Electronic Supplementary Information

Reversible hydrogen-bonded polymerization regulated by allosteric metal templation

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1. Materials, methods, and abbreviations

General

All chemicals, reagents and solvents were purchased from commercial suppliers and used, unless otherwise stated, without further purification. If needed, solvents were dried by literature known procedures. All yields were given as isolated yields. **N1**[S1], **1**[S2], and **2**[S3] were prepared according to literature procedure.

NMR spectroscopy

The ^{1}H NMR and ^{13}C NMR spectra were recorded with a Bruker AVANCE III (400 MHz or 600 MHz) spectrometer and calibrated against the residual proton signal or natural abundance carbon resonance of the used deuterated solvent from tetramethylsilane (TMS) as the internal standard. The chemical shifts δ are indicated in ppm and the coupling constants J in Hz. The multiplicities are given as s (singlet), d (doublet), dd (doublet of doublets), t (triplet), and m (multiplet).

Diffusion Ordered Spectroscopy (DOSY) were carried out at 298 K on a Bruker AVANCE III 600 spectrometer. The ledbpgp2s pulse sequence from Bruker Biospin was selected for the DOSY NMR by using gradients varied linearly from 5% up to 95% in 32 steps, with 16 scans per step. The diffusion time (Δ) was set at 20 ms, and the gradient length (δ) was set at 2 ms. Heptakis(2,3,6-tri-O-methyl)-β-cyclodextrin (peralkylated β-CD) was used as internal standard if necessary.

Mass spectrometry

Low-resolution electrospray ionization mass spectra (LR-ESI-MS) were obtained on LCMS2020. High-resolution electrospray ionization mass spectra (HR-ESI-MS) were recorded on an Agilent Technologies 6540 UHD Accurate-Mass. High-resolution mass spectra (HRMS) of **M3**+KPF_6 were measured on a Q-Exactive™ HF/UltiMate™ 3000 RSLCnano using a Nano roFlow meter with ProFlow technology in positive mode.

Melting point determination

The melting points were measured on a Haineng MP100 automatic melting point instrument.

Scanning electron microscopy (SEM)

SEM investigations were carried out on a ZEISS SUPRA 55 instrument.

Viscometry

Viscosity measurements were carried out with Ubbelohde micro viscometers (Shanghai Liangjing Glass Instrument Factory, 0.40 mm inner diameter) at 298 K in chloroform and acetonitrile.

X-ray crystal

Single crystals suitable for X-ray diffraction were selected and mounted in inert oil in cold gas stream and their X-ray diffraction intensity data was collected on a Rigaku XtaLAB Synergy diffractometer equipped with a Hypix6000HE detector, using Mo Kα radiation (λ = 0.7107 Å).

Abbreviations

UPy = 2-ureido-4[1H]-pyrimidinone

B18C6 = benzo-18-crown-6

DMSO = dimethyl sulfoxide

M = mol/L

br = broad

Ar = aromatic group

2. Concentration-dependent ^{1}H NMR

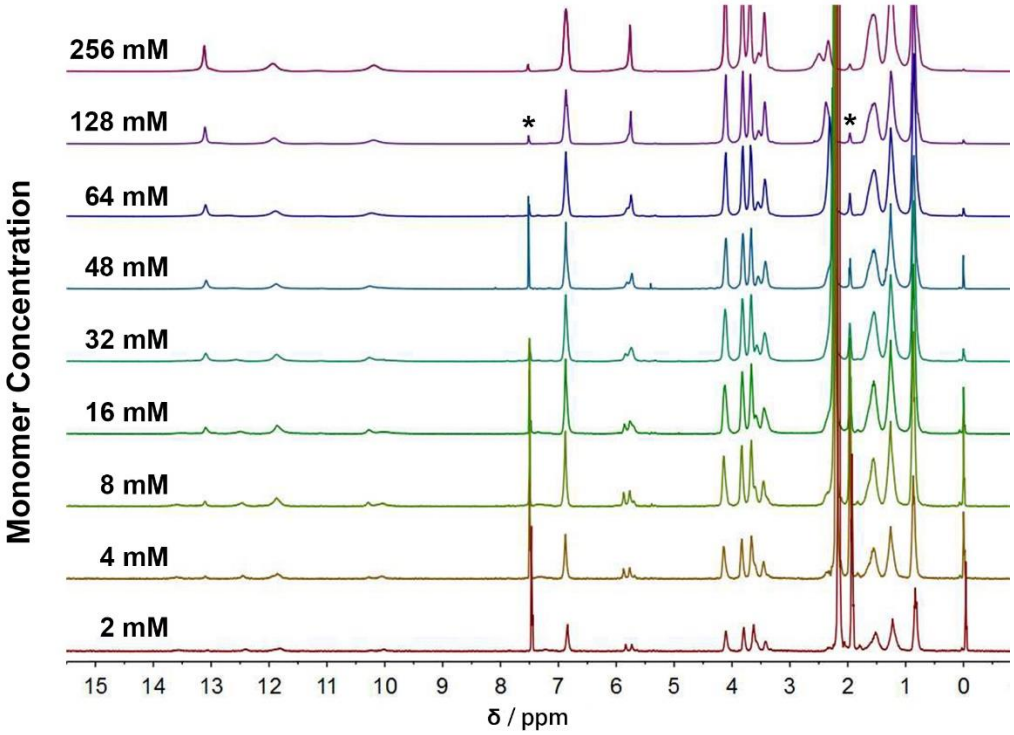


Fig. S1. ^{1}H NMR spectra (300 MHz, $CDCl_3/CD_3CN$ = 1:1, v/v, 298 K) of **M1** at different monomer concentrations. The asterisk symbols indicate solvent peaks.

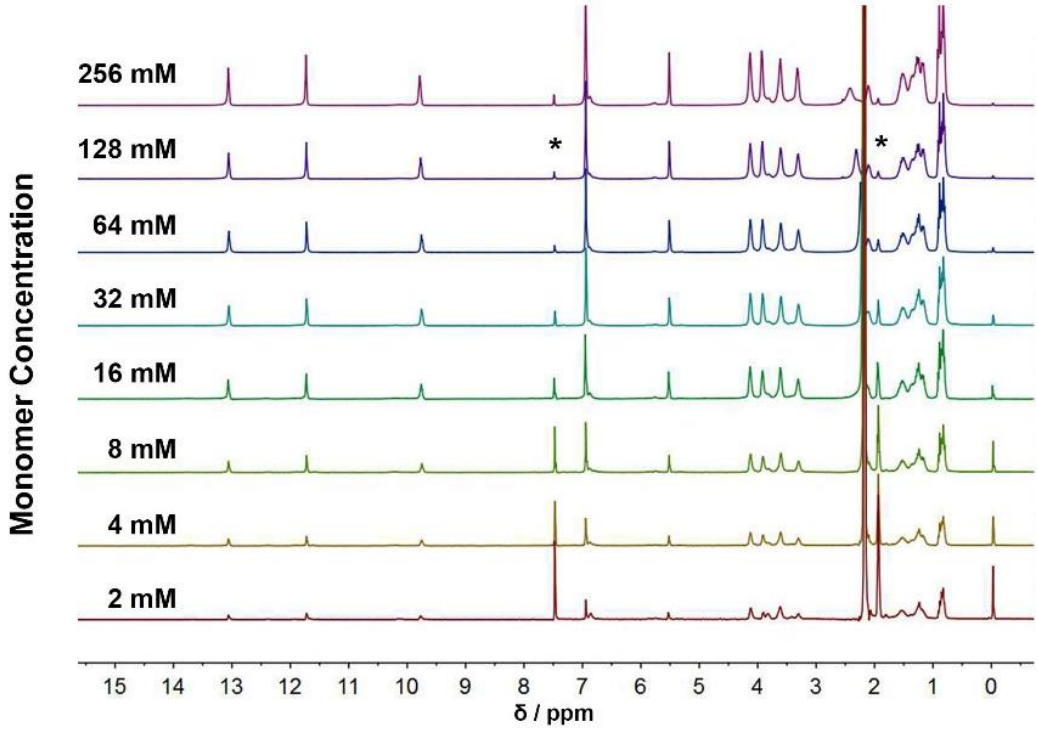


Fig. S2. ^{1}H NMR spectra (300 MHz, $CDCl_3/CD_3CN$ = 1:1, v/v, 298 K) of **M1** with equal molar of KPF_6 at different monomer concentrations. The asterisk symbols indicate solvent peaks.

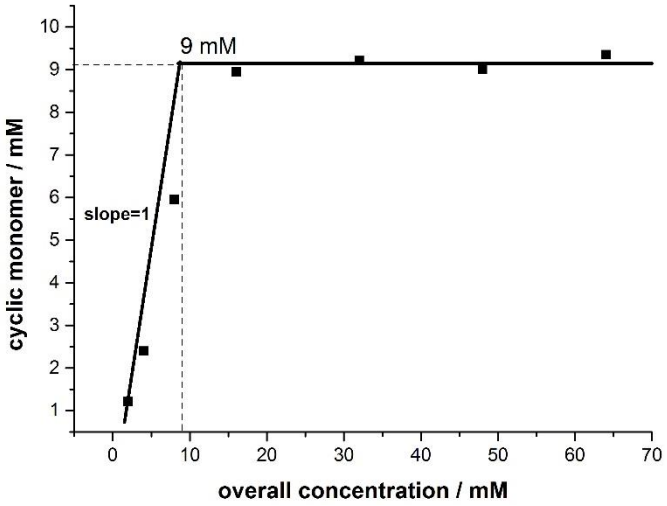


Fig. S3. Concentration of cyclic monomers in $CDCl_3/CD_3CN$=1/1 (v/v) solutions versus increasing concentration of monomer **M1**, calculated from the ^1H NMR spectra. H_3 in **M1** was used for calculation.

3. DOSY experiments

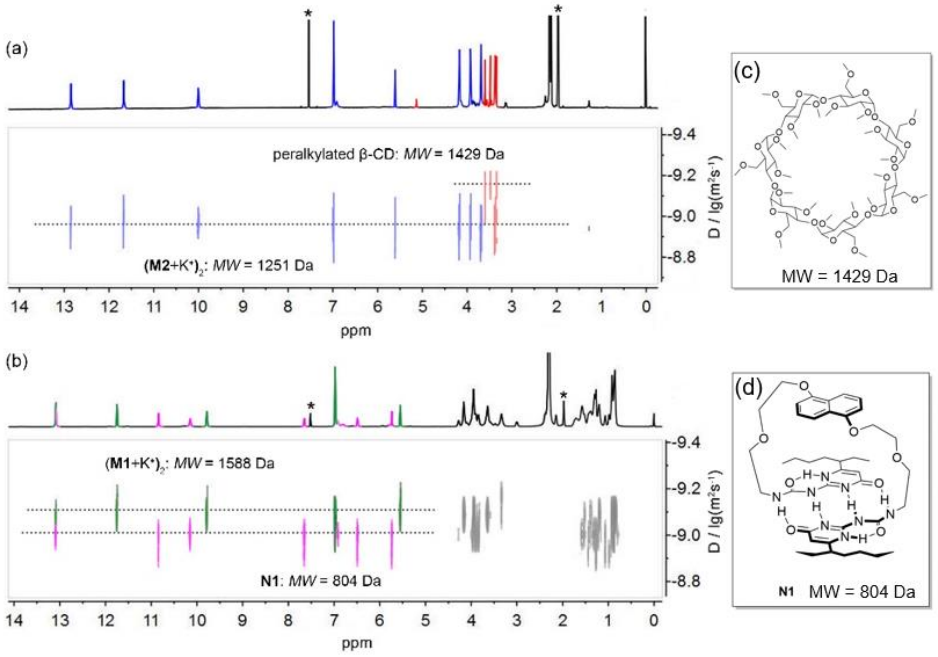


Fig. S4. Two DOSY spectra (600 MHz, $CDCl_3/CD_3CN$ = 1:1, v/v, 298 K) of (a) **M2**⊃K^+ complex (16 mM) with the addition of permethylated β-CD as the internal standard and (b) **M1**⊃K^+ complex (8 mM) with the addition of **N1**[S1] as the internal standard. Chemical structures of (c) permethylated β-CD and (d) a highly stable cyclic monomer of **N1**. The red peaks stand for proton signals from permethylated β-CD and the blue peaks belong to **M2**. The magenta peaks stand for peaks belonging to **M1** and the green peaks represent peaks from **N1**. Asterisk symbols represent solvent peaks.

By comparing the diffusion coefficients of a smaller methyl-substituted analogue (**M2**⊃K^+)$_n$ (when n = 1, *MW* = 626 Da, 1.15 × 10^{-9} m^2 s^{-1}) and permethylated β-CD (6.76 × 10^{-10} m^2 s^{-1}, Figure S4a), as well as (**M1**⊃K^+)$_n$ (7.94 × 10^{-10} m^2 s^{-1}, at 8 mM) and a highly stable UPy-based cyclic monomer **N1**[S1] (1.02 × 10^{-9} m^2 s^{-1}, *MW* = 804 Da, Figure S4b), it can be concluded that K^+ templates the formation of a dimeric species (**M1**⊃K^+)$_2$ (*MW* = 1588 Da).

Moreover, by employing the Stokes-Einstein equation (R_h = k_BT/(6πηD)), the diffusion coefficients that were experimentally obtained could be converted to an approximate hydrodynamic radius (or Stokes radius).[S4] k_B is the Boltzmann's constant and T is the temperature. The viscosity coefficient η of a mixed solution of $CHCl_3$ and CH_3CN (v/v = 1/1) is obtained from literature report (η = 0.22 cP).[S5] Taking a solution of **M2** (8 mM, $CHCl_3$/ CH_3CN, v/v = 1/1) for example, R_h can be calculated by the following equation:

$$R_h = \frac{k_B T}{6\pi\eta D} = \frac{1.38 \times 10^{-23} \times 298}{6 \times 3.14 \times 0.22 \times 10^{-3} \times 1.15 \times 10^{-9}} = 0.86\ nm$$

We have obtained a crystal structure of **M3**⊃K^+ (vide infra). Inspired by this structure, we prepared a molecular model of (**M2**⊃K^+)$_2$ (Figure S4). According to Stokes−Einstein equation assuming a spherical molecule, we measured the longest distance (diameter) in **M2**⊃K^+ dimer by simplifying the supramolecular dimer to a geometric sphere and a spherical radius of 0.85 nm (Figure S5, $r = 16.963\ Å \div 2 = 0.85\ nm$) was shown, which was in good agreement with the experimental value.

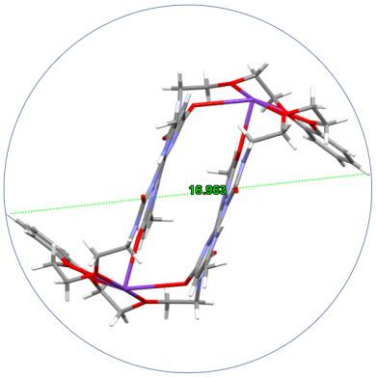


Fig. S5. A molecular model of **M2**

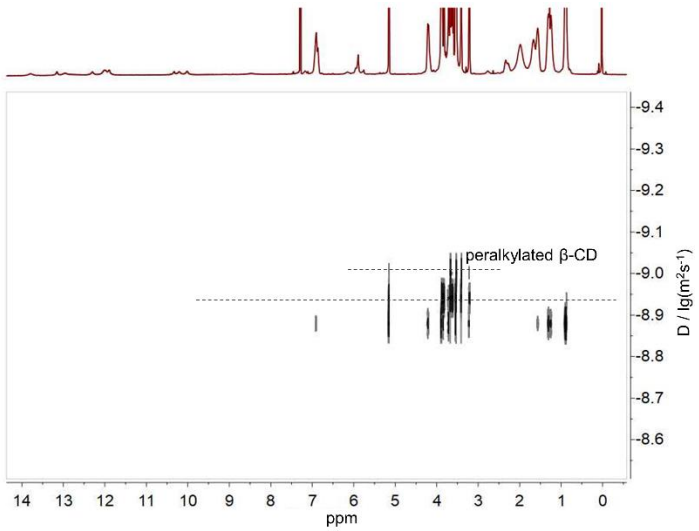


Fig. S6. DOSY spectrum (600 MHz, $CDCl_3$, 298 K) of **M1** in 4 mM.

By using the Stokes-Einstein equation (η of $CHCl_3$ is 0.54 cP), the size of cyclic monomer was estimated as follows:

$$R_h = \frac{k_B T}{6\pi\eta \mathrm{D}} = \frac{1.38 \times 10^{-23} \times 298}{6 \times 3.14 \times 0.54 \times 10^{-3} \times 1.15 \times 10^{-9}} = 0.46\ nm$$

which shows that the hydrodynamic radius of cyclic monomer was nearly half of the cyclic dimer (0.86 nm).

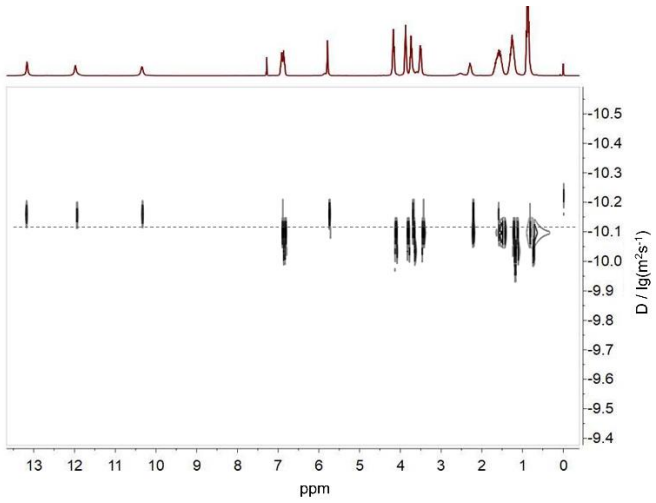


Fig. S7. DOSY spectrum (600 MHz, $CDCl_3$, 298 K) of **M1** in 128 mM.

Furthermore, the size of supramolecular polymer at 128 mM (D = 7.58×10^{-11} $m^2\ s^{-1}$) was estimated as follows:

$$R_h = \frac{k_B T}{6\pi\eta \mathrm{D}} = \frac{1.38 \times 10^{-23} \times 298}{6 \times 3.14 \times 0.22 \times 10^{-3} \times 7.58 \times 10^{-11}} = 5.3\ nm$$

4. Mass spectrometry of M1+KPF_6

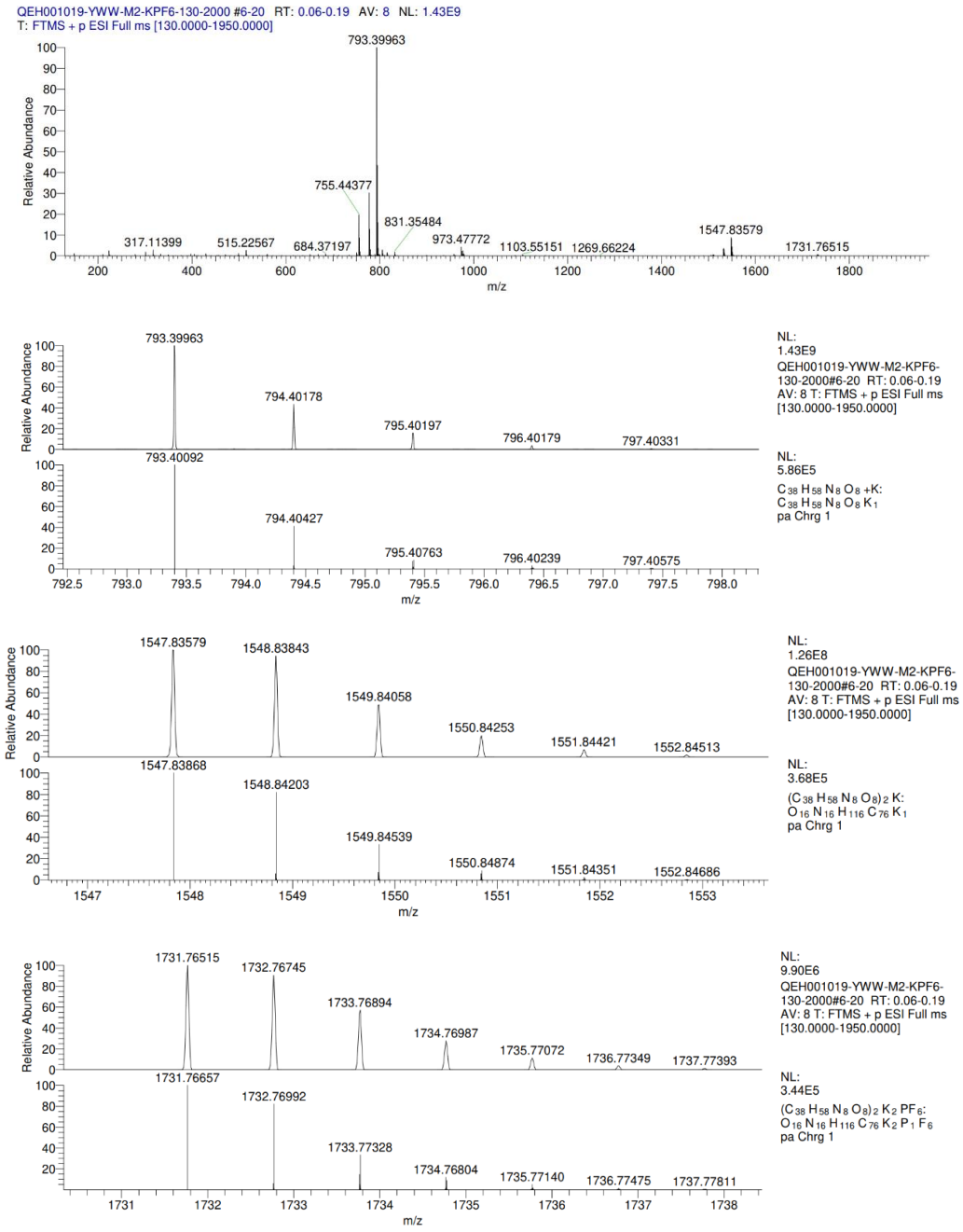


Fig. S8. HR-MS (ESI, positive mode, $CHCl_3/CH_3CN$ = 1:5, v/v) of **M3** + KPF_6

The formation of dimer was also confirmed by high-resolution ESI-MS, with the signals being clearly observed at m/z = 793.3996, which correspond to $[2\mathbf{M1} + 2K]^{2+}$ (calculated as 793.4009). And m/z =1731.7651, which correspond to $[2\mathbf{M1} + KPF_6 + K]^{+}$ (calculated as 1731.7666). Other peaks: m/z calcd for $[\mathbf{M1} + H]^{+}$ = 755.4456, found = 755.4437; $[2\mathbf{M1} + K]^{+}$ = 1547.8387, found = 1547.8357.

5. Crystallographic data for M3⊃K^+

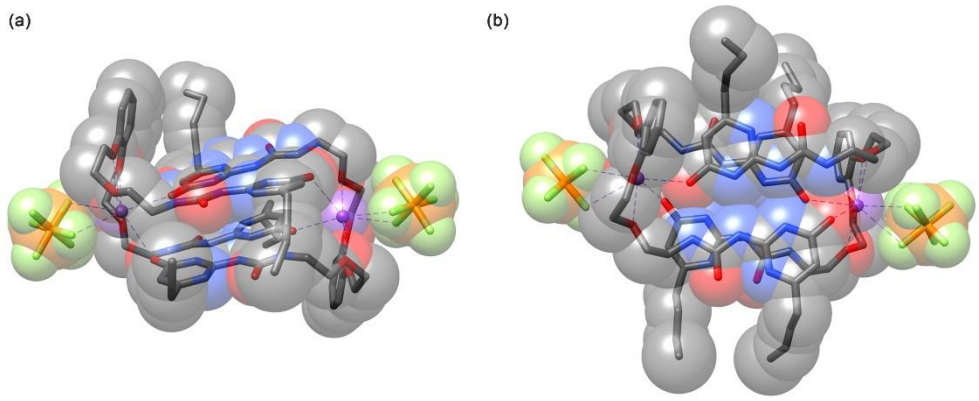


Table S1 Crystal data and structure refinement parameter for **M3**

CCDC number	1962895
Empirical formula	$C_{64}H_{92}F_{12}K_2N_{16}O_{16}P_2$
Formula weight / g mol^{-1}	1709.67
Temperature / K	159.99(10)
Crystal system	monoclinic
Space group	$P2_1/n$
a / Å	14.5377(3)
b / Å	16.9875(3)
c / Å	31.4097(5)
α / °	90
β / °	92.689(2)
γ / °	90
Volume / $Å^3$	7748.4(2)
Z	4
ρ_{calc} / g cm^{-3}	1.456
μ / mm^{-1}	0.266
F / 000	3537.0
Crystal size / mm^3	0.25 × 0.2 × 0.2
Index ranges	$-18 \le h \le 17$, $-22 \le k \le 22$, $-32 \le l \le 39$
Reflections collected	89281
Independent reflections	18990 [R_{int} = 0.0292, R_{sigma} = 0.0285]
Data/restraints/parameters	18990/36/1102
Goodness-of-fit on F^2	1.087
Final *R* indices [$I > 2\text{sigma}(I)$]	R_1 = 0.0612, wR_2 = 0.1874
R indices (all data)	R_1 = 0.0887, wR_2 = 0.2077
Largest diff. peak / hole / e·$Å^{-3}$	0.73/-0.64

6. The complexation of K^+ with M4

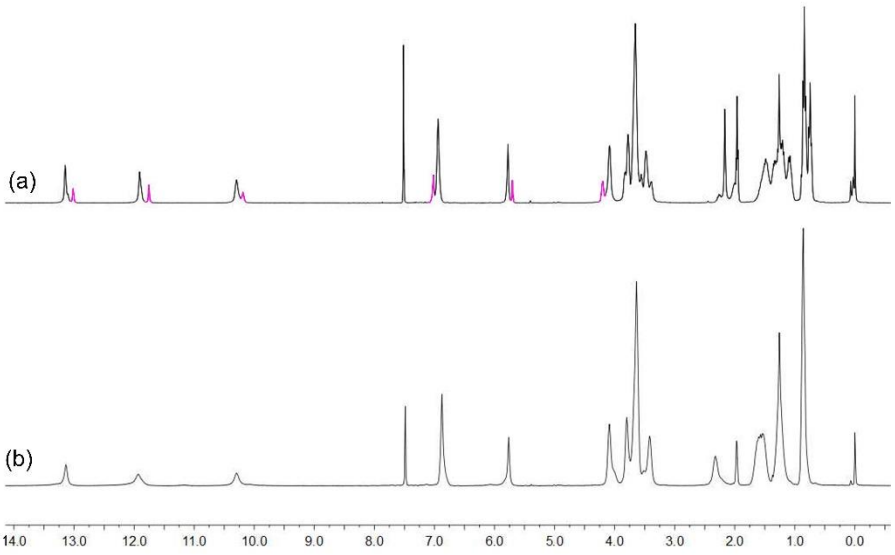


Fig. S9. ^{1}H NMR spectra (300 MHz, $CDCl_3/CD_3CN$ = 1/1, v/v, 298 K) of (a) **M4** + KPF_6 and (b) **M4**. Complexed species are labeled in pink.

7. Topological transformation monitored by ^{1}H NMR

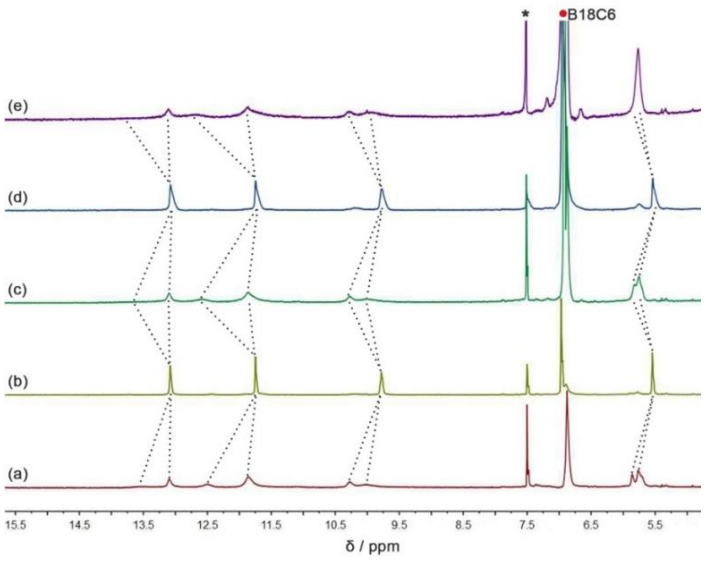


Fig. S10. Partial ^{1}H NMR spectra (300 MHz, $CDCl_3/CD_3CN$ = 1/1, v/v, 298 K) of (a) **M1** (16 mM), (b) after addition of 1 equiv. KPF_6 (16 mM), (c) after addition of 1 equiv. B18C6 (16 mM), (d) after addition of 1 equiv. KPF_6 (16 mM), and (e) after addition of 1 equiv. B18C6 (16 mM). The asterisk symbols indicate solvent peaks and the red dot stand for another proton signals in B18C6.

Firstly, the reversible topological transformation was realized by benzo-18-crown-6 (B18C6). The process was monitored by ^{1}H NMR. A solution of **M1** ($CDCl_3/CD_3CN$ = 1/1, v/v, 16 mM) at lower concentration was prepared, in which cyclic monomer and linear supramolecular polymer co-existed. Thus, two sets of peaks were appeared (Figure S8a). After the addition of 1 equiv. of KPF_6, there are only discrete cyclic dimers, resulting in one set of sharp peaks in ^{1}H NMR (Figure S8b). After the addition of 1 equiv. B18C6, these discrete cyclic dimers were transformed back into cyclic monomer and linear supramolecular polymer, resulting in the recovery of two sets of peaks in ^{1}H NMR (Figure S8c). This process can be repeated again (Figure S8d and 8e).

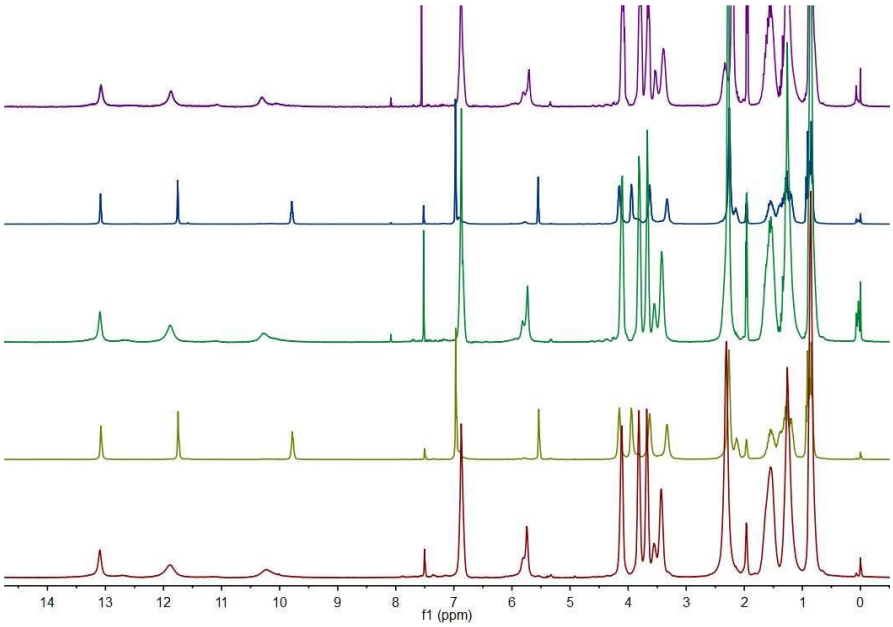
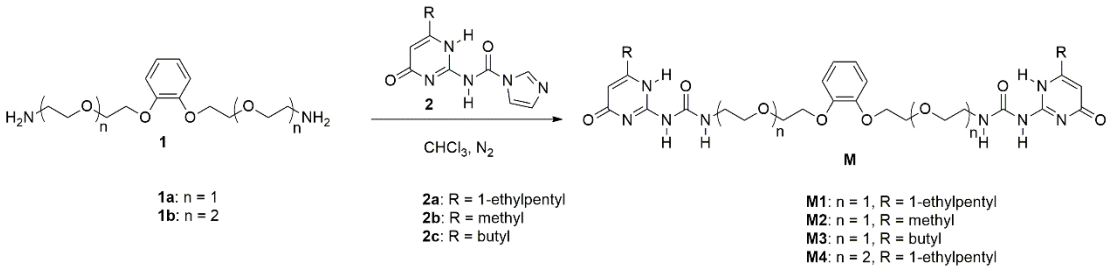


Fig. S11. ^{1}H NMR spectra (300 MHz, $CDCl_3/CD_3CN$ = 1:1, v/v, 298 K) of (a) **M1** (128 mM), (b) after addition of 1 equiv. KPF_6, (c) after washing with water and supplementing with CD_3CN, (d) repeating the process of (b), and (e) repeating the process of (c).

Secondly, the reversible topological transformation was realized by water extraction. The process was also monitored by ^{1}H NMR. A solution of **M1** (0.5 mL, $CDCl_3/CD_3CN$ = 1/1, v/v, 128 mM) at a relatively high concentration was prepared, in which linear supramolecular polymers were predominant. Thus, only one set of broad peaks was appeared (Figure S9a). After the addition of 1 equiv. of KPF_6, the linear supramolecular polymers were transformed into discrete cyclic dimers, resulting in one set of sharp peaks and changes of chemical shifts in ^{1}H NMR (Figure S9b). After washing with water (0.5 mL × 2), K^+ ions were extracted into water phase and linear supramolecular polymers were recovered in organic solution, resulting in the recovery of one set of broad peaks in ^{1}H NMR (Figure S9c). Herein, CD_3CN was appropriately supplemented because part of the CD_3CN was also extracted into the aqueous phase. This reversible transformation processes can be repeated again (Figure S9d and 9e).

8. Synthetic procedures and characterizations



Scheme S1 Synthetic route of **M1**-**M4**

8.1 Synthesis of Compound **M1**

Imidazolide **2a** (0.94 g, 3.09 mmol) and **1a** (0.40 g, 1.41 mmol) were dissolved in dry $CHCl_3$ (30 mL) and this solution was stirred for 12 h under nitrogen at room temperature. To the reaction mixture $CHCl_3$ (20 mL) was added and the organic layer was washed with 1 M HCl (50 mL), saturated $NaHCO_3$ (50 mL), brine (50 mL), dried over anhydrous $MgSO_4$ and concentrated under reduced pressure. The resulting residue was subjected to column chromatography over silica gel (eluent: $CHCl_3$/MeOH = 100:1, v/v) to afford compound **M1** as a colorless viscous solid (0.90 g, 85%). ^{1}H NMR (300 MHz, $CDCl_3$): δ 13.16 (br s, 2H, N*H*), 11.98 (br s, 2H, N*H*), 10.34 (br s, 2H, N*H*), 6.86 (d, *J* = 18.6 Hz, 4H, Ar-*H*), 6.14-5.35 (m, 2H, alkylidene-*H*), 4.17 (m, 4H, OCH_2), 4.06-3.78 (m, 4H, OCH_2), 3.80-3.22 (m, 8H, OCH_2), 2.29 (m, 2H, C*H*(CH_2)$_2$), 1.81-1.35 (m, 8H, CH_2), 1.35-1.12 (m, 8H, CH_2), 1.03-0.68 (m, 12H, CH_3) ppm. ^{13}C NMR (75 MHz, DMSO-d_6): δ 170.7, 161.1, 154.4, 151.6, 148.4, 121.3, 114.4, 105.1, 69.4, 68.9, 68.3, 47.9, 39.2, 32.9, 29.1, 26.5, 22.2, 13.9, 11.8 ppm. ESI-MS ($C_{38}H_{58}N_8O_8$): *m/z* calcd for $[M + H]^+$ = 755.45, found = 755.35 (81%); $[M + Na]^+$ = 777.43, found = 777.30 (100%); HR-ESI-MS ($C_{38}H_{58}N_8O_8$): *m/z* calcd for $[M + H]^+$ = 755.4450, found = 755.4441.

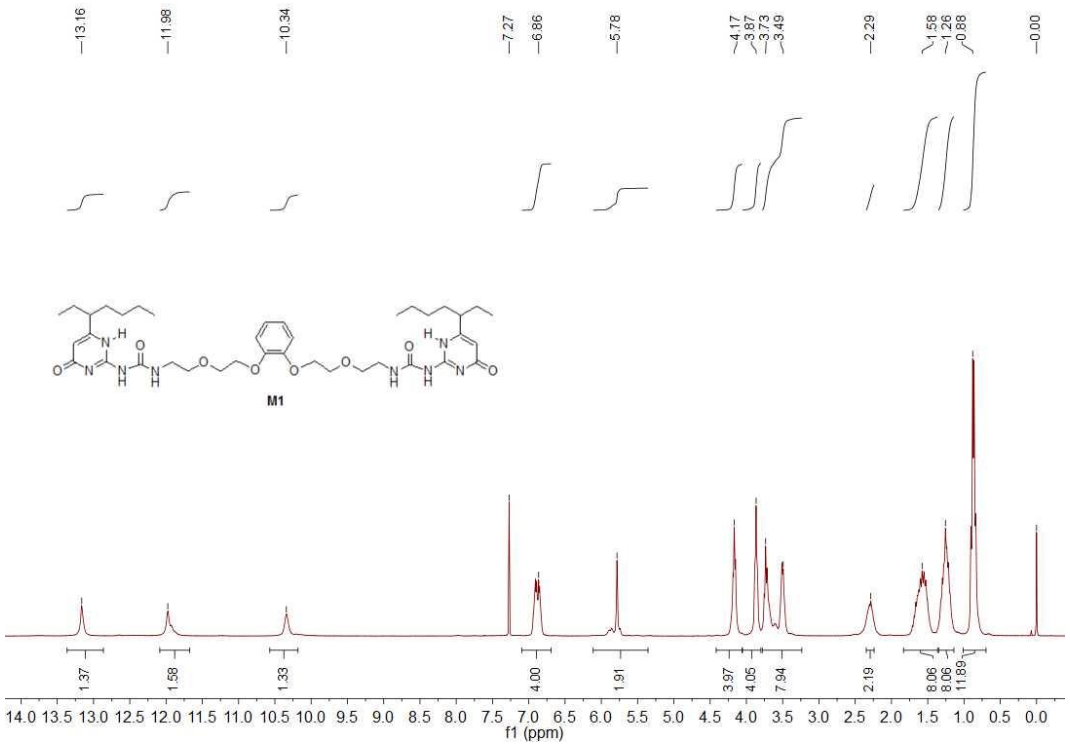


Fig. S12. ^{1}H NMR (300 MHz, $CDCl_3$) spectrum for **M1**

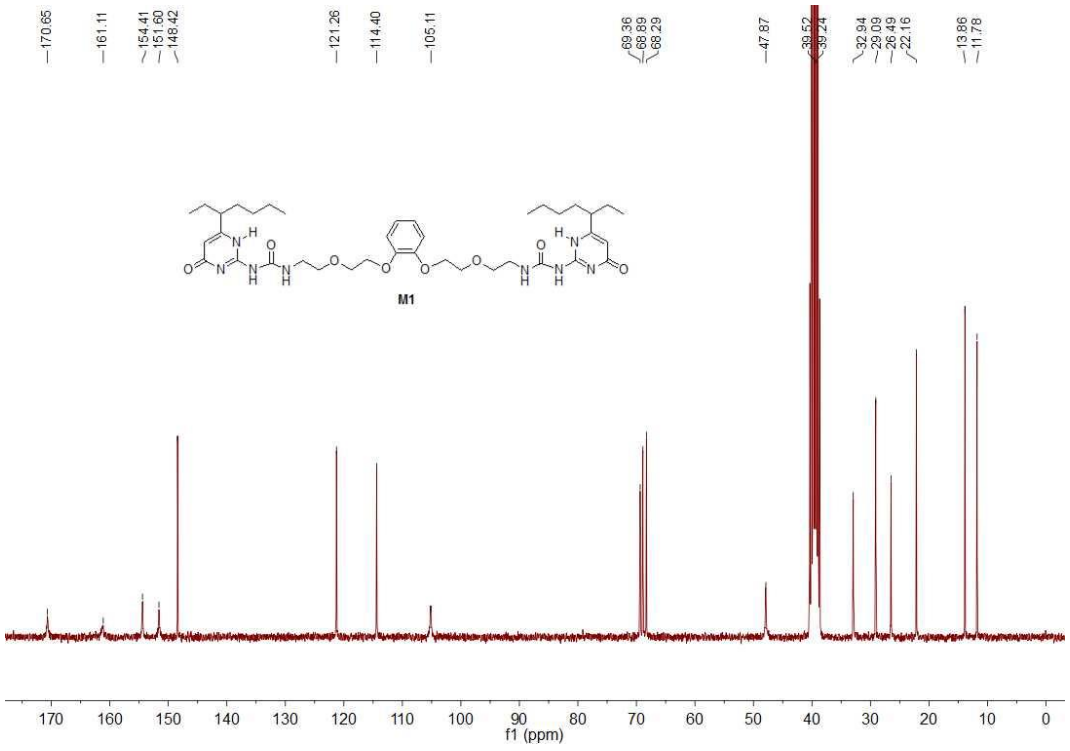


Fig. S13. ^{13}C NMR (75 MHz, DMSO-d_6) spectrum for **M1**

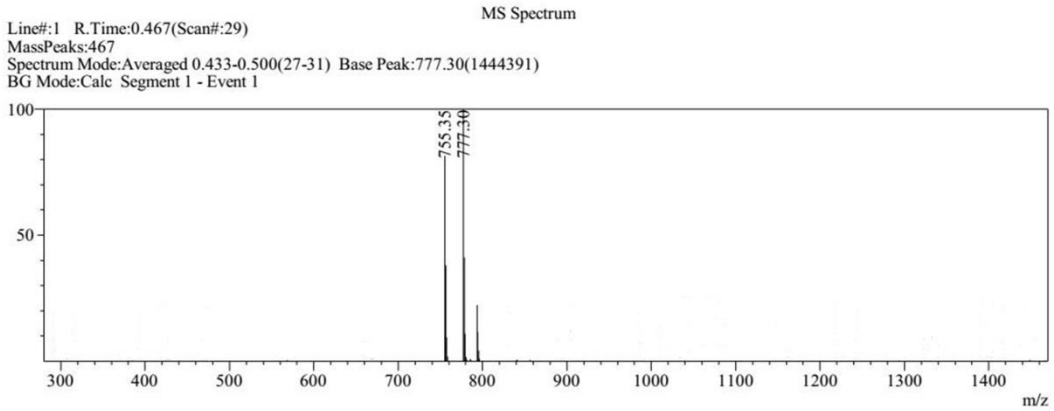


Fig. S14. Electrospray ionization mass spectrum of **M1**

8.2 Synthesis of Compound **M2**

Imidazolide **2b** (0.61 g, 2.79 mmol) and compound **1a** (0.36 g, 1.27 mmol) were dissolved in dry $CHCl_3$ (30 mL) and this solution was stirred for 12 h under nitrogen at room temperature. To the reaction mixture $CHCl_3$ (20 mL) was added and the organic layer was washed with 1 M HCl (50 mL), saturated $NaHCO_3$ (50 mL), brine (50 mL), dried over anhydrous $MgSO_4$ and concentrated under reduced pressure. The resulting residue was subjected to column chromatography over silica gel (eluent: $CHCl_3$/MeOH = 100:1, v/v) to afford compound **M2** as a white solid (0.60 g, 81%). m.p.: 235-237 °C. ^{1}H NMR (300 MHz, DMSO-d_6): δ [ppm] = 11.50 (br s, 2H, N*H*), 9.79 (br s, 2H, N*H*), 7.65 (br s, 2H, N*H*), 7.01-6.92 (m, 2H, Ar-*H*), 6.90-6.83 (m, 2H, Ar-*H*), 5.75(s, 2H, alkylidene-*H*), 4.10-4.07 (m, 4H, OCH_2), 3.76-3.73 (m, 4H, OCH_2), 3.59-3.55 (t, J = 5.4 Hz, 4H, OCH_2), 3.35-3.32 (m, 4H, OCH_2), 2.07 (s, 6H, CH_3). ^{13}C NMR (75 MHz, DMSO-d_6): δ [ppm] = 179.3, 161.8, 155.0, 151.5, 148.5, 121.4, 114.4, 104.7, 69.4, 69.0, 68.4, 39.2, 23.1. ESI-MS ($C_{26}H_{34}N_8O_8$): *m/z* calcd for $[M + H]^+$ = 587.60, found = 587.09 (46%); $[M + Na]^+$ = 609.59, found = 609.05 (100%); HR-ESI-MS ($C_{26}H_{34}N_8O_8$): *m/z* calcd for $[M + H]^+$ = 587.2572, found = 587.2511; $[M + Na]^+$ = 609.2392, found = 609.2391.

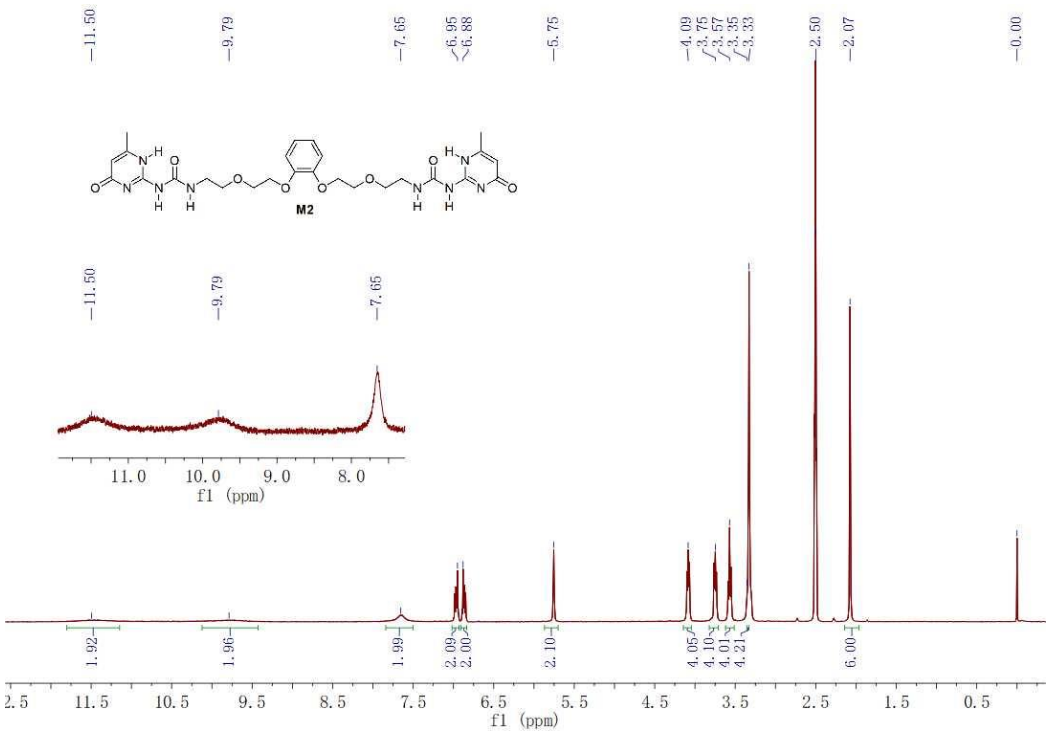


Fig. S15. ^{1}H NMR (300 MHz, DMSO-d_6) spectrum for **M2**

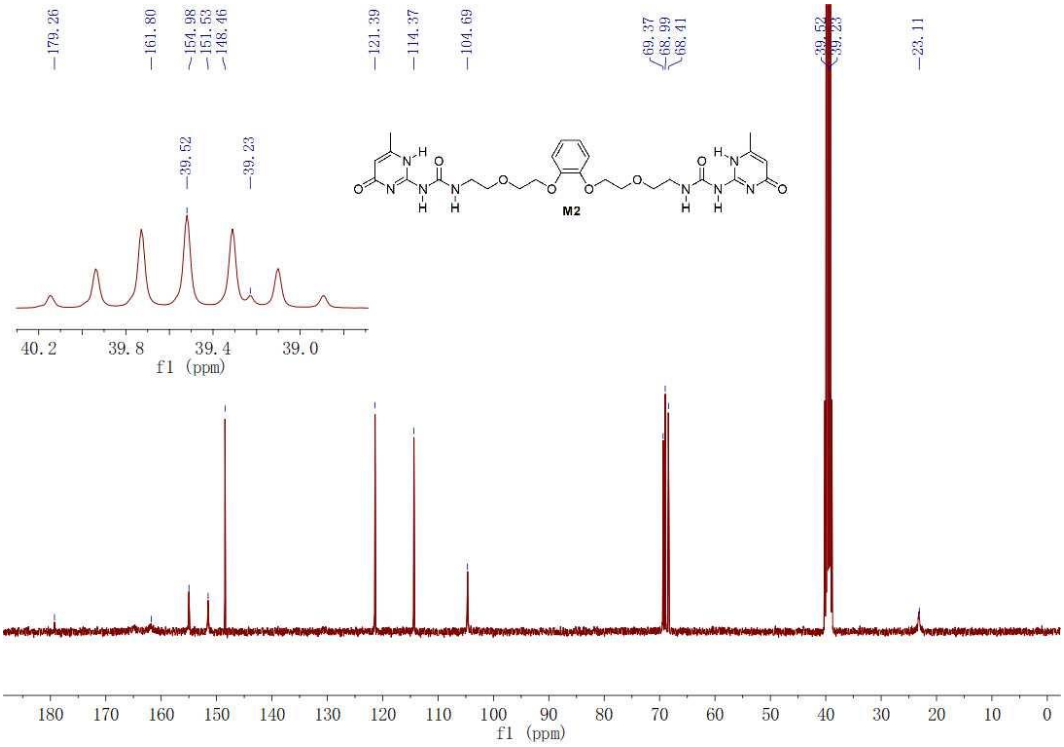


Fig. S16. ^{13}C NMR (75 MHz, DMSO-d_6) spectrum for **M2**

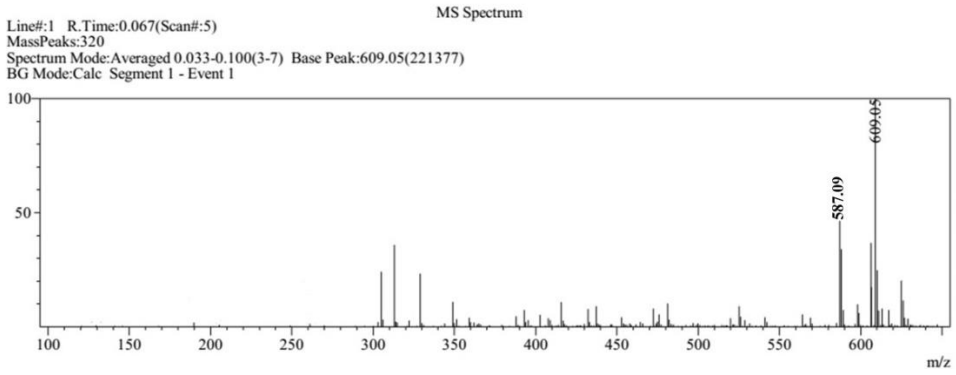


Fig. S17. Electrospray ionization mass spectrum ($CHCl_3/CH_3CN$ 1:5) of **M2**

8.3 Synthesis of Compound **M3**

Imidazolide **2c** (0.20 g, 0.78 mmol) and compound **1a** (0.10 g, 0.35 mmol) were dissolved in dry $CHCl_3$ (15 mL) and this solution was stirred for 12 h under nitrogen at room temperature. To the reaction mixture $CHCl_3$ (15 mL) was added and the organic layer was washed with 1 M HCl (30 mL), saturated $NaHCO_3$ (30 mL), brine (30 mL), dried over anhydrous $MgSO_4$ and concentrated under reduced pressure. The resulting residue was subjected to column chromatography over silica gel (eluent: $CHCl_3$/MeOH = 100:1, v/v) to afford compound **M3** as a white solid (0.18 g, 75%). m.p.: 148-150 °C. ^{1}H NMR (300 MHz, DMSO-d_6): δ [ppm] = 11.43 (br s, 2H, N*H*), 9.70 (br s, 2H, N*H*), 7.60 (br s, 2H, N*H*), 6.98-6.93 (m, 2H, Ar-*H*), 6.89-6.84 (m, 2H, Ar-*H*), 5.75(s, 2H, alkylidene-*H*), 4.13-4.07 (m, 8H, OCH_2), 3.76-3.73 (m, 4H, OCH_2), 3.57 (t, J = 5.3 Hz, 4H, OCH_2), 3.35-3.32 (m, 4H, OCH_2), 2.33 (t, J = 7.5 Hz, 4H, CH_2CH$_2$CH$_2$CH$_3$), 1.57-1.47 (m, 4H, CH$_2$CH_2CH$_2$CH$_3$), 1.33-1.20 (m, 4H, CH$_2$CH$_2$CH_2CH$_3$), 0.86 (t, J = 7.3 Hz, 6H, CH$_2$CH$_2$CH$_2$CH_3). ^{13}C NMR (75 MHz, $CDCl_3$): δ [ppm] = 173.0, 157.0, 154.7, 152.3, 149.3, 121.6, 114.9, 105.7, 69.8, 69.6, 69.3, 39.8, 32.5, 29.0, 22.2, 13.8. ESI-MS ($C_{32}H_{46}N_8O_8$): *m/z* calcd for $[M + H]^+$ = 671.76, found = 671.10 (36%); $[M + Na]^+$ = 693.75, found = 693.05 (90%); HR-ESI-MS ($C_{32}H_{46}N_8O_8$): *m/z* calcd for $[M + Na]^+$ = 693.3331, found = 693.3335.

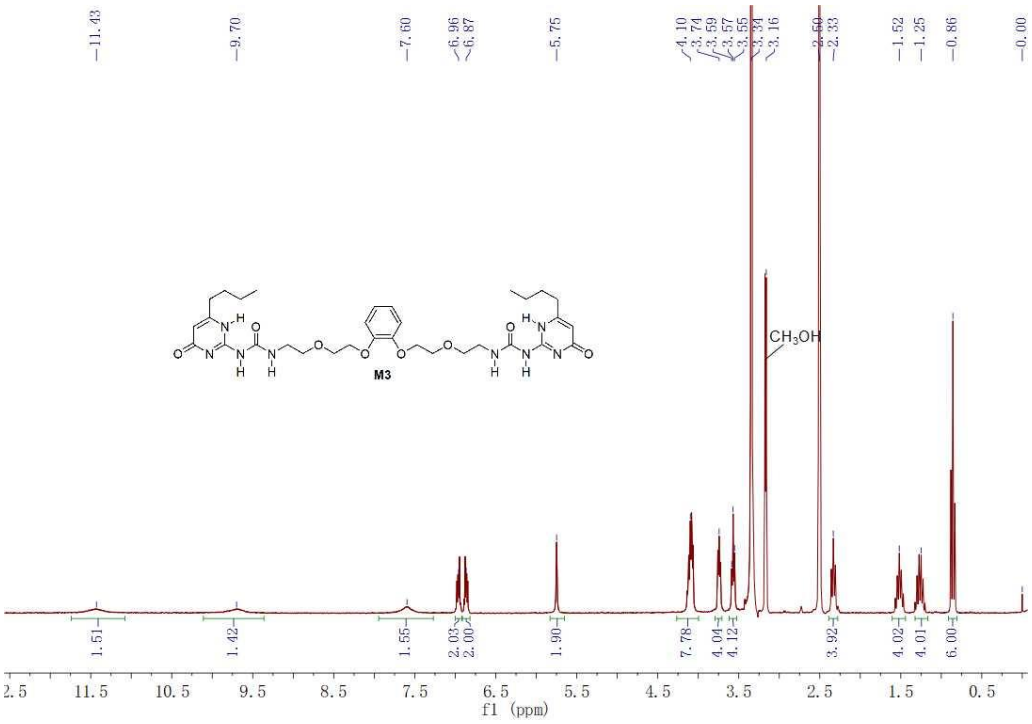


Fig. S18. ^{1}H NMR (300 MHz, DMSO-d_6) spectrum for **M3**

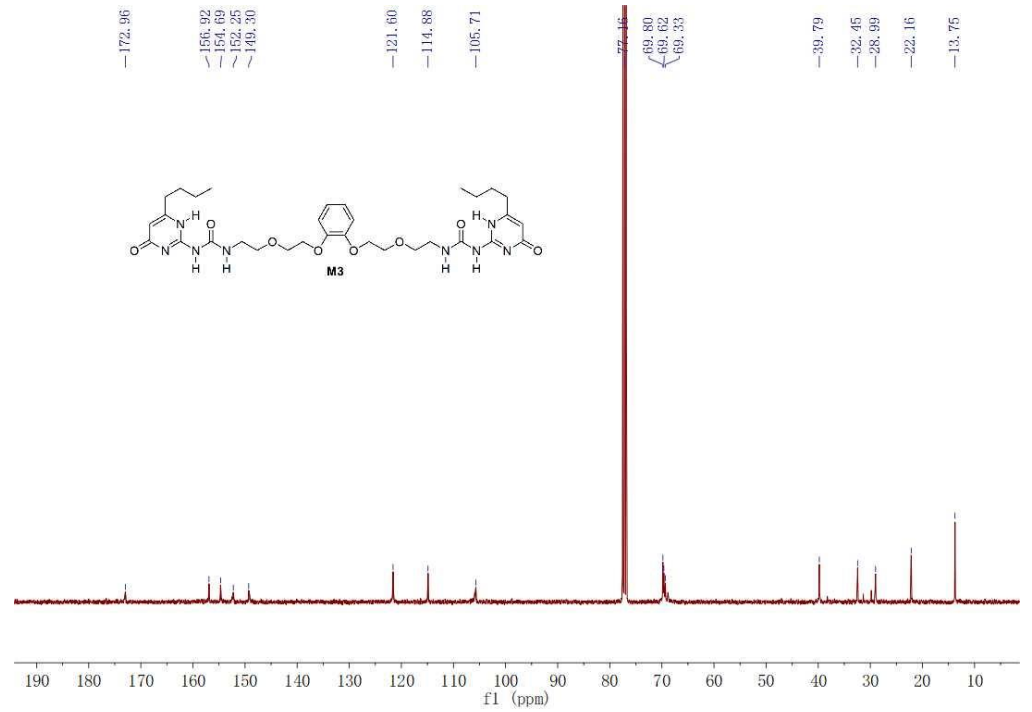


Fig. S19. ^{13}C NMR (75 MHz, $CDCl_3$) spectrum for **M3**

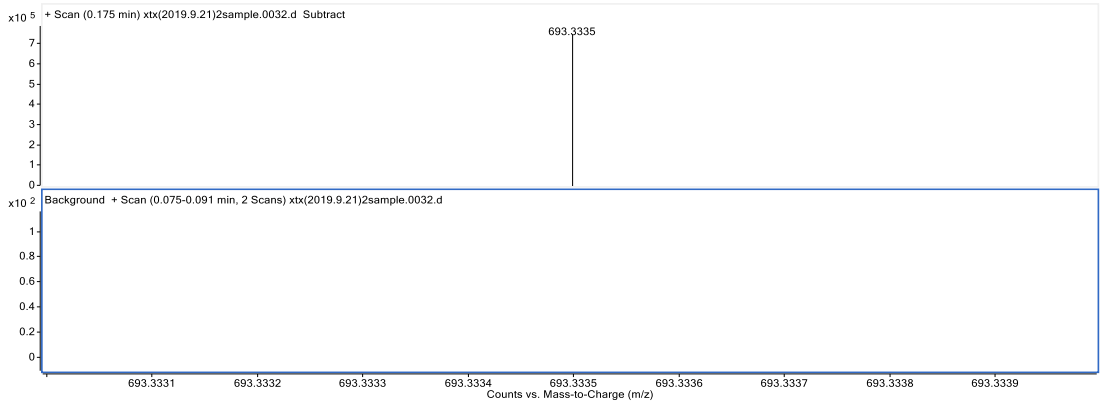


Fig. S20. HR-MS (ESI, positive mode, $CHCl_3/CH_3CN$ = 1:5, v/v) of **M3**

8.4 Synthesis of Compound **M4**

Imidazolide **2a** (1.79 g, 5.9 mmol) and **1b** (1.00 g, 2.7 mmol) were dissolved in dry $CHCl_3$ (30 mL) and this solution was stirred for 12 h under nitrogen at room temperature. To the reaction mixture $CHCl_3$ (20 mL) was added and the organic layer was washed with 1 M HCl (50 mL), saturated $NaHCO_3$ (50 mL), brine (50 mL), dried over anhydrous $MgSO_4$ and concentrated under reduced pressure. The resulting residue was subjected to column chromatography over silica gel (eluent: $CHCl_3$/MeOH = 100:1, v/v) to afford compound **M4** as a colorless viscous solid (1.76 g, 77%). ^{1}H NMR (300 MHz, $CDCl_3$): δ 13.17 (br s, 2H, N*H*), 11.97 (br s, 2H, N*H*), 10.32 (br s, 2H, N*H*), 6.84 (d, *J* = 33.5 Hz, 4H, Ar-*H*), 5.79 (s, 2H, alkylidene-*H*), 4.21-3.98 (m, 4H, OCH_2), 3.92-3.80 (m, 4H, OCH_2), 3.77-3.61 (m, 12H, OCH_2), 3.56-3.42 (m, 4H, OCH_2), 2.35-2.20 (m, 2H, C*H*(CH_2)$_2$), 1.70-1.46 (m, 8H, CH_2), 1.33-1.25 (m, 8H, CH_2), 0.90-0.84 (m, 12H, CH_3) ppm. ^{13}C NMR (75 MHz, $CDCl_3$): δ 173.0, 157.0, 155.4, 154.8, 149.0, 121.6, 115.0, 106.3, 70.8, 70.4, 69.8, 69.5, 68.8, 45.3, 39.5, 32.9, 29.3, 26.6, 22.5, 13.9, 11.7 ppm. ESI-MS ($C_{42}H_{66}N_8O_{10}$): *m/z* calcd for $[M - H]^-$ = 841.48, found = 841.15; $[M + Na]^+$ = 865.48, found = 865.20 (100%); HR-ESI-MS ($C_{42}H_{66}N_8O_{10}$): *m/z* calcd for $[M + H]^+$ = 843.4980, found = 843.4966.

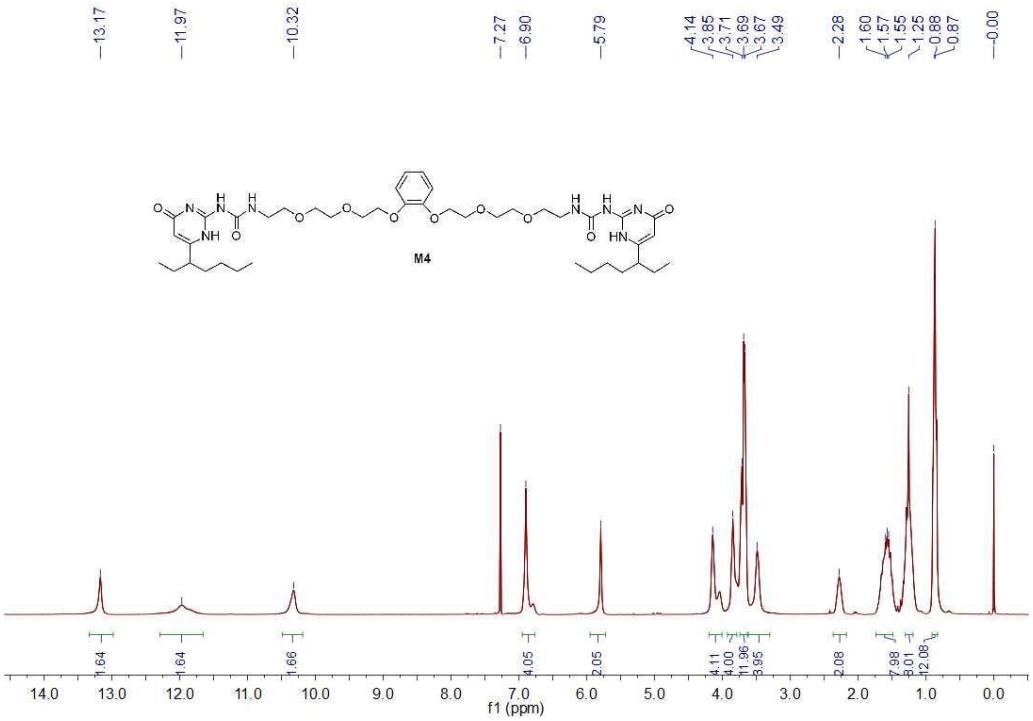


Fig. S21. ^{1}H NMR (300 MHz, $CDCl_3$) spectrum for **M4**

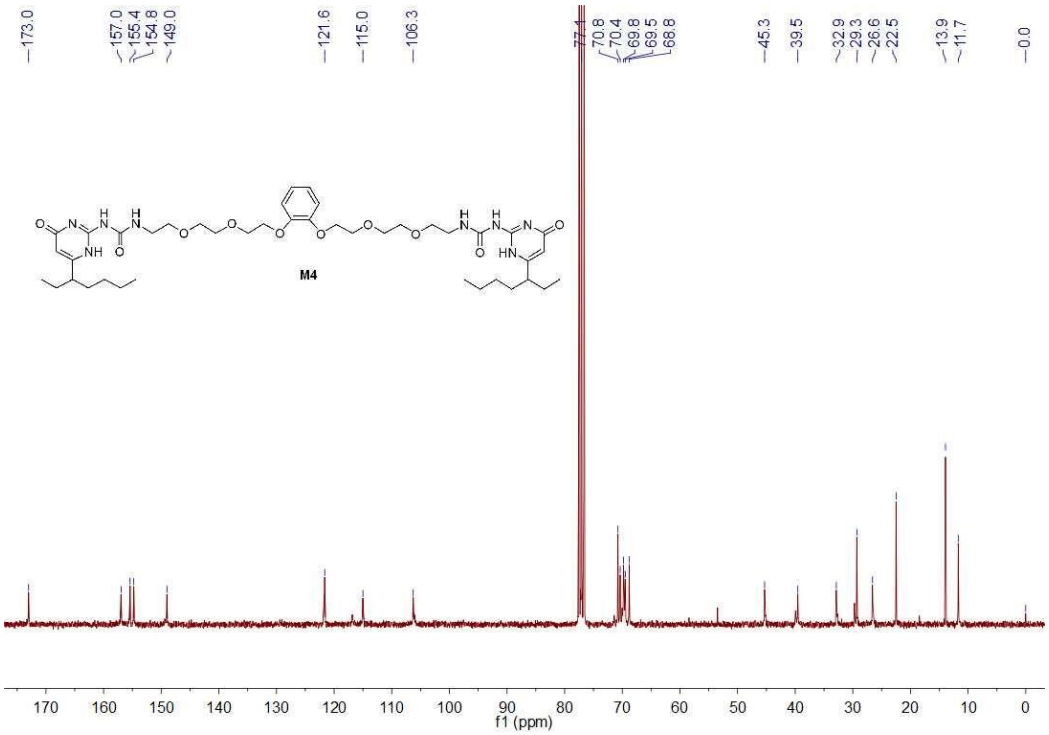


Fig. S22. ^{13}C NMR (75 MHz, $CDCl_3$) spectrum for **M4**

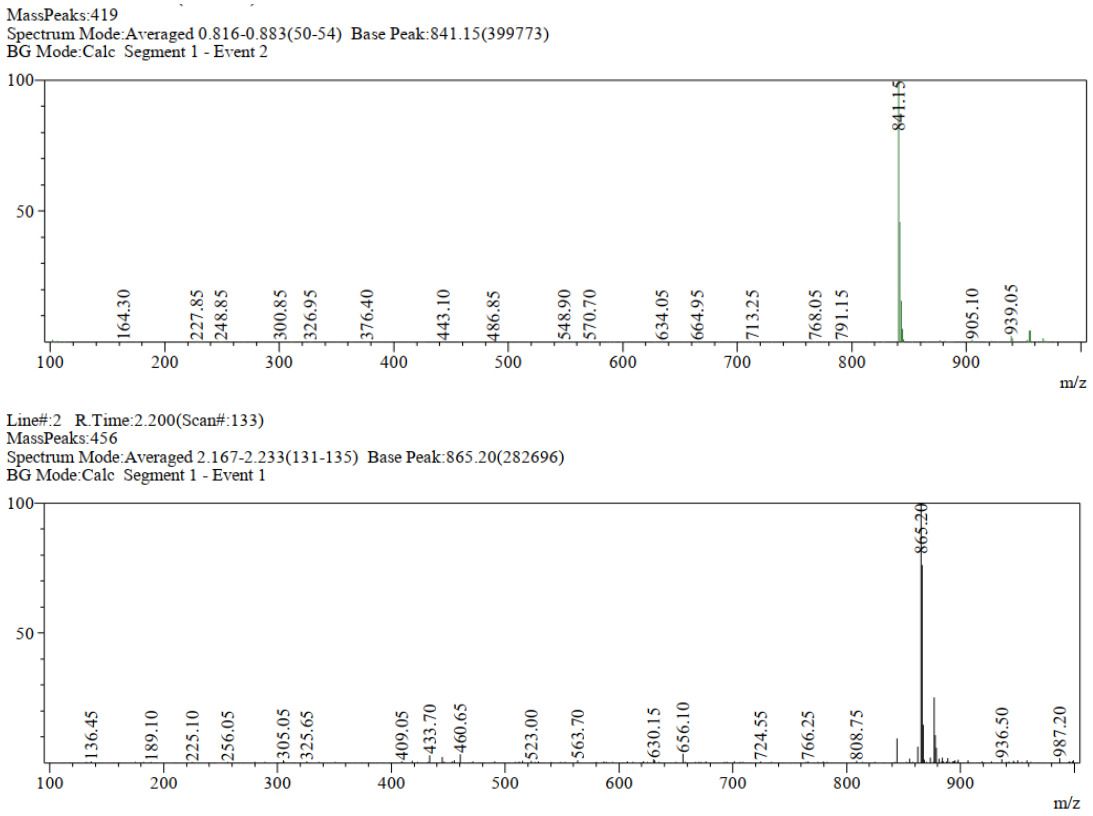


Fig. S23. Electrospray ionization mass spectrum ($CHCl_3/CH_3CN$ 1:5) of **M4**

9. References

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