Synthesis, Structure Elucidation, and Functionalization of Sulfonamide Catenanes

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Section A. Materials and general methods.

All reagents were commercially available and used as supplied without further purification. Deuterated solvents were purchased from Cambridge Isotope Laboratory. Compounds **B** and **C** were prepared according to the published procedures.[S1-S3]

All solvents were dried according to standard procedures and all of them were degassed under N_2 for 30 minutes before use. All reactions were carried out under inert N_2 atmosphere. ^{1}H NMR; ^{13}C NMR spectra were recorded on Bruker 400 MHz Spectrometer (^{1}H: 400 MHz) and Bruker 500 MHz Spectrometer (^{1}H: 500 MHz; ^{13}C: 126 MHz) at 298 K. The ^{1}H and ^{13}C NMR chemical shifts are reported relative to residual solvent signals. 2D-NMR spectra (^{1}H-^{1}H COSY, NOESY) were recorded on Bruker 400 MHz Spectrometer (^{1}H: 400 MHz) and Bruker 500 MHz Spectrometer (^{1}H: 500MHz) at 298 K.

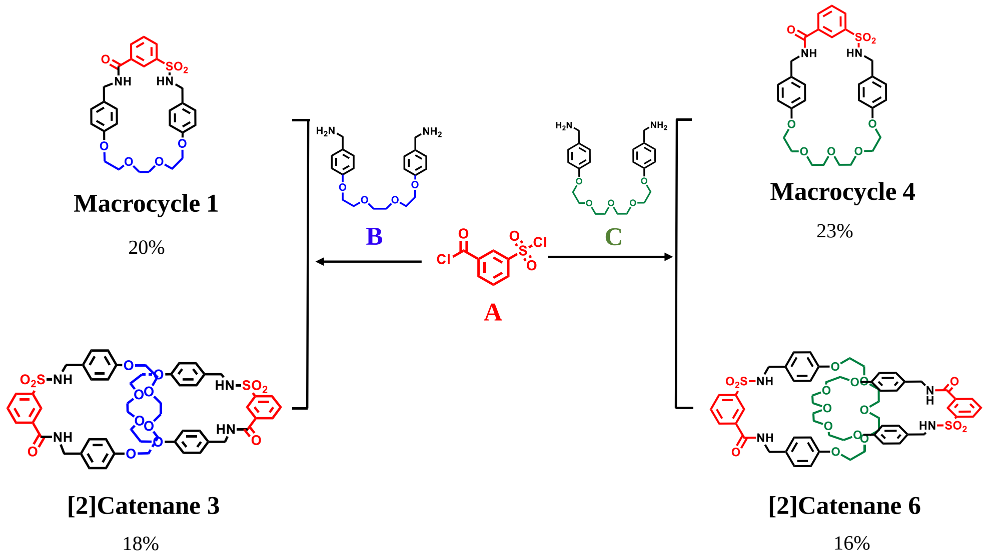
ESI-MS was conducted on Waters Synapt G2-Si mass spectrometer with traveling wave ion mobility. The IM-MS experiments for complexes were performed under the following conditions: ESI capillary voltage, 3.0 kV; sample cone voltage, 20 V; extraction cone voltage, 1.0 V; source temperature 100 ºC; desolvation temperature, 120 ºC; cone gas flow, 10 L/h; desolvation gas flow, 700 L/h (N_2); source gas control, 0 mL/min; trap gas control, 2 mL/min; Helium cell gas control, 100 mL/min; ion mobility (IM) cell gas control, 30 mL/min; sample flow rate, 5 μL/min; IM traveling wave height, 25 V; and IM traveling wave velocity, 1000 m/s.

UV-vis spectra and steady-state fluorescence spectra were recorded in a quartz cell (light path 10 mm) on a Shimadzu UV2700 UV-visible spectrophotometer and a Shimadzu RF-6000 fluorescence spectrophotometer.

All calculations were performed with the Gaussian 09 program.[S4] The B3LYP functional was utilized for geometry optimization. [S5-S7] The 6-31G* basis set was considered for all atoms.

Section B. Synthesis and characterization of [2]catenanes 3 and 6.

Scheme S1. The synthesis route of [2]catenanes **3** and **6**.



Synthesis of macrocycle 1 and [2]catenane 3: **B** (0.360 g, 1.00 mmol, 1 eq.) in $CHCl_3$ (dry, 40 mL) and **A** (0.239 g, 1.00 mmol, 1 eq.) in $CHCl_3$ (dry, 40 mL) were added simultaneously *via* syringe pump to NEt_3 (0.7 mL, 5 mmol, 5 eq.) in $CHCl_3$ (dry, 160 mL) over 4 h at room temperature under N_2 before stirring for an additional 16 h. The reaction mixture was washed with 1 M HCl (aq.) (100 mL), 1 M KOH (aq.) (100 mL) and brine (100 mL), dried ($MgSO_4$) and the solvent removed *in vacuo*. The solution was concentrated and the residue was purified by column chromatography (SiO_2; DCM/Acetone = 10:1 for **1**, DCM/Acetone = 5:1 for **3**). Both **1** and **3** were obtained as white solids.

Macrocycle 1 (120 mg, 20%): ^{1}H NMR (500 MHz, DMSO-d_6) δ 9.12-9.14 (t, J = 5.0 Hz, 1H), 8.23 (s, 1H), 8.15-8.17 (t, J = 5.0 Hz, 1H), 7.98-8.00 (d, J = 10.0 Hz, 1H), 7.83-7.85 (d, J = 10.0 Hz, 2H), 7.53-7.56 (t, J = 5.0 Hz, 1H), 7.24-7.26 (d, J = 10.0 Hz, 2H), 6.94-6.95 (d, J = 10.0 Hz, 2H), 6.84-6.86 (d, J = 10.0 Hz, 2H), 6.45-6.47 (d, J = 10.0 Hz, 2H), 4.41-4.42 (d, J = 5.0 Hz, 2H), 4.14-4.15 (m, 2H), 4.08-4.09 (d, J = 5.0 Hz, 2H), 3.72-3.74 (m, 4H), 3.58-3.62 (m, 4H), 3.52-3.53 (m, 2H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 164.69, 158.04, 157.86, 142.28, 135.12, 132.34, 130.87, 129.56, 129.46, 129.36, 129.06, 128.85, 126.13, 115.35, 114.16, 70.70, 70.22, 69.31, 69.20, 67.99, 67.43, 46.23, 42.50, 31.17. HRMS (ESI-TOF): Calculated for [**1** + Na]$^+$: 549.1666; Found: 549.1672.

[2]Catenane 3 (108 mg, 18%): ^{1}H NMR (500 MHz, DMSO-d_6) δ 9.17-9.20 (t, J = 10.0 Hz, 2H), 8.25 (s, 2H), 8.14-8.16 (t, J = 5.0 Hz, 2H), 8.06-8.08 (d, J = 10.0 Hz, 2H), 7.87-7.88 (d, J = 5.0 Hz, 2H), 7.61-7.64 (t, J = 10.0 Hz, 2H), 7.23-7.25 (d, J = 10.0 Hz, 4H), 7.04-7.06 (d, J = 10.0 Hz, 4H), 6.89-6.90 (d, J = 5.0 Hz, 4H), 6.73-6.74 (d, J = 5.0 Hz, 4H), 4.41-4.42 (d, J = 5.0 Hz, 4H), 4.04-4.06 (m, 4H), 3.94-3.98 (m, 8H), 3.68-3.73 (m, 8H), 3.58-3.59 (m, 8H). ^{13}C NMR (126 MHz, DMSO-d_6) δ

165.13, 158.03, 157.60, 141.68, 135.50, 131.93, 131.21, 129.76, 129.41, 128.56, 128.38, 126.98, 125.95, 114.76, 114.57, 69.97, 69.31, 67.97, 67.53, 56.30, 46.12, 43.07, 42.68, 32.38, 31.93, 30.30. HRMS (ESI-TOF): Calculated for [**3** + Na]$^+$: 1075.3440; Found: 1075.3991.

Synthesis of macrocycle 4 and [2]catenane 6: **C** (0.404 g, 1.00 mmol, 1 eq.) in $CHCl_3$ (dry, 40 mL) and **A** (0.239 g, 1.00 mmol, 1 eq.) in $CHCl_3$ (dry, 40 mL) were added simultaneously via syringe pump to NEt_3 (0.7 mL, 5 mmol, 5 eq.) in $CHCl_3$ (dry, 160 mL) over 4 h at room temperature under N_2 before stirring for an additional 16 h. The reaction mixture was washed with 1 M HCl (aq) (100 mL), 1 M KOH (aq) (100 mL) and brine (100 mL), dried ($MgSO_4$) and the solvent removed *in vacuo*. The solution was concentrated and the residue was purified by column chromatography (SiO_2; DCM/Acetone = 10:1 for **4**, DCM/Acetone = 5:1 for **6**). Both **4** and **6** were obtained as white solids.

Macrocycle 4 (147 mg, 23%): ^{1}H NMR (500 MHz, DMSO-d_6) δ 9.12-9.15 (t, J = 10.0 Hz, 1H), 8.22 (s, 1H), 8.13-8.15 (t, J = 5.0 Hz, 1H), 7.99-8.01 (d, J = 10.0 Hz, 1H), 7.83-7.84 (d, J = 5.0 Hz, 2H), 7.54-7.57 (t, J = 10.0 Hz, 1H), 7.25-7.27 (d, J = 10.0 Hz, 2H), 6.91-6.93 (d, J = 10.0 Hz, 2H), 6.87-6.88 (d, J = 5.0 Hz, 2H), 6.50-6.52 (d, J = 10.0 Hz, 2H), 4.41-4.42 (d, J = 10.0 Hz, 2H), 4.06-4.09 (m, 4H), 3.73-3.78 (d, 4H), 3.53-3.63 (m, 10H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 164.81, 157.95, 157.84, 142.05, 135.18, 132.18, 130.98, 129.54, 129.37, 129.13, 128.85, 126.03, 114.77, 114.18, 70.59, 70.44, 70.31, 70.26, 69.27, 67.78, 67.45, 46.26, 42.52. HRMS (ESI-TOF): Calculated for [**4** + Na]$^+$: 593.1928; Found: 593.1912.

[2]Catenane 6 (103 mg, 16%): ^{1}H NMR (500 MHz, DMSO-d_6) δ 9.18-9.20 (t, J = 5.0 Hz, 2H), 8.26 (s, 2H), 8.14-8.16 (t, J = 5.0 Hz, 2H), 8.06-8.07 (d, J = 5.0 Hz, 2H), 7.88-7.89 (d, J = 5.0 Hz, 2H), 7.61-7.65 (t, J = 10.0 Hz, 2H), 7.23-7.25 (d, J = 10.0 Hz, 4H), 7.06-7.07 (d, J = 5.0 Hz, 4H), 6.88-6.90 (d, J = 10.0 Hz, 4H), 6.74-6.76 (d, J = 10.0 Hz, 4H), 4.41-4.42 (d, J = 5.0 Hz, 4H), 4.03-4.05 (t, J = 5.0 Hz, 4H), 3.94-3.98 (m, 8H), 3.68-3.71 (m, 8H), 3.53-3.55 (m, 16H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 165.16, 158.05, 157.92, 141.65, 135.52, 131.91, 131.22, 129.77, 129.65, 129.41, 129.18, 128.65, 128.41, 126.98, 125.96, 114.75, 114.57,114.26, 70.40, 70.31, 69.38, 69.35, 67.60, 67.54, 46.12, 42.70. HRMS (ESI-TOF): Calculated for [**6** + Na]$^+$: 1163.3964; Found: 1163.3986.

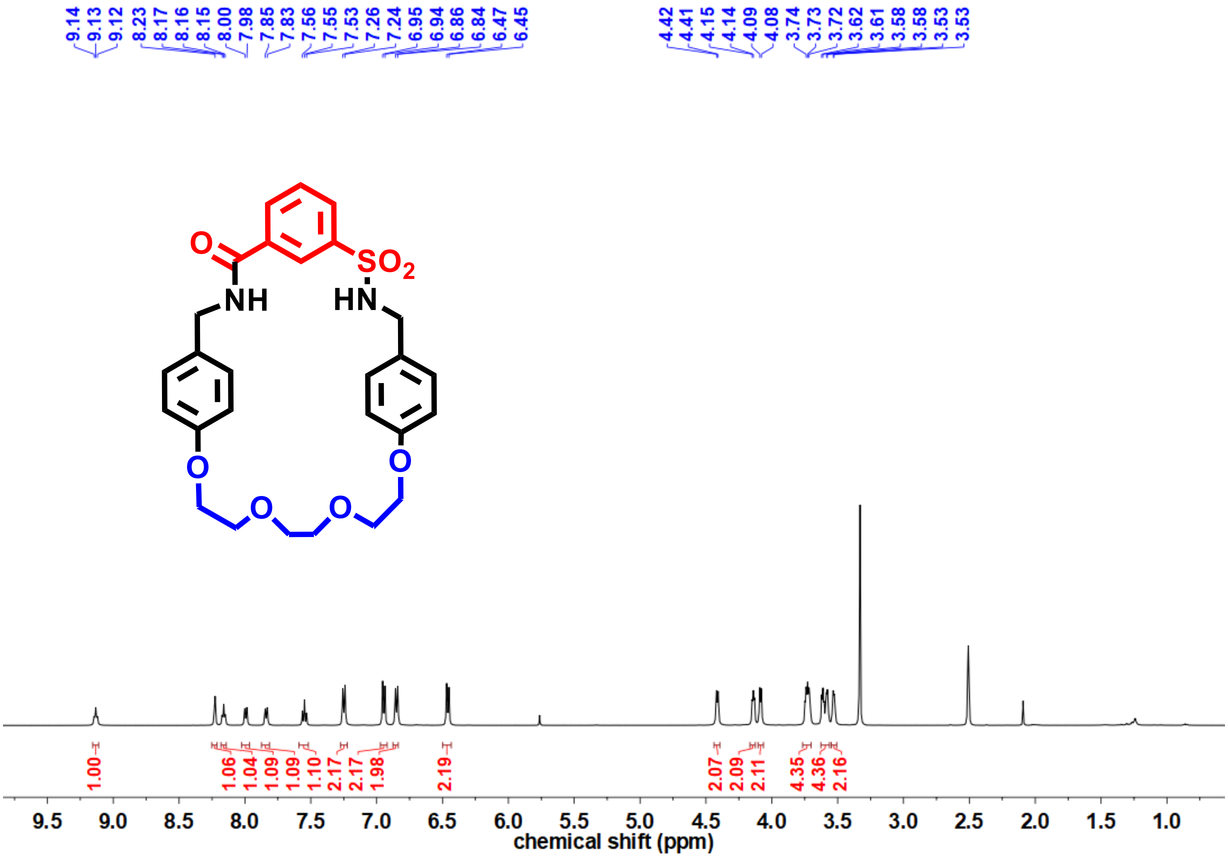


Figure S1. ^{1}H NMR spectrum (DMSO-d_6, 298 K, 500 MHz) of **1**.

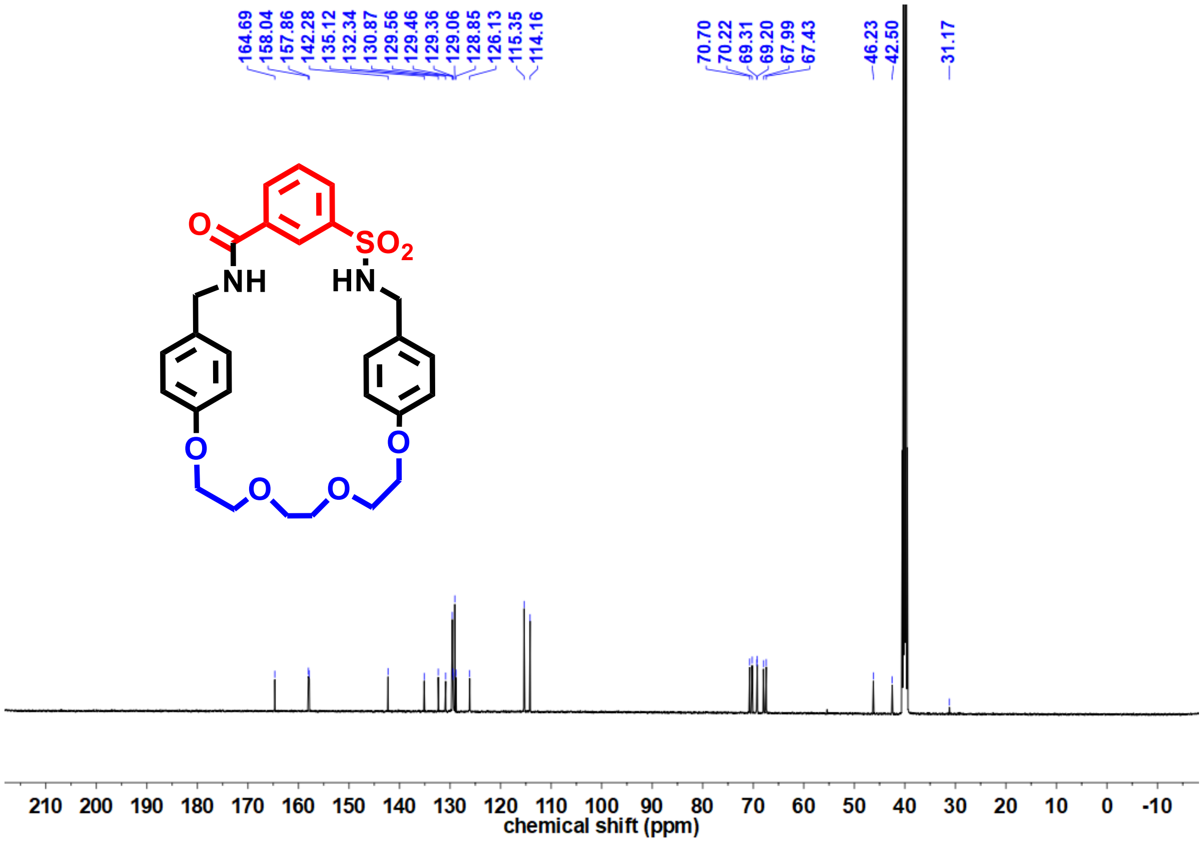


Figure S2. ^{13}C NMR spectrum (DMSO-d_6, 298 K, 126 MHz) of **1**.

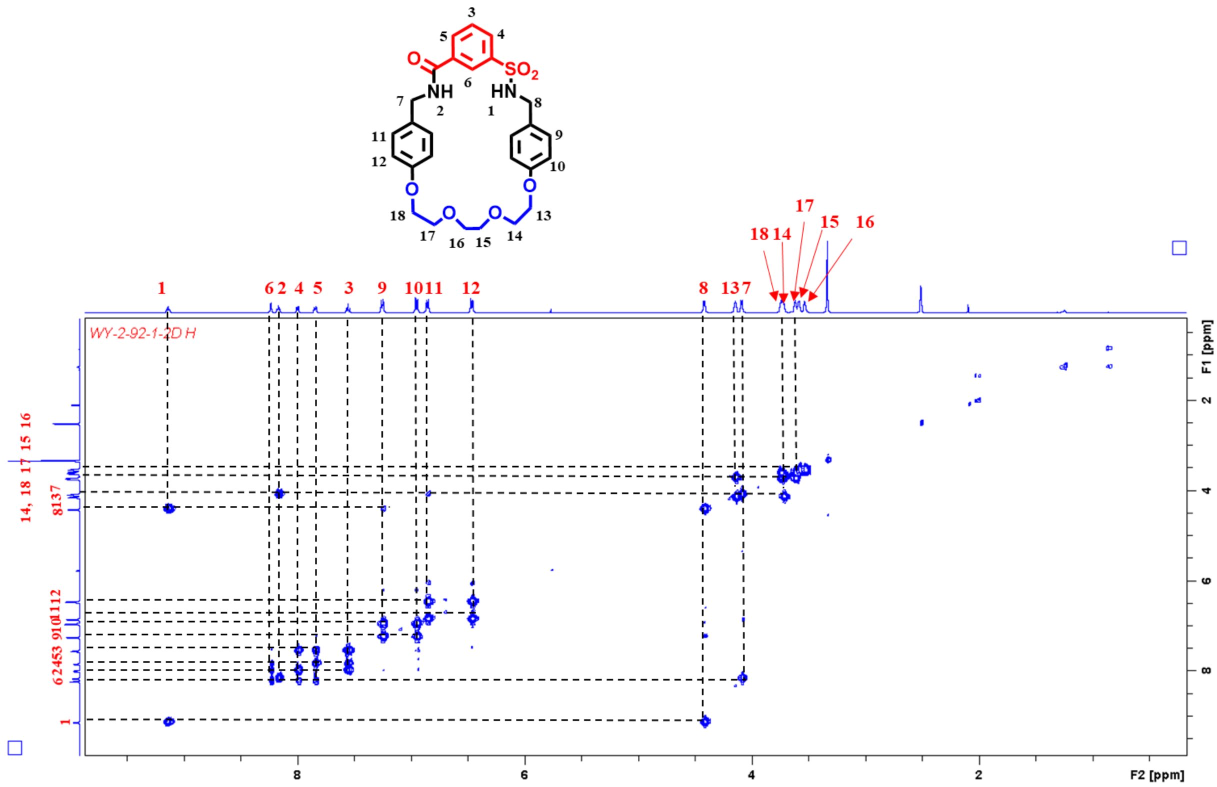


Figure S3. 2D ^{1}H-^{1}H COSY spectrum (DMSO-d_6, 298 K, 500 MHz) of **1**.

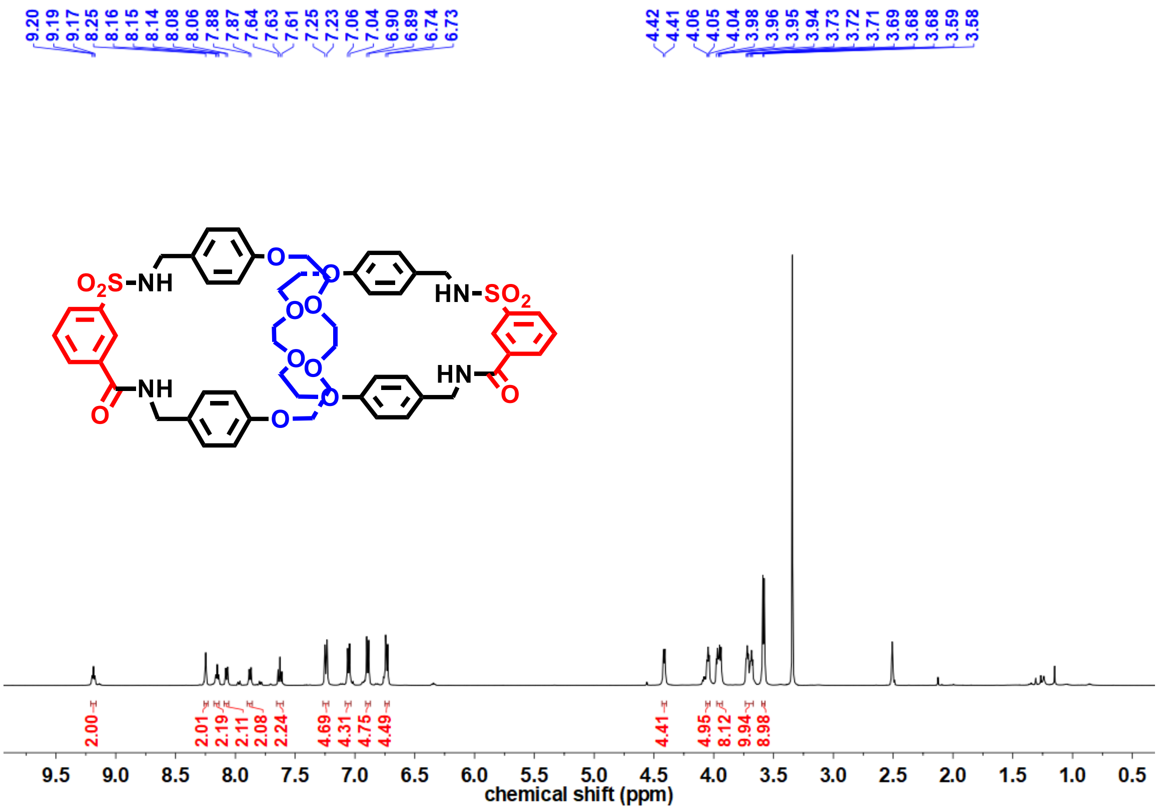


Figure S4. ^{1}H NMR spectrum (DMSO-d_6, 298 K, 500 MHz) of **3**.

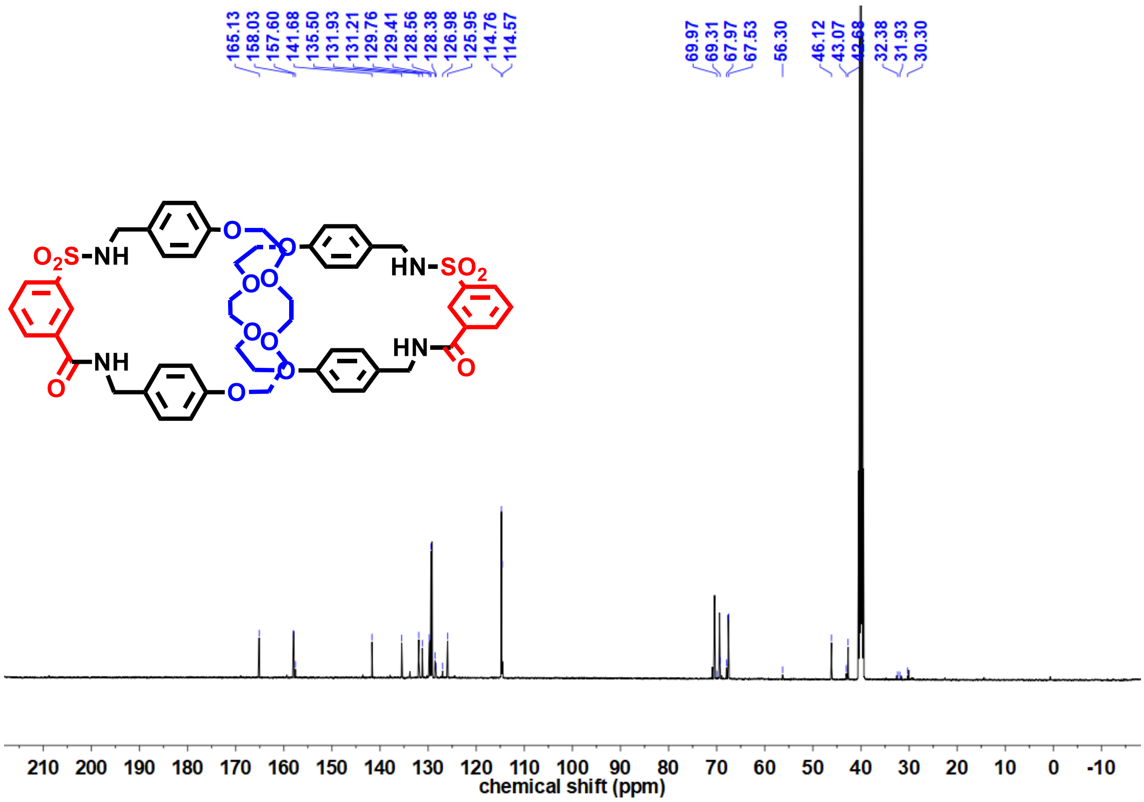


Figure S5. ^{13}C NMR spectrum (DMSO-d_6, 298 K, 126 MHz) of **3**.

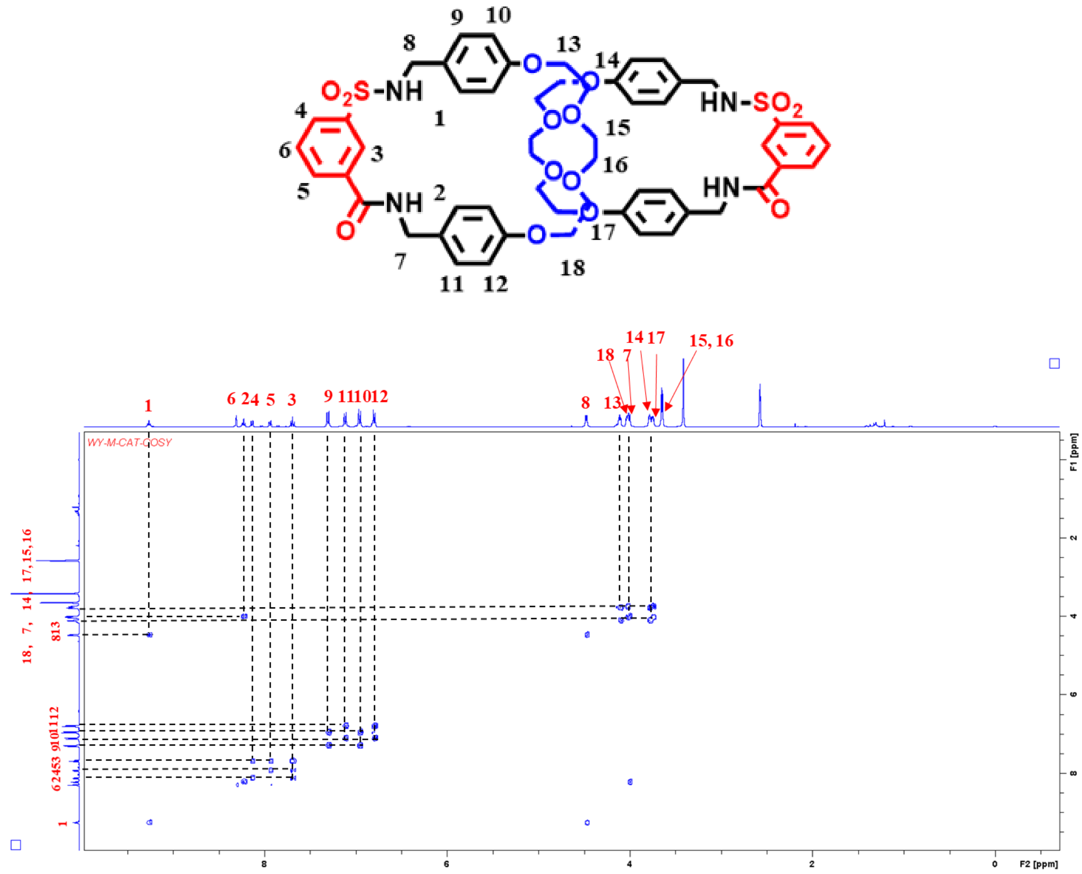


Figure S6. 2D ^{1}H-^{1}H COSY spectrum (DMSO-d_6, 298 K, 500 MHz) of **3**.

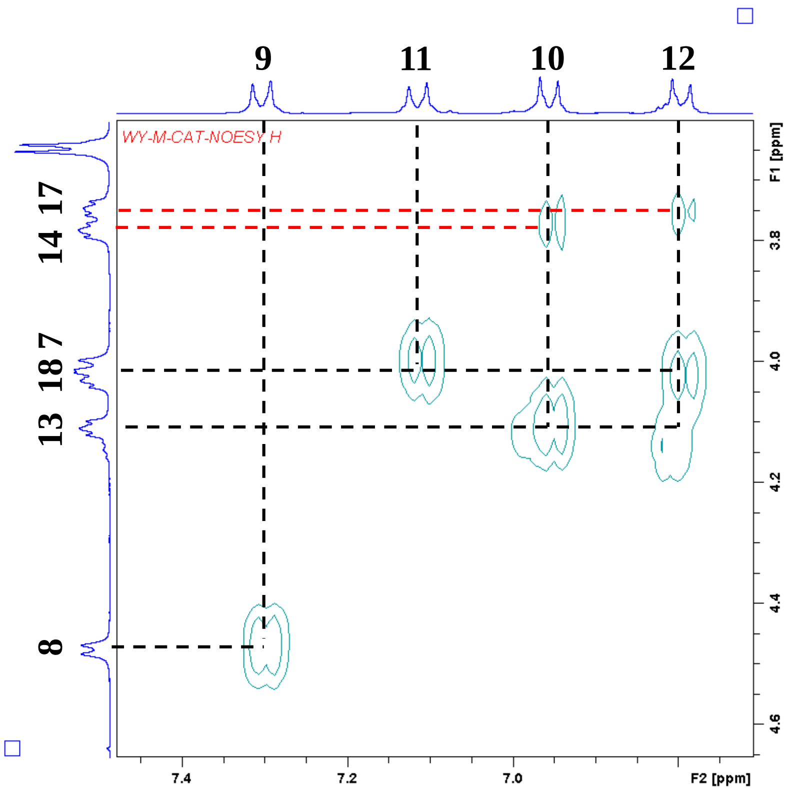


Figure S7. Partial 2D ^{1}H-^{1}H NOESY spectrum (DMSO-d_6, 298 K, 500 MHz) of **3**.

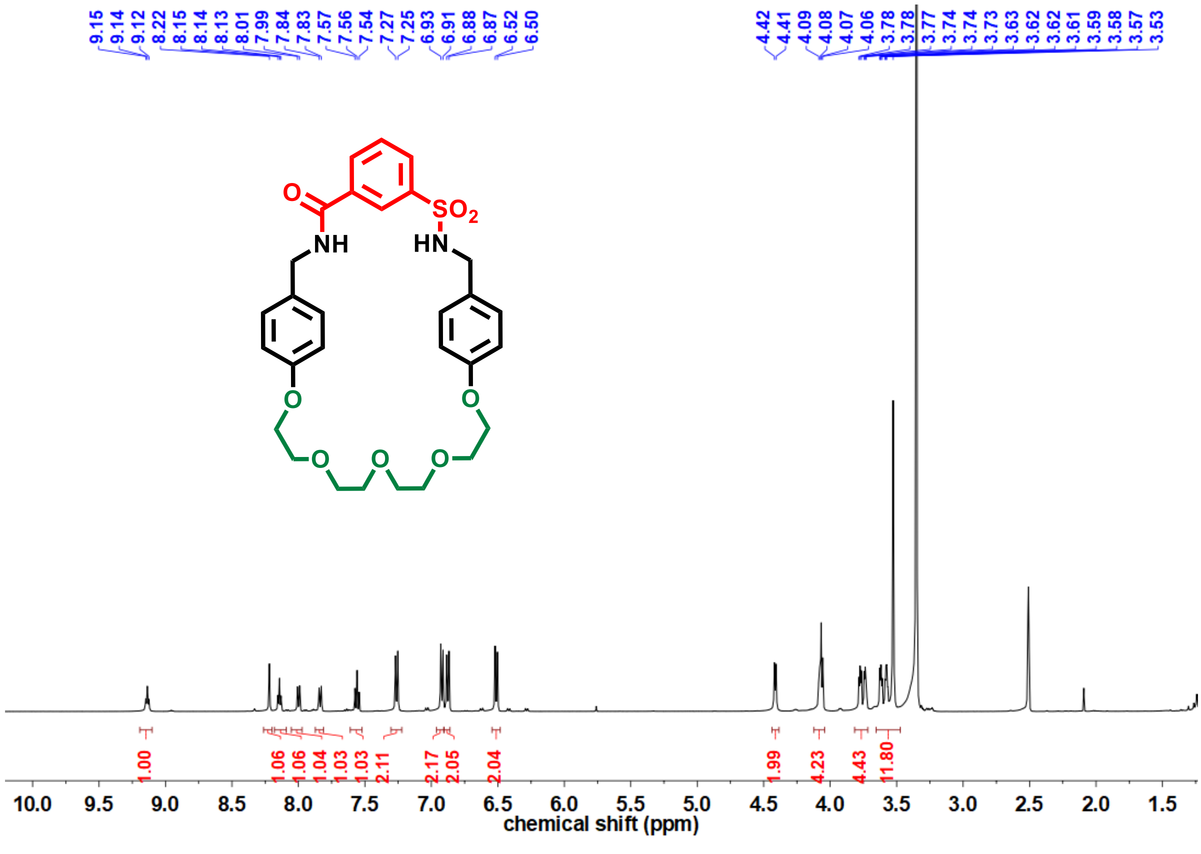


Figure S8. ^{1}H NMR spectrum (DMSO-d_6, 298 K, 500 MHz) of **4**.

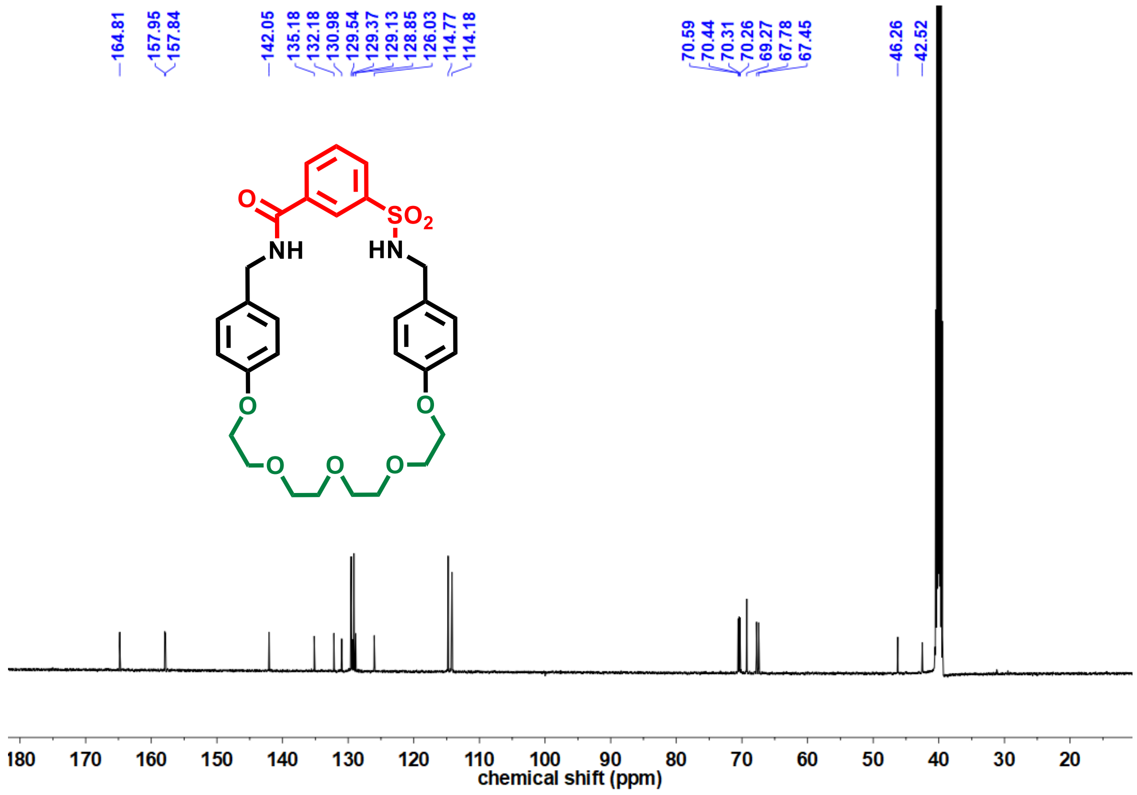


Figure S9. ^{13}C NMR spectrum (DMSO-d_6, 298 K, 126 MHz) of **4**.

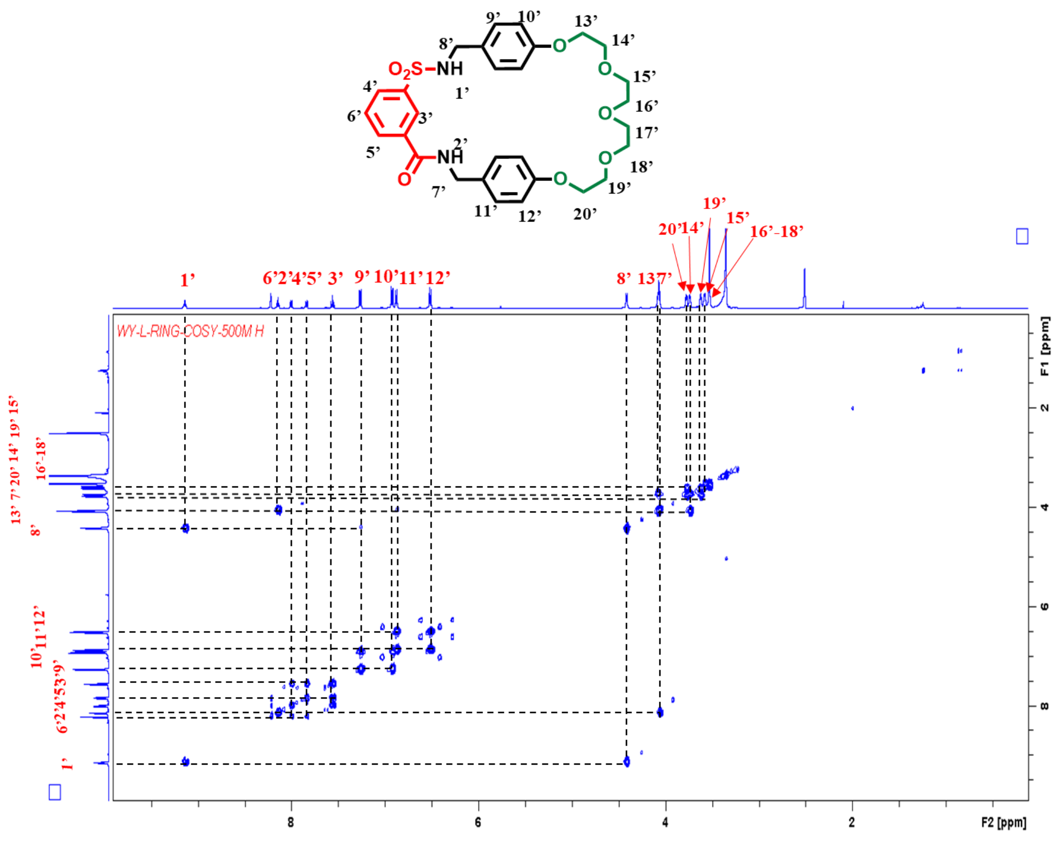


Figure S10. 2D ^{1}H-^{1}H COSY spectrum (DMSO-d_6, 298 K, 500 MHz) of **4**.

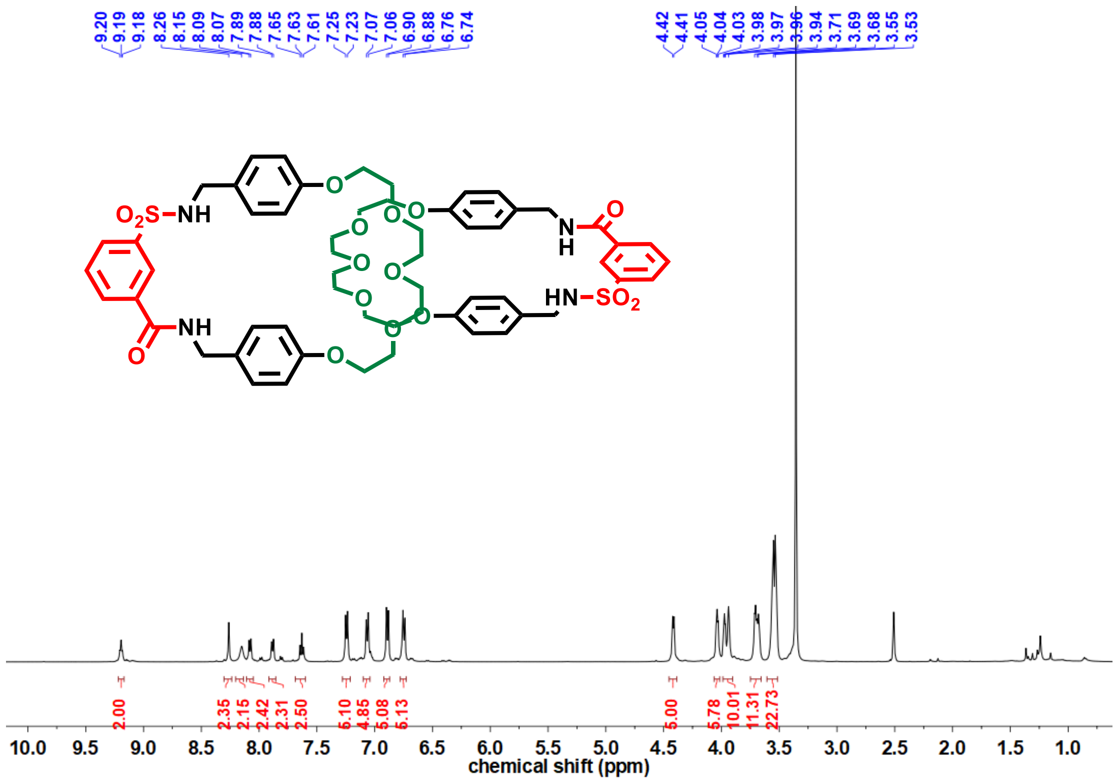


Figure S11. ^{1}H NMR spectrum (DMSO-d_6, 298 K, 500 MHz) of **6**.

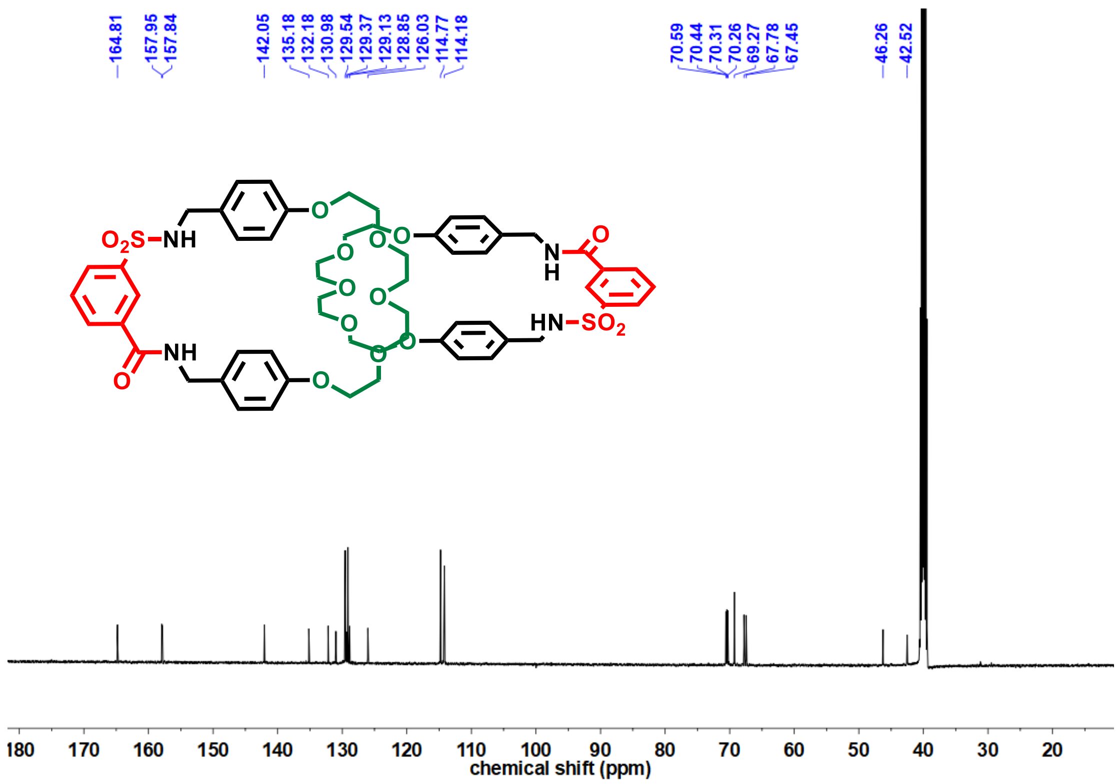


Figure S12. ^{13}C NMR spectrum (DMSO-d_6, 298 K, 126 MHz) of **6**.

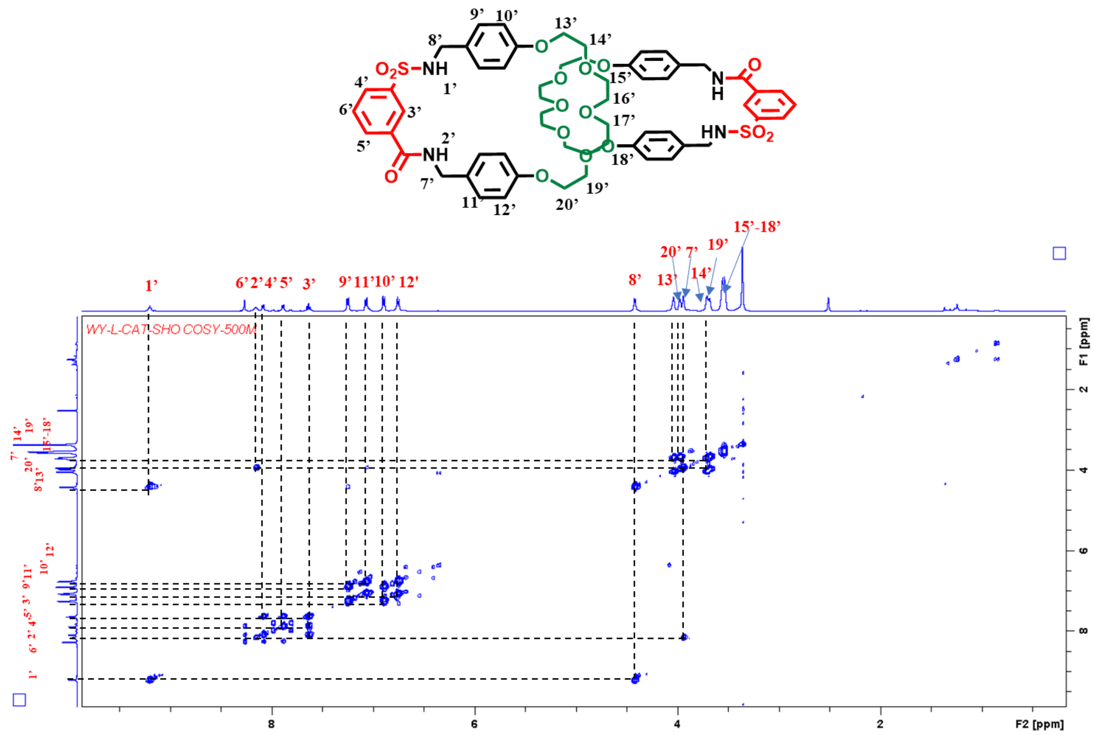


Figure S13. 2D ^1H-^1H COSY spectrum (DMSO-d_6, 298 K, 500 MHz) of **6**.

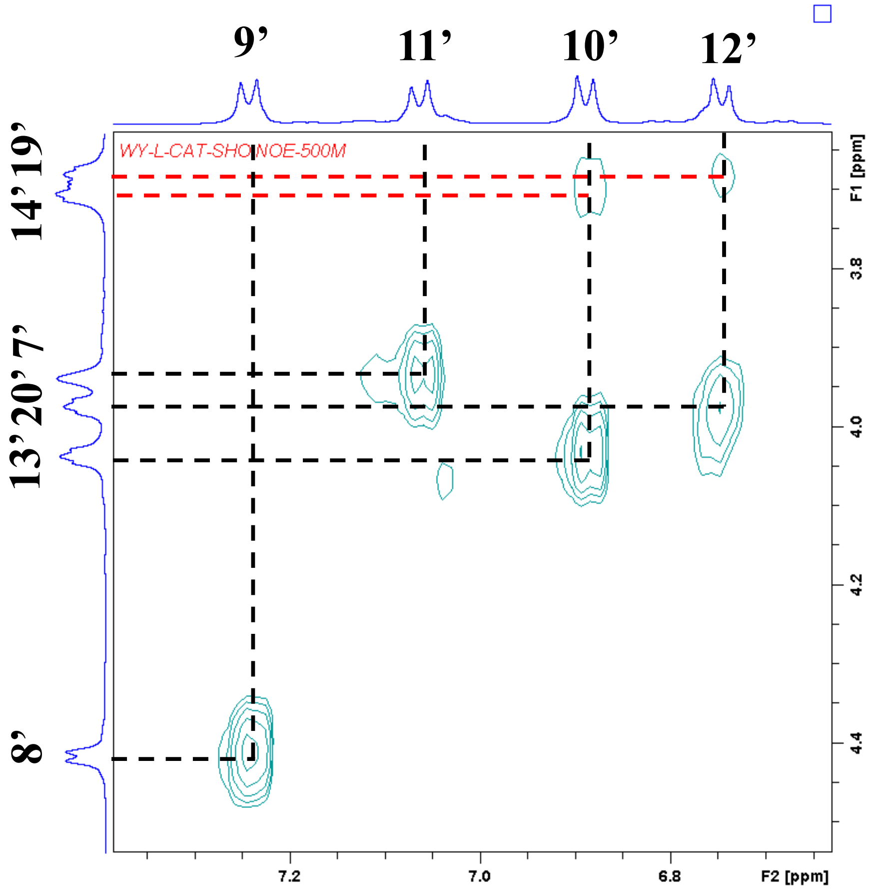
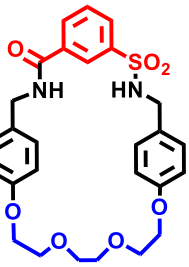


Figure S14. Partial 2D ^1H-^1H NOESY spectrum (DMSO-d_6, 298 K, 500 MHz) of **6**.



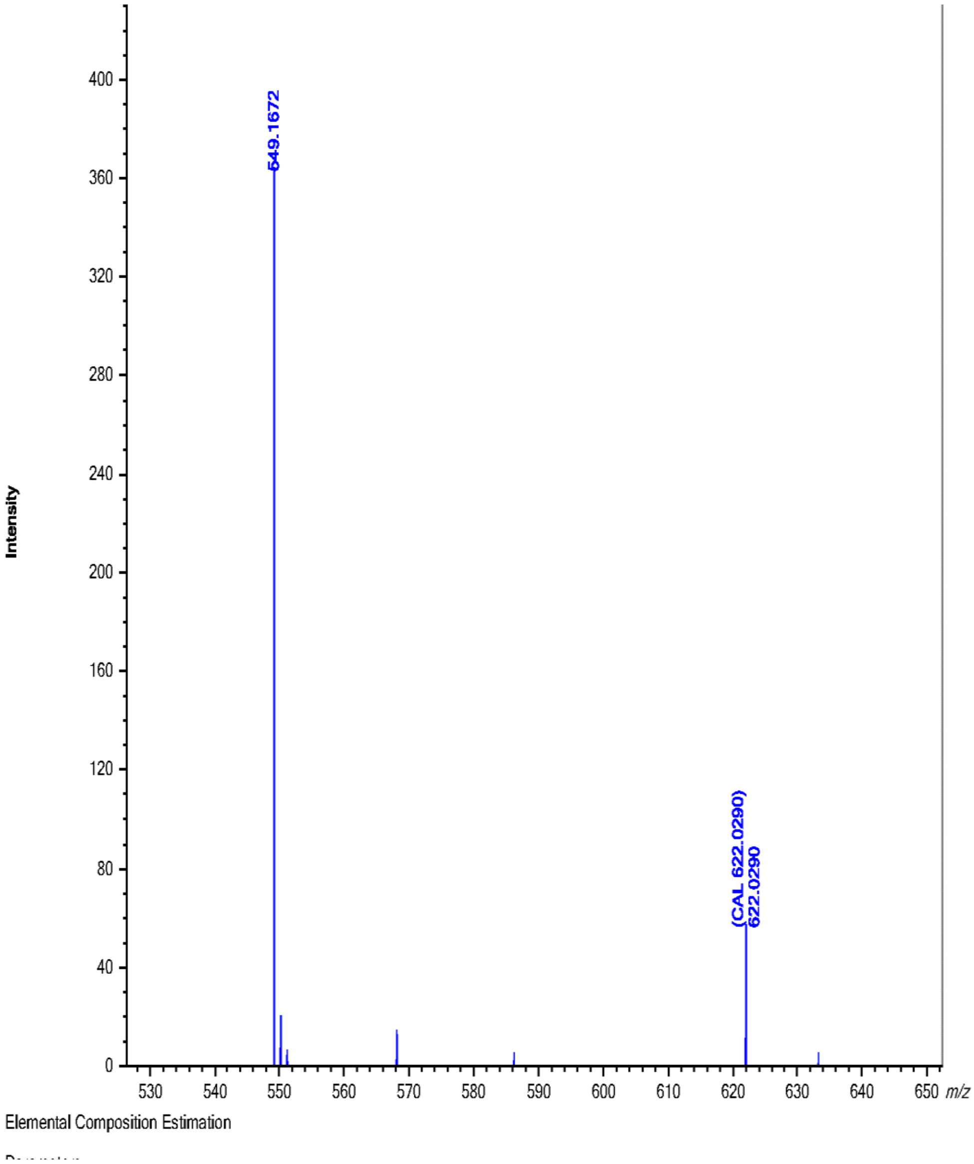
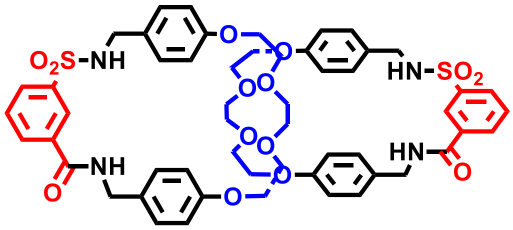


Figure S15. HRMS (ESI-TOF-MS) spectrum of **1**.



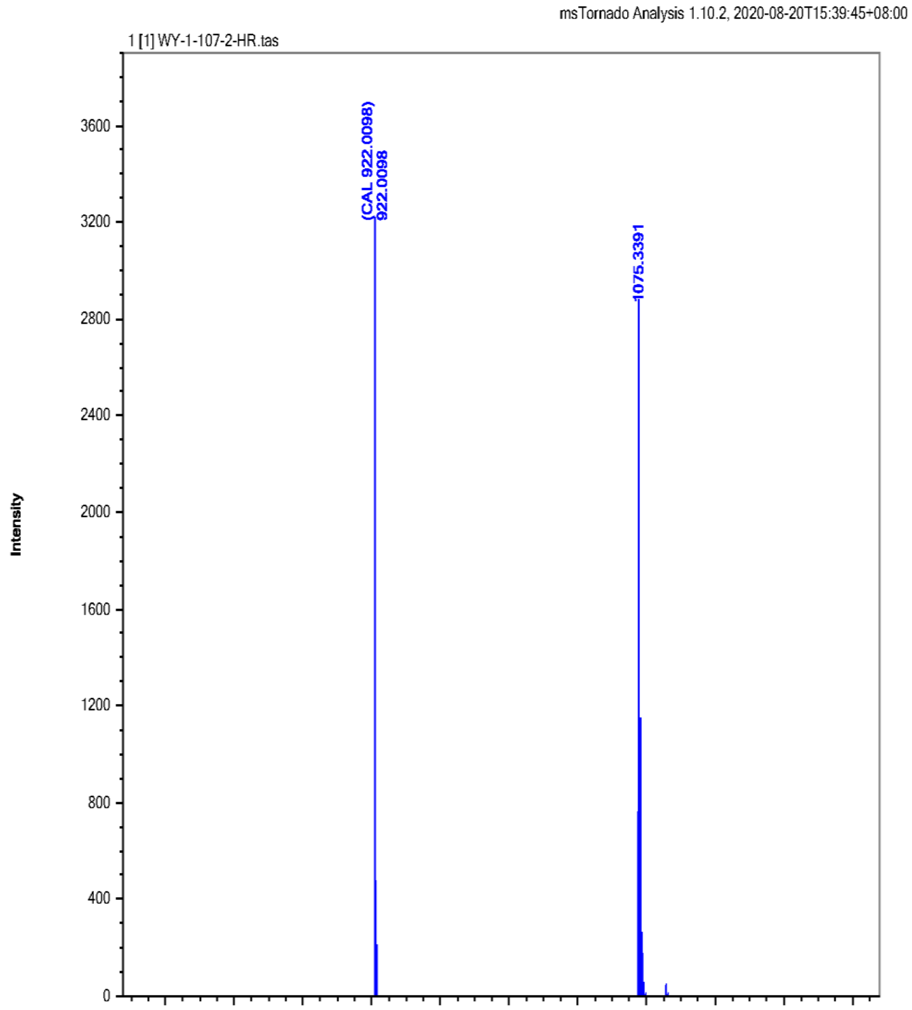
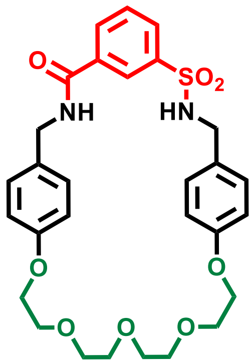


Figure S16. HRMS (ESI-TOF-MS) spectrum of **3**.



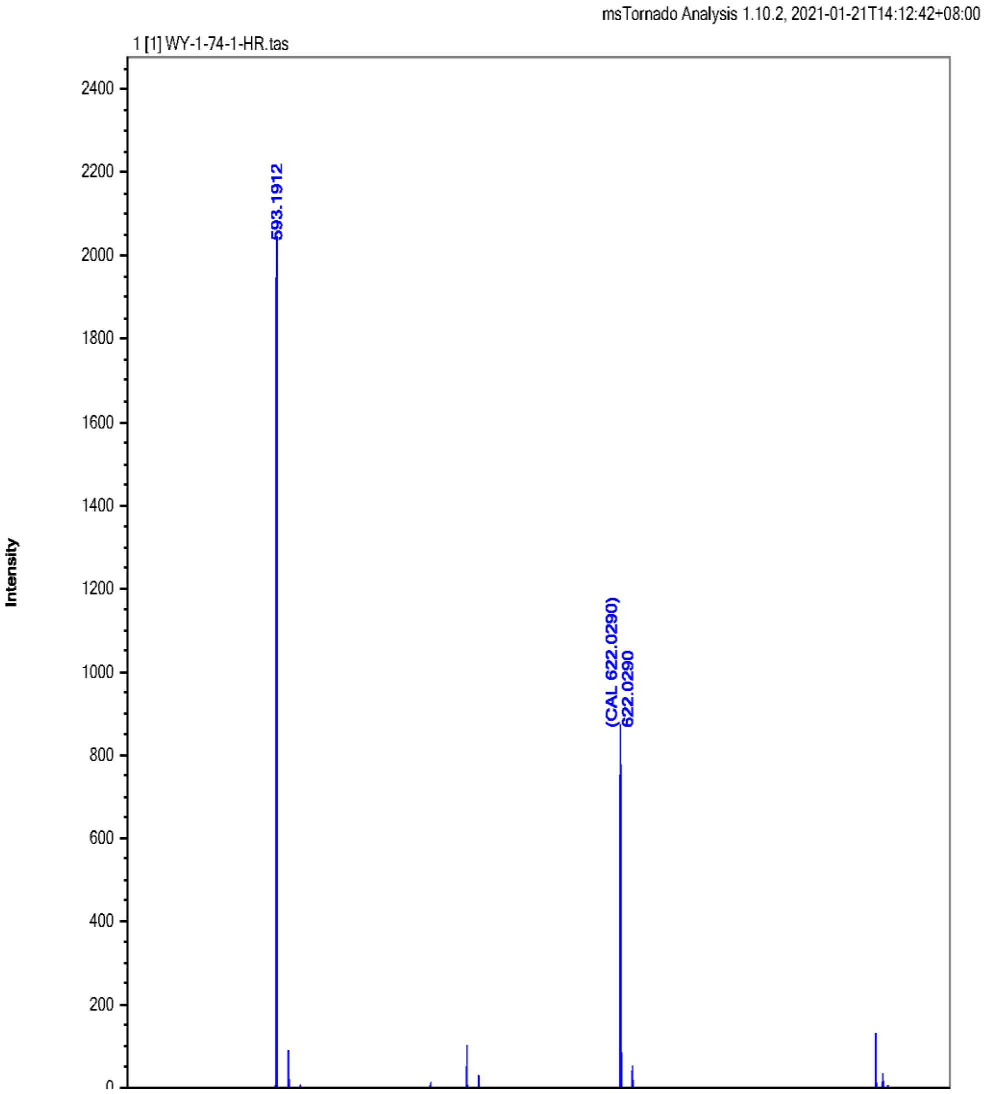
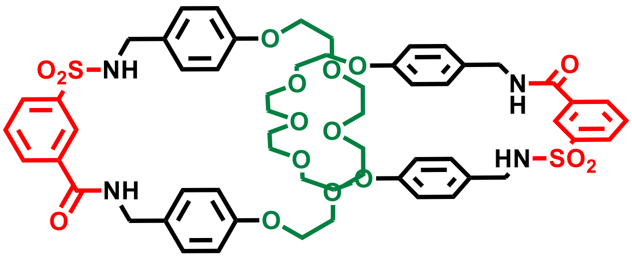


Figure S17. HRMS (ESI-TOF-MS) spectrum of **4**.



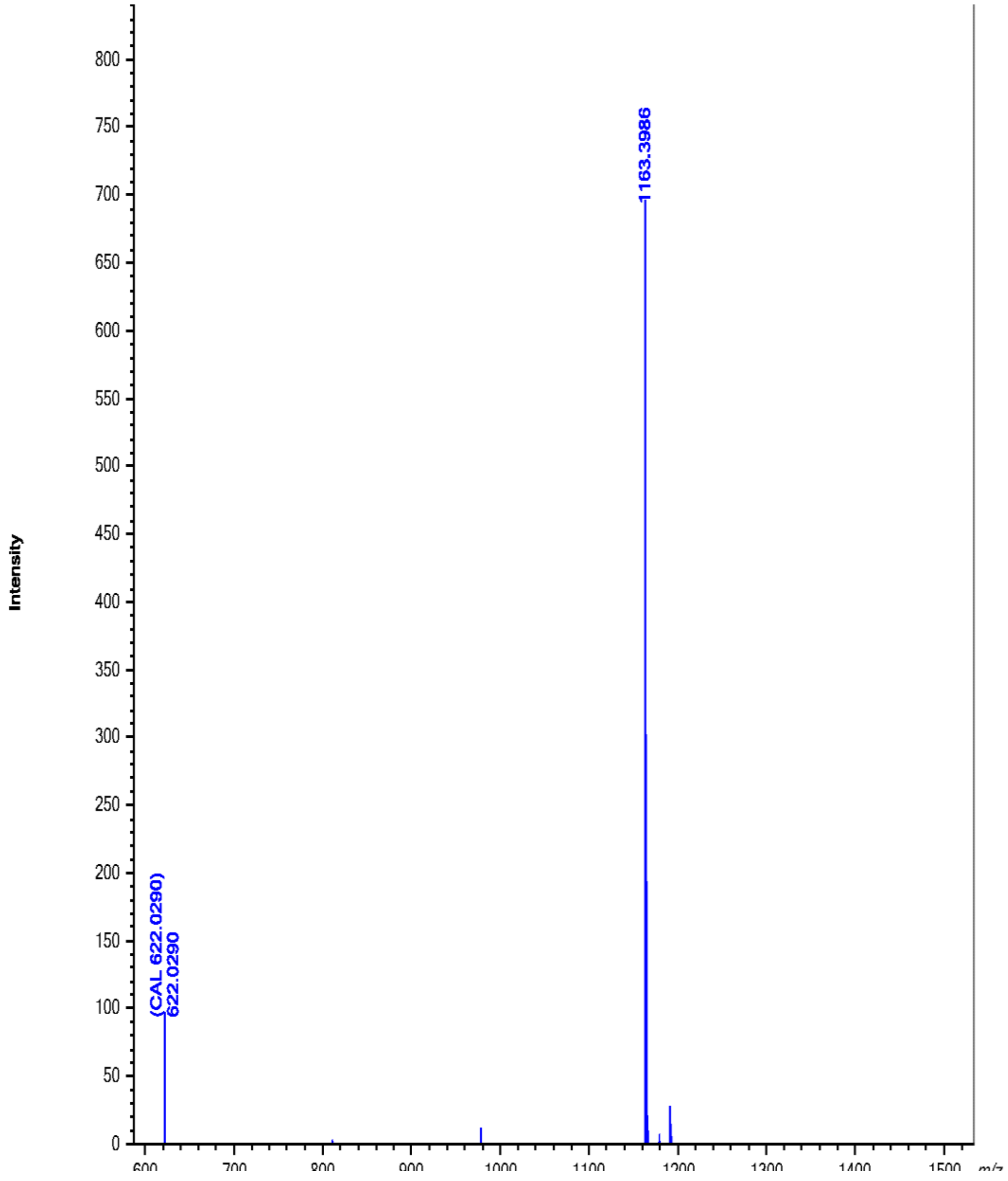


Figure S18. HRMS (ESI-TOF-MS) spectrum of **6**.

Section C. CID/IMS measurements of [2]catenanes 3 and 6.

Figure S19. ESI-TOF-MS spectrum of **3.**

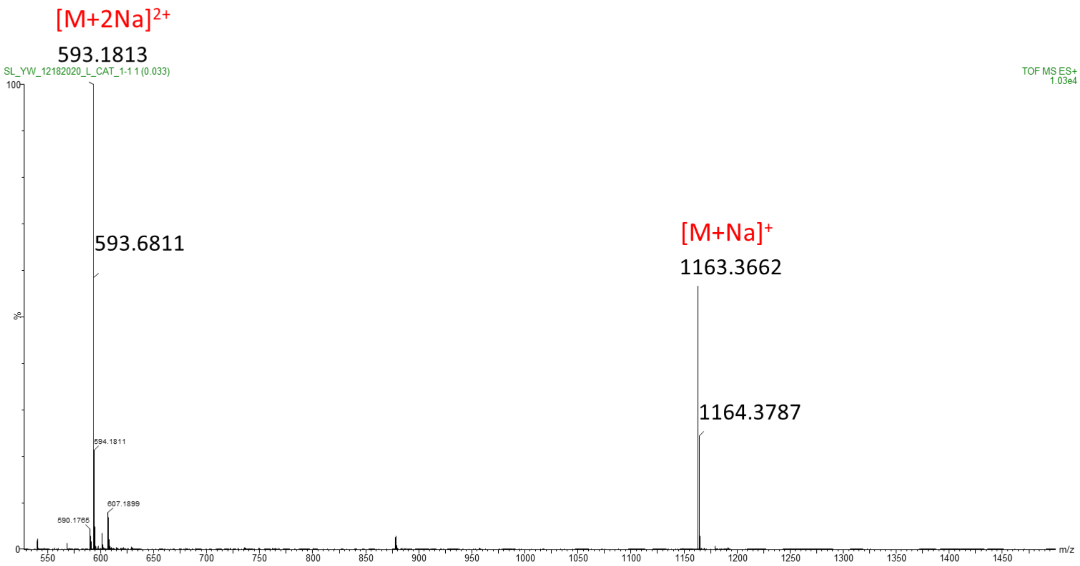


Figure S20. ESI-TOF-MS spectrum of **6.**

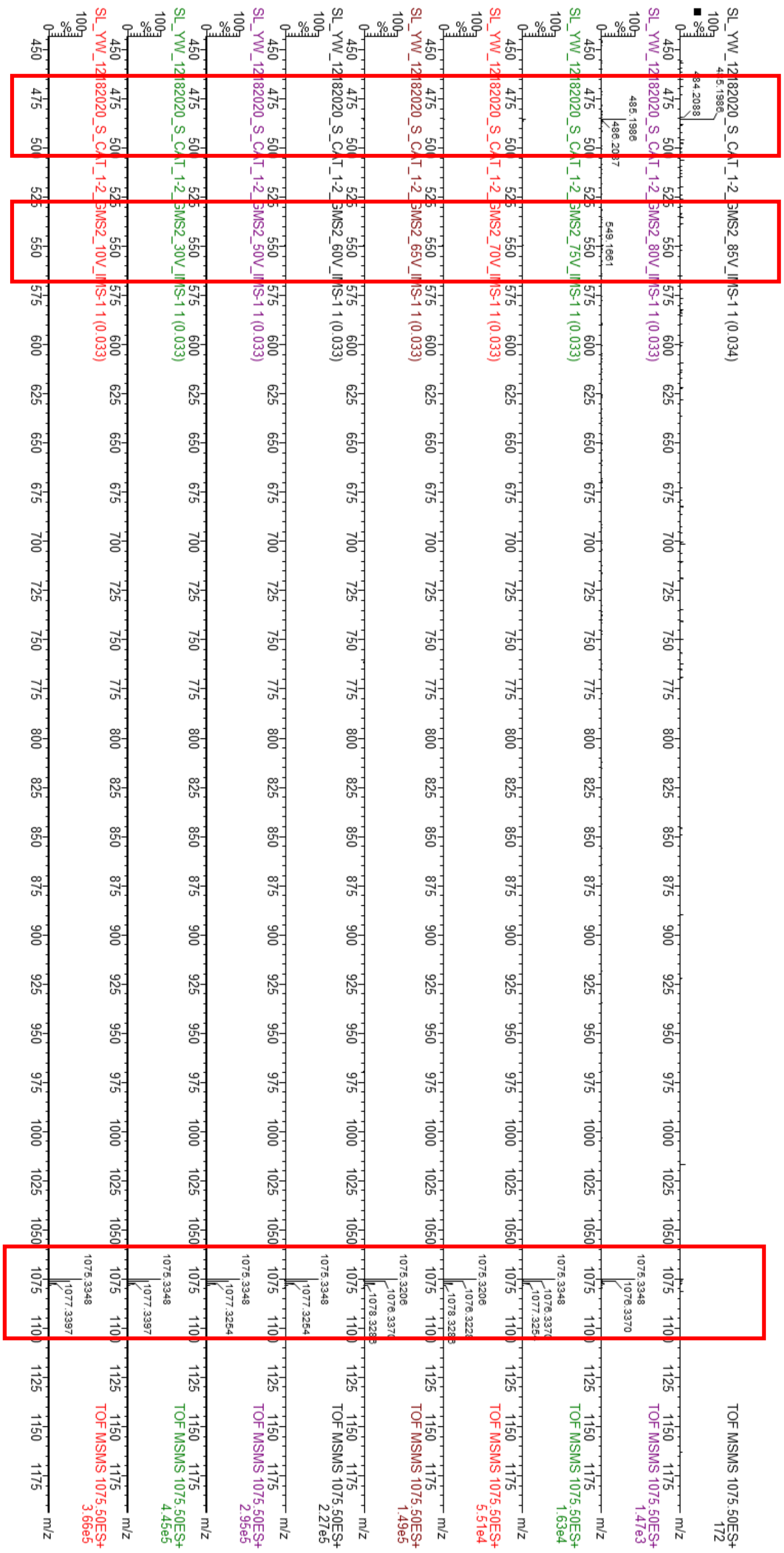


Figure S21. Full gMS^2 mass spectrum of **3** at 10 - 85V collision voltage in the mass selected CID/IMS experiments.

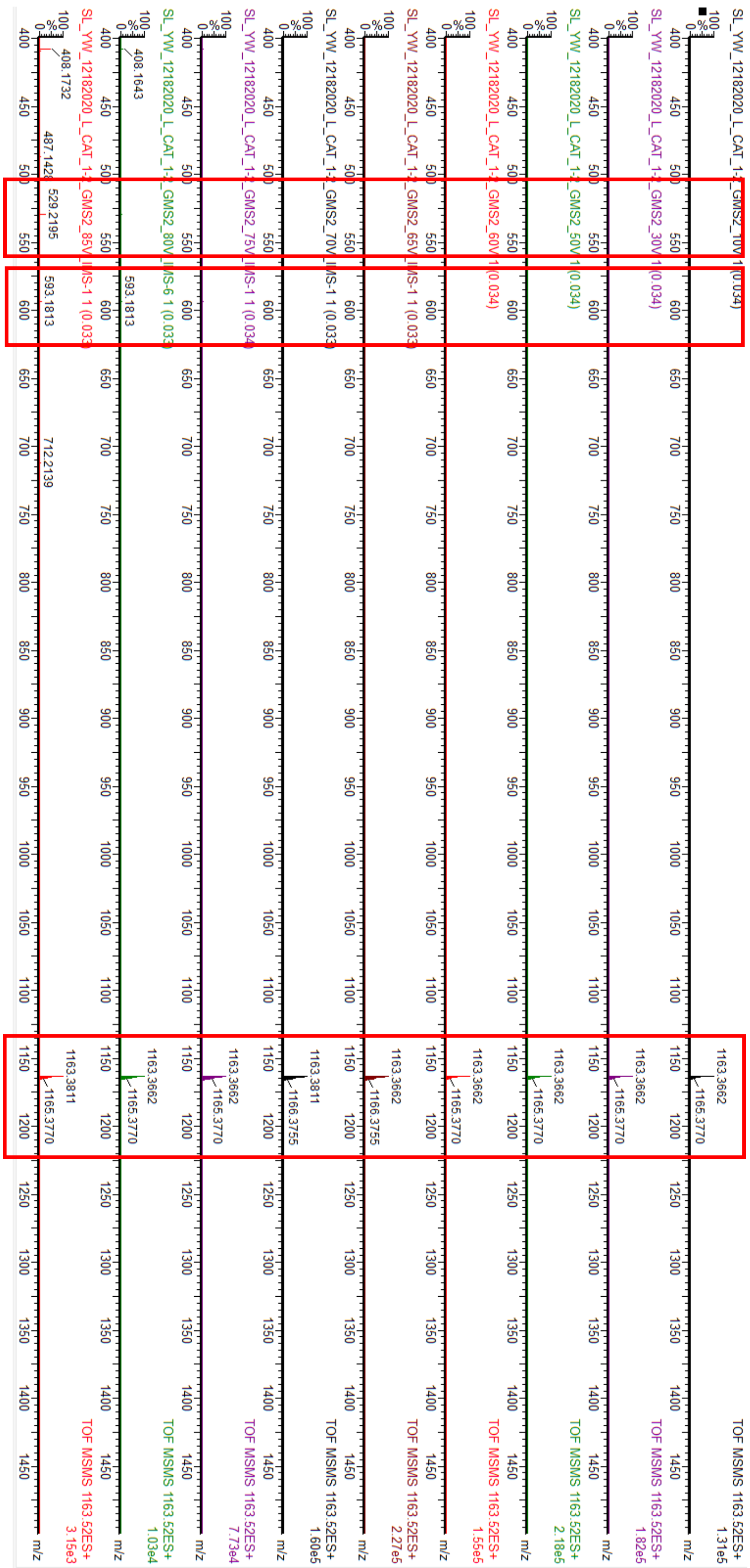


Figure S22. Full gMS^2 mass spectrum of **6** at 10 - 85V collision voltage in the mass selected CID/IMS experiments.

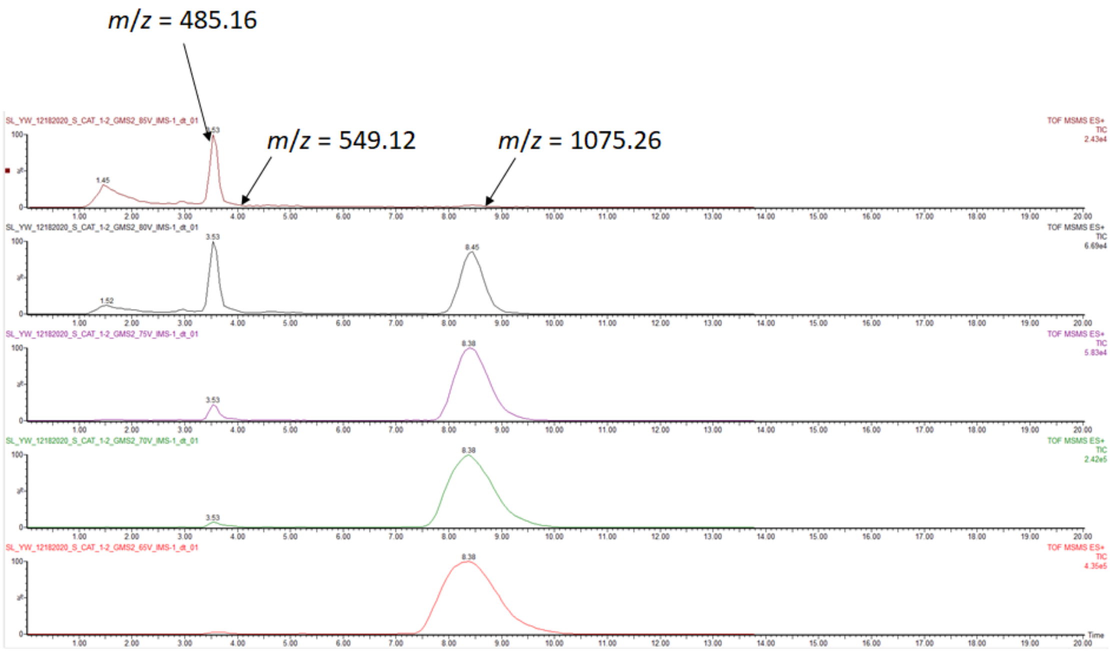


Figure S23. Normalized arrival time distributions of the species formed from [2]catenane **3** at 65 - 85 V collision voltage.

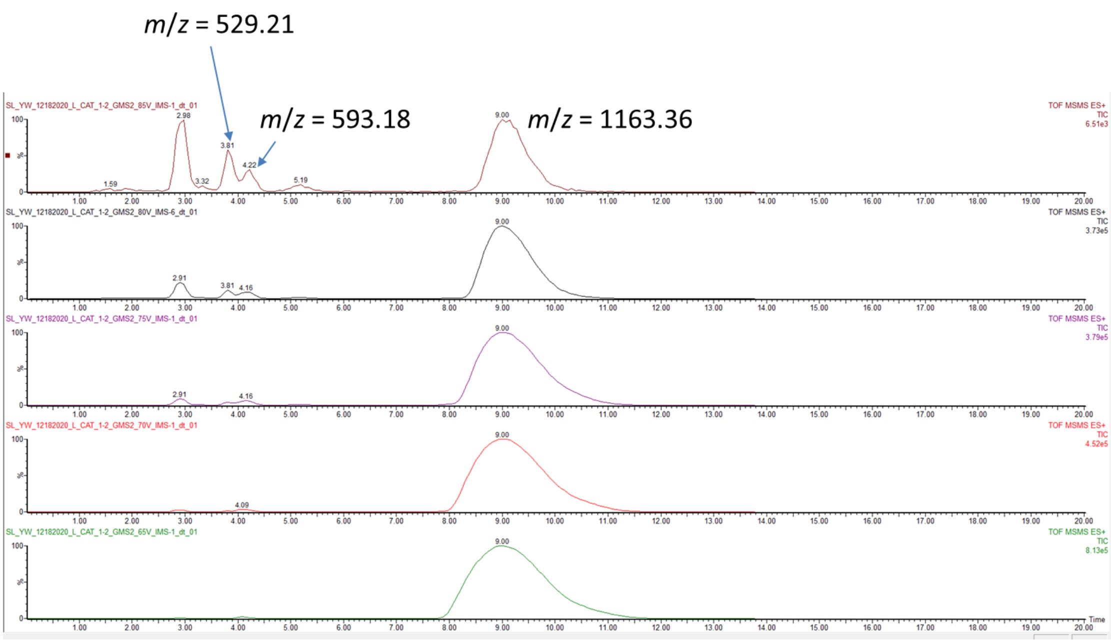


Figure S24. Normalized arrival time distributions of the species formed from [2]catenane **6** at 65 - 85 V collision voltage.

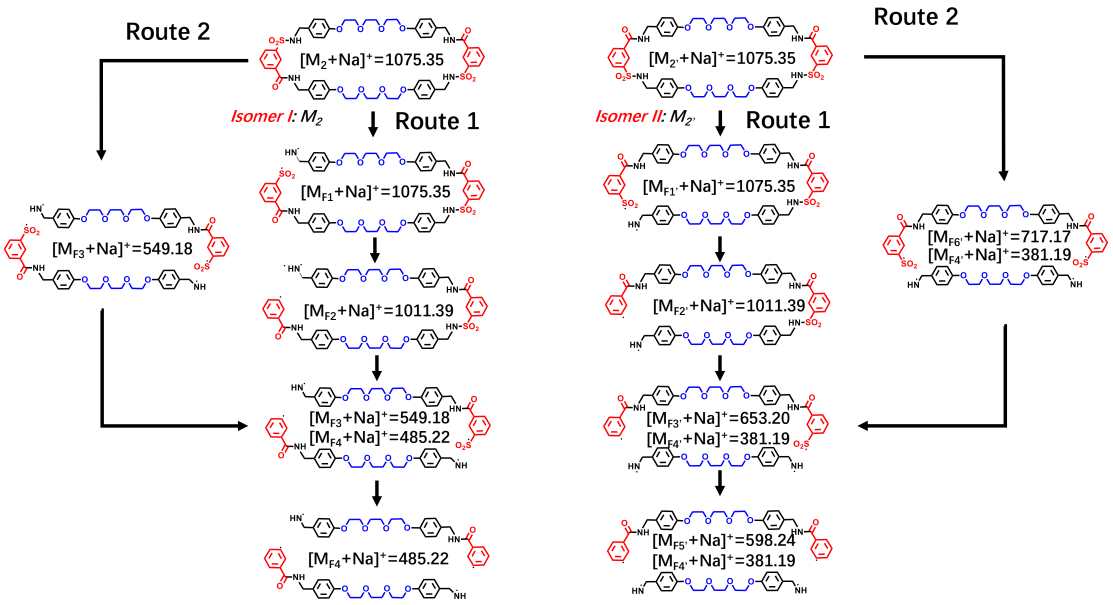


Fig. S25. Possible fragmentation pathways of the two isomers of macrocycle **2** and the expected *m/z* values of the corresponding sodiated *pseudo*-molecular ions.

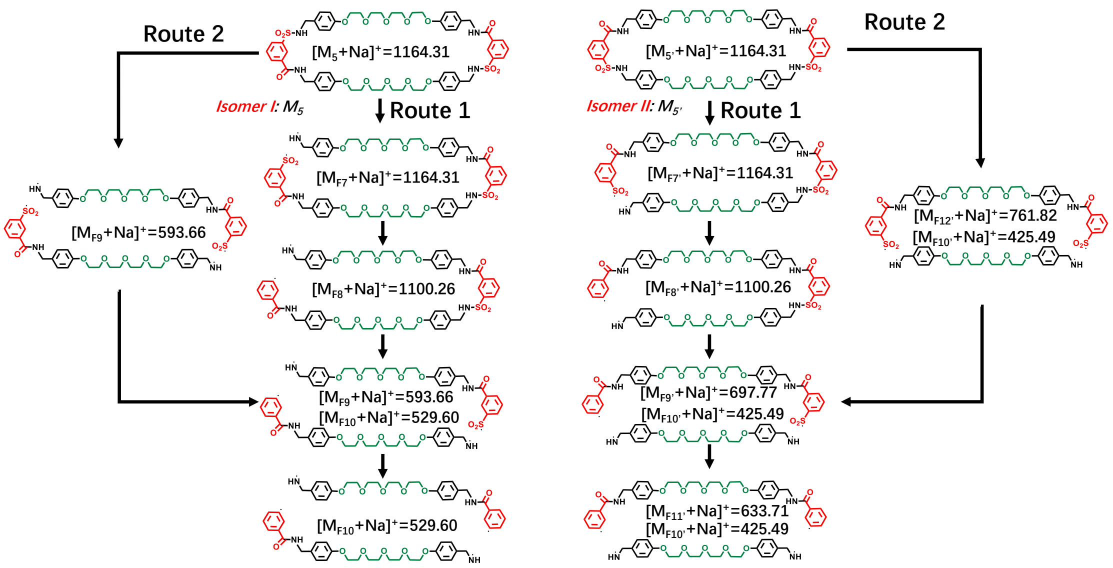


Fig. S26. Possible fragmentation pathways of the two isomers of macrocycle **5** and the expected *m/z* values of the corresponding sodiated *pseudo*-molecular ions.

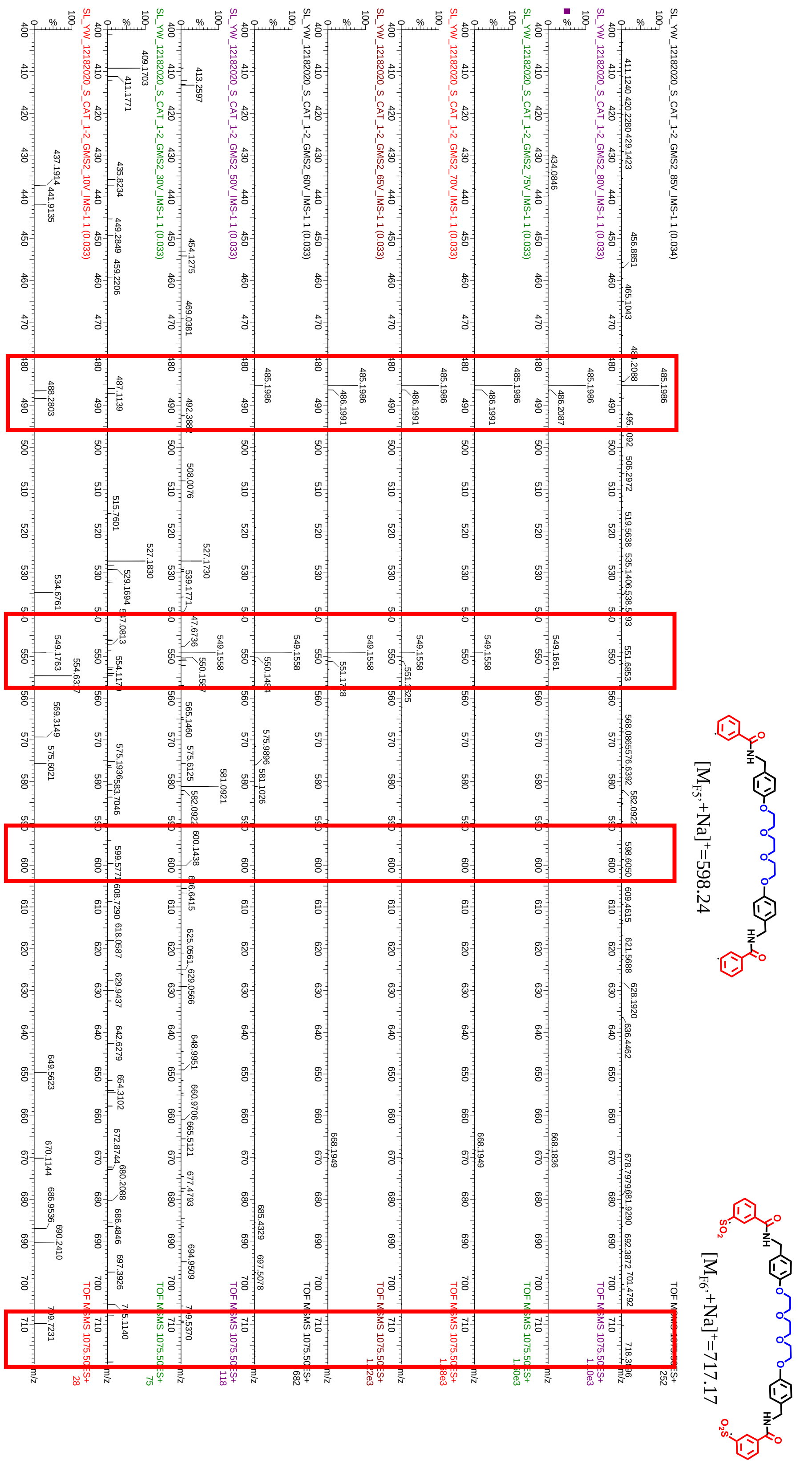


Figure S27. Partial gMS^2 mass spectrum of **3** at 10 - 85V collision voltage in the mass selected CID/IMS experiments in which the characteristic peaks of macrocycle **2** were not observed.

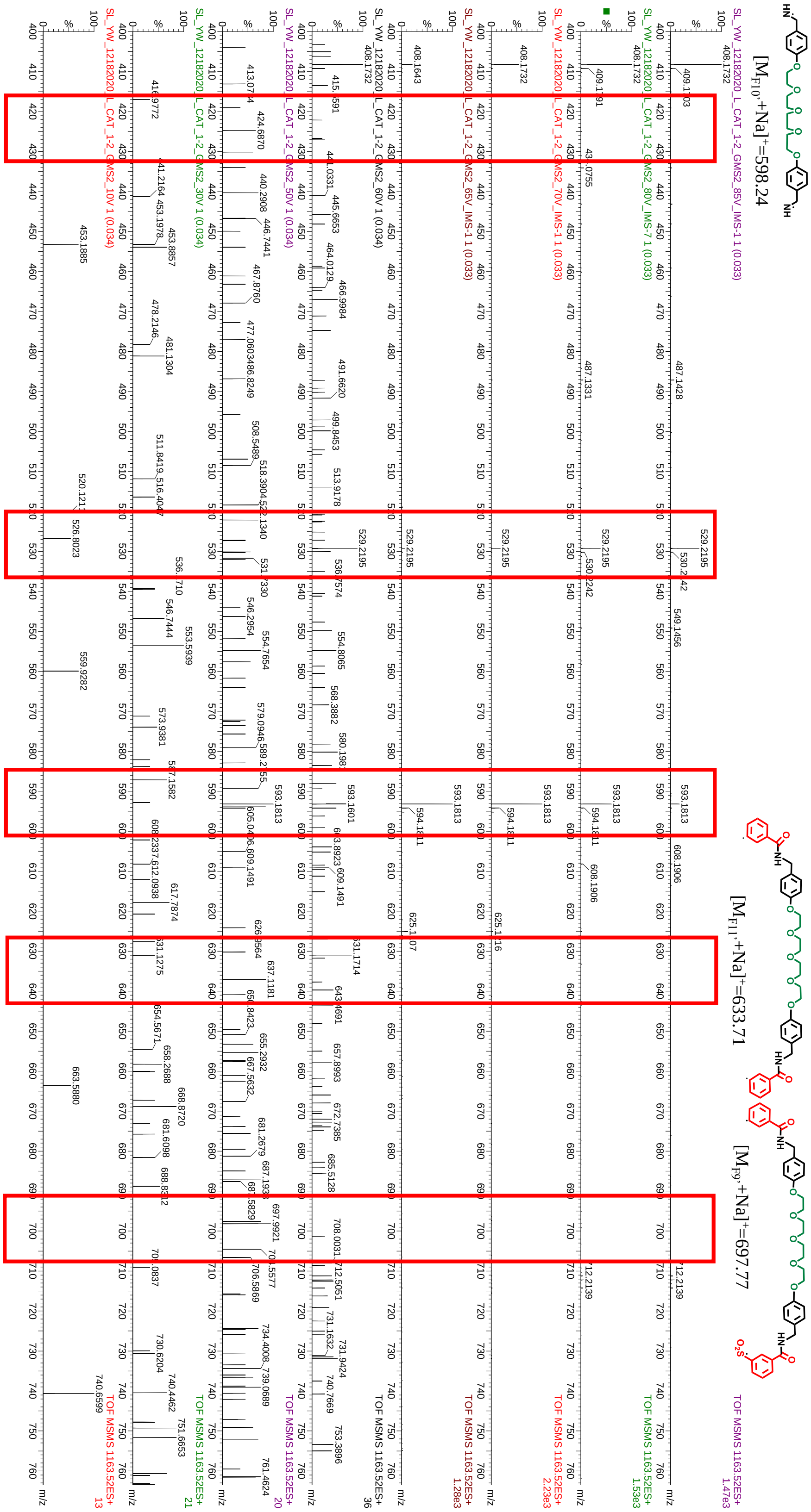
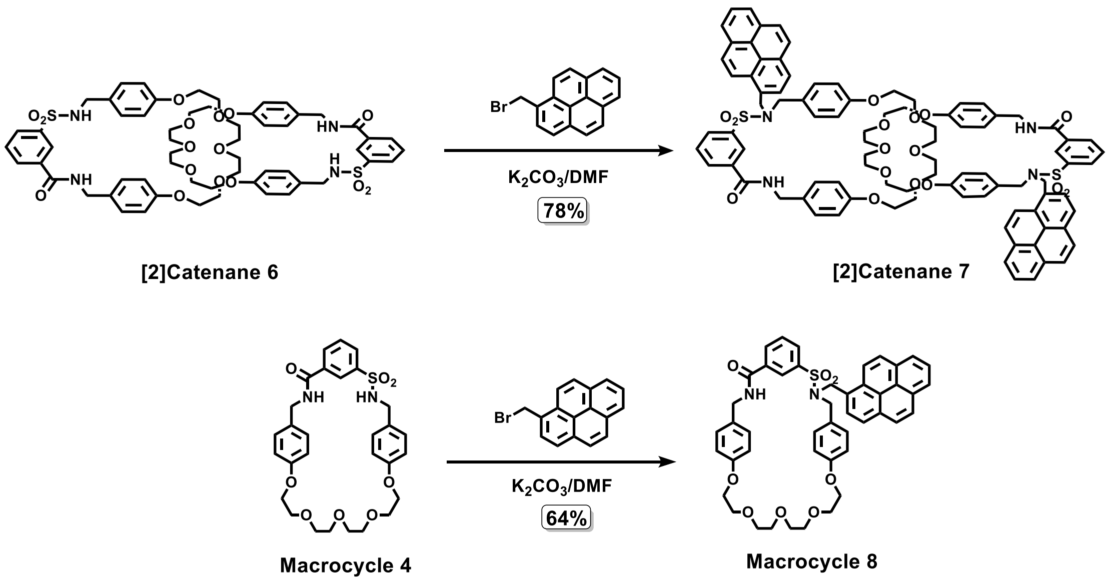


Figure S28. Partial gMS^2 mass spectrum of **6** at 10 - 85V collision voltage in the mass selected CID/IMS experiments in which the characteristic peaks of macrocycle **5** were not observed.

Section D. Synthesis and photophysical properties of pyrene-functionalized [2]catenane 7 and macrocycle 8.

Scheme S2. The synthesis route of pyrene-functionalized [2]catenane **7** and macrocycle **8**.



Synthesis of the [2]catenane 7: K_2CO_3 (15 mg, 0.108 mmol, 2.5 eq.) was added to a solution of [2]catenane **6** (50 mg, 0.043 mmol, 1 eq.) in DMF (20 mL) and then the suspension was stirred at room temperature for 30 min. 1-(Bromomethyl)pyrene (127 mg, 0.430 mmol, 10 eq.) was added and then the mixture was heated at 50℃ for 48 h. After cooling to room temperature, then evaporating the organic solvent under reduced pressure, the residue was partitioned between H_2O (20 mL) and CH_2Cl_2 (3 × 20 mL); the combined organic phases were dried ($MgSO_4$) and concentrated. The residue was purified chromatographically (SiO_2; EtOAc/DCM = 1:4) to afford **7** as a white solid (52 mg, 78%). ^{1}H NMR (500 MHz, CD_2Cl_2) δ 7.86-8.15 (m, 22H), 7.69-7.71 (d, J = 10.0 Hz, 2H), 7.43-7.47 (t, J = 10.0 Hz, 2H), 7.11-7.12 (d, J = 10.0 Hz, 4H), 7.02-7.05 (t, J = 7.5 Hz, 2H), 6.72-6.74 (d, J = 10.0 Hz, 4H), 6.65-6.66 (d, J = 5.0 Hz, 4H), 6.25-6.26 (d, J = 5.0 Hz, 4H), 4.98 (s, 4H), 4.38-4.39 (d, J = 5.0 Hz, 4H), 4.20 (s, 4H), 3.92-3.93 (m, 4H), 3.70-3.71 (m, 4H), 3.54-3.59 (m, 20H). ^{13}C NMR (126 MHz, CD_2Cl_2) δ 165.46, 158.19, 157.81, 140.03, 153.62, 131.46, 131.17, 131.09, 130.55, 130.45, 129.66, 129.43, 129.37, 129.09, 128.34, 127.73, 127.70, 127.68, 127.41, 127.20, 125.98, 125.41, 125.26, 124.54, 124.41, 124.30, 122.82, 114.55, 113.82, 70.65, 70.60, 69.52, 69.37, 67.49, 67.23, 51.01, 50.08, 43.37. HRMS (ESI-TOF): Calculated for [**7** + Na]$^+$: 1591.5529; Found: 1591.5511.

Synthesis of the macrocycle 8: K_2CO_3 (15 mg, 0.110 mmol, 1.2 eq.) was added to a solution of macrocycle **4** (50 mg, 0.088 mmol, 1 eq.) in DMF (20 mL) and then the suspension was stirred at room temperature for 30 min. 1-(Bromomethyl)pyrene (127 mg, 0.430 mmol, 5 eq.) was added and then the mixture was heated at 50°C for 48 h. After cooling to room temperature, then evaporating the organic solvent under reduced pressure, the residue was partitioned between H_2O (20 mL) and CH_2Cl_2 (3 × 20 mL); the combined organic phases were dried ($MgSO_4$) and concentrated. The residue was purified chromatographically (SiO_2; EtOAc/DCM = 1:6) to afford **8** as a white solid (44 mg, 64%). ^{1}H NMR (500 MHz, CD_2Cl_2) δ 7.97-8.21 (m, 11H), 7.91-7.93 (d, J = 10.0 Hz, 1H), 7.49-7.52 (t, J = 10.0 Hz, 1H), 7.23-7.25 (d, J = 10.0 Hz, 2H), 6.89-6.90 (d, J = 5.0 Hz, 2H), 6.55-6.57 (d, J = 10.0 Hz, 2H), 6.43-6.45 (t, J = 5.0 Hz, 1H), 6.41-6.43 (d, J = 10.0 Hz, 2H), 5.12 (s, 2H), 4.48-4.49 (d, J = 5.0 Hz, 2H), 4.26 (s, 2H), 4.08-4.10 (m, 2H), 3.76-3.80 (m, 4H), 3.63-3.68 (m, 4H), 3.57-3.60 (m, 6H). ^{13}C NMR (126 MHz, CD_2Cl_2) δ 165.01, 158.43, 158.23, 140.65, 135.50, 131.35, 131.30, 131.21, 130.68, 130.60, 129.85, 129.61, 129.45, 129.39, 129.12, 128.41, 127.85, 127.70, 127.57, 127.35, 127.30, 126.11, 125.41, 125.36, 125.07, 124.77, 124.71, 124.47, 122.66, 114.88, 114.12, 70.76, 70.71, 70.59, 70.54, 69.52, 69.44, 67.77, 67.39, 49.89, 49.14, 43.34. HRMS (ESI-TOF): Calculated for [**8** + Na]$^+$: 807.2711; Found: 807.2731.

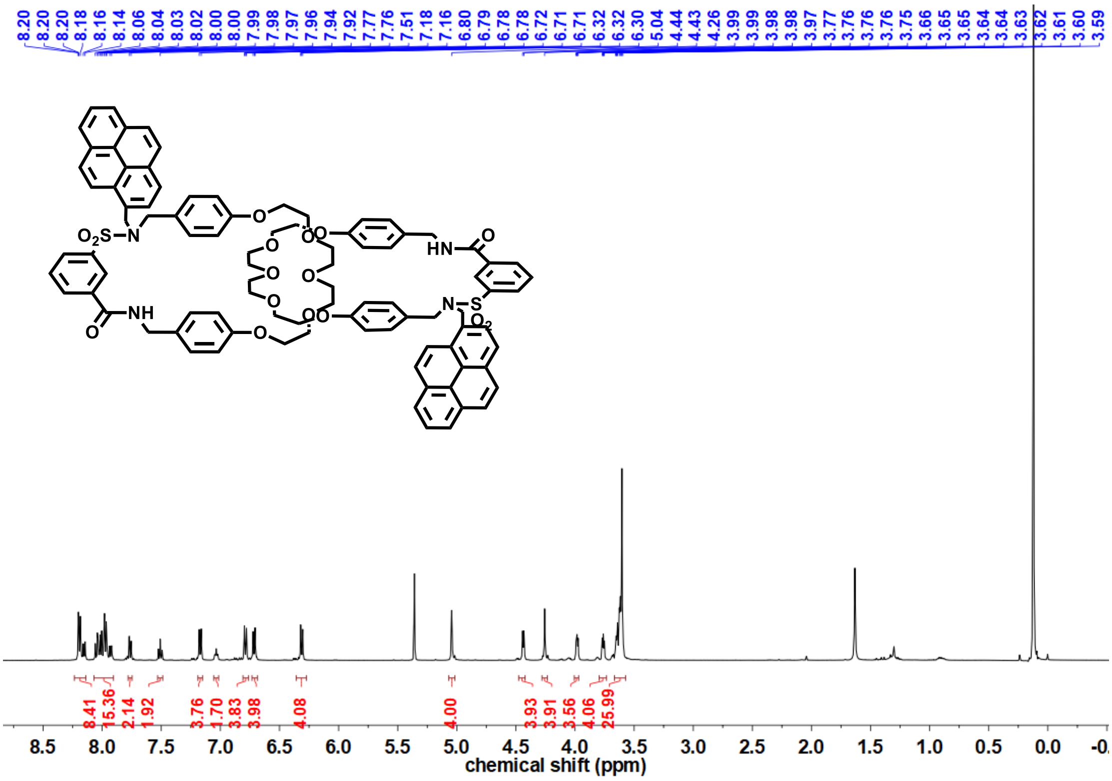


Figure S29. [1]H NMR spectrum (CD_2Cl_2, 298 K, 500 MHz) of **7**.

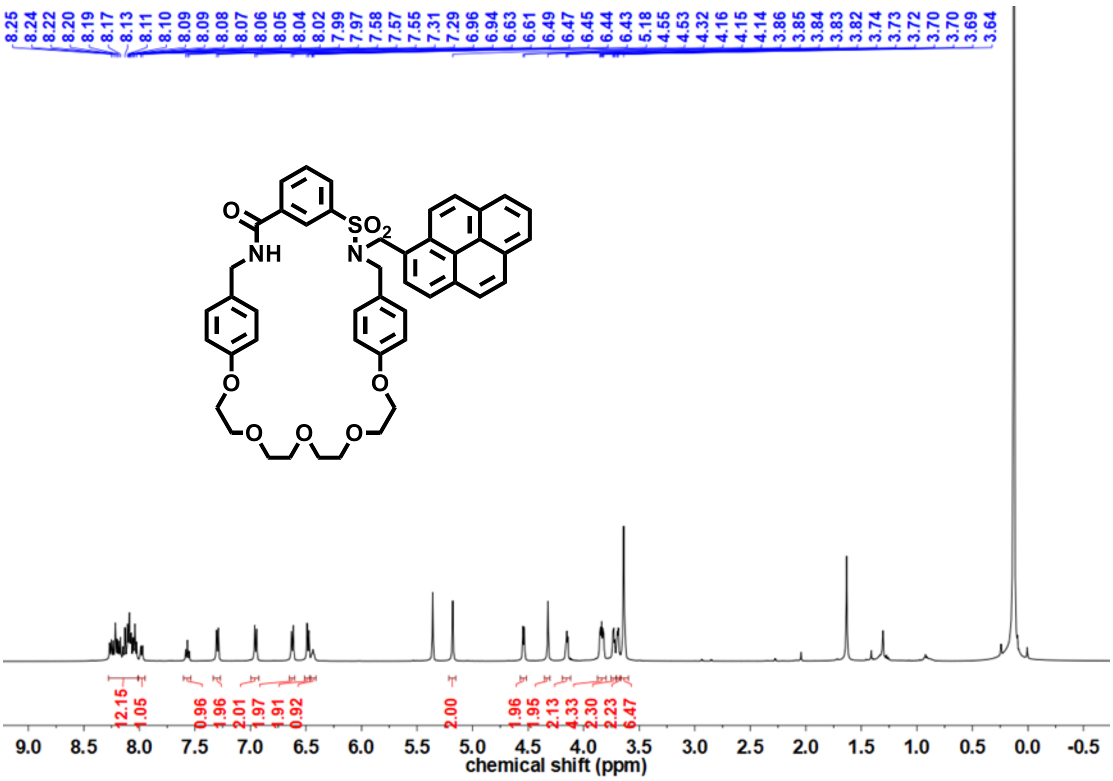


Figure S30. [1]H NMR spectrum (CD_2Cl_2, 298 K, 500 MHz) of **8**.

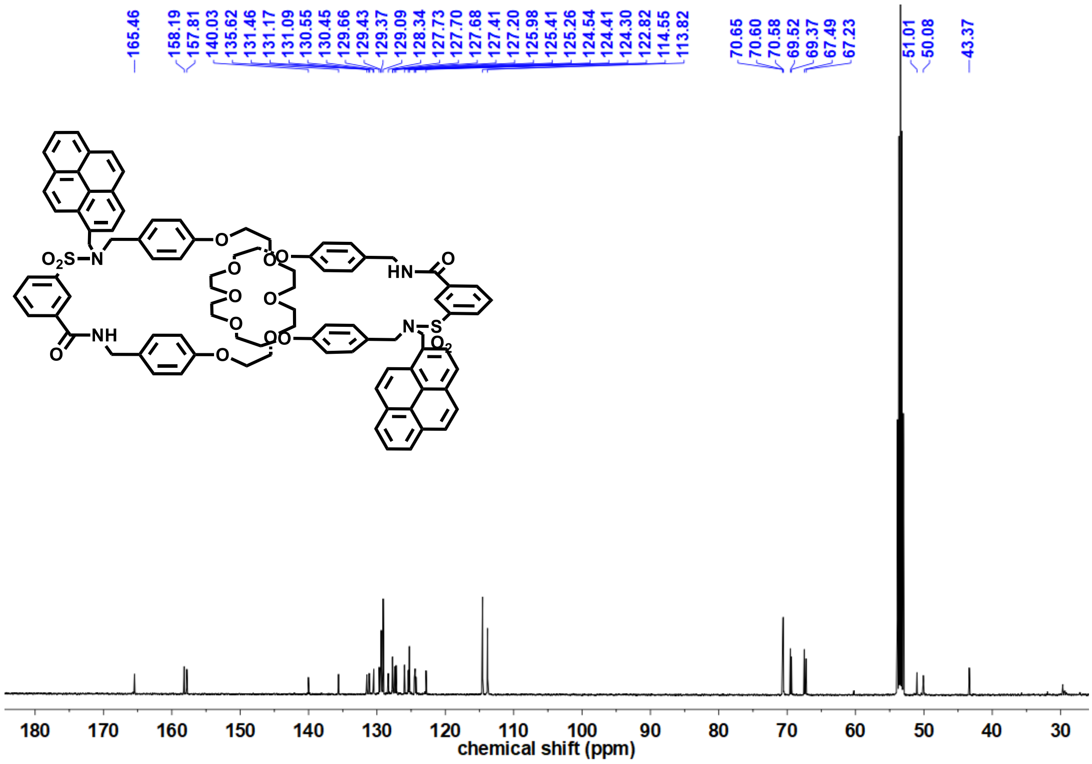


Figure S31. ^{13}C NMR spectrum (CD_2Cl_2, 298 K, 126 MHz) of **7**.

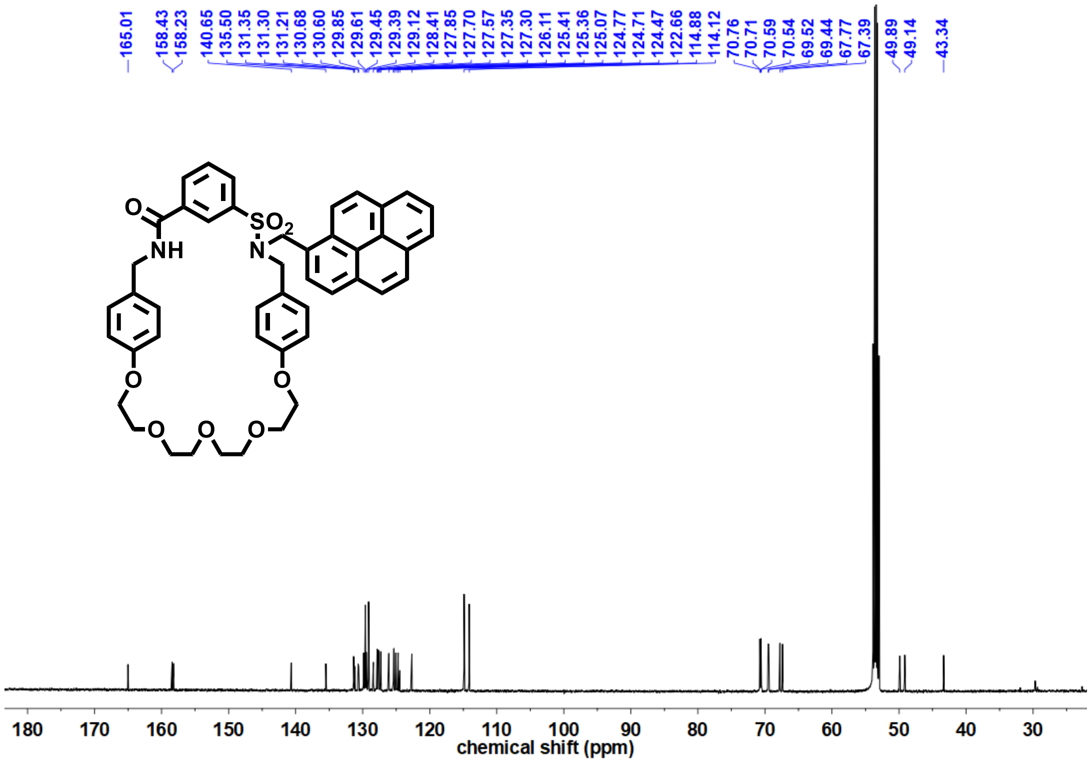
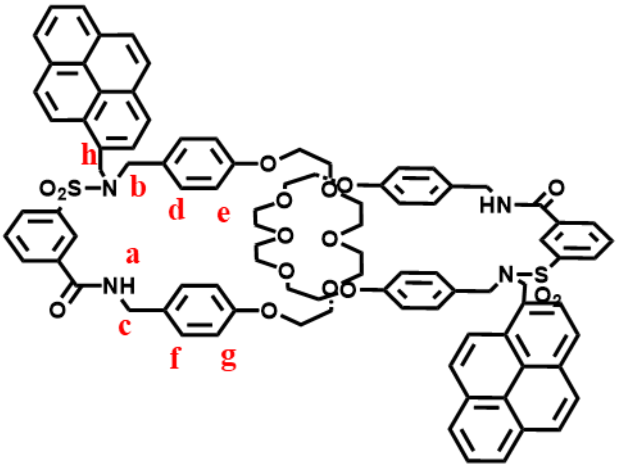


Figure S32. ^{13}C NMR spectrum (CD_2Cl_2, 298 K, 126 MHz) of **8**.



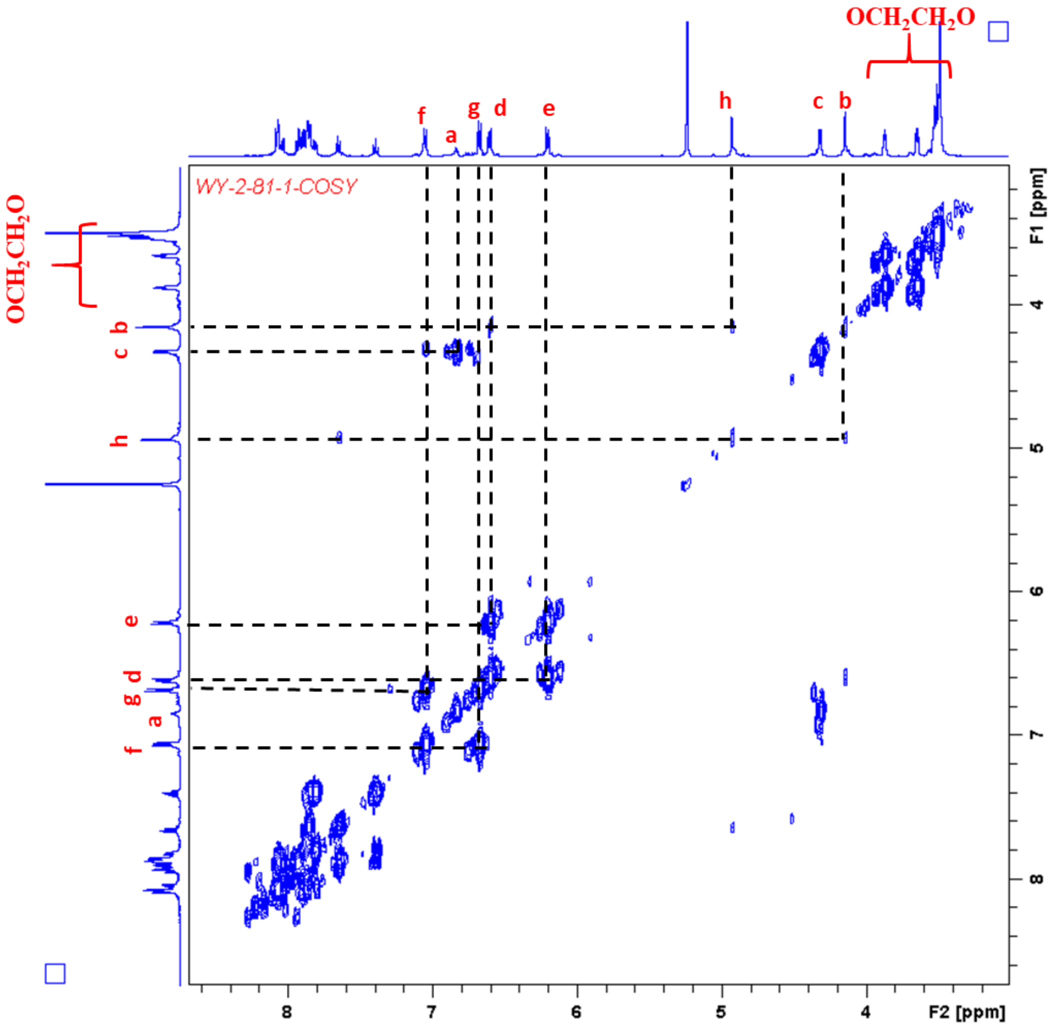


Figure S33. 2D ^{1}H-^{1}H COSY spectrum (CD_2Cl_2, 298 K, 400 MHz) of **7**.

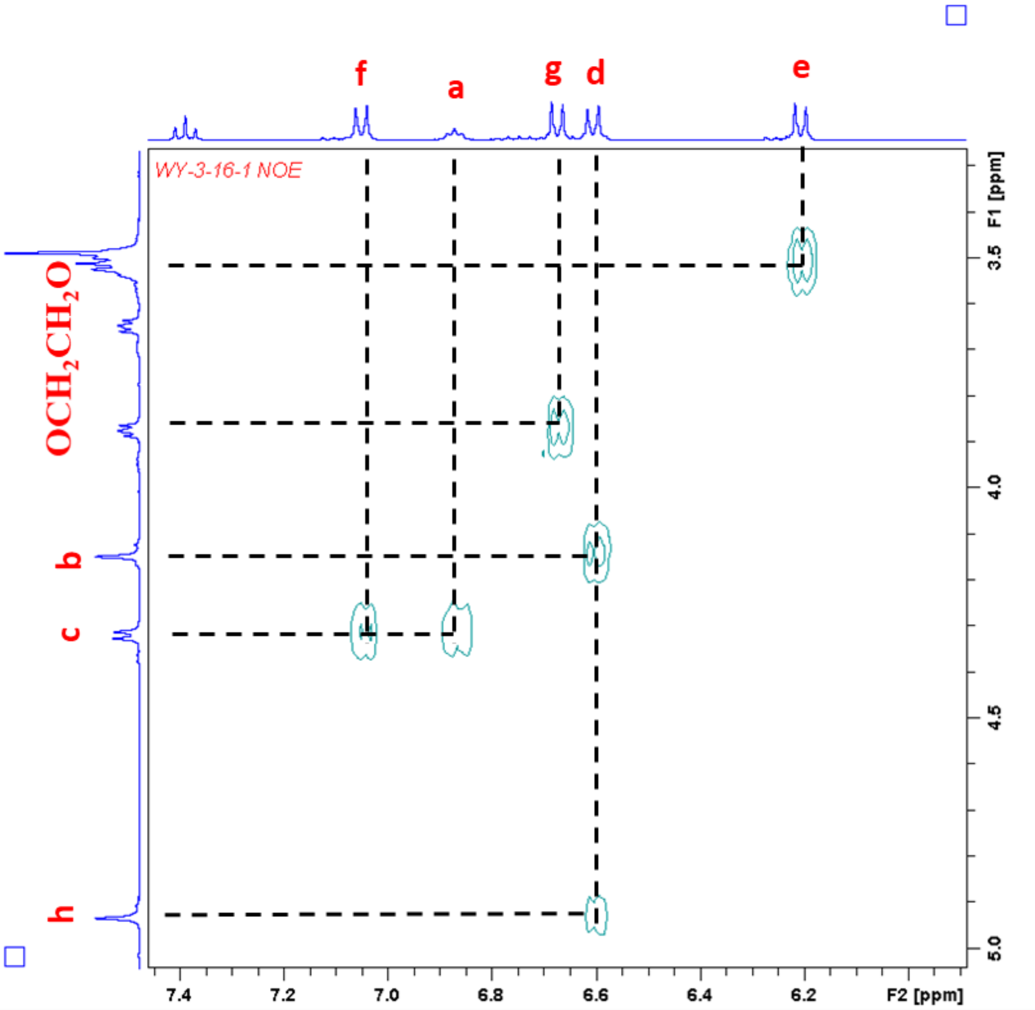


Figure S34. Partial 2D ^1H-^1H NOESY spectrum (CD_2Cl_2, 298 K, 400 MHz) of **7**.

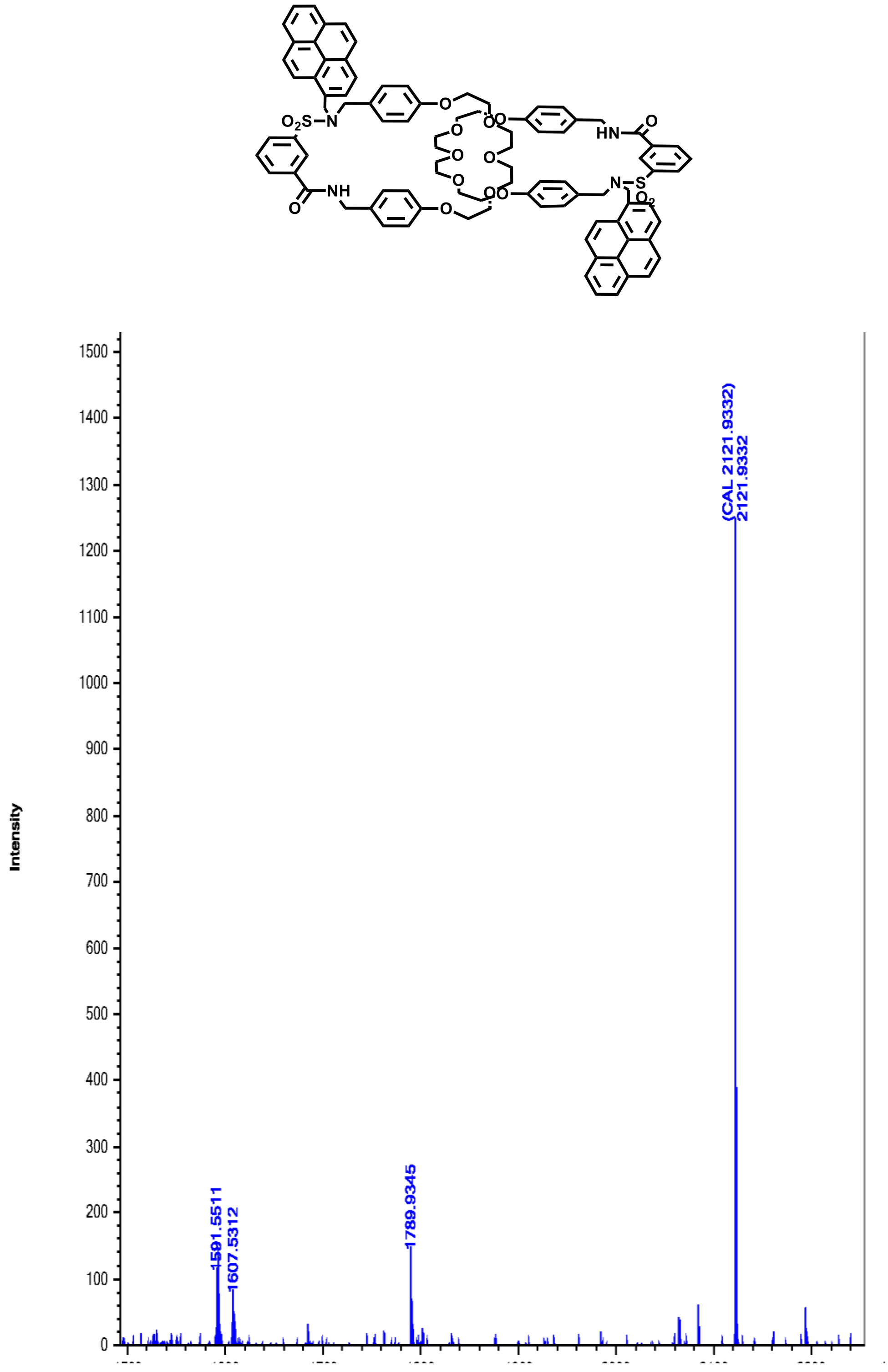
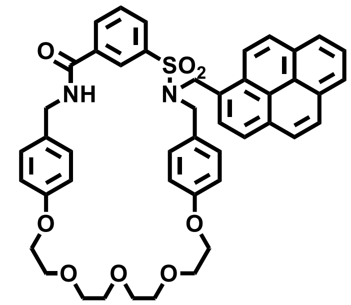


Figure S35. HRMS (ESI-TOF-MS) spectrum of **7**.



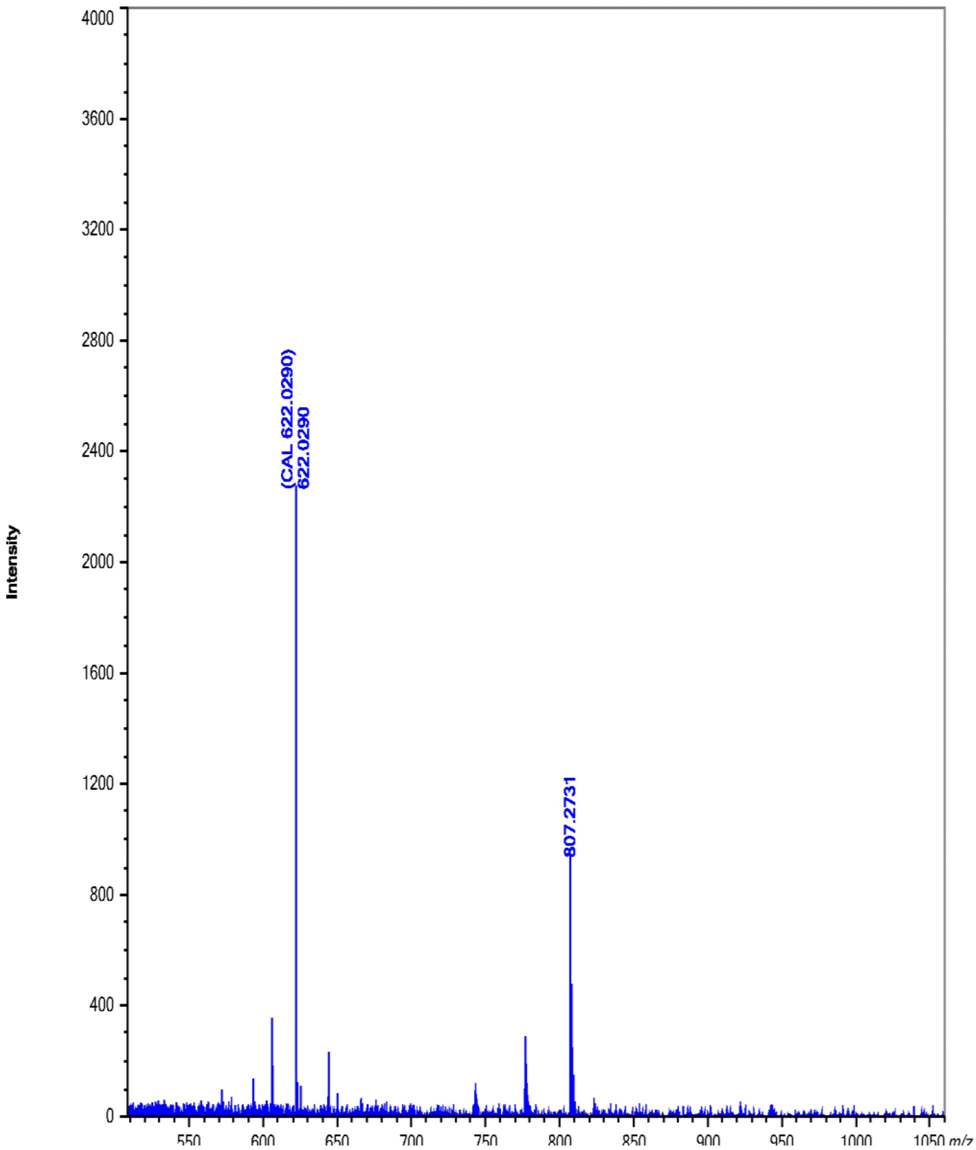


Figure S36. HRMS (ESI-TOF-MS) spectrum of **8**.

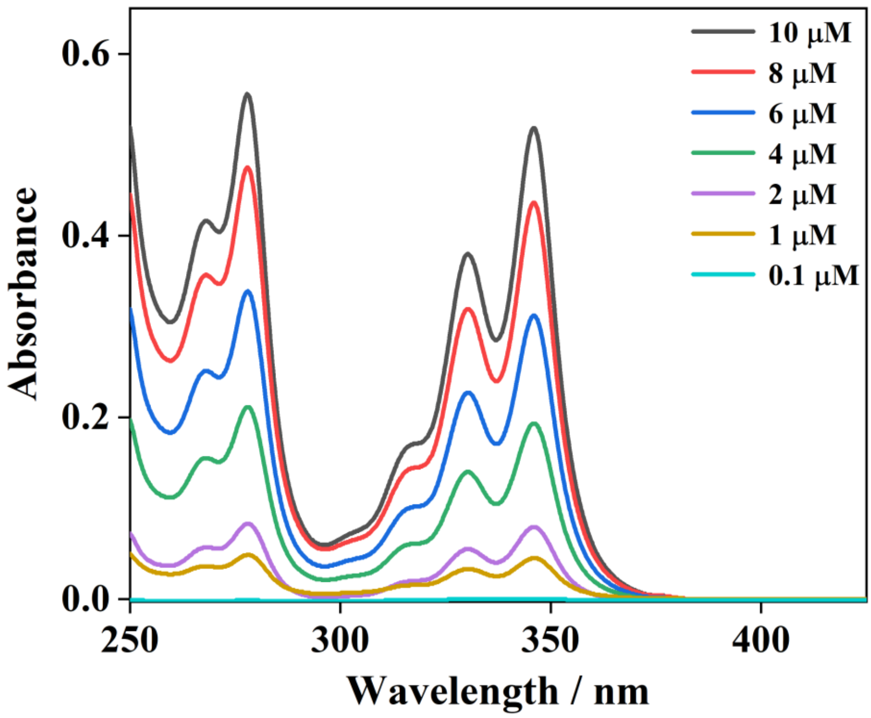


Figure S37. UV−vis absorption spectra of **7** in DCM at different concentration.

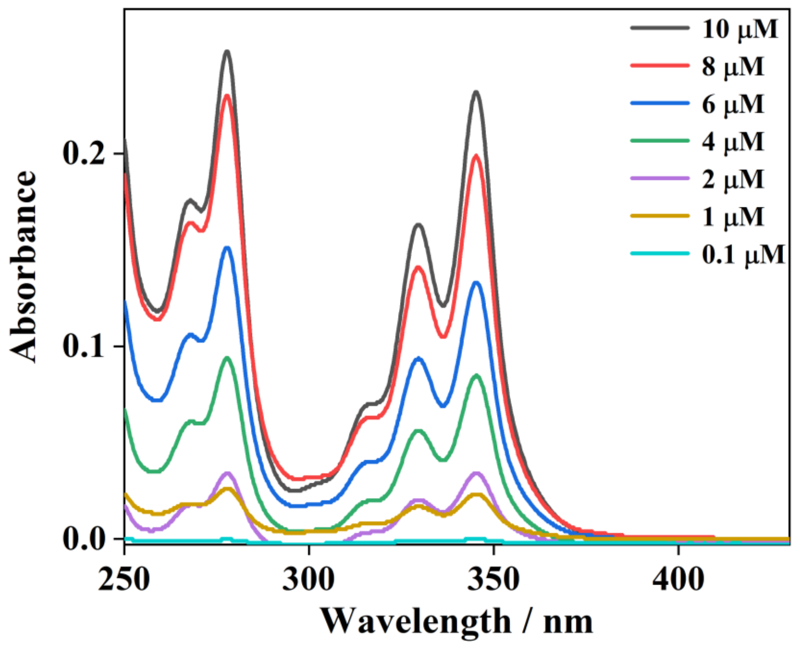


Figure S38. UV−vis absorption spectra of **8** in DCM at different concentration.

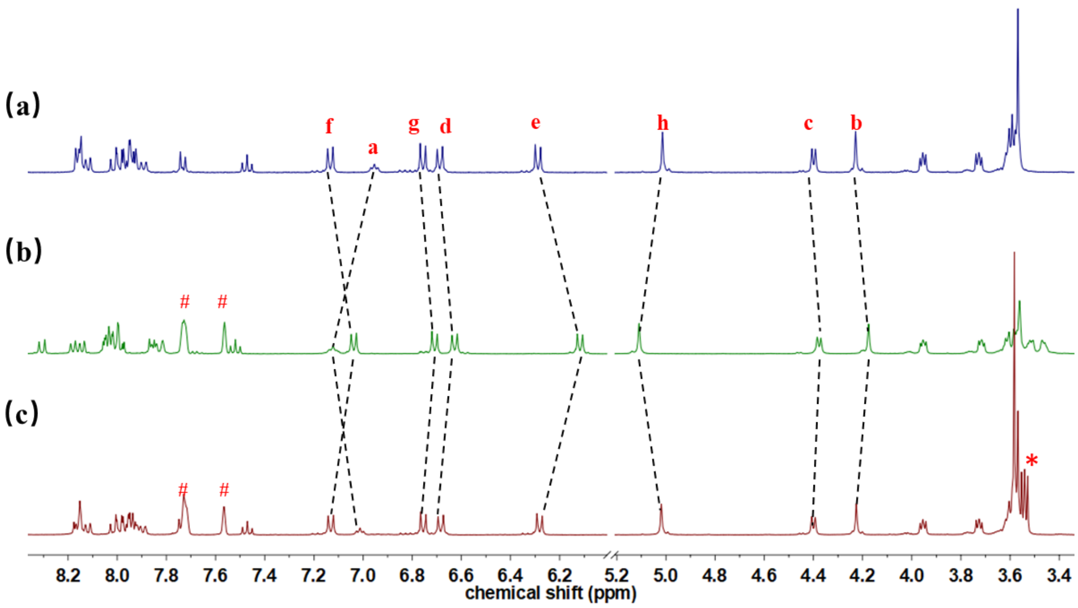


Figure S39. Partial ^{1}H NMR spectra (400 MHz, CD_2Cl_2, 298 K) of (a) the [2]catenane **7** and (b) the solution in (a) after the addition of 1 equiv. of NaTFPB, and (c) the solution in (b) after the addition of 1 equiv. of [2.2.2]cryptand. #: Signals for the TFPB anion; *: Signals for the [2.2.2]cryptand.

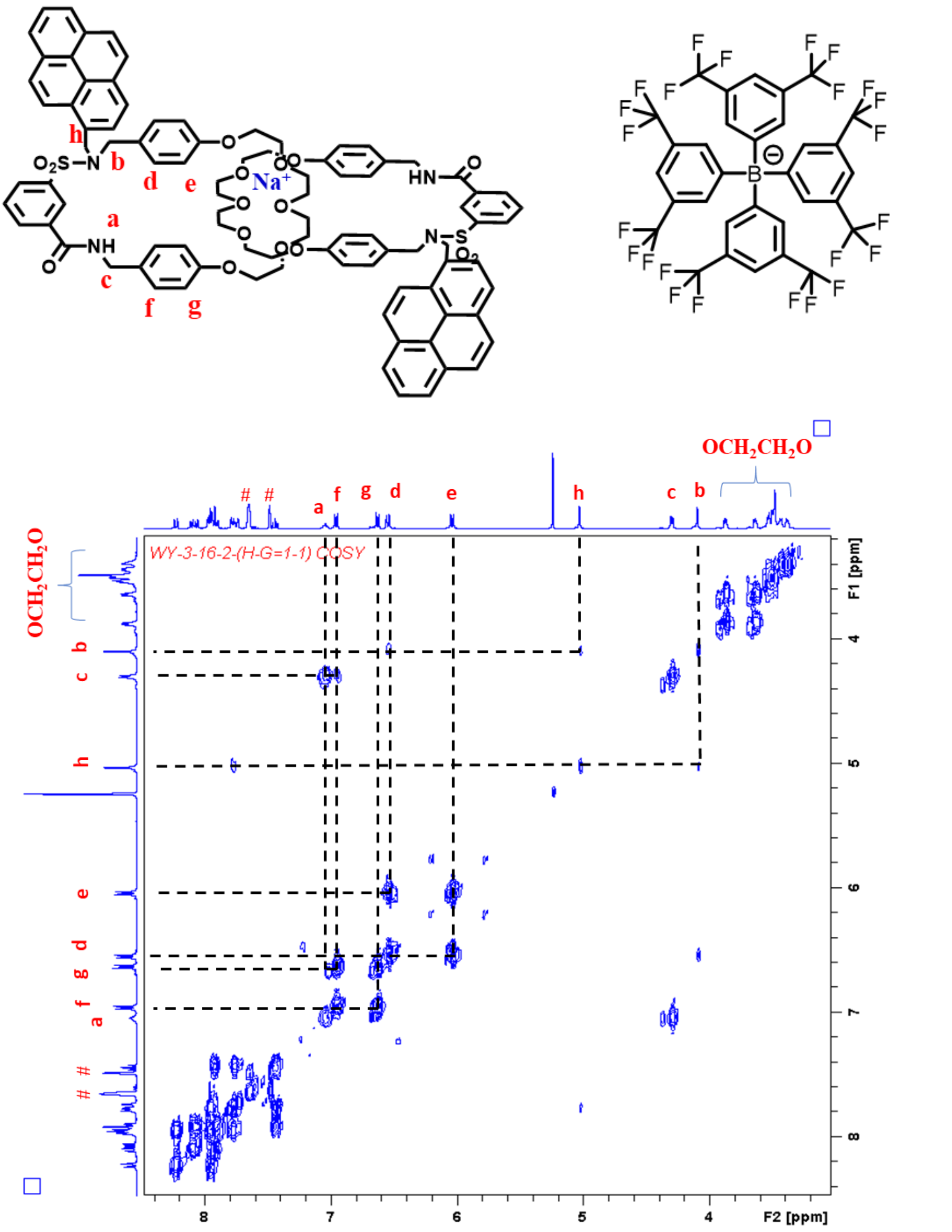


Figure S40. Partial 2D ^{1}H-^{1}H COSY spectrum (CD_2Cl_2, 298 K, 400 MHz) of **7** ⊃ Na^+ (1 eq.). #: Signals for the TFPB anion.

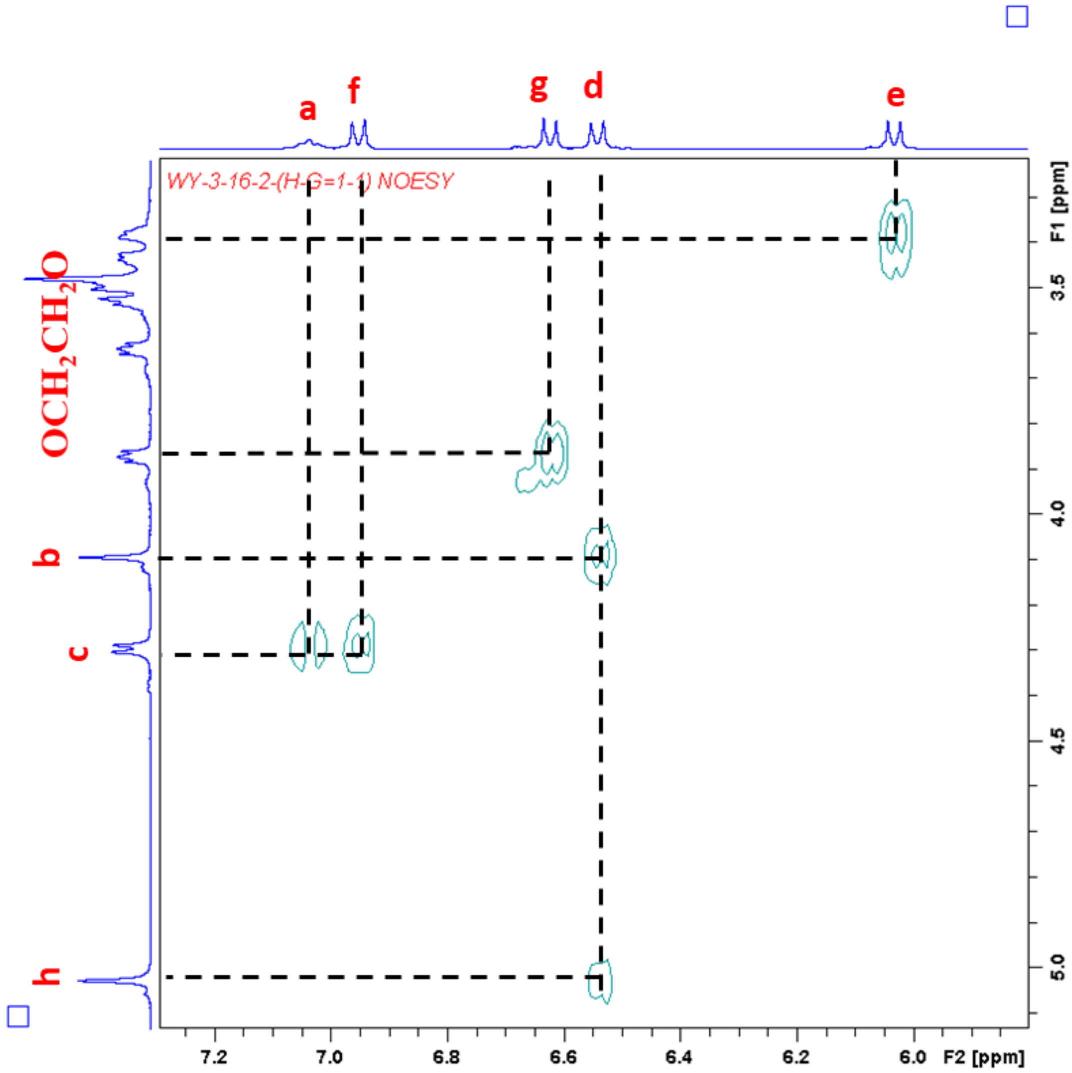


Figure S41. Partial 2D ^{1}H-^{1}H NOESY spectrum (CD_2Cl_2, 298 K, 400 MHz) of **7** ⊃ Na^+ (1 eq.).

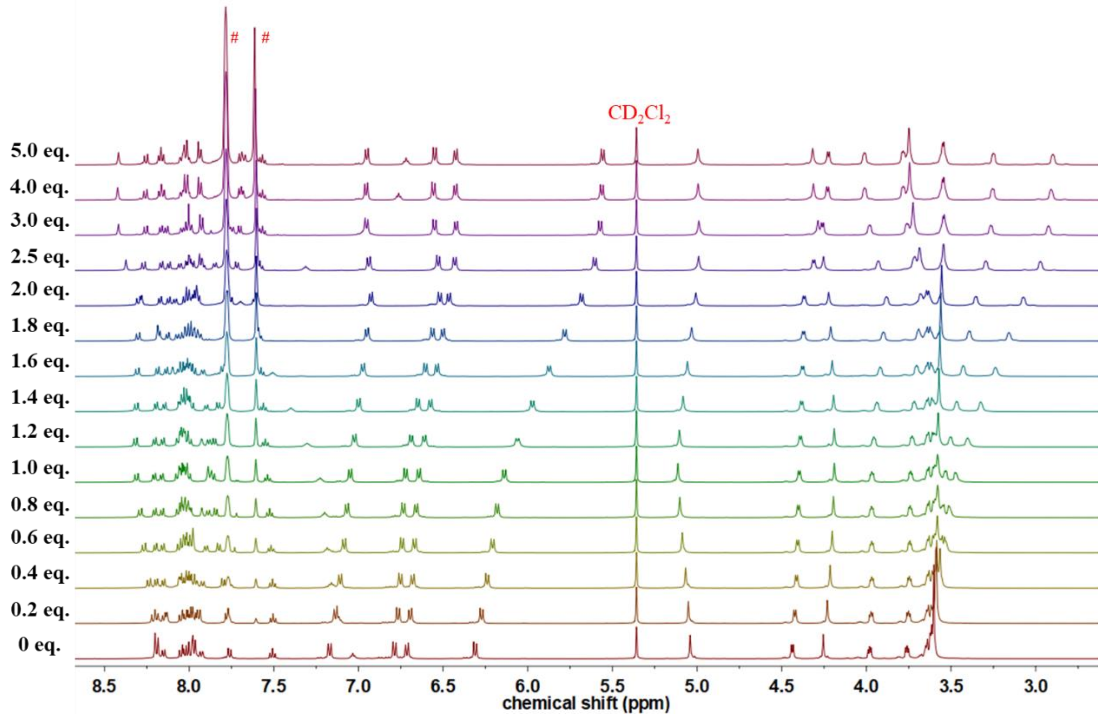


Figure S42. Stacked ^{1}H NMR spectra (500 MHz, 298K) of [2]catetane 7 (10 mM) titrated by Na^{+} (0 -5.0 equiv.) in CD_2Cl_2. #: Signals for the TFPB anion.

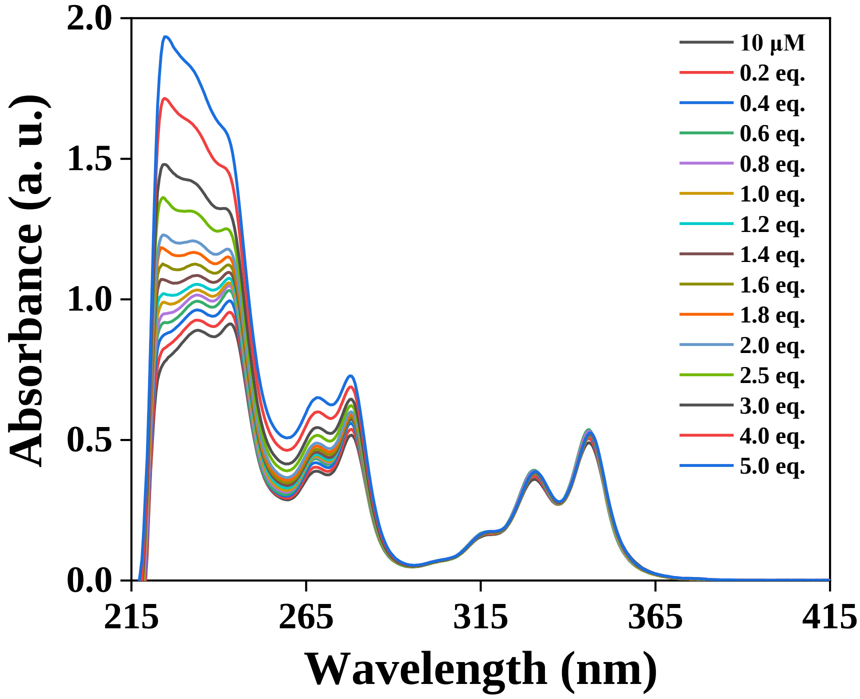


Figure S43. Stacked plots of UV−vis absorption spectra of [2]catetane 7 (10 μM) titrated by Na^{+} (0 -5.0 equiv.) in DCM.

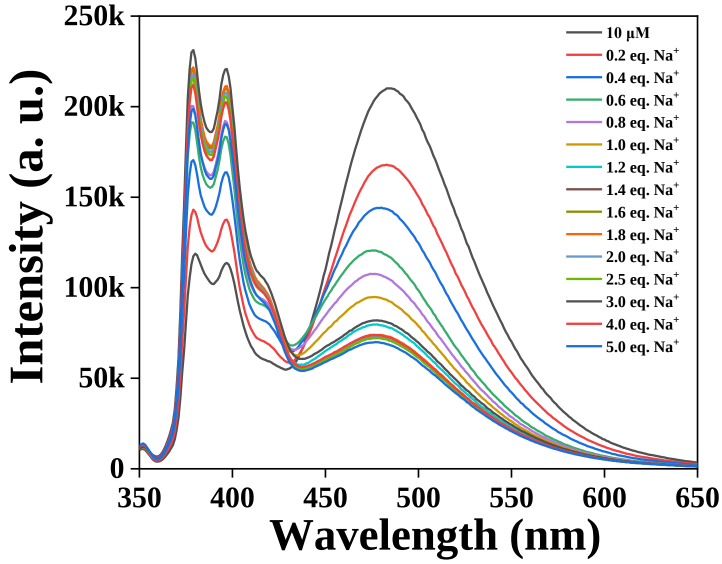


Figure S44. Stacked plots of emission spectra of [2]catetane **7** (10 μM) titrated by Na^+ (0 -5.0 equiv.) in DCM. (Excitation, 330 nm; emission, 485 nm.)

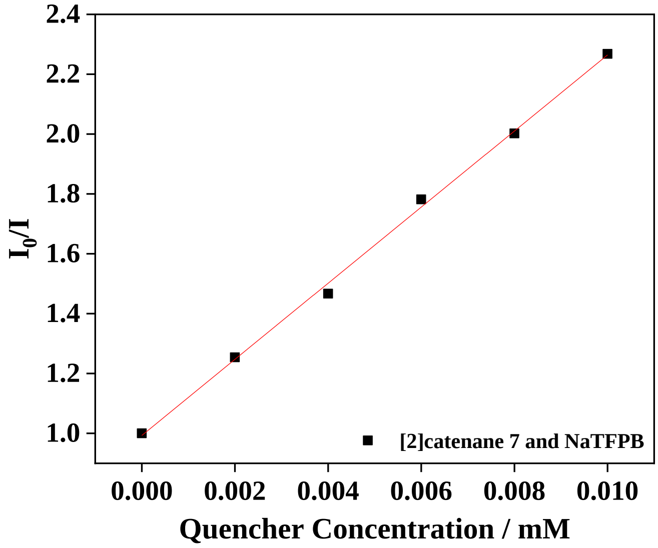
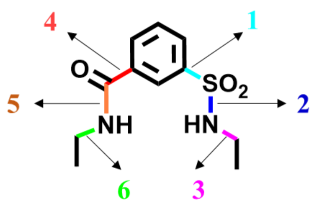


Figure S45. The Stern-Völmer plots of [2]catenane **7** titration with NaTFPB. (According to previous reports: *J. Am. Chem. Soc.* 2004, **126**, 14736; *J. Am. Chem. Soc.* 2017, **139**, 1554, the quenching constant (*K*sv) was calculated based on the fluorescence quenching titration results and the Stern-Völmer equation. In accordance with the Stern-Völmer equation, the measured absorbance I_0/I at 485 nm varied as a function of concentration (mM) in a linear relationship (R^2 = 0.9982), suggesting 1:1 stoichiometry of the interaction between Na^+ and the host **7** in the range of not more than 1.0 eq. Na^+. The *K*sv constant was calculated as 127129±2707 M^{-1} with NaTFPB.)

Section E. DFT results and computational details

In order to verify the possibility of the bond breaking position of [2]catenanes **3** and **6**, we established model compound **S1**, and calculated the bond energies of its 6 chemical bonds.

Table S1. Bond energy analysis of radical fragments for model compound **S1**.



S1

	ΔH_{S1} (kcal/mol)	$\Delta H_{radical1}$ (kcal/mol)	$\Delta H_{radical2}$ (kcal/mol)	Bond energy[a] (kcal/mol)
S1	-1161.8			
Bond [1]		-683.0	-478.7	71.6
Bond [2]		-134.4	-1027.3	53.6
Bond [3]		-79.1	-1082.6	79.2
Bond [4]		-247.8	-913.9	95.6
Bond [5]		-134.4	-1027.3	90.5
Bond [6]		-79.1	-1082.6	87.0

[a] (Bond energy (ΔH) = $\Delta H_{radical1}$ + $\Delta H_{radical2}$ - ΔH_{S1})

Cartesian Coordinates for All of the Calculated Structures

S1, $E_{(SCF\ Done)}$=-1161.819322

C	-0.790583000	-1.090276000	0.190757000
C	-0.874779000	-2.433616000	-0.172760000
C	0.283580000	-3.086730000	-0.603278000
C	1.496316000	-2.404188000	-0.651847000
C	1.580728000	-1.062072000	-0.250618000

C	0.421923000	-0.398929000	0.162583000
H	-1.826645000	-2.950028000	-0.109875000
H	0.235730000	-4.131233000	-0.897068000
H	2.402633000	-2.890926000	-0.996269000
H	0.434832000	0.649352000	0.441939000
C	2.935232000	-0.402035000	-0.320873000
O	3.809317000	-0.836046000	-1.066465000
N	-2.652131000	0.667579000	-0.659071000
H	-3.112759000	0.038282000	-1.317709000
N	3.113669000	0.683783000	0.490223000
H	2.409845000	0.891103000	1.184506000
C	4.365499000	1.430031000	0.545064000
H	4.834586000	1.285500000	1.527911000
H	5.019737000	0.974786000	-0.201070000
C	-3.438370000	1.904199000	-0.445843000
H	-4.428618000	1.689474000	-0.019577000
H	-2.890196000	2.507632000	0.280500000
C	-3.578232000	2.647535000	-1.771787000
H	-4.127762000	2.051612000	-2.510928000
H	-4.132650000	3.580015000	-1.620610000
H	-2.595385000	2.888199000	-2.188873000
C	4.165938000	2.921390000	0.267698000
H	3.487206000	3.378841000	0.998093000
H	5.124120000	3.449831000	0.328005000
H	3.746738000	3.078422000	-0.731517000
S	-2.265244000	-0.224783000	0.734282000
O	-3.293505000	-1.237827000	1.010248000
O	-1.887283000	0.760658000	1.752641000

Bond [1] radical$_1$, $E_{(SCF\ Done)}$=-683.007342

N	-0.473687000	-0.527649000	-0.126392000
H	-0.504565000	-1.425654000	0.349881000
C	-1.549543000	0.428072000	0.167834000
H	-1.451261000	0.827860000	1.187057000
H	-1.437036000	1.273133000	-0.516731000
C	-2.909005000	-0.237794000	-0.026989000
H	-3.038753000	-1.088433000	0.653099000
H	-3.708798000	0.479772000	0.184645000
H	-3.025051000	-0.598116000	-1.053825000
S	1.120909000	0.008588000	-0.281225000
O	1.971590000	-1.057644000	0.304896000
O	1.190662000	1.425882000	0.161998000

Bond [1] radical$_2$, $E_{(SCF\ Done)}$=-478.697923

C	2.398018000	-1.564952000	-0.094284000
C	3.445889000	-0.675154000	-0.001669000
C	3.106404000	0.686413000	0.073976000
C	1.768609000	1.080008000	0.058790000
C	0.736482000	0.134167000	-0.018078000
C	1.061855000	-1.235666000	-0.111181000
H	4.483887000	-0.996424000	0.007006000
H	3.892199000	1.434904000	0.142151000
H	1.495317000	2.128788000	0.102253000
H	0.292491000	-1.993899000	-0.232953000
C	-0.680383000	0.649167000	-0.027414000
O	-0.938029000	1.797565000	-0.378174000
N	-1.640687000	-0.237574000	0.380453000
H	-1.345555000	-1.105353000	0.803994000

C	-3.056052000	0.105248000	0.438833000
H	-3.385944000	0.129450000	1.486788000
H	-3.134612000	1.121419000	0.047200000
C	-3.924324000	-0.863909000	-0.366324000
H	-3.829170000	-1.892194000	0.004370000
H	-4.980370000	-0.580441000	-0.291336000
H	-3.638194000	-0.855686000	-1.423140000

Bond [2] radical$_1$, $E_{(SCF\ Done)}$=-134.420739

N	1.325532000	-0.269507000	-0.114431000
H	1.197598000	-1.088545000	0.502410000
C	0.140391000	0.543678000	0.045651000
H	0.202623000	1.049124000	1.028726000
H	0.159096000	1.338847000	-0.710277000
C	-1.185712000	-0.231967000	-0.026386000
H	-1.249722000	-0.977389000	0.775973000
H	-2.039087000	0.448299000	0.073397000
H	-1.277303000	-0.754054000	-0.984798000

Bond [2] radical$_2$, $E_{(SCF\ Done)}$=-1027.313097

C	1.660186000	0.250795000	-0.084557000
C	2.131502000	1.561575000	-0.014147000
C	1.197279000	2.596525000	0.061020000
C	-0.167843000	2.313523000	0.054185000
C	-0.628161000	0.990309000	-0.007281000
C	0.299623000	-0.053124000	-0.098561000
H	3.198118000	1.758296000	-0.004866000
H	1.538462000	3.625646000	0.123739000
H	-0.906197000	3.107352000	0.091600000

H	-0.008496000	-1.089016000	-0.191704000
C	-2.122848000	0.777078000	-0.007470000
O	-2.882634000	1.680203000	-0.345987000
N	-2.552705000	-0.457156000	0.389008000
H	-1.885249000	-1.098665000	0.793013000
C	-3.964805000	-0.821053000	0.444252000
H	-4.262603000	-0.967307000	1.491393000
H	-4.513239000	0.043091000	0.064383000
C	-4.273513000	-2.075304000	-0.375473000
H	-3.703985000	-2.941177000	-0.016030000
H	-5.338159000	-2.323634000	-0.300556000
H	-4.028187000	-1.920606000	-1.431206000
S	2.851252000	-1.104925000	-0.275232000
O	4.135543000	-0.649282000	0.325129000
O	2.168331000	-2.350550000	0.174495000

Bond [3] radical$_1$, $E_{(SCF\ Done)}$=-79.091826

C	0.795448000	0.000004000	-0.023361000
H	1.354029000	-0.927709000	0.051459000
H	1.354368000	0.927439000	0.051671000
C	-0.694382000	0.000074000	-0.000706000
H	-1.109783000	-0.886012000	-0.496804000
H	-1.095416000	-0.003514000	1.029165000
H	-1.109591000	0.889328000	-0.491090000

Bond [3] radical$_2$, $E_{(SCF\ Done)}$=-1082.601244

C	-1.430842000	0.412352000	-0.054133000
C	-1.824538000	1.751021000	-0.079851000
C	-0.836865000	2.736315000	-0.042889000

C	0.509533000	2.379053000	0.007510000
C	0.897434000	1.031904000	0.001096000
C	-0.087440000	0.038670000	-0.018100000
H	-2.876862000	2.008566000	-0.132657000
H	-1.120713000	3.784345000	-0.055506000
H	1.289306000	3.132013000	0.050913000
H	0.162095000	-1.016411000	0.014387000
C	2.377538000	0.739151000	0.047204000
O	3.168914000	1.580070000	0.464739000
N	-3.050079000	-1.041209000	1.555019000
H	-3.771092000	-1.782537000	1.571428000
N	2.760544000	-0.492888000	-0.401753000
H	2.078255000	-1.078144000	-0.862192000
C	4.152666000	-0.929037000	-0.418817000
H	4.487149000	-1.040069000	-1.459234000
H	4.728157000	-0.115058000	0.026233000
C	4.361318000	-2.236406000	0.347938000
H	3.763916000	-3.052115000	-0.077623000
H	5.414050000	-2.537441000	0.303482000
H	4.079075000	-2.120222000	1.399376000
S	-2.675959000	-0.866166000	-0.074685000
O	-3.878912000	-0.348496000	-0.743141000
O	-2.053010000	-2.122041000	-0.521130000

Bond [4] radical$_1$, $E_{(SCF\ Done)}$=-247.75747

C	-1.428708000	0.313629000	-0.302894000
O	-1.881091000	-0.739681000	0.072973000
N	-0.209297000	0.838585000	-0.086778000
H	-0.003001000	1.721585000	-0.531865000

C	0.879481000	0.134937000	0.611641000
H	1.349864000	0.836775000	1.310754000
H	0.402410000	-0.651831000	1.201283000
C	1.917968000	-0.455167000	-0.343273000
H	2.388386000	0.325654000	-0.952682000
H	2.709194000	-0.962681000	0.220828000
H	1.454504000	-1.182531000	-1.017496000

Bond [4] radical$_2$, $E_{(SCF\ Done)}$=-913.90945

C	-1.019279000	0.115089000	0.107429000
C	-1.922003000	0.682763000	-0.793383000
C	-3.202667000	0.137067000	-0.925128000
C	-3.579796000	-0.972424000	-0.153670000
C	-2.637967000	-1.474810000	0.721133000
C	-1.365209000	-0.989937000	0.904216000
H	-1.621802000	1.550127000	-1.370864000
H	-3.909644000	0.577506000	-1.623450000
H	-4.572298000	-1.404914000	-0.245245000
H	-0.660366000	-1.408620000	1.615419000
N	1.572190000	-0.330671000	-0.503626000
H	1.507853000	-0.163428000	-1.508289000
C	2.978623000	-0.442770000	-0.055151000
H	3.543182000	0.480583000	-0.247829000
H	2.956567000	-0.595720000	1.025636000
C	3.638650000	-1.627133000	-0.756596000
H	3.666827000	-1.485988000	-1.844172000
H	4.672028000	-1.737570000	-0.410566000
H	3.097915000	-2.555097000	-0.545905000
S	0.619253000	0.834788000	0.283406000

O	0.624930000	2.100496000	-0.464009000
O	1.008100000	0.791271000	1.695639000

Bond [5] radical$_1$, $E_{(SCF\ Done)}$=-134.420735

N	1.325303000	-0.269646000	-0.114592000
H	1.196998000	-1.088014000	0.503155000
C	0.140424000	0.543793000	0.045720000
H	0.202716000	1.048726000	1.029056000
H	0.158946000	1.339081000	-0.710079000
C	-1.185480000	-0.231966000	-0.026384000
H	-1.249928000	-0.977284000	0.776060000
H	-2.038953000	0.448288000	0.072696000
H	-1.276568000	-0.754240000	-0.984763000

Bond [5] radical$_2$, $E_{(SCF\ Done)}$=-1027.254423

C	0.232970000	-0.606739000	-0.028858000
C	0.573849000	-1.267287000	-1.213083000
C	1.867451000	-1.138767000	-1.723052000
C	2.807614000	-0.358487000	-1.052225000
C	2.456516000	0.294150000	0.141282000
C	1.161776000	0.167560000	0.660775000
H	-0.164905000	-1.880395000	-1.718823000
H	2.138942000	-1.651680000	-2.641115000
H	3.818160000	-0.246895000	-1.433520000
H	0.891348000	0.654910000	1.591447000
C	3.447705000	1.122622000	0.873658000
O	4.580866000	1.343413000	0.569686000
N	-2.336873000	0.149945000	-0.437278000
H	-3.226021000	-0.331426000	-0.572708000

C	-2.485883000	1.585135000	-0.127391000
H	-2.935700000	1.739769000	0.861534000
H	-1.480609000	2.019395000	-0.099734000
C	-3.315267000	2.259502000	-1.217035000
H	-4.327861000	1.840055000	-1.262360000
H	-3.409691000	3.330098000	-1.007665000
H	-2.848569000	2.135194000	-2.199164000
S	-1.428001000	-0.794097000	0.632307000
O	-1.875841000	-2.169346000	0.394024000
O	-1.421195000	-0.211467000	1.979006000

Bond [6] radical$_1$, $E_{(SCF\ Done)}$=-79.091825

C	0.795387000	0.000009000	-0.023346000
H	1.353851000	-0.927775000	0.051477000
H	1.354525000	0.927332000	0.051580000
C	-0.694358000	0.000102000	-0.000710000
H	-1.109727000	-0.884617000	-0.499252000
H	-1.095328000	-0.006294000	1.029184000
H	-1.109496000	0.890692000	-0.488655000

Bond [6] radical$_2$, $E_{(SCF\ Done)}$=-1082.288786

C	-0.081621000	0.871431000	0.055256000
C	-0.538816000	2.069199000	-0.495015000
C	-1.888474000	2.188527000	-0.842785000
C	-2.758994000	1.123226000	-0.635438000
C	-2.289643000	-0.075091000	-0.073819000
C	-0.941723000	-0.203781000	0.276994000
H	0.155411000	2.890735000	-0.635752000
H	-2.254965000	3.116842000	-1.270583000

H	-3.809184000	1.198047000	-0.898675000
H	-0.575627000	-1.127873000	0.710124000
C	-3.248784000	-1.185879000	0.160745000
O	-4.427145000	-1.152601000	-0.229300000
N	2.214224000	-0.385046000	-0.618216000
H	2.460314000	0.130957000	-1.463102000
N	-2.764171000	-2.346951000	0.715548000
H	-3.553181000	-2.849146000	1.141253000
C	3.297323000	-1.299245000	-0.190750000
H	4.221237000	-0.753127000	0.046209000
H	2.959926000	-1.787166000	0.725611000
C	3.551970000	-2.327136000	-1.290306000
H	3.890817000	-1.849068000	-2.217733000
H	4.333915000	-3.025721000	-0.973631000
H	2.642921000	-2.895513000	-1.510192000
S	1.645739000	0.724683000	0.530870000
O	2.262022000	2.042473000	0.323288000
O	1.719972000	0.049201000	1.828753000

Section F. References

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