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Supporting Information

Copper Metallogel as Potential Drug Carrier for Anti-Inflammatory Drugs

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Experimental Sections

Materials and Instruments used

All chemicals and reagents were purchased from Sigma Aldrich and used without further purification. The IR spectral studies were performed on Agilent Technologies FTIR spectrometer. UV-vis studies were carried out on SHIMADZU Uv-2450 spectrophotometer using quartz cuvettes. Powder X-ray diffraction (PXRD) data were collected on Rigaku Smart Lab 9 KW rotating anode Powder X-ray Diffractometer at room temperature. The thermo gravimetric analysis was carried out using NETZSCH STA 449F1 JUPITER SERIES under N_2 atmosphere and at a heating rate of 10° K/ min. FESEM data was collected on Nova Nano SEM 450 JFEI USA (S.E.A) PTE LTD.

Synthesis of CuBTC gel

A DMF solution (700 µl) of copper (II) nitrate trihydrate (72.5 mg) was added drop wise to a solution (700 µl DMF) of benzene tricarboxylic acid (52.5 mg) containing equimolar amount of NEt_3.The stirring was continued for 5 minutes in ice bath and gel formation takes place. The **CuBTC** gel was kept undisturbed for 10-15 minutes in ice bath and was then kept at low temperature for 12 h. The CuBTC gel was further dried in vacuo. The obtained yield of **CuBTC** material was 92%.

Method of drug loaded gels formation

Anti-inflammatory drugs were loaded into metal organic gel by single step in-situ method. In this method metal and drug were added to the ligand solution with catalytic amount of NEt_3 simultaneously in a single step.

Synthesis of CuBTC@5FU

DMF solution (700 µl) of copper (II) nitrate trihydrate (72.5 mg) and 5-Fluorouracil (17.5 mg in 100 µl DMF) was added dropwise to a solution (700 µl DMF) of benzene tricarboxylic acid (52.5 mg) containing equimolar amount of NEt_3. The stirring was continued for 5 minutes in ice bath and gel formation took place. The **CuBTC@5FU** gel was kept undisturbed for 10-15 minutes in ice bath and further kept at low temperature for 12 h. The **CuBTC@5FU** gel was dried in vacuo and was used for further characterization. The obtained yield of **CuBTC@5FU** material was 88%.

Synthesis of CuBTC@PN

CuBTC@PN was synthesized by the same protocol as described for the synthesis of **CuBTC@5FU** except that Phenidone was used instead of 5-fluorouracil. The obtained yield of **CuBTC@PN** material was 80%.

Synthesis of CuBTC@IBP

CuBTC@IBP was synthesized by the same protocol as described for the synthesis of **CuBTC@5FU** except that ibuprofen was used instead of 5-fluorouracil. The obtained yield of **CuBTC@IBP** material was 90%.

Synthesis of CuBTC@CP

CuBTC@CP was synthesized by the same protocol as described for the synthesis of **CuBTC@5FU** except that cisplatin was used instead of 5-fluorouracil. The obtained yield of **CuBTC@CP** material was 96%.

Drug loading efficiency

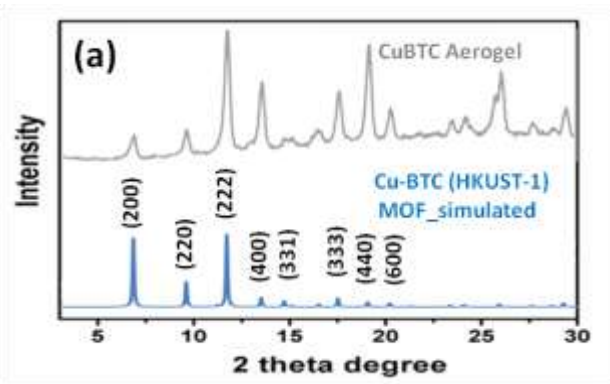
Drug loading efficiencies were calculated by the eq (1).

$$\text{Drug loading efficiency} = \frac{\text{Amount of loaded drug(mg)}}{\text{Amount of Feuded drug(mg)}} \text{ X } 100 \quad \ldots\ldots\ldots\ldots\ldots (1)$$

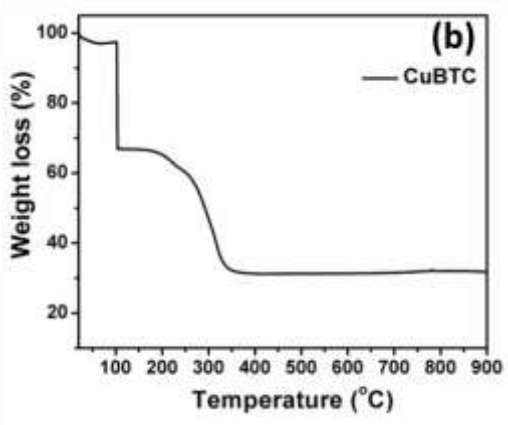
Drug releasing Method

Drug releasing study was carried out through sample and separate (SS) method. Drug release was monitored via physically separating the drug particles from the release media, followed by its analysis. Physical separation between the release media and drug particles was carried out with the help of syringe filters. After sampling, an equal amount of fresh release media was added to the set-up so that sink conditions were maintained during the duration of *in vitro* drug release study. The supernatant was used for analysis by UV Spectroscopy and the corresponding drug release percentage was calculated through eq. (2) at two different pH i.e 5.2 and 7.2 for 72 h.

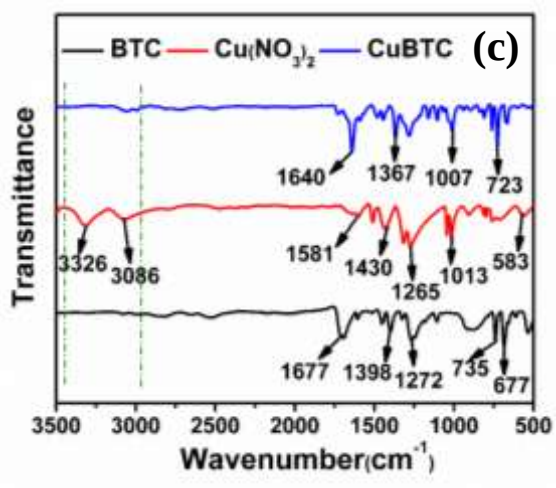
$$\text{Percentage drug release} = \frac{\text{Absorbance of Drug (at time t=t) - absorbance of Drug (at time t=0)}}{\text{Absorbance of Drug (at time t=t)}} \times 100 \quad \ldots\ldots\ldots\ldots\ldots (2)$$



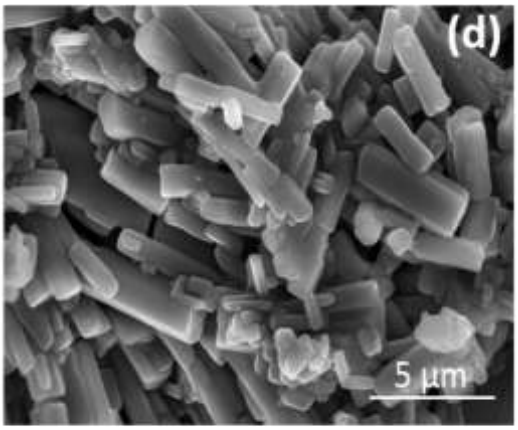
(a) Overlay PXRD patterns of CUBTC and Cu-BTC (HKUST-1)



(b) TGA of CuBTC



(c) FTIR spectrum of CuBTC



(d) FESEM Image of CuBTC

Figure S1: Overlay PXRD patterns of CuBTC and Cu-BTC (HKUST-1) (a) TGA (b) FTIR(c) and(d) FESEM of CuBTC

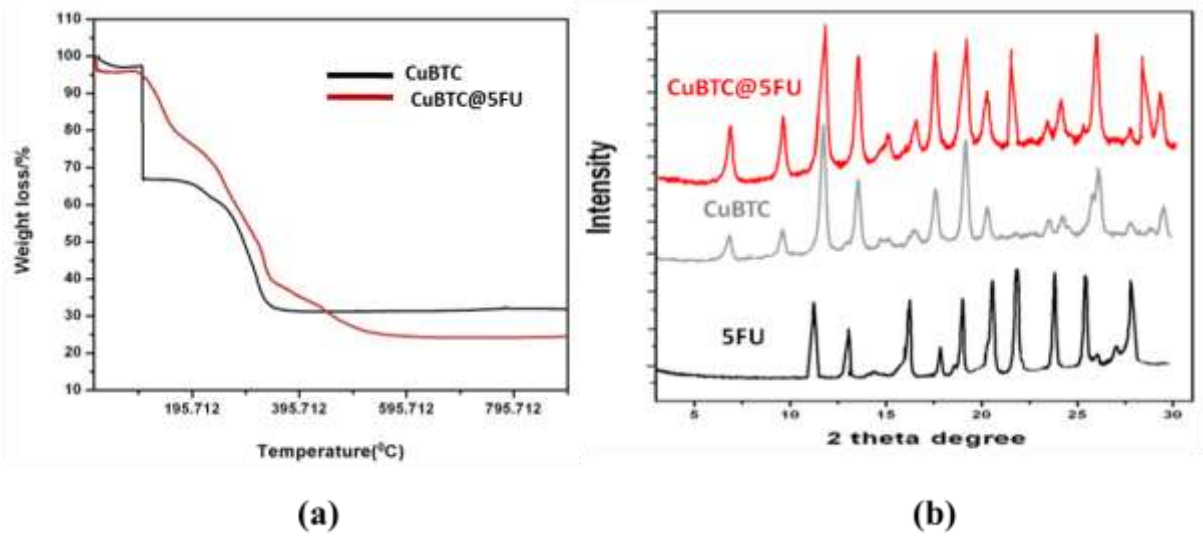


Figure S2: (a) TGA Spectra of CuBTC and CuBTC@5FU (b) Overlay PXRD patterns of 5FU, CuBTC and CuBTC@5FU.

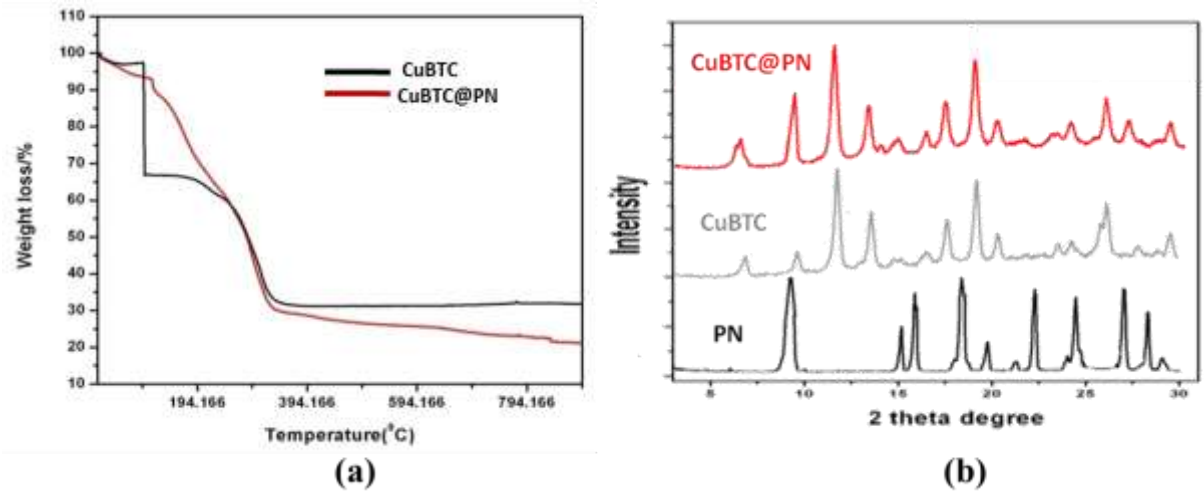


Figure S3: (a) TGA Spectra of CuBTC and CuBTC@PN (b) Overlay PXRD patterns of PN, CuBTC and CuBTC@PN.

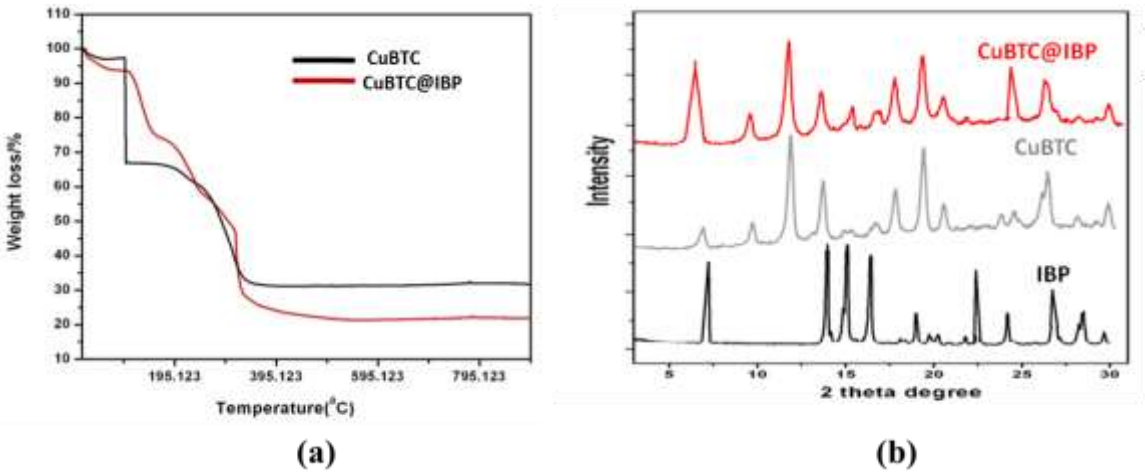


Figure S4: (a) TGA Spectra of CuBTC and CuBTC@IBP (b) Overlay PXRD patterns of IBP, CuBTC and CuBTC@IBP.

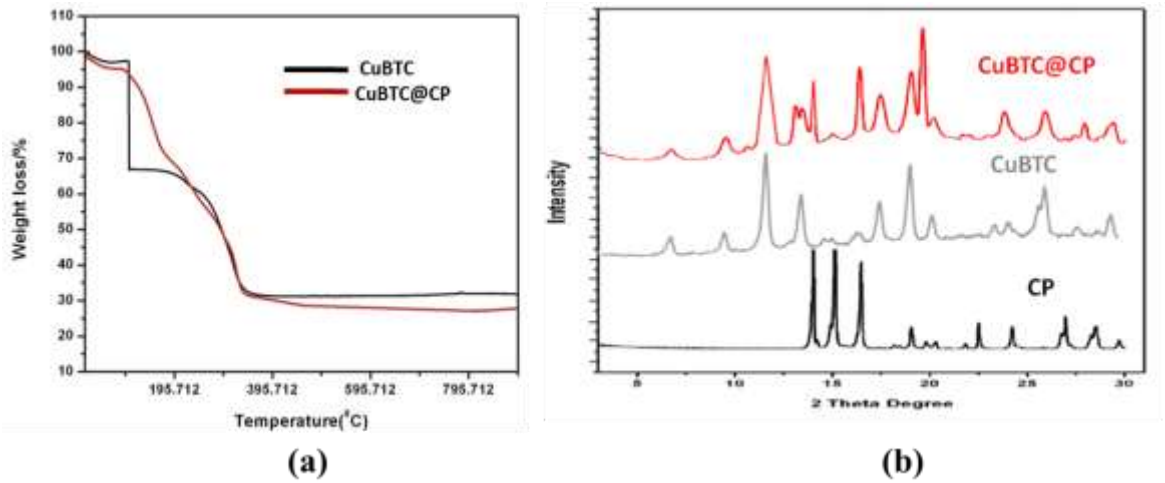


Figure S5: (a) TGA Spectra of CuBTC and CuBTC@5CP (b) Overlay PXRD patterns of CP, CuBTC and CuBTC@CP.