

Supplementary Materials

Inhibition of *C. albicans* dimorphic switch by Cobalt(II) Complexes with Ligands Derived from Pyrazoles and Dinitrobenzoate: Synthesis, Characterization and Biological Activity

1. Characterization of ligands L1-L6

1.1 Bis(3,5-dimethyl-1-pyrazol-1-yl)methane (L1)

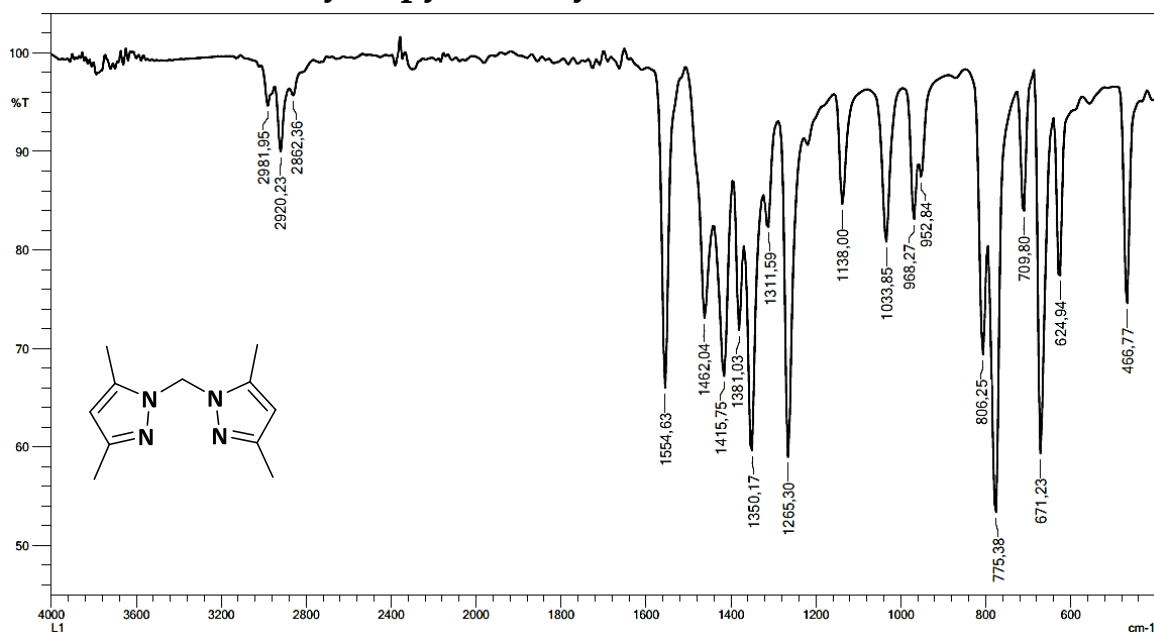


Figure S1. IR spectrum of L1.

1.2 Bis(3,5-dimethyl-4-nitro-1-pyrazol-1-yl)methane (L2)

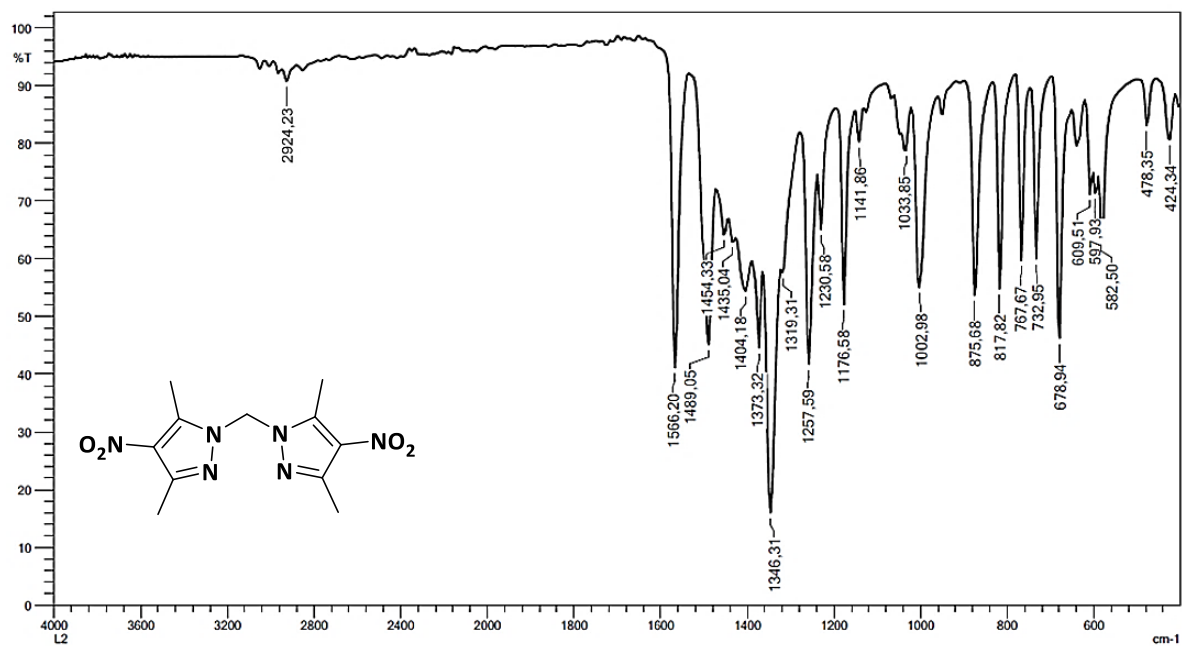


Figure S2. IR spectrum of L2.

1.3 2,6-bis(3,5-dimethylpyrazol-1-yl)methylpyridine (L3)

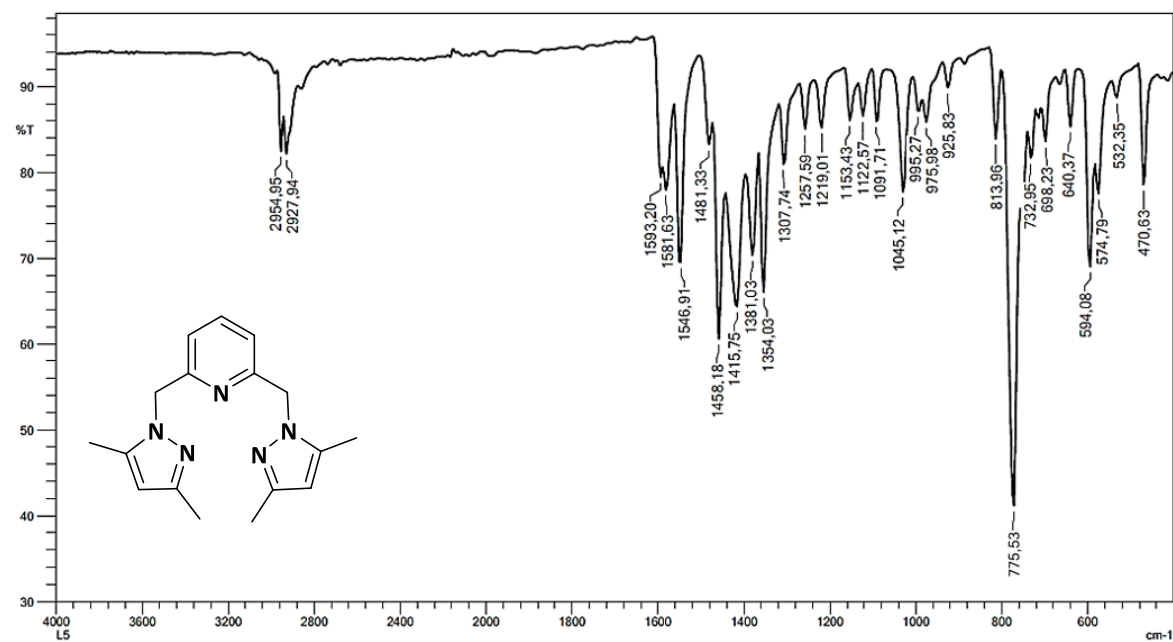


Figure S3. IR spectrum of L3.

1.4 2,6 bis (4-nitro-3,5-dimethylpyrazol-1-ylmethyl)pyridine (L4)

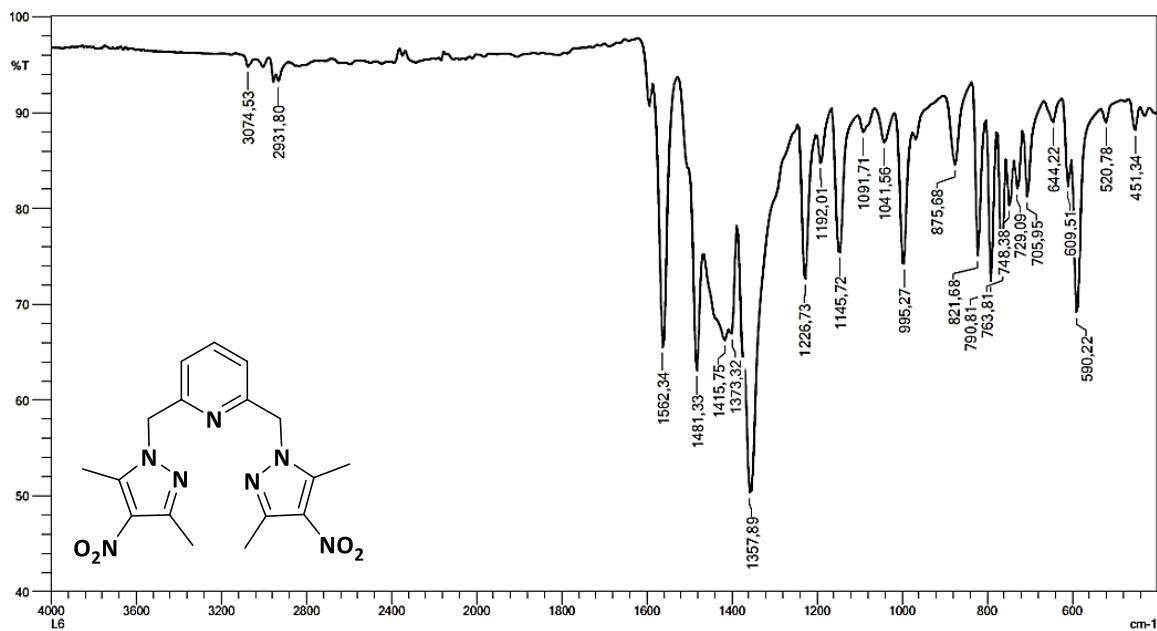


Figure S4. IR spectrum of L4.

1.5 3,5-bis(3,5-dimethylpyrazol-1-ylmethyl)toluene (L5)

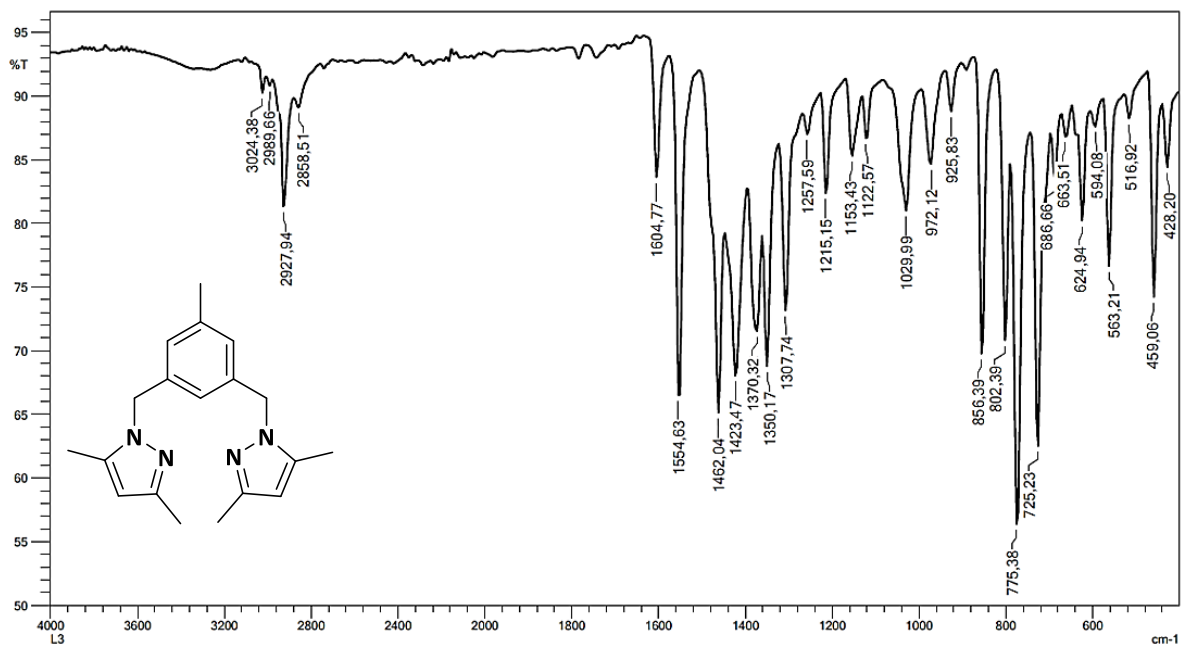


Figure S5. IR spectrum of L5.

1.6 3,5-bis(3,5-dimethyl-4-nitropyrazol-1-ylmethyl)toluene (L6)

^1H NMR (400 MHz, CDCl_3) δ 6.86 (s, 2H), 6.70 (s, 1H), 5.18 (s, 4H), 2.54 (s, 6H), 2.53 (s, 6H), 2.31 (s, 3H).

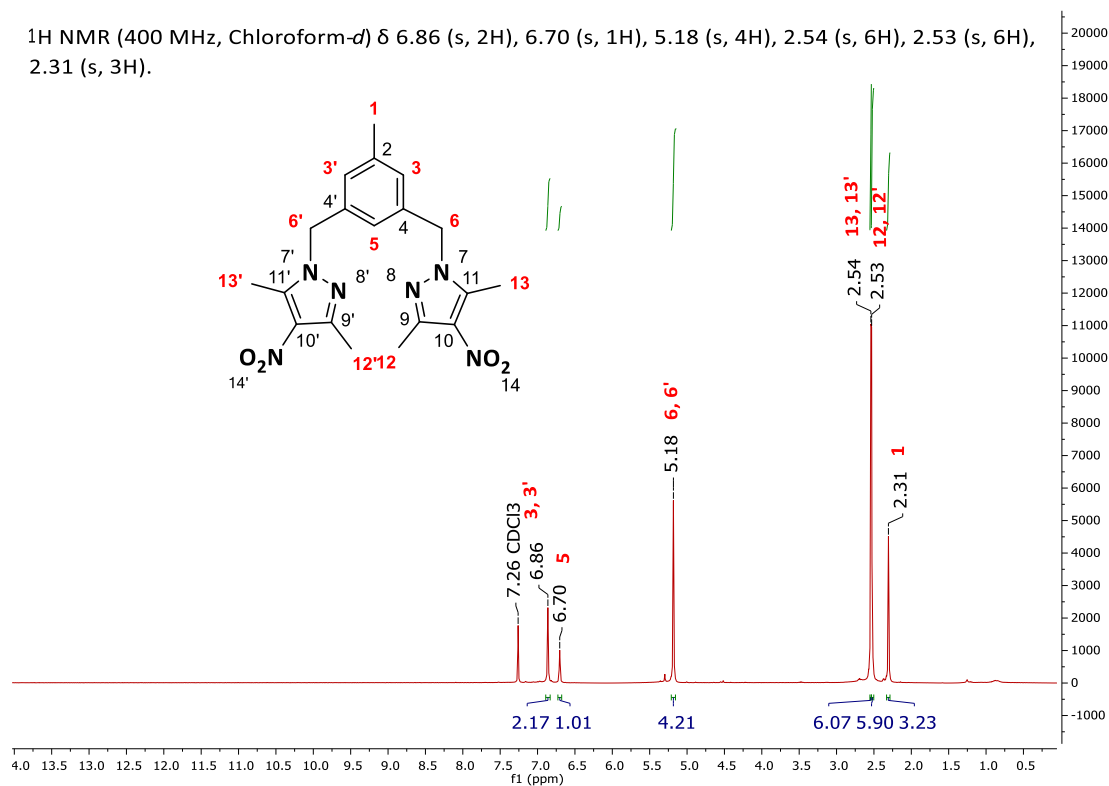


Figure S6. ^1H RMN spectrum of L6.

^{13}C NMR (100 MHz, CDCl_3) δ 146.37, 140.31, 140.08, 135.90, 131.52, 127.47, 122.50, 53.31, 21.42, 14.18, 11.73.

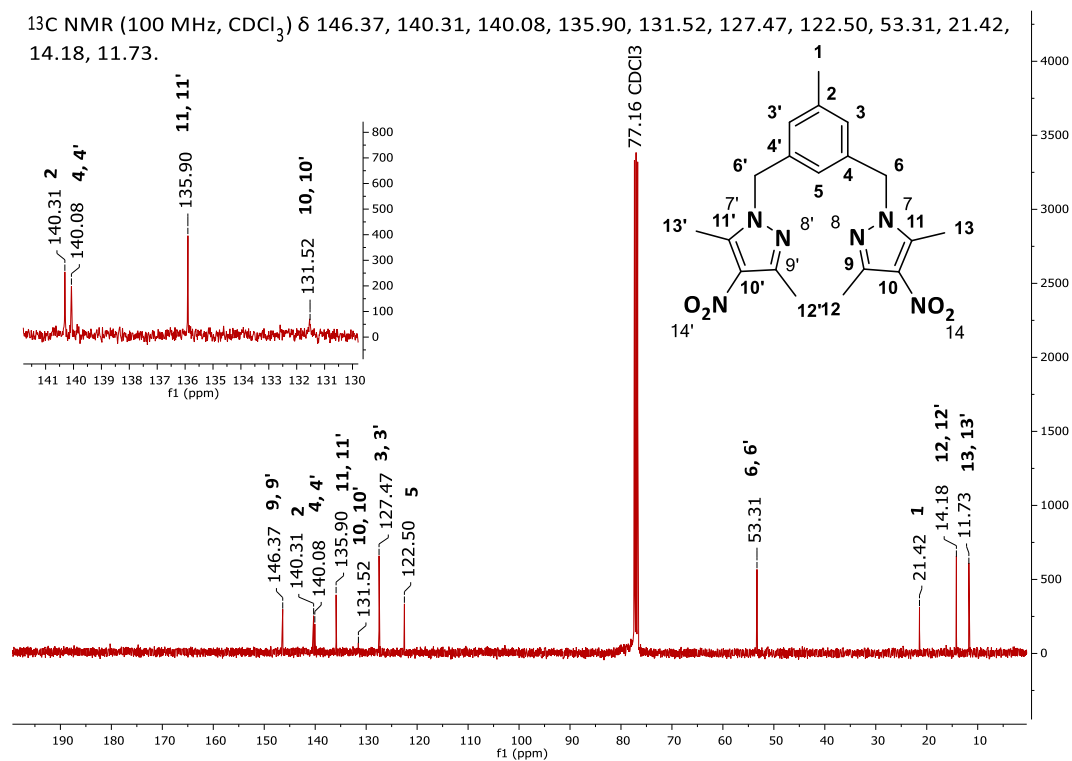


Figure S7. ^{13}C RMN spectrum of L6.

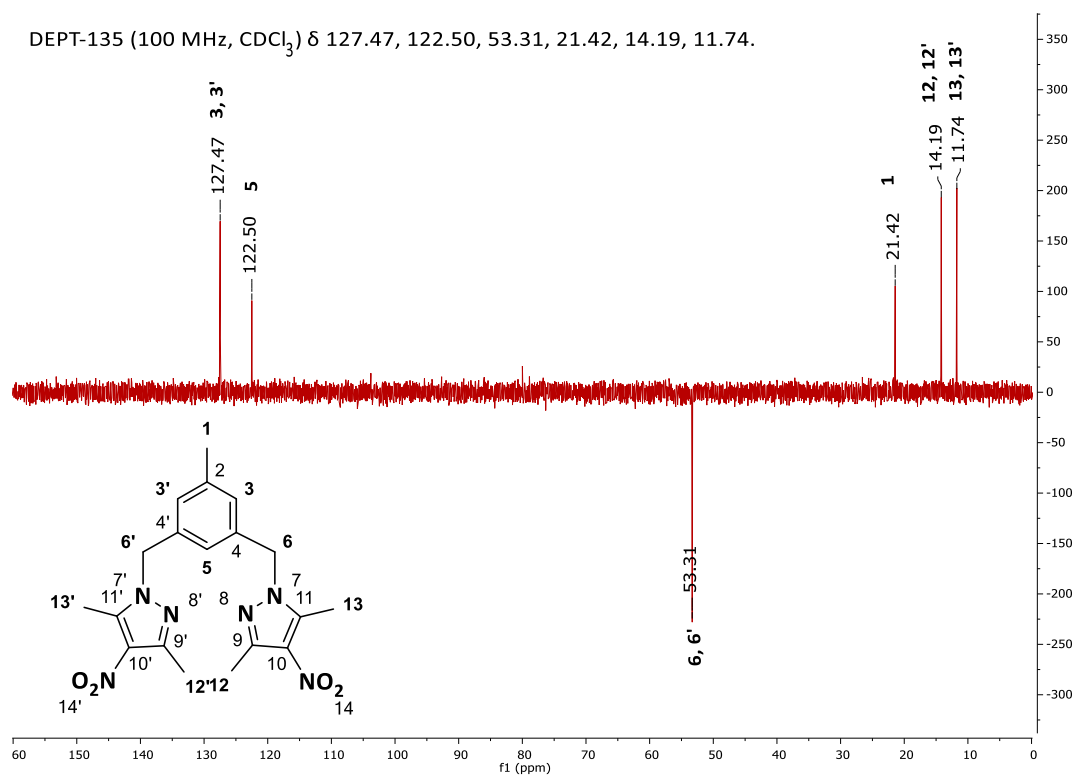


Figure S81. DEPT-135 spectrum of L6.

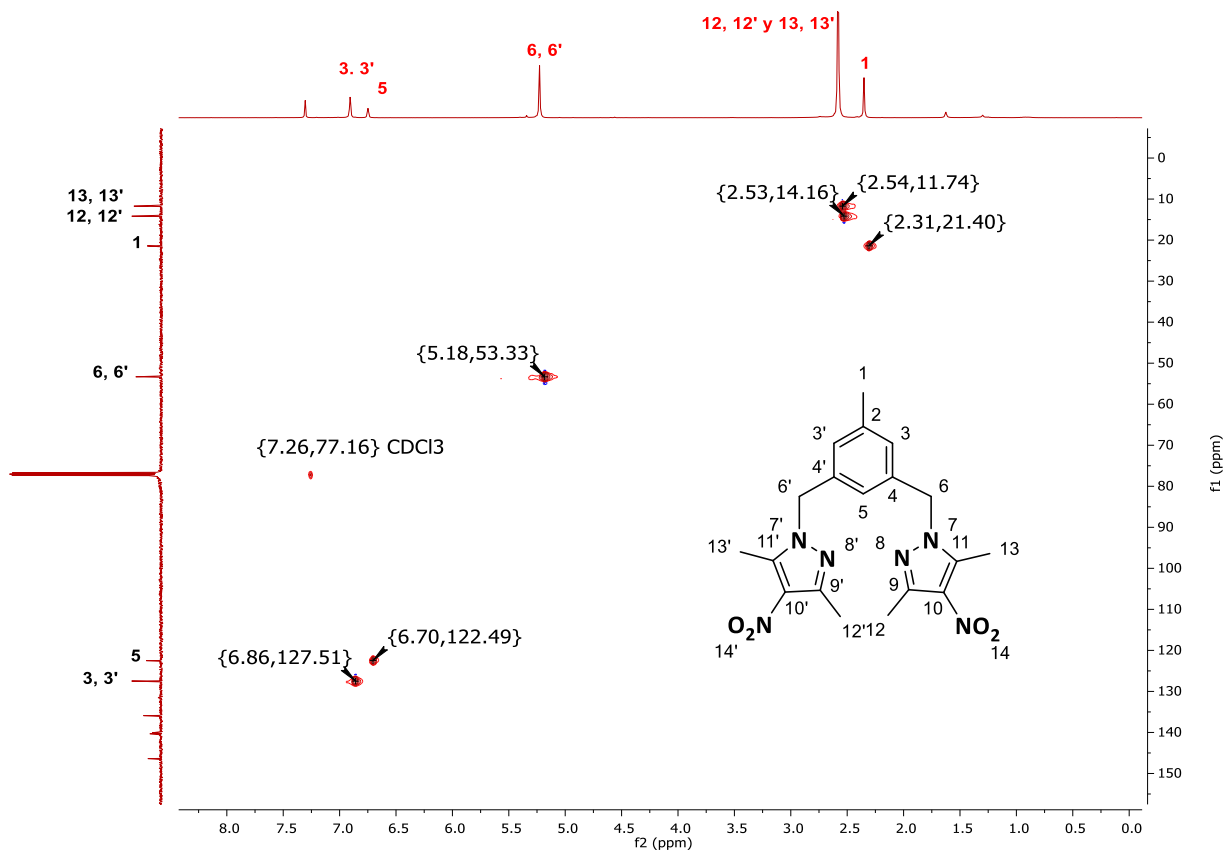


Figure S92. HSQC spectrum of L6.

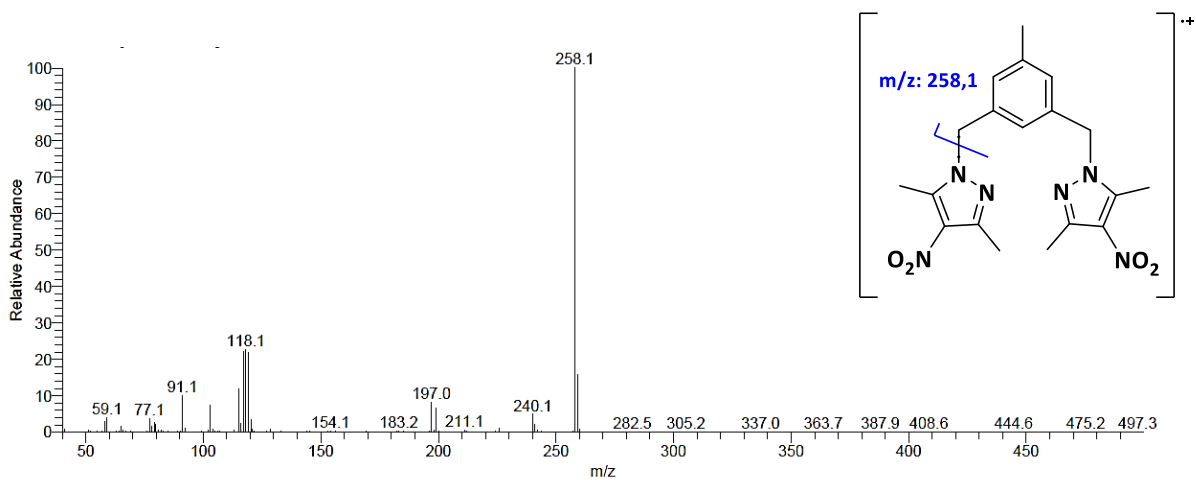


Figure S10. GC-MS spectrum of L6.

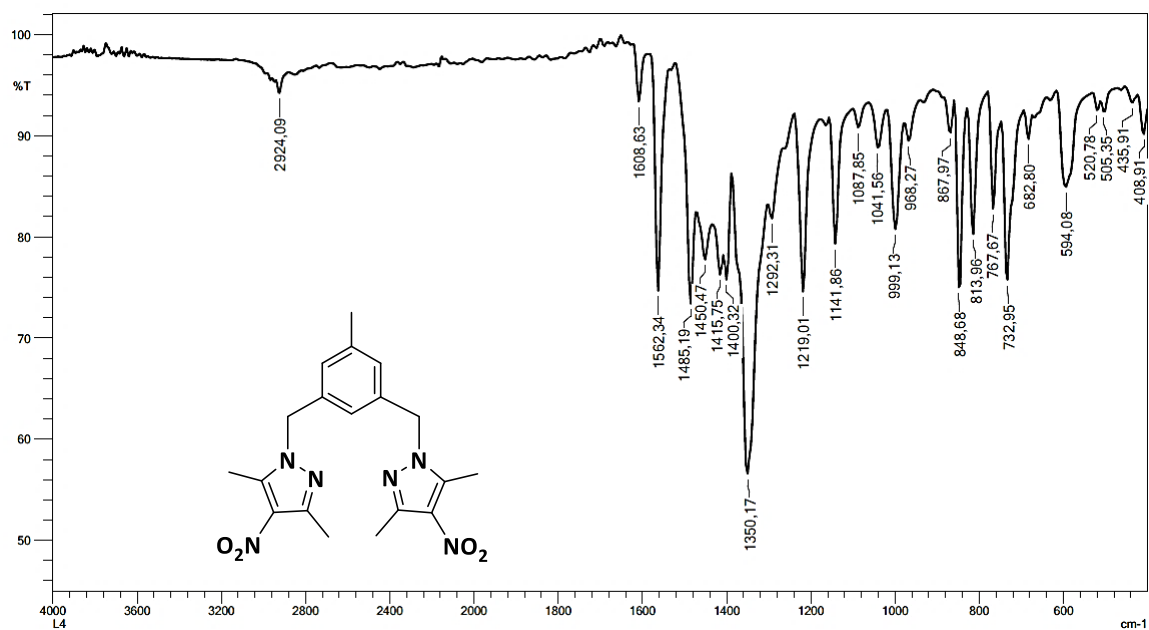


Figure S113. IR spectrum of L6.

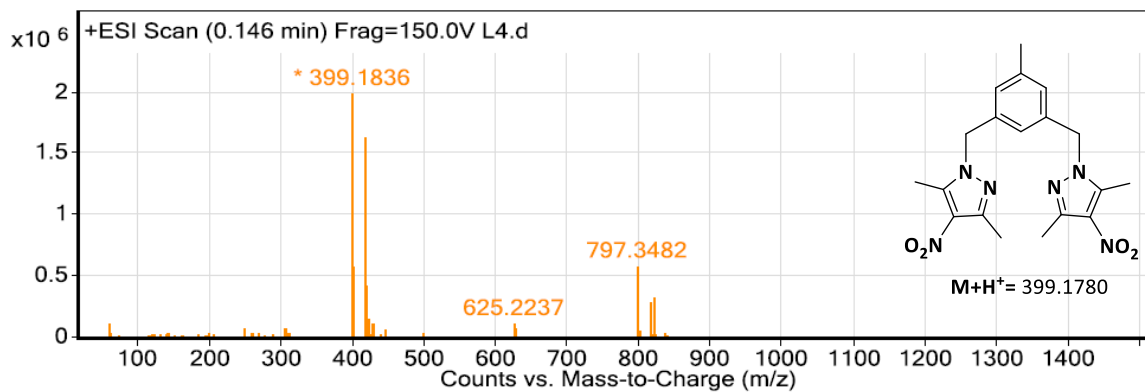


Figure S12. HRMS spectrum of L6.

2. Characterization of Complexes (1-7)

2.1 Bis(dinitrobenzoate-O, O ') of Co(II)

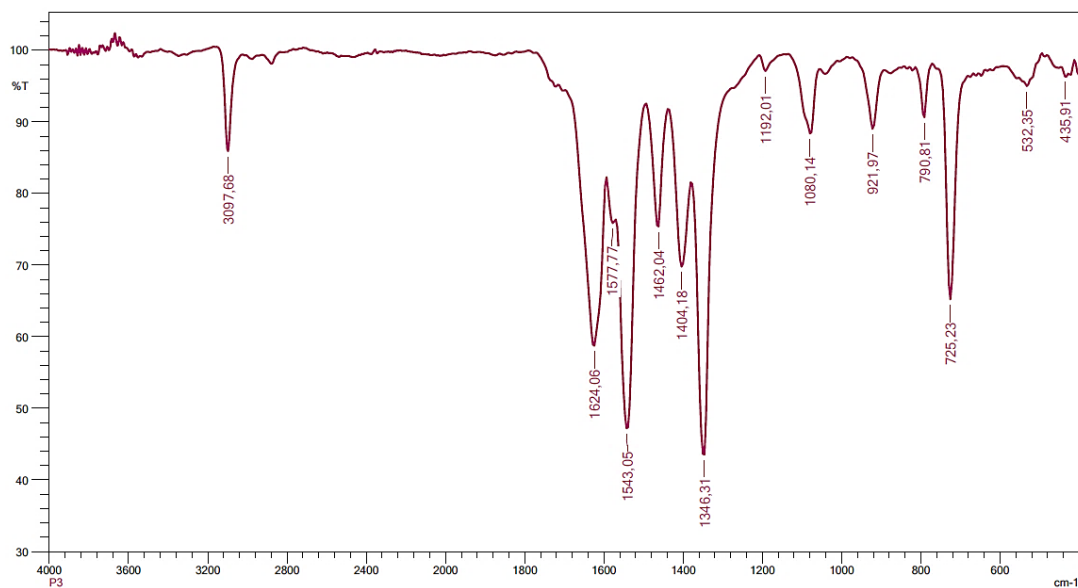


Figure S13. IR spectrum of 1.

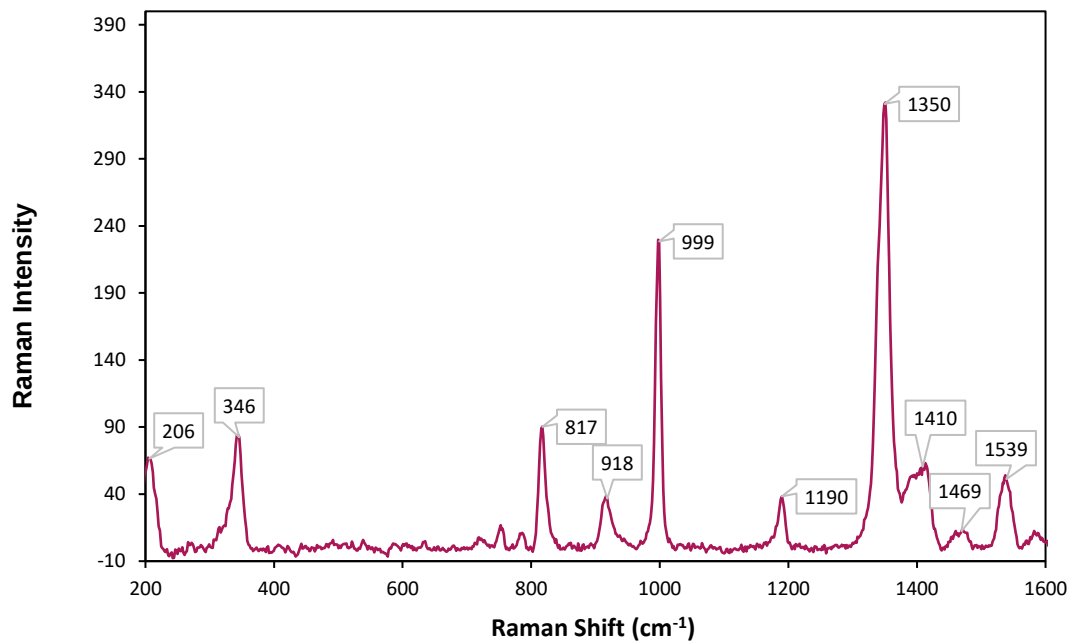


Figure S14. Raman spectrum of 1.

2.2 Dinitrobenzoate[bis(3,5-dimethylpyrazol-1-yl)methane] of Co(II)

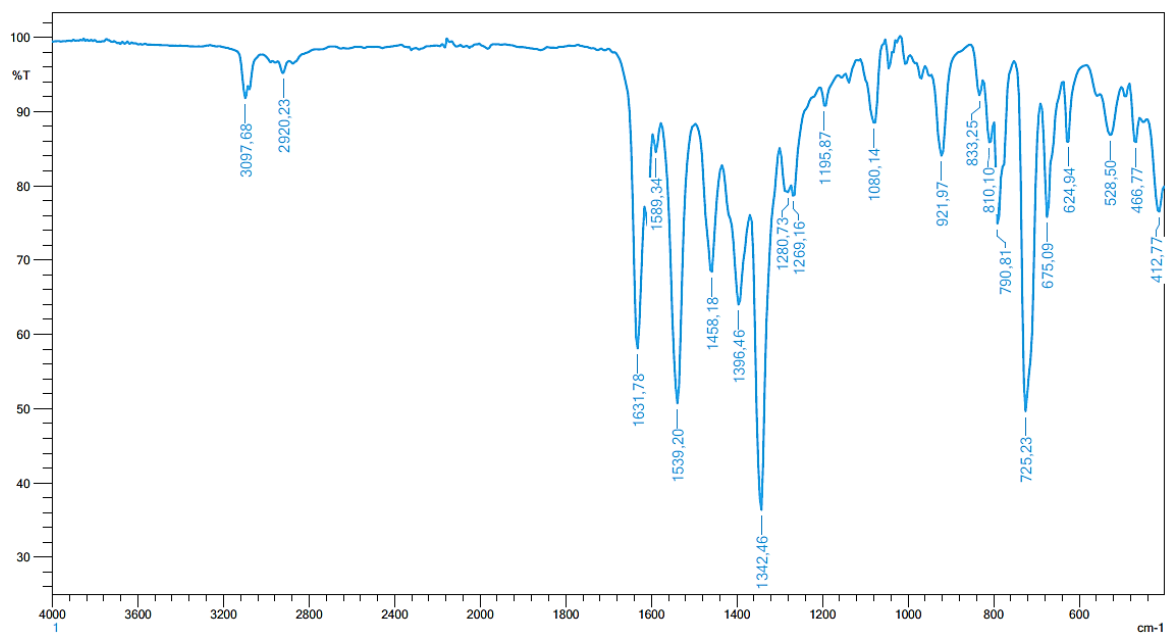


Figure S15. IR spectrum of 2.

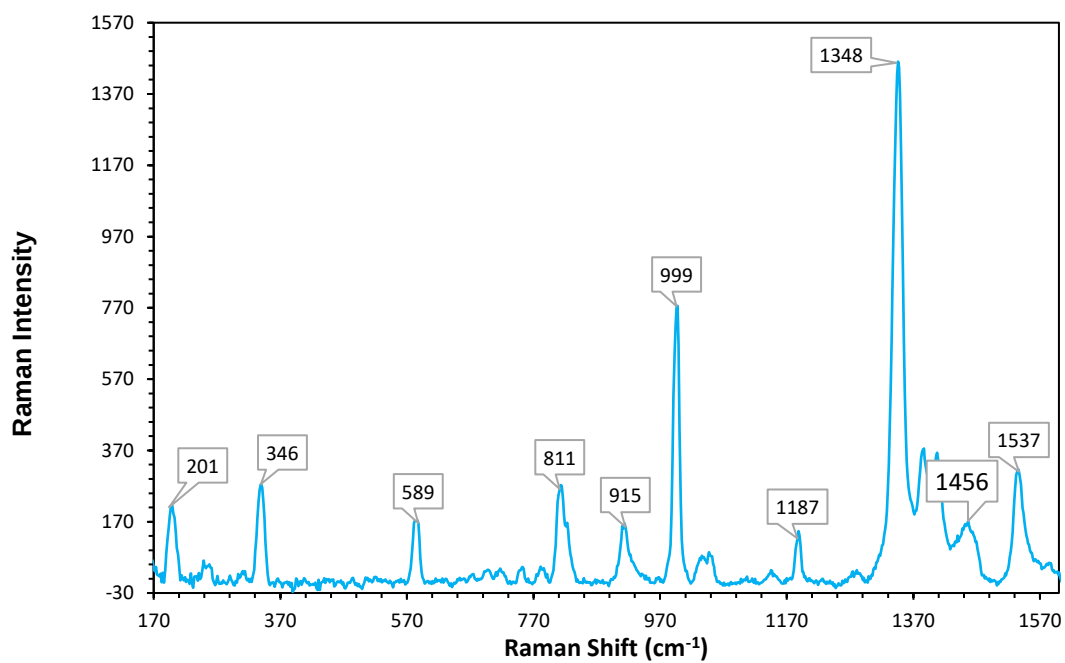


Figure S16. Raman spectrum of 2.

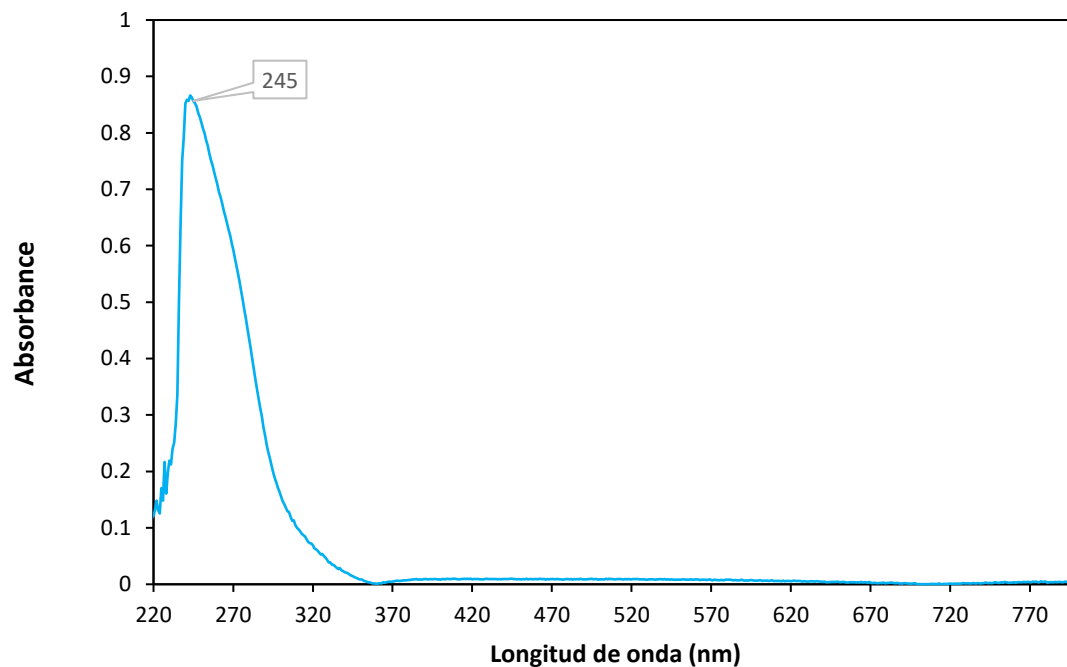


Figure S17. UV-Vis spectrum of 2.

2.3 Dinitrobenzoate[bis(3,5-dimethyl-4-nitro-1-pyrazol-1-yl)methane] of Co(II)

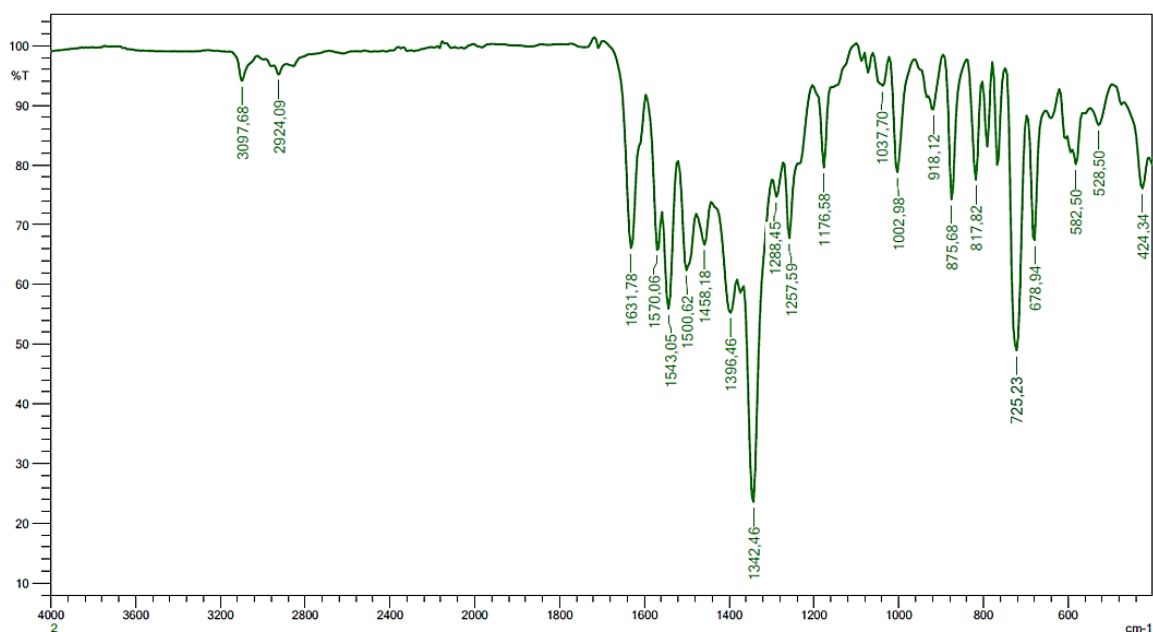


Figure S18. IR spectrum of 3.

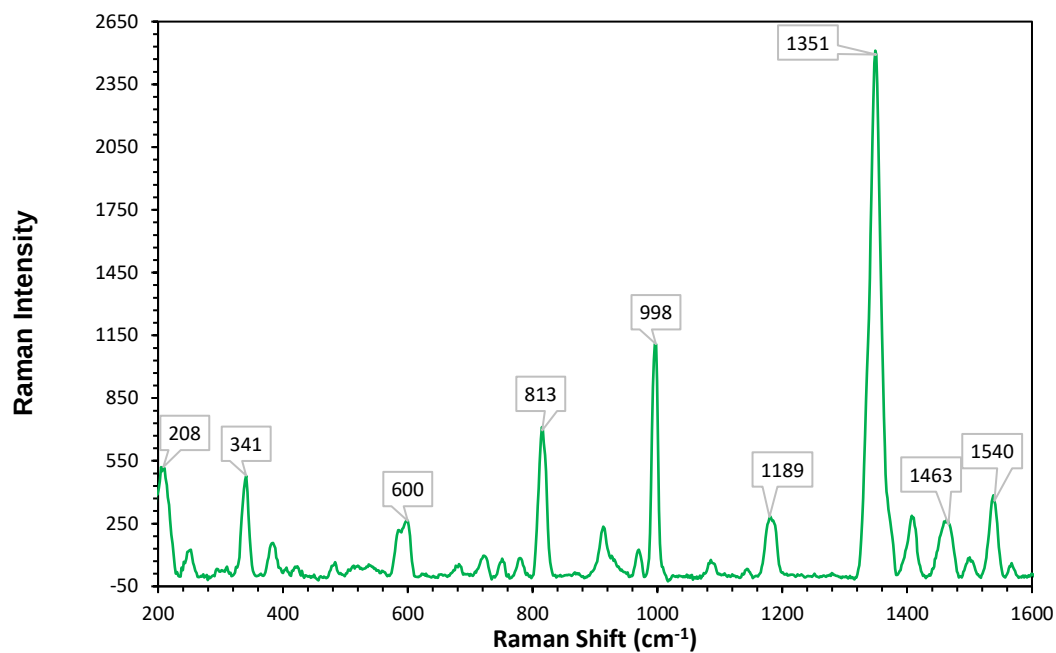


Figure S194. Raman spectrum of 3.

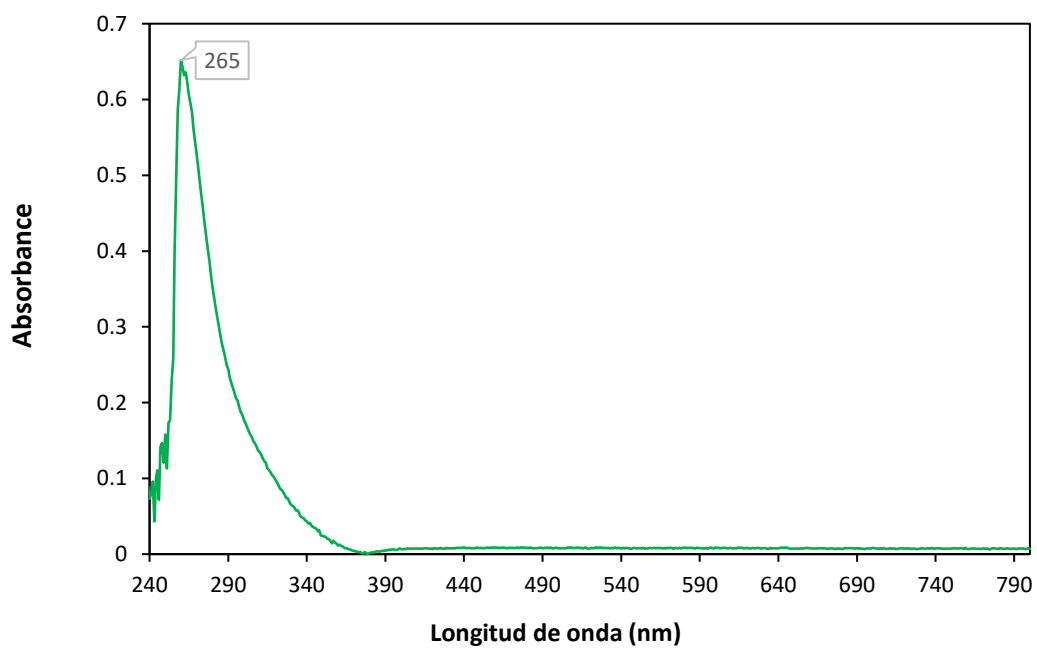


Figure S20. UV-Vis spectrum of 3.

2.4 [2,6-bis(3,5-dimethylpyrazol-1-ylmethyl)pyridine] of Co(II)

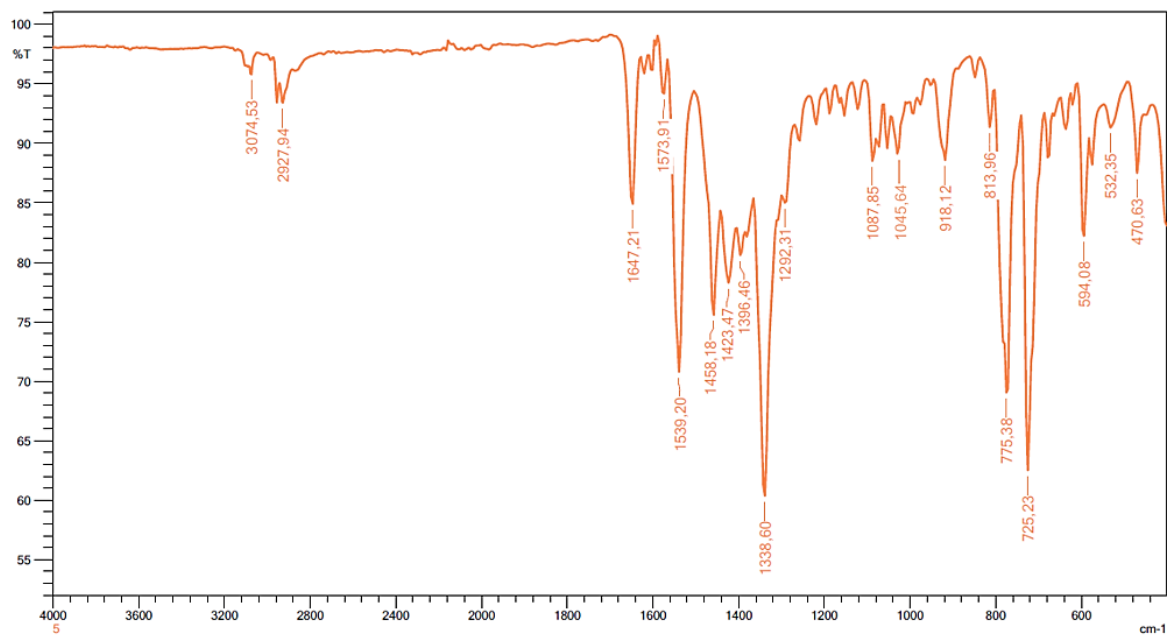


Figure S21. IR spectrum of 4.

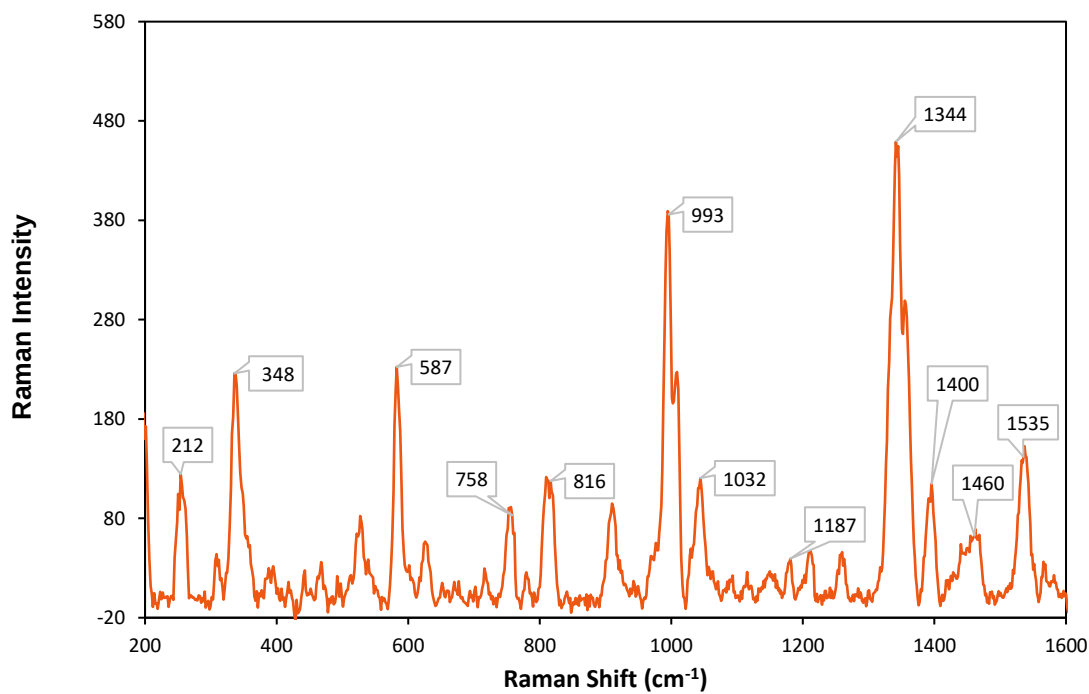


Figure S22. Raman spectrum of 4.

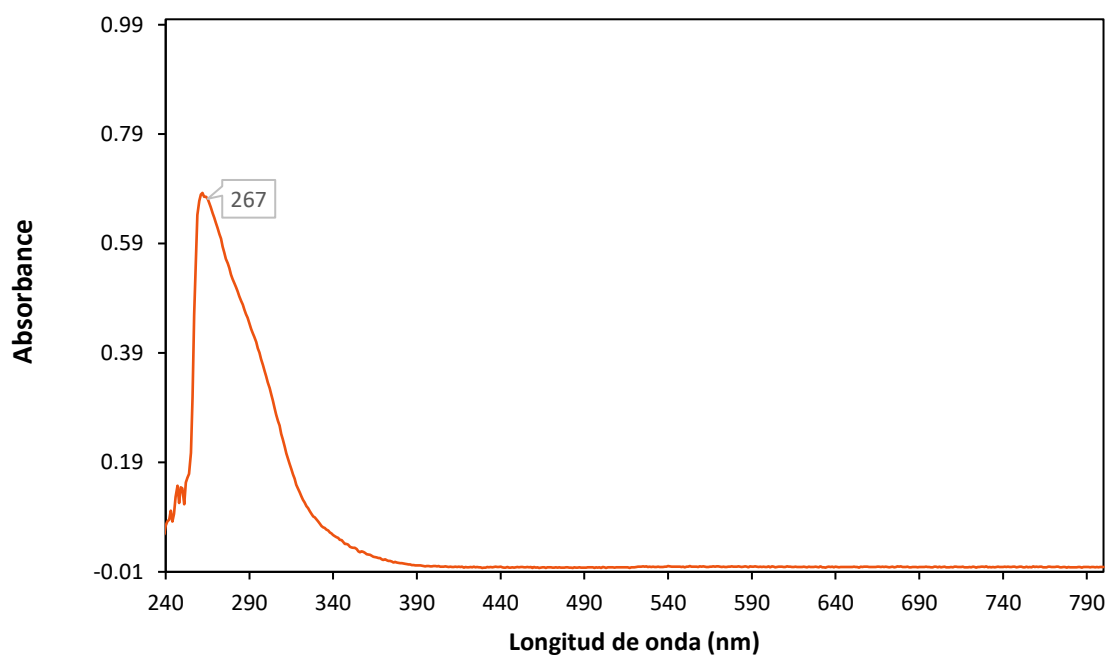


Figure S23. UV-Vis spectrum of 4.

2.5 [2,6-bis(4-nitro-3,5-dimethylpyrazol-1-ylmethyl)pyridine] of Co(II)

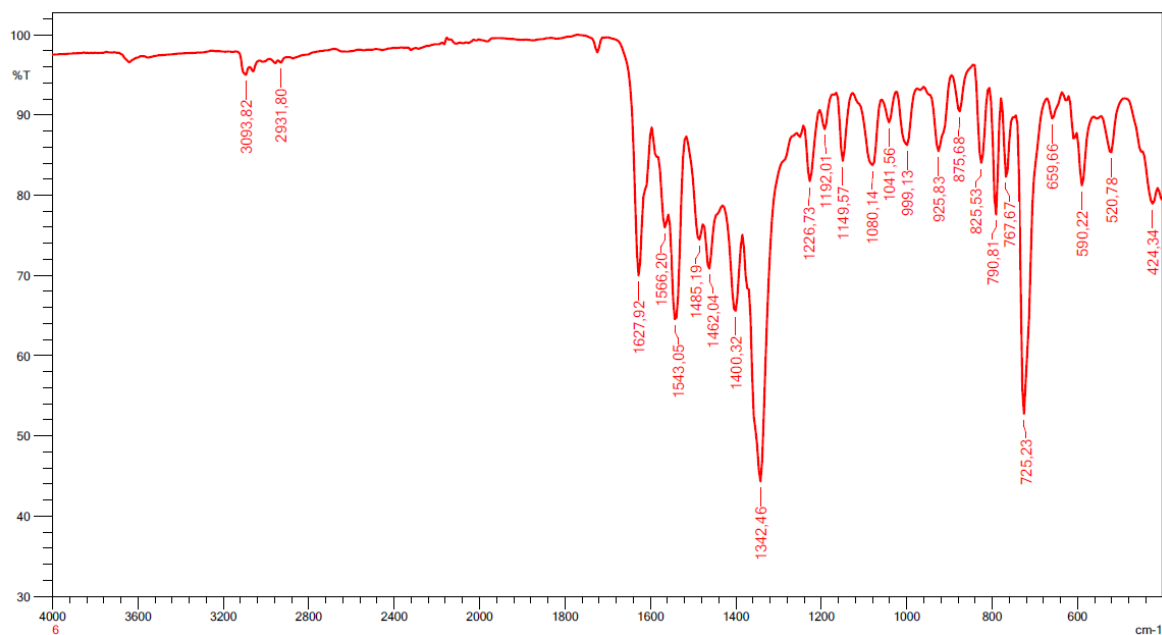


Figure S24. IR spectrum of 5.

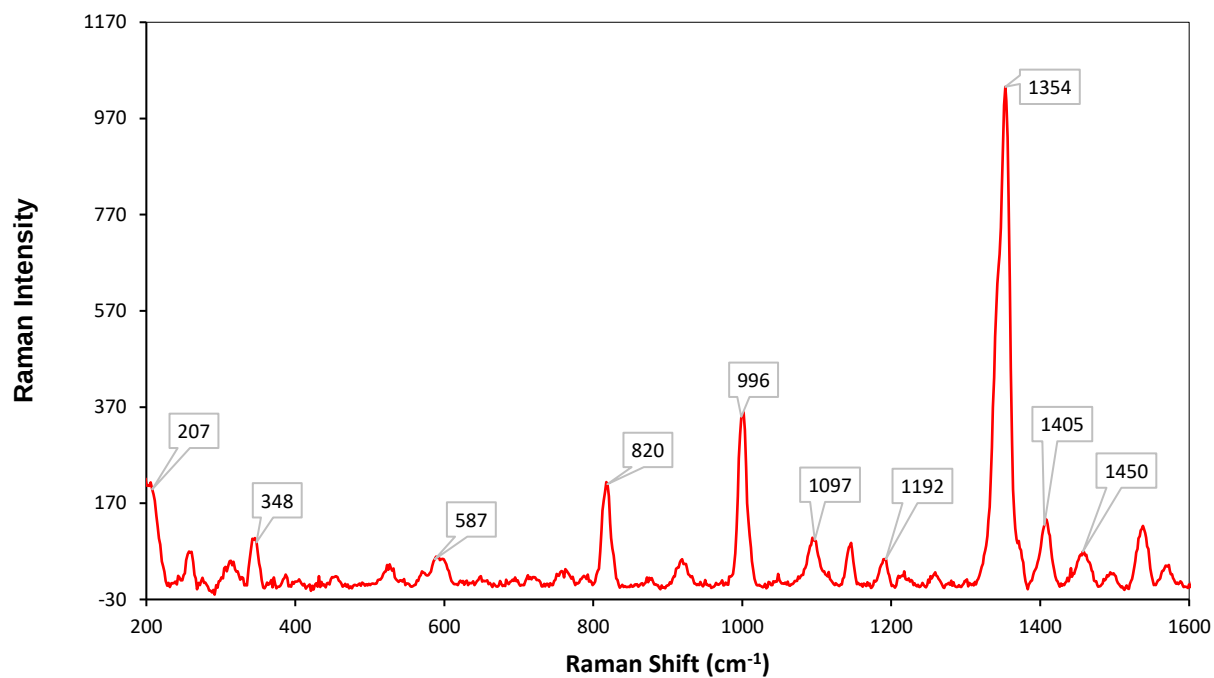


Figure S25. Raman spectrum of 5.

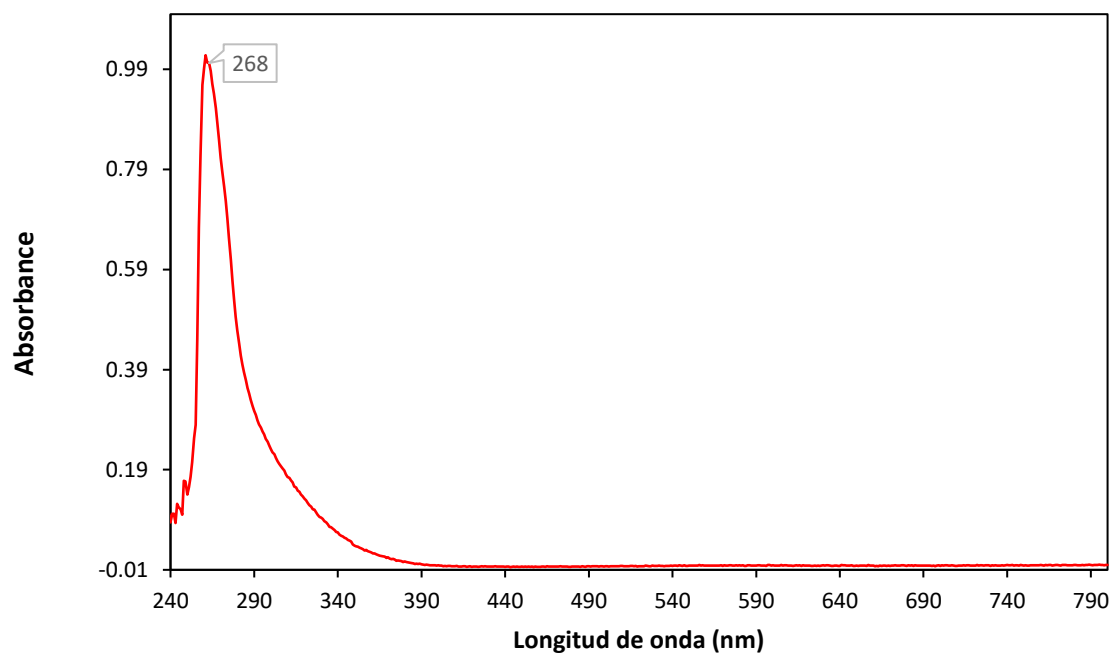


Figure S26. UV-Vis spectrum of 5.

2.6 Dinitrobenzoate[3,5-bis(3,5-dimethylpyrazol-1-ylmethyl)toluene] of Co(II)

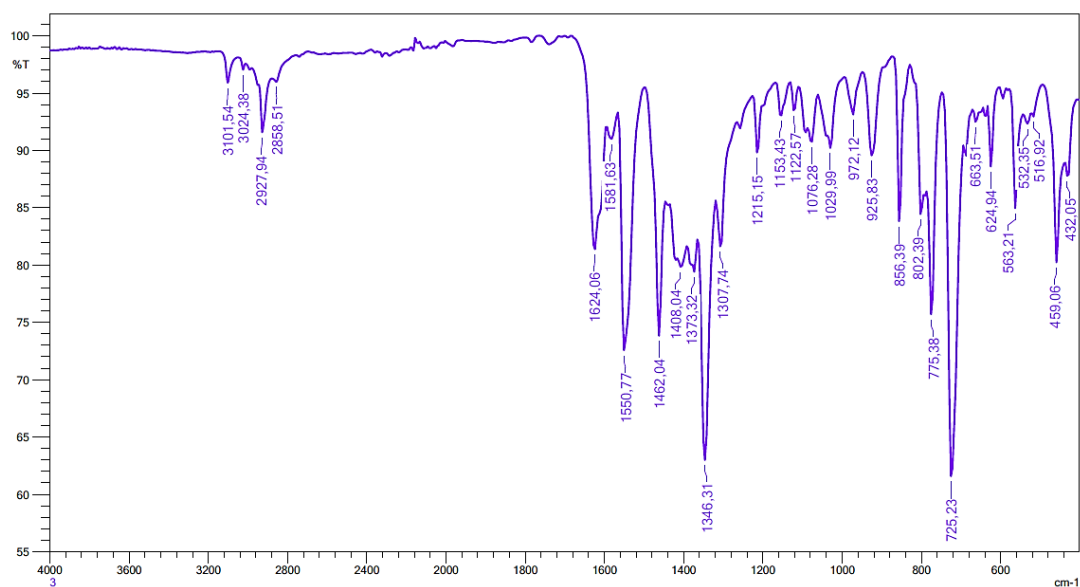


Figure S27. IR spectrum of 6.

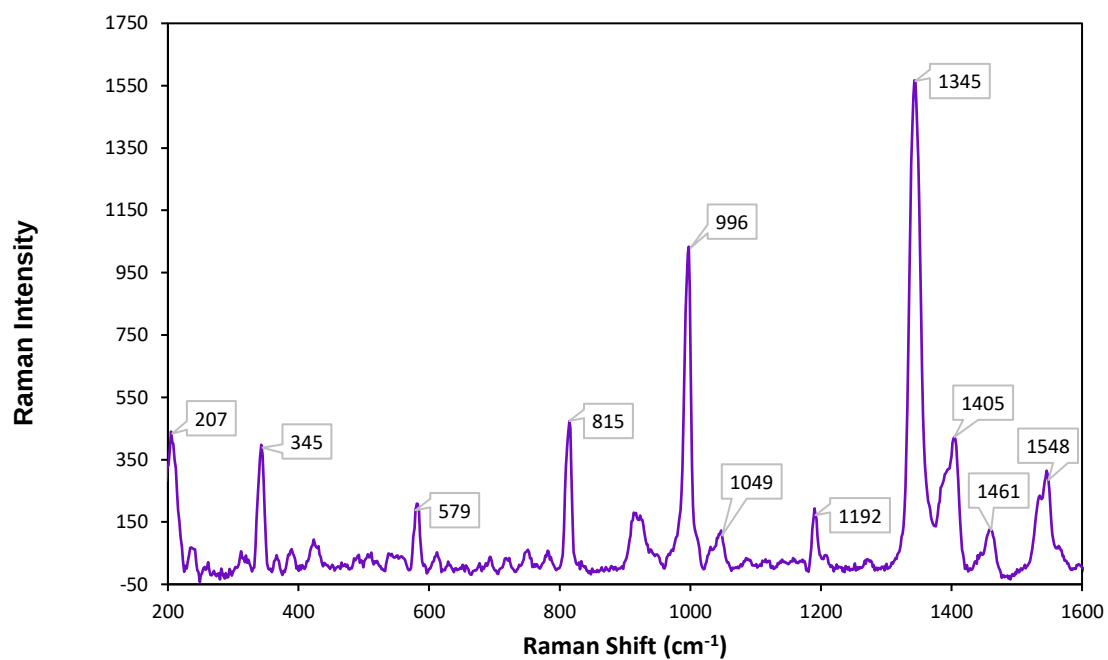


Figure S28. Raman spectrum of 6.

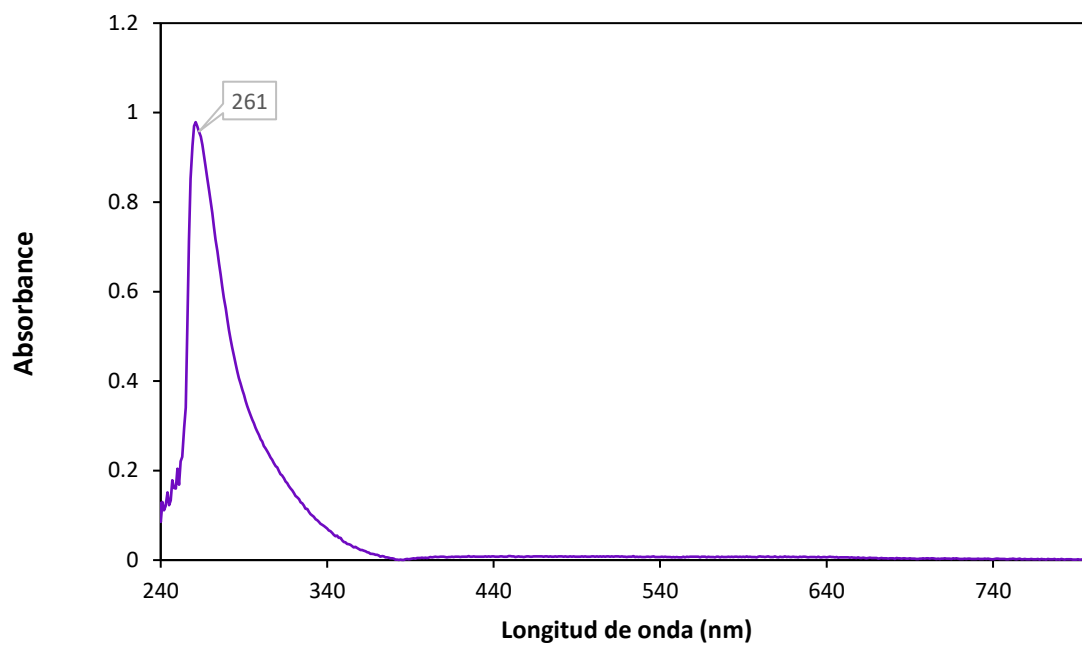


Figure S29. UV-Vis spectrum of 6.

2.7 Dinitrobenzoate[3,5-bis(3,5-dimethyl-4-nitropyrazol-1-ylmethyl) toluene] of Co(II)

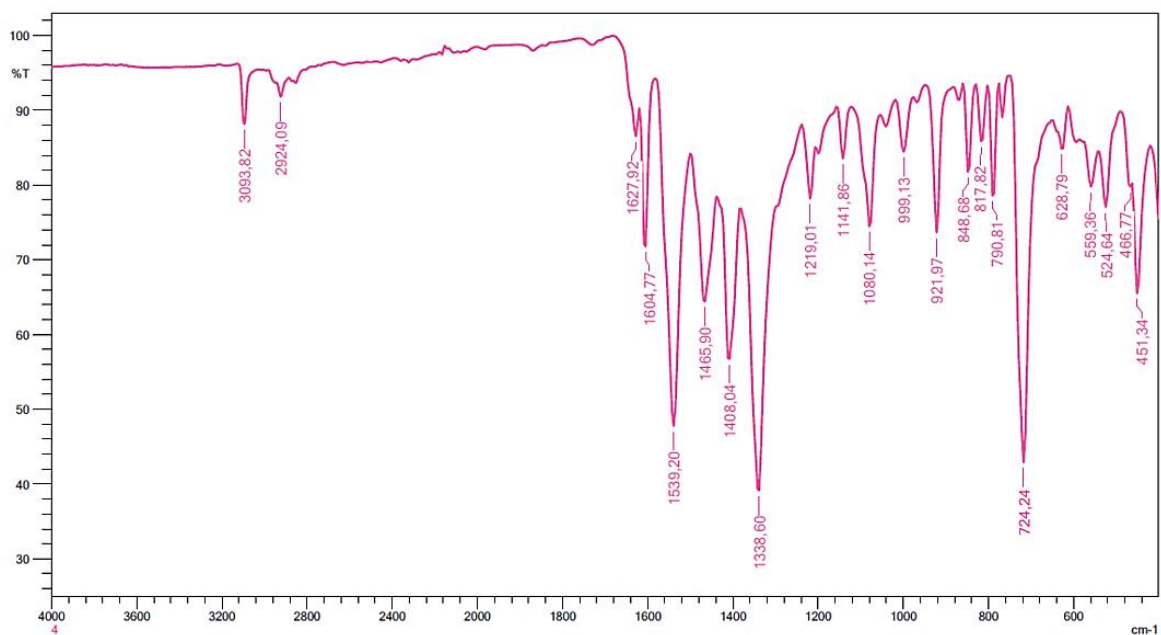


Figure S30. IR spectrum of 7.

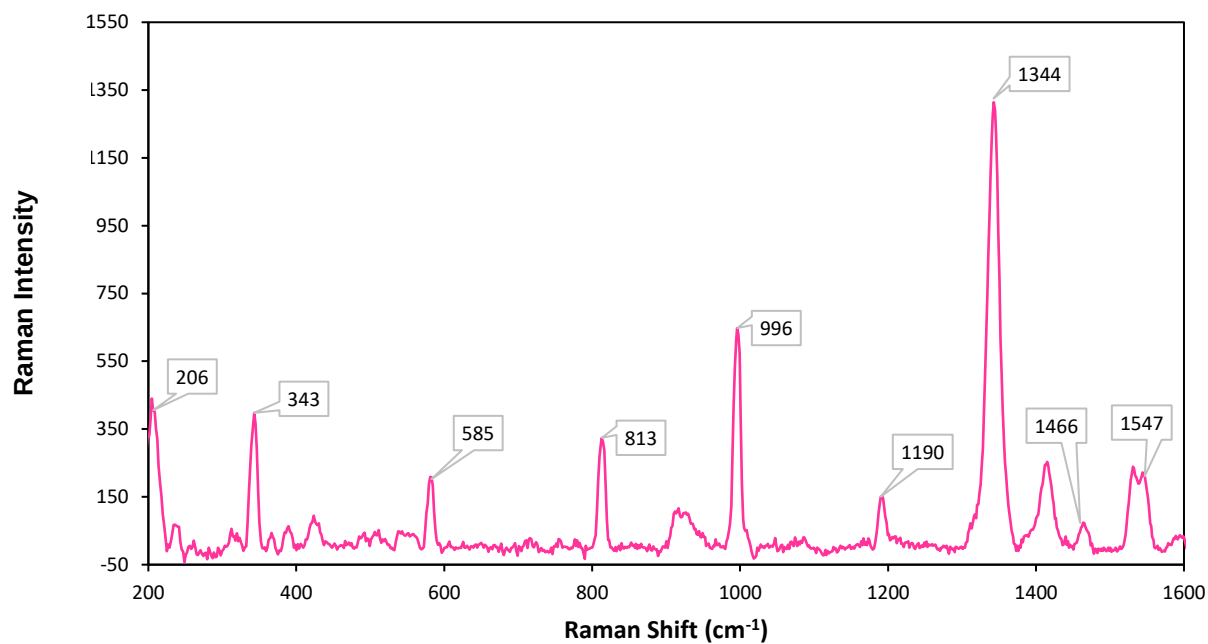


Figure S31. Raman spectrum of 7.

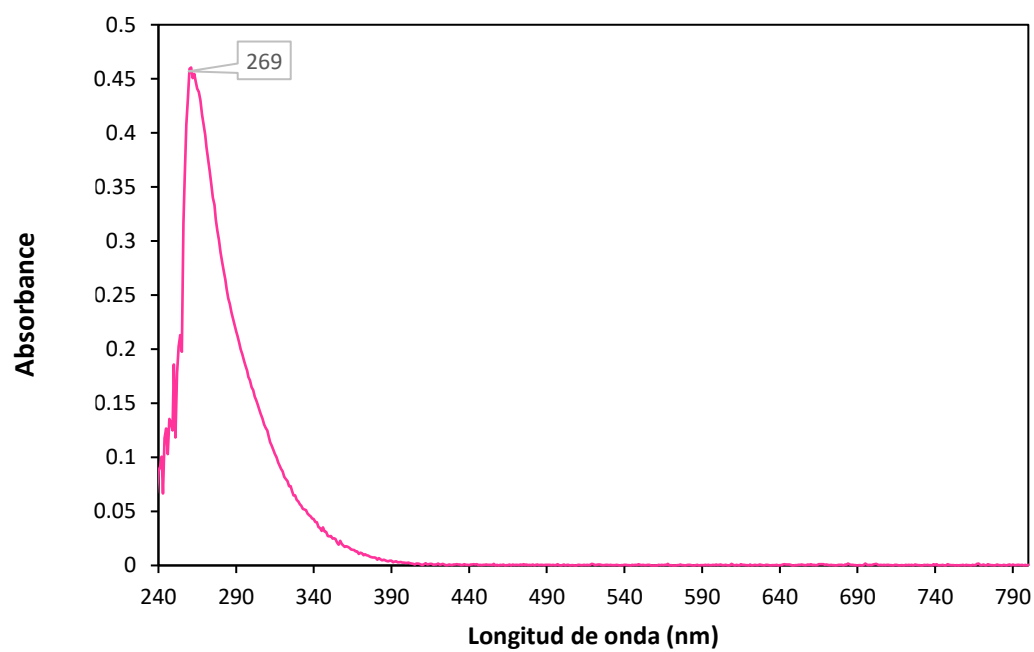


Figure S32. UV-Vis spectrum of 7.

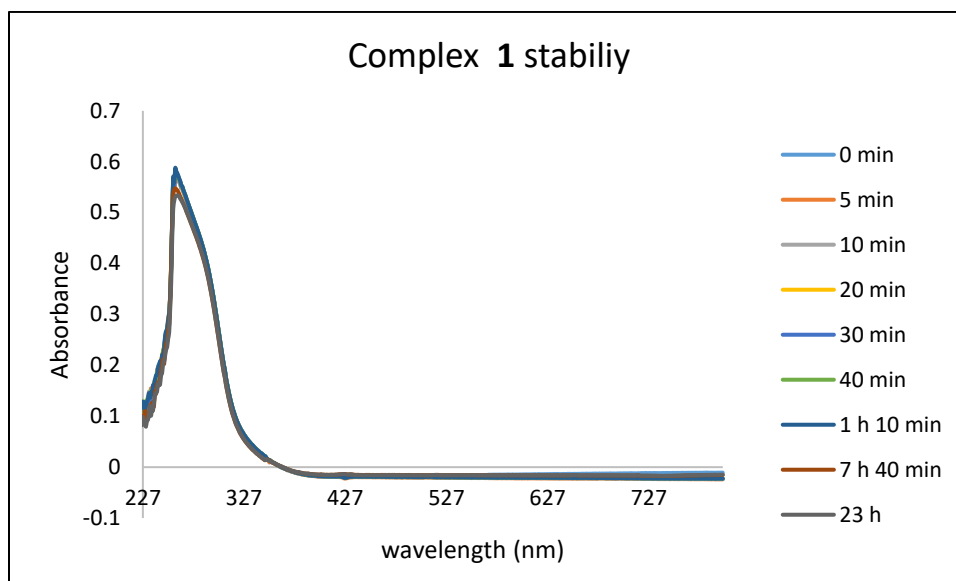


Figure S33. Stability study in solution for complex 1. (In DMSO; 3×10^{-5} M)

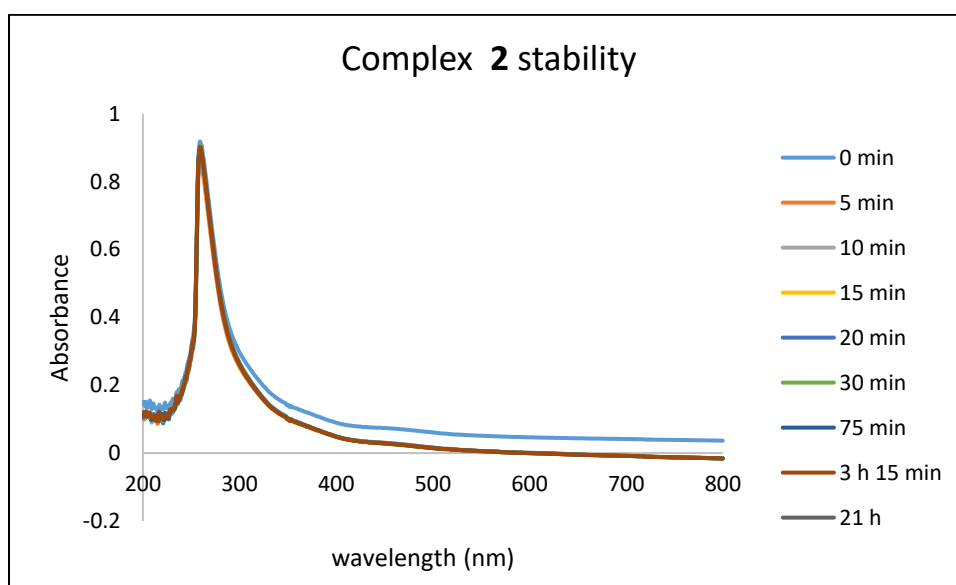


Figure S34. Stability study in solution for complex 2. (In DMSO; 3×10^{-5} M)

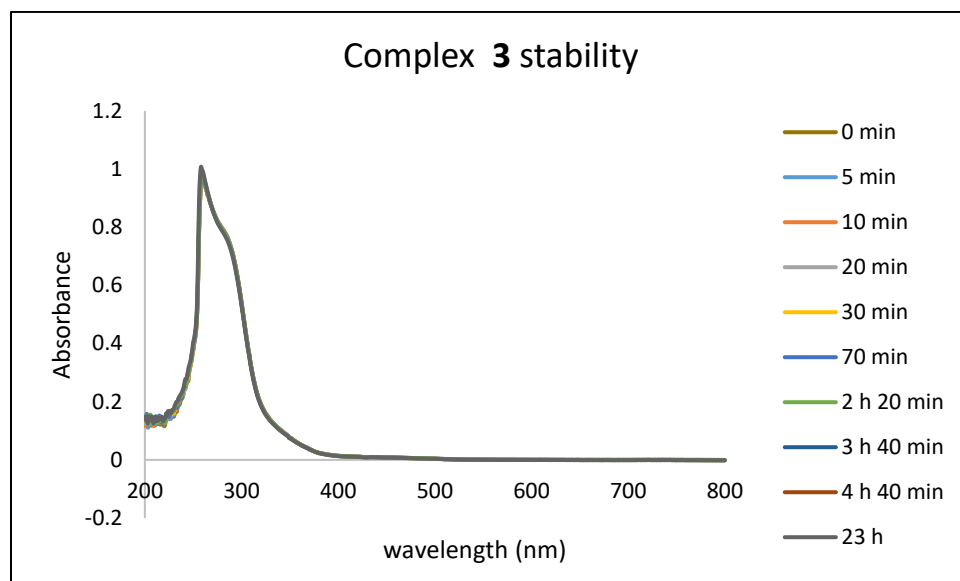


Figure S35. Stability study in solution for complex 3. (In DMSO; 3×10^{-5} M)

Table S1. Selected bands of the IR spectra (cm⁻¹) for **L1-L6** and **1-7**. **ν**: stretching; **as**: asymmetrical; **s**: symmetrical; **δ**: flexion; **op**: out of the plane; **Pz**: pyrazole.

Comp.	ν_{CH₃} (C-H)	ν(C=C)	ν(C=N)	δAnillo Pz	ν_{as}(NO₂)	ν_s(NO₂)	ν_{as}(COO⁻)	ν_s(COO⁻)	δ_{op}(C-NO₂)
7	-	1543	-	-	1462	1346	1624	1577	725
L1	2920	1554	1381	806	-	-	-	-	-
2	2920	1539	1396	810	1458	1342	1631	1589	725
L2	2924	1566	1373	817	1489	1346	-	-	732
3	2924	1543	1396	817	1500	1342	1631	1570	725
L3	2927	1546	1381	813	-	-	-	-	-
4	2927	1539	1396	813	1458	1338	1647	1573	725
L4	2931	1562	1373	821	1481	1357	-	-	729
5	2931	1543	1400	825	1485	1342	1627	1566	725
L5	2927	1554	1370	802	-	-	-	-	-
6	2927	1550	1373	802	1462	1346	1624	1581	725
L6	2924	1562	1400	813	1485	1350	-	-	732
7	2924	1539	1408	817	1465	1338	1627	1604	725