

## Functionalization of 3D porous copper(II) Metal-organic framework and its capacity for loading and delivery of Ibuprofen drug

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### Supplementary Information

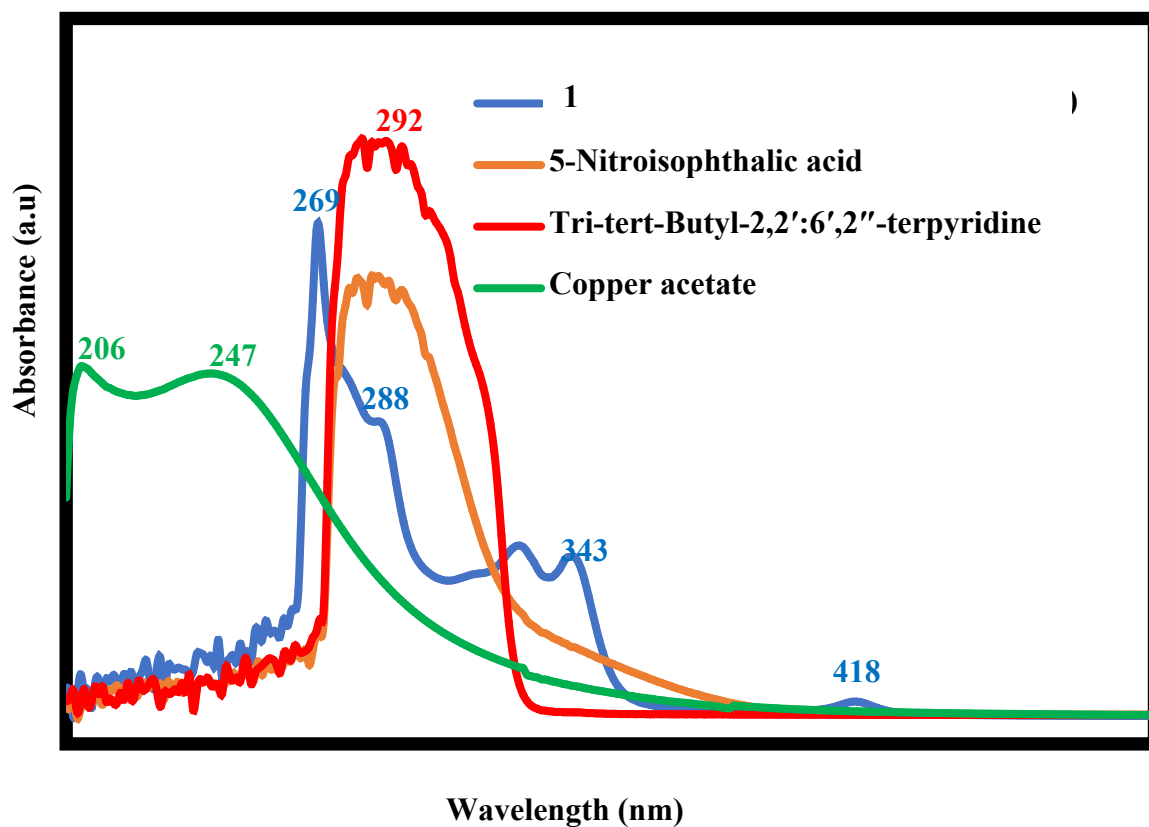


Figure S1: Electronic Spectra of 4,4',4''-Tri-tert-Butyl-2,2':6',2''-terpyridine, 5-Nitroisophthalic acid,  $\text{Cu}(\text{CH}_3\text{COO})_2 \cdot \text{H}_2\text{O}$  and **1**.

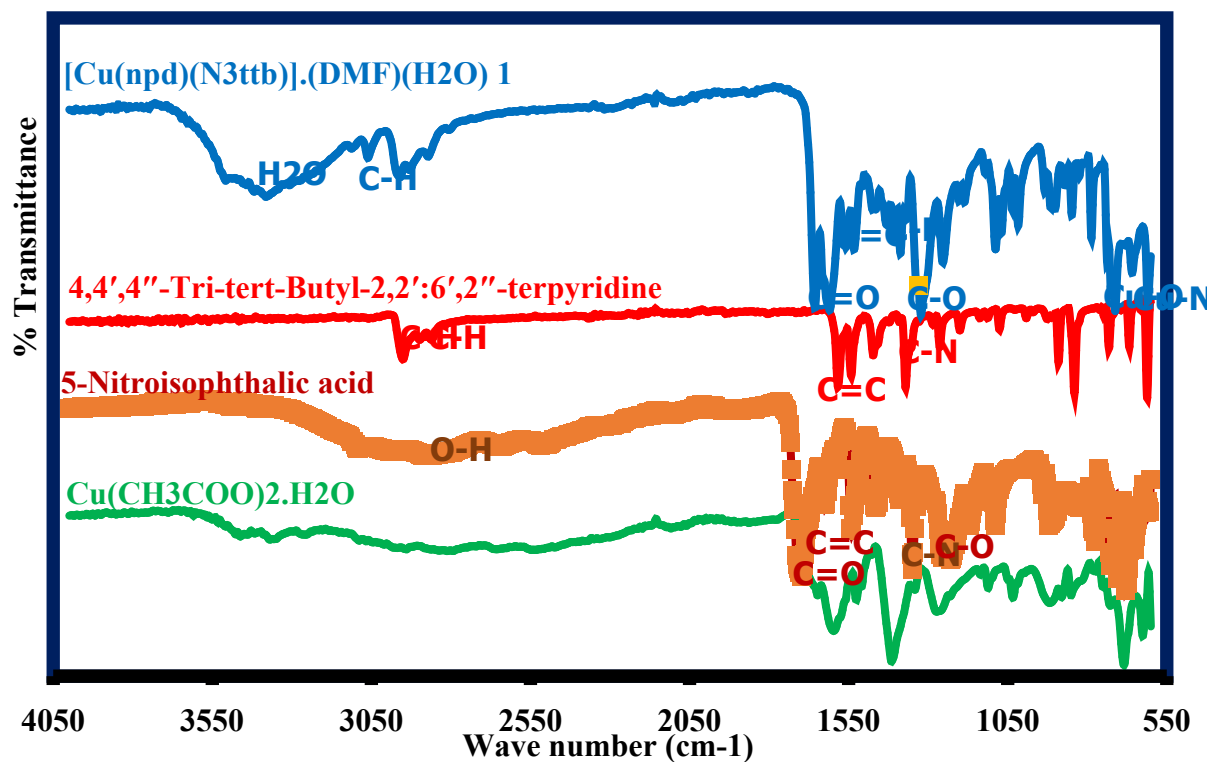


Figure S2: FT-IR spectra of 4,4',4''-Tri-tert-Butyl-2,2':6',2''-terpyridine, 5-Nitroisophthalic acid, Cu(CH<sub>3</sub>COO)<sub>2</sub>.H<sub>2</sub>O and 1.

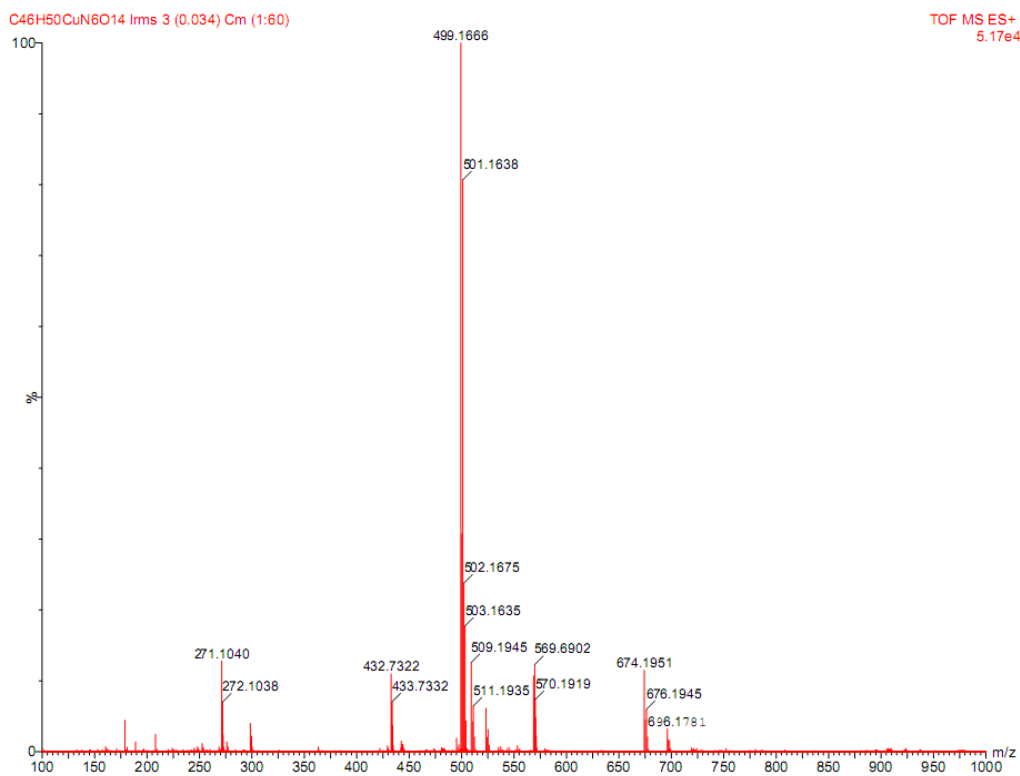


Figure S3: Mass spectra of 1.

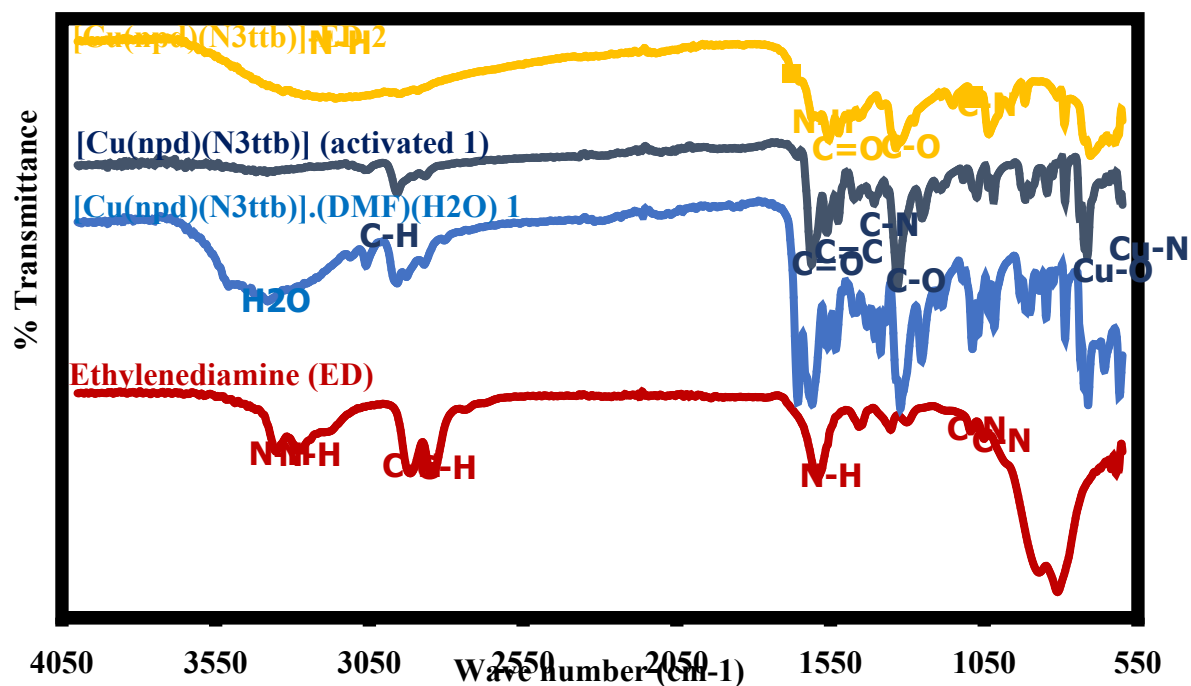


Figure S4: Comparison of the FT-IR spectra of ethylenediamine, as-synthesized, activated, and functionalized MOFs

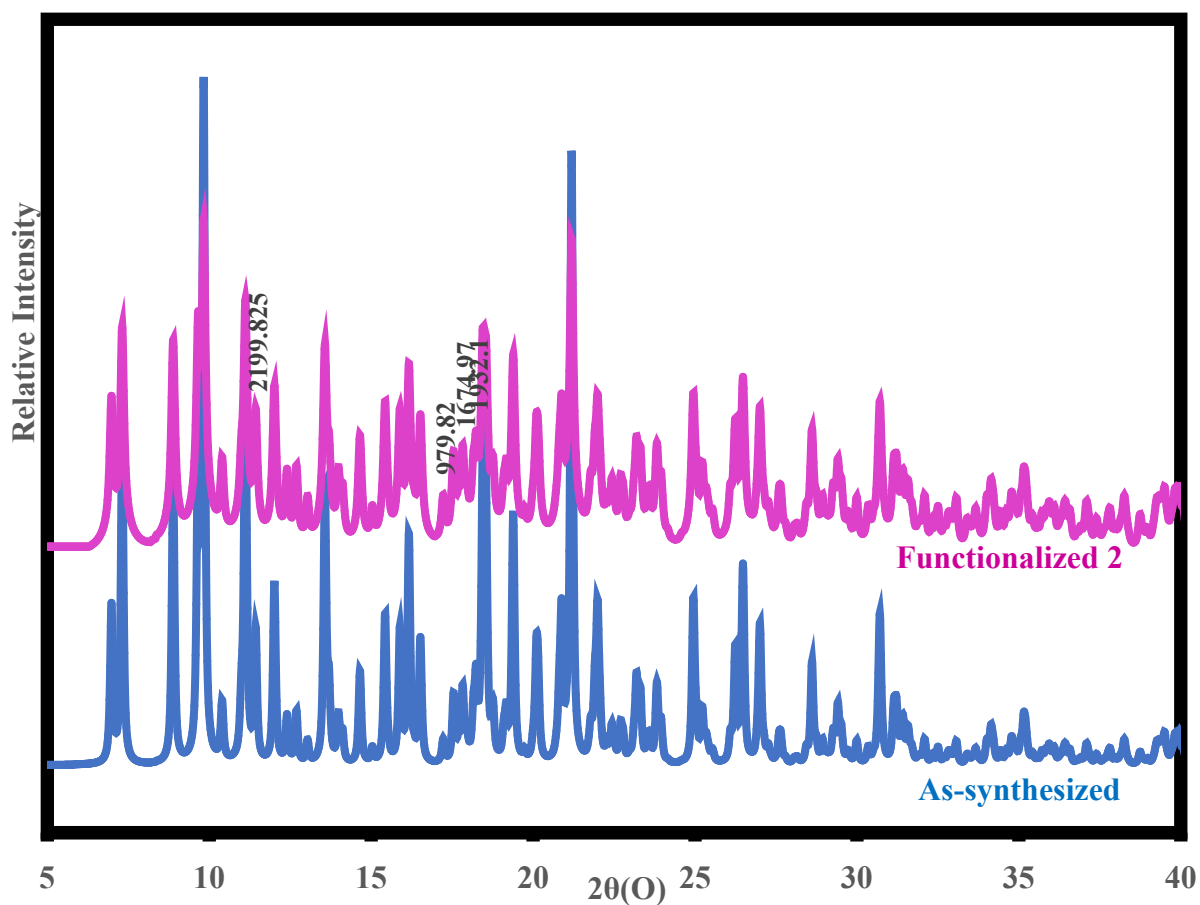


Figure S5: Comparison of the PXRD spectra of as-synthesized 1 and functionalized MOFs 2

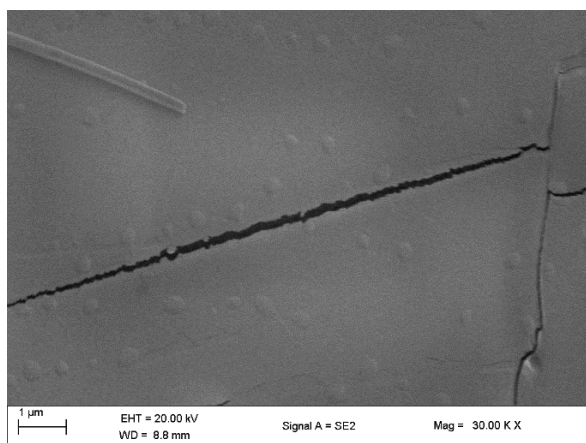
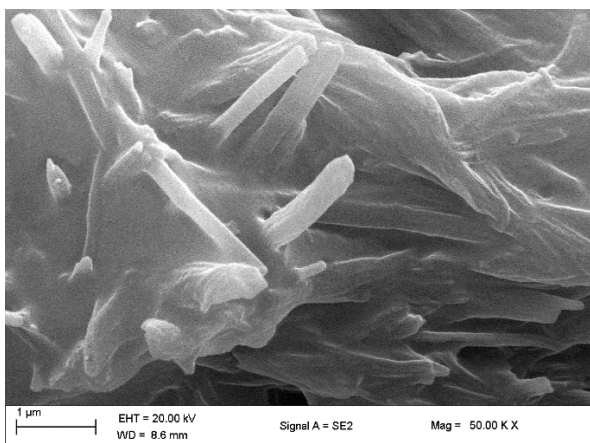


Figure S6: SEM images of **1** at different magnification

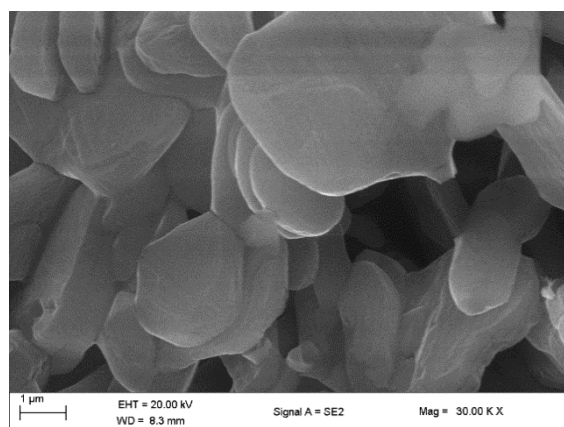
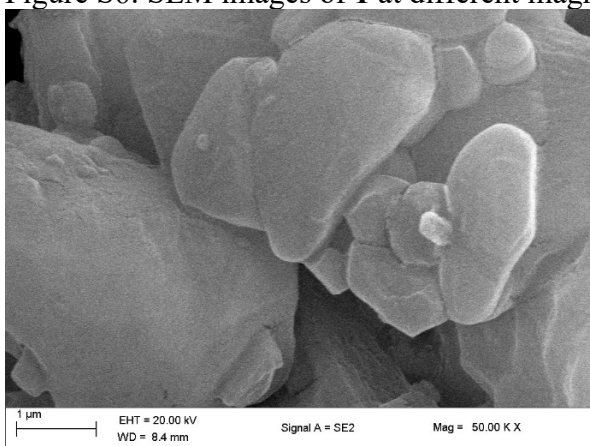


Figure S7: SEM images of **2** at different magnification

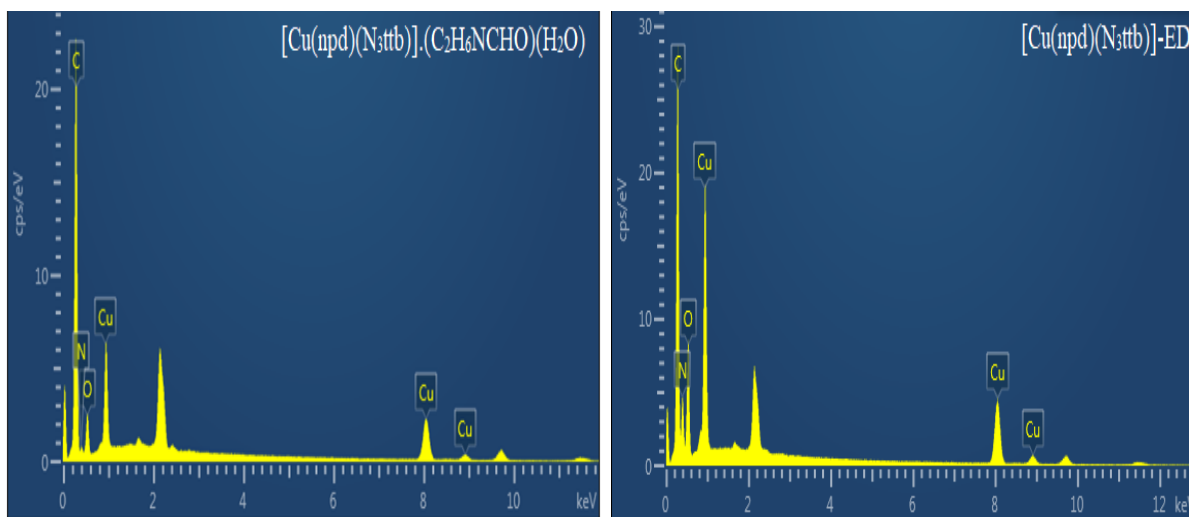


Figure S8: EDX Spectra of **1** and **2**

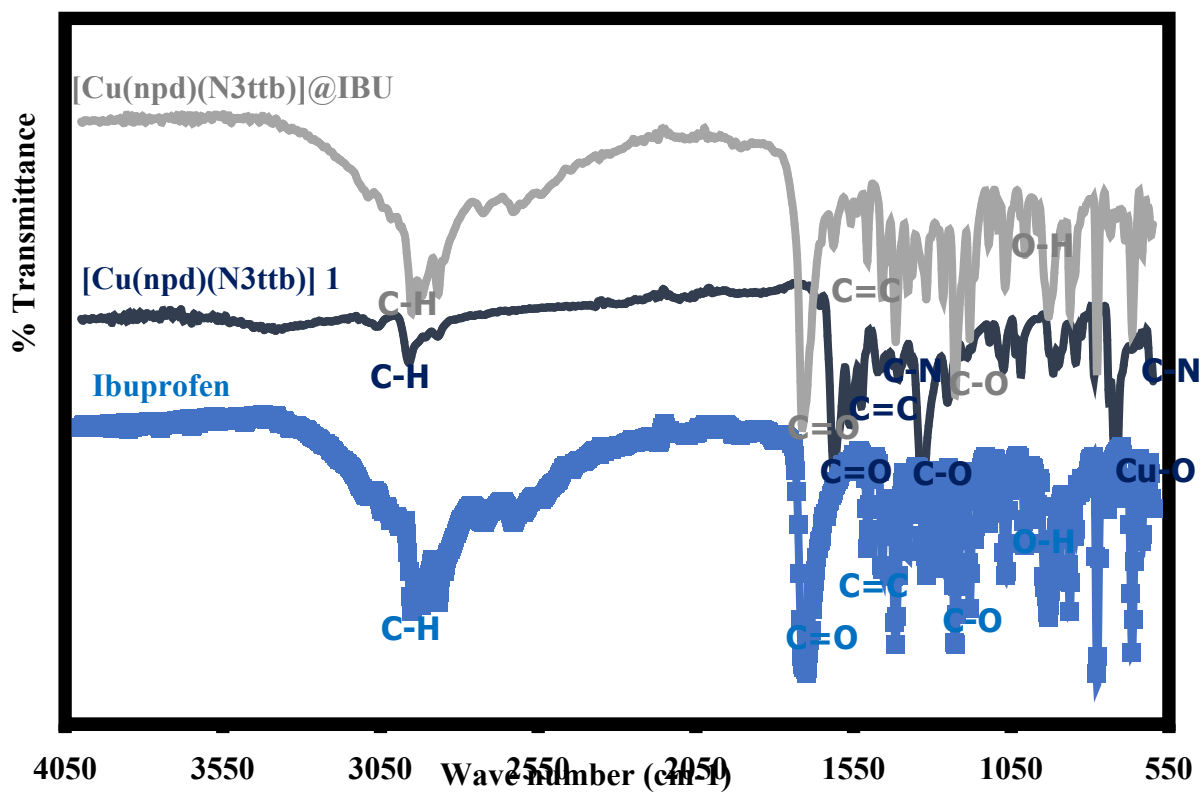


Figure S9: Infrared spectra of **1** before and after loading of Ibuprofen.

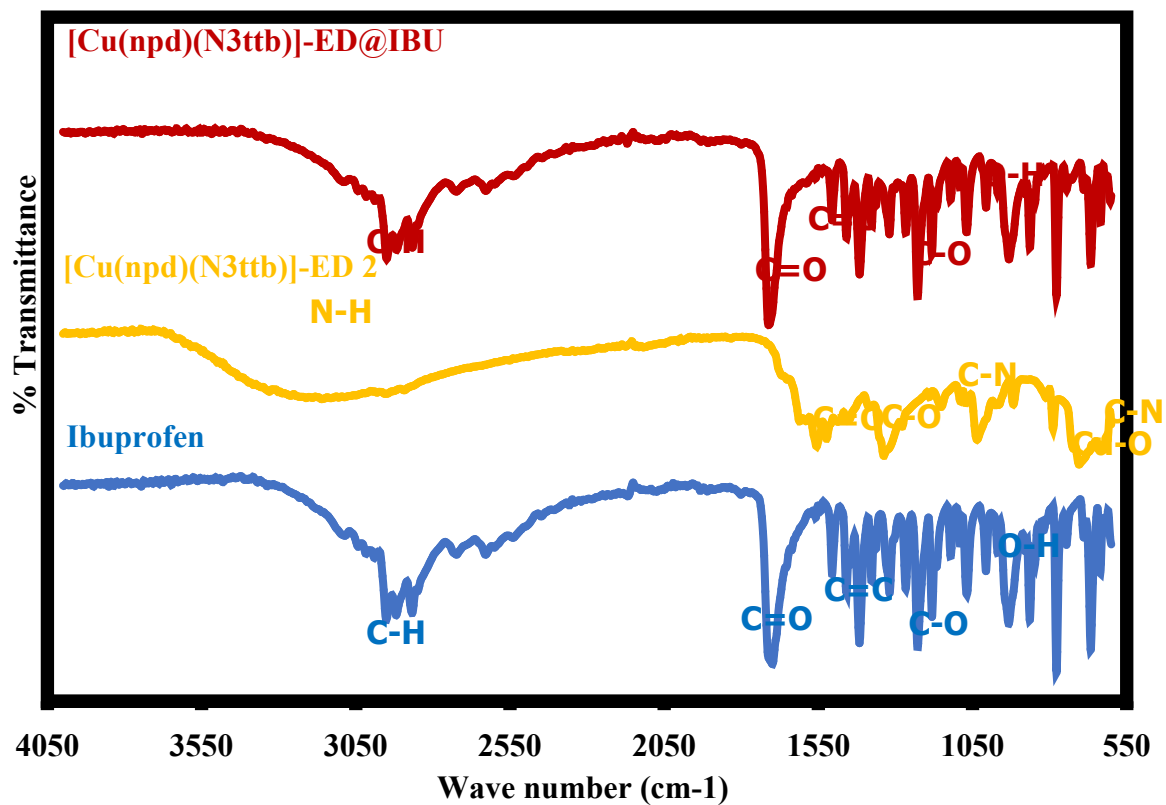


Figure S10: Infrared spectra of **2** before and after loading of Ibuprofen.

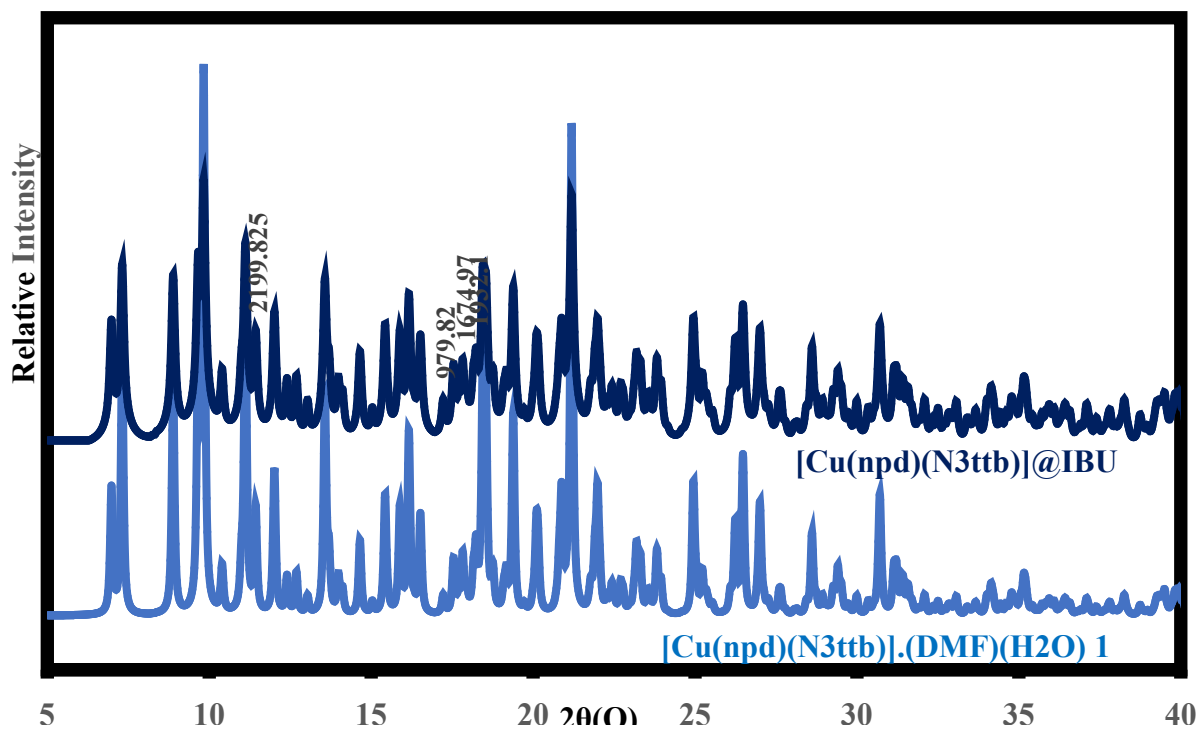


Figure S11: PXRD spectra of **1** before and after loading of Ibuprofen.

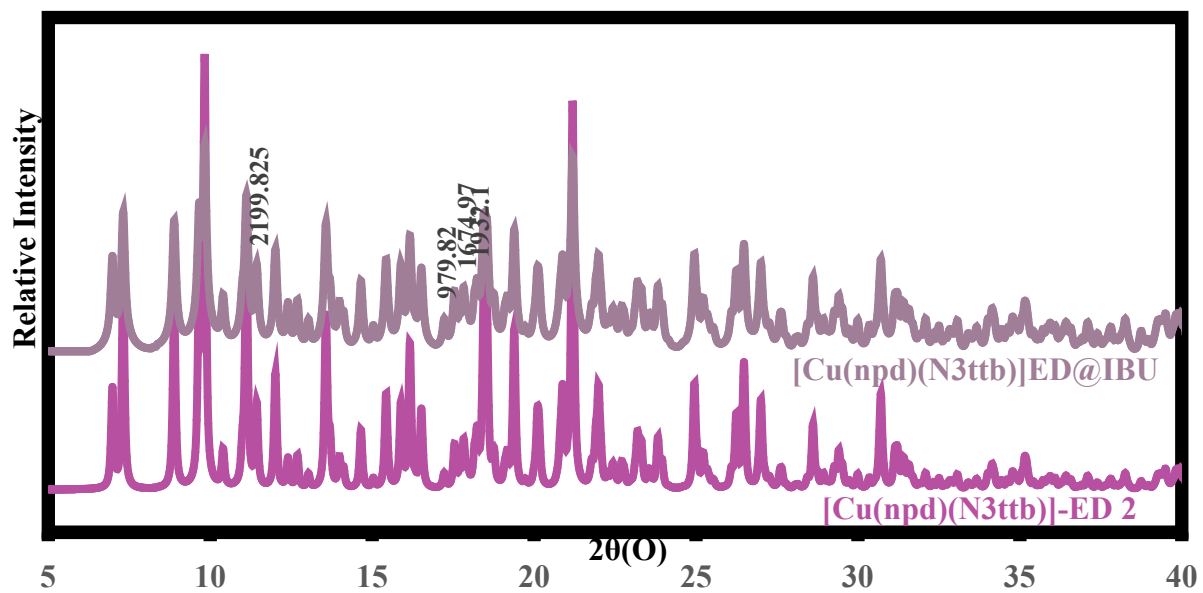
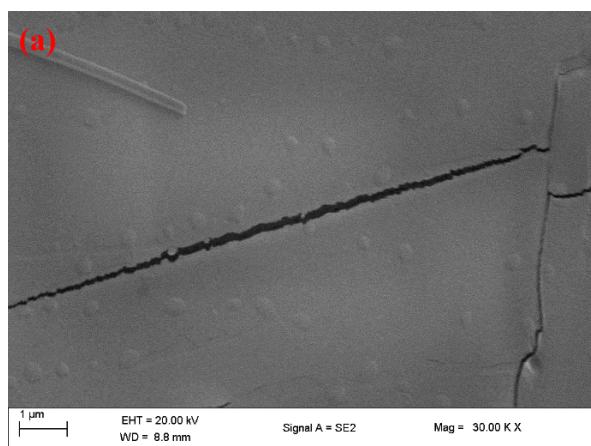
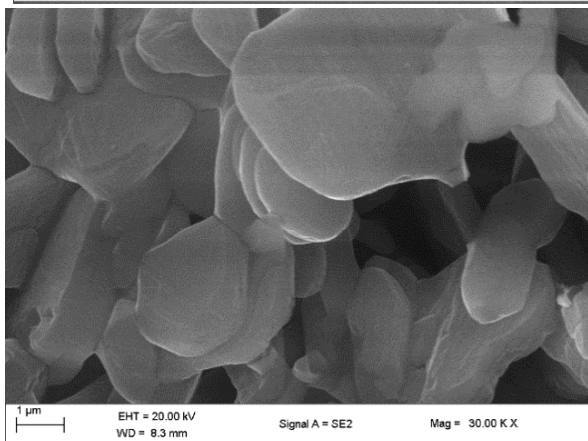


Figure S12: PXRD spectra of **2** before and after loading of Ibuprofen.



(b)



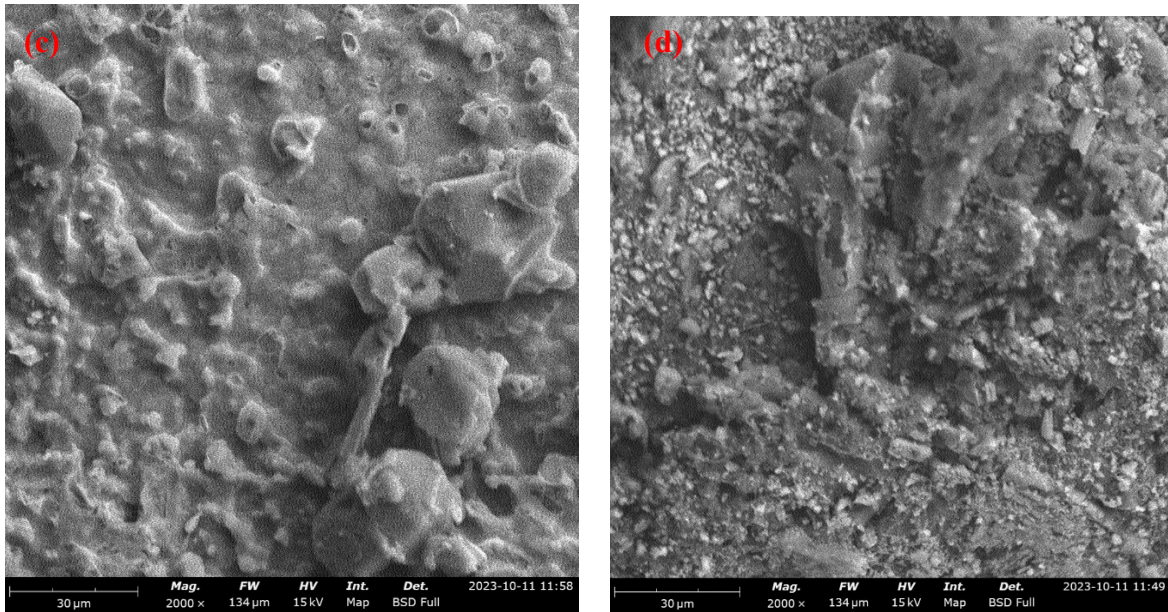


Figure S13: SEM Image of (a)  $[\text{Cu}(\text{npd})(\text{N}_3\text{ttb})].(\text{C}_2\text{H}_6\text{NCHO})(\text{H}_2\text{O})$  (b)  $[\text{Cu}(\text{npd})(\text{N}_3\text{ttb})]\text{-ED}$  (c)  $[\text{Cu}(\text{npd})(\text{N}_3\text{ttb})]\text{@IBU}$  (d)  $[\text{Cu}(\text{npd})(\text{N}_3\text{ttb})]\text{-ED@IBU}$

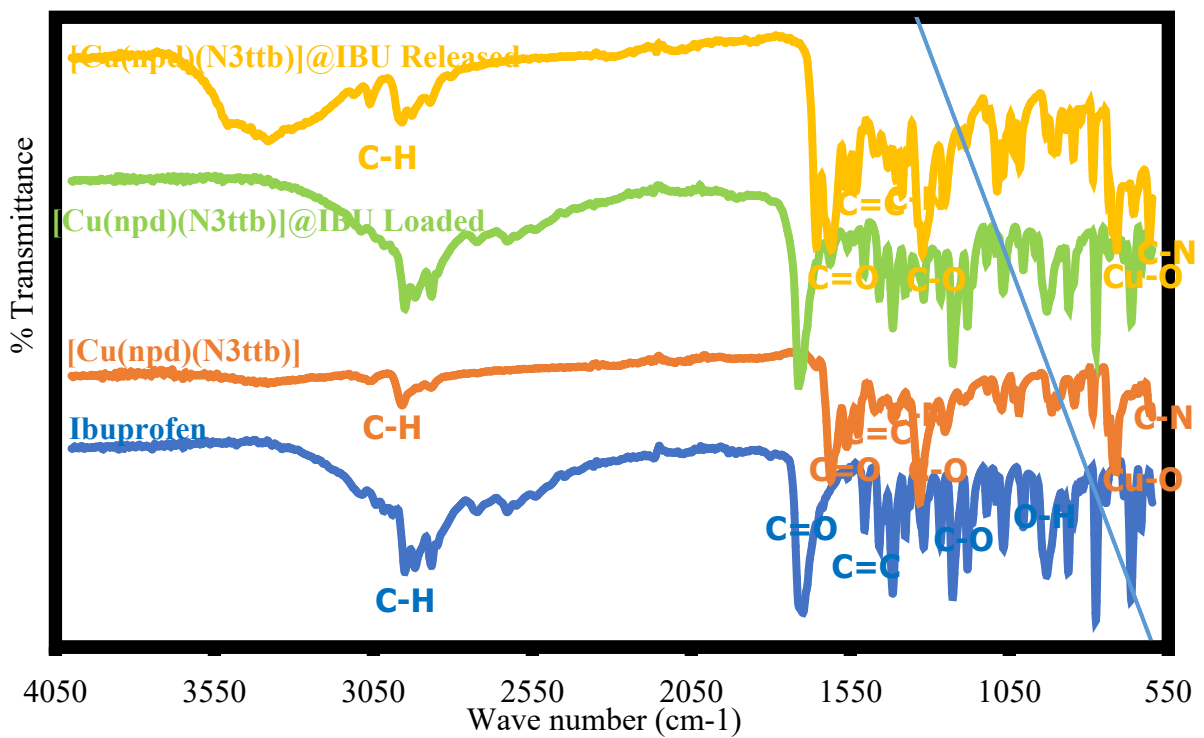


Figure S14: Infrared spectra of  $[\text{Cu}(\text{npd})(\text{N}_3\text{ttb})]\text{@IBU}$  (Loading and released)



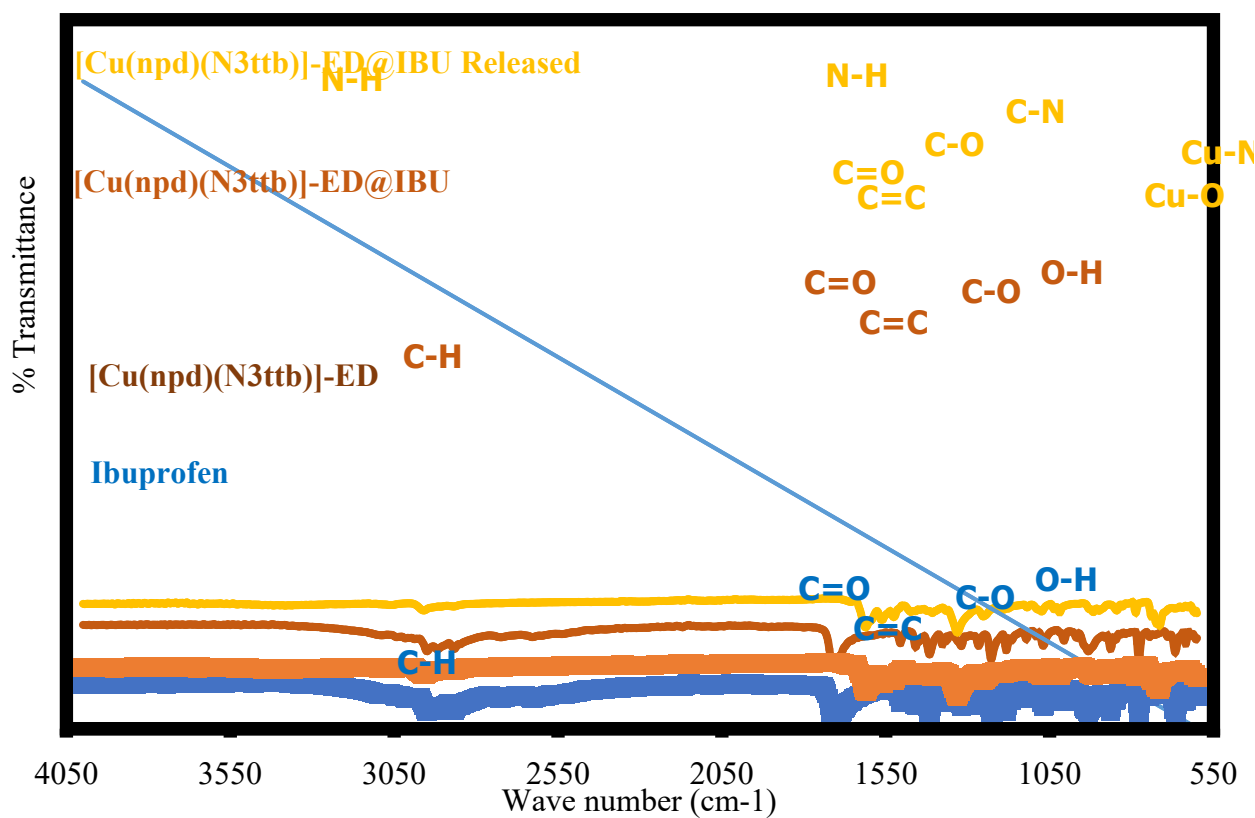


Figure S15: Infrared spectra of [Cu(npd)(N<sub>3</sub>ttb)]-ED@IBU (Loading and released).

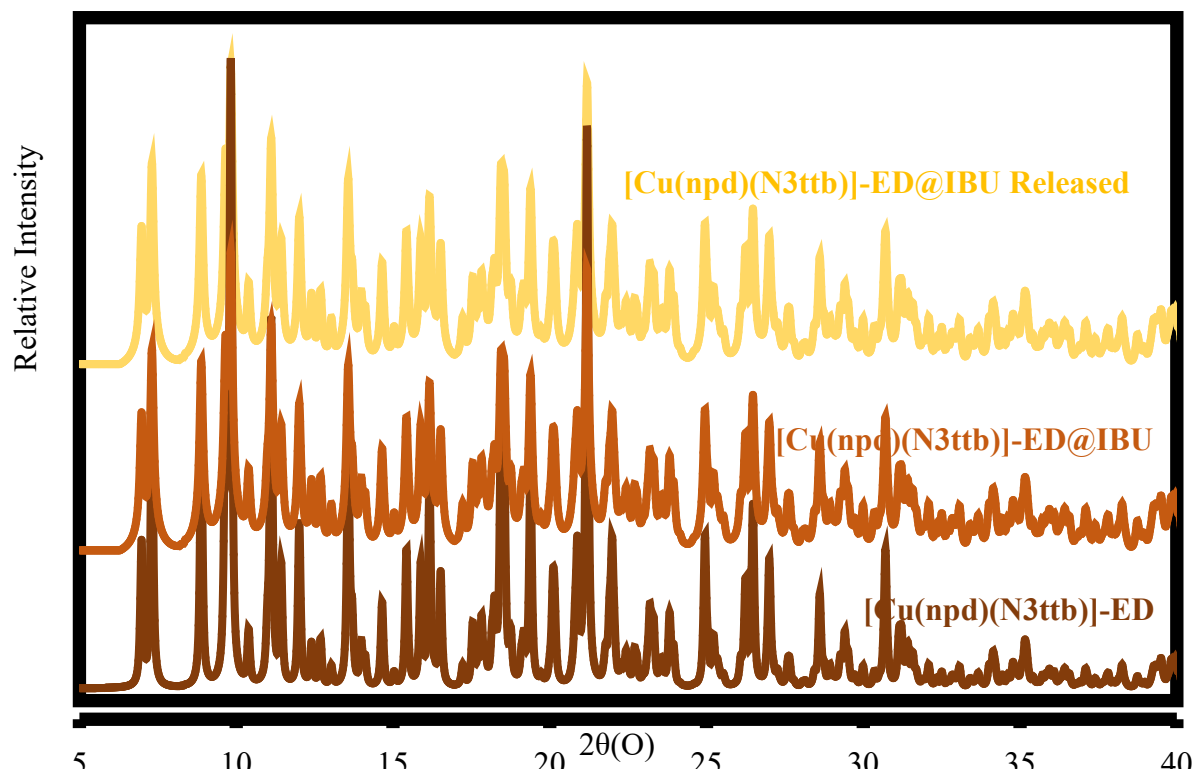


Figure S16: Comparison of the PXRD spectra of [Cu(npd)(N<sub>3</sub>ttb)]-ED@IBU (Loaded and released) MOFs.

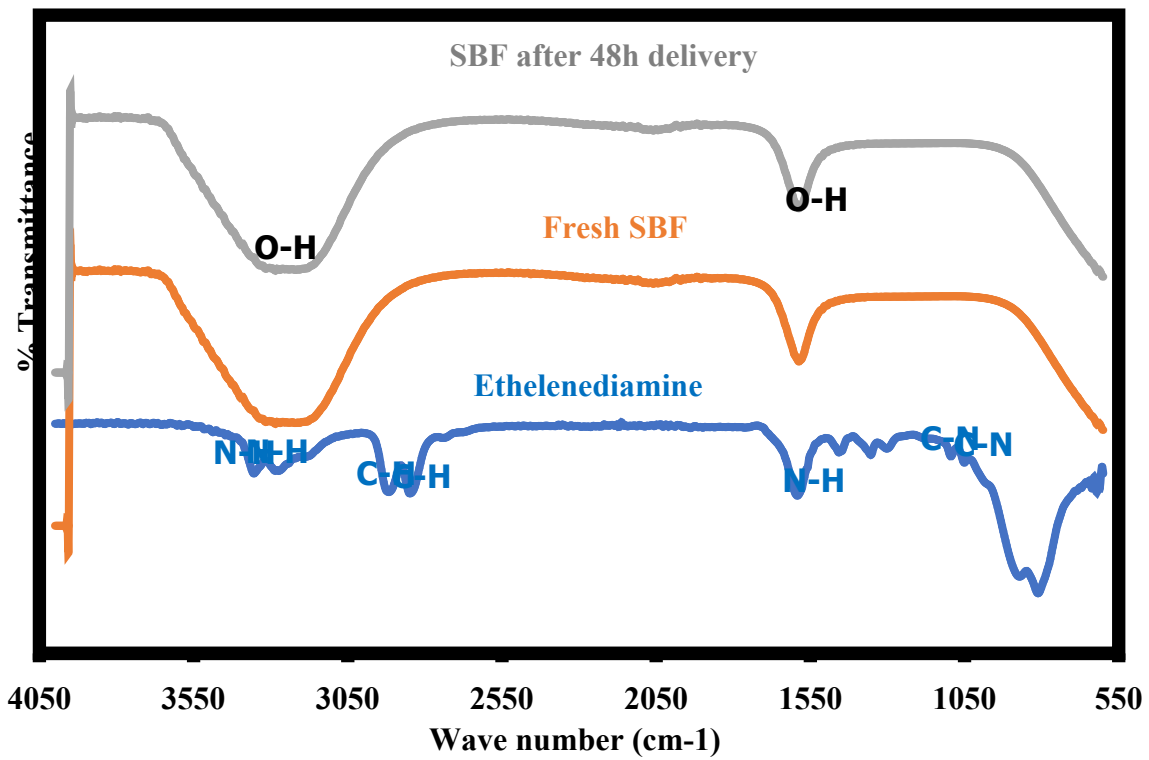


Figure S17: Comparison of the FT-IR spectra of Ethylenediamine and Simulated body fluid.

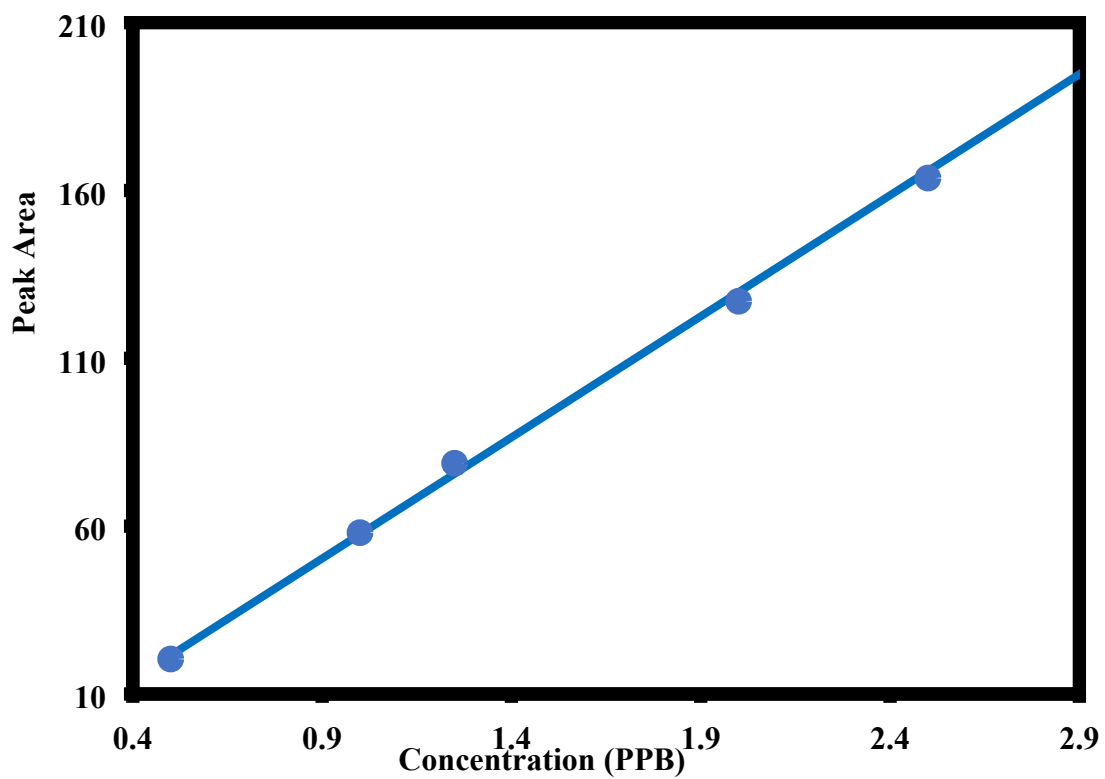


Figure S18: Calibration plot of standard ethylenediamine by HPLC method.

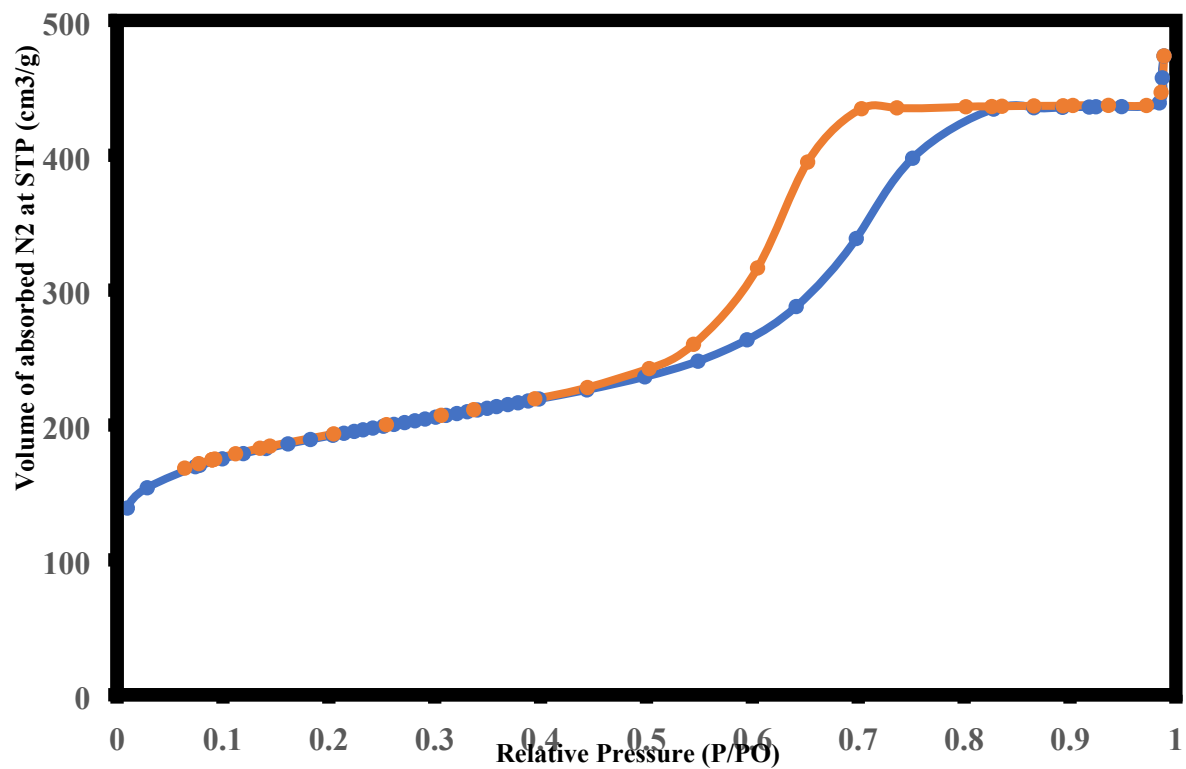


Figure S19: Nitrogen adsorption-desorption isotherm plot for 1

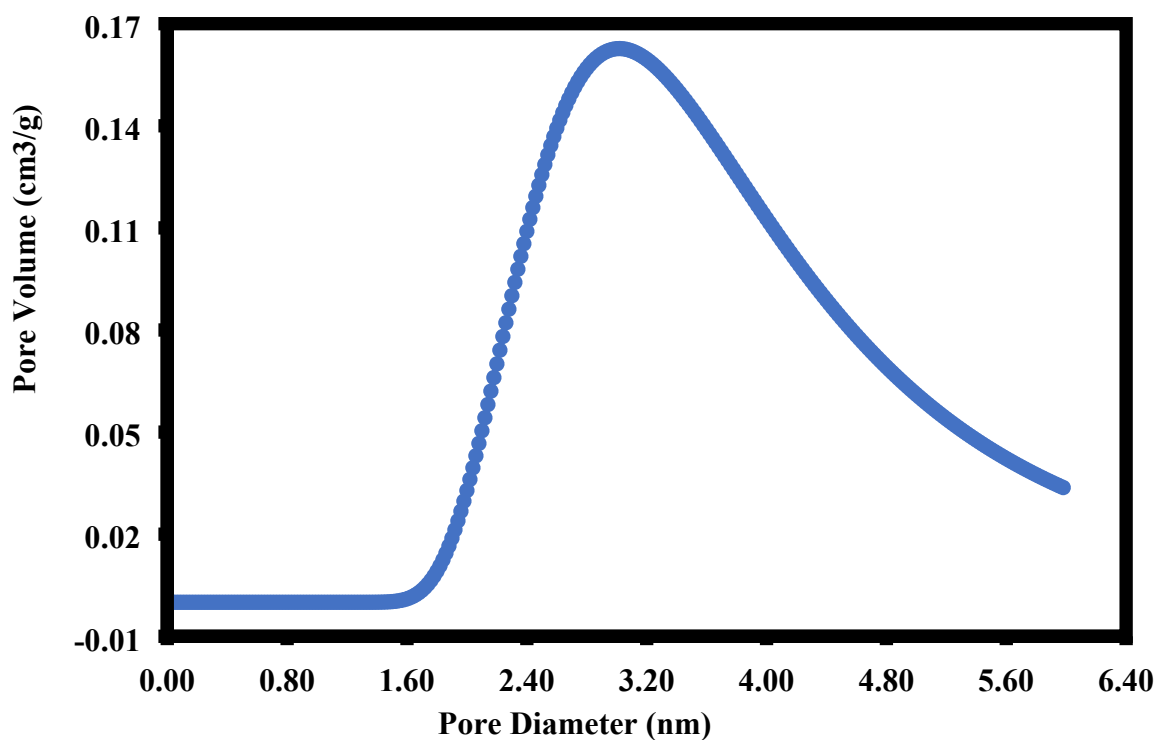


Figure S20: Pore size distribution for 1

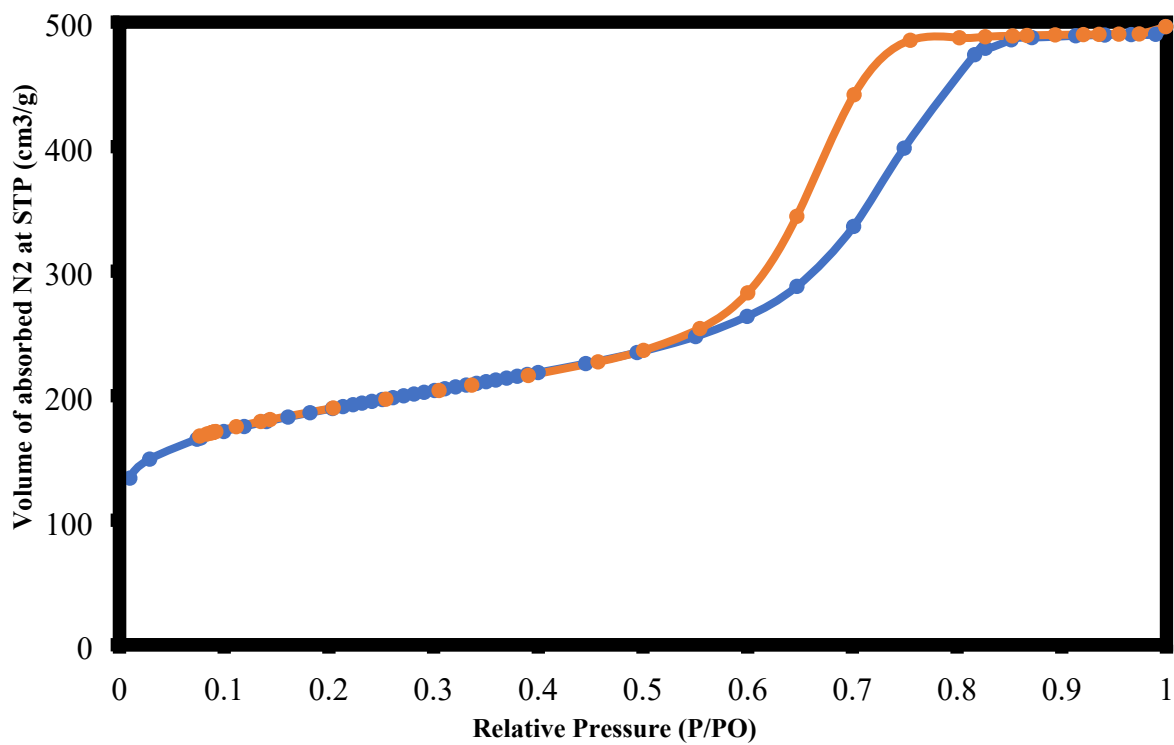


Figure S21: Nitrogen adsorption-desorption isotherm plot for **2**

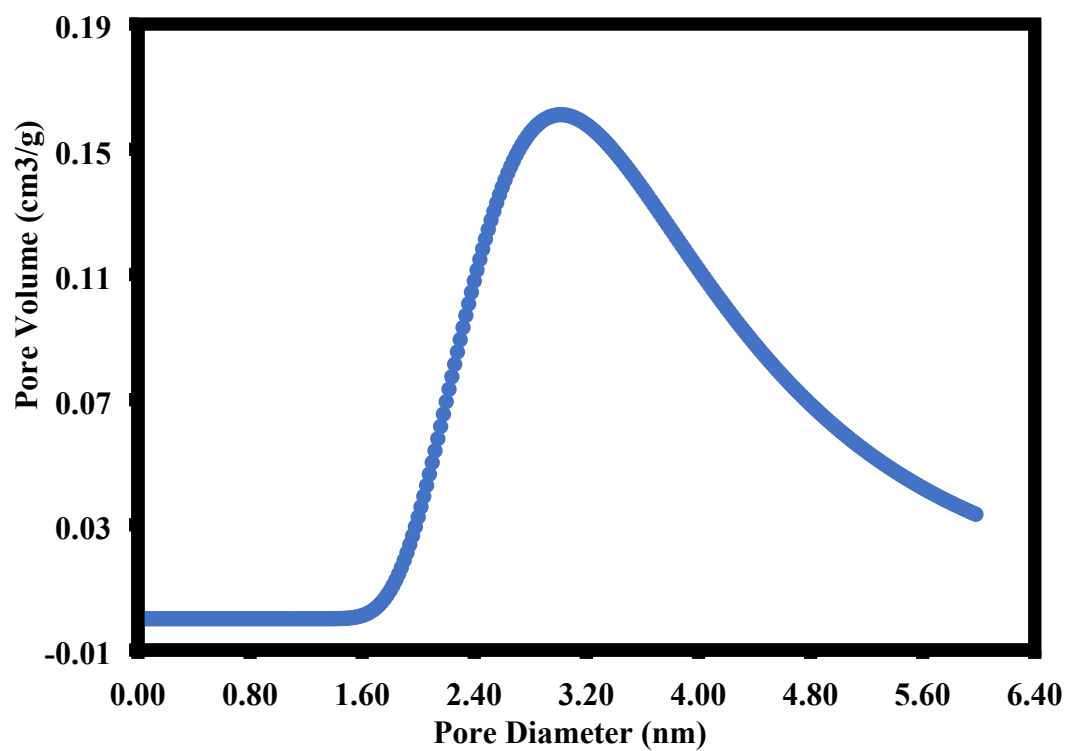


Figure S22: Pore size distribution for **2**

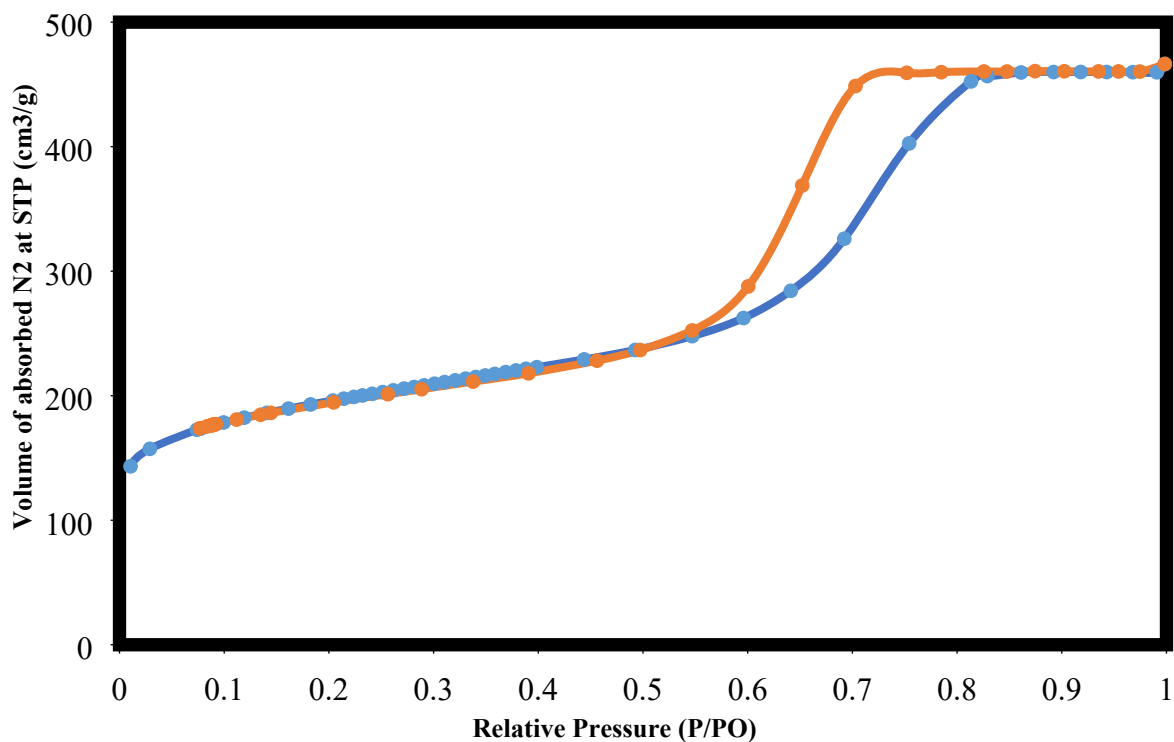


Figure S23: Nitrogen adsorption-desorption isotherm plot for [Cu(npd)(N<sub>3</sub>ttb)]@IBU

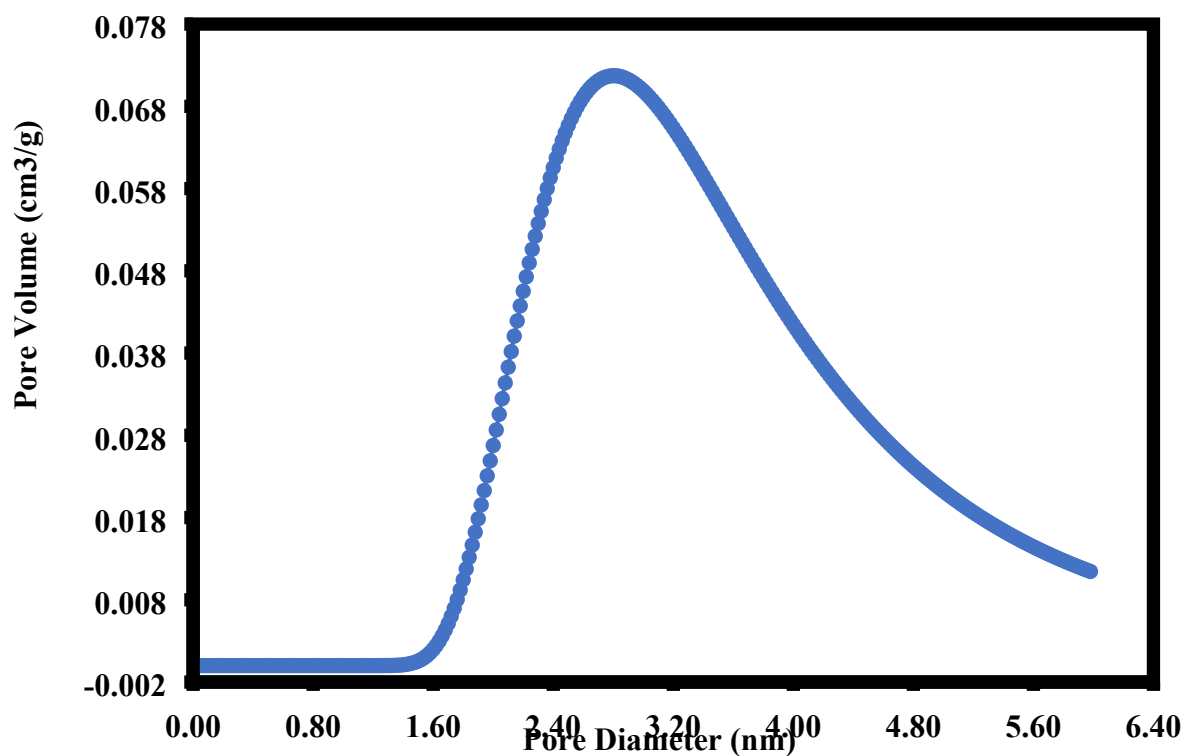


Figure S24: Pore size distribution for [Cu(npd)(N<sub>3</sub>ttb)]@IBU

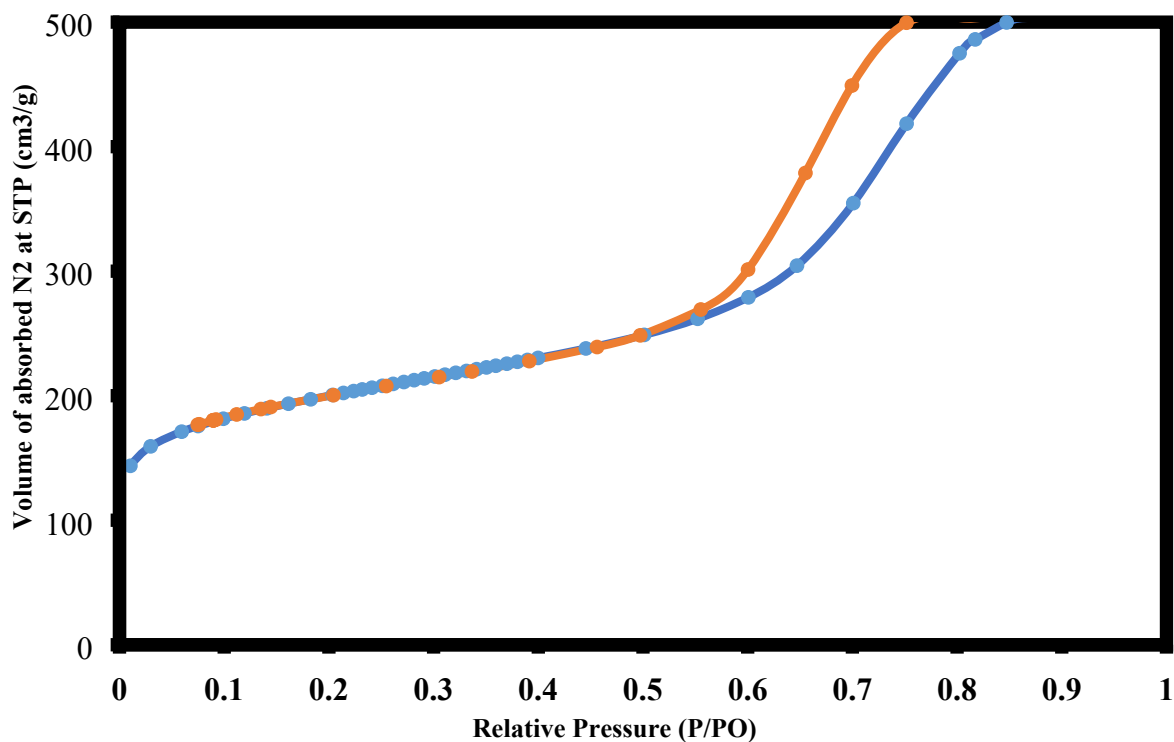


Figure S25: Nitrogen adsorption-desorption isotherm plot for [Cu(npd)(N<sub>3</sub>ttb)]-ED@IBU

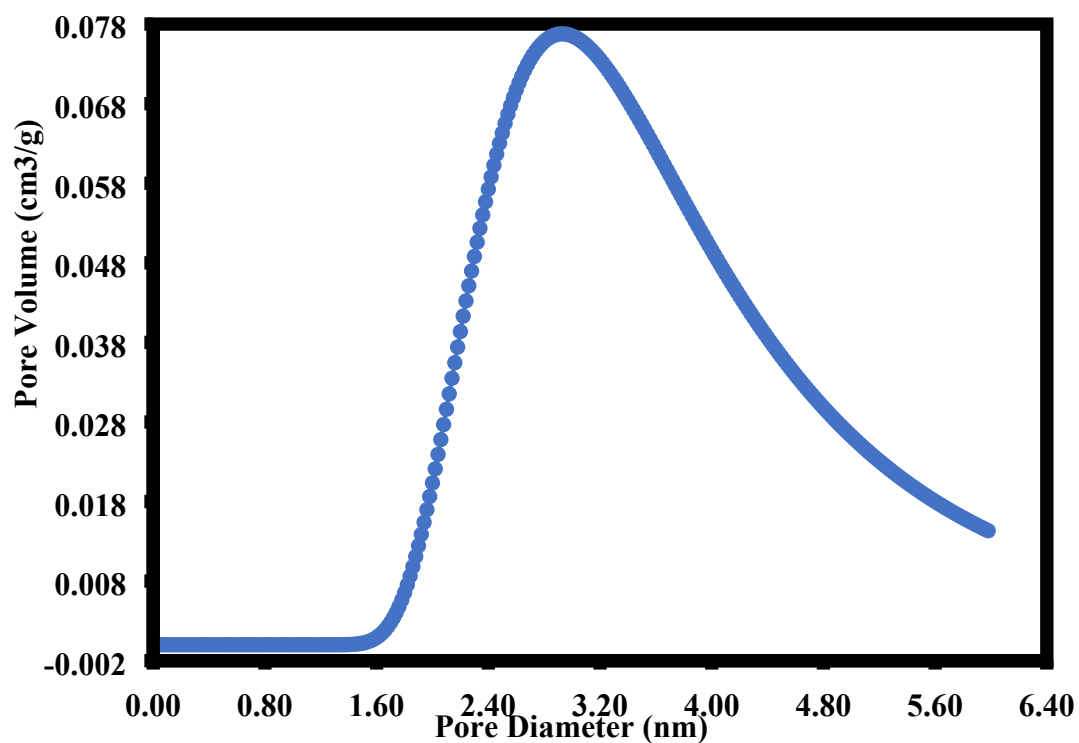


Figure S26: Pore size distribution for [Cu(npd)(N<sub>3</sub>ttb)]-ED@IBU

Table T1: Elemental composition of **1** and **2**.

ELEMENT	[Cu(npd)(N <sub>3</sub> ttb)].(C <sub>2</sub> H <sub>6</sub> NCHO)(H <sub>2</sub> O)		[Cu(npd)(N <sub>3</sub> ttb)]-ED	
	Wt%	Wt% Sigma	Wt%	Wt% Sigma
Carbon	66.17	0.60	44.28	0.35
Nitrogen	10.14	0.75	24.45	0.48
Oxygen	11.51	0.25	19.68	0.25
Copper	12.18	0.17	11.56	0.13
Total	100		100	

Table T2: Comparison of the loading of Ibuprofen in different MOFs. <sup>59–67</sup>

<b>S/No</b>	<b>MOFs</b>	<b>Loading Capacity (mg/g)</b>	<b>Author</b>
1	2	1,530.2	<b>This Research</b>
2	1	916.4	<b>This Research</b>
3	[Zn(BDC)(H <sub>2</sub> O) <sub>2</sub> ] <sub>n</sub>	445.0	62
4	MIL-100	347.0	59
5	MIL-100(Fe)	330.0	63
6	MIL-100	330.0	60
7	MIL-53	220.0	60
8	MIL-53(Cr)	220.0	64
9	MIL-53(Fe)	210.0	64
10	MIL-53	190	65
11	MIL-47	120	65
12	MOF-2	70.0	66
13	MOF-3	50.0	66
14	MOF-1	25.0	66
15	MOF-4	10.0	66



Table T3: Conc. of Cu<sup>2+</sup> (ppb)

<b>Time (h)</b>	<b>Concentration (ppb)</b>
0	0.00
3	0.02
6	0.00
12	0.05
24	0.01
48	0.01

Table T4: Conc. of Ethylenediamine (ppb)

<b>Time (h)</b>	<b>Concentration (ppb)</b>
0	0.00
3	0.00
6	0.00
12	0.00
24	0.00
48	0.00

Table T5: BET surface area & pore volume comparison of **1** and **2** before & after drug Loading.

<b>MOFs</b>	<b>Surface Area (m<sup>2</sup>/g)</b>	<b>Pore Volume (cc/g)</b>	<b>Volume Filled (%)</b>
[Cu(npd)(N <sub>3</sub> ttb)].(C <sub>2</sub> H <sub>6</sub> NCHO)(H <sub>2</sub> O)	527.645	0.466	0.00
[Cu(npd)(N <sub>3</sub> ttb)]@IBU	211.494	0.191	59.01
[Cu(npd)(N <sub>3</sub> ttb)]-ED	497.591	0.425	0.00
[Cu(npd)(N <sub>3</sub> ttb)]-ED@IBU	235.505	0.213	49.88