Different coordination abilities of 1,7- and 4,7-phenanthroline in the reactions with copper(II) salts: structural characterization and biological evaluation of the reaction products

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Abstract

The reactions between equimolar amounts of CuX_2 (X = NO_3^- and $CF_3SO_3^-$) and two aromatic nitrogen-containing heterocycles differing in the position of nitrogen atoms, 1,7- and 4,7-phenanthroline (1,7- and 4,7-phen), were performed in ethanol/methanol at room temperature. When CuX_2 salts were mixed with 4,7-phen, two copper(II) complexes, $[Cu(NO_3)_2(4,7\text{-}Hphen)_2](NO_3)_2$ (**1**) and $[Cu(CF_3SO_3)(4,7\text{-}phen)_2(H_2O)_2]CF_3SO_3$ (**2**), were formed. On the other hand, in the reaction of CuX_2 salts with 1,7-phen, only 1,7-$HphenNO_3$ (**3a**/**b**) and 1,7-$HphenCF_3SO_3$ (**4**) were obtained as the final products. The obtained products **1 – 4** were characterized by spectroscopic and X-ray diffraction techniques. In the copper(II) complexes **1** and **2**, the coordination geometry around the Cu(II) ion is distorted octahedral and square pyramidal, respectively. The antimicrobial potential of the copper(II) complexes **1** and **2** and corresponding compounds used for their synthesis were assessed against four different bacterial species and *Candida albicans*, displaying moderate growth inhibiting activity. The cytotoxic properties of the investigated complexes were also evaluated against the normal human lung fibroblast cell line (MRC-5) indicating moderate, yet more pronounced cytotoxicity than antimicrobial properties.

Keywords: Copper(II), Phenanthroline, Structural characterization, Antimicrobial activity, Cytotoxicity

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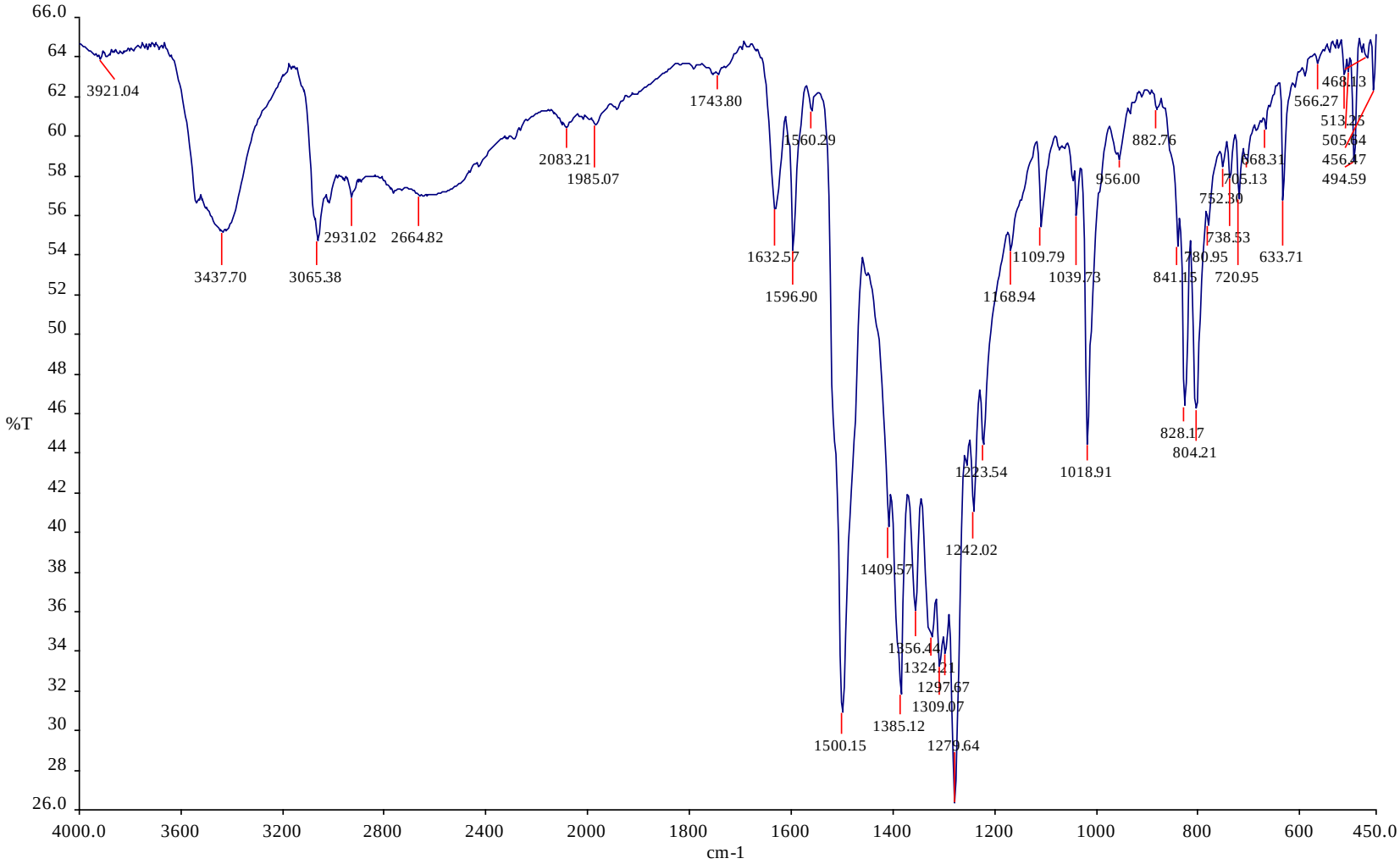
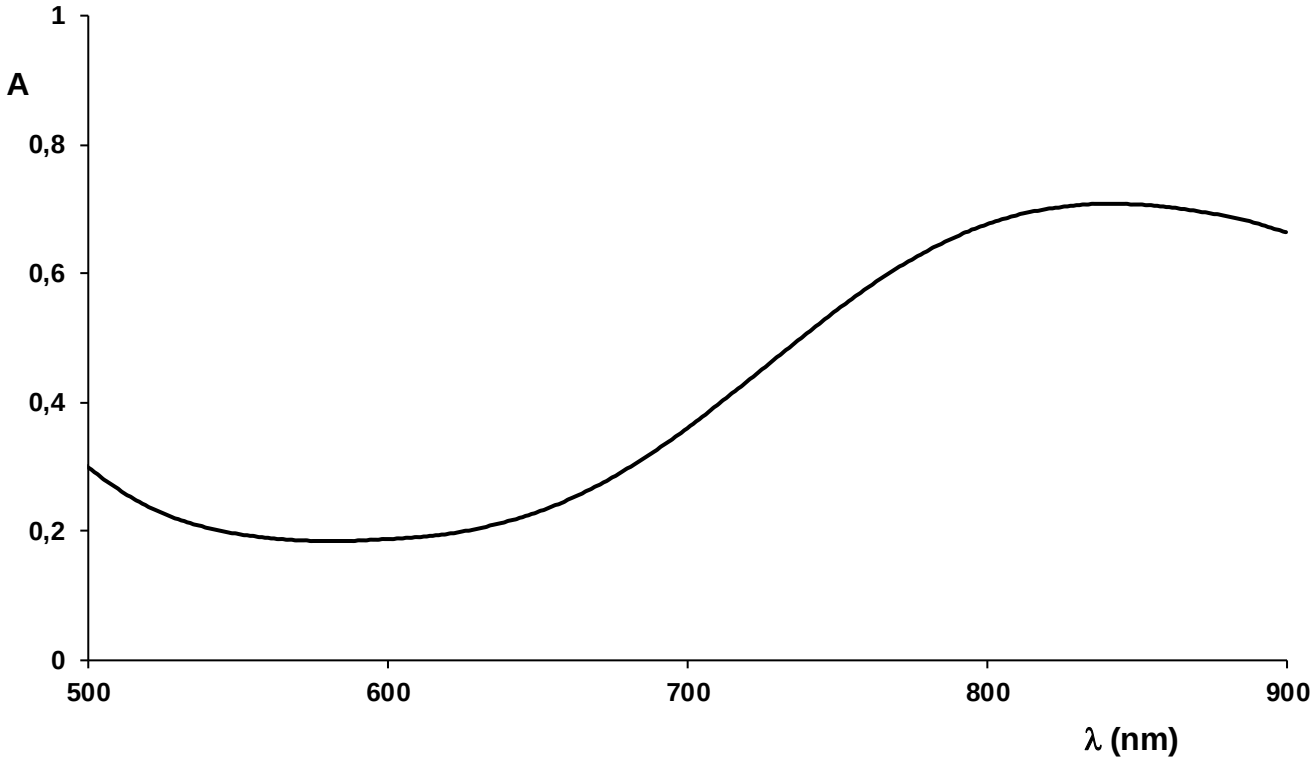
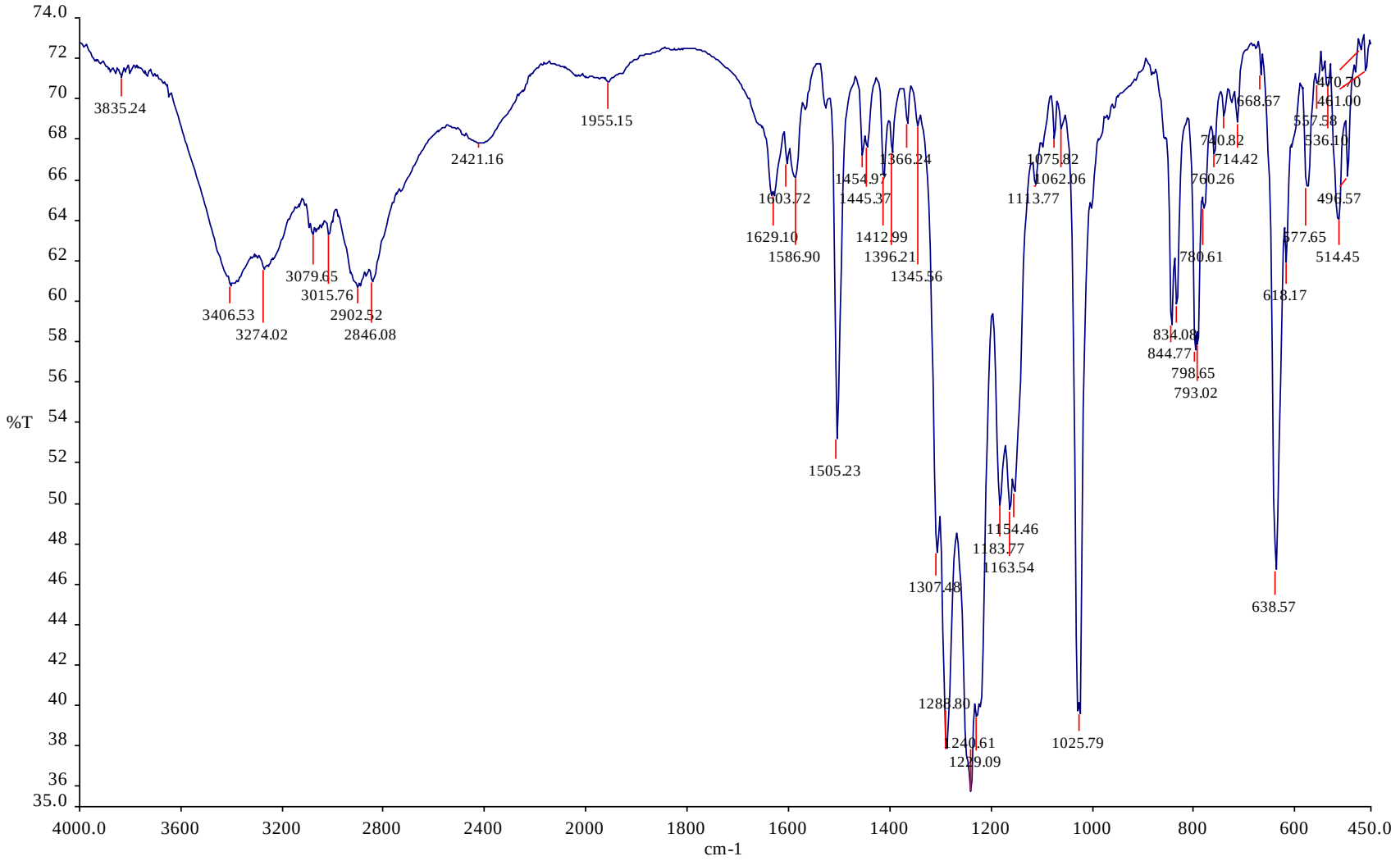
IR spectrum of **1**



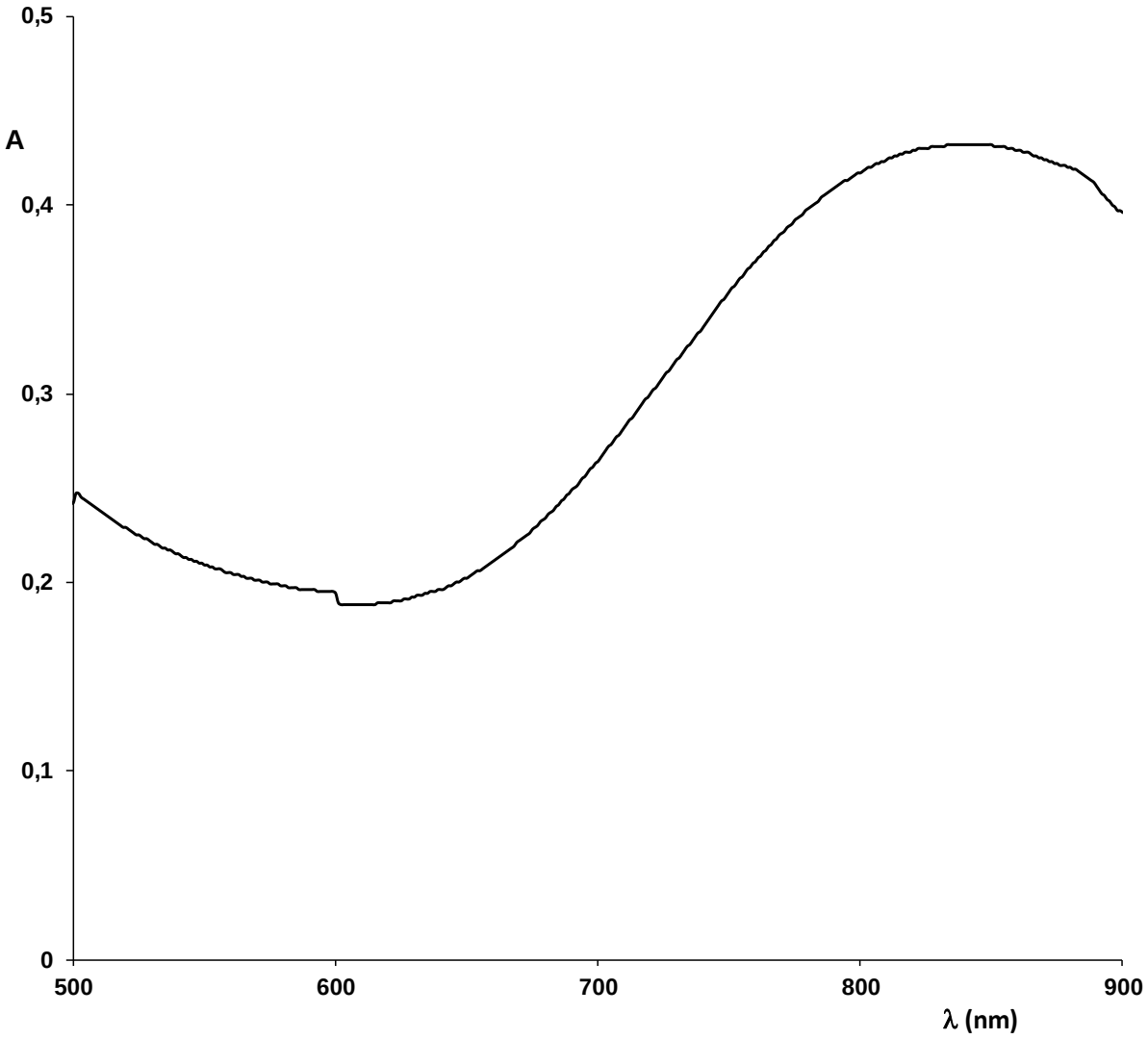
UV-Vis spectrum of **1** (DMSO)



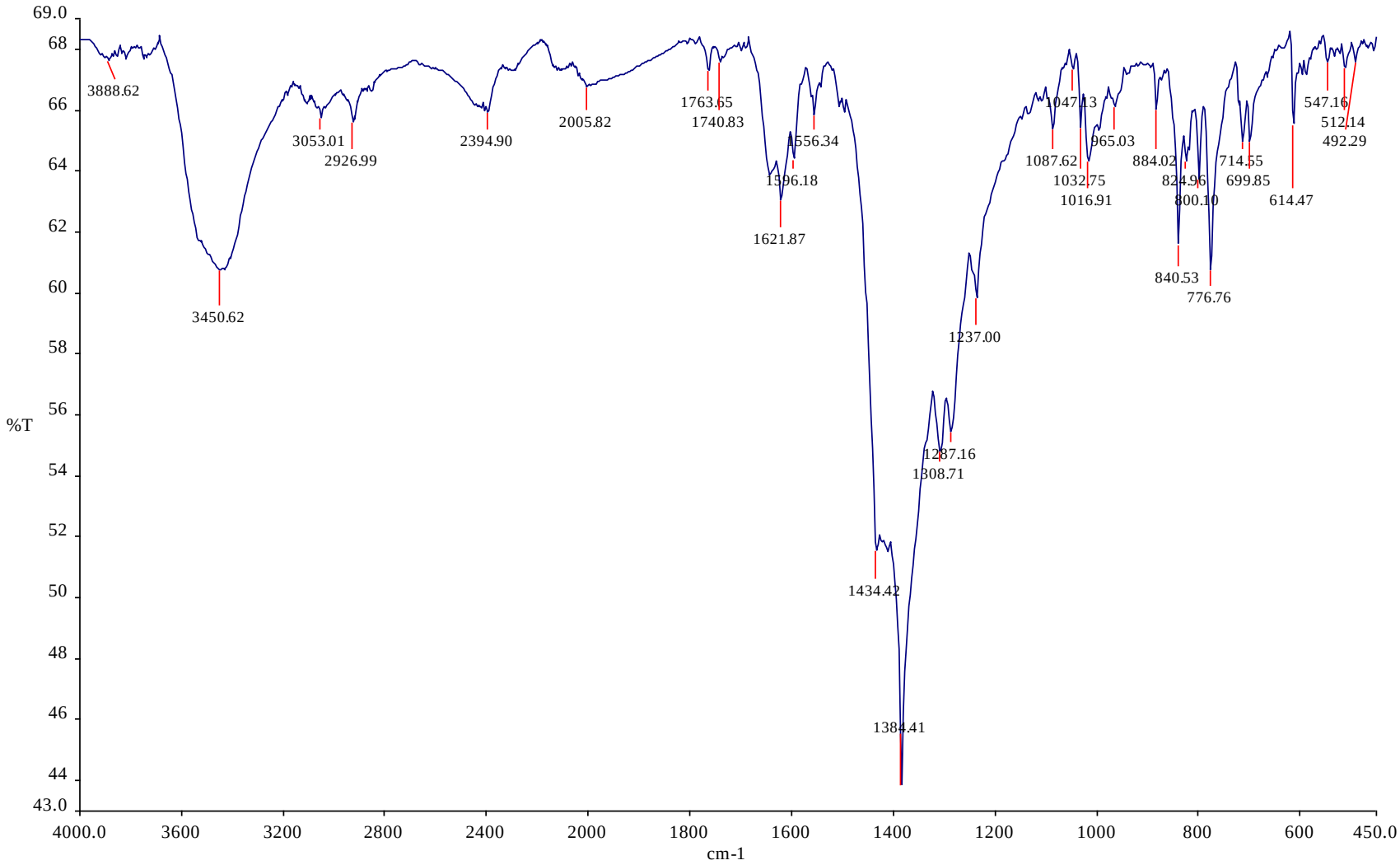
IR spectrum of **2**



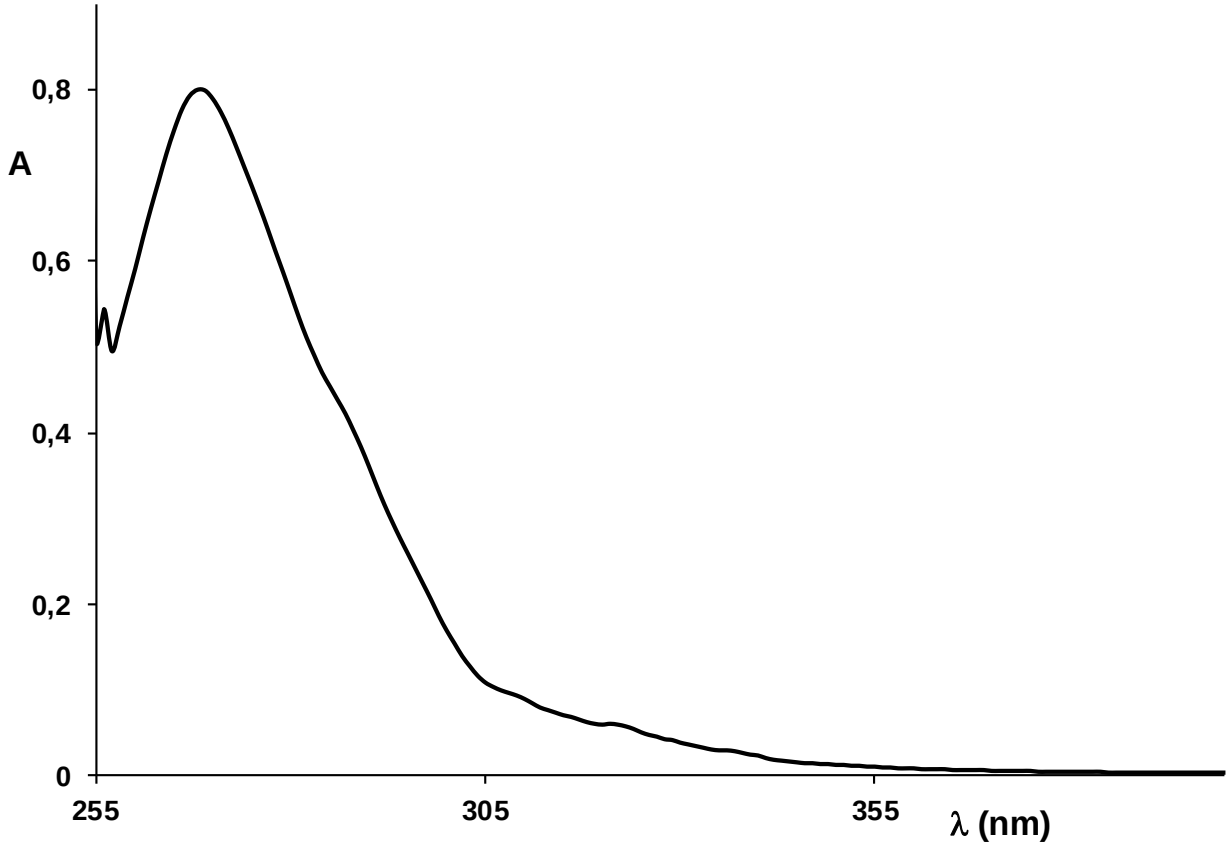
UV-Vis spectrum of **2** (DMSO)



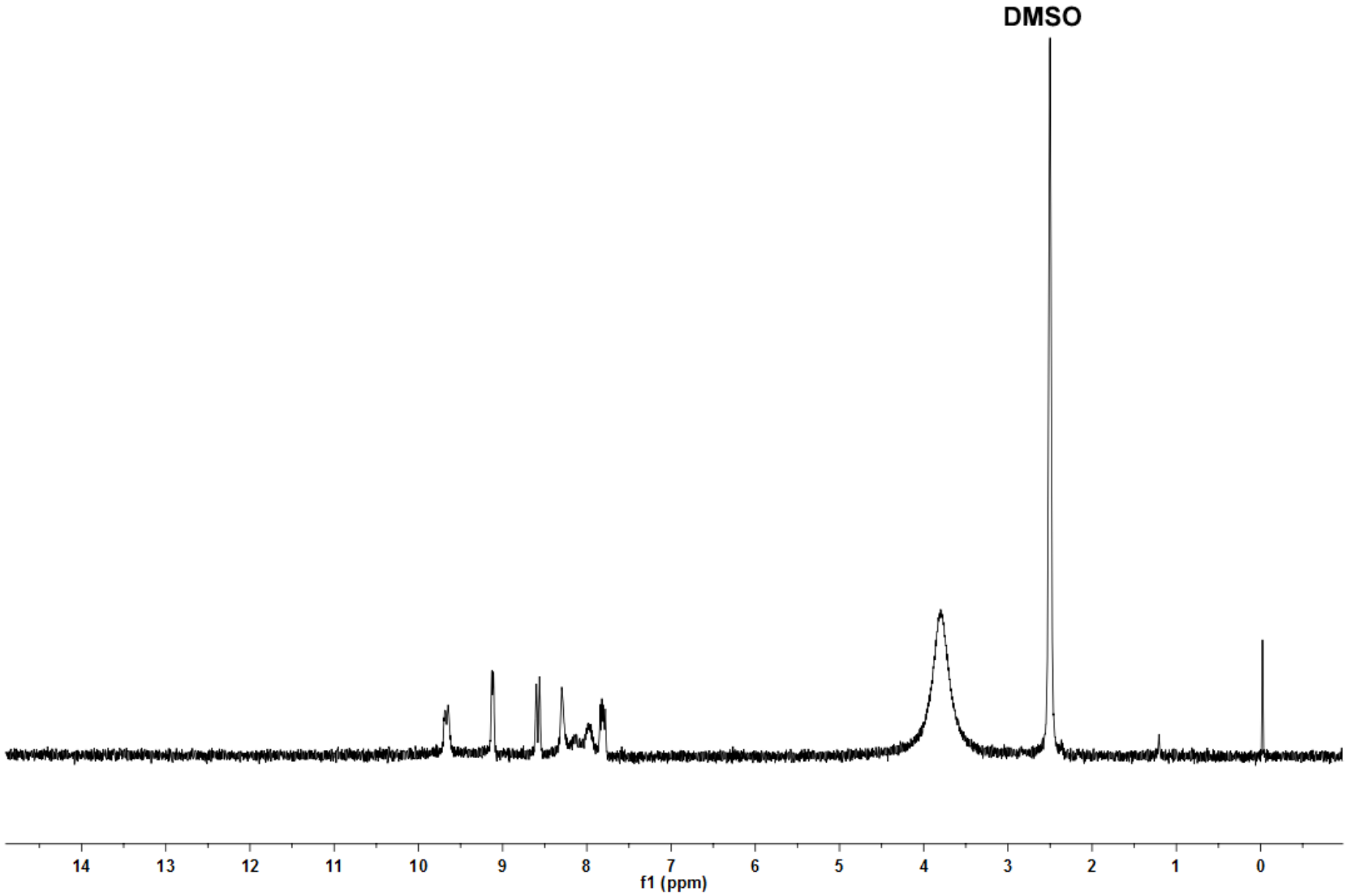
IR spectrum of **3a**



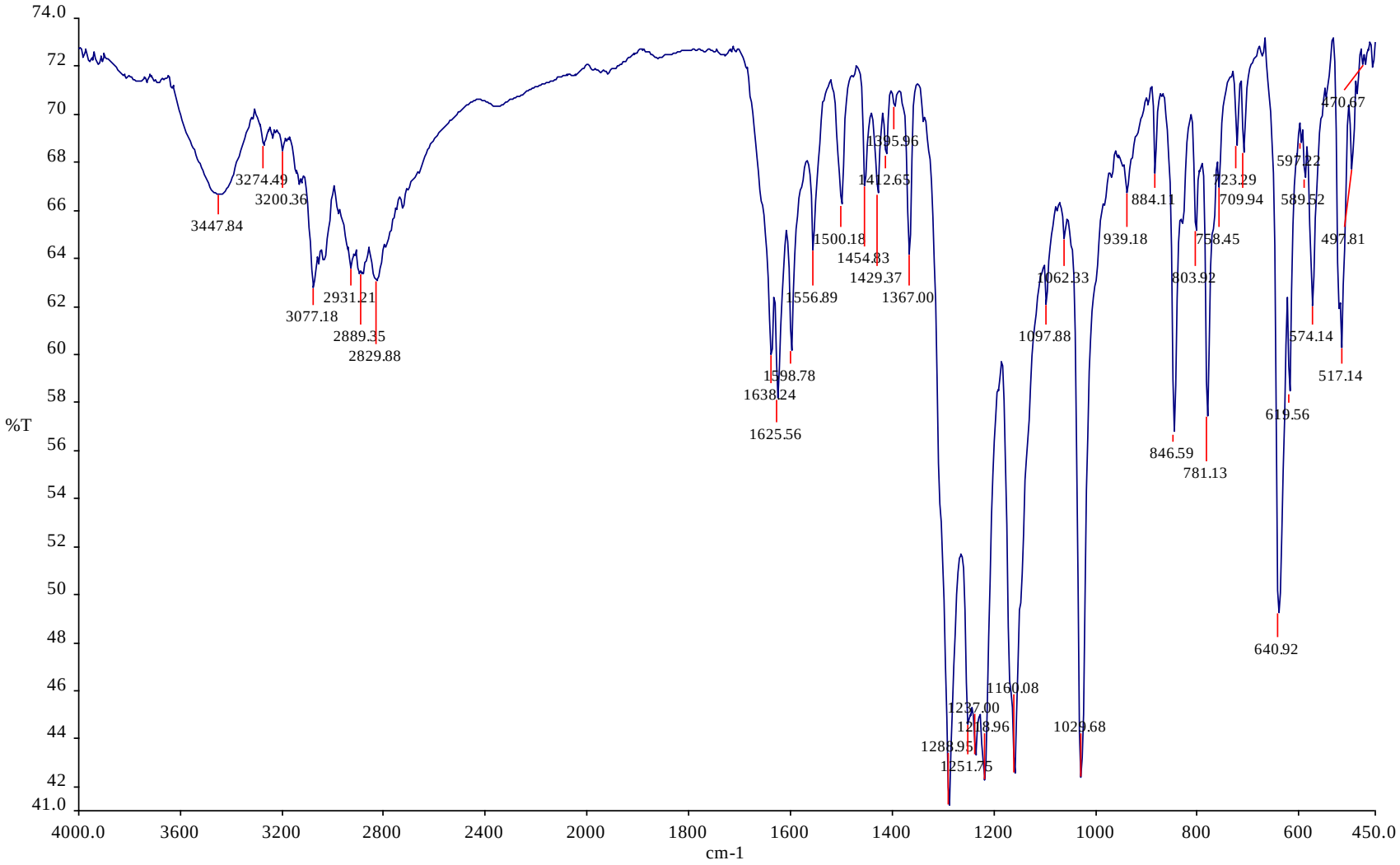
UV-Vis spectrum of **3a** (DMSO)



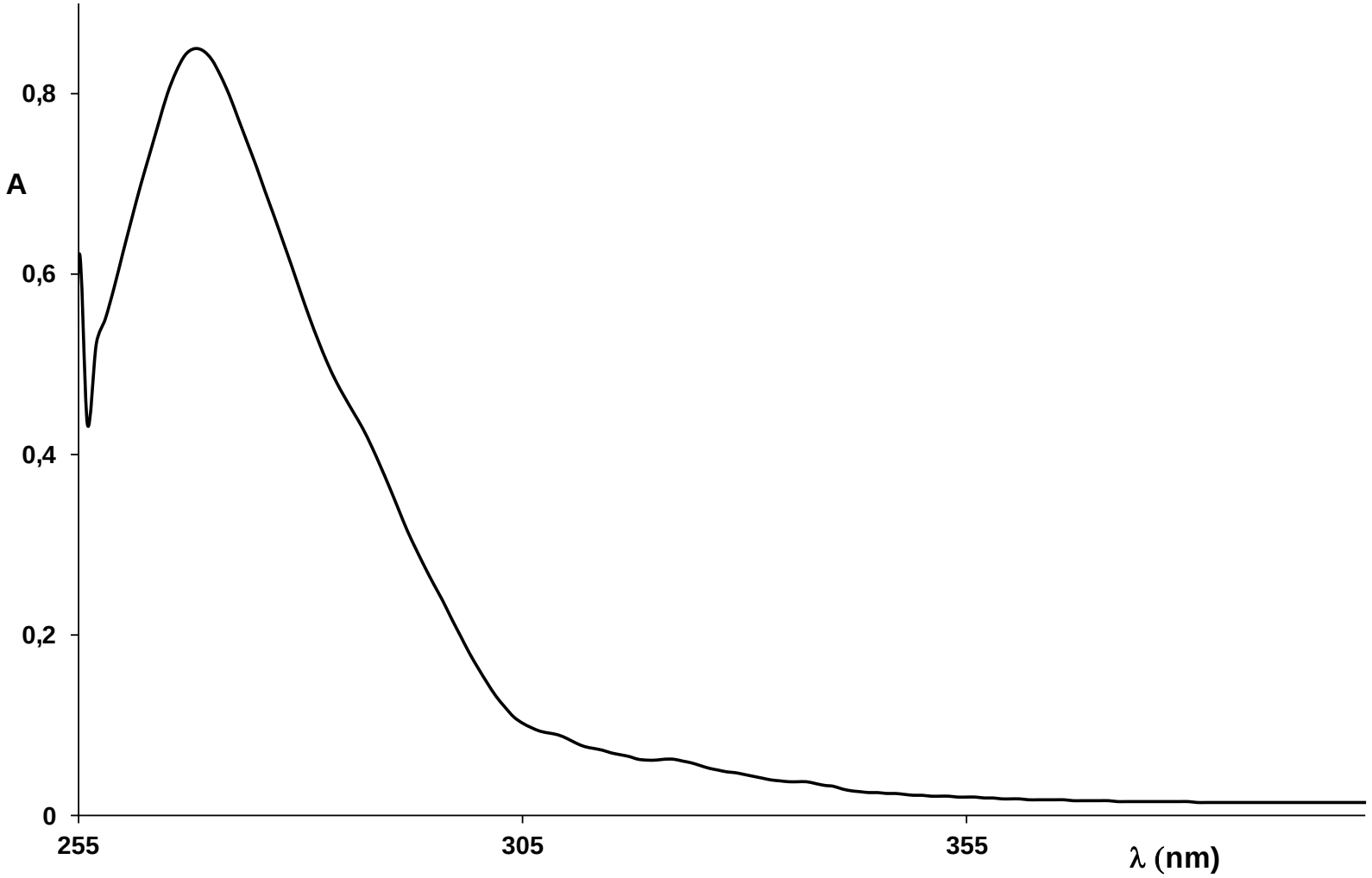
^{1}H NMR spectrum of **3a** (200 MHz, DMSO-d_6)



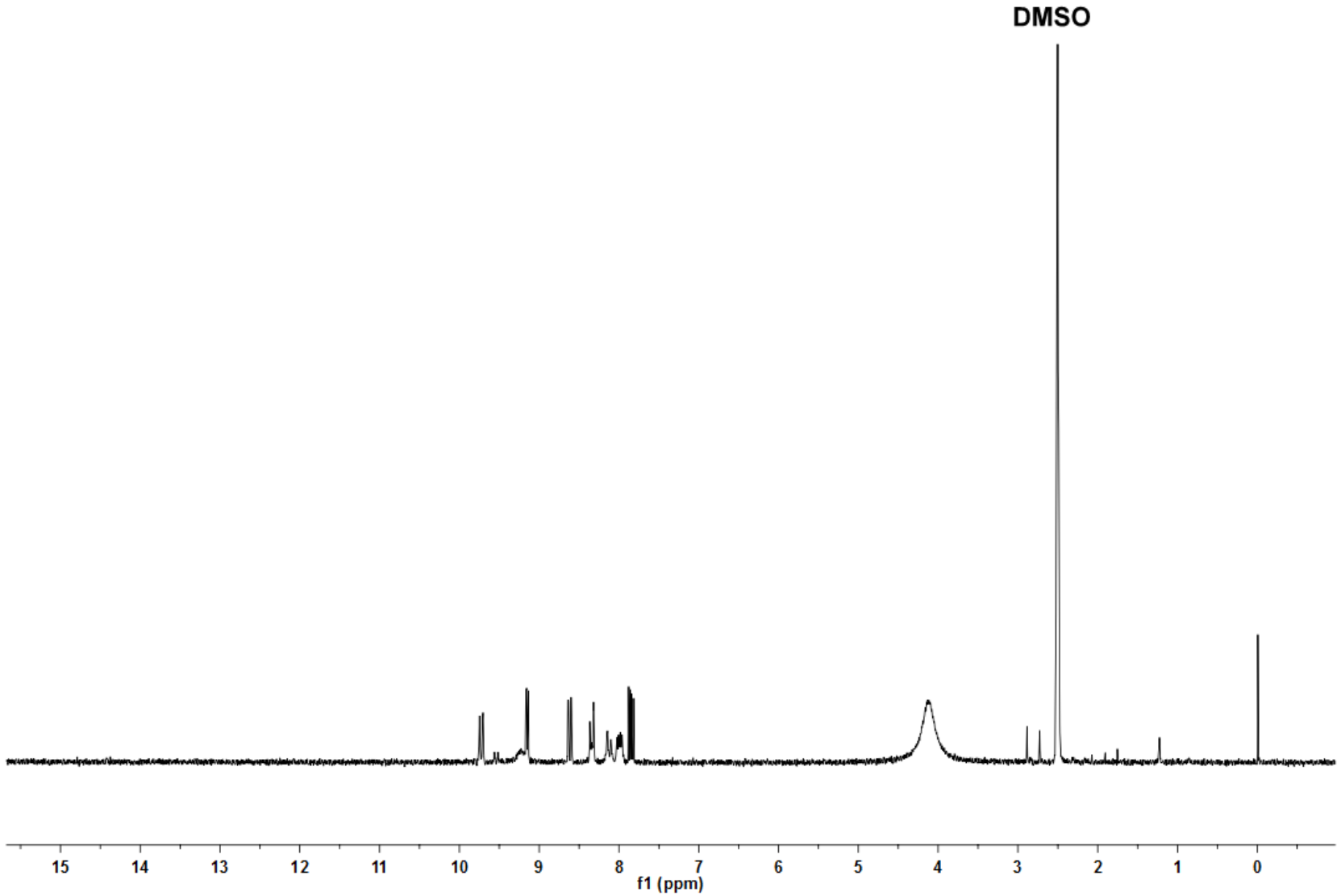
IR spectrum of **4**



UV-Vis spectrum of **4** (DMSO)



^{1}H NMR spectrum of **4** (200 MHz, DMSO-d_6)



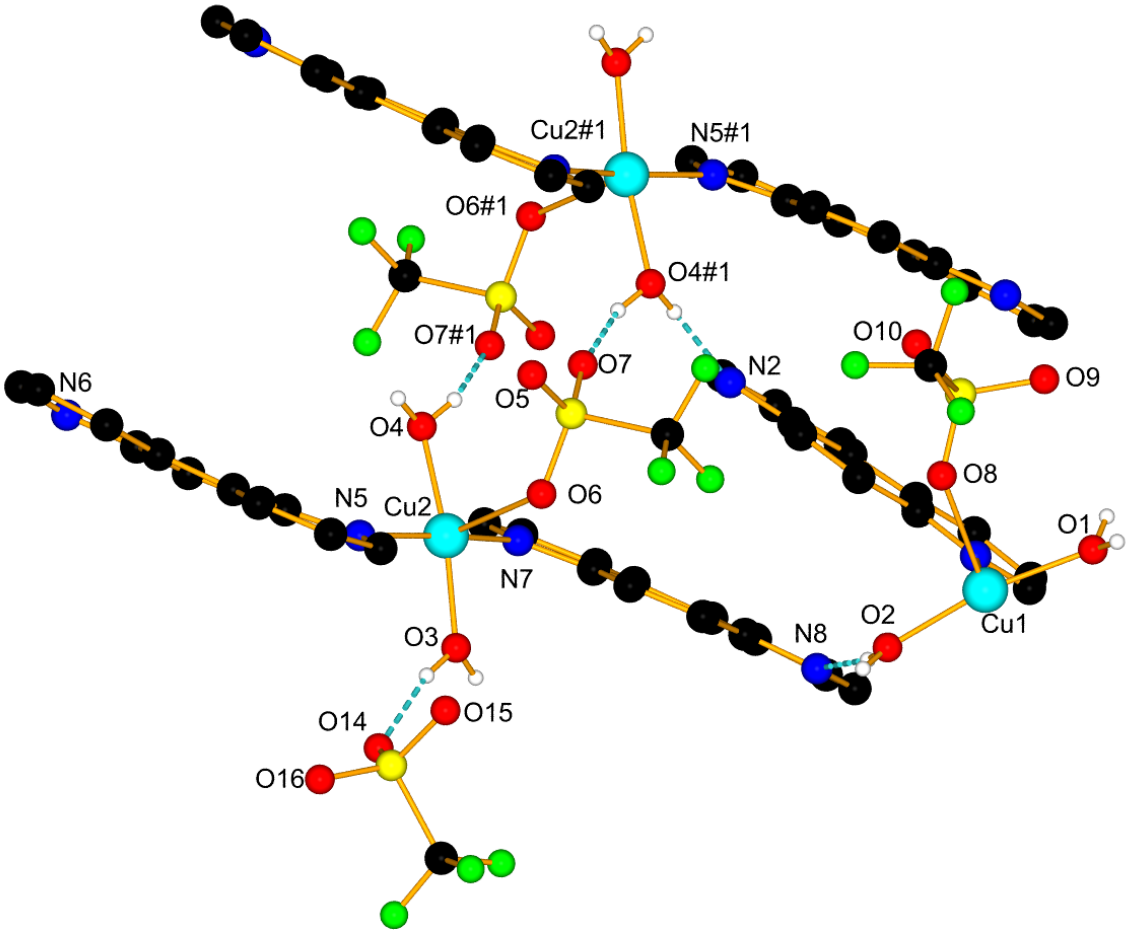


Fig. S1. Molecular structure of **2**. Some hydrogen atoms and partitioning of counter-ions are omitted for clarity. Hydrogen bonds are drawn as dashed blue lines, #1: −*x*+1, −*y*+1, −z+1.

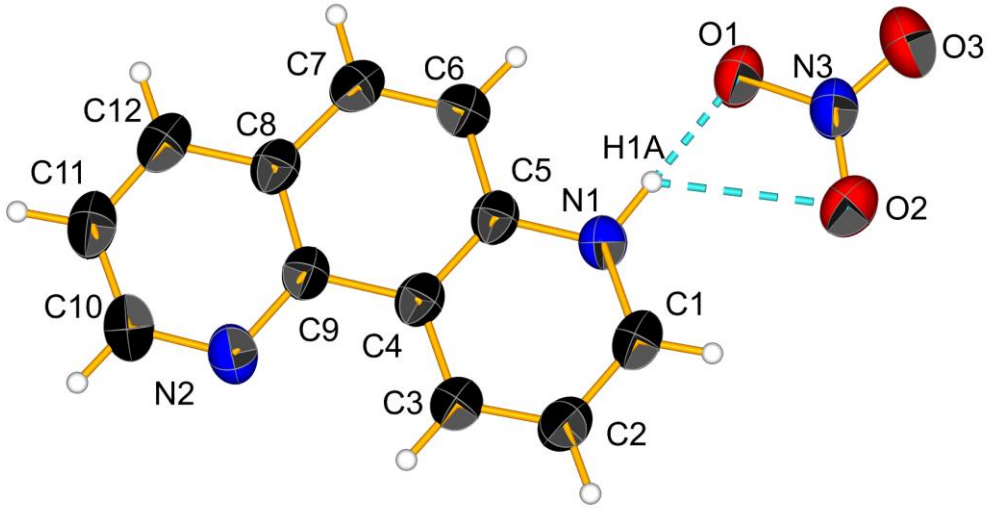


Fig. S2. Molecular structure of **3b**. Displacement ellipsoids are drawn at 50% probability level and H atoms are represented by spheres of arbitrary size.

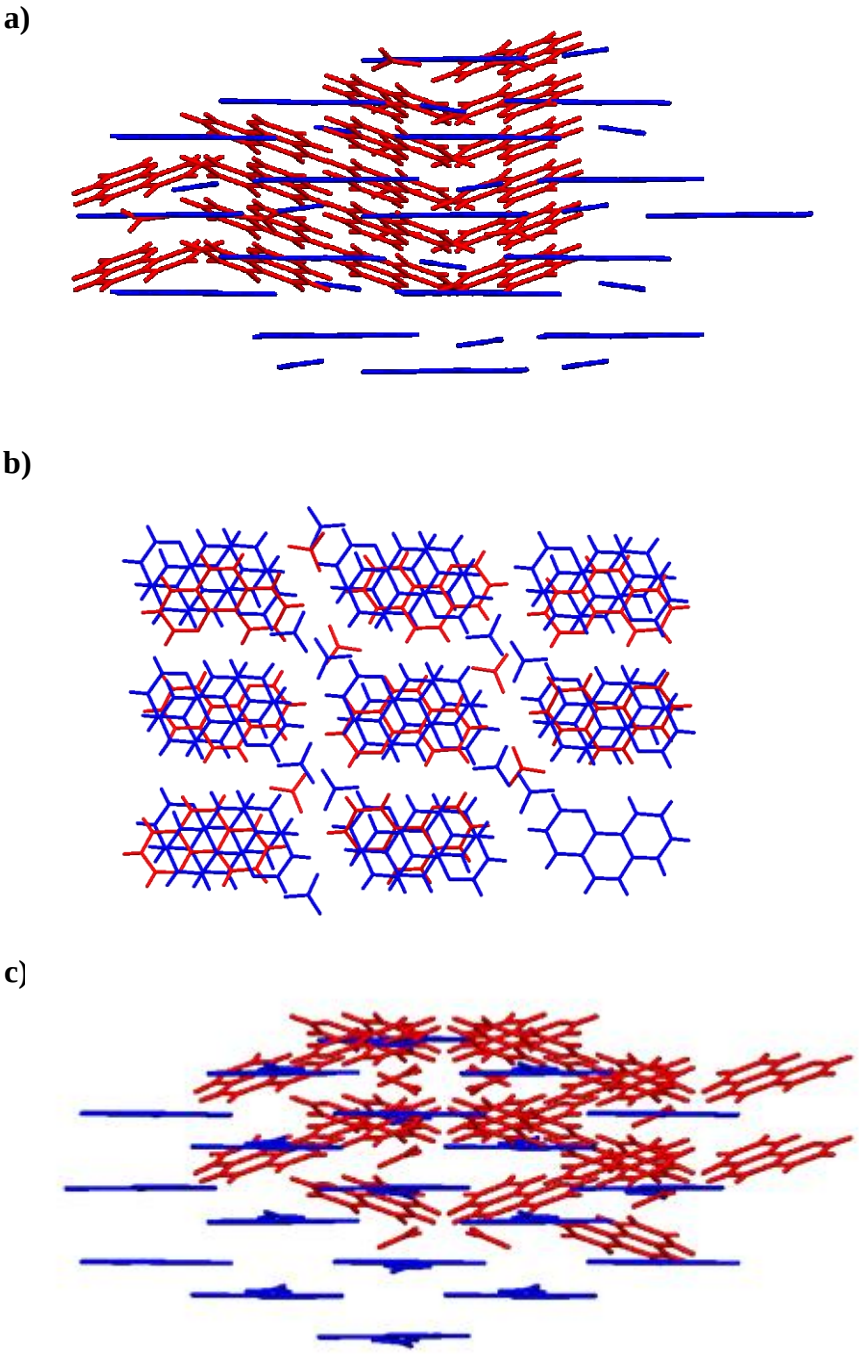


Fig. S3. The overlay of the packing of the **3a** (red) and **3b** (blue) along the *a* **(a)**, *b* **(b)** and *c* **(c)** axis.