

Supplementary Information

Manganese(I) Based $NN\cap SS$ Bis-chelated Homo-Binuclear Metallacycles: Synthesis, Spectral, Crystallographic, Anticancer potential and Molecular docking studies

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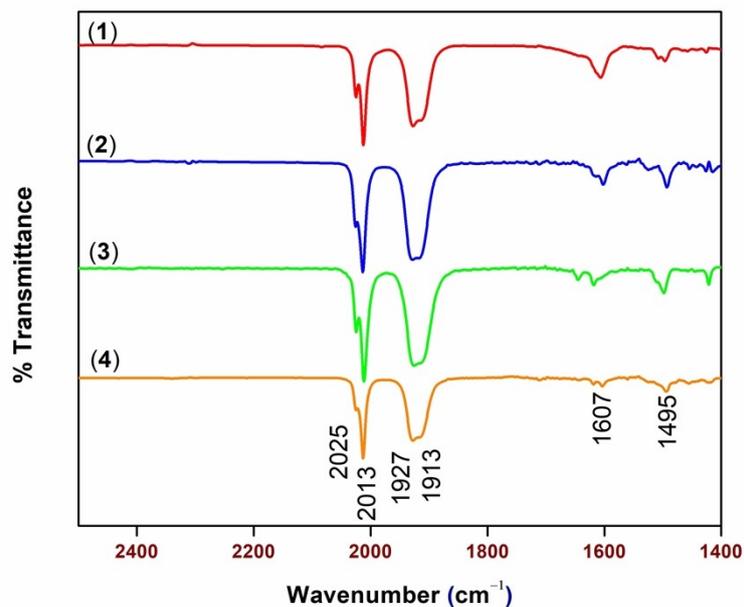


Fig. S1. Stacked IR spectra of compounds 1–4 in CH_2Cl_2 .

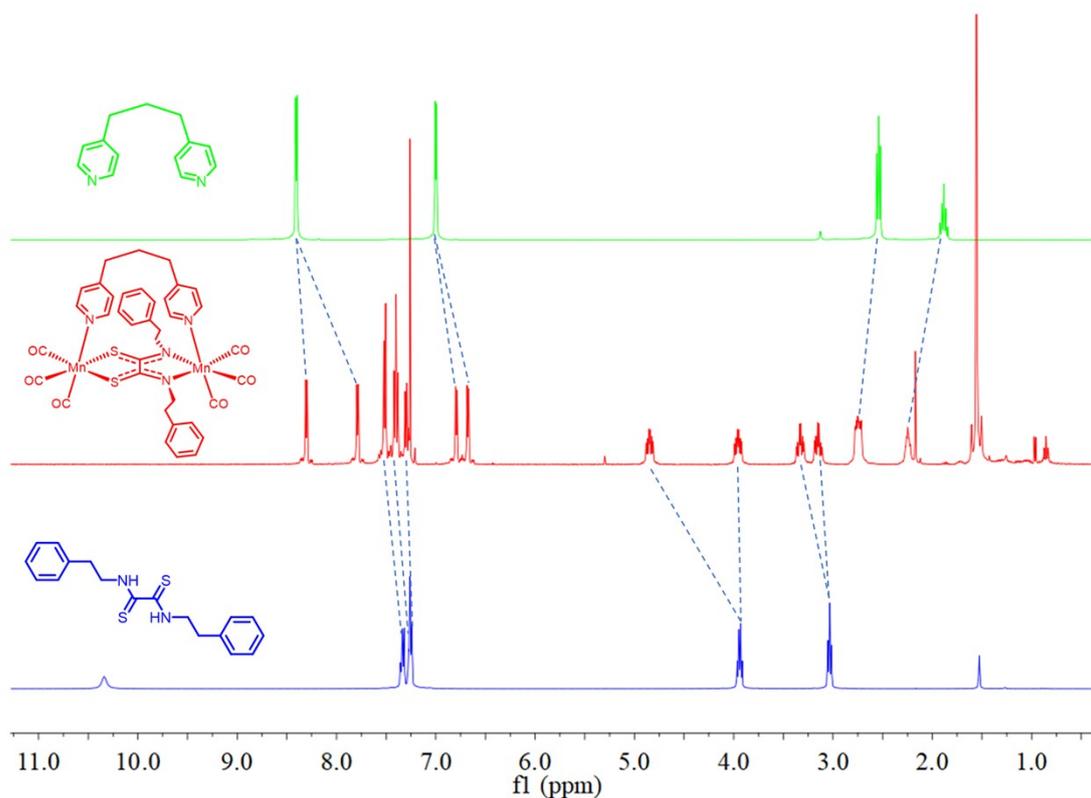


Fig. S2. Stacked ^1H NMR spectra of N,N' -diphenyldithioamide (dpdto) (blue), compound 4 (red) and 1,3-bis(4-pyridyl)propane (L') (green).

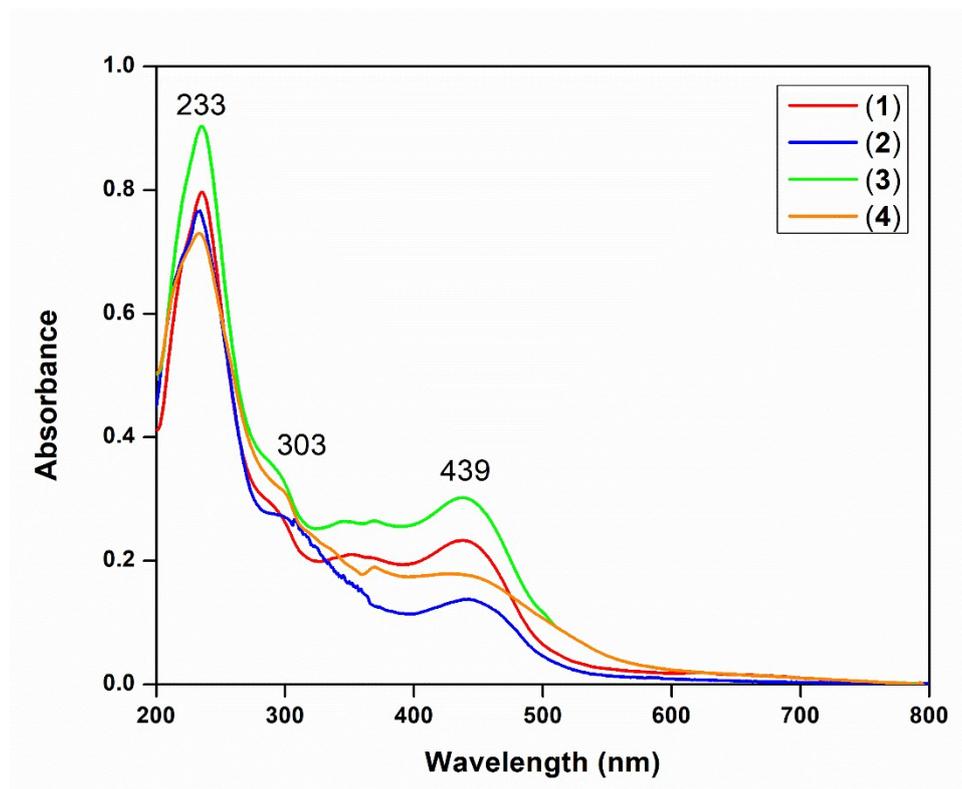


Fig. S3. Overlay UV-Vis absorption spectra of compounds **1–4** in CH₂Cl₂.

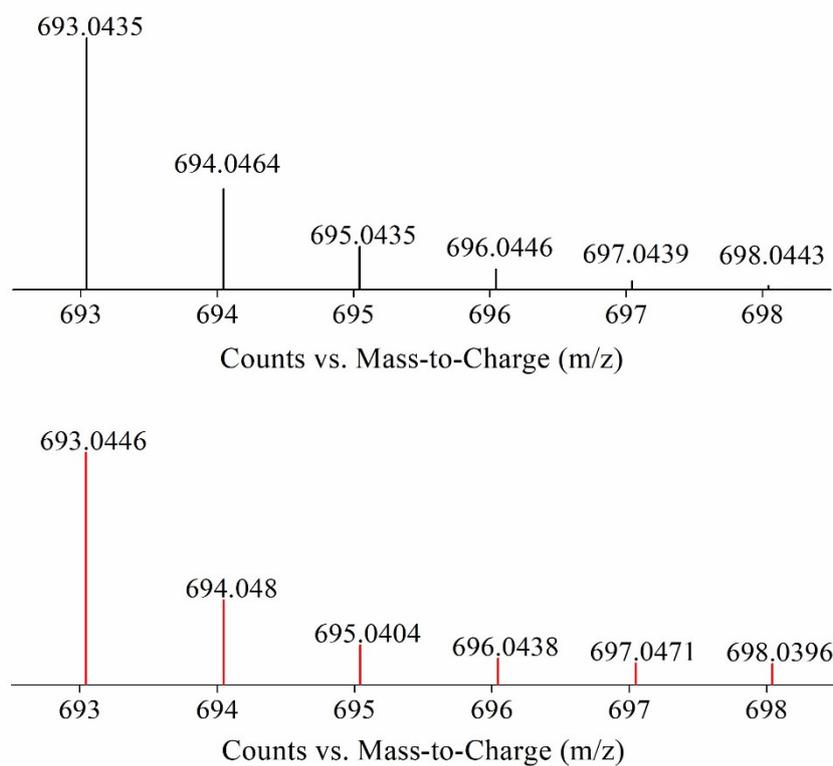


Fig. S4. ESI-MS theoretical (bottom) and experimental (top) isotopic distribution patterns of $[(\text{CO})_3\text{Mn}(\mu\text{-}\eta^4\text{-dbudt})(\mu\text{-bpe})\text{Mn}(\text{CO})_3]$ (**1**): $[\text{M} + \text{H}]^+$.

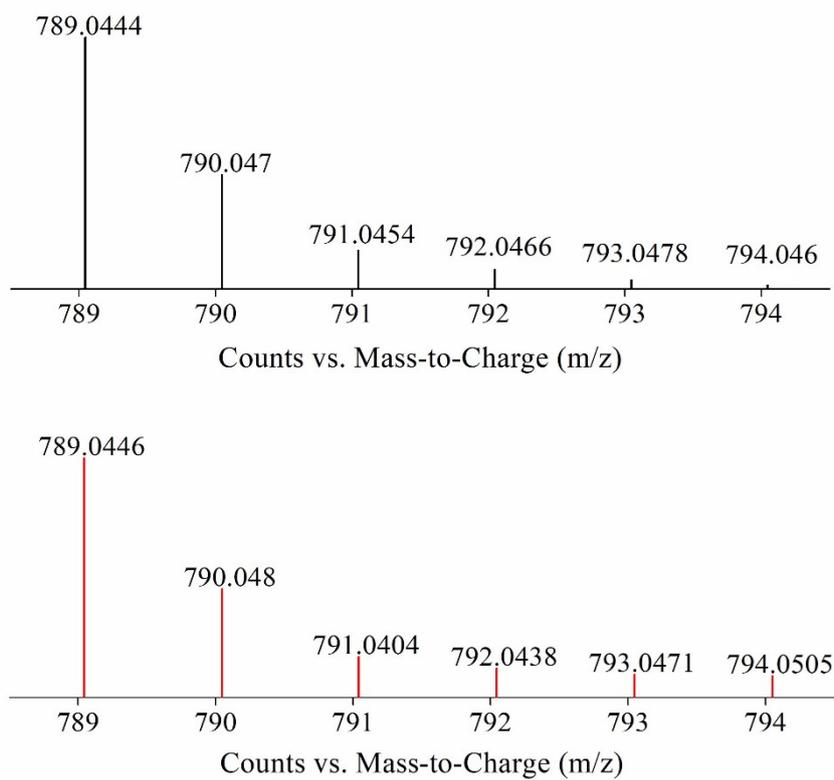


Fig. S5. ESI-MS theoretical (bottom) and experimental (top) isotopic distribution patterns of $[(\text{CO})_3\text{Mn}(\mu\text{-}\eta^4\text{-dpedt})(\mu\text{-bpe})\text{Mn}(\text{CO})_3]$ (**2**): $[\text{M} + \text{H}]^+$.

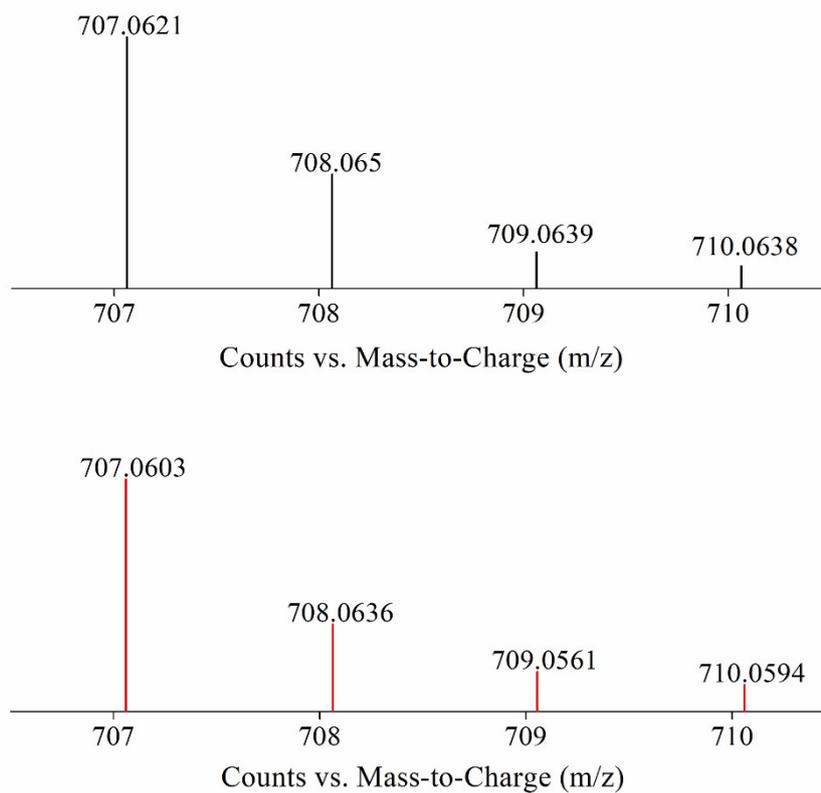


Fig. S6. ESI-MS theoretical (bottom) and experimental (top) isotopic distribution patterns of $[(\text{CO})_3\text{Mn}(\mu\text{-}\eta^4\text{-dbudt})(\mu\text{-bpp})\text{Mn}(\text{CO})_3]$ (**3**): $[\text{M} + \text{H}]^+$.

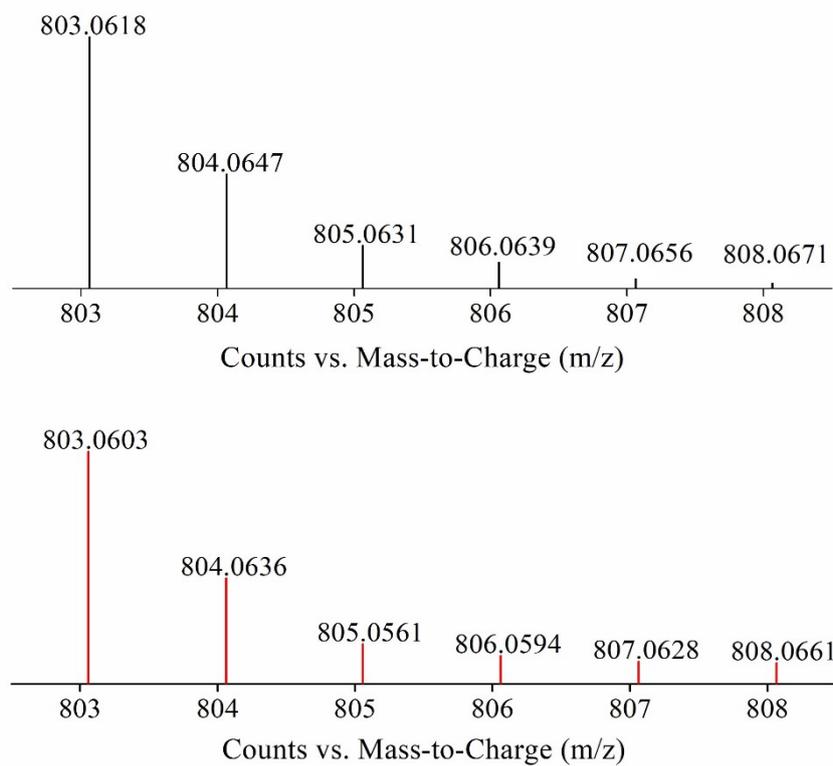


Fig. S7. ESI-MS theoretical (bottom) and experimental (top) isotopic distribution patterns of $[(\text{CO})_3\text{Mn}(\mu\text{-}\eta^4\text{-dpedt})(\mu\text{-bpp})\text{Mn}(\text{CO})_3]$ (**4**): $[\text{M} + \text{H}]^+$.

Table S1. Molecular docking results and parameters of the metallacycle **4** with epidermal growth factor receptor tyrosine kinase and human matrix metalloproteinase-9 (MMP-9)

Protein	PDB ID	Vina score (kcal/mol)	Cavity volume (Å ³)	Docking center (x, y, z)	Docking size (x, y, z)
epidermal growth factor receptor tyrosine kinase	1M17	-9.6	991	36, 8, 51	24, 24, 24
human matrix metalloproteinase-9	1L6J	-9.4	382	38, 24, 23	24, 24, 24

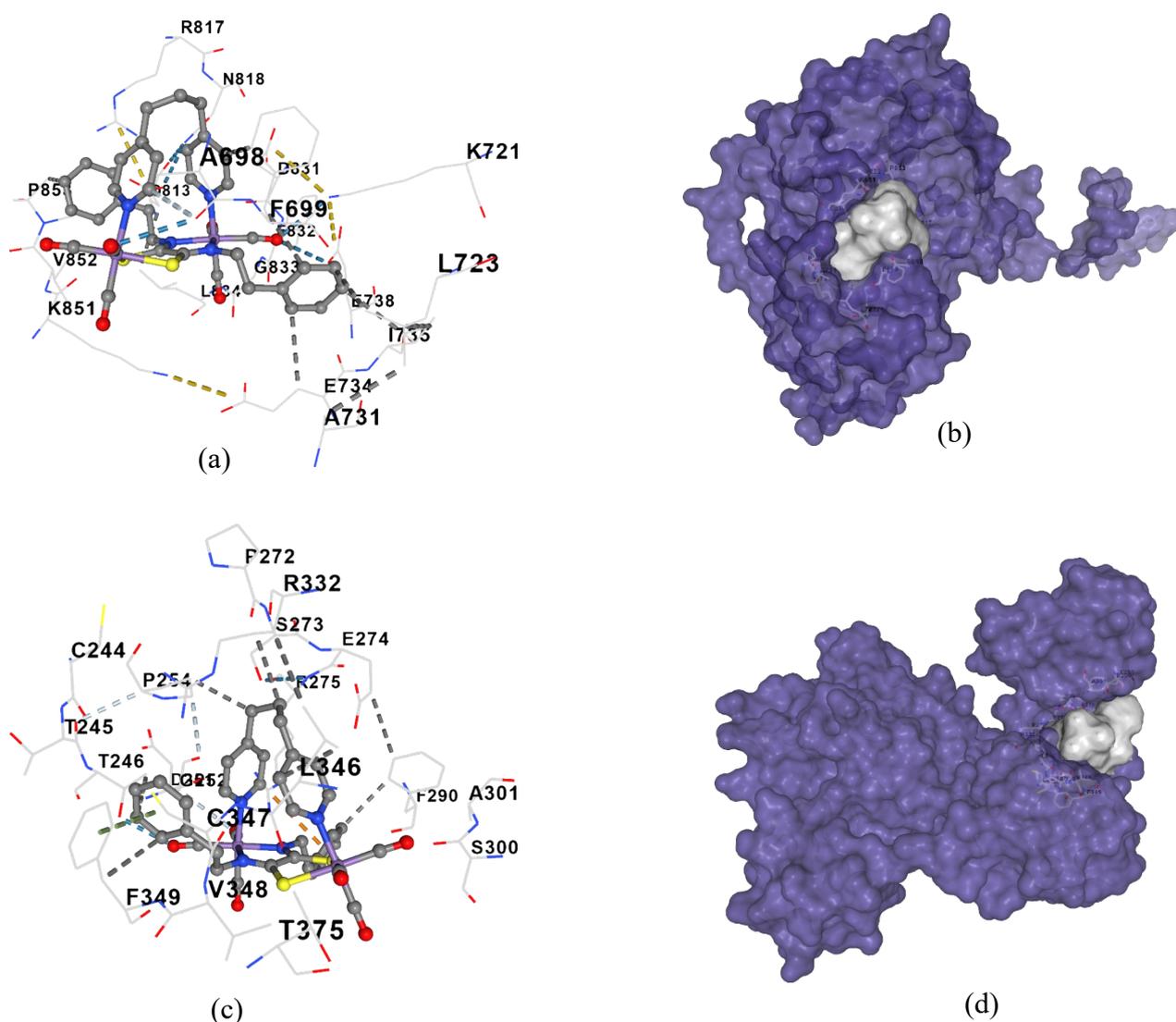


Fig. S8. (a) Binding mode of metallacycle **4** at the epidermal growth factor receptor tyrosine kinase (PDB ID: 1M17) active site, (b) Cavity surface of epidermal growth factor receptor tyrosine kinase in complex with **4**.), (c) Binding mode of metallacycle **4** at the human matrix metalloproteinase-9 (PDB ID: 1L6J) active site, (d) Cavity surface of human matrix metalloproteinase-9 in complex with **4**.

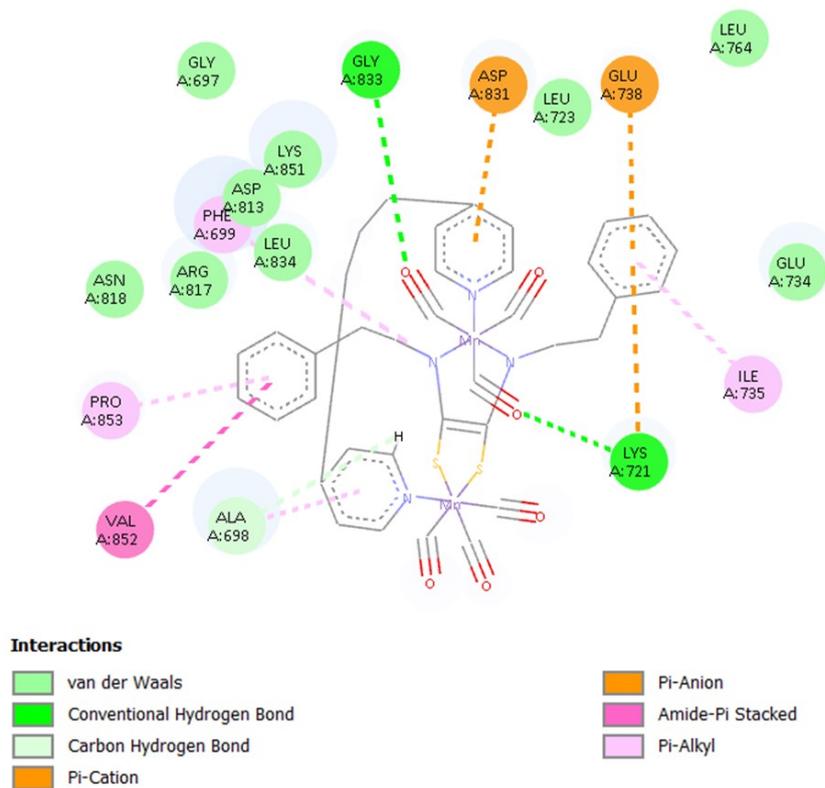


Fig. S9. Ligand–protein interactions involving amino acid residues for metallacycle **4** with EGFR (PDB ID: 1M17) in 2D.

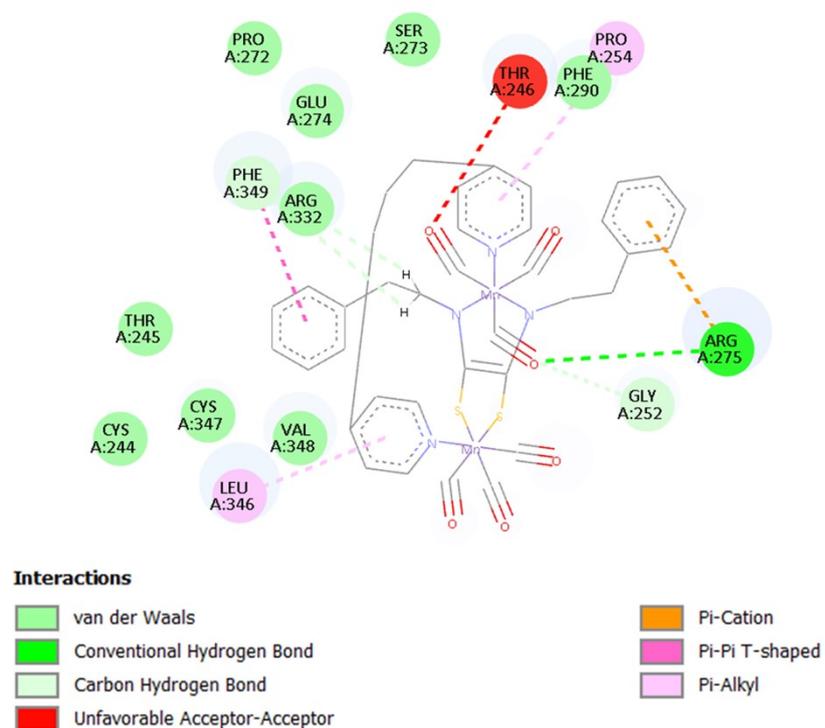


Fig. S10. Ligand–protein interactions involving amino acid residues for metallacycle **4** with MMP-9 (PDB ID: 1L6J) in 2D.

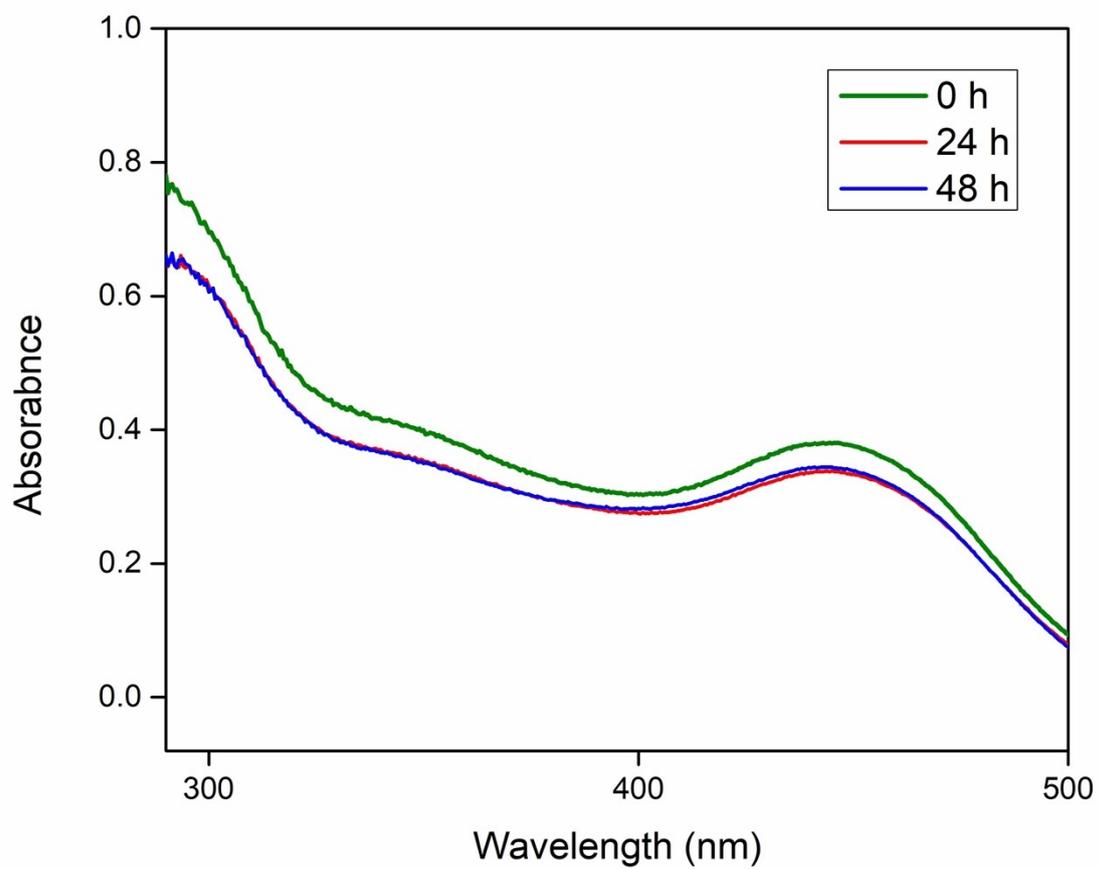


Fig. S11. Time-dependent UV-visible absorption spectra of **2** in 0.1 % DMSO/DMEM.

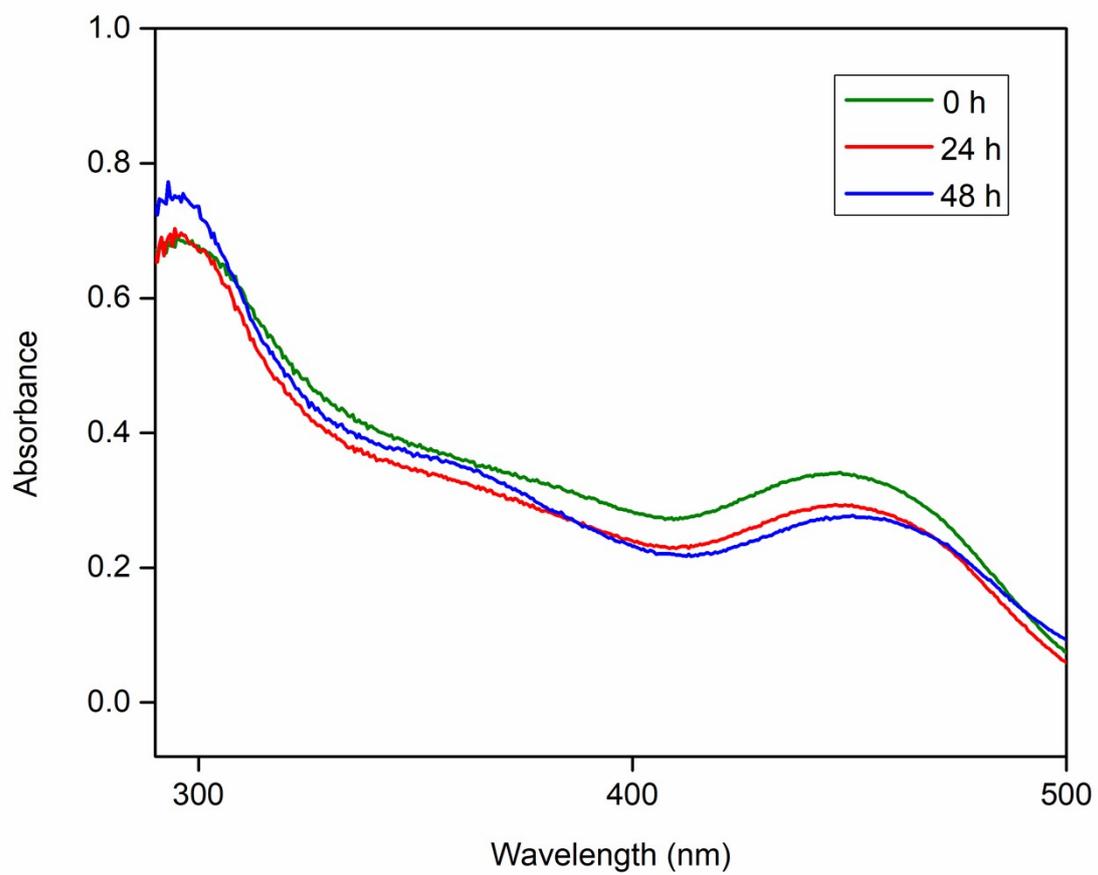


Fig. S12. Time-dependent UV-visible absorption spectra of **4** in 0.1 % DMSO/DMEM.

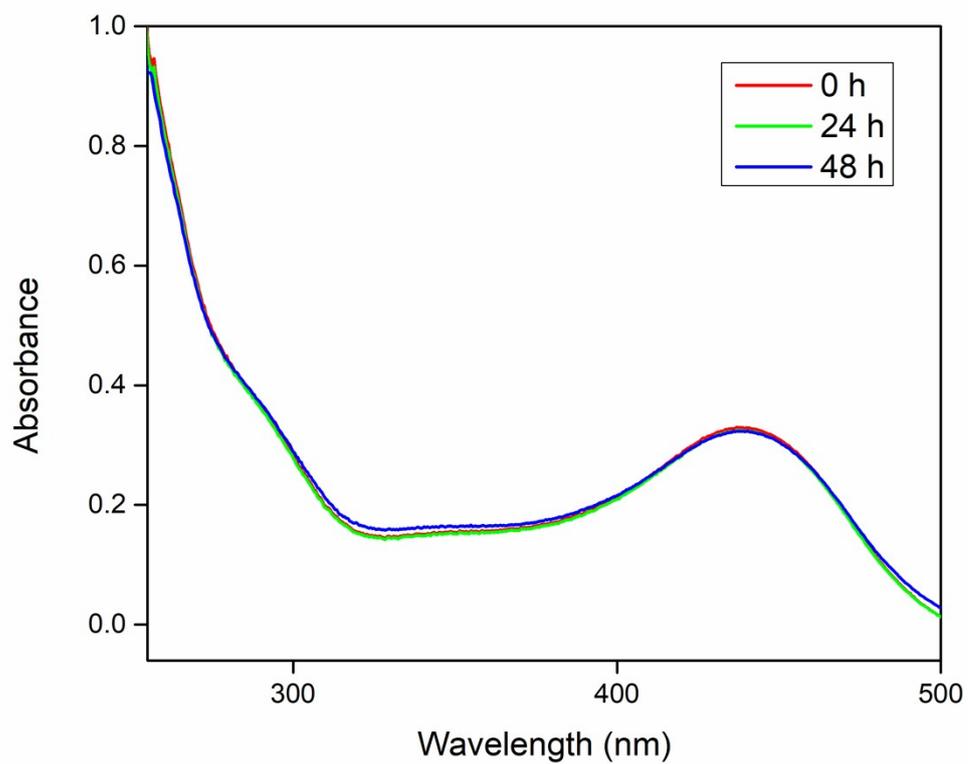


Fig. S13. Time-dependent UV-visible absorption spectra of **2** in DMSO.

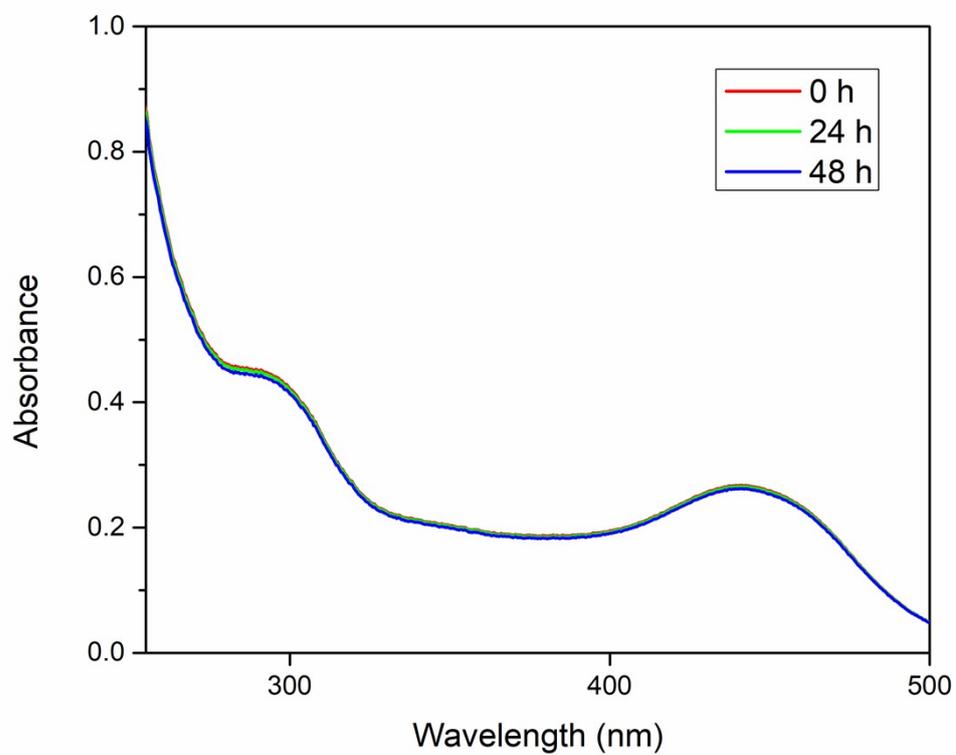


Fig. S14. Time-dependent UV-visible absorption spectra of **4** in DMSO.

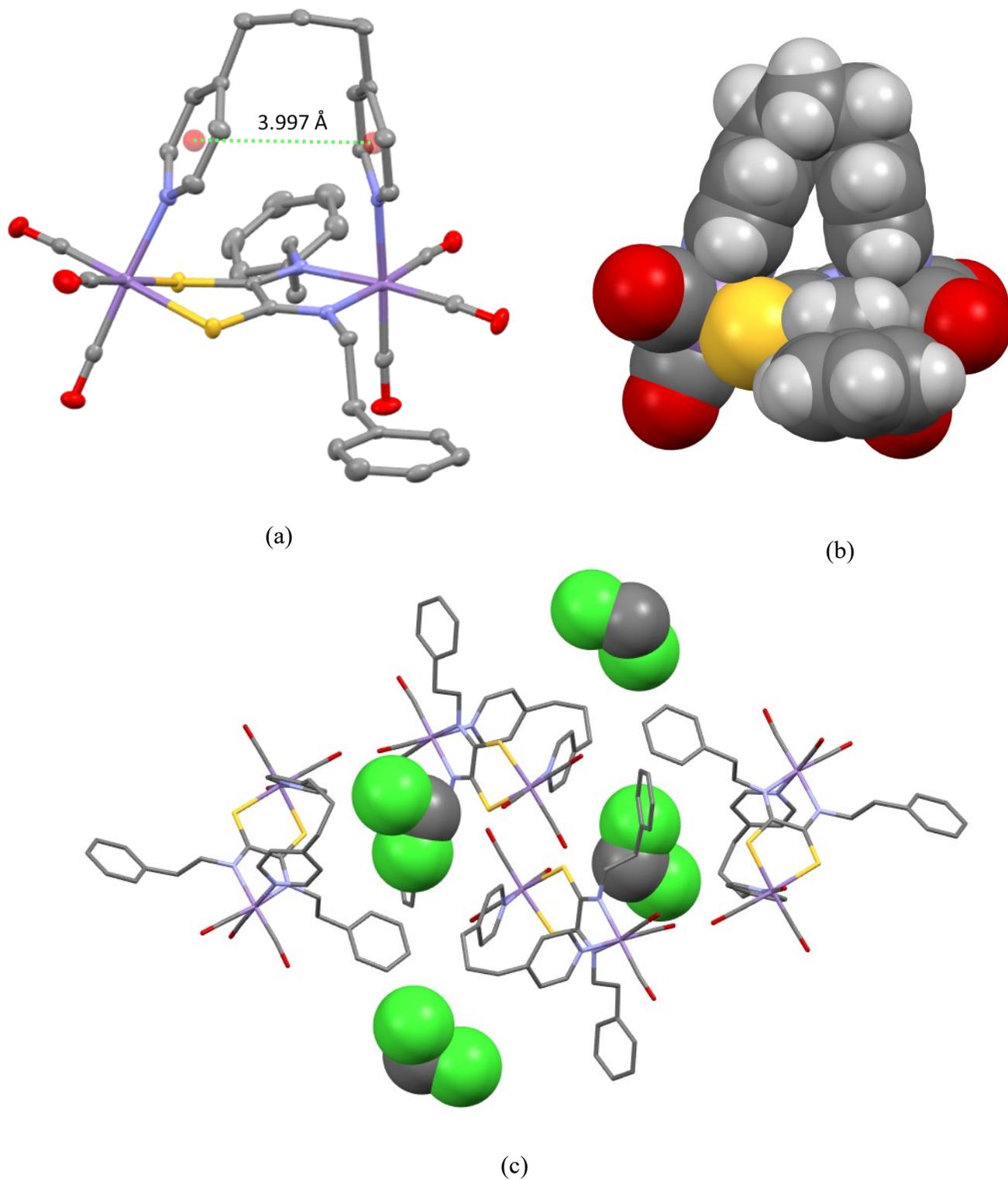


Fig. S15. (a) Ellipsoid representation of **4** centroid \cdots centroid distance between the two pyridyl groups of the bpp ligand. (b) Space filling model of **4**. (c) Packing diagram of **4**·CH₂Cl₂ viewed along *a* axis showing a CH₂Cl₂ molecule present outside (space filling representation).

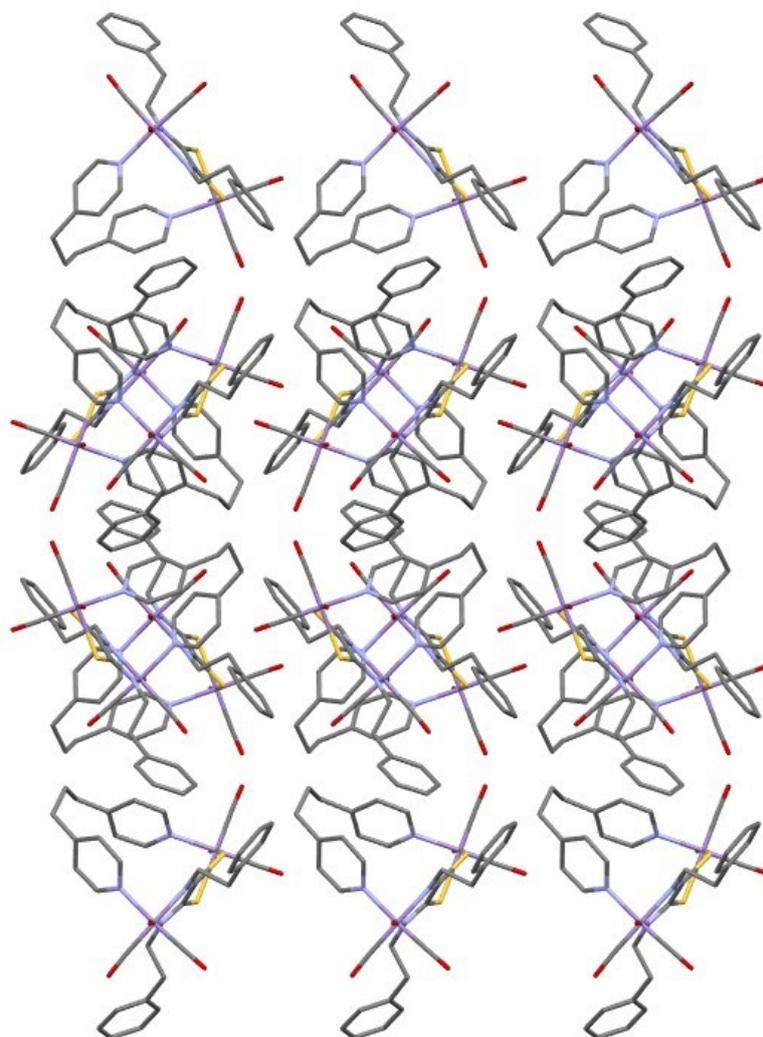


Fig. S16. Packing diagram of **4** in stick representation viewed along *c* axis showing zig-zag chain formation.

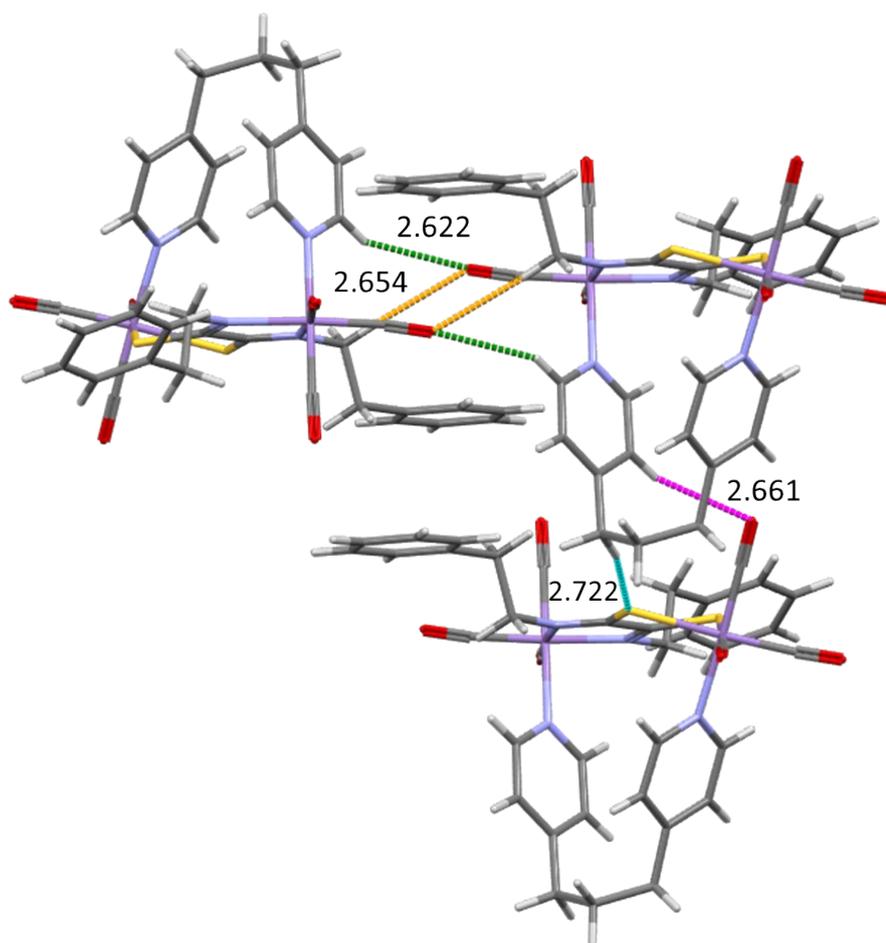


Fig. S17. Stick representation of **4** showing intermolecular hydrogen bonding C–H \cdots C \equiv O (green, yellow and magenta dotted lines) and C–H \cdots C=S (blue dotted lines).