Electronic Supplementary Material (ESI) for Chemical Communications

Supplementary Information:

Targeted synthesis of a 2D ordered porous organic framework for drug release

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1. Instruments

The thermogravimetric analysis (TGA) was performed using a Netzch Sta 449c thermal analyzer system at the heating rate of 10 ^{o}C/min in air atmosphere. The FTIR spectra were measured using a Nicolet Impact 410 Fourier transform infrared spectrometer. The nitrogen adsorption isotherm was measured on an Autosorb iQ_2 adsorptometer, Quantachrome Instruments. The XRD was performed by a Riguku D/MAX2550 diffractometer using CuKα radiation, 40 kV, 200 mA with scanning rate of 0.4 ^{o}/min. TEM micrographs was recorded using a FEI Tecnai G^2 F20 s-twin D573 with an acceleration voltage of 300 kV. SEM micrographs were performing on JEOL-JSM-6300 under an accelerating voltage of 20-30 kV. Samples were sputtered with a thin film of Pt.

2. Materials

All starting materials were purchased from commercial suppliers and used without further purification unless otherwise noted. The piperazine was purchased from Aldrich, Cyanuric chloride was purchased from Alfa Aesar.

3. Synthesis

The synthesis was carried out from polymerization of CC and piperazine in homogeneous solution phase. Typically, triazine trichloride (51.7 mg, 0.6 mmol) was dissolved in 10 mL of THF and cooled to 0 °C before piperazine (73.8 mg, 0.4 mmol) and 0.85 mL of N,N-diisopropyl ethylamine were added. After stirring at 0 °C for 4 h, system raised to the room temperature and then refluxed overnight.

4. Elemental analysis

Elemental analysis calcd (%) for $C_9H_{12}N_6$: C 52.95, H 5.88, N 41.17; found: C 53.26, H 5.67, N 41.07.

5. IR study of the Polymer PAF-6

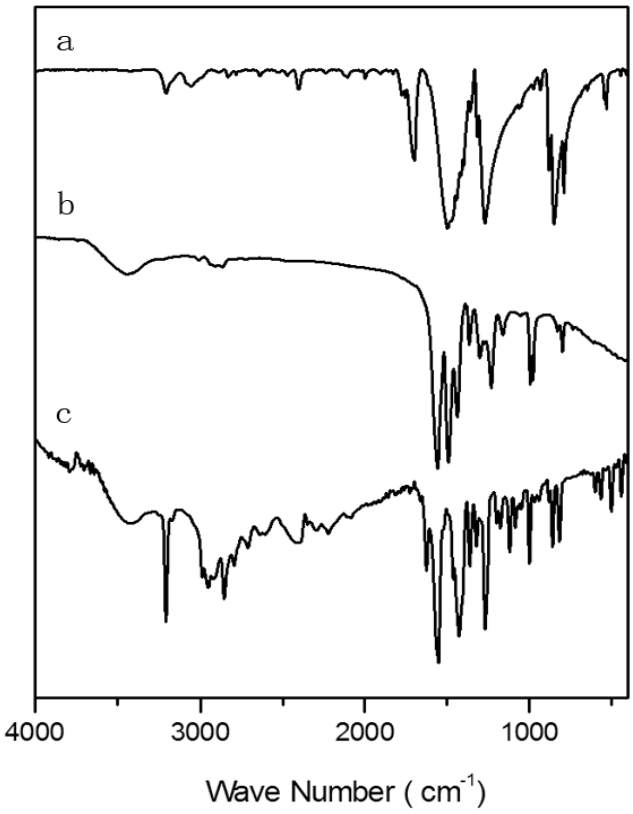

Fig. s1. FTIR spectra of cyanuric chloride（a）, PAF-6 (b) and piperazine (c) from 400-4000 cm^{-1}.

6. Simulated structure of PAF-6

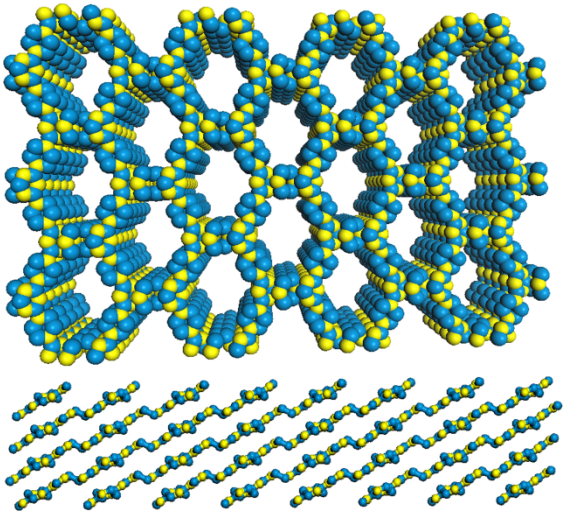

Fig. s2 Simulated structure of PAF-6 along [001] and [100] direction (structure is based on field-force calculation and crystal lattice parameters; C blue, N yellow, H atoms are omitted for clarity).

7. TGA trace of the PAF-6

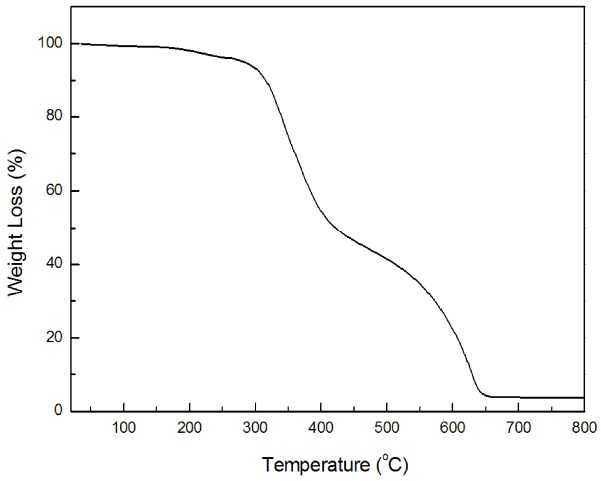

Fig. s3. TGA trace for an activated sample of PAF-6 under air atmosphere.

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8. Viability of cells in the presence of PAF-6 using MTT assay

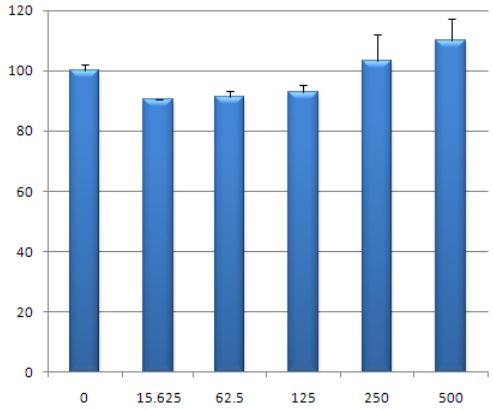

Fig. s4 Cell viability measured using the MTT assays at concentrations that increase from left to right: 0, 15.6, 62.5, 125, 250 and 500 μg/mL.

The viability of cells in the presence of PAF-6 was investigated using 3-[4,5-dimethylthialzol-2-yl]-2,5-diphenyltetrazolium bromide (MTT, Sigma) assay. For MTT assay, HeLa cells were seeded into 96-well plates at a density of 1×10^4 per well in 100 μL of media and grown overnight. The cells were then incubated with various concentrations of PAF-6 for 48 h. Following this incubation, cells were incubated in media containing 0.5 mg mL^{-1} of MTT for 4 h. The precipitated formazan violet crystals were dissolved in 100 μL of 10 % SDS in 10 mmol HCl solution at 37 °C overnight. The absorbance was measured at 570 nm by multi-detection microplate reader (SynergyTM HT, BioTek Instruments Inc, USA). The assay was carried out in triplicate in the above manner.

9. Drug loading and release

The loading of the drug was carried out by the immersion of PAF-6 in ibuprofen hexane solution with a certain concentration. A typical procedure for loading ibuprofen in PAF-6 was as follows: 200 mg of PAF-6 was suspended in 10mL of 0.1 M ibuprofen hexane solution under stirring for 6 h while preventing the evaporation of hexane. The drug-loaded sample was separated from the solution by vacuum filtration, washed with hexane, and dried at room temperature. Filtrate (1.0 mL) was sucked and properly diluted to determine the drug-loading amount by UV-Vis spectrophotometer.

After the drug-loaded samples (50 mg) transfering to semipermeable bag, the release rate was obtained by soaking the drug-loaded samples in 200 mL of simulated body fluid (PBS, pH = 7.4, buffer solution) at predetermined time intervals, 3 mL samples were withdrawn and analyzed for ibuprofen content at 222 nm using UV-Vis spectrophometer immediately. Then the samples were added back to the system to keep the volume constant.