Electronic Supplementary Material (ESI) for Dalton Transactions.

Metal-organic framework based drug delivery systems as smart carriers for release of poorly soluble drugs hydrochlorothiazide and dapsone

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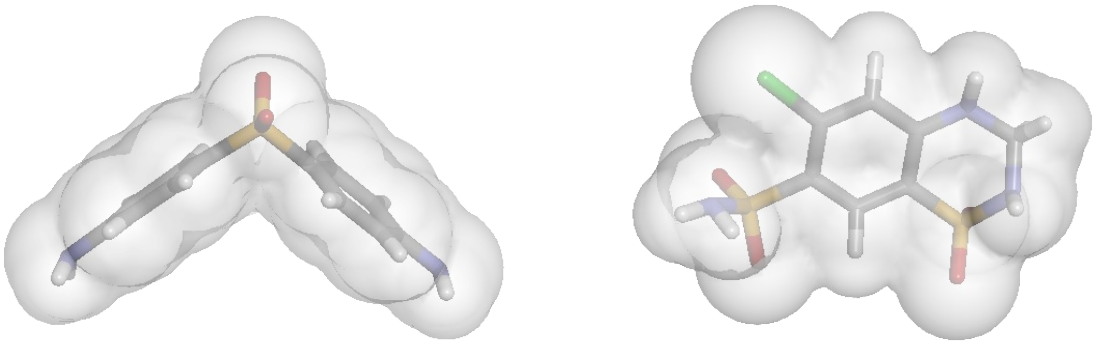


Dapsone Hydrochlorothiazide

Fig. S1 The structure of Dapsone and Hydrochlorothiazide after adding the van der Waals radii. The molecular size of DAP and HCT is estimated to be approximately 12.3 x 6.4 Å and 11.2 x 7.5 Å, respectively, which enables the facile encapsulation of the drugs in the MOF.[1,2]

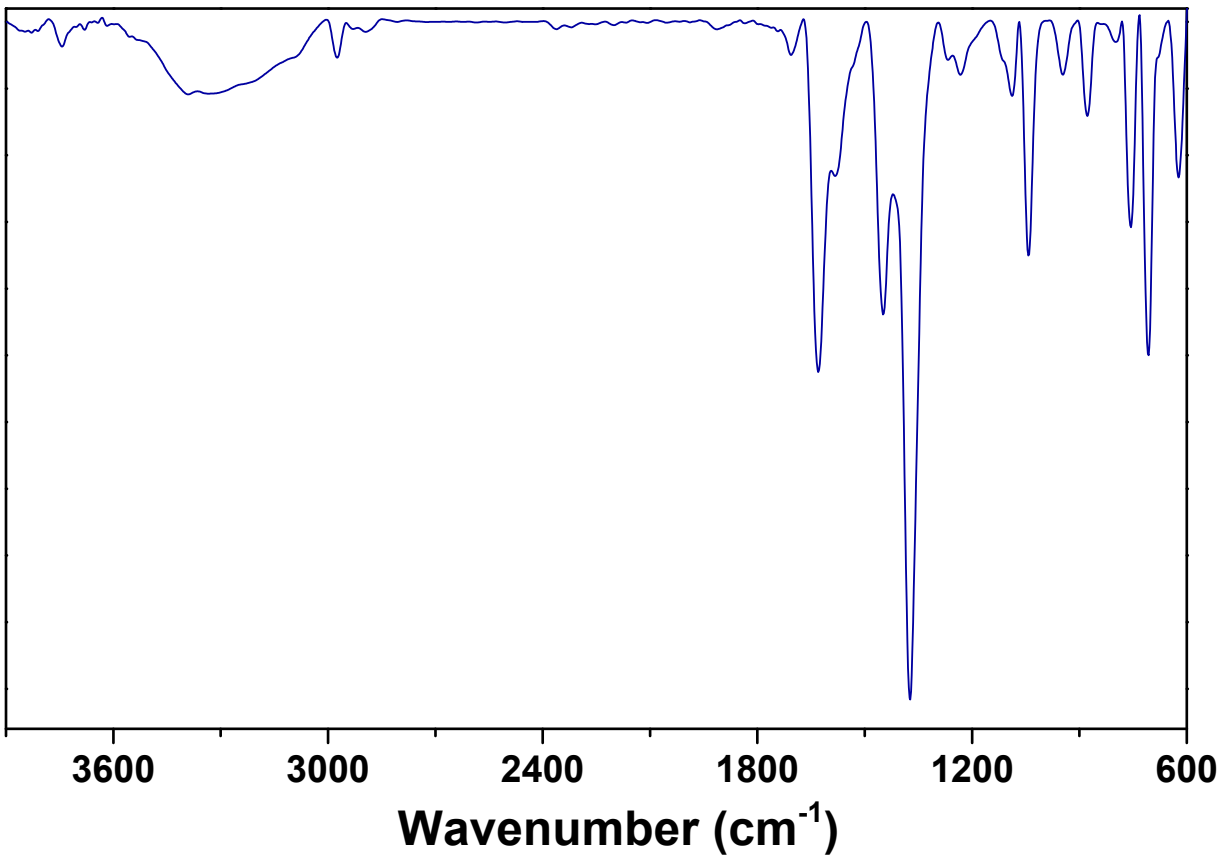


Fig. S2 FTIR spectrum of MIL-100(Fe).

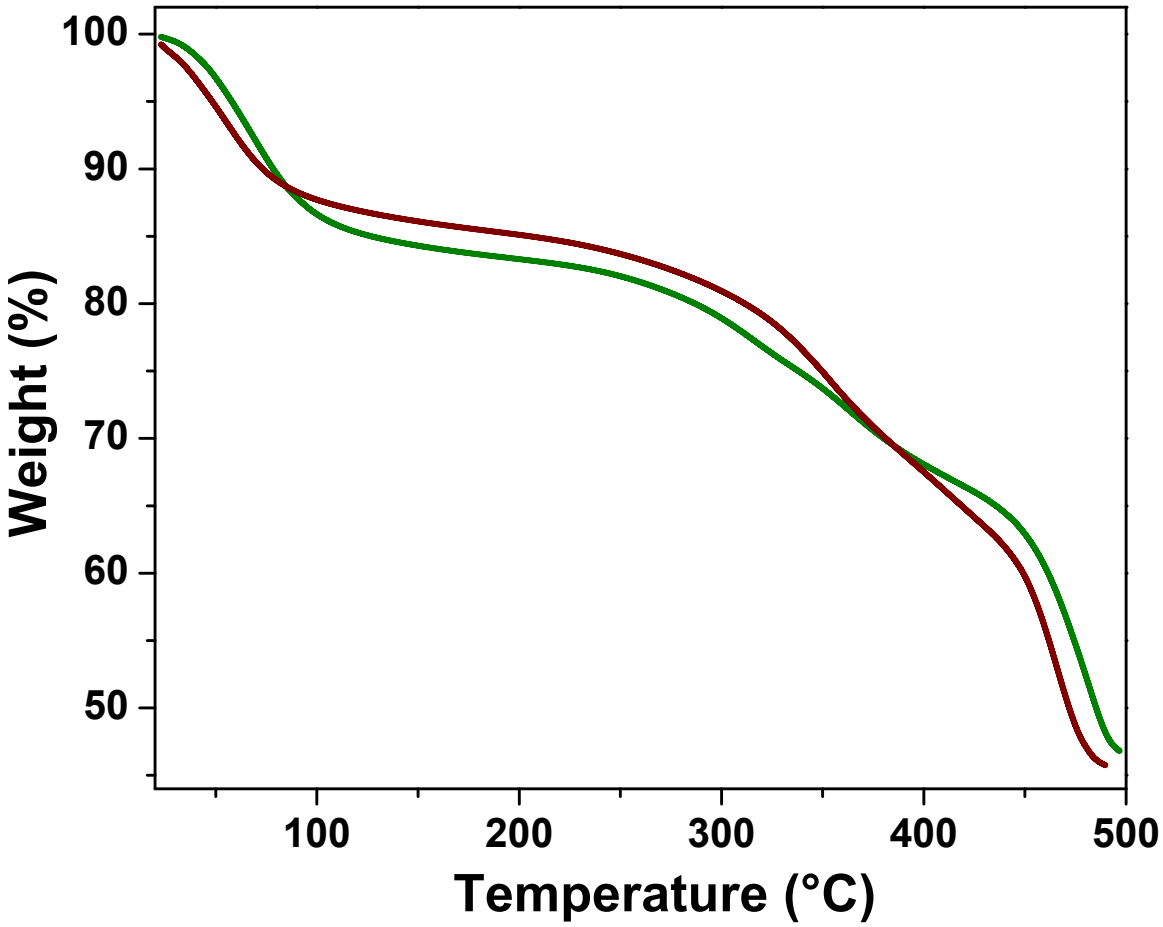


Fig. S3 TGA plot of MIL-100(Fe) (olive) and HCT@MIL-100(Fe) (wine).

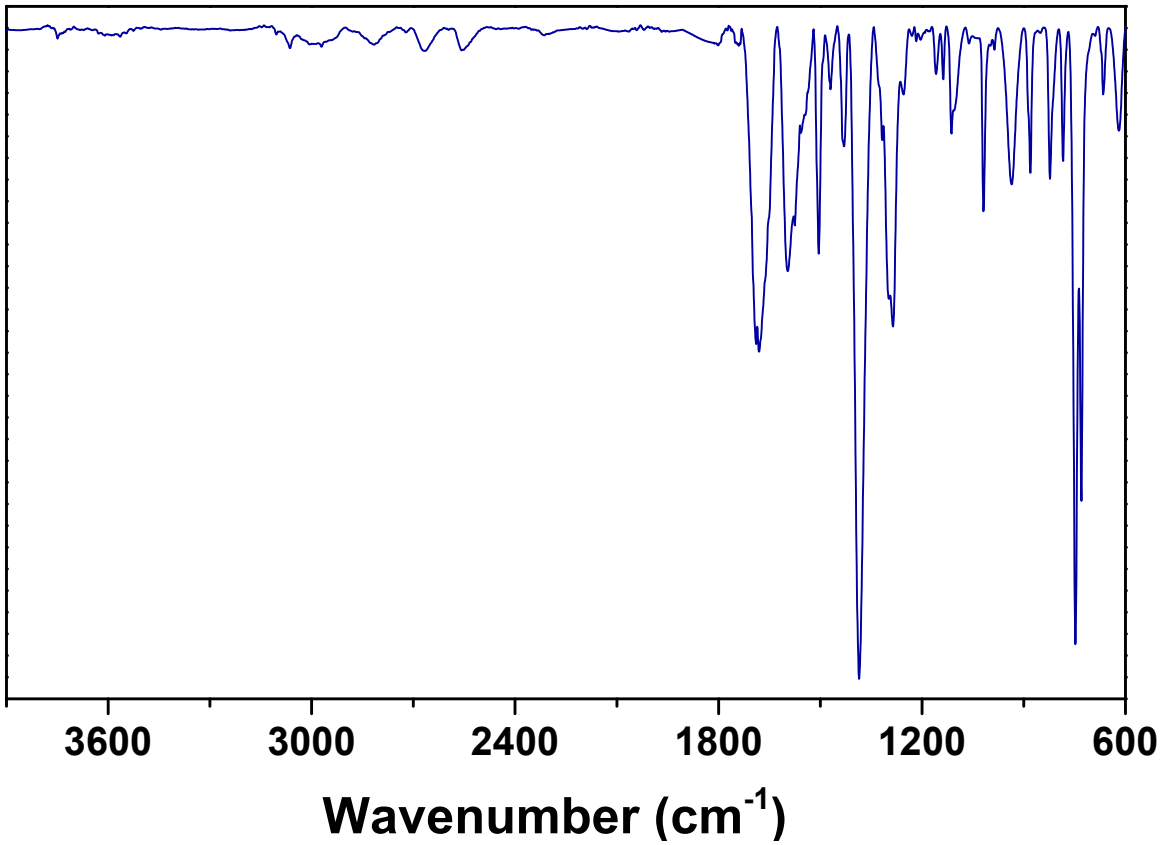


Fig. S4 FTIR spectrum of MIL-53(Fe).

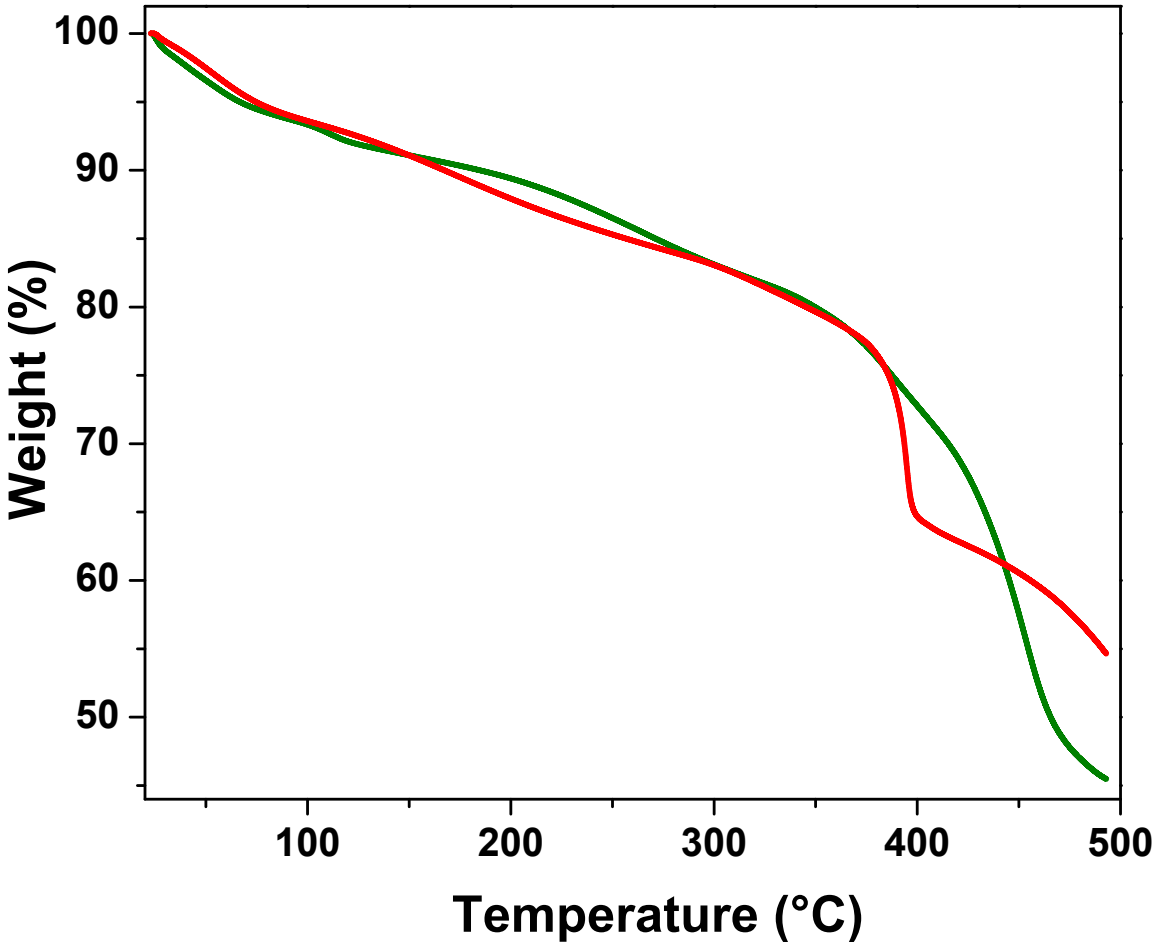


Fig. S5 TGA plot of MIL-53(Fe) (green) and DAP@MIL-53(Fe) (red).

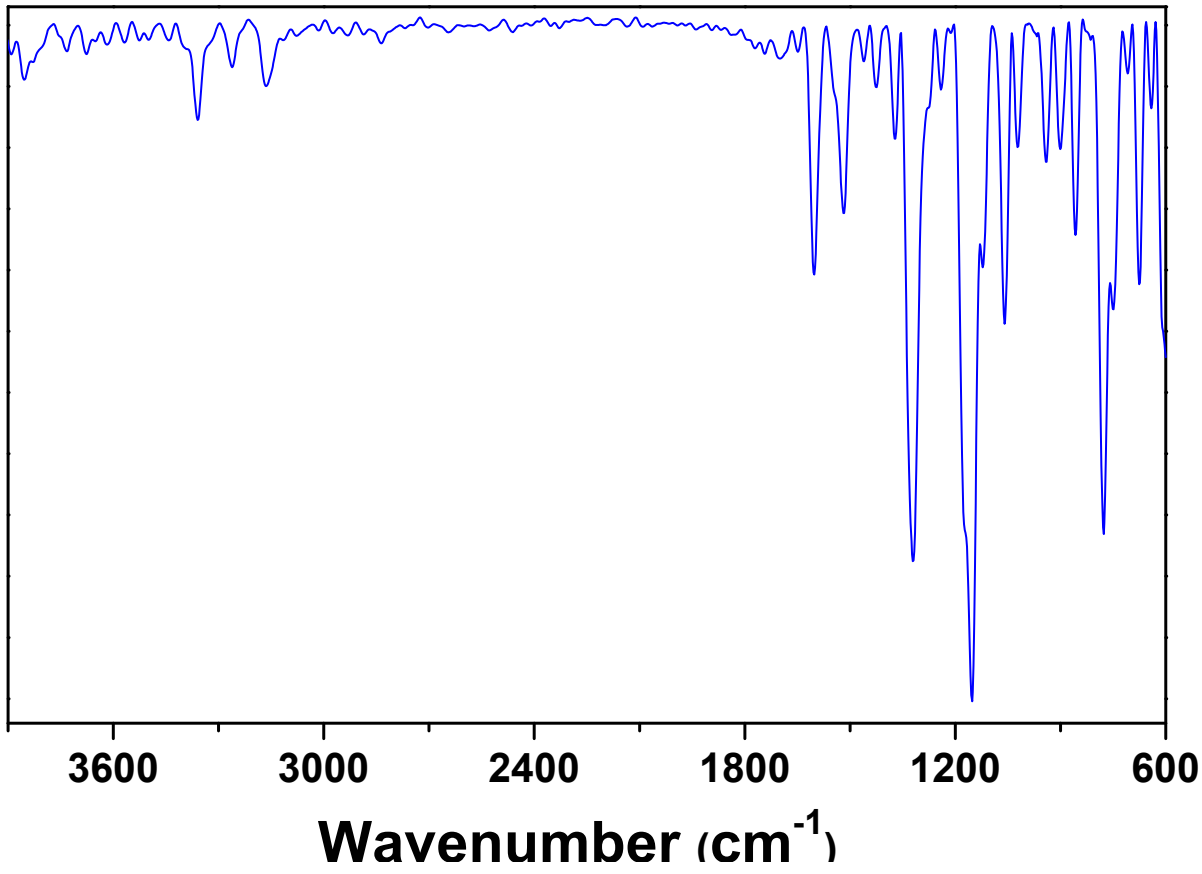


Fig. S6 FTIR spectrum of Hydrochlorothiazide (HCT).

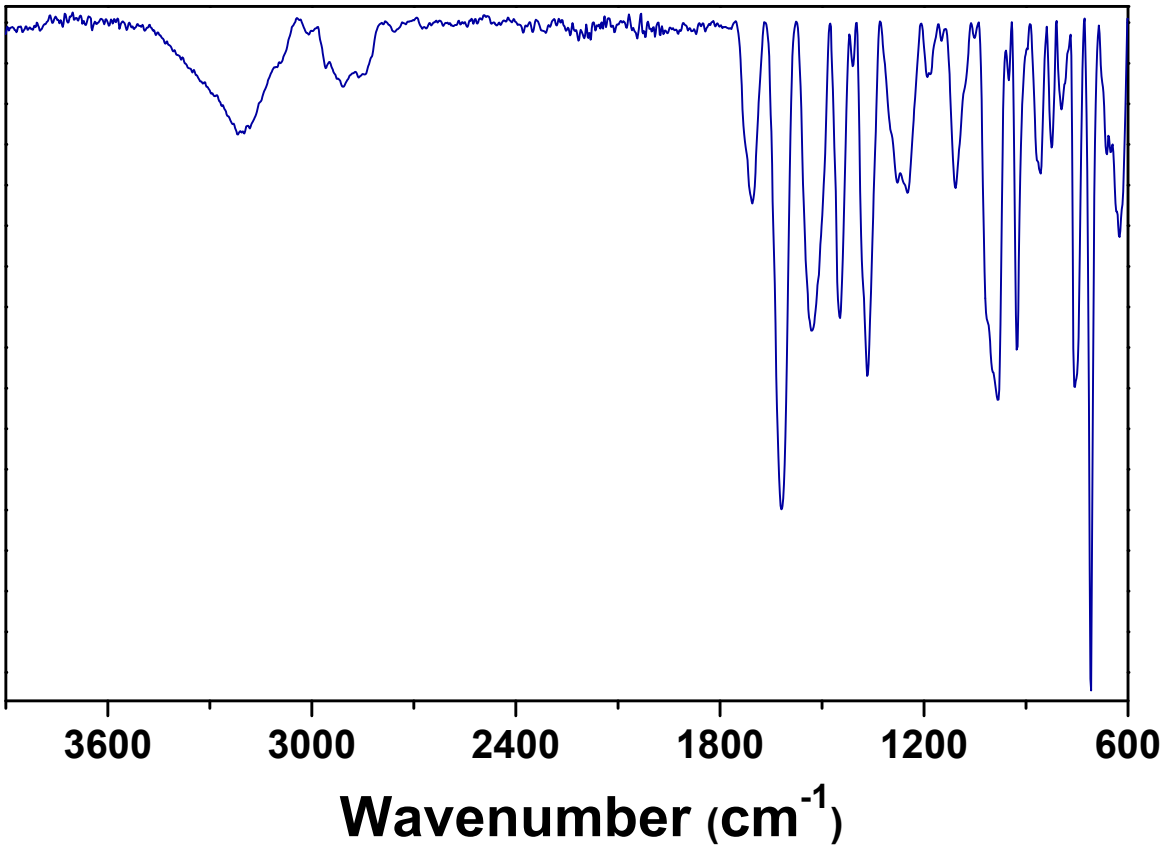


Fig. S7 FTIR spectrum of HCT@MIL-100(Fe).

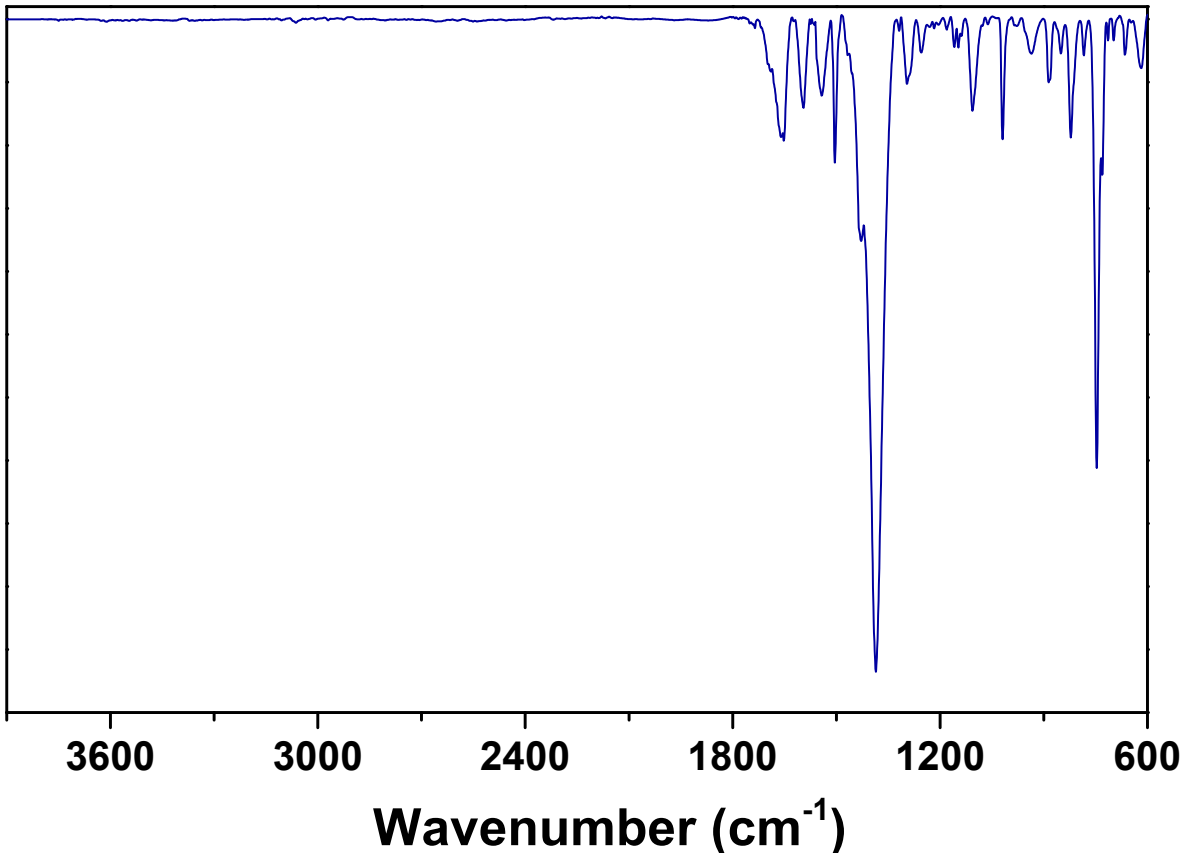


Fig. S8 FTIR spectrum of DAP@MIL-53(Fe).

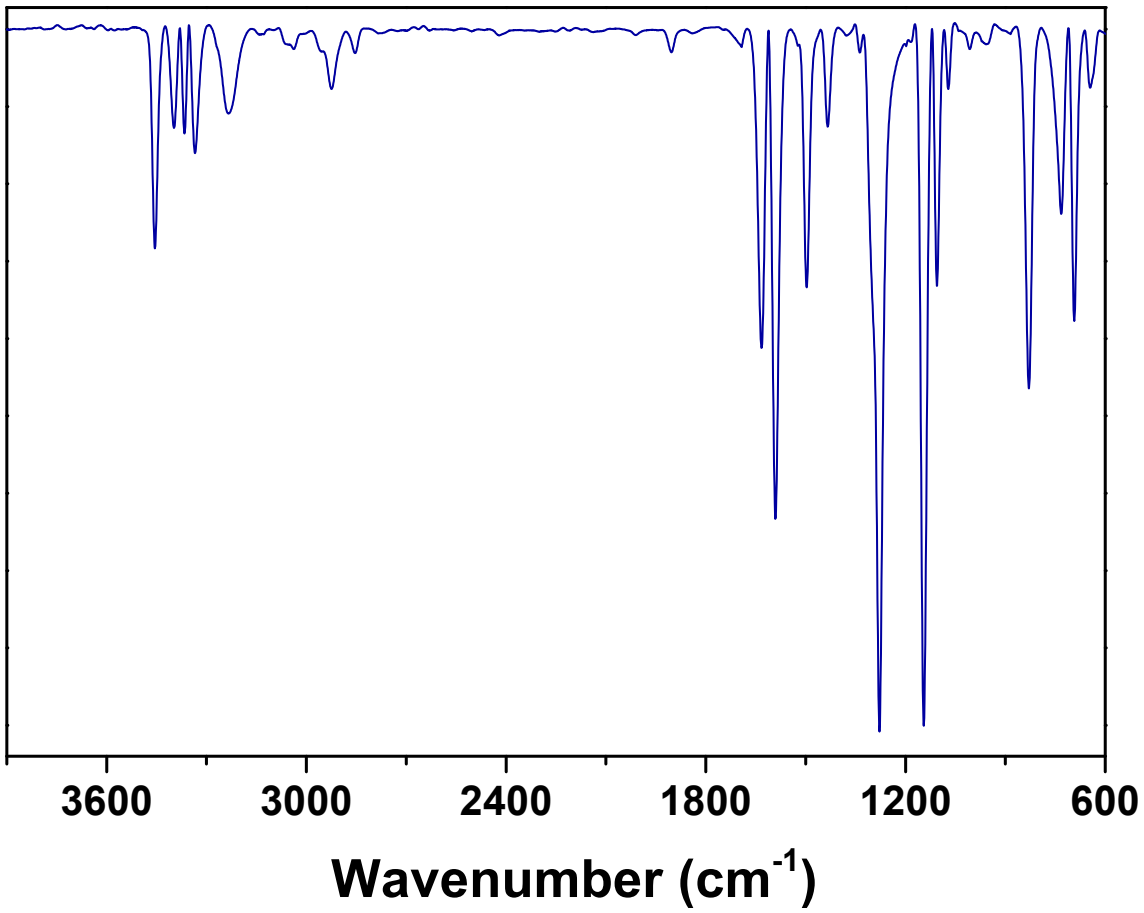


Fig. S9 FTIR spectrum of Dapsone (DAP).

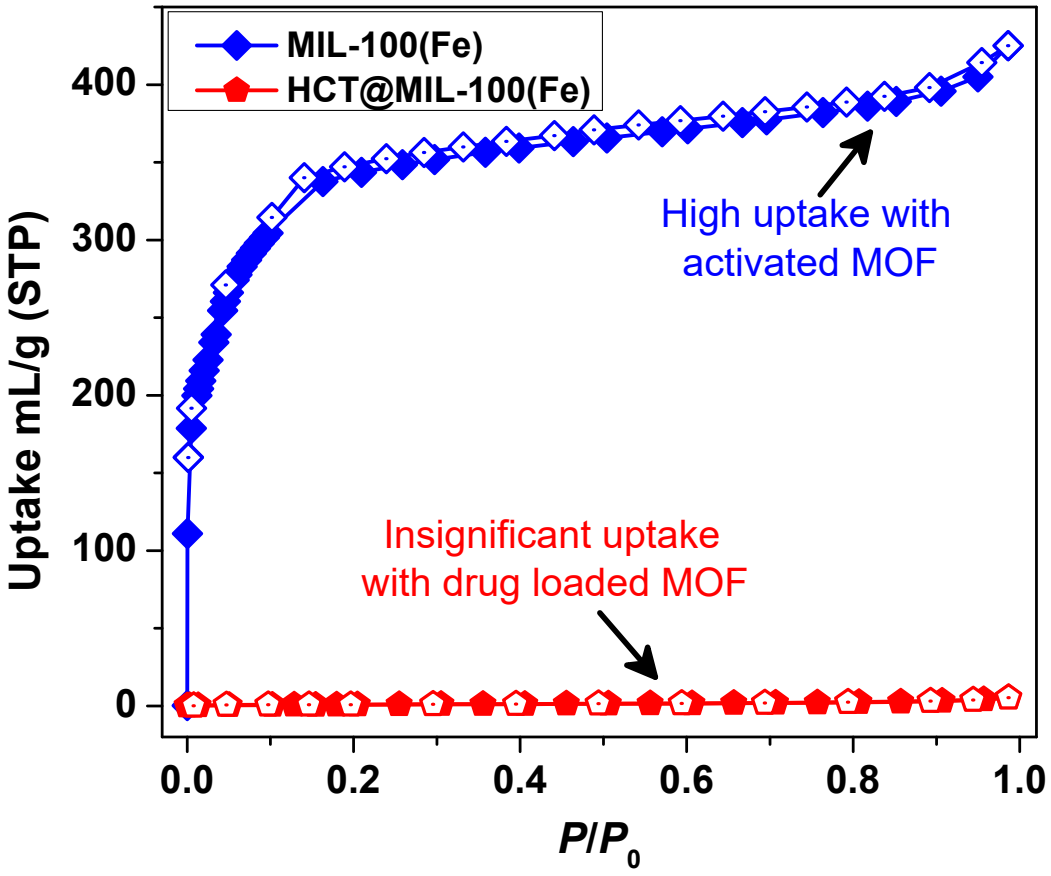


Fig. S10 Nitrogen adsorption isotherms measured at 77 K for MIL-100(Fe) (blue) and HCT@MIL-100(Fe) (red). Adsorption curve is represented with closed symbols and desorption by open symbols. P_0 is the saturated vapor pressure of nitrogen at the measurement temperatures.

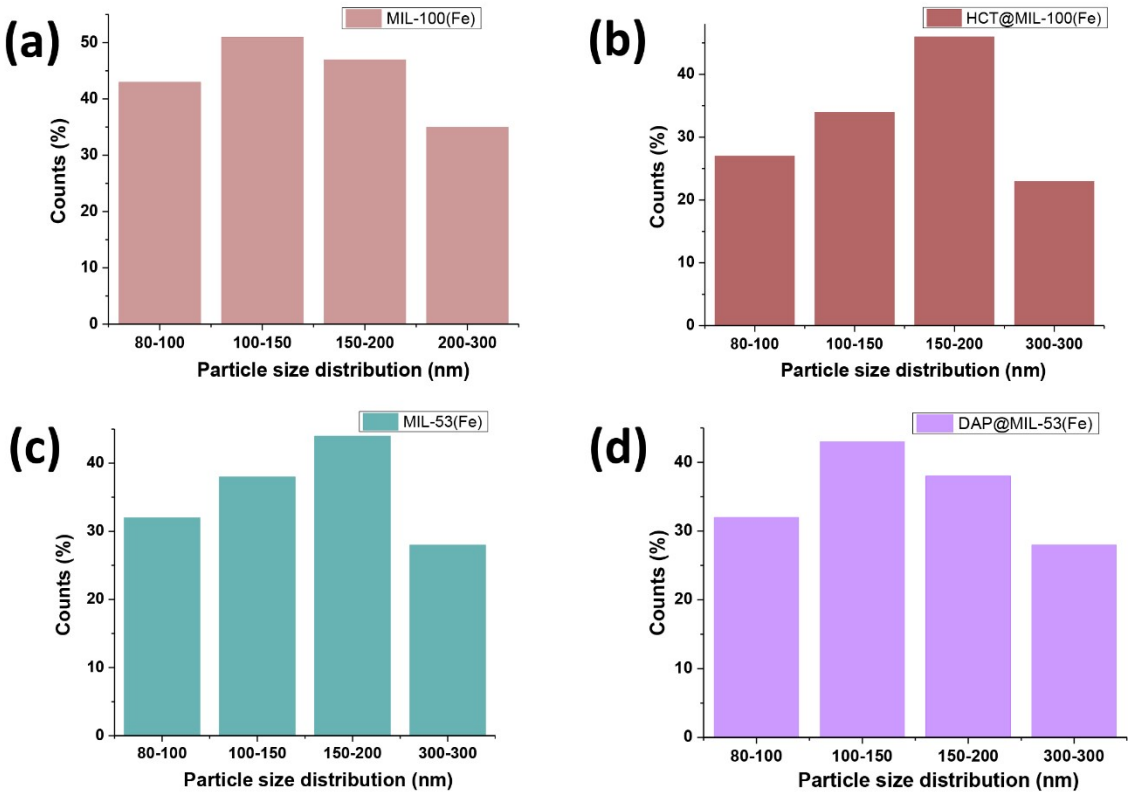


Fig. S11 Histogram of particle size distribution of (a) MIL-100(Fe), (b) HCT@MIL-100(Fe), (c) MIL-53(Fe), (d) DAP@MIL-53(Fe).

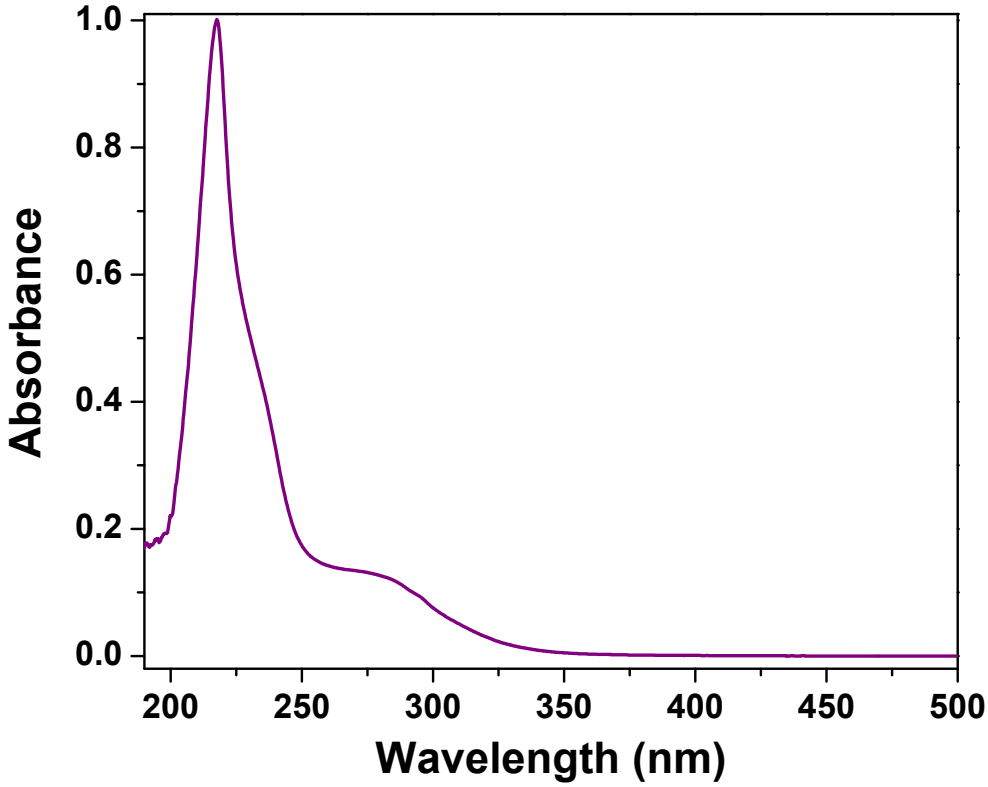


Fig. S12 UV-Vis absorption plot of HCT@MIL-100(Fe) showing the maximum HCT loaded in MIL-100(Fe).

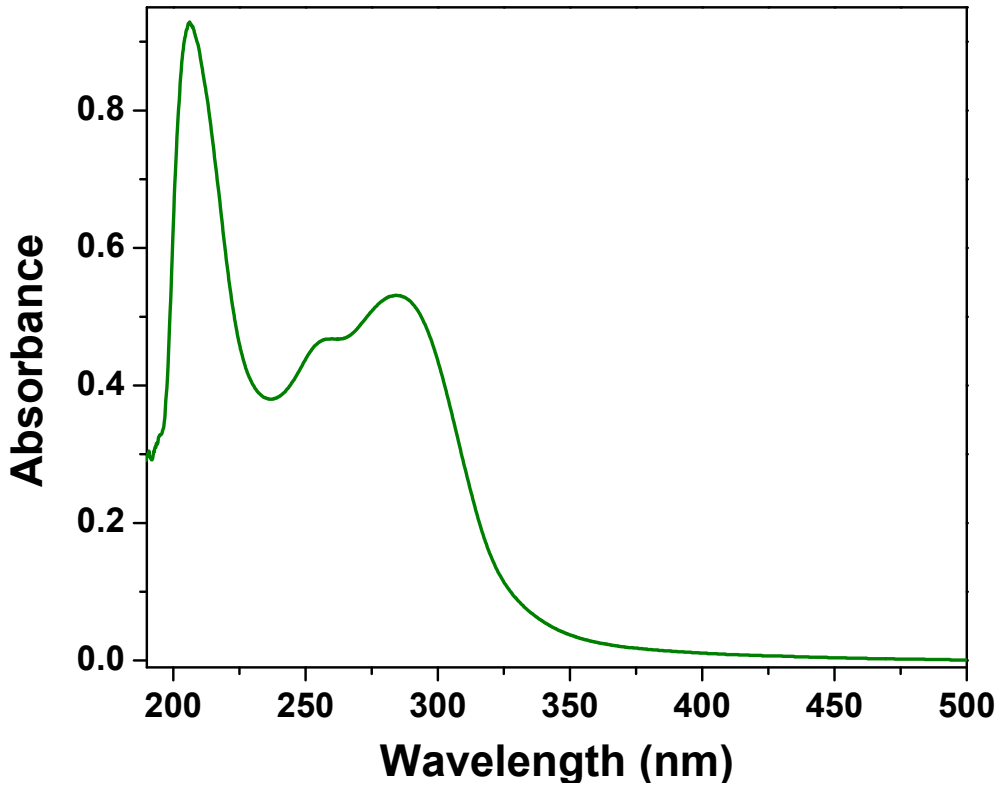


Fig. S13 UV-Vis absorption plot of DAP@MIL-53(Fe) showing the maximum DAP loaded in MIL-53(Fe).

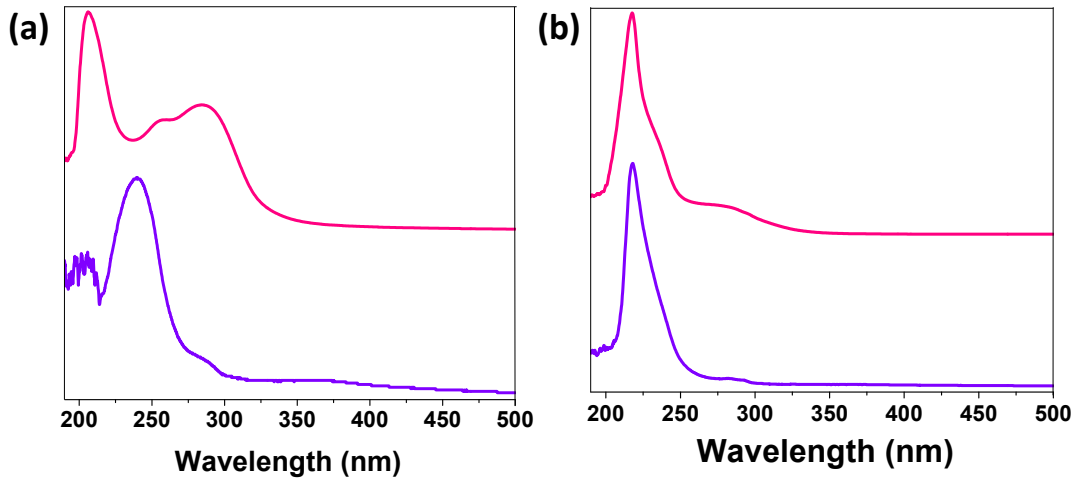


Fig. S14 UV-vis absorbance spectra of (a) 1,4-benzenedicarboxylic acid (purple), DAP@MIL-53(Fe) (pink), and (b) 1,3,5-benzenetricarboxylic acid (purple), HCT@MIL-100(Fe) (pink).

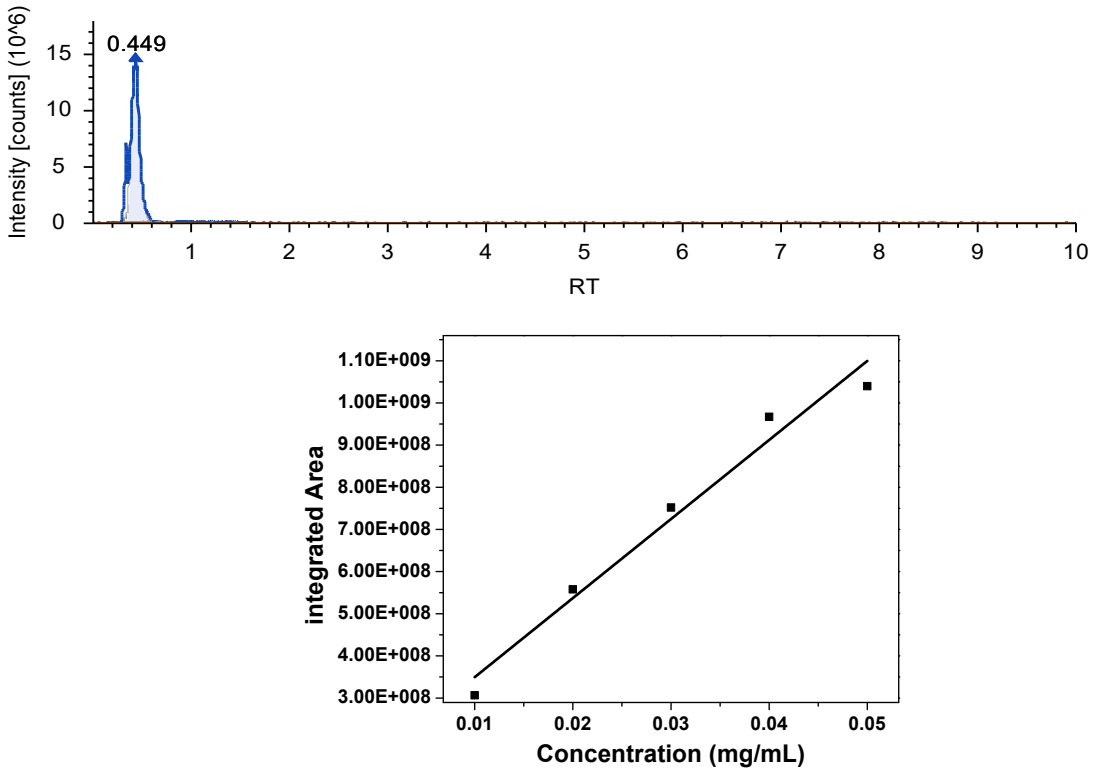


Fig. S15 Calibration curve and chromatograms by LC-MS of hydrochlorothiazide.

The analyte is determined using a thermoscientific Q Exactive Plus and UHPLC+ focused instrument. C-18 reverse-phase column (1.7 µm, 2.1 x 50 mm) was used. The mobile phase consisted of 50% solution (v/v) of acetonitrile (ACN) and H_2O. The injection volume was set at 1 ppm with a flow rate of 0.3 mL min-1 and the column temperature was fixed at 37 ℃. Several ACN solution of hydrochlorothiazide were taken as standard. The standard calibration curve showed a decent correlation coefficient ≥ 0.986. The chromatogram of standard solutions showed a retention time of 0.449 min. Upon calculation it has shown that 236 mg (23.6 %) of hydrochlorothiazide has been encapsulated per gram of MIL-100(Fe) which is very much similar to the results obtained by UV-vis spectroscopy. In case of DAP encapsulated MOF, these is no peak at 286 nm in spectra of terephthalic acid, therefore we concluded that BDC does not interfere with the quantification of dapsone encapsulated in MIL-53(Fe).

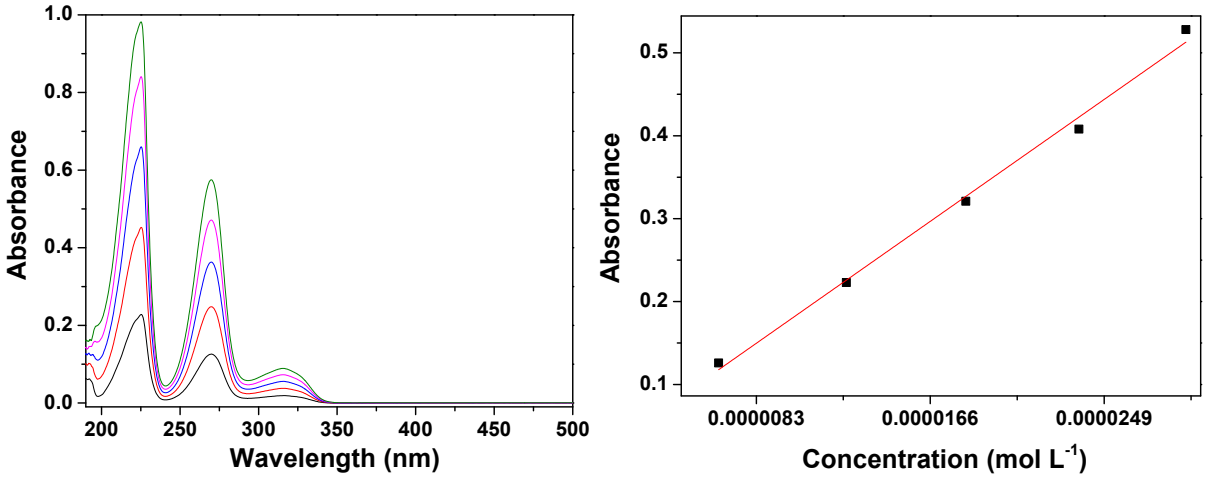


Fig. S16 UV-Vis absorption plot and calibration curve for epsilon calculation of hydrochlorothiazide.

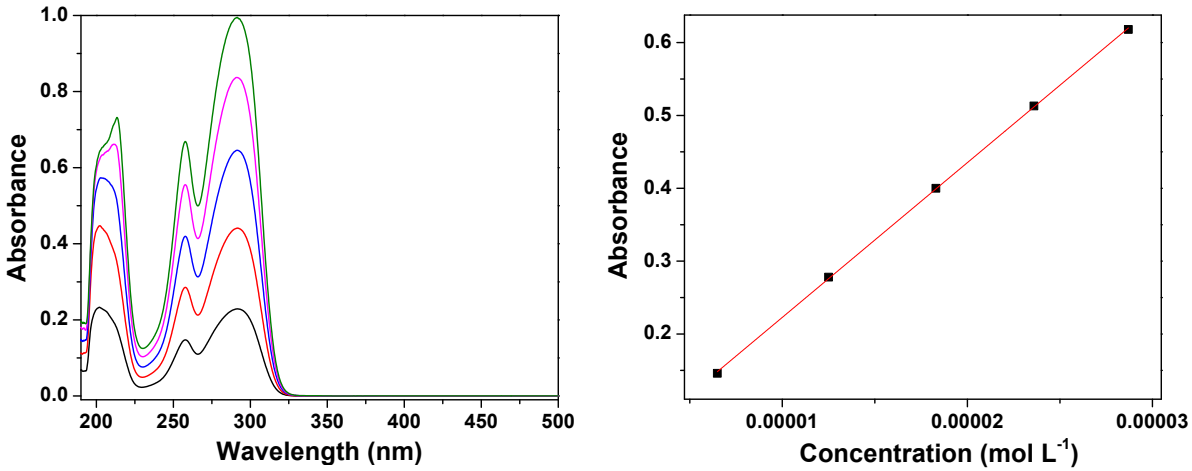


Fig. S17 UV-Vis absorption plot and calibration curve for epsilon calculation of dapsone.

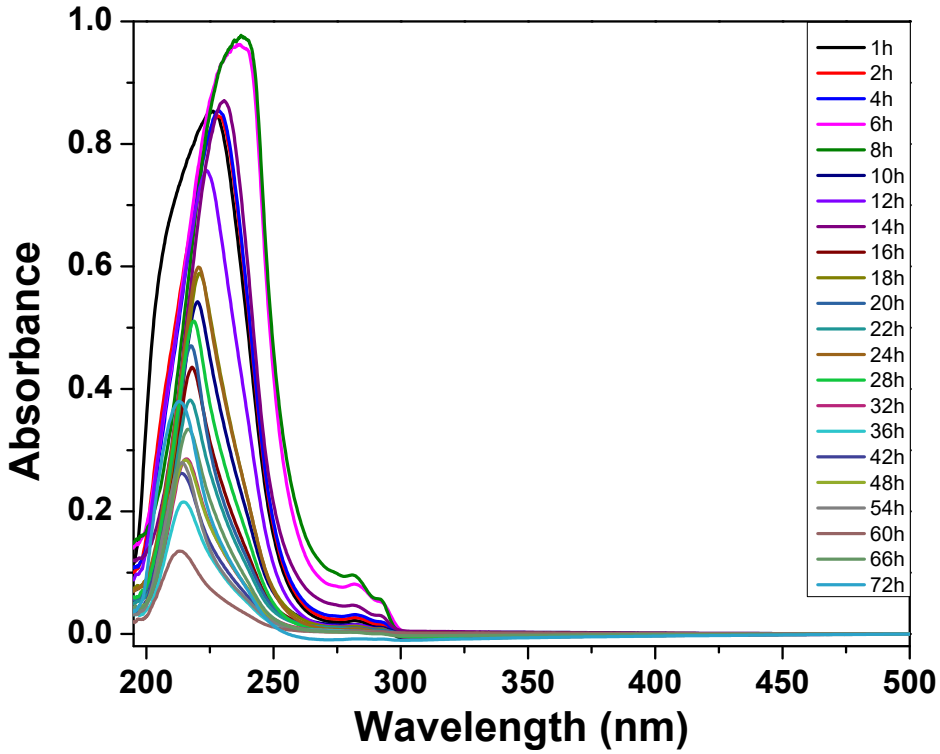


Fig. S18 UV-Vis absorbance plot of HCT release from HCT@MIL-100(Fe) for a time period of 72 hours.

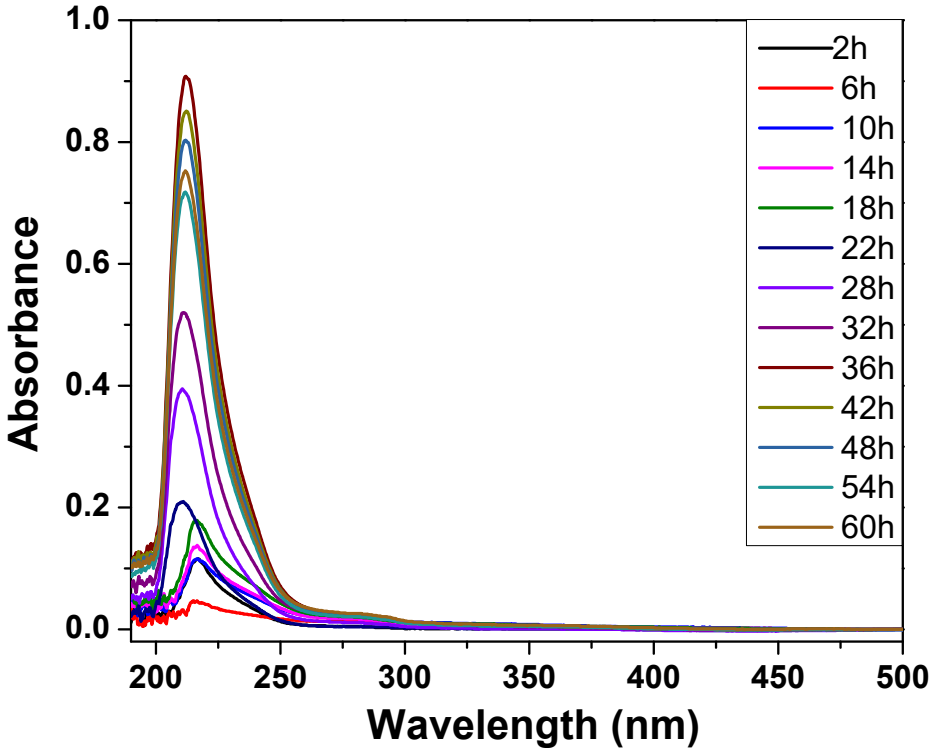


Fig. S19 UV-vis spectra of MIL-100(Fe) release in phosphate buffer of pH 7.4.

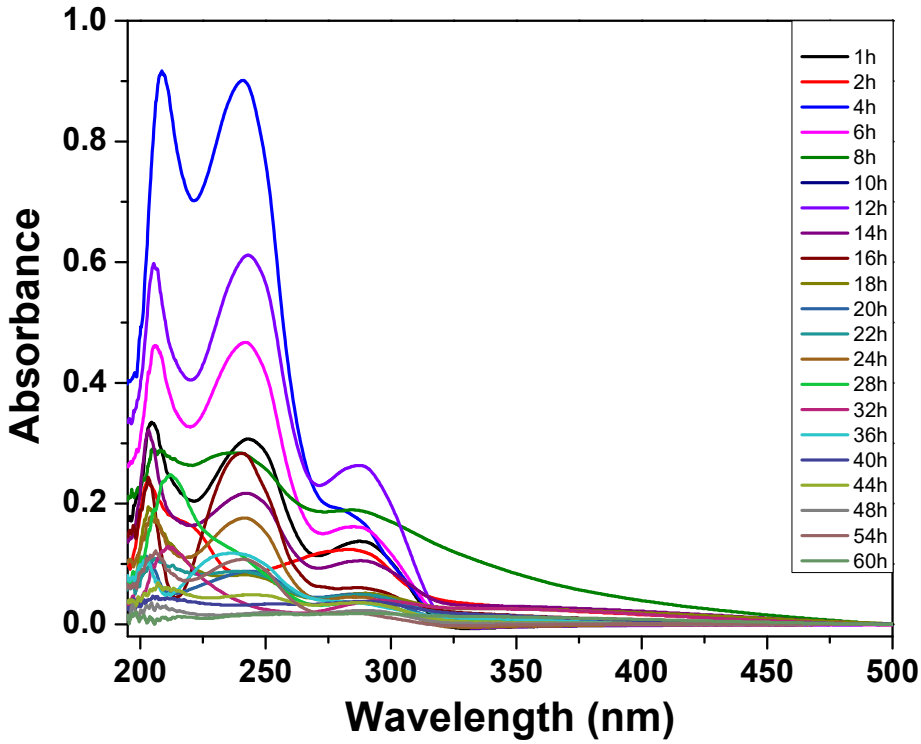


Fig. S20 UV-Vis absorbance plot of DAP release from DAP@MIL-53(Fe) for a time period of 72 hours.

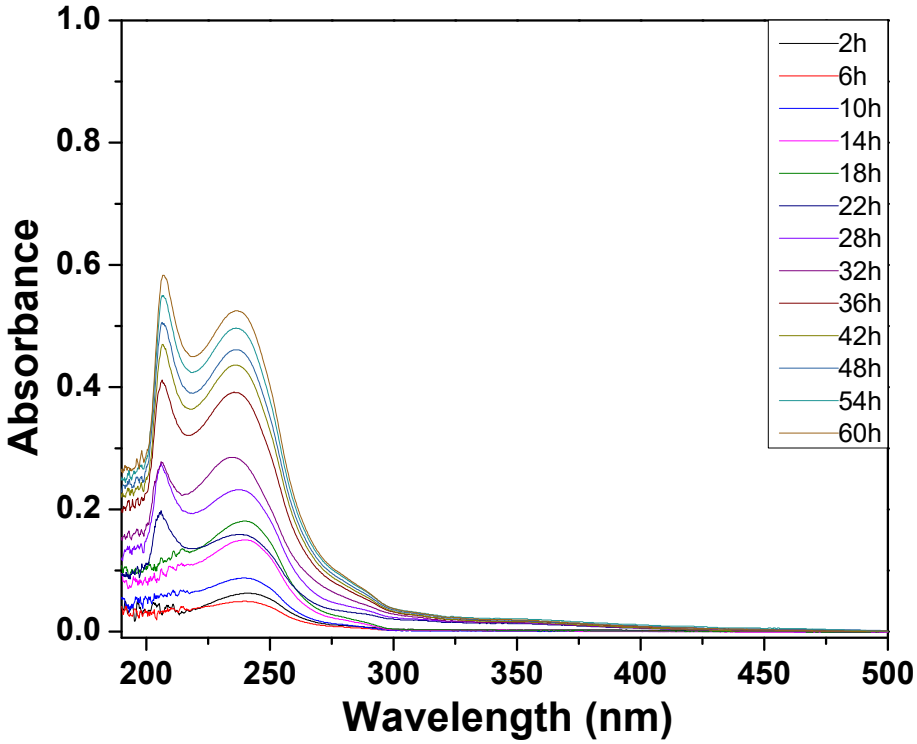
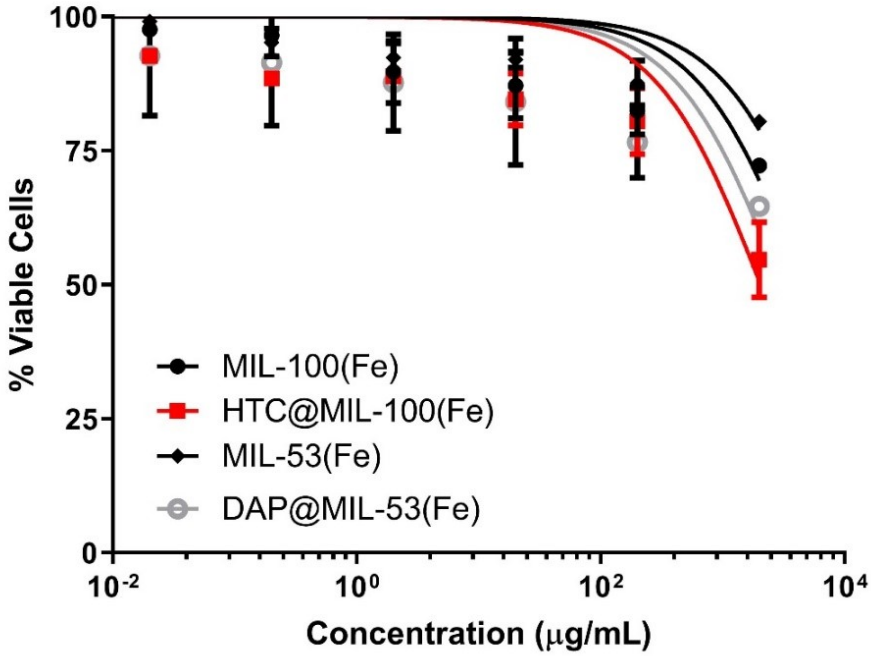


Fig. S21 UV-vis spectra of MIL-53(Fe) release in phosphate buffer of pH 7.4.



Samples	MIL-100(Fe)	HCT@MIL-100(Fe)	MIL-53(Fe)	DAP@MIL-53(Fe)
IC50	4539	2051	7436	2995

Fig. S22 IC50 values of the test compounds treated to A549 cells.

References

1. P. l. D. et o. Dideberg, *Acta Cryst.*, 1972, **B28**, 2340.

2. D. E. Braun, H. Krüger, V. Kahlenberg, U. J. Griesser, *Cryst. Growth Des.*, 2017, **17**, 5054.