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Supporting Information

A range of surfactant-accelerated hydrogels based on terpyridine-based assembly via strong dipole-dipole interactions

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Contents

1. General information

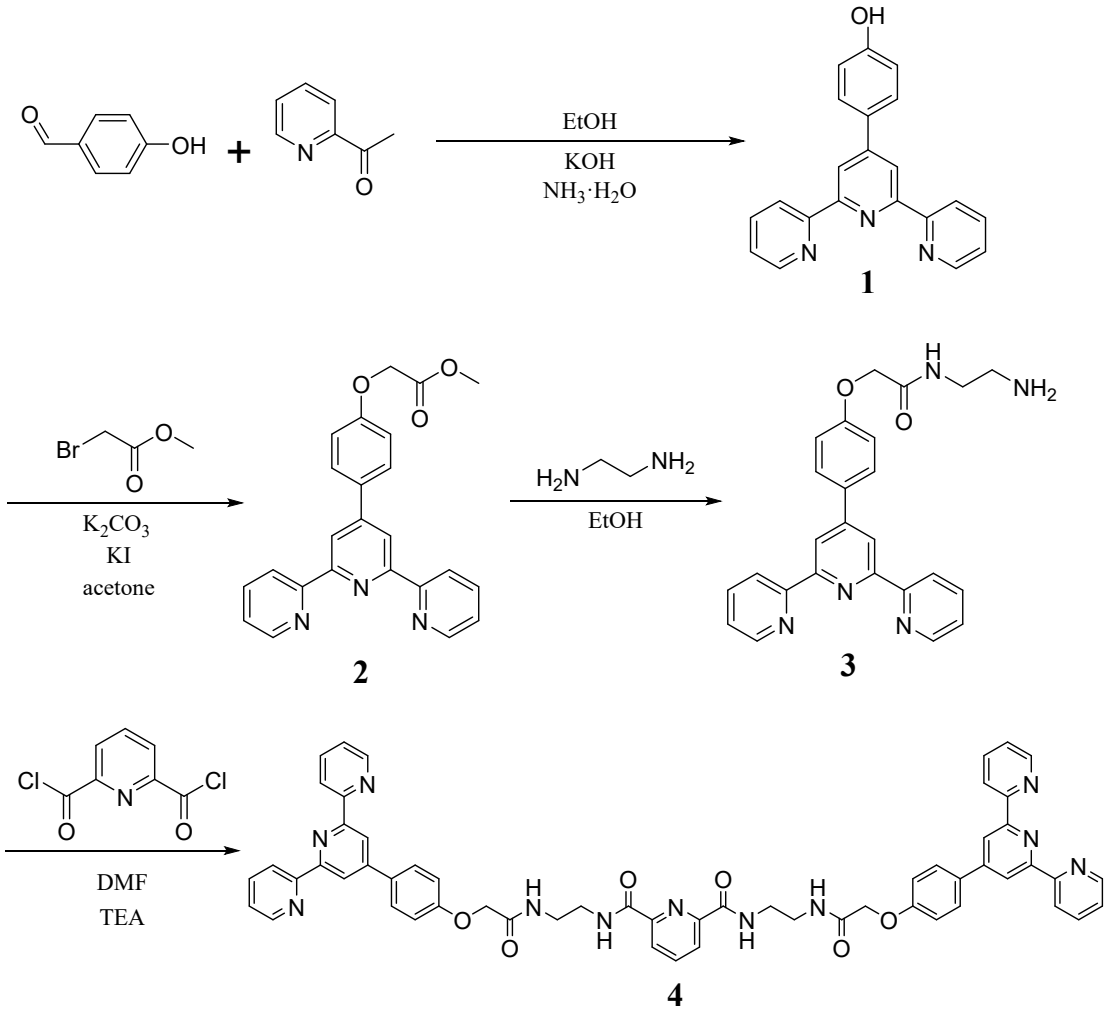
^{1}H NMR and ^{13}C NMR spectra were recorded at 500 MHz and 125 MHz, respectively. Chemical shifts were reported in ppm from the solvent resonance as the internal standard (DMSO-d_6: δ_H = 2.50 ppm, δ_C = 39.52 ppm; D_2O: δ_H = 4.79 ppm). Multiplicity was indicated as follows: s (singlet), d (doublet), dd (doublet of doublet), m (multiplet). Coupling constants were reported in Hertz (Hz). High resolution mass spectrometry (HRMS) spectra were obtained by using time-of-flight (TOF) QII with electrospray ionization. HPLC analysis was carried out on a Wufeng instrument. Fluorescence curves for the solutions and titrations were explored on a Hitachi F-7000 spectrometer. UV-vis (ultraviolet−visible spectroscopy) absorption spectra were recorded by using a UV-vis 2550 spectroscope (Shimadzu). Scanning electron microscopy (SEM) images of DA-BET@surfactant xerogels were obtained by using FE-SEM S-4800 (Hitachi) instruments. The X-ray diffraction (XRD) data of xerogels were acquired by using a Rigaku D/MAX-2500 diffractometer (Cu target; λ = 1.542 Å). All theoretical calculations were performed at the density functional theory (DFT) level using the Gaussian 16 A.03 software package.

2. Materials

DMF was distilled from CaH_2; 4-Hydroxybenzaldehyde, sodium dodecyl sulfate (SDS) and hexadecyl sulfobetaine (SB3C16) were purchased from Shanghai Bide pharmaceutical technology co. ltd; 2,6-pyridinedicarboxylic acid chloride, 2-acetylpyridine, methyl bromoacetate, hexadecyl trimethyl ammonium bromide (CTAB), tetrabutylammonium bromide (TBAB), tetrabutylammonium chloride (TBAC), triton X-100, span 60, betaine, N-Dodecyl-N, N-dimethyl-3-ammonio-1-propanesulfonate (Anzergent 3-12), tetramethylammonium bromide (TMAB), tetraethylammonium bromide (TEAB), tetrapropylammonium bromide (TPAB), tetramethylammonium chloride (TMAC), tetraethylammonium chloride (TEAC) and tetrapropyl ammonium chloride (TPAC) were purchased from Shanghai Aladdin

reagent co. ltd; oleylamine was purchased from Shanghai McLean biochemical technology co. ltd; sodium dodecyl sulfonate (SLS) and sodium dodecyl benzenesulfonate (SDBS) were purchased from Tianjin Hengxing chemical reagent preparation co. ltd. All purchased reagents were used without further purification. Analytical thin layer chromatography was performed on 0.20 mm silica gel plates. Silica gel (200–300 mesh) (from Qingdao Haiyang Chem. Company, Ltd.) was used for flash chromatography.

3. Synthesis data of DA-BET



Scheme S1. The synthesis procedure of DA-BET

The compounds **1**, **2** and **3** were synthesized according to a previously published literature[1, 2].

Synthesis of compound **4**

Compound 3 (2.65 g, 6.23 mmol) and 8 mL Et_3N were dissolved into 80 mL DMF in a 250 mL round-bottom flask. 2,6-Pyridinedicarboxylic acid chloride (0.6 g, 2.94 mmol) in 5 mL DMF was added dropwise to the above solution under N_2 at 0 °C, and continued stirring at 0 °C for 0.5 h. The mixture was then stirred at 100 °C for 16 h. After completion of the reaction (monitored by TLC), the crude mixture was poured into water, extracted with dichloromethane, saturated sodium chloride solution and the organic layer was dried over Na_2SO_4, concentrated under reduced pressure. The residue was purified by column chromatography on silica gel (eluting with 50:1 dichloromethane/methanol) to give product **4** as a white solid (1.01g, 31.1% yield). [determined by **HPLC** analysis Pronaos EP-C18, methanol, 254 nm UV detector, 1.0 mL/min]; Mp: 289.5 – 290.6 ℃. **^{1}H NMR** (500 MHz, DMSO-d_6) ,δ: 8.77 (d, *J* = 4.0 Hz), 8.69 (s), 8.68 (d, *J* = 7.9 Hz), 8.27 (d, *J* = 5.2 Hz), 8.10 (s), 8.06 (d, *J* = 1.7 Hz), 8.04 (s), 8.03 (d, *J* = 1.8 Hz), 7.93 (d, *J* = 8.8 Hz), 7.54 (dd, *J* = 7.0, 5.2 Hz), 7.18 (d, *J* = 8.8 Hz), 4.58 (s), 3.25 – 3.21 (m). **^{13}C NMR** (125 MHz, DMSO-d_6), δ: 168.52, 163.40, 158.77, 155.47, 155.02, 149.26, 148.71, 148.41, 139.49, 137.36, 130.21, 128.05, 124.41, 124.08, 120.87, 117.30, 115.47, 66.97, 39.94, 38.36. **HRMS** (ESI) found：m/z 982.3778 $[M + H]^+$; cal. for $C_{57}H_{47}N_{11}O_6$ + H 982.3784.

References

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4. Preparation of the supramolecular hydrogel

Bis-terpyridine derivative DA-BET (25 mg mL^{-1}), surfactant (molar ratio was 1:2, 1:4, 1:6, 1:8 or 1:10), and deionized water were added into a screw-top glass vial. The mixture was subjected to ultrasonic treatment for 5 minutes, followed by heating at 130 °C for 3 to 5 minutes. After cooling the mixture to room temperature, a supramolecular hydrogel was obtained.

The supramolecular hydrogels formed by DA-BET with different surfactants can be seen in Table S1.

5. Characterization of the supramolecular hydrogel

Table S1. The gelation properties of DA-BET (25 mg mL^{-1}) with different surfactants (molar ratio was 1:2, 1:4, 1:6, 1:8 or 1:10) in deionized water

Surfactants	n (D: s) 1:2	n (D: s) 1:4	n (D: s) 1:6	n (D: s) 1:8	n (D: s) 1:10
Cetrimonium Bromide (CTAB)	G	G	G	G	G
Tetrabutylammonium bromide (TBAB)	G	G	G	G	G
Tetrabutylammonium chloride (TBAC)	G	G	G	G	G
Sodium dodecyl sulfate (SDS)	S	PG	G	G	G
Sodium lauryl sulfonate (SLS)	G	G	G	G	G
Sodium dodecyl benzene sulfonate (SDBS)	PG	G	G	G	G
Span 60	I	I	I	PG	G
Triton X-100	S	PG	PG	PG	PG
Oleylamine	I	I	I	I	I
Betaine	G	G	G	G	G
SB3C16	G	G	G	G	G
Anzergent 3-12	G	G	G	G	G

Note: G: gel; PG: partial gel; I: insoluble; S: solution. n (D: s): molar ratio of DA-BET to surfactants. All the hydrogels are prepared through sonication-heating-cooling process.

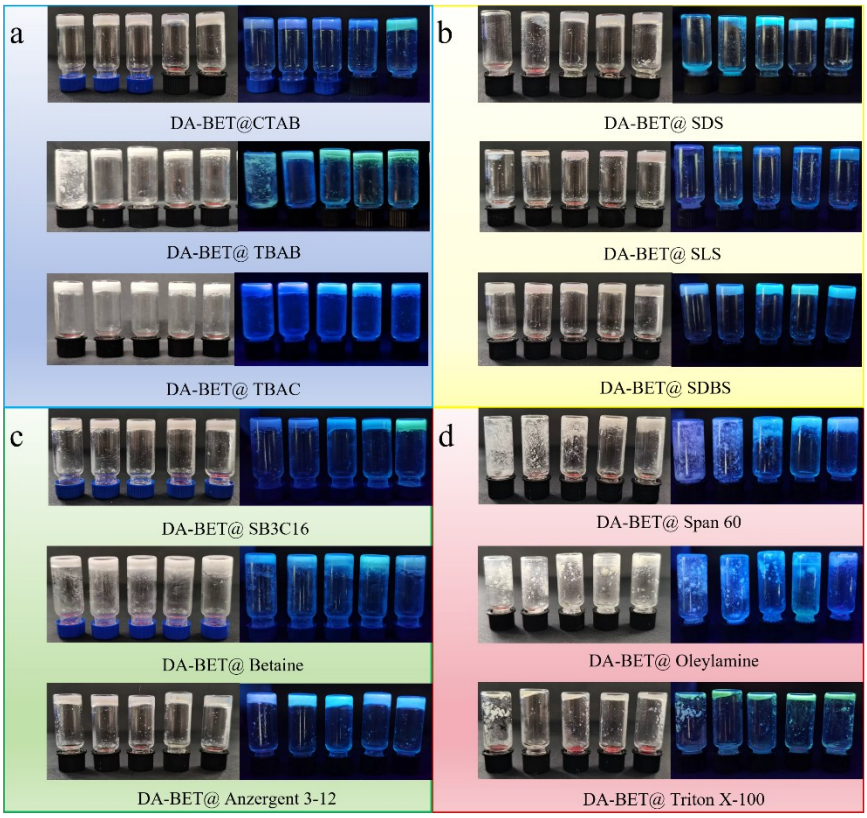

Fig. S1. Photos of hydrogels formed by DA-BET with different surfactants (a) cationic surfactants, (b) anionic surfactants, (c) zwitterionic surfactants and (d) neutral surfactants in light and in dark (irradiated by 365 nm).

Table S2. The gelation properties of DA-BET (25 mg mL^{-1}) and surfactants with different carbon chain lengths (molar ratio is 1:10) in deionized water.

Surfactants	n (D: s) 1:10
TMAC	I
TEAC	PG
TPAC	G
TBAC	G
TMAB	I
TEAB	PG
TPAB	G
TBAB	G

Note: G: gel; PG: partial gel; I: insoluble. n (D: s): molar ratio of DA-BET to surfactants. All the hydrogels are prepared through sonication-heating-cooling process.

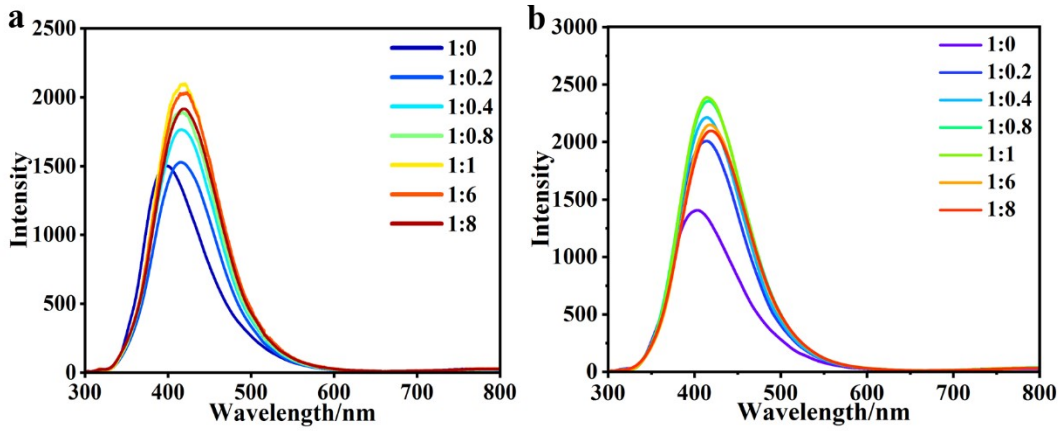

Fig. S2. The fluorescence titrations spectrums of DA-BET aqueous solution (1×10^{-5} mol L^{-1}) with (a) SLS (molar ratios are 1:0 to 1:8), (b) SB3C16 (molar ratios are 1:0 to 1:8).

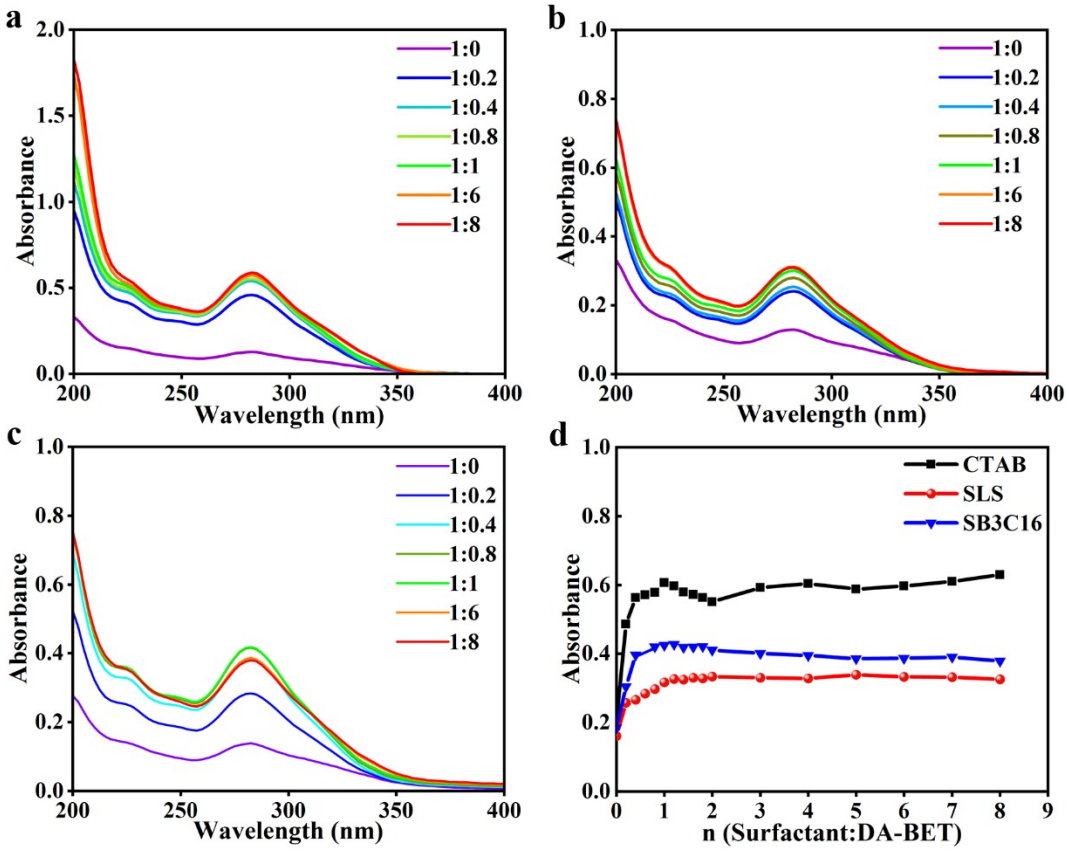

Fig. S3. The UV-vis titrations spectra of DA-BET aqueous solution (1×10^{-5} mol L^{-1}) with (a) CTAB (molar ratios are 1:0 to 1:8), there is an increase in the absorbance peak at 282 nm and a shoulder at approximately 320 nm, suggesting an enhanced solubility of DA-BET in water. (b) SLS (molar ratios are 1:0 to 1:8). (c) SB3C16 (molar ratios are 1:0 to 1:8). (d) Job's plot diagrams of UV titration experiment of DA-BET with CTAB, SLS and SB3C16.

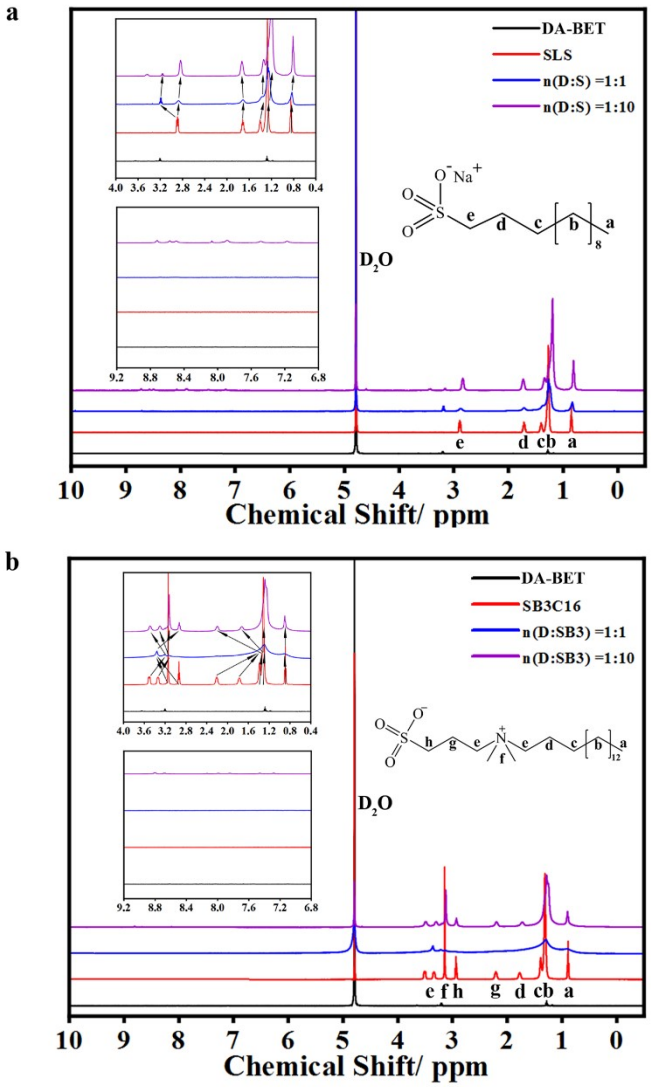

Fig. S4. (a) ^{1}H NMR spectra (500 MHz, D_2O) of SLS, and DA-BET in the presence of 0, 1, 10 molar ratios of SLS. When the molar ratio of DA-BET and SLS is 1:1, H_a shifts from 0.86 ppm to 0.84 ppm, H_b shifts from 1.28 ppm to 1.26 ppm, H_c shifts from 1.41 ppm to 1.38 ppm, H_d shifts from 1.73 ppm to 1.72 ppm, H_e shifts from 2.90 ppm to 2.88 ppm, respectively. As the molar ratio of DA-BET and SLS rise to 1:10, the H signals shift to lower magnetic field (H_d shifts from 1.72 ppm to 1.74 ppm), and the nuclear magnetic resonance signal of the terpyridine region in DA-BET become clearer. (b) ^{1}H NMR spectra (500 MHz, D_2O) of SB3C16, and DA-BET in the presence of 0, 1, 10 molar ratios of SB3C16. When the molar ratio of DA-BET and SB3C16 is 1:1, all the signals of Hs on SB3C16 are weakened, with H_a, H_b, H_c, H_d, and H_g merges into one multiplet, while H_e, H_f, and H_g merges into another multiplet. When the molar ratio of DA-BET and SB3C16 is 1:10, it can be observed that all signals of Hs on SB3C16 show a slight shift towards the high-field, while the signals of Hs on terpyridine in DA-BET can be observed in the low-field region.

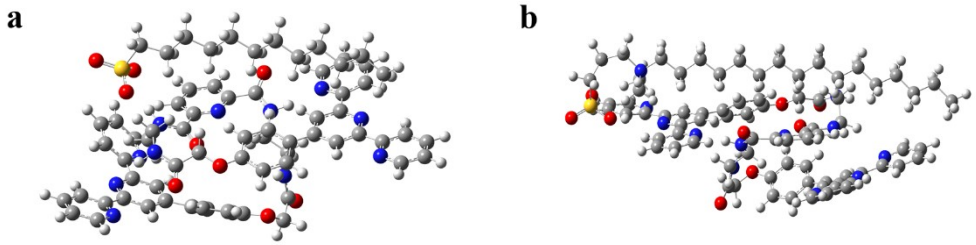

Fig. S5. (a) Intermolecular complexes between (a) DA-BET and SLS. (b) DA-BET and SB3C16.

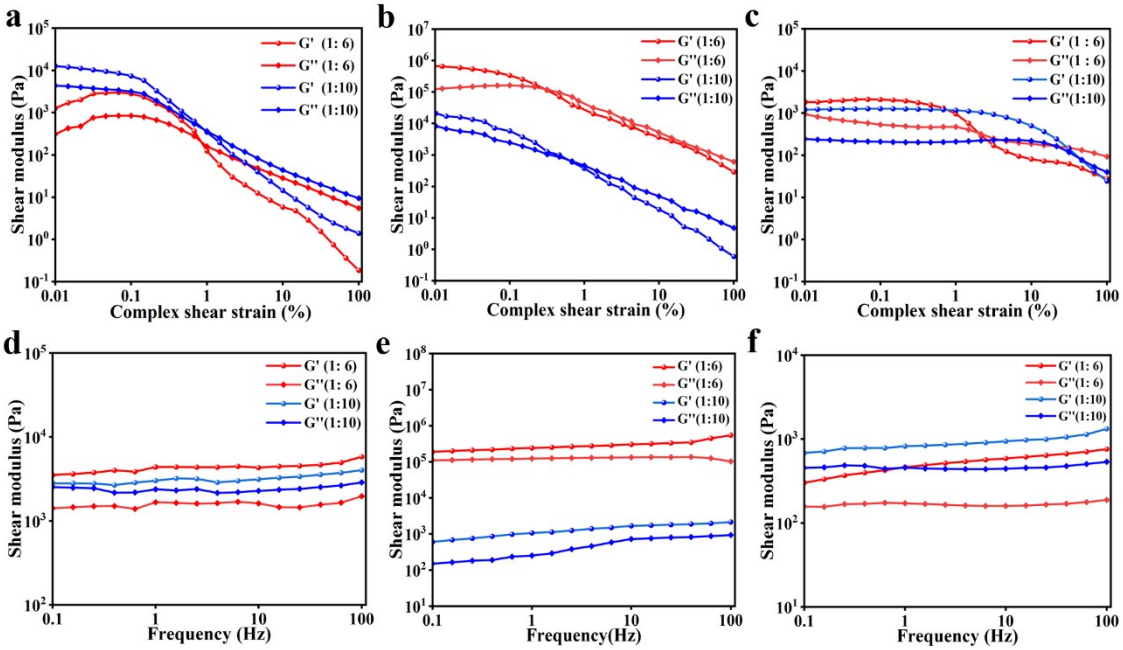

Fig. S6. Oscillatory rheology measurements of the DA-BET@surfactant hydrogels with different molar ratios of surfactant (DA-BET, 25 mg/mL). Dynamic strain sweep measurement of (a) DA-BET@CTAB hydrogel angular frequency at 10 rad/s; (b) DA-BET@SLS hydrogel angular frequency at 10 rad/s; the initial strength of anionic surfactant contained hydrogels are about three orders of magnitude higher than that of cationic surfactants. (c) DA-BET@SB3C16 hydrogel angular frequency at 10 rad/s. A higher concentration of zwitterionic surfactant makes it easier for the gel to maintain its state, but once the strain reaches around 46%, the gel collapses. And frequency sweep experiment of (d) DA-BET@CTAB hydrogel under a strain of 0.1%; (e) DA-BET@SLS hydrogel under a strain of 0.1%; (f) DA-BET@SB3C16 hydrogel under a strain of 0.1%. G′ is bigger than G″ within all the frequency range, showing frequency-dependent viscoelastic behavior, indicating that they possess characteristics of both dynamic and gel phases.

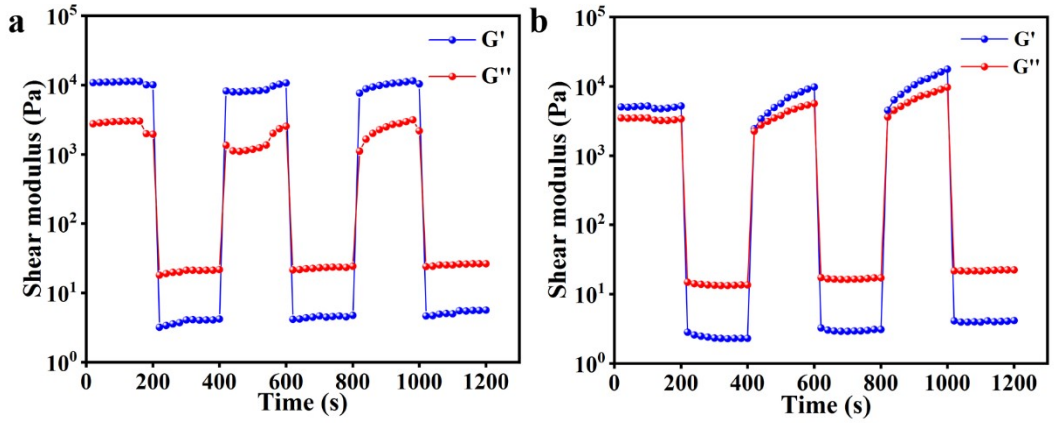

Fig. S7. Recovery test for the DA-BET@CTAB hydrogel, by applying alternating strain amplitudes of 0.1 % and 100 % (a and b). (a) n (DA-BET: CTAB) = 1:6. (b) n (DA-BET: CTAB) = 1:10. When the strain > 100%, the gel transforms into a sol with G″ > G′. When the strain is released, the sol recovers to the initial gel state with a value of 97% within 200 s. Notably, the value of recovered G' of supramolecular gel (DA-BET: CTAB = 1: 10) seems higher than that of the original one.

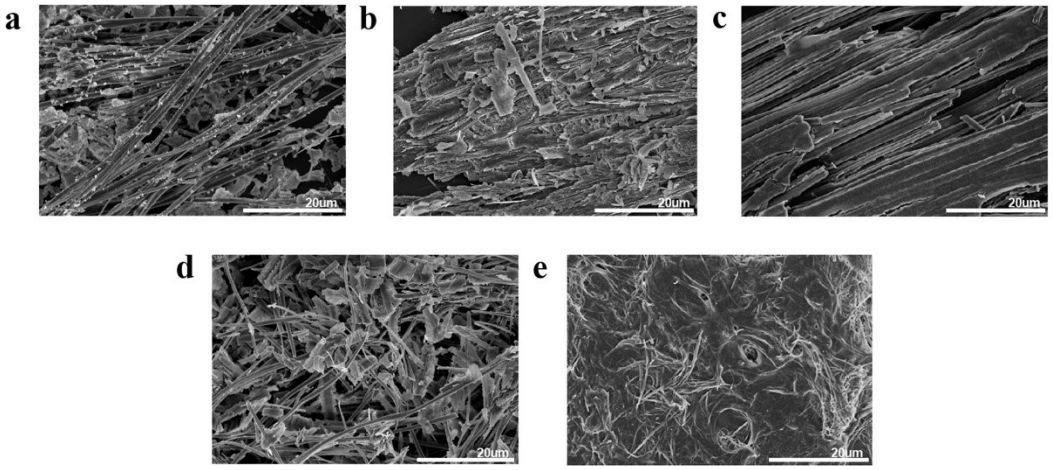

Fig. S8. SEM images of (a) DA-BET@CTAB hydrogel with molar ratio of 1:6; SEM images of DA-BET@SLS hydrogel (b, c) and DA-BET@SB3C16 hydrogel (d, e) with molar ratio of (b) 1:6, (c) 1:10, (d) 1:6 and (e) 1:10. DA-BET: 25 mg mL^{-1}. Scale bar: 20 μm.

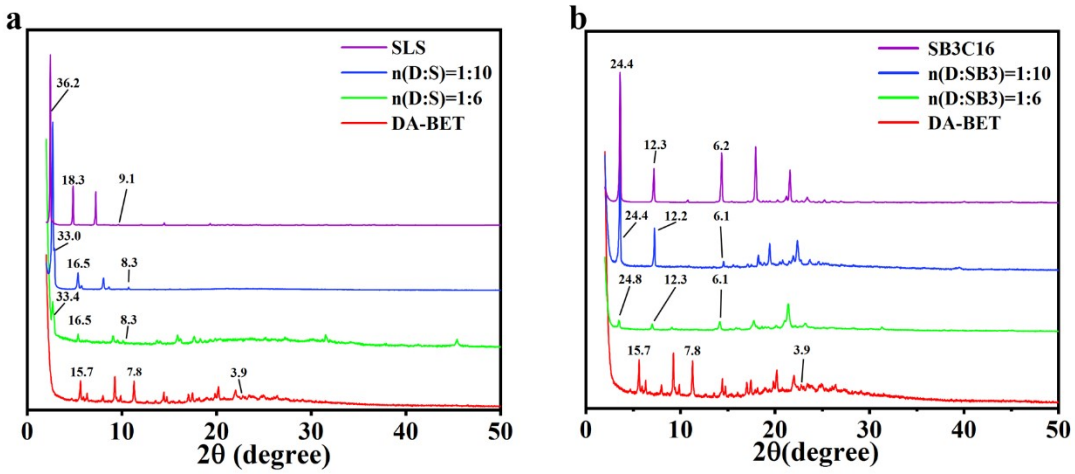

Fig. S9. XRD pattern of (a) SLS, and DA-BET in the presence of 0, 6, 10 molar ratios of SLS, the peaks at 33.4, 16.5, 8.3 Å (the molar ratio of DA-BET and SLS is 1:6, mass fraction of SLS is 62.5 wt%) and peaks at 33.0, 16.5, 8.3 Å (the molar ratio of DA-BET and SLS is 1:10, mass fraction of SLS is 73.5 wt%) are with the ratio of 1:1/2:1/4, indicating a lamellar structure of xerogels which formed by DA-BET and SLS, and (b) SB3C16, and DA-BET in the presence of 0, 6, 10 molar ratios of SB3C16, the peaks at 24.8, 12.3, 6.1 Å (the molar ratio of DA-BET and SB3C16 is 1:6, mass fraction of SB3C16 is 70.6 wt%) and peaks at 24.4, 12.2, 6.1 Å (the molar ratio of DA-BET and SB3C16 is 1:10, mass fraction of SB3C16 is 80.0 wt%) are with the ratio of 1:1/2:1/4, indicating a lamellar structure of the aggregation.

6. Datas of DFT calculations

6.1 Details of DFT calculations: All theoretical calculations are performed using the Gaussian 16 A.03 package[1] based on the density functional theory (DFT). The geometry optimizations and frequency calculations at each stable point are performed using the PBEPBE[2,3]-D3[4]/def2SVP[5,6] basis set. All calculated configuration frequencies are positive values, confirming that they are stable points. The views of various molecular conformations and the molecular electrostatic potential (MEP) maps are generated using Gauss View 6.0.16 software. Interacting molecules between DA-BET and various surfactant molecules are predicted according to the MEP, then the stable configurations are optimized and the interaction energies are determined.

1. M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li. M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewshi, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr. J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Lyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman and D. J. Fox, Gaussian 16, Revision A. 03; Gaussian. Inc.: Wallingford, CT, 2016.

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6. F. Weigend, *Phys. Chem. Chem. Phys*. 2006, **8**, 1057.

6.2 Datas of DFT calculations: The sum of electronic and zero-point energies of DA-BET, CTAB, SLS, SB3C16, and DA-BET combined with CTAB, SLS, and SB3C16 are as follows: E_D (hartree) = -3247.050353, E_C (hartree) = -801.586990, E_{SL} (hartree) = -1094.184847, E_{SB} (hartree) = -1502.682944, $E_{D\text{-}C}$ (hartree) = -4048.687253, $E_{D\text{-}SL}$ (hartree) = -4341.334706, $E_{D\text{-}SB}$ (hartree) = -4749.822783, respectively. The interaction energies between DA-BET and surfactants are calculated by the following equation (S represents surfactant):

$$E_{exD\text{-}S} = E_D + E_S - E_{D\text{-}S}$$

Table S3. Zero-point correction of molecular electronic energy and interaction energy

Surfactant	E_S (hartree)	$E_{D\text{-}S}$ (hartree)	$E_{exD\text{-}S}$ (hartree)	$E_{exD\text{-}S}$ (kcal/mol)
CTAB	-801.586990	-4048.687253	0.04991	31.3
SLS	-1094.184847	-4341.334706	0.099506	62.4
SB3C16	-1502.682944	-4749.822783	0.089486	56.2

Cartesian coordinates

DA-BET

C	4.37400100	-4.64225200	-0.92579000
C	5.50163600	-5.47494200	-1.01067500
C	6.77262100	-4.88089800	-1.00496600
C	6.86722400	-3.48707900	-0.92807900
C	5.68220800	-2.72361200	-0.86010200
N	4.45842200	-3.30195600	-0.84659400
H	7.68280500	-5.49796500	-1.06441000
H	3.34631500	-5.05199900	-0.92067900
H	5.37679000	-6.56603800	-1.07460900
H	7.83205300	-2.96216000	-0.92308100
C	5.75490200	-1.23286700	-0.79628600
C	4.62138900	-0.45155300	-1.08907100
C	7.01300700	0.64794300	-0.32882600
C	4.67344200	0.95303300	-0.94480500
H	3.70068800	-0.96537200	-1.39357200
N	6.93496700	-0.69143100	-0.43911000
C	5.91310500	1.49926800	-0.55597300
H	6.07232700	2.57970100	-0.43858400
C	8.33246000	1.22813200	0.06496200
C	9.43326200	0.38770500	0.34115200
C	10.65143100	0.97155300	0.70632300
H	9.30009000	-0.70003700	0.26553900
C	9.58363100	3.12021600	0.49582000
C	10.73666500	2.37021900	0.78648300
H	11.52704400	0.34179900	0.92842900
H	9.61090500	4.22381700	0.55054000
H	11.67312400	2.87386700	1.06953500
N	8.41350600	2.57342700	0.14537900
C	3.46867700	1.79090800	-1.14999600
C	3.30904000	3.03791000	-0.49187500
C	2.39792000	1.34643200	-1.95557100
C	2.13683700	3.78525200	-0.61586400
H	4.10757700	3.41238300	0.16609600
C	1.21647200	2.08285000	-2.09418000
H	2.48223600	0.39562000	-2.50217900
C	1.06904600	3.31214200	-1.41323400
H	2.00749400	4.73377100	-0.07596300
H	0.40378900	1.66364900	-2.69836700
O	-0.04693900	4.08720600	-1.45837200
C	-1.15114900	3.56236700	-2.17609900
H	-1.34806000	2.51222800	-1.86985200
H	-0.94116200	3.55578700	-3.27307300
C	-2.40135500	4.40196300	-1.91827000
O	-2.40489800	5.43136100	-1.25555700

N	-3.54521100	3.90802500	-2.53134700
H	-4.37334300	4.45985800	-2.28536500
C	-3.77176200	2.51690600	-2.90708900
H	-4.55705500	2.47557900	-3.68996000
H	-2.85528100	2.09926300	-3.36387700
C	-4.16816900	1.66978600	-1.67239900
H	-5.23032700	1.83799800	-1.41330100
H	-3.56696000	2.05610100	-0.82521400
N	-3.92180200	0.23724100	-1.77365500
H	-4.69502700	-0.39707000	-1.56323800
C	-2.63046800	-0.20841000	-1.62901300
O	-1.67990800	0.57780800	-1.60746900
C	-2.38107700	-1.69743200	-1.49701600
C	-3.32467000	-2.70190000	-1.78566600
C	-2.93426600	-4.04447700	-1.64700200
H	-4.34224500	-2.45788900	-2.12641500
C	-0.74984400	-3.26040300	-0.98778100
C	-1.62655700	-4.33745200	-1.24870500
H	-3.65226200	-4.85238700	-1.85270900
H	-1.24796200	-5.36494600	-1.15578500
N	-1.12823000	-1.98431600	-1.10549200
C	0.71453100	-3.56959500	-0.71878200
O	1.14016800	-4.69015200	-1.04529200
N	1.52697600	-2.60315900	-0.20672400
H	2.53958600	-2.82642000	-0.30580300
C	1.21800100	-1.30429000	0.38265700
H	1.11182000	-0.52030100	-0.40046100
H	0.23992600	-1.33088000	0.89982900
C	2.33471400	-0.92809800	1.36961300
H	2.28801900	-1.54003800	2.29273600
H	3.32631600	-1.13299100	0.90847700
N	2.24576000	0.46173800	1.77249800
H	2.01667900	1.16908300	1.06727800
C	2.44109300	0.85744200	3.06112200
O	2.78427500	0.11021000	3.97700400
C	2.17937800	2.35264800	3.34025900
H	1.93128200	2.43156600	4.42059200
H	3.11093400	2.92686500	3.15899400
O	1.19318700	2.97106000	2.51924800
C	-0.07120000	2.45585100	2.53226300
C	-0.46327000	1.34267000	3.30852900
C	-1.00766100	3.07354800	1.67577000
C	-1.72255500	0.77146700	3.10399400
H	0.21746300	0.88133800	4.03651100

C	-2.27738300	2.51585300	1.52345500
H	-0.71383500	3.95690800	1.09032600
C	-2.64089300	1.31391200	2.17955700
H	-1.99412300	-0.12666400	3.67899400
H	-2.97682500	3.00271200	0.82804700
C	-3.86396500	0.57186900	1.80865800
C	-3.84584400	-0.83942700	1.77220900
C	-5.05217800	1.20095600	1.38126100
C	-4.96070500	-1.54595000	1.28742700
H	-2.95705600	-1.41802000	2.05760900
C	-6.11643300	0.41710300	0.89158100
H	-5.16693500	2.29351200	1.39117200
N	-6.07288300	-0.92995000	0.83761200
C	-4.91259200	-3.03640100	1.20648500
C	-5.98144900	-3.76453500	0.63887500
C	-3.71838900	-4.97121600	1.60947700
C	-5.88304400	-5.15930300	0.56807400
H	-6.85861800	-3.21636500	0.26832300
C	-4.72694600	-5.78423200	1.06145200
H	-2.79189200	-5.42497100	2.00509000
H	-6.70071700	-5.75466900	0.13252700
H	-4.60459700	-6.87710400	1.02642800
C	-7.35445500	1.07313400	0.37472900
C	-8.54310700	0.33145000	0.19697000
C	-8.36764100	3.00439400	-0.39134600
C	-9.67904000	0.98625200	-0.29247500
H	-8.54532600	-0.73681100	0.45328100
C	-9.59720400	2.35491300	-0.59387500
H	-8.26166400	4.07965000	-0.62293000
H	-10.62224400	0.43600600	-0.43406000
H	-10.46467000	2.91129300	-0.97902200
N	-3.80299200	-3.63834100	1.68393000
N	-7.27318400	2.38879000	0.07630500

CTAB

N	-8.63889100	0.08019100	-0.00002700
C	-7.26780800	-0.61485900	0.00012900
H	-7.27161700	-1.27084300	0.89403300
H	-7.27150900	-1.27096400	-0.89369200
C	-6.04209600	0.28812500	0.00014400
H	-6.03518000	0.94839300	0.89318100
H	-6.03526000	0.94855300	-0.89278300
C	-4.75492700	-0.55537900	0.00002300
H	-4.75131500	-1.22597800	0.88821500

H	-4.75137800	-1.22584000	-0.88827400
C	-3.48264200	0.29944600	0.00004700
H	-3.49071700	0.97162800	0.88766900
H	-3.49073600	0.97170800	-0.88751500
C	-2.19381900	-0.52913400	-0.00000600
H	-2.18893200	-1.20244300	0.88695500
H	-2.18897700	-1.20239300	-0.88700800
C	-0.91886700	0.32073000	-0.00000800
H	-0.92585100	0.99462300	0.88671700
H	-0.92585700	0.99463200	-0.88672600
C	0.37197800	-0.50449800	-0.00001800
H	0.37761000	-1.17875700	0.88649900
H	0.37759100	-1.17876100	-0.88653300
C	1.64771000	0.34384000	-0.00003100
H	1.64097200	1.01836400	0.88638500
H	1.64097200	1.01834100	-0.88646500
C	2.93943400	-0.47990500	-0.00002100
H	2.94551400	-1.15455200	0.88633200
H	2.94550800	-1.15458200	-0.88635200
C	4.21547100	0.36792200	-0.00003800
H	4.20875400	1.04272700	0.88624500
H	4.20876600	1.04267800	-0.88635900
C	5.50766000	-0.45505600	-0.00000800
H	5.51396600	-1.12987300	0.88628400
H	5.51397000	-1.12993000	-0.88625600
C	6.78378400	0.39262600	-0.00003000
H	6.77694500	1.06754500	0.88620900
H	6.77696200	1.06747400	-0.88632400
C	8.07624800	-0.42993600	0.00001500
H	8.08243700	-1.10481600	0.88633900
H	8.08245000	-1.10489100	-0.88625300
C	9.35255500	0.41727600	-0.00001100
H	9.34625100	1.09251200	0.88628800
H	9.34627200	1.09242900	-0.88637500
C	-9.70229300	-0.98722000	0.00027600
H	-9.58601400	-1.61213300	0.90399800
H	-10.69803800	-0.50797900	0.00040900
H	-9.58634800	-1.61231000	-0.90336900
C	-8.80362200	0.93297200	-1.22970100
H	-8.05880800	1.74680400	-1.21633600
H	-8.65717300	0.30403600	-2.12652100
H	-9.82220700	1.36139200	-1.23377000
C	-8.80358900	0.93361700	1.22922900
H	-8.65685800	0.30517900	2.12636200

H	-8.05889700	1.74755300	1.21531200
H	-9.82225000	1.36181900	1.23321300
C	10.64629600	-0.40482200	0.00004200
H	10.64891800	-1.07894300	0.88596200
H	10.64893500	-1.07902800	-0.88581300
C	11.91452100	0.45090000	0.00001400
H	11.95780300	1.10871800	0.89353100
H	12.83178000	-0.17192000	0.00005500
H	11.95782300	1.10863000	-0.89356700

DA-BET@CTAB

C	6.89695300	6.01384900	-0.48608000
C	7.31691700	7.35383200	-0.48310100
C	6.34189700	8.36009600	-0.54952600
C	4.99388600	7.99211900	-0.62989900
C	4.65994200	6.62186000	-0.64310500
N	5.60270100	5.65422700	-0.55861000
H	6.62900300	9.42294100	-0.54362700
H	7.61797400	5.17708000	-0.42943900
H	8.38846800	7.59492900	-0.42460500
H	4.18600700	8.73376800	-0.68942800
C	3.23155300	6.19869800	-0.75456900
C	2.90425200	4.88266200	-1.13700700
C	0.99899900	6.76045400	-0.53021100
C	1.55263700	4.47831100	-1.17824600
H	3.72366300	4.19030600	-1.36896800
N	2.29365000	7.12186500	-0.47254100
C	0.58749400	5.45428500	-0.86526800
H	-0.49286200	5.25696300	-0.89106700
C	-0.02469700	7.80149900	-0.21413700
C	0.36684600	9.10719700	0.15164400
C	-0.62582300	10.05191600	0.43682200
H	1.43773700	9.34544200	0.20581700
C	-2.26019200	8.34131400	-0.01871800
C	-1.97247100	9.66720800	0.35003900
H	-0.35226500	11.07864500	0.72494600
H	-3.30933200	8.00259200	-0.09512500
H	-2.78670000	10.37548300	0.56399300
N	-1.32022600	7.42878600	-0.29354500
C	1.17730100	3.07922600	-1.50674300
C	-0.04405300	2.51471200	-1.06351600
C	2.04863900	2.23758100	-2.23171100
C	-0.36716400	1.18059600	-1.32402600
H	-0.74435600	3.12370200	-0.47331600

C	1.74303400	0.89774200	-2.49556900
H	3.00202100	2.63259000	-2.61101900
C	0.52694600	0.35439000	-2.03593100
H	-1.30827200	0.75462300	-0.94796400
H	2.48849500	0.28492600	-3.01480500
O	0.15011500	-0.95541100	-2.21684600
C	1.11349300	-1.80174300	-2.82671800
H	2.09892900	-1.70117900	-2.31799200
H	1.26503900	-1.52273000	-3.89804500
C	0.64300300	-3.24853600	-2.77788800
O	-0.52119300	-3.56113600	-2.48124600
N	1.57834500	-4.18104500	-3.12120800
H	1.23374600	-5.14438200	-3.06391300
C	3.02478700	-3.97707900	-3.19792800
H	3.44823600	-4.72421900	-3.89838200
H	3.23715900	-2.98320400	-3.63381400
C	3.67627600	-4.08076100	-1.79627500
H	3.78946300	-5.13749800	-1.48799600
H	2.96132800	-3.62156800	-1.08349800
N	4.94980100	-3.39552900	-1.65971000
H	5.74910500	-3.93027800	-1.31369200
C	4.94639100	-2.02685700	-1.53030300
O	3.90732800	-1.37711500	-1.69308100
C	6.24298300	-1.32680500	-1.19037200
C	7.51393900	-1.92645100	-1.27947900
C	8.64256200	-1.15001000	-0.96907200
H	7.64036000	-2.97200800	-1.59867700
C	7.15163000	0.70190200	-0.55035200
C	8.46701100	0.18776200	-0.60605900
H	9.64878700	-1.59213800	-1.01609700
H	9.30904500	0.85976600	-0.38928200
N	6.07560500	-0.04239500	-0.82820100
C	6.97934900	2.19669700	-0.32948400
O	7.94938200	2.93084800	-0.57351800
N	5.76863500	2.69318800	0.04862000
H	5.68946000	3.72697600	-0.07663600
C	4.57512600	2.02384300	0.54540300
H	3.91166000	1.70665500	-0.29210100
H	4.83922200	1.08804800	1.07438700
C	3.82379900	2.98285600	1.48560700
H	4.31577500	3.05816400	2.47589500
H	3.83053100	4.00800000	1.05421500
N	2.46061400	2.54311200	1.71178300
H	1.93398100	2.15529000	0.92344300

C	1.86595600	2.59707400	2.93679800
O	2.37153700	3.09306100	3.94094100
C	0.46887100	1.94384000	3.01018600
H	0.30042200	1.66798800	4.07291500
H	-0.30501900	2.68282700	2.71876800
O	0.28057800	0.83363000	2.13000600
C	1.15518000	-0.21218600	2.23255300
C	2.14648400	-0.33400600	3.23032600
C	1.06241800	-1.19511200	1.22669500
C	3.09382800	-1.36030400	3.13743400
H	2.22828200	0.39275600	4.04992700
C	1.98548400	-2.23959500	1.17857200
H	0.31190100	-1.07286300	0.43590100
C	3.05602700	-2.31471000	2.09837500
H	3.89231800	-1.41307900	3.89293100
H	1.91967500	-2.96832100	0.35795500
C	4.17627700	-3.25826800	1.88353600
C	5.50199700	-2.81450600	2.06099200
C	3.99634300	-4.57470400	1.41125700
C	6.57488900	-3.66313700	1.72891200
H	5.73712300	-1.79610900	2.39949900
C	5.12719800	-5.35723800	1.09913100
H	2.99765300	-5.00942200	1.26687100
N	6.39011100	-4.90716900	1.24438300
C	7.97645600	-3.16612300	1.86342900
C	9.07087100	-3.96879800	1.47555400
C	9.37119000	-1.43037300	2.47237700
C	10.36456800	-3.44771900	1.60358600
H	8.88073100	-4.97783300	1.08459000
C	10.52543600	-2.14910800	2.11109900
H	9.45743300	-0.40547100	2.87539100
H	11.23973800	-4.04911100	1.31265300
H	11.52209500	-1.69884200	2.23035600
C	4.96370300	-6.74412300	0.56906100
C	6.03820400	-7.65907500	0.61158100
C	3.58460000	-8.31099400	-0.42375900
C	5.84294200	-8.95260800	0.11391200
H	6.99580400	-7.33514700	1.04150100
C	4.58815100	-9.29395500	-0.41457800
H	2.58707600	-8.54154200	-0.83958700
H	6.65941900	-9.69047400	0.14257000
H	4.38755700	-10.29934700	-0.81336500
N	8.13117700	-1.91889600	2.35471100
N	3.75787800	-7.06826800	0.04943700

N	-3.32943800	-2.54164500	-0.86182100
C	-4.59079800	-2.15233300	-0.09733900
H	-4.59681100	-2.78637800	0.81260300
H	-4.42787700	-1.10602900	0.23201500
C	-5.91150900	-2.27587600	-0.84614600
H	-6.07553300	-3.32018100	-1.18673700
H	-5.90797000	-1.63776300	-1.75497400
C	-7.08565500	-1.85589500	0.05265300
H	-7.09643300	-2.48903600	0.96810000
H	-6.92566600	-0.81320500	0.40799700
C	-8.44468000	-1.95148400	-0.64886000
H	-8.60139300	-2.99380000	-1.00795100
H	-8.43204900	-1.31727800	-1.56400400
C	-9.62052800	-1.53746000	0.24174900
H	-9.63085700	-2.17294400	1.15627400
H	-9.45931600	-0.49660600	0.60362100
C	-10.98252300	-1.62733000	-0.45409800
H	-11.14196700	-2.66775400	-0.81833800
H	-10.97180700	-0.99045300	-1.36778700
C	-12.15873200	-1.21612100	0.43732500
H	-12.16875000	-1.85417400	1.35027800
H	-11.99690400	-0.17665200	0.80342300
C	-13.52208600	-1.30240000	-0.25609800
H	-13.68285600	-2.34150000	-0.62386100
H	-13.51215600	-0.66305800	-1.16821500
C	-14.69805400	-0.89338100	0.63660600
H	-14.70778800	-1.53364300	1.54811500
H	-14.53585600	0.14506800	1.00567300
C	-16.06215900	-0.97727600	-0.05561700
H	-16.22364000	-2.01543200	-0.42588400
H	-16.05260200	-0.33600700	-0.96645100
C	-17.23791100	-0.56993600	0.83811500
H	-17.24738700	-1.21185300	1.74851200
H	-17.07553900	0.46779900	1.20922900
C	-18.60238600	-0.65235900	0.14643900
H	-18.76412800	-1.68992700	-0.22544600
H	-18.59288500	-0.00977100	-0.76350100
C	-19.77806600	-0.24616100	1.04080100
H	-19.78714100	-0.88921000	1.95047200
H	-19.61544300	0.79116700	1.41310900
C	-21.14280100	-0.32766400	0.34975500
H	-21.30531200	-1.36500500	-0.02313000
H	-21.13388400	0.31566700	-0.55995400
C	-2.14063900	-2.32707600	0.04044200

H	-2.23677000	-2.98019000	0.92632900
H	-1.23302100	-2.57320400	-0.53891600
H	-2.11577500	-1.26956600	0.35912600
C	-3.14639000	-1.69092100	-2.09256900
H	-3.95403000	-1.91158000	-2.81110700
H	-3.18332900	-0.62702100	-1.79635700
H	-2.15575500	-1.93298300	-2.52152600
C	-3.36257600	-3.99285200	-1.26629100
H	-2.39778300	-4.23125000	-1.75048400
H	-3.51156500	-4.60860600	-0.36052200
H	-4.19604100	-4.15433600	-1.97124100
C	-22.31964200	0.07808000	1.24419600
H	-22.32520600	-0.56573000	2.15237400
H	-22.15363200	1.11416100	1.61608500
C	-23.67746900	-0.00662700	0.54430900
H	-23.88762300	-1.03928600	0.19438100
H	-24.50696700	0.29275500	1.21636400
H	-23.71441400	0.65506700	-0.34664700

SLS

C	-9.53689900	-0.58342800	-0.00000300
H	-9.55598000	-1.24319100	-0.89320700
H	-9.55598300	-1.24319100	0.89320200
H	-10.47688200	0.00563000	-0.00000500
C	-8.29863600	0.31562500	0.00000000
H	-8.32538200	0.98962700	-0.88575400
H	-8.32538400	0.98962700	0.88575300
C	-6.97631100	-0.45959300	0.00000200
H	-6.94655800	-1.13458100	0.88616400
H	-6.94655800	-1.13458500	-0.88615800
C	-5.72960600	0.43071300	0.00000100
H	-5.75987800	1.10547800	0.88616700
H	-5.75987800	1.10547500	-0.88616700
C	-4.40812400	-0.34454800	0.00000100
H	-4.37789800	-1.01938200	-0.88601300
H	-4.37789900	-1.01938000	0.88601700
C	-3.16122200	0.54574500	0.00000000
H	-3.19199700	1.22071100	0.88609500
H	-3.19199800	1.22071000	-0.88609500
C	-1.83939600	-0.22899200	0.00000000
H	-1.80924700	-0.90409700	-0.88586900
H	-1.80924700	-0.90409700	0.88587100
C	-0.59148100	0.66013500	0.00000000
H	-0.62274200	1.33546000	0.88614900

H	-0.62274200	1.33545900	-0.88614900
C	0.73029300	-0.11434000	0.00000000
H	0.76249700	-0.78964100	-0.88553500
H	0.76249700	-0.78964000	0.88553600
C	1.98181400	0.77054900	0.00000000
H	1.95207900	1.44601400	0.88687200
H	1.95207800	1.44601300	-0.88687400
C	3.29316700	-0.02082200	0.00000000
H	3.34323300	-0.69096300	-0.88673300
H	3.34323400	-0.69096200	0.88673400
C	4.55606700	0.82811100	-0.00000100
H	4.63300100	1.47211900	0.90162100
H	4.63300100	1.47211800	-0.90162400
S	6.08169400	-0.23560000	0.00000000
O	5.94764200	-1.03986900	1.26637800
O	5.94764200	-1.03987200	-1.26637700
O	7.21090800	0.75398300	-0.00000100

DA-BET@SLS

C	-5.07541600	3.68363100	2.03050200
C	-6.29618900	4.32344600	2.30517500
C	-7.48760300	3.62905500	2.04441400
C	-7.41910900	2.33929800	1.50428200
C	-6.15112700	1.77670700	1.24685500
N	-5.00661200	2.44080400	1.52635100
H	-8.46479900	4.09357100	2.25066700
H	-4.09674600	4.17332100	2.19678300
H	-6.30366800	5.34440000	2.71496700
H	-8.31491400	1.75146000	1.26178400
C	-6.02682900	0.43357800	0.60873600
C	-4.77580200	0.01100600	0.13059300
C	-7.03115400	-1.50310700	-0.13232500
C	-4.62654400	-1.25165100	-0.48279600
H	-3.92977900	0.69602800	0.24612700
N	-7.14291200	-0.30838200	0.48072100
C	-5.80878900	-2.01270500	-0.61503800
H	-5.82944300	-2.99466800	-1.10598100
C	-8.28639400	-2.29484300	-0.30375100
C	-9.50956900	-1.82096200	0.22191700
C	-10.66808900	-2.57937100	0.02543900
H	-9.51191600	-0.86843600	0.76866500
C	-9.31440500	-4.17582400	-1.16416700
C	-10.57736700	-3.78651000	-0.68579400
H	-11.63504100	-2.23279200	0.42282500

H	-9.20115900	-5.12116900	-1.72614600
H	-11.46174300	-4.41586700	-0.86709600
N	-8.19911900	-3.45856800	-0.98306400
C	-3.30187700	-1.71954100	-0.94709600
C	-3.05366000	-3.07601900	-1.28296900
C	-2.21066000	-0.82472300	-1.05006100
C	-1.79631600	-3.50437600	-1.70723600
H	-3.86042100	-3.81870900	-1.19595300
C	-0.94009200	-1.23719500	-1.45718800
H	-2.33895300	0.24036300	-0.80998600
C	-0.71889500	-2.59045200	-1.80383000
H	-1.61013700	-4.55671300	-1.96693600
H	-0.12293800	-0.50541300	-1.44952800
O	0.46484800	-3.08693600	-2.22837100
C	1.52484000	-2.14901900	-2.36439400
H	1.68991300	-1.59200600	-1.40789800
H	1.26542800	-1.40006700	-3.14859000
C	2.82534400	-2.85991700	-2.72136800
O	2.95106700	-4.08246100	-2.72559500
N	3.86327900	-2.00141500	-3.01974800
H	4.75791600	-2.49480100	-3.10821700
C	3.90825100	-0.57562900	-2.70658400
H	4.57002900	-0.06888300	-3.43880000
H	2.90368600	-0.13639900	-2.85555100
C	4.37502300	-0.29036900	-1.25027300
H	5.47017900	-0.13376400	-1.22475100
H	4.14275400	-1.19798900	-0.66305500
N	3.74729900	0.83546000	-0.59610000
H	4.26790300	1.75701800	-0.63712500
C	2.58643100	0.65803500	0.08664400
O	1.95805100	-0.41736200	0.10846700
C	2.06295500	1.85316700	0.85364800
C	2.90678700	2.86355700	1.34930400
C	2.33018600	3.94345400	2.03510900
H	3.99021200	2.85898400	1.16985900
C	0.18371100	2.90196900	1.69203200
C	0.94227300	3.97884000	2.20088400
H	2.98355400	4.75713900	2.38357100
H	0.42288500	4.81632700	2.68840700
N	0.72898800	1.86566000	1.03961100
C	-1.32490400	2.96027000	1.78501300
O	-1.90021100	4.06166600	1.71644200
N	-2.01272400	1.78961000	1.91561300
H	-3.04155400	1.90703800	1.82731900

C	-1.49628600	0.44815400	2.16848700
H	-1.12278100	-0.02596200	1.23634300
H	-0.61219300	0.49253700	2.83527200
C	-2.59509700	-0.41909400	2.80395000
H	-2.72056200	-0.20117100	3.88316300
H	-3.57096200	-0.20555700	2.31421900
N	-2.29972400	-1.83228200	2.69190400
H	-2.09357100	-2.22152700	1.76623700
C	-2.24047000	-2.66504300	3.76796800
O	-2.46276900	-2.33592400	4.93337200
C	-1.91193700	-4.13050900	3.42679300
H	-1.34842000	-4.55084500	4.28797700
H	-2.87093000	-4.68410200	3.34946900
O	-1.24834500	-4.33990300	2.19073700
C	0.07945400	-3.99346200	2.10351400
C	0.79691900	-3.32529100	3.11610300
C	0.72535300	-4.32927400	0.89769900
C	2.13340700	-2.97054400	2.88960100
H	0.32545700	-3.05264000	4.07046000
C	2.06103300	-3.98226300	0.69244500
H	0.15078100	-4.84208100	0.11432900
C	2.79140100	-3.27804000	1.68070600
H	2.67639300	-2.43575400	3.68304200
H	2.51652800	-4.22326900	-0.28015100
C	4.16691600	-2.79833200	1.41106500
C	4.63692500	-1.59380900	1.97427900
C	5.01982400	-3.44858400	0.49202800
C	5.87087700	-1.05522000	1.55497000
H	4.02316800	-0.98819900	2.65428900
C	6.25979000	-2.86413300	0.16905000
H	4.73653900	-4.38003200	-0.01662100
N	6.67478100	-1.68892400	0.68014700
C	6.23234200	0.33908800	1.95100300
C	7.12242300	1.09274000	1.15686900
C	5.77172700	2.16480700	3.28032300
C	7.27302800	2.45844800	1.42010700
H	7.61231200	0.61371000	0.29859200
C	6.58726500	3.01167400	2.51063500
H	5.21446200	2.56862700	4.14576900
H	7.85415000	3.10231700	0.74293700
H	6.62704700	4.09139600	2.70916100
C	7.15370700	-3.50851500	-0.83863800
C	8.41566000	-2.94541300	-1.13940500
C	7.46589600	-5.19302200	-2.38894600

C	9.21240900	-3.55791700	-2.11233300
H	8.72667100	-2.04003600	-0.59999600
C	8.73242200	-4.70836700	-2.75964100
H	7.04941100	-6.09409700	-2.87573900
H	10.19937800	-3.14025600	-2.36699700
H	9.32189100	-5.22071100	-3.53521400
N	5.57408700	0.86830400	3.00511500
N	6.69611300	-4.61832900	-1.45729600
C	-9.08519100	0.53084400	-2.78754200
H	-8.66414500	-0.49485400	-2.73179600
H	-9.35032900	0.81998800	-1.74876300
H	-10.02464700	0.47694600	-3.37533700
C	-8.07912200	1.51105900	-3.39647100
H	-7.83080300	1.19604000	-4.43539800
H	-8.54429800	2.51835400	-3.49460100
C	-6.78861700	1.62722300	-2.57999600
H	-7.04234700	1.96266700	-1.55015100
H	-6.34495200	0.61358900	-2.45511100
C	-5.73258800	2.56837100	-3.16758700
H	-6.15481400	3.59629800	-3.25298800
H	-5.49625600	2.25549300	-4.21086000
C	-4.43901600	2.61080100	-2.34729900
H	-4.03390200	1.57672400	-2.26761700
H	-4.66970800	2.91605400	-1.30206300
C	-3.34802600	3.52522900	-2.91190100
H	-3.73575100	4.56706200	-2.98966700
H	-3.11489500	3.21509500	-3.95694600
C	-2.06149800	3.51561500	-2.08006800
H	-1.72728200	2.46051200	-1.94644100
H	-2.27327200	3.88690700	-1.05206900
C	-0.90271100	4.31797600	-2.68484400
H	-1.20180900	5.38552900	-2.79683900
H	-0.70239500	3.95251200	-3.71897300
C	0.37529700	4.21524200	-1.84989500
H	0.59965700	3.13752800	-1.68052300
H	0.18039600	4.62338000	-0.83295200
C	1.62955800	4.88183100	-2.43327900
H	1.47151600	5.97966000	-2.53701200
H	1.81331100	4.49975300	-3.46399800
C	2.83736300	4.58671900	-1.53937100
H	2.91121800	3.48461400	-1.42614800
H	2.64235300	4.97461300	-0.51899000
C	4.20959900	5.08500400	-1.97139800
H	4.30502400	6.19003500	-1.94868900

H	4.51034700	4.72086800	-2.97539000
S	5.49297900	4.44026400	-0.80986400
O	5.06102800	4.92352000	0.55039500
O	5.37117900	2.92355200	-0.96882100
O	6.81010800	4.95506800	-1.28230900

SB3C16

C	15.30817900	-0.19914300	-0.00832900
H	15.36928400	-0.86387700	-0.89573300
H	15.37306200	-0.84709800	0.89113600
H	16.20642500	0.45097900	-0.01633500
C	14.01438700	0.61752000	-0.01327000
H	13.99855500	1.29988900	0.86619600
H	13.99474500	1.28310900	-0.90542900
C	12.74610300	-0.24322900	-0.00238500
H	12.76213200	-0.90976400	0.89038900
H	12.75858800	-0.92694800	-0.88212700
C	11.44454100	0.56462300	-0.00765700
H	11.42843100	1.23062300	-0.90058200
H	11.43218000	1.24832300	0.87184800
C	10.17749100	-0.29649500	0.00363100
H	10.19277700	-0.96201400	0.89688400
H	10.18967700	-0.98066900	-0.87546500
C	8.87605500	0.51174800	-0.00267800
H	8.86023300	1.17678800	-0.89625500
H	8.86366400	1.19632600	0.87607300
C	7.60927700	-0.34972600	0.00927500
H	7.62438900	-1.01396300	0.90345500
H	7.62203300	-1.03505400	-0.86888400
C	6.30777600	0.45839200	0.00126700
H	6.29202300	1.12190500	-0.89339600
H	6.29480300	1.14422600	0.87897600
C	5.04150000	-0.40380800	0.01410700
H	5.05619300	-1.06614800	0.90964300
H	5.05495900	-1.09066400	-0.86279100
C	3.73999500	0.40427200	0.00366300
H	3.72426100	1.06560300	-0.89251300
H	3.72599300	1.09169400	0.88000700
C	2.47466300	-0.45929700	0.01760000
H	2.48863200	-1.11898800	0.91497200
H	2.48894700	-1.14795300	-0.85774400
C	1.17343300	0.34928400	0.00393000
H	1.15762000	1.00752200	-0.89429100
H	1.15783400	1.03836200	0.87871000

C	-0.08992600	-0.51710100	0.01916500
H	-0.07759400	-1.17289400	0.91904400
H	-0.07529100	-1.20726200	-0.85464000
C	-1.38944000	0.29454400	0.00144000
H	-1.40522000	0.94830500	-0.89931100
H	-1.40724100	0.98409800	0.87507900
C	-2.64968800	-0.58442500	0.01788100
H	-2.62515800	-1.22909900	0.92168700
H	-2.62386800	-1.26368200	-0.86052900
C	-3.90847900	0.27637300	0.00179300
H	-3.91872100	0.93283600	-0.89157500
H	-3.93631400	0.93759900	0.89137300
N	-5.24648000	-0.44935200	-0.00920700
C	-6.36179300	0.63521300	0.04279200
H	-6.13136100	1.32265000	-0.79708400
H	-6.18132900	1.18215100	0.99117900
C	-7.77263200	0.10394600	-0.03832100
H	-8.00902400	-0.61896200	0.77420500
H	-7.98340100	-0.41398100	-0.99870900
C	-8.83112300	1.19275800	0.08002100
H	-8.80759700	1.91980500	-0.75686000
H	-8.79822100	1.72965700	1.04981400
S	-10.47940300	0.28724400	-0.00237000
O	-11.49839000	1.36737000	0.11368700
O	-10.38389800	-0.39241300	-1.34116900
O	-10.36781000	-0.64456000	1.17476100
C	-5.39872900	-1.26049200	-1.26285300
H	-6.38759000	-1.74934700	-1.25614500
H	-5.33225100	-0.58498100	-2.13513200
H	-4.60073100	-2.02151900	-1.30854600
C	-5.37548600	-1.34621800	1.18744900
H	-5.20329100	-0.74906800	2.10142300
H	-6.39739100	-1.76191500	1.20948000
H	-4.63588300	-2.16265400	1.12151000

DA-BET@SB3C16

C	-4.02449400	-2.66047600	-2.48278600
C	-5.21927000	-3.01065600	-3.13579800
C	-6.34450400	-2.19254900	-2.95057500
C	-6.24601700	-1.07842800	-2.10712700
C	-5.00957200	-0.80888700	-1.47935400
N	-3.91669100	-1.58250000	-1.68724400
H	-7.30632600	-2.41689300	-3.43728400
H	-3.10186100	-3.26199000	-2.58587700

H	-5.25451100	-3.90182600	-3.78005200
H	-7.11895200	-0.43999600	-1.90824200
C	-4.87647500	0.35500100	-0.55315900
C	-3.65006600	0.66823100	0.05890400
C	-5.91153700	2.17967700	0.43340400
C	-3.52605100	1.85295300	0.81976100
H	-2.79273000	0.00624700	-0.10425400
N	-5.98931700	1.08281200	-0.34243200
C	-4.69328100	2.62319000	0.99347700
H	-4.71226000	3.54535700	1.59077000
C	-7.18497900	2.90506000	0.71790500
C	-8.42400400	2.38280900	0.28889300
C	-9.59889100	3.06184700	0.63809300
H	-8.48057500	1.44911100	-0.28749800
C	-8.21089500	4.70254400	1.73540200
C	-9.49383000	4.25354100	1.36978800
H	-10.56529900	2.61890300	0.35371100
H	-8.09281500	5.63815500	2.31242200
H	-10.38654000	4.82599800	1.66478000
N	-7.08375500	4.04755000	1.43384900
C	-2.21064200	2.25877200	1.36810400
C	-1.85995600	3.62372800	1.52663000
C	-1.22959100	1.29686700	1.69359000
C	-0.59129100	4.00306100	1.96777500
H	-2.58792700	4.40556000	1.26175100
C	0.04547800	1.65810300	2.14260700
H	-1.46397400	0.22548500	1.60554800
C	0.38166200	3.02437500	2.27718400
H	-0.31427700	5.06278000	2.06003700
H	0.77610600	0.86663100	2.34826300
O	1.59471800	3.48229500	2.68301800
C	2.60153100	2.50775200	2.89881800
H	2.68828600	1.84416400	2.01113300
H	2.35042500	1.86690300	3.77882500
C	3.94392200	3.19053100	3.16052300
O	4.07672400	4.39921100	3.29442300
N	5.01068400	2.30915300	3.27486500
H	5.90000500	2.80223800	3.40207700
C	5.07277500	0.96159400	2.72736100
H	5.81619700	0.37042900	3.30149700
H	4.10140800	0.45214200	2.87438100
C	5.42507800	0.97219800	1.21592500
H	6.51427900	1.08964700	1.06731400
H	4.94122100	1.86903000	0.78325300

N	4.96244800	-0.18556600	0.46871300
H	5.64770000	-0.79675600	0.02266600
C	3.63422300	-0.27314800	0.13903700
O	2.82723500	0.58438900	0.50945000
C	3.14444400	-1.48447100	-0.62976500
C	3.92333400	-2.60773900	-0.96658900
C	3.29132900	-3.69507600	-1.59363900
H	4.99857800	-2.65907200	-0.74092300
C	1.22619000	-2.45398100	-1.49588500
C	1.91765400	-3.63396400	-1.85008500
H	3.87546900	-4.58463600	-1.87265700
H	1.35764600	-4.46590300	-2.29975800
N	1.83207800	-1.42003500	-0.90617000
C	-0.28117900	-2.40445100	-1.67554500
O	-0.90478100	-3.47947500	-1.73413500
N	-0.91076800	-1.19845700	-1.72732600
H	-1.95015000	-1.28670600	-1.68877900
C	-0.37830500	0.16160800	-1.73501900
H	-0.14837000	0.50042500	-0.69990500
H	0.59082800	0.20189500	-2.26676100
C	-1.39226200	1.11447500	-2.39129400
H	-1.33751500	1.08438300	-3.49815500
H	-2.42854200	0.80959100	-2.12751300
N	-1.15256800	2.48588800	-1.98570300
H	-0.86232100	2.67333100	-1.02076700
C	-1.26629100	3.53104700	-2.85214100
O	-1.66007900	3.43276000	-4.01366300
C	-0.83214900	4.90024600	-2.28745600
H	-0.56006200	5.53038700	-3.16126400
H	-1.69236600	5.37628400	-1.77398500
O	0.20795800	4.85705500	-1.31418200
C	1.40519600	4.30917900	-1.67728000
C	1.67599800	3.77632400	-2.95735500
C	2.39714500	4.25189400	-0.67496300
C	2.85994600	3.06346700	-3.16885800
H	0.95461100	3.86395400	-3.78081100
C	3.59352600	3.57878700	-0.92326500
H	2.19587700	4.68747100	0.31458900
C	3.82467400	2.90998600	-2.15028700
H	3.03239100	2.60738100	-4.15550800
H	4.33432600	3.51856200	-0.11260100
C	4.93886500	1.95060100	-2.30384000
C	4.72726500	0.74516400	-3.00796700
C	6.19508200	2.10796900	-1.68120900

C	5.72216600	-0.24830900	-3.01872900
H	3.77170200	0.51964500	-3.50026100
C	7.12914500	1.05245500	-1.72401200
H	6.45966300	3.01867800	-1.12657900
N	6.89670900	-0.10765800	-2.37180600
C	5.45933500	-1.54883000	-3.70448200
C	6.41421400	-2.58911500	-3.67349300
C	3.98437400	-2.84742200	-4.91768000
C	6.10793400	-3.80332300	-4.29966300
H	7.36871200	-2.41803100	-3.15699700
C	4.86466500	-3.94441300	-4.93587300
H	2.99677800	-2.91880400	-5.40798500
H	6.83261000	-4.63248800	-4.29300200
H	4.57952600	-4.88007900	-5.43966600
C	8.42535000	1.16514900	-0.98947300
C	9.45600500	0.22086900	-1.19332500
C	9.69225100	2.30653700	0.57216500
C	10.64613500	0.35493300	-0.46929100
H	9.29622900	-0.59099100	-1.91567800
C	10.77573500	1.42245300	0.43331700
H	9.75292500	3.15505900	1.27739500
H	11.46651000	-0.36678300	-0.60465000
H	11.69376400	1.56909300	1.02172000
N	4.26699200	-1.68322600	-4.32297800
N	8.54671000	2.18563800	-0.11158200
C	12.33198900	-1.58350700	2.67713200
H	12.21606300	-0.67381900	2.05197000
H	12.53086300	-2.43185400	1.98860200
H	13.23559300	-1.44433800	3.30433400
C	11.08318000	-1.83524300	3.52436900
H	11.24828700	-2.72093700	4.17797900
H	10.92339900	-0.98007700	4.21887300
C	9.81146200	-2.05417300	2.69693800
H	9.97396100	-2.90268800	1.99297800
H	9.63327800	-1.16427600	2.05019000
C	8.56220400	-2.33024500	3.54015100
H	8.39020400	-1.47590200	4.23447300
H	8.74474800	-3.21195700	4.19554200
C	7.29764500	-2.56833300	2.71072300
H	7.46459100	-3.42656600	2.02022000
H	7.13109000	-1.68712400	2.04745800
C	6.02751900	-2.81810700	3.53339000
H	5.87621400	-1.96801700	4.23809400
H	6.16539100	-3.71569200	4.17732200

C	4.78120700	-2.97184000	2.65809200
H	4.89901400	-3.85675200	1.99197300
H	4.73488400	-2.09712800	1.97638400
C	3.44368900	-3.06849100	3.39887100
H	3.38939100	-2.26536800	4.16974100
H	3.38392400	-4.02730100	3.96182600
C	2.24530800	-2.93592300	2.45150600
H	2.34903200	-3.66593600	1.61684500
H	2.27799900	-1.93484500	1.96743400
C	0.87673600	-3.11497500	3.10887600
H	0.78298000	-2.40903300	3.96613700
H	0.80606700	-4.13387100	3.55381600
C	-0.29511100	-2.89534300	2.14590100
H	-0.19708400	-3.57145000	1.26698700
H	-0.23509900	-1.86579100	1.72391700
C	-1.66189300	-3.10886000	2.80226500
H	-1.73299300	-2.47887700	3.71872600
H	-1.73322200	-4.16174900	3.15950000
C	-2.84937800	-2.79964700	1.88851700
H	-2.75573100	-3.36860600	0.93696000
H	-2.81552700	-1.72899000	1.58834600
C	-4.20701700	-3.08797100	2.54044500
H	-4.26721300	-2.56118200	3.51979900
H	-4.28457600	-4.17405900	2.77465500
C	-5.37933800	-2.65578900	1.65213500
H	-5.27170900	-3.14753500	0.66410300
H	-5.29628400	-1.56575000	1.46516800
C	-6.73208300	-2.98610900	2.27516400
H	-6.80443400	-2.55494700	3.29463900
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H	-9.22652600	-4.03988200	2.10248400
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C	-11.15976100	-2.38302500	0.51352900
H	-12.26269100	-2.37257200	0.59759900
H	-10.87764100	-3.28473600	-0.06613300
S	-10.87774500	-0.87631300	-0.57466800
O	-12.03748800	-0.88360000	-1.49805500
O	-10.82824900	0.24883100	0.43491400
O	-9.52992800	-1.07878800	-1.25116900

C	-7.91536400	-0.95986300	1.47294900
H	-8.86012900	-0.56220100	1.05966300
H	-7.76425200	-0.59230000	2.50501300
H	-7.09440100	-0.62037600	0.82044900
C	-7.94240900	-3.04791800	0.12284200
H	-8.09099300	-4.14028800	0.20291400
H	-8.71649100	-2.53161000	-0.48983500
H	-6.96991100	-2.83136200	-0.34394300

7. Application of the supramolecular hydrogel

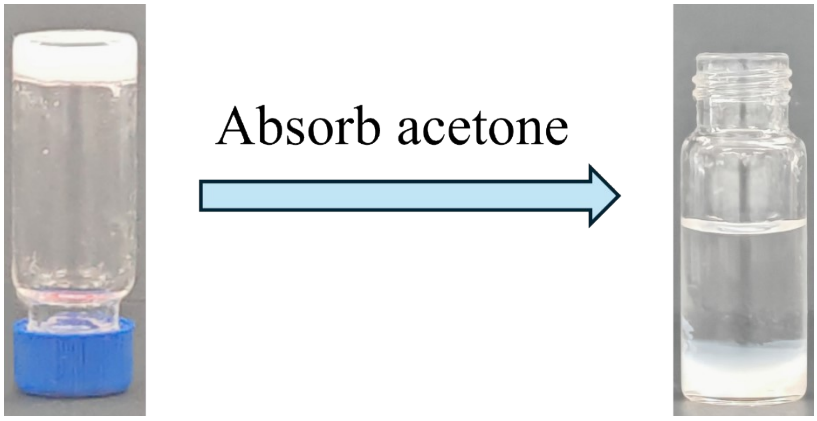

Fig.S10 The photographs show the hydrogel absorbing acetone until equilibrium is reached. After absorbing acetone, a layer of liquid is observed floating on the gel surface, where phase separation is clearly visible.

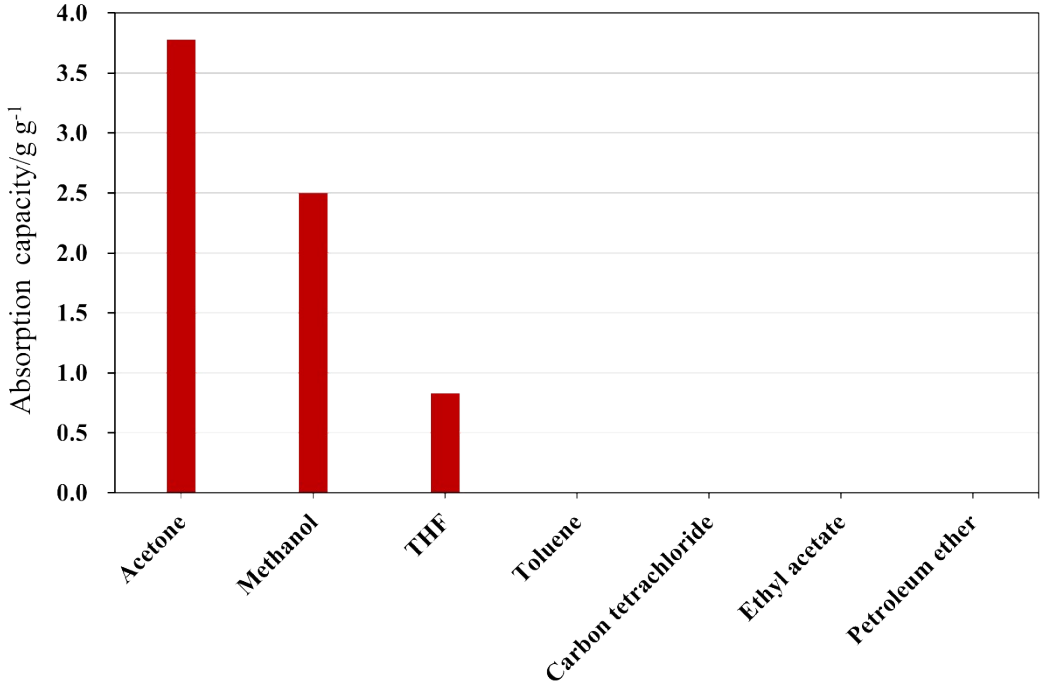

Fig.S11 The absorption capacity (g g^{-1}) of the hydrogels toward seven tested organic solvents at room temperature. The gel placed in an open vial is exposed to organic solvent vapors in a closed flask for one week.

Table S4 The mass variations of hydrogels and surface-bound liquids during acetone and methanol absorption are investigated.

Mass / Organic solvents	M_0	M_1
Acetone	0.2102 g	0.9609 g
Methanol	0.2007 g	0.7019 g

M_0, the initial mass of hydrogel before absorption of acetone or methanol; M_1: Total masses of the hydrogel and the liquid after adsorption equilibrium.

8. Spectra of compound 4

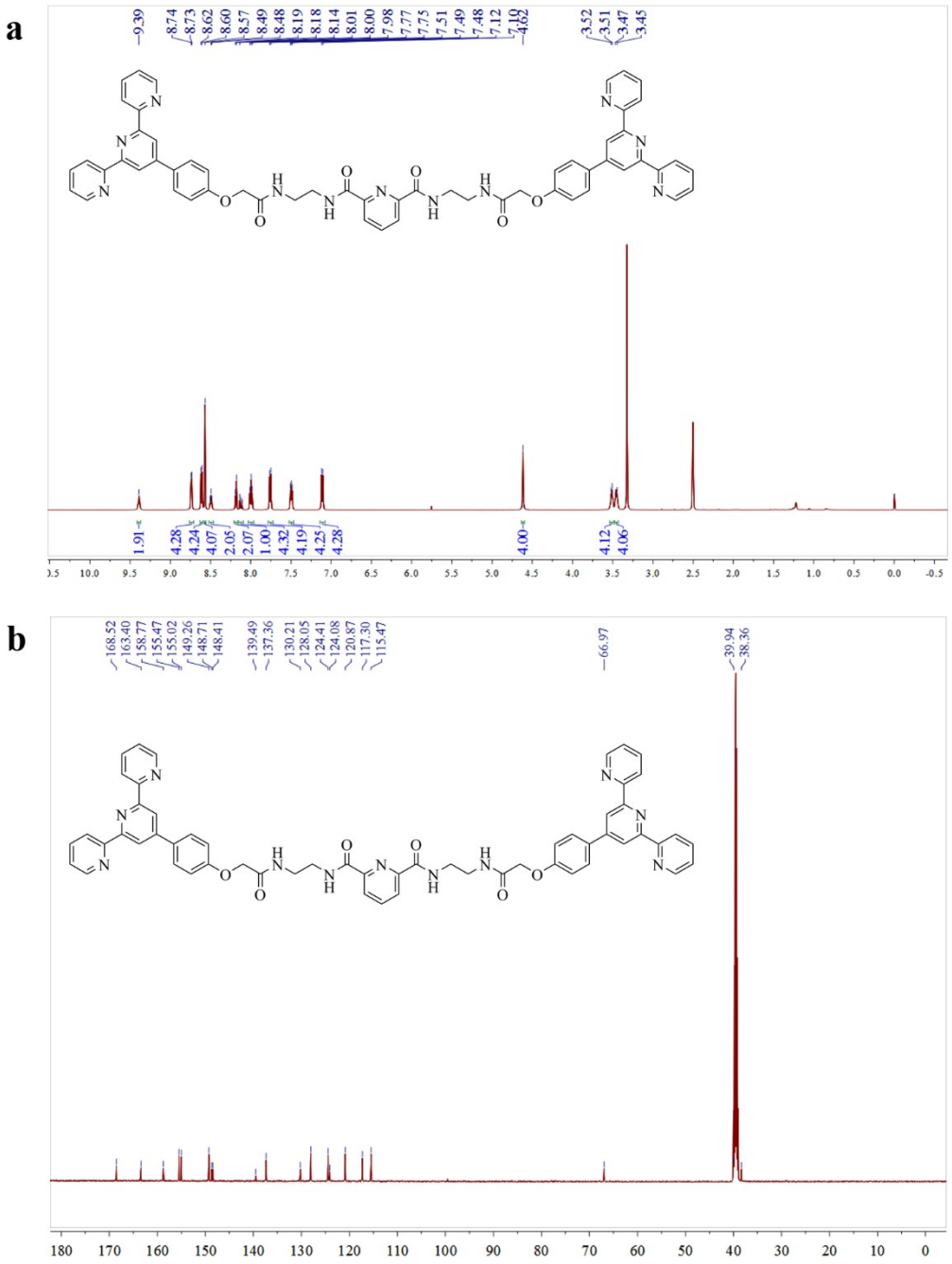

Fig. S12 (a) ^{1}H NMR spectra of compound **4**. (b) ^{13}C NMR spectra of compound **4**.

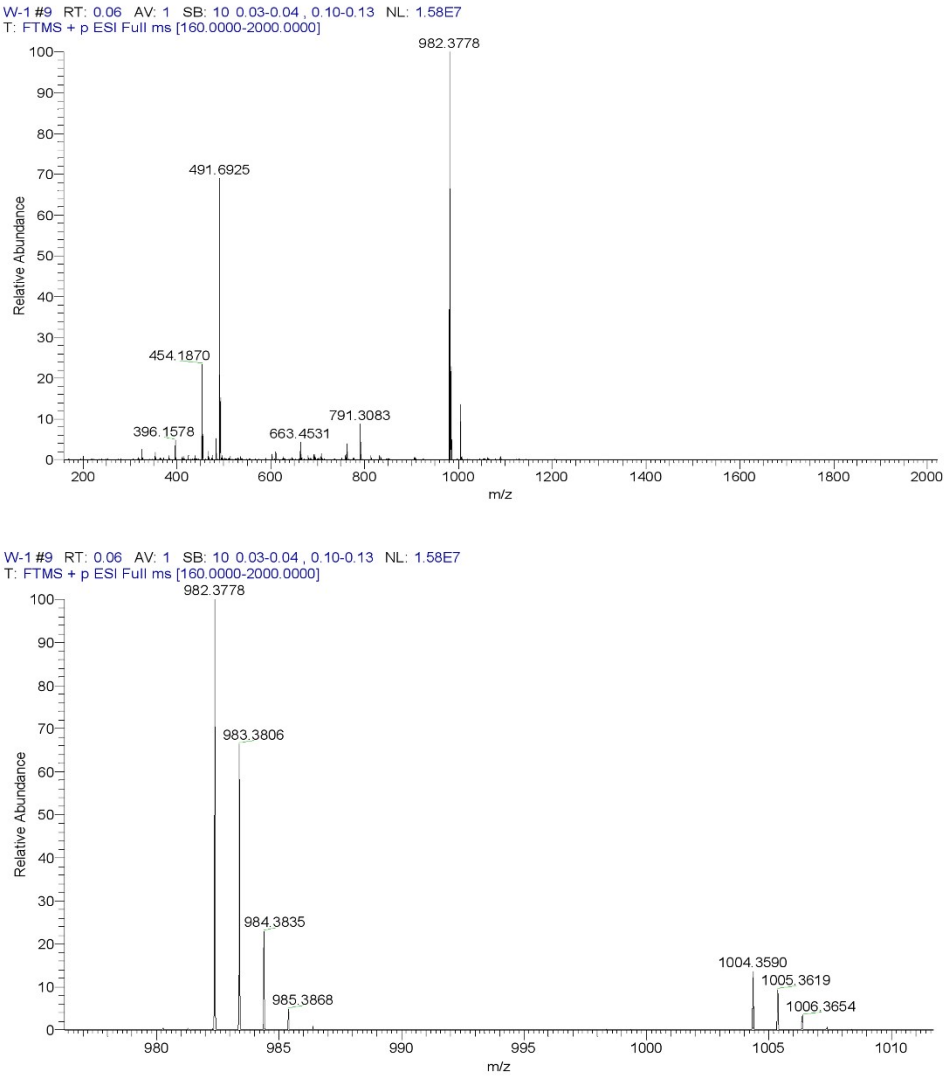

Fig. S13 HRMS spectra of compound **4**.

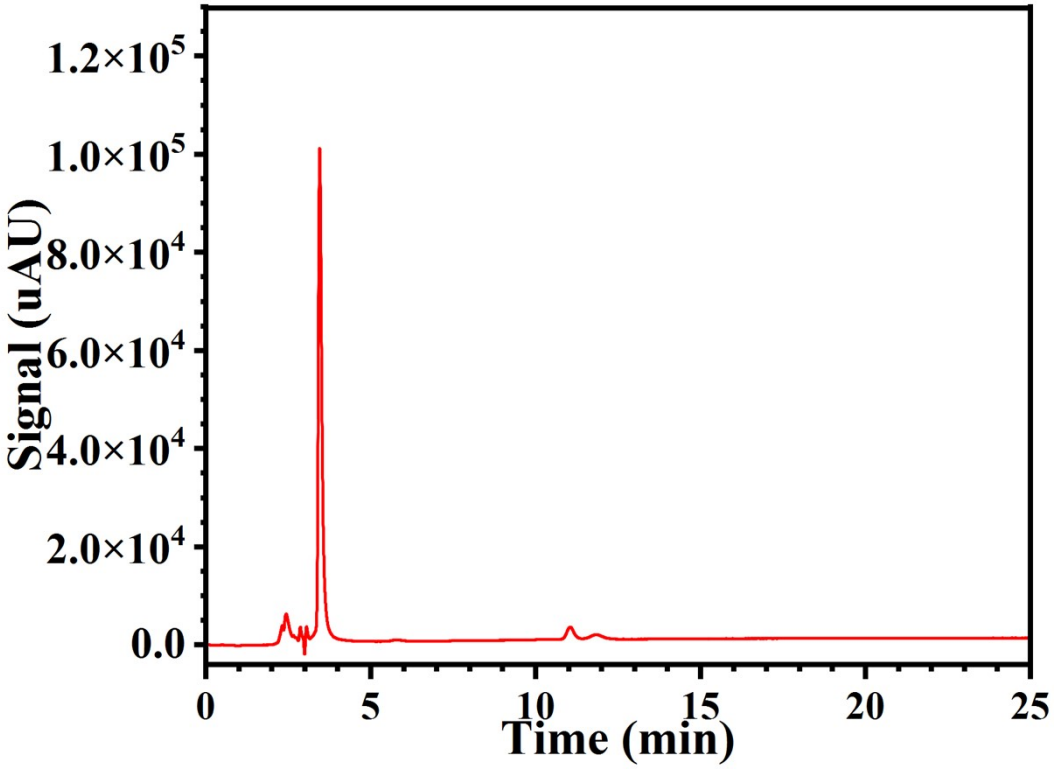

Fig. S14 HPLC spectra of compound **4**.