Electronic Supplementary Information (ESI)

A pH-/thermo-responsive hydrogel formed from N,N’-dibenzoyl-
L-cystine: property, self-assembly structure and release behavior
of SA

Jinlian Zhong, Hongyu Fu, Xinjian Jia, Haoxiang Lou, Tiantian Wan, Haiqing Luo,
Huijin Liu, Dichang Zhong*, Xuzhong Luo’

Key Laboratory of Organo-Pharmaceutical Chemistry of Jiangxi Province, Gannan
Normal University, Ganzhou, 341000, China. E-mail: luoxuzhong@hotmail.com;
zhong_dichang@hotmail.com

1. Synthesis of xerogels

After the DBC gel containing NaCl was completely exchanged by water
molecules, the corresponding DBC xerogel was obtained by drying the gel in a
vacuum oven at 60 °C for 24 h.

2. Growth of DBC Crystal

First, 10.0 mg of DBC was mixed with 5 mL of the NaOH solution (0.5 mg/L)
until the solid was completely dissolved. And then, the mixture was adjusted to a
given pH with aqueous HCl solutions until obtaining a stable hydrogel at ambient
temperature. After five days, colorless crystals suitable for single-crystal X-ray
diffraction analysis were finally obtained by filtration.
3. SEM

Fig. S1 SEM images of DBC hydrogels: (a) 7.0 g/L; (b) 8.0 g/L; (c) 9.0 g/L; (d) 10.0 g/L

4. Rheological behavior of hydrogels

Fig. S2 The stress sweep of DBC gel formed by varying concentration (2.0 g/L, 3.0 g/L, 5.0 g/L, 6.0 g/L)
Fig. S3 Rheological measurements of DBC hydrogels with the mode of frequency sweep for $G'$ and $G''$ (gelator concentrations: 2.0 g/L, 3.0 g/L, 5.0 g/L and 6.0 g/L).

5. Date of differential scanning calorimetry (DSC)

Fig. S4 DSC thermograms of DBC hydrogels prepared at various gelator concentrations (gelator concentrations: 1.5 g/L, 2.0 g/L, 3.0 g/L, 4.0 g/L, 5.0 g/L and 6.0 g/L).
6. Structure of DBC Crystal

Table S1. Crystal data and structure refinement for DBC.

| Compound | DBC |
|----------|-----|
| Formula  | C_{20}H_{20}N_{2}O_{7}S_{2} |
| F_w.     | 464.5 |
| Crystal system | Monoclinic |
| Space group | P2_1 |
| a (Å)    | 10.8180(11) |
| b (Å)    | 9.0405(9) |
| c (Å)    | 10.9871(11) |
| α (°)    | 90 |
| β (°)    | 90.798(3) |
| γ (°)    | 90 |
| V (Å³)   | 1074.44(19) |
| Z        | 2 |
| D_c (g·cm⁻³) | 1.436 |
| Reflections/ unique | 5104/4073 |
| R(int)   | 0.0388 |
| GoF on F² | 1.043 |
| R₁[I ≥ 2σ(I)] | 0.0472 |
| wR₂[I ≥ 2σ(I)] | 0.1149 |
Table S2. Selected bond distances (Å) and angles (°) for DBC.

| Bond/Angle Description | Distance/Angle (Å/°) |
|-------------------------|----------------------|
| C13—O5                  | 1.198(3)             |
| C13—O4                  | 1.322(3)             |
| C13—C12                 | 1.514(3)             |
| O6—C14                  | 1.228(3)             |
| N2—C14                  | 1.334(3)             |
| C14—C15                 | 1.494(3)             |
| N1—C7                   | 1.329(3)             |
| N1—C8                   | 1.451(3)             |
| C15—C16                 | 1.382(4)             |
| C15—C20                 | 1.388(4)             |
| C16—C17                 | 1.384(4)             |
| C7—O1                   | 1.224(3)             |
| C8—C9                   | 1.516(3)             |
| O5—C13—O4               | 123.4(2)             |
| O5—C13—C12              | 124.3(2)             |
| O4—C13—C12              | 112.2(2)             |
| C14—N2—C12              | 122.1(2)             |
| O6—C14—N2               | 121.3(2)             |
| O6—C14—C15              | 121.8(2)             |
| N2—C14—C15              | 116.9(2)             |
| C7—N1—C8                | 124.1(2)             |
| C16—C15—C20             | 119.3(2)             |
| C16—C15—C14             | 123.1(2)             |
| C20—C15—C14             | 117.6(2)             |
| C15—C16—C17             | 119.7(3)             |
| O1—C7—N1                | 121.4(3)             |
| C10—S2                  | 1.808(3)             |
| C3—C2                   | 1.354(4)             |
| C3—C4                   | 1.364(4)             |
| C20—C19                 | 1.378(4)             |
| C9—O3                   | 1.197(3)             |
| C9—O2                   | 1.311(3)             |
| C5—C6                   | 1.373(4)             |
| C5—C4                   | 1.377(4)             |
| C17—C18                 | 1.370(5)             |
| C1—C2                   | 1.378(4)             |
| C1—C6                   | 1.390(4)             |
| C18—C19                 | 1.358(5)             |
| O1—O7Wi                 | 7.6384(39)           |
| C13—C12—C11             | 111.24(18)           |
| C8—C10—S2               | 115.79(16)           |
| C2—C3—C4                | 119.4(3)             |
| C19—C20—C15             | 119.8(3)             |
| O3—C9—O2                | 125.4(2)             |
| O3—C9—C8                | 122.3(2)             |
| C6—C5—C4                | 120.6(2)             |
| C18—C17—C16             | 120.5(3)             |
| C3—C4—C5                | 120.7(3)             |
| C2—C1—C6                | 120.3(3)             |
| C19—C18—C17             | 120.0(3)             |
| C3—C2—C1                | 120.8(3)             |
7. Release behavior of DBC hydrogel

Fig. S5 Release kinetics: (a) different SA concentrations from the DBC hydrogels (3.0 g/L) at 25 °C; (b) SA from the DBC hydrogels formed by different concentrations at 25 °C.