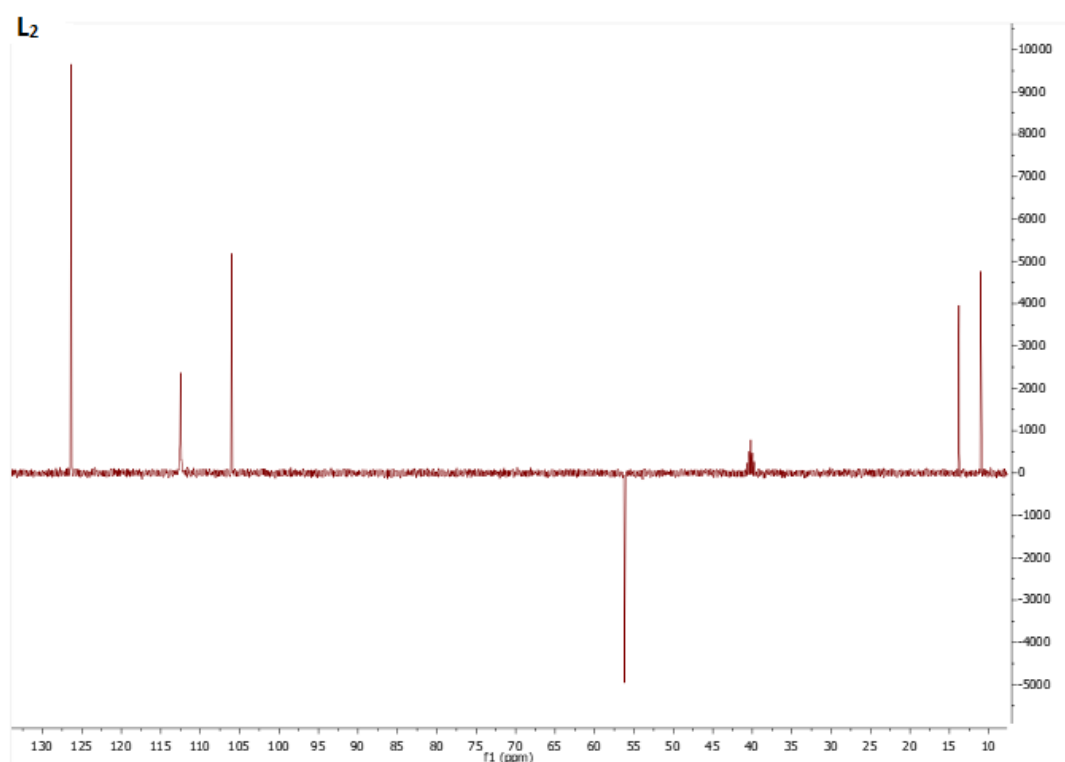


Figure S6. DEPT- 135 NMR spectrum of L₂ in DMSO (400 MHz).

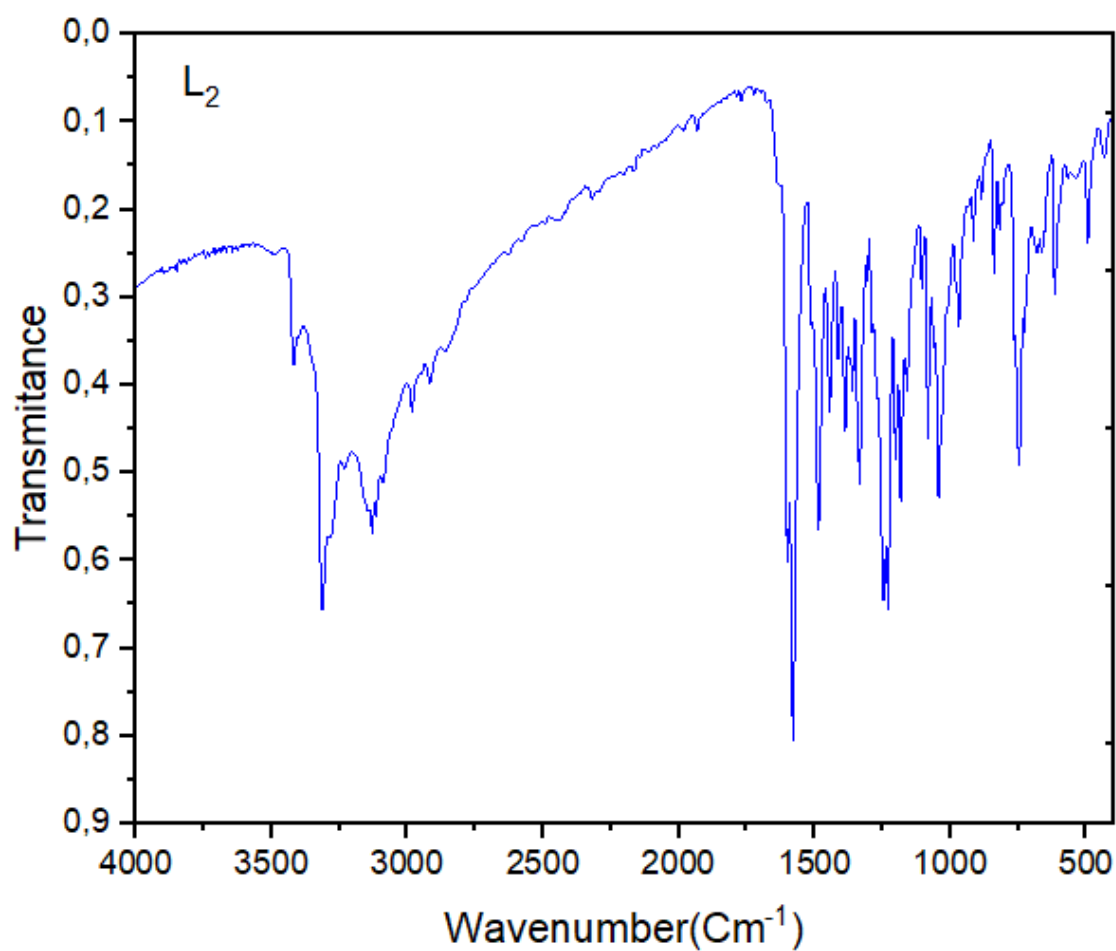
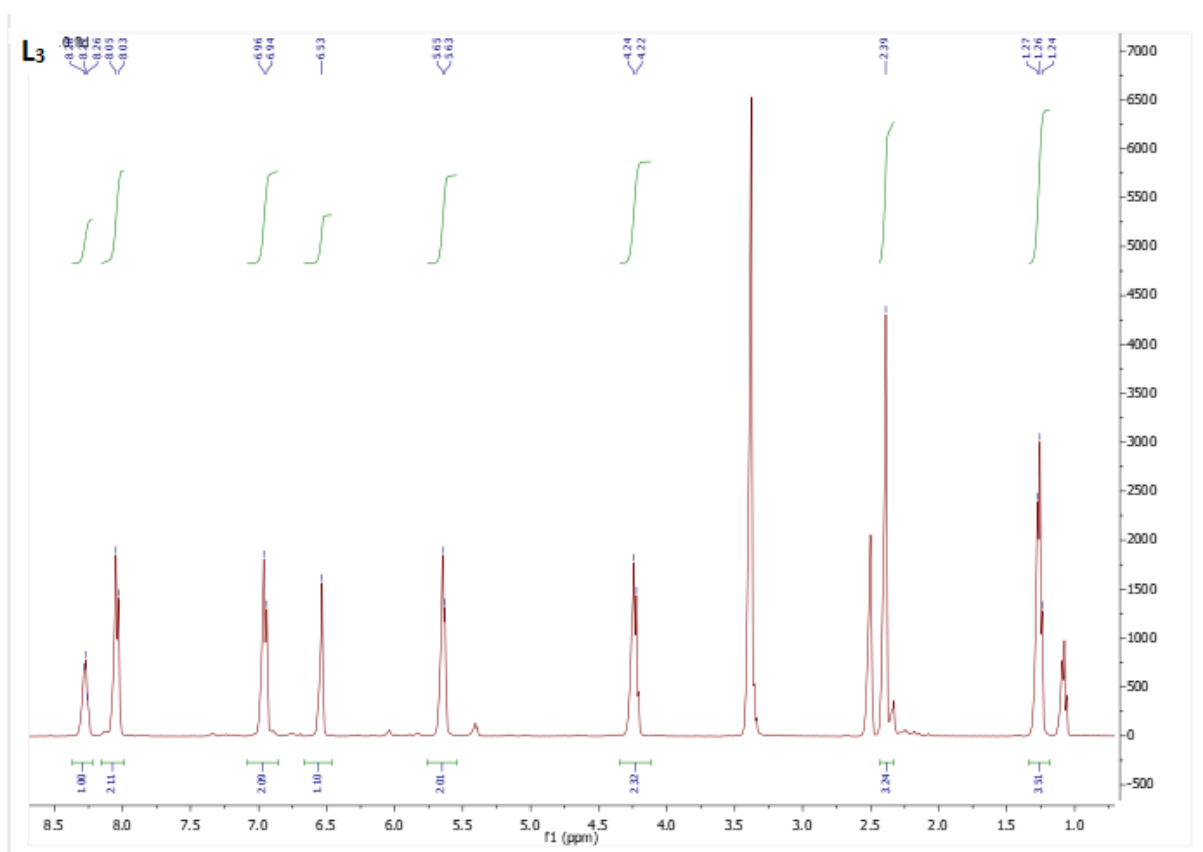
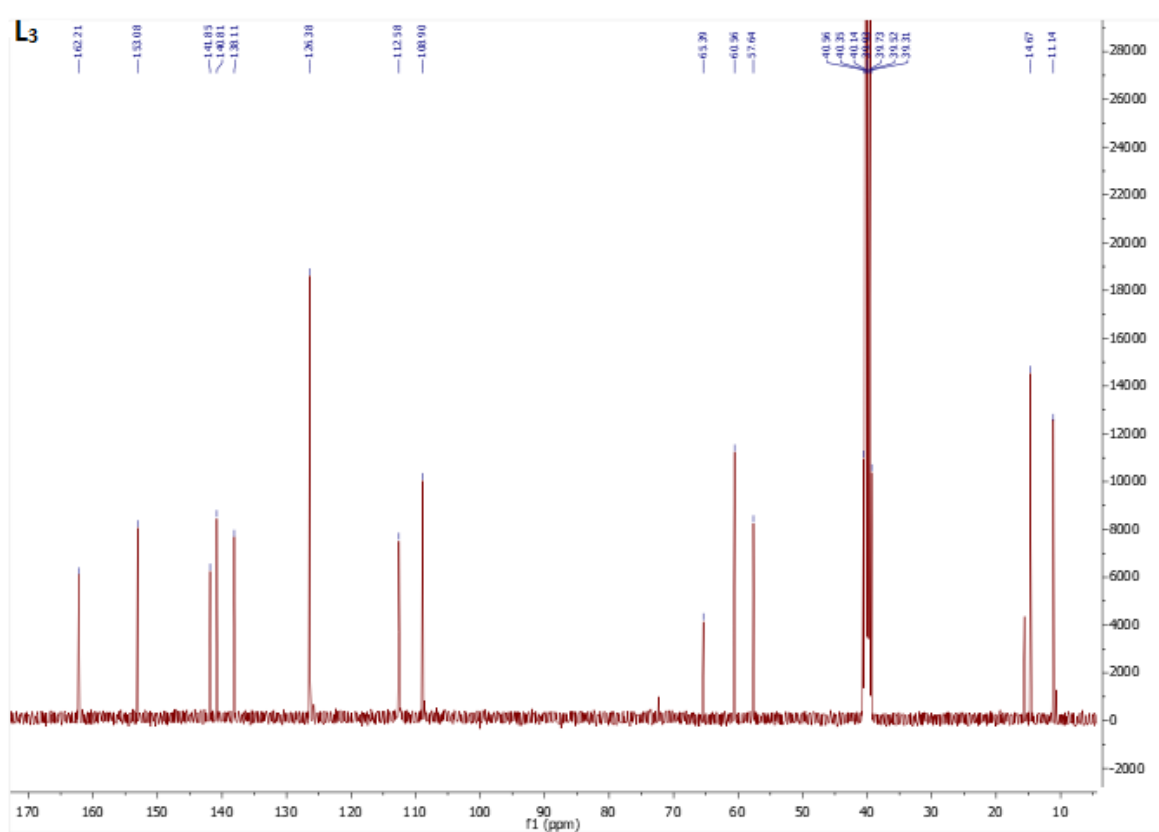


Figure S7. FT-IR spectrum of L₂.

Figure S8. ¹H NMR spectrum of L3 in DMSO (400 MHz).Figure S9. ¹³C NMR spectrum of L3 in DMSO (400 MHz).

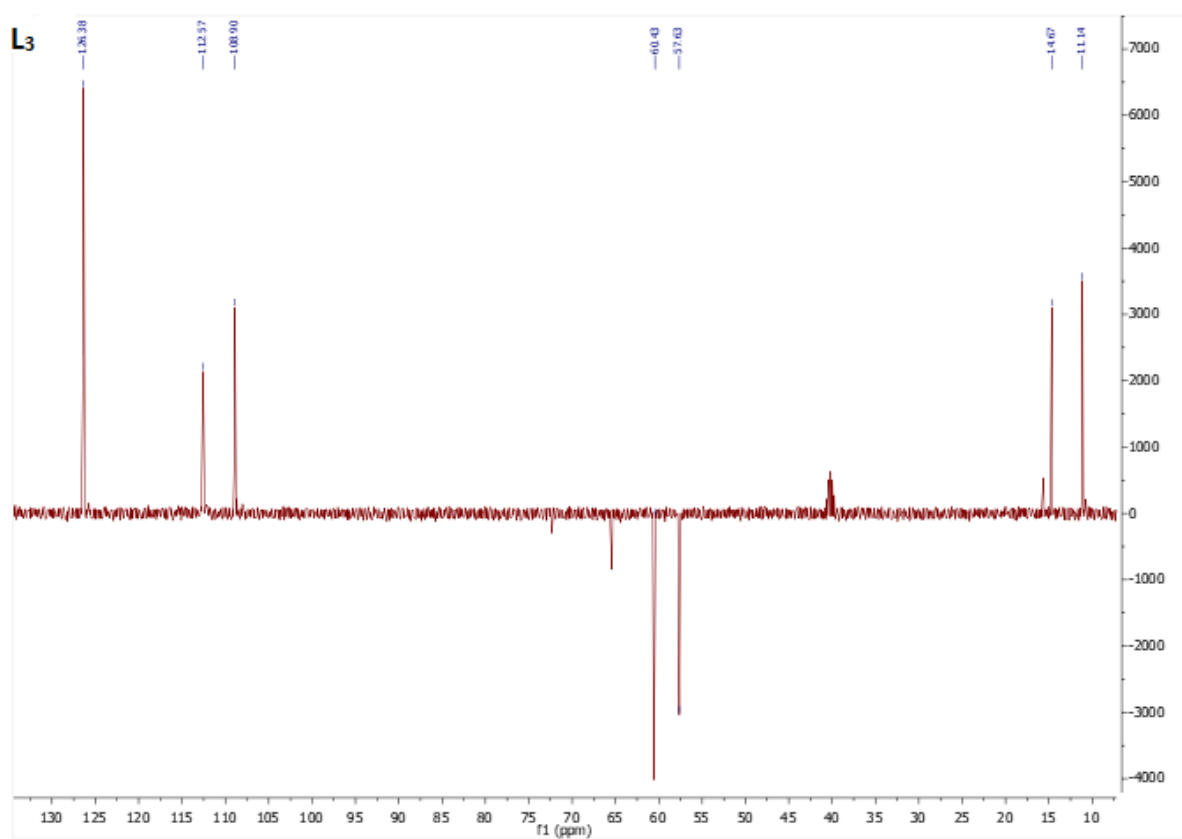


Figure S10. DEPT- 135 NMR spectrum of L₃ in DMSO (400 MHz).

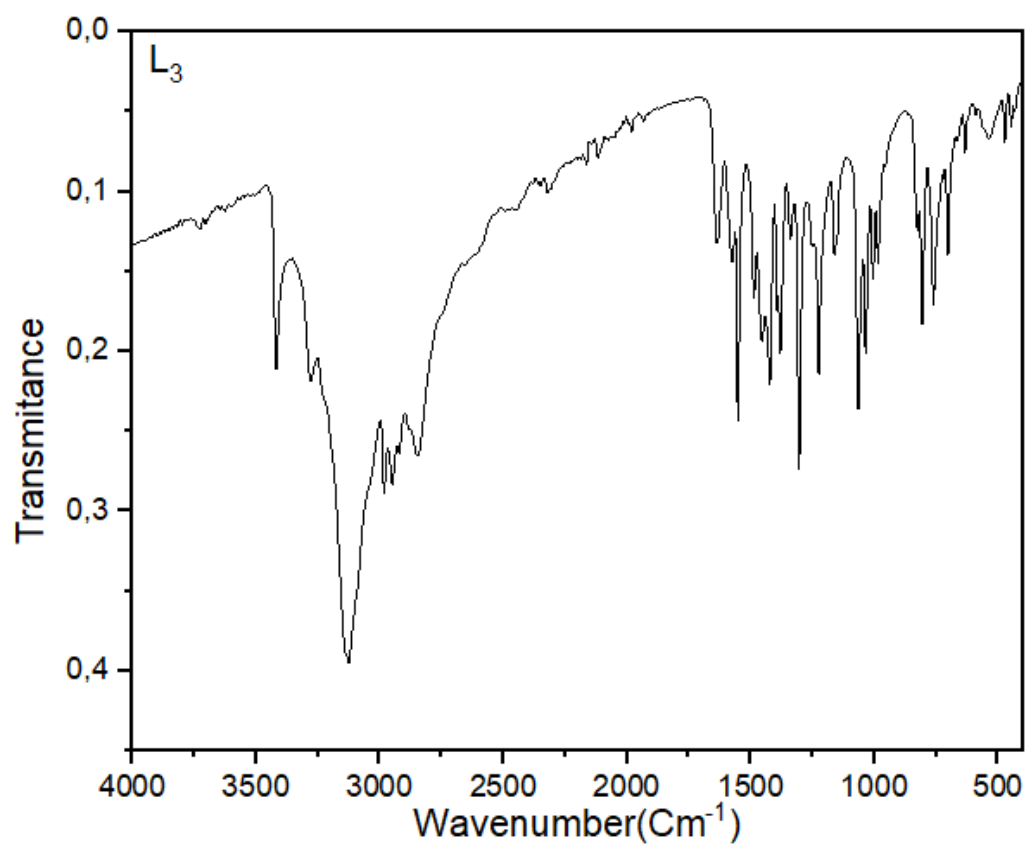


Figure S11. FT-IR spectrum of L₃.

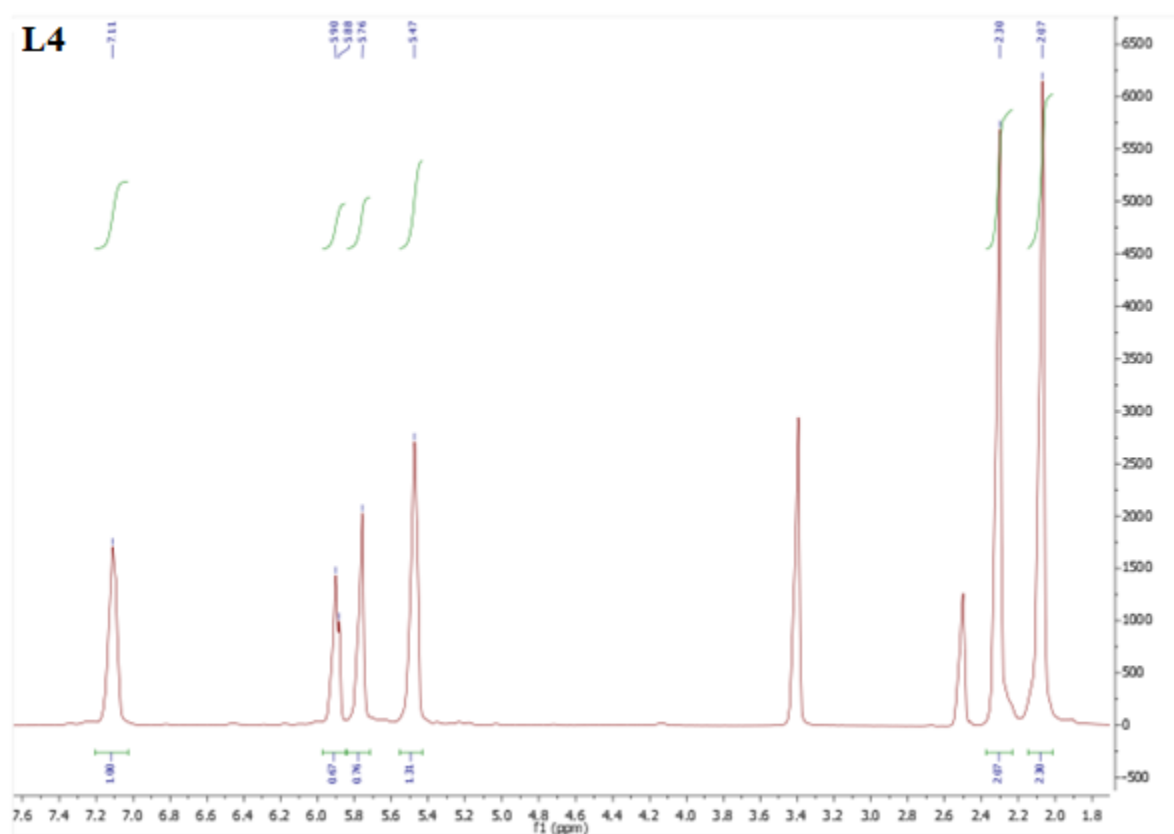


Figure S12. ^1H NMR spectrum of L4 in DMSO (400 MHz).

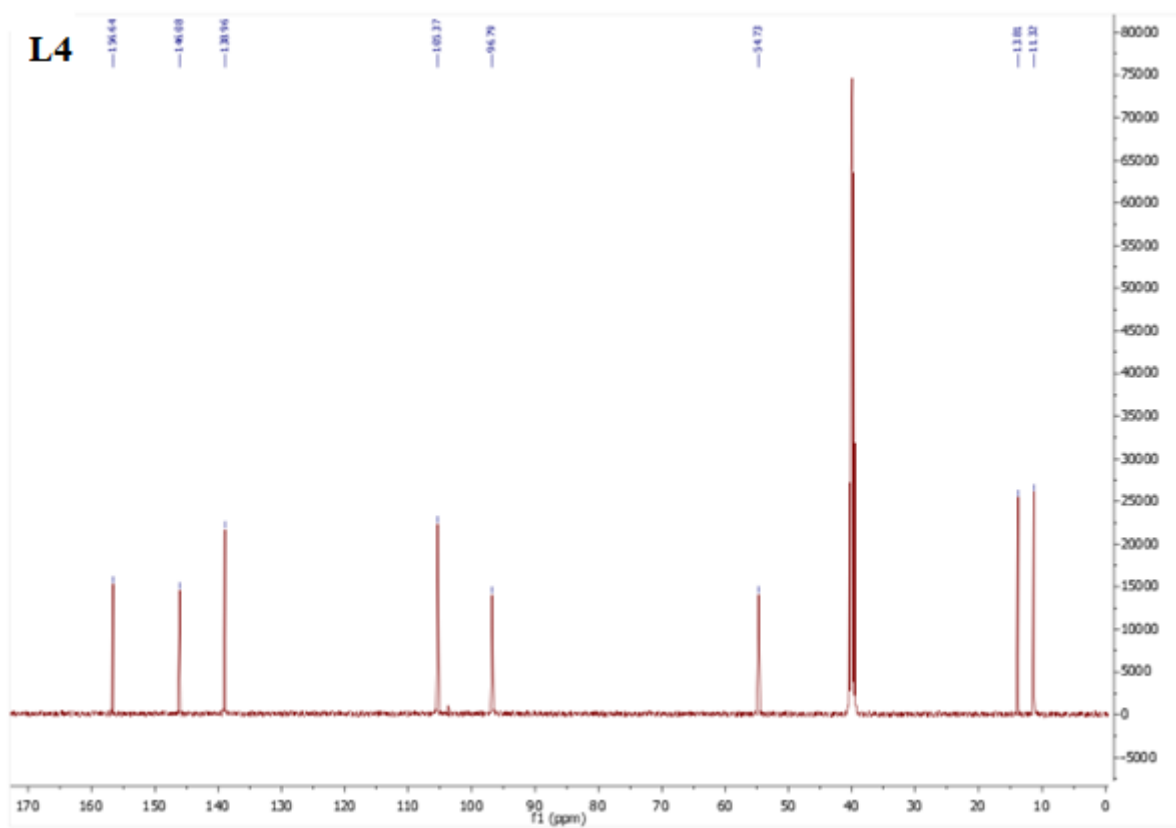


Figure S13. ^{13}C NMR spectrum of L4 in DMSO (400 MHz).

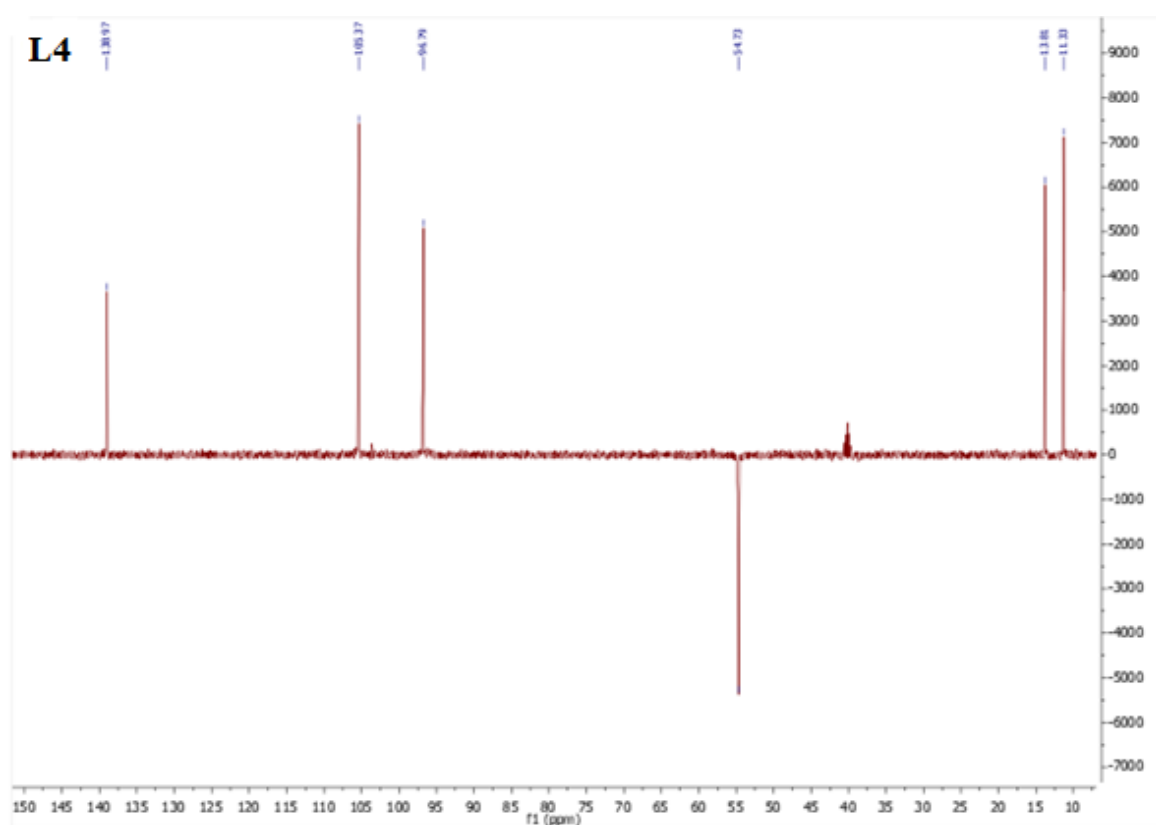


Figure S14. ^{13}C NMR spectrum of L4 in DMSO (400 MHz).

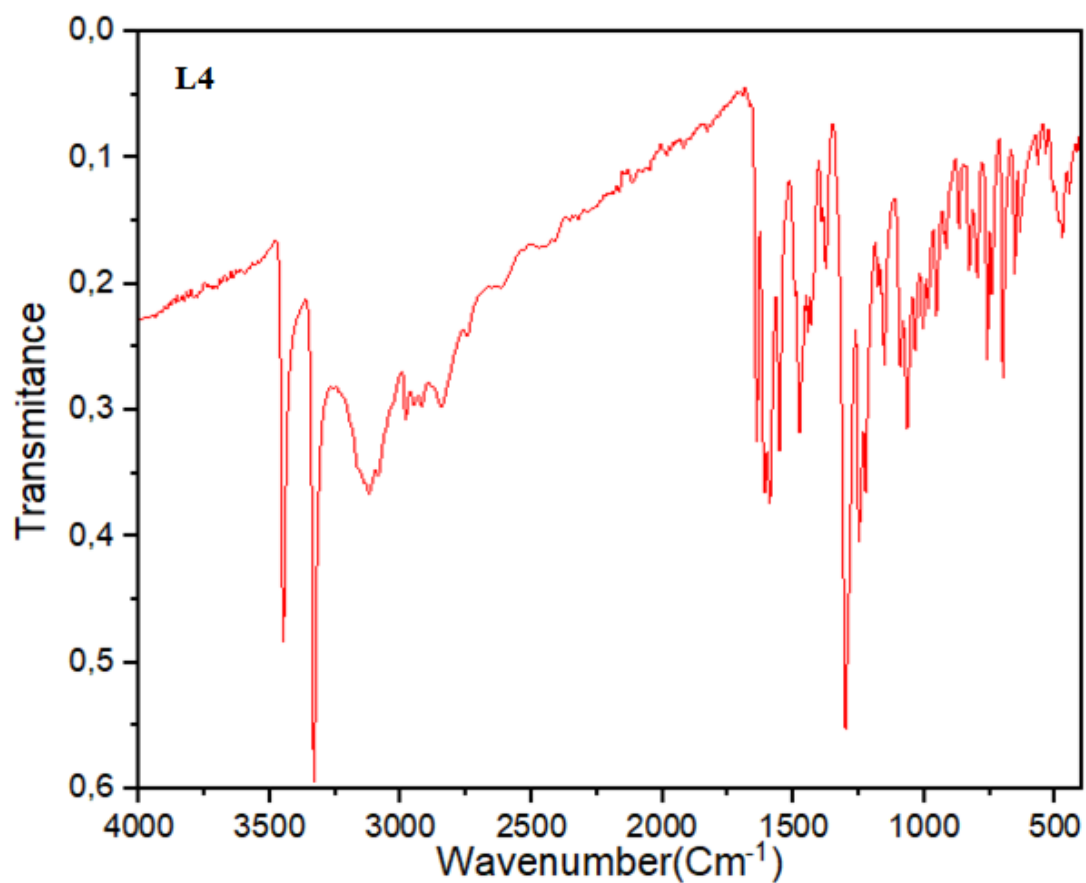


Figure S15. FT-IR spectrum of L4.

2. Effect of concentration

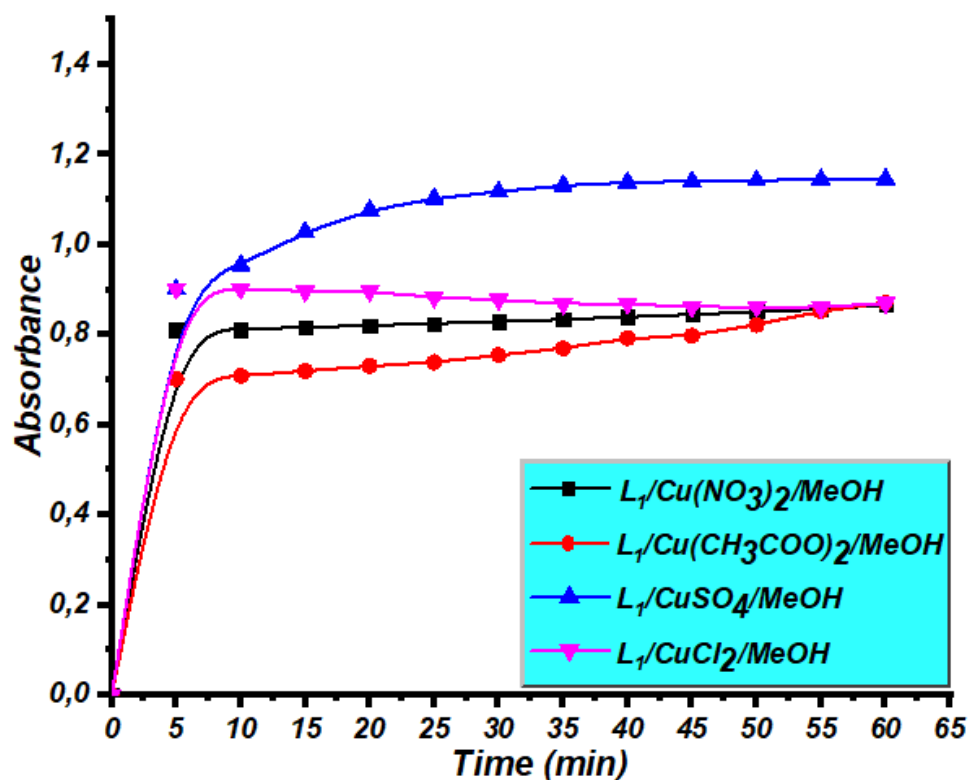


Figure S16. Absorbance evolution of *o*-quinone in presence of complexes formed by L_1 and different copper salts in MeOH.

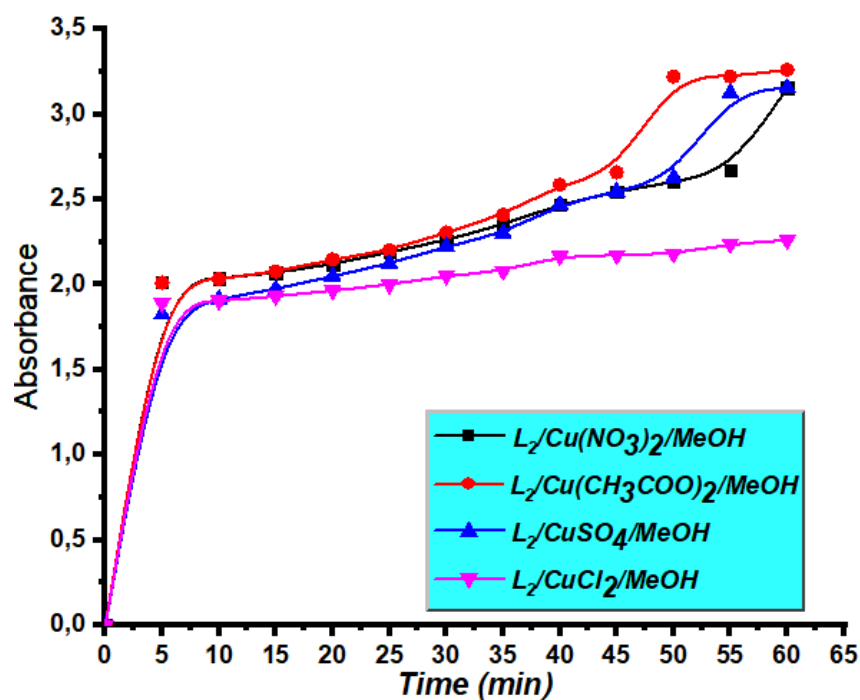


Figure S17. Absorbance evolution of *o*-quinone in presence of complexes formed by L_2 and different copper salts in MeOH.

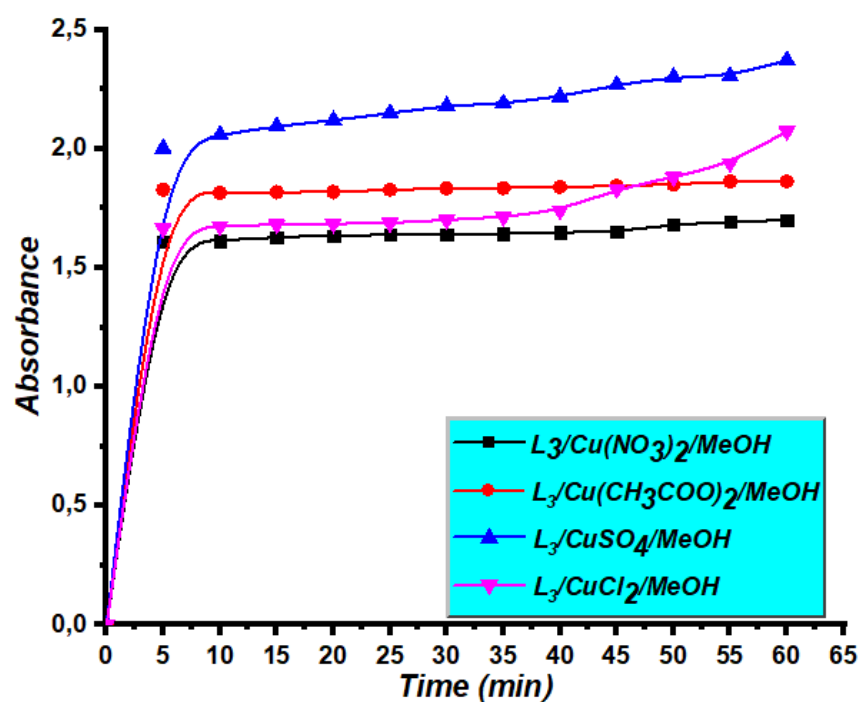


Figure S18. Absorbance evolution of *o*-quinone in presence of complexes formed by L_3 and different copper salts in MeOH.

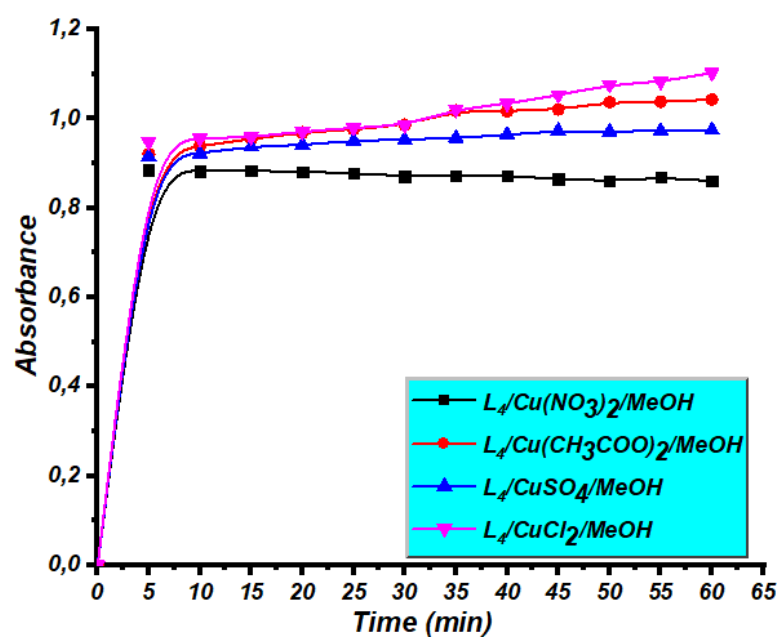


Figure S19. Absorbance evolution of *o*-quinone in presence of complexes formed by L_4 and different copper salts in MeOH.

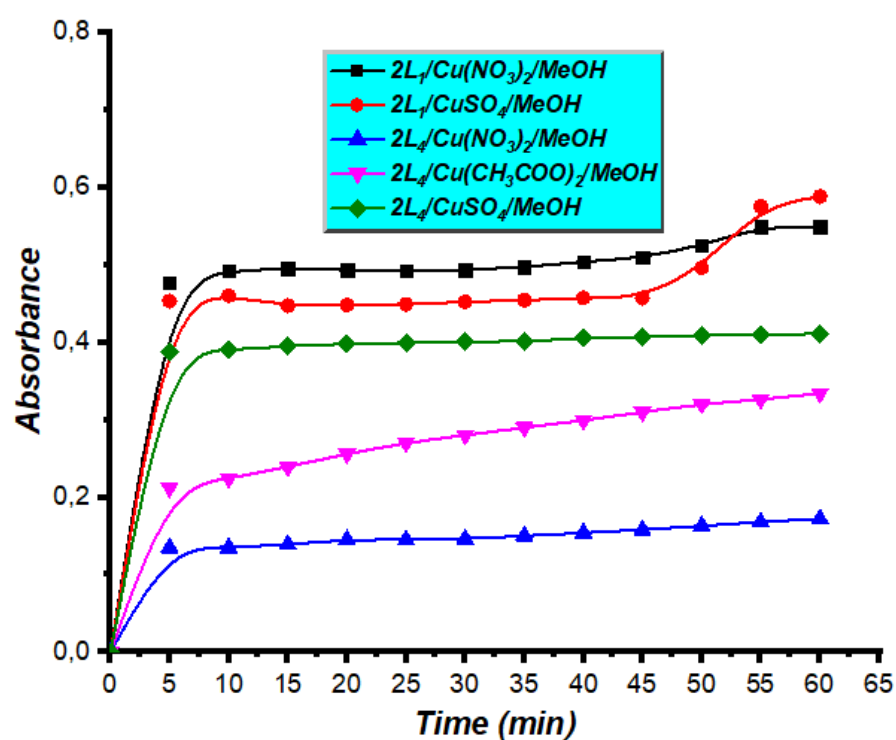


Figure S20. Absorbance evolution of *o*-quinone in presence of complexes formed by L_1 and L_4 with different copper salts in MeOH.

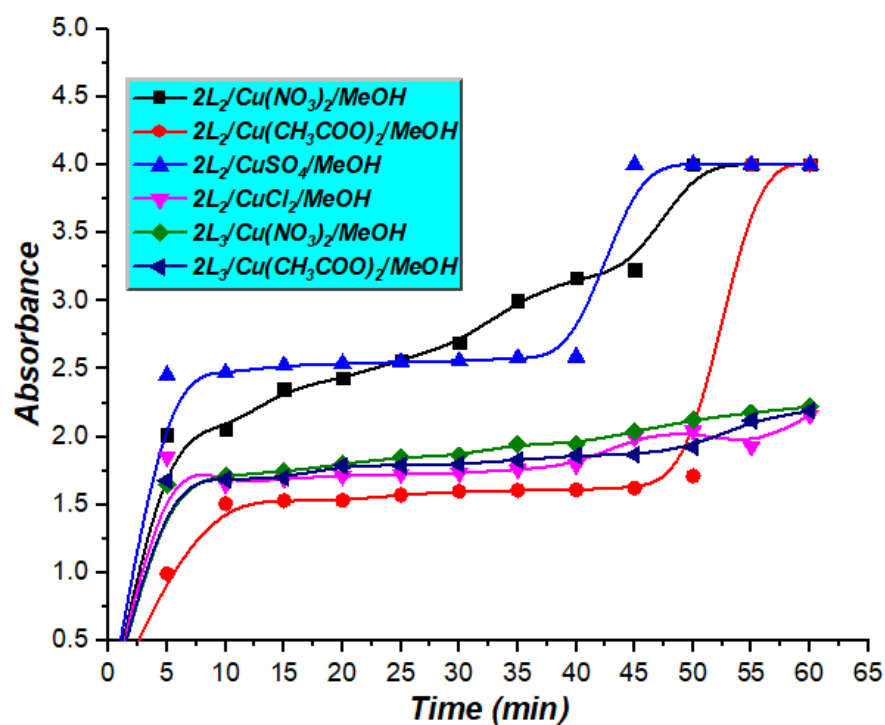


Figure S21. Absorbance evolution of *o*-quinone in presence of complexes formed by L_2 and L_3 with different copper salts in MeOH.

3. Solvent effect

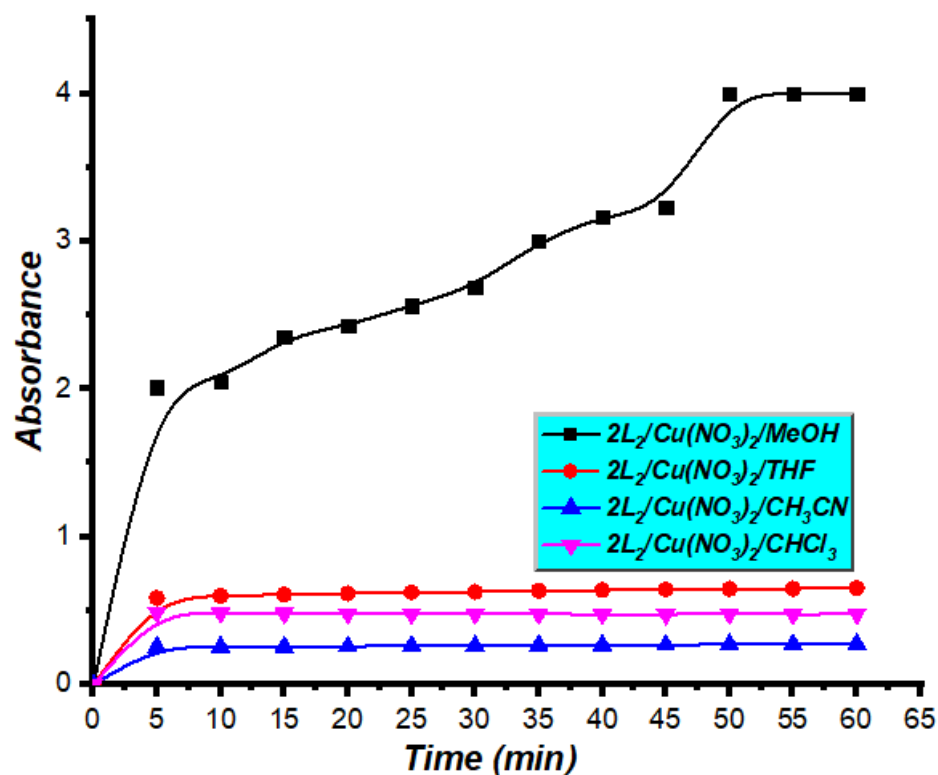


Figure S22. Absorbance evolution of *o*-quinone in presence of complexes formed by $2L_2/Cu(NO_3)_2$ in different solvents.

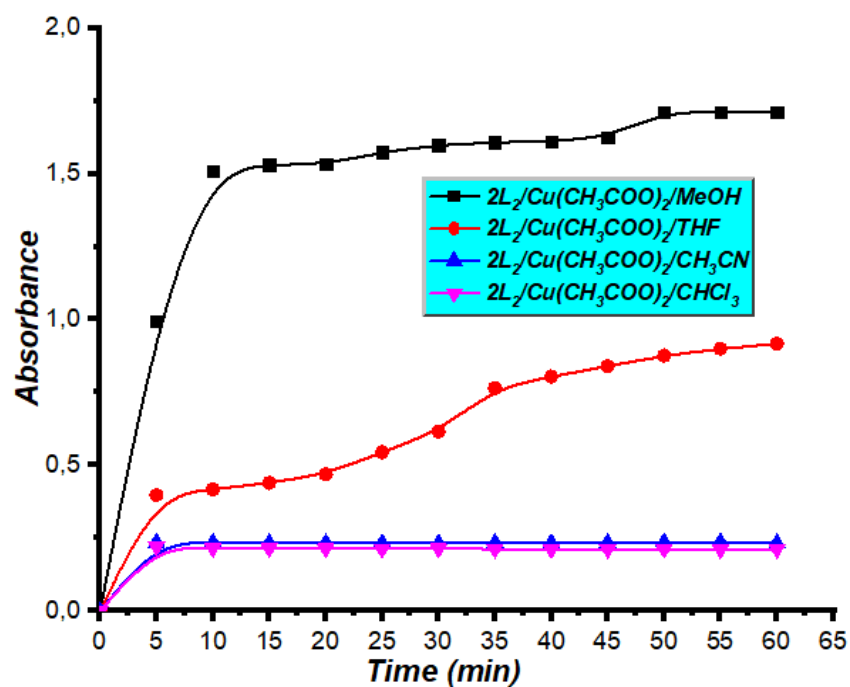


Figure S23. Absorbance evolution of *o*-quinone in presence of complexes formed by $2L_2/Cu(CH_3COO)_2$ in different solvents.

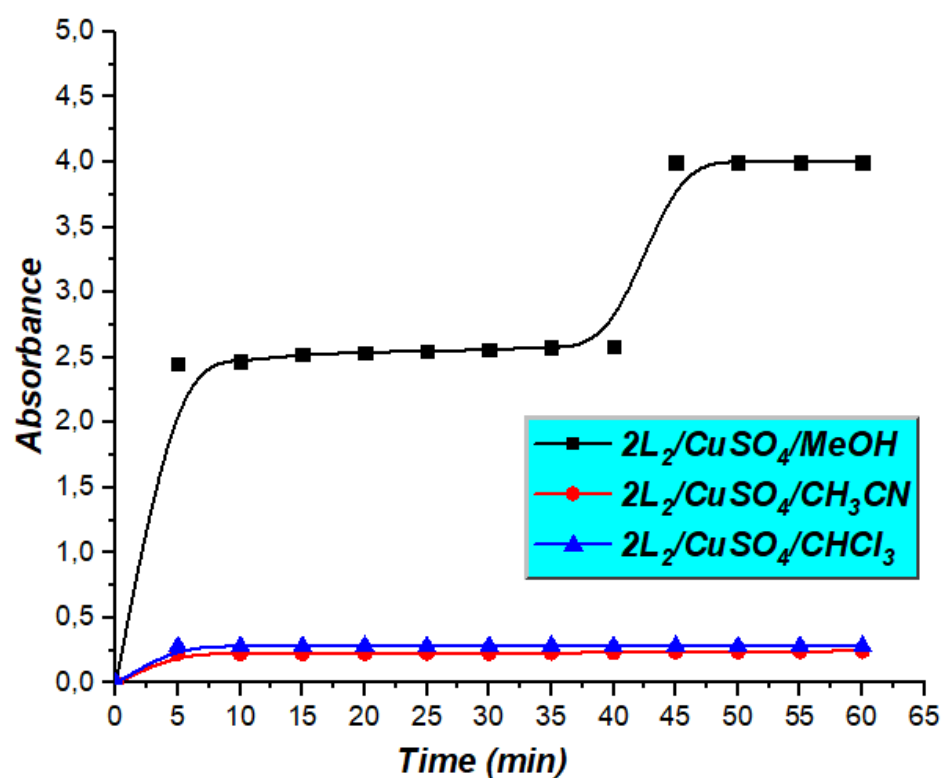


Figure S24. Absorbance evolution of *o*-quinone in presence of complexes formed by 2L₂/CuCuSO₄ in different solvents.

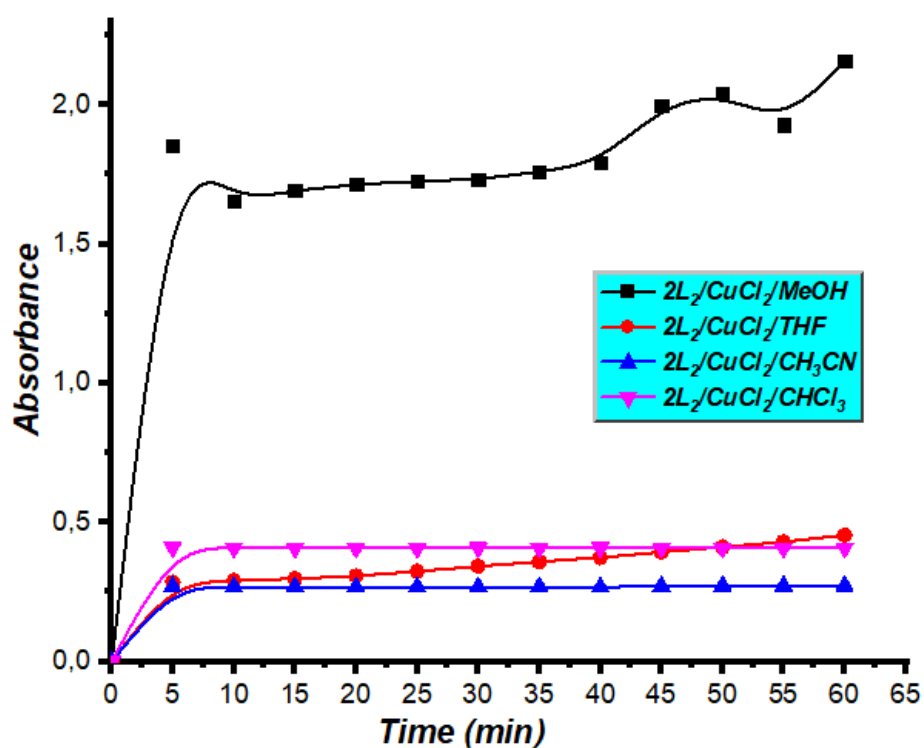
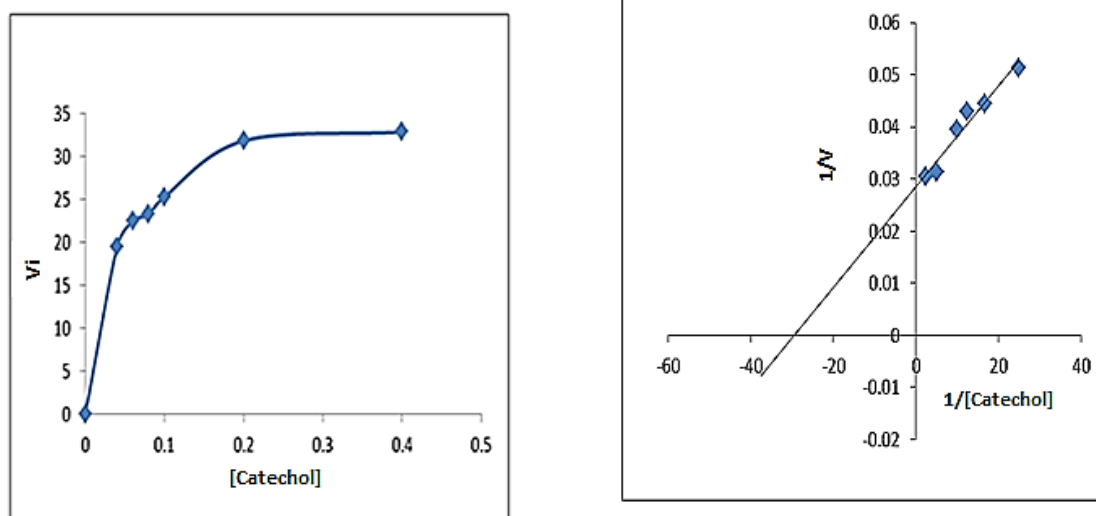
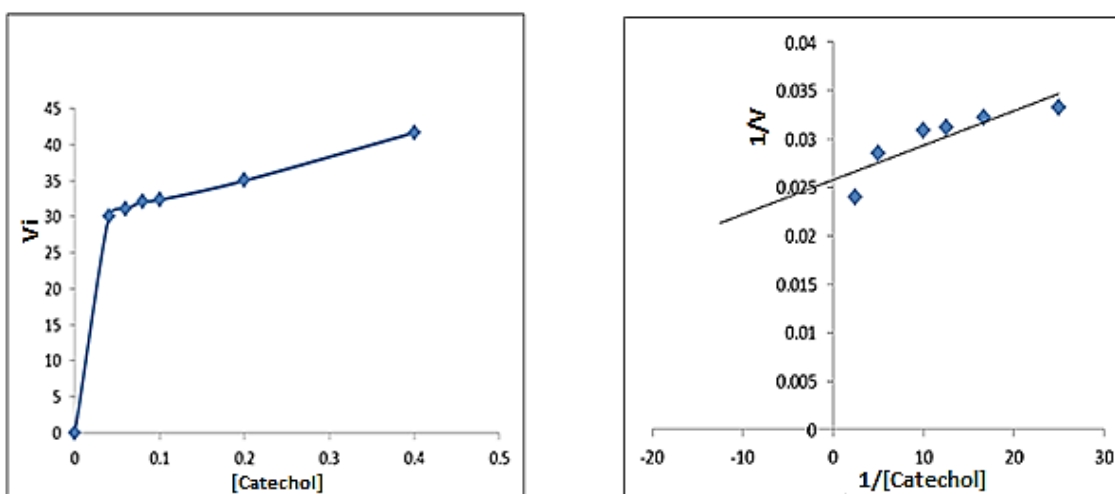
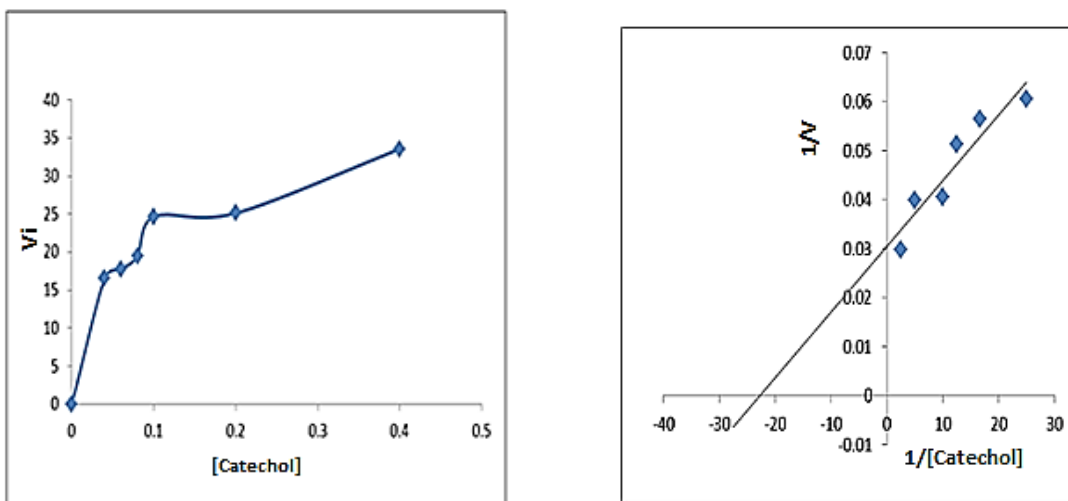


Figure S25. Absorbance evolution of *o*-quinone in presence of complexes formed by 2L₂/CuCl₂ in different solvents.

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 $2L_2/CuSO_4$.