Electronic Supplementary Material (ESI) for CrystEngComm.

Supporting Information

Series of Highly stable Cd(II)-based coordination polymers for sensitive and selective detection of nitrofuran antibiotics

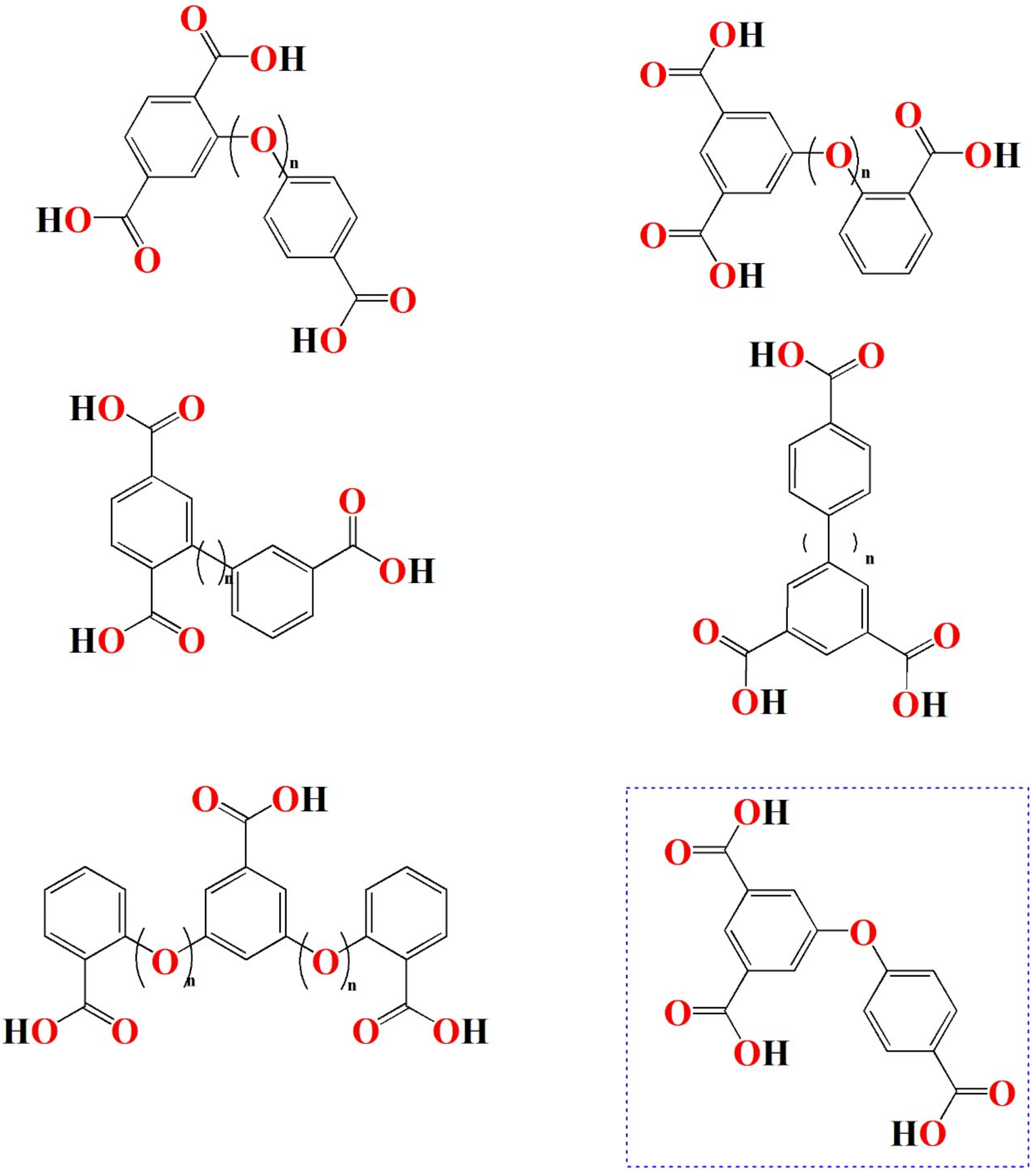
Experimental

Materials and Method

All the reagents to perform synthesis obtained from commercial sources were of analytical grade. The ligand 5-(4′-carboxylphenoxy)isophthalic acid, 3,6-bis(imidazol-1-yl)-9H-carbazole, 1,1'-(1,4-butanediyl)bis(imidazole), 1,4-bis(1-imidazoly)benzene, 2-imidazol-1-ylpyridine was purchased from chemical company and used without further purification. Powder X-ray diffraction (PXRD) data were collected using Bruker ADVANCE X-ray diffractometer with Cu-Kα radiation (λ=1.5418 Å) at 50 kV, 20 mA with a scanning rate of 6°/min and a step size of 0.02°. Fourier transform infrared (FT-IR) spectra for both the MOFs as KBr discs were recorded on Nicolet Impact 750 FTIR in the range of 400-4000 cm^{-1}. Thermogravimetric analyses (TGA) were performed under nitrogen atmosphere from room temperature to 900 °C at a heating rate of 10 °C min^{-1}. The photocatalytic investigations were carried out using Shimadzu UV-Vis 2501PC recording spectrophotometer.Nitrogen adsorption-desorption measurements were performed at 77 K in a liquid nitrogen bath on a Micromeritics ASAP 3020 analyzer. The sample was first degassed at 80 °C for 10 h to remove the adsorbed solvents before measurement. The Brunauer-Emmett-Teller (BET) method was used to calculate the specific surface areas (S_{BET}).

X-ray Crystallography

The single crystal X-ray diffraction data for both the MOFs were collected on a Bruker SMART APEX diffractometer which was equipped with graphite monochromated MoKα radiation (λ = 0.71073 Å) by using an ω-scan technique. The structures were solved by direct method (SHLEXS-2014) and refined using the full-matrix least-square procedure based on F^2 (Shelxl-2014). All the hydrogen atoms were generated geometrically and refined isotropically using a riding model. All nonhydrogen atoms were refined with anisotropic displacement parameters. Crystallographic details and selected bond dimensions for **1-4** are listed in Tables S1 and S2, respectively. CCDC numbers: 2102107- 2102110.



Scheme S1 representative tricarboxylate linker as confirmed by a search of the Cambridge Structural Database

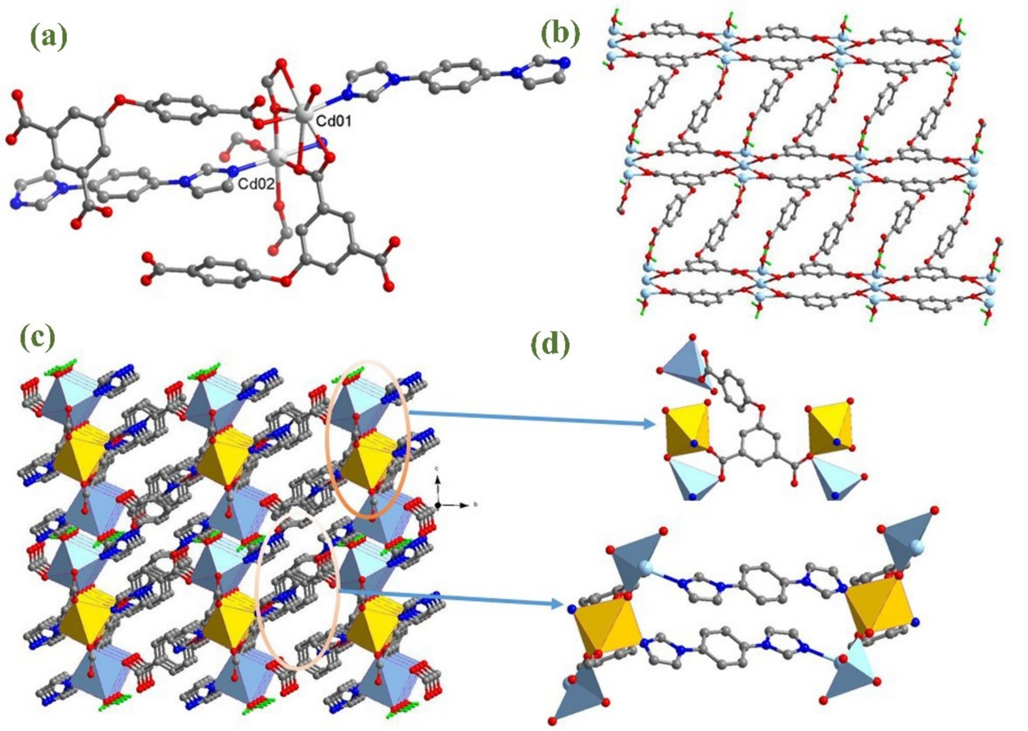


Figure S1 (a) the coordination geometry of the Cd(II) centers in 3, (b) 2D layer built by tricarboxylate and metal center; (c) 3D network; (d) different coordination modes of two coligands.

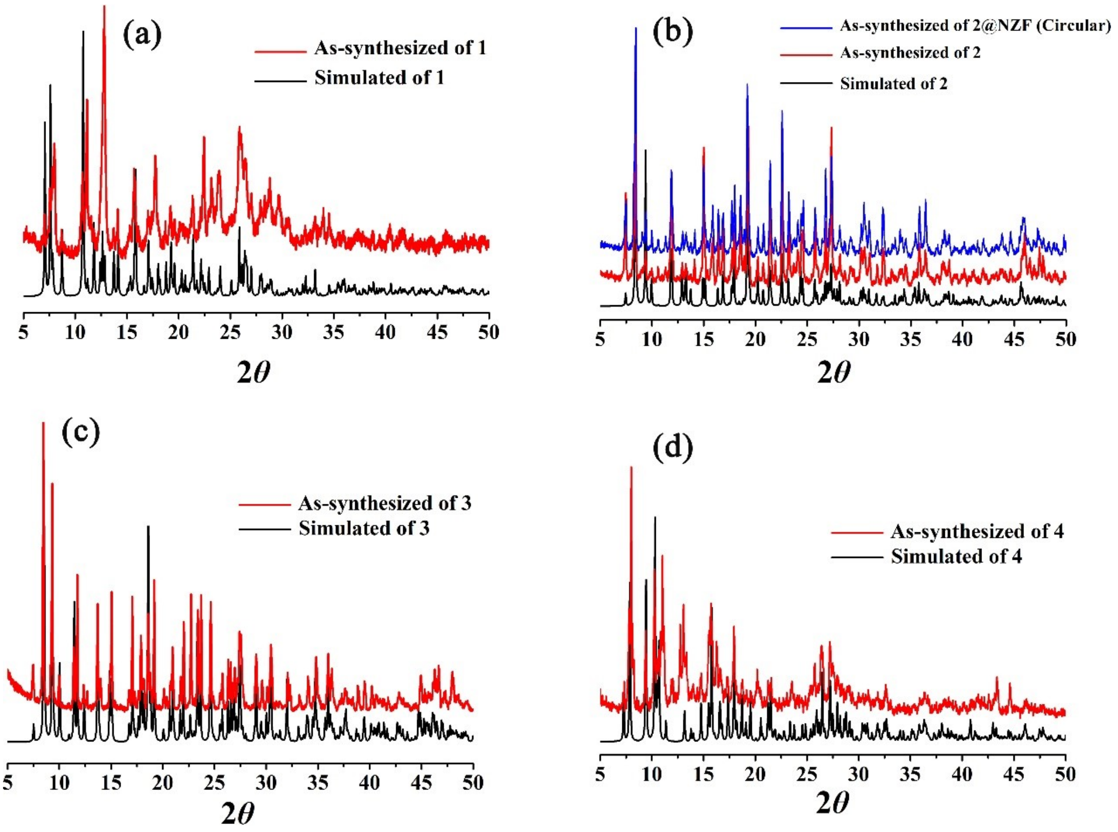


Figure S2 view of the different patterns of as-synthesized MOFs for **1-4**.

Thermogravimetric analysis

Thermal stability of compounds **1-4** was evaluated by thermogravimetric analysis (TGA) under nitrogen atmosphere. As shown in Fig. S3, compound **1** loses its lattice and two coordinated water molecules (exptl, 4.6%; calcd, 4.9%) in the 155-306 °C temperature range. The dehydrated sample remains stable up to 365 °C followed by the decomposition. For MOF **2**, there is one distinct thermal effect in the 37-260 °C range that corresponds to the removal of 2 lattice and 2 coordinated H_2O molecules (exptl, 5.2%; calcd, 5.0%). A dehydrated sample remains stable up to ~329 °C. Similarly, MOF **3** shows the loss of two coordinated water molecules between 34 and 306 °C (exptl, 2.4%; calcd, 2.5%) and a dehydrated sample remains stable up to ~340 °C. For **4**, a dehydrated sample remains stable up to ~285 °C.

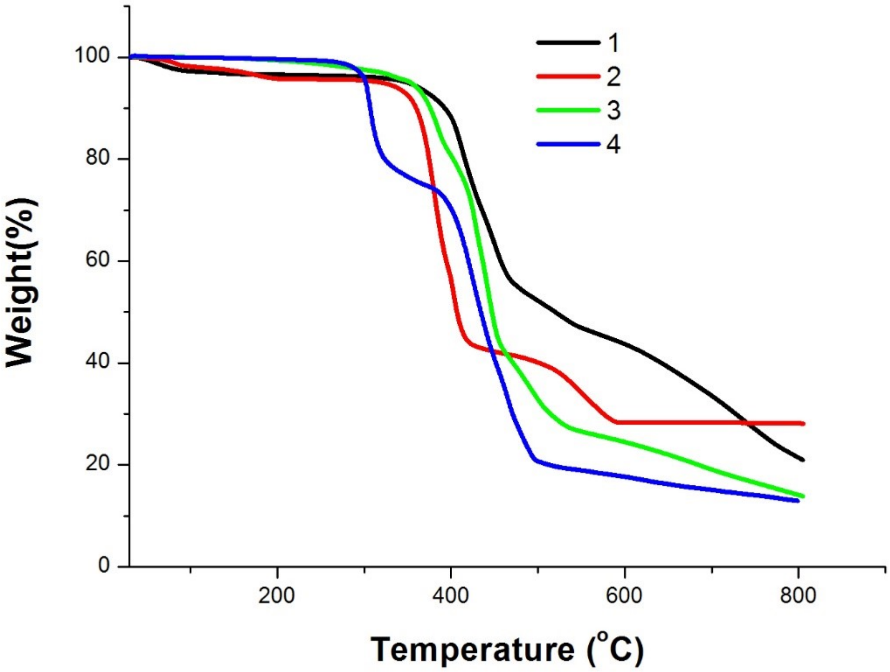


Figure S3 TGA curves of compounds **1-4**.

The IR spectra of **1-4** are determined in the frequency range of 400–4000 cm^{-1}, as shown in Fig. S4. The bands around 3258 cm^{-1} for **1-3** are characteristic of the vibrations of hydroxyl groups. The bands around 1628 and 1499 cm^{-1} for **1-4** are characteristic of the asymmetric and symmetric vibrations of carboxyl groups. The strong peaks at 1320 cm^{-1} for **1-4**, indicate the $\nu_{C–N}$ stretching vibrations of the N-donor linker.

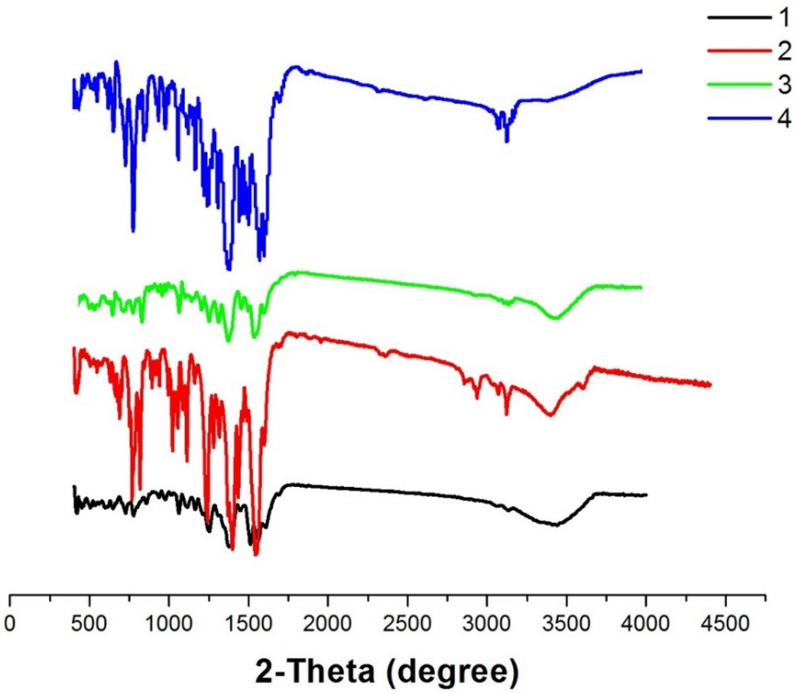


Figure S4 IR spectra of compounds **1-4**.

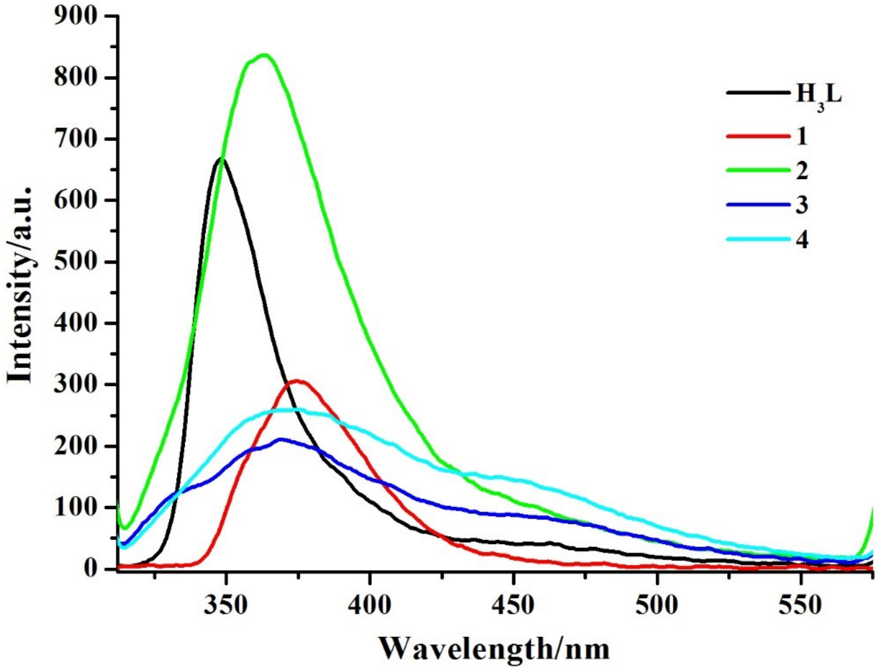


Fig. S5 photoluminescence spectra of **1-4** and the H$_3$L ligand was recorded at room temperature.

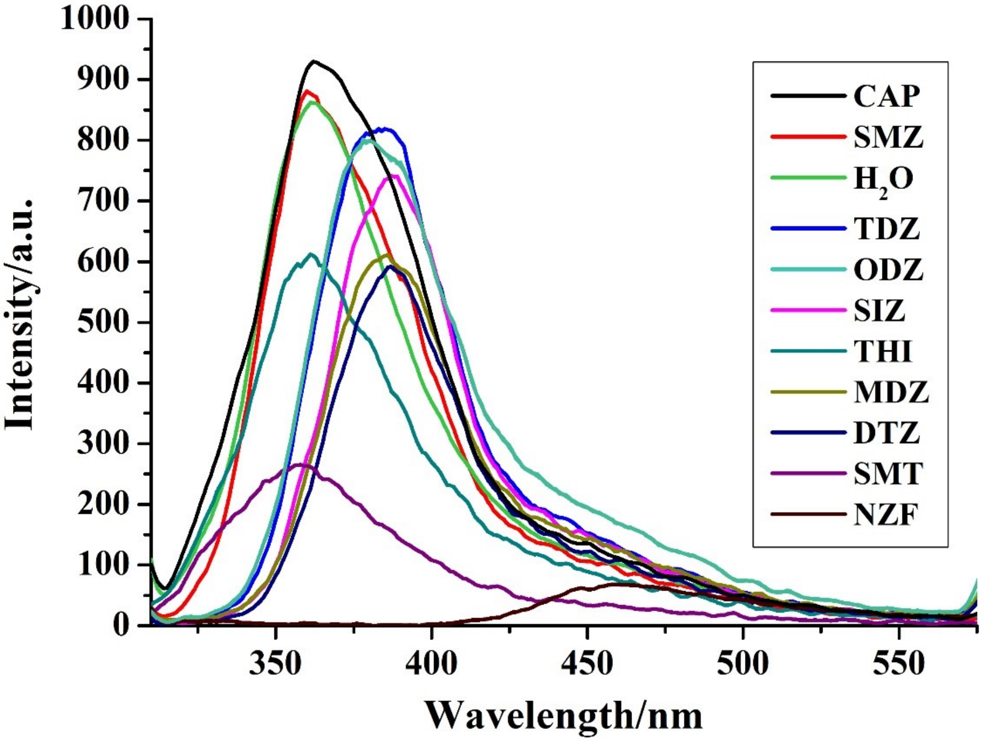


Fig. S6 photoluminescence spectra of **2** in the presence of different antibiotics was recorded at room temperature.

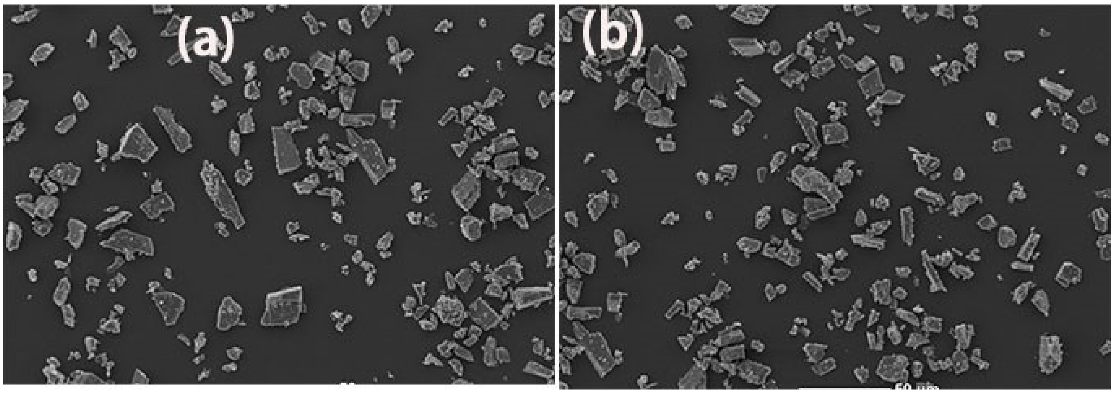


Fig. S7 Comparison of sample morphology changes before and after the probe in **2**.

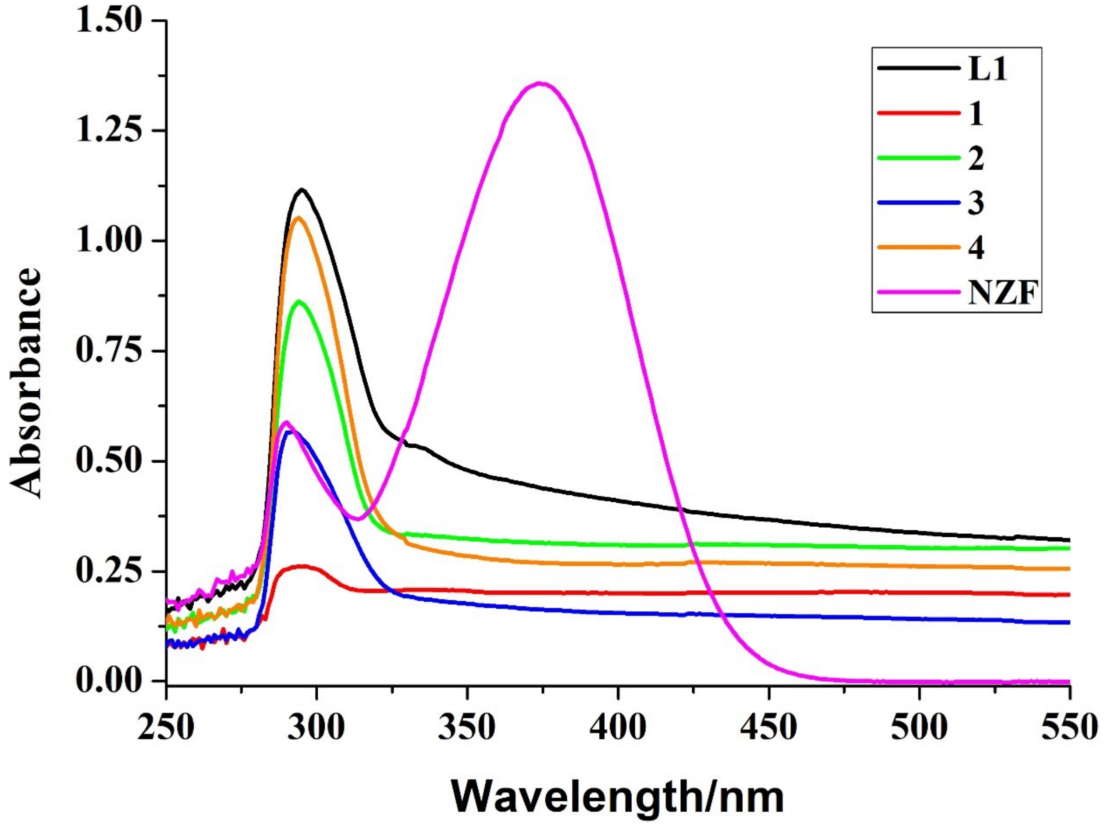


Fig. S8 The UV-vis spectra of the NFZ antibiotic, MOFs **1-4** and H_3L at room temperature.