Supporting Information

Probing Rotaxane Dynamics with ^{19}F NMR/MRI: Unveiling the Roles of Mechanical Bond and Steric Hindrance

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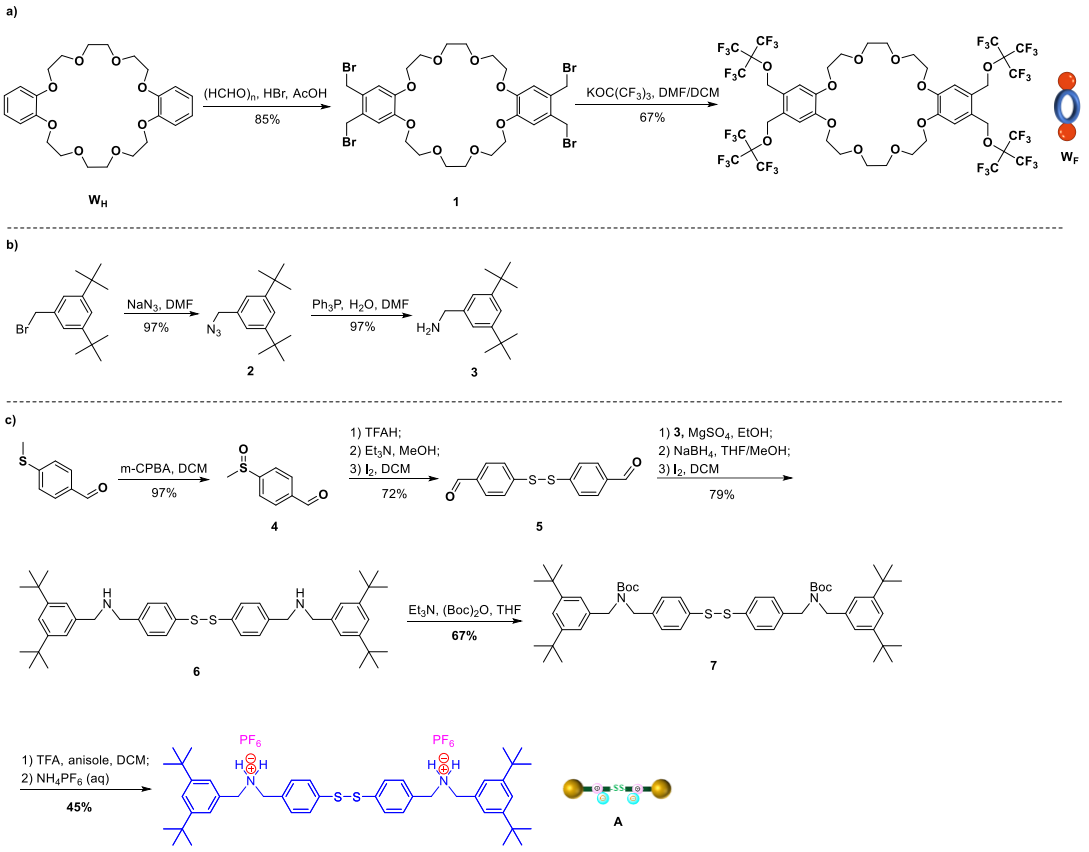
1. General information

^{1}H, ^{13}C and ^{19}F NMR spectra were recorded on Bruker 400 MHz or 500 MHz spectrometers. Chemical shifts were in ppm and coupling constants (*J*) were in Hertz (Hz). ^{1}H NMR spectra were referenced to deuterated solvents: $CDCl_3$ (s, 7.26 ppm), CD_3CN (s, 1.94 ppm). ^{13}C NMR spectra were referenced to solvent carbons (77.16 ppm for $CDCl_3$, 1.32 ppm for CD_3CN). ^{19}F NMR spectra were referenced to 2% perfluorobenzene (s, -164.90 ppm). The splitting patterns for ^{1}H NMR spectra were denoted as follows: s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet), b (broad), and combinations thereof. High-resolution mass spectra (HRMS) were recorded on a Thermo Fisher Scientific Q Exactive Focus. MALDI-ICR mass spectra were recorded on a 9.4 T SolariX FT-ICR-MS using the single MS mode for positive ions with dithranol as a matrix.

2. Synthesis and characterization of compounds



Scheme S1. Synthesis of fluorinated wheel $\mathbf{W_F}$, stopper **3**, and axle **A**.

Crown ether **1**

Dibenzo 24-crown-8 ($\mathbf{W_H}$, 0.50 g, 1.11 mmol), paraformaldehyde (0.30 g, 9.99 mmol), and hydrobromic acid (33% water solution) in acetic acid (8.00 mL) were stirred at 60 °C until all the solids dissolved (about 1 day). The mixture was then left to stand without stirring for another 2 days to allow the precipitation of a white product. The solid was collected by filtration, washed consecutively with water, ethanol, and diethyl ether, and then air-dried. Crown ether **1** was obtained as a white solid (0.78 g, yield 85%), which was directly used in the next step without further purification [1].

Fluorinated wheel $\mathbf{W_F}$

A mixture of crown ether **1** (1.22 g, 1.49 mmol) and potassium perfluoro-*tert*-butoxide (2.45 g, 8.94 mmol) in a mixture of *N, N*-dimethyl formaldehyde/dichloromethane (DMF/DCM, 1/1, 20 mL) were stirred overnight at room temperature. After thin-lay chromatography (TLC) showed that the reaction was completed, water (150 mL) was added to the reaction mixture which was extracted

with ethyl acetate (EA, 2 × 60 mL). The organic layers were collected, dried over anhydrous sodium sulfate, and evaporated under reduced pressure. The residue was purified by flash column chromatography on silica gel (petroleum ether (PE)/EA = 2/1) to give fluorinated wheel $\mathbf{W_F}$ as a white wax (1.43 g, yield 67%). ^{1}H NMR (500 MHz, CD_3CN) δ 7.01 (s, 4H), 5.11 (s, 8H), 4.17 – 4.09 (m, 8H), 3.83 – 3.77 (m, 8H), 3.67 (s, 8H). ^{19}F NMR (471 MHz, CD_3CN) δ -71.31.

Compound **2**

To a solution of 3,5-di-*tert*-butylbenzyl bromide (5.00 g, 17.65 mmol) in N, N-dimethylformamide (DMF, 80 mL) was added sodium azide (1.38 g, 21.18 mmol) and the mixture was stirred under an atmosphere of nitrogen at 80 °C for 5 h. The reaction mixture was cooled to room temperature, diluted with water (100 mL), and extracted with EA (2 × 80 mL). The combined organic layers were washed with brine (3 × 100 mL), dried with anhydrous sodium sulfate, and concentrated under reduced pressure. The residue was purified by flash column chromatography on silica gel (PE) to give compound **2** as a colorless oil (4.20 g, yield 97%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41 (s, 1H), 7.15 (s, 2H), 4.35 (s, 2H), 1.35 (s, 18H).

Stopper **3**

To a solution of compound **2** (4.20 g, 17.12 mmol) in tetrahydrofuran (THF, 80 mL) was added triphenylphosphine (6.28 g, 23.96 mmol). The mixture was stirred at 30 ℃ for 1 h, and water (1.54 mL, 85.59 mmol) was added to the reaction. The reaction mixture was stirred at room temperature overnight. After removal of the solvent under reduced pressure, the residue was purified by flash column chromatography on silica gel (dichloromethane/methanol (DCM/MeOH) = 10/1) to give stopper **3** as a yellow oil (3.65 g, yield 97%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.33 (s, 1H), 7.16 (d, J = 1.6 Hz, 2H), 3.87 (s, 2H), 1.33 (s, 18H).

Compound **4**

At 0 ℃, a solution of 3-chloroperoxybenzoic acid (1.47 g, 8.52 mmol) in DCM (20 mL) was slowly added to a solution of 4-(methylthio) benzaldehyde (1.00 g, 6.57 mmol) in DCM (10 mL), and the resulting mixture was stirred at 0 ℃ for 1 h. Then the mixture was allowed to warmed to room temperature and stirred overnight. The reaction was quenched with 100 mL of saturated sodium bicarbonate solution and extracted with DCM (3×100 mL). The combined organic layers were washed with brine, dried over anhydrous $MgSO_4$, and concentrated *in vacuo*. The residue was purified by flash column chromatography on silica gel (DCM:EA = 1:1) to give compound **4** as a

white solid (1.07 g, yield 97%) .^{1}H NMR (600 MHz, $CDCl_3$) δ 10.05 (s, 1H), 8.01 (d, *J* = 7.3 Hz, 2H), 7.79 (d, *J* = 7.5 Hz, 2H), 2.75 (s, 3H).

Compound **5**

Step 1: Under an atmosphere of nitrogen, compound **4** (654.0 mg, 3.89 mmol) was dispersed in trifluoroacetic acid anhydride (12.7 mL, 58.31 mmol), the reaction was refluxed at 40 ℃ for 30 min. Then, the solvent was removed under reduced pressure, and an ice-cooled mixture of triethylamine (Et_3N, 12 mL) and MeOH (12 mL) was added. After removing the solvent, the residue was dissolved in 15 mL of DCM, and 60 mL of saturated NH_4Cl solution was added. The organic layer was washed with brine 3 times, dried over anhydrous $MgSO_4$, and concentrated under reduced pressure to give a yellow oil.

Step 2: The yellow oil was dissolved in DCM (15 mL), and I_2 (1.18 g, 4.65 mmol) was added. The resulting mixture was stirred at room temperature for 4 h. Then the reaction was quenched with 1 M $Na_2S_2O_3$ (80 mL) and extracted with DCM (3 × 30 mL). The organic layers were dried over anhydrous $MgSO_4$. After removal of the solvent under reduced pressure, the residue was purified by flash column chromatography on silica gel (petroleum ether: ethyl acetate = 10: 1) to give compound **5** as a white solid (348.1 mg, yield 72%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.95 (s, 2H), 7.82 (d, *J* = 8.5 Hz, 2H), 7.62 (d, *J* = 8.4 Hz, 2H).

Compound **6**

Step 1: To a solution of stopper **3** (398 mg, 1.81 mmol) in 15 mL of EtOH was added compound **5** (249 mg, 0.91 mmol) and anhydrous $MgSO_4$ (546 mg, 4.54 mmol) under an atmosphere of nitrogen, the resulting reaction was refluxed at 80℃ for 24 h. Then, the solvent was removed under reduced pressure, and the residue was dissolved in 20 mL of MeOH/THF (v/v = 1/1). $NaBH_4$ (171.1 mg, 4.52 mmol) was slowly added to the solution, and the reaction mixture was stirred overnight at room temperature. Then the reaction was quenched with saturated NH_4Cl aqueous solution, and extracted with DCM (3×50 mL). The combined organic layers were dried over anhydrous $MgSO_4$. The solvent was removed under reduced pressure to give a yellow oil.

Step 2: The yellow oil was dissolved in DCM (10 mL), and I_2 (461.0 mg, 1.82 mmol) was added. The resulting mixture was stirred at room temperature for 4 h, washed with 1 M $Na_2S_2O_3$ (40 mL), extracted with DCM (3 × 50 mL), and the combined organic layers were dried over anhydrous $MgSO_4$. After removal of the solvent under reduced pressure, the residue was purified

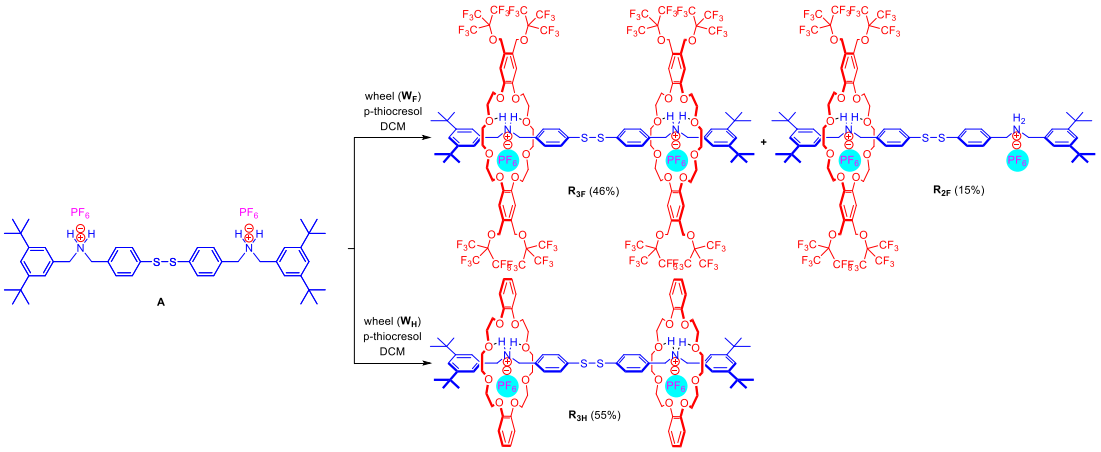
by flash column chromatography on silica gel (DCM:MeOH = 80:1) to give compound **6** as a yellow solid (490.0 mg, yield 79%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.47 (d, *J* = 8.0 Hz, 4H), 7.32 (s, 2H), 7.30 (d, *J* = 7.9 Hz, 4H), 7.15 (s, 4H), 3.80 (s, 4H), 3.78 (s, 4H), 1.32 (s, 36H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 150.8, 139.8, 139.0, 135.5, 129.0, 128.0, 122.3, 121.1, 53.7, 52.7, 34.8, 31.5.

Compound **7**

Under an atmosphere of nitrogen, Et_3N (0.96 mL, 6.92 mmol) was added to the solution of compound **6** (2.05 g, 3.01 mmol) in THF (50 mL) at 0°C, the resulting mixture was stirred for 10 min. Then di-*tert*-butyl dicarbonate (1.73 mL, 7.52 mmol) was slowly added to the mixture, and the resulting mixture was stirred at 40°C overnight. After removal of the solvent under reduced pressure, the residue was purified by flash column chromatography on silica gel (PE:EA = 40:1) to give compound **7** as a yellow solid (1.77 g, yield 67%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.36 (d, *J* = 6.8 Hz, 4H), 7.23 (s, 2H), 7.10 (s, 2H), 7.04 (s, 2H), 6.97 (s, 2H), 6.93 (s, 2H), 4.31 (s, 4H), 4.23 (s, 4H), 1.41 (s, 18H), 1.22 (s, 36H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 155.9, 150.9, 137.8, 137.5, 137.0, 136.8, 135.7, 130.6, 128.7, 128.2, 127.8, 122.2, 121.8, 121.2, 80.0, 50.2, 49.8, 49.1, 48.7, 34.7, 31.4, 28.4.

Axle **A**

To a solution of compound **7** (1.68 g, 1.91 mmol) in DCM (25 mL) was added trifluoroacetic acid (2.92 mL, 38.10 mmol) and anisole (2.07 mL, 19.05 mmol). The reaction mixture was stirred at room temperature for 12 h. After removal of the solvent, the residue was dissolved in MeOH (30 mL) and a saturated aqueous solution of NH_4PF_6 (20 mL, 91.78 mmol) was added. The resulting mixture was further stirred at room temperature for 5 h. After removal of the solvent in vacuo, the mixture was extracted with dichloromethane (3×100 mL), and washed with brine. The combined organic layers were concentrated under reduced pressure to give the crude product, which was purified by recrystallization from diethyl ether, giving Axle **A** as a white solid (1.20 g, yield 65%). ^{1}H NMR (500 MHz, CD_3CN) δ 7.61 (d, *J* = 10.0 Hz, 4H), 7.52 (s, 2H), 7.44 (d, *J* = 10.0 Hz, 4H), 7.28 (s, 4H), 4.20 (s, 4H), 4.17 (s, 4H), 1.31 (s, 36H). ^{13}C NMR (126 MHz, CD_3CN) δ 152.8, 139.1, 132.3, 130.9, 130.8, 128.3, 125.3, 124.6, 53.0, 51.7, 35.6, 31.5. ^{19}F NMR (471 MHz, CD_3CN) δ -72.56, -74.06.



Scheme S2. Synthesis of rotaxanes $\mathbf{R_{3F}}$, $\mathbf{R_{2F}}$, and $\mathbf{R_{3H}}$.

[3]Rotaxane $\mathbf{R_{3F}}$

Wheel $\mathbf{W_F}$ (400 mg, 0.28 mmol) and Axle **A** (100 mg, 0.10 mmol) were dissolved in DCM (3 mL), and *p*-toluenethiol (1 mg, 0.01 mmol) was added to the solution. The reaction mixture was stirred overnight at room temperature. After removal of the solvent under reduced pressure, the residue was purified by flash column chromatography on silica gel (DCM:MeOH = 20:1) to give [3]Rotaxane $\mathbf{R_{3F}}$ and [2]Rotaxane $\mathbf{R_{2F}}$ as white solids ($\mathbf{R_{3F}}$:183 mg, yield 46%; $\mathbf{R_{2F}}$: 36 mg, yield 15%). Note: A higher yield of $\mathbf{R_{2F}}$ (100 mg, yield 40%) could be obtained when 1.0 equivalent of $\mathbf{W_F}$ (150 mg, 0.10 mmol) is applied.

$\mathbf{R_{3F}}$: ^{1}H NMR (500 MHz, CD_3CN) δ 7.37 (s, 2H), 7.21 (s, 4H), 7.18 (d, J = 8.0 Hz, 4H), 7.04 (d, J = 8.0 Hz, 4H), 6.87 (s, 8H), 5.10 (q, J = 10.7 Hz, 16H), 4.84 (t, J = 7.5 Hz, 4H), 4.47 (t, J = 7.5 Hz, 4H), 4.11 – 4.00 (m, 16H), 3.83 – 3.76 (m, 8H), 3.69 – 3.65 (m, 8H), 3.65 – 3.60 (m, 8H), 3.58 – 3.50 (m, 8H), 1.11 (s, 36H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 151.4, 147.7, 137.4, 131.4, 130.2, 129.9, 127.6, 126.7, 123.4, 123.1, 120.4 (q, J = 293.6 Hz), 113.4, 80.3-79.2 (m), 70.5, 69.8, 68.5, 68.2, 53.0, 52.3, 34.6, 31.1. ^{19}F NMR (471 MHz, CD_3CN) δ -71.26, -72.62, -74.13. MALDI-ICR-MS m/z: $[M\text{-}PF_6+H]^+$ calculated for $C_{132}H_{135}F_{78}O_{24}N_2PS_2^+$, 3708.7338; found, 3708.7097.

$\mathbf{R_{2F}}$: ^{1}H NMR (500 MHz, CD_3CN) δ 7.43 (d, J = 8.3 Hz, 2H), 7.40 (s, 1H), 7.35 (s, 2H), 7.34 (s, 1H), 7.25 (d, J = 8.3 Hz, 2H), 7.23 – 7.20 (m, 4H), 7.17 (d, J = 8.4 Hz, 2H), 6.89 (s, 4H), 5.09 (q, J = 10.0 Hz, 8H), 4.82 (t, J = 7.5 Hz, 2H), 4.53 (t, J = 7.5 Hz, 2H), 4.11 – 4.00 (m, 8H), 3.87 (d, J = 8.8 Hz, 4H), 3.83 – 3.75 (m, 4H), 3.73 – 3.66 (m, 4H), 3.65 – 3.59 (m, 4H), 3.57 – 3.50 (m, 4H), 1.29 (s, 18H), 1.10 (s, 18H). ^{13}C NMR (126 MHz, CD_3CN) δ 151.6, 147.8, 137.6, 131.5, 130.4, 130.1, 127.7, 126.8, 123.6, 120.4 (q, J = 289.8 Hz), 113.6, 80.5-79.3 (m), 70.7, 70.0, 68.6, 68.4,

53.2, 52.5, 34.8, 31.2, 29.9. ^{19}F NMR (471 MHz, CD_3CN) δ -71.20, -72.65, -74.15. MALDI-ICR-MS m/z: $[M\text{-}PF_6]^+$ calculated for $C_{88}H_{98}F_{36}O_{12}N_2S_2^+$, 2122.5986; found, 2122.1292.

[3]Rotaxane $\mathbf{R_{3H}}$

Wheel $\mathbf{W_H}$ (250 mg, 0.56 mmol) and Axle **A** (100 mg, 0.10 mmol) were dissolved in DCM (3 mL), and *p*-toluenethiol (1 mg, 0.01 mmol) was added to the solution. The reaction mixture was stirred overnight at room temperature. After removal of the solvent under reduced pressure, the residue was purified by flash column chromatography on silica gel (DCM:MeOH = 20:1) to give [3]Rotaxane $\mathbf{R_{3H}}$ as a white solid (105 mg, yield 55%) [2]. ^{1}H NMR (500 MHz, CD_3CN) δ 7.44 (s, 2H), 7.33 (d, *J* = 1.5 Hz, 4H), 7.13 (d, *J* = 8.3 Hz, 4H), 6.96 (d, *J* = 8.3 Hz, 4H), 6.85 – 6.77 (m, 8H), 6.76 – 6.62 (m, 8H), 4.75 – 4.67 (m, 4H), 4.66 – 4.57 (m, 4H), 4.11 – 3.90 (m, 16H), 3.84 – 3.65 (m, 16H), 3.64 – 3.54 (m, 8H), 3.52 – 3.42 (m, 8H), 1.19 (s, 36H).

3. HPLC analysis

Purity analysis using high performance liquid chromatography (HPLC) was performed with Shimadzu LC-20A analytical HPLC system equipped with an Amethyst C18-H reversed phase column (particle size 5.0 μm, column dimension 4.6×250 mm), mobile phase A consisted of 0.1% (v/v) TFA in Milli Q water and mobile phase B consisted of 0.1% (v/v) TFA in acetonitrile. The conditions for analytical HPLC were as follows: flow rate 1.0 mL/min, detection wavelength 254 nm, gradient B/A 50-95%, v/v, 35 min linear gradient.

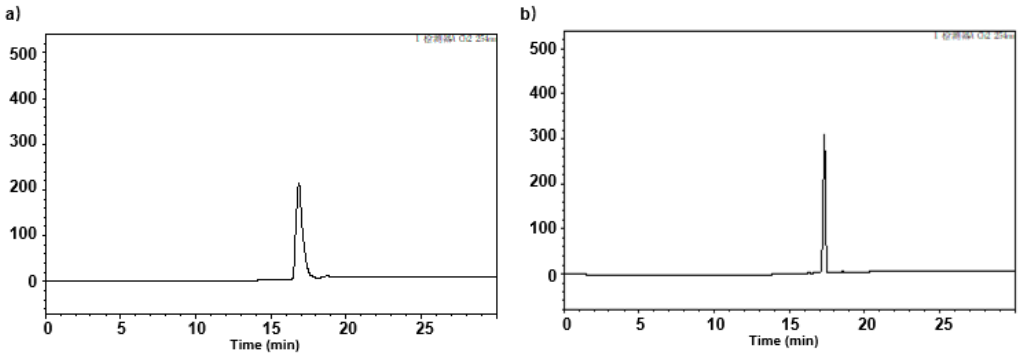


Figure S1 HPLC chromatograms of Rotaxanes $\mathbf{R_{2F}}$ (a) and $\mathbf{R_{3F}}$ (b) in acetonitrile (1 mg/mL).

4. NMR analysis of $\mathbf{R_{2F}}$, $\mathbf{R_{3F}}$, and $\mathbf{R_{3H}}$

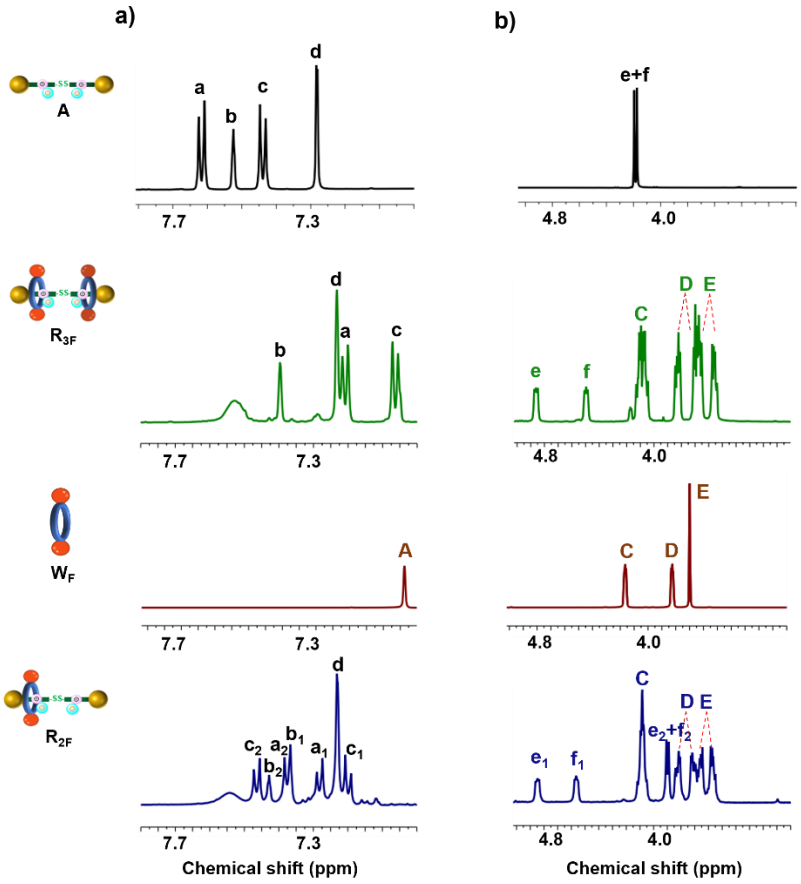


Figure S2 An expanded view of 7.8-7.0 ppm (a) and 5.0-3.0 ppm region (b) of ^{1}H NMR spectra of **A**, **R$_{3F}$**, **W$_{F}$**, and **R$_{2F}$**.

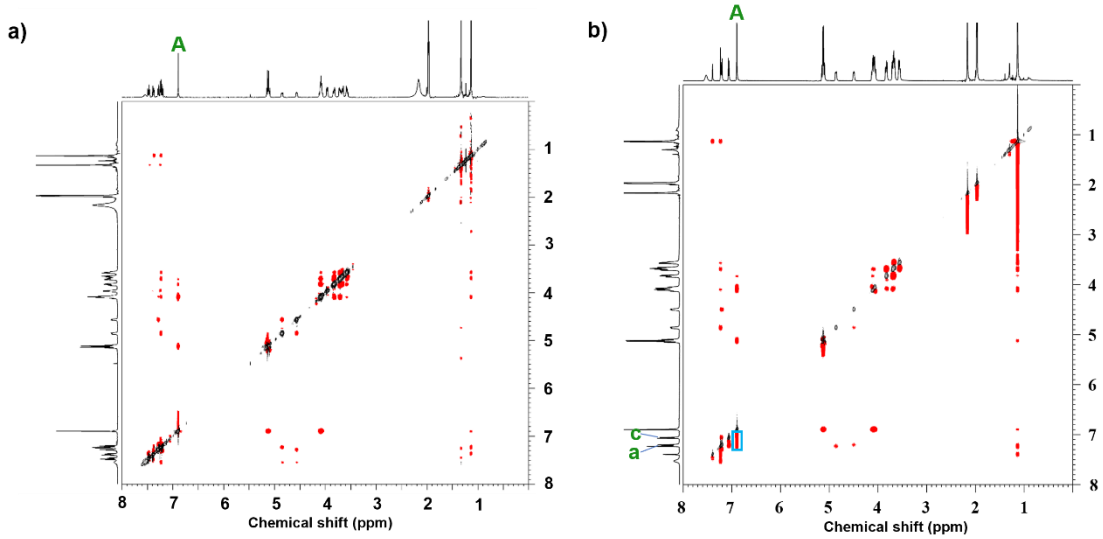


Figure S3 ^{1}H-^{1}H ROESY NMR spectra of **R$_{2F}$** (a) and **R$_{3F}$** (b). NMR conditions: 2.5 mM in CD_3CN at 298 K, 600 MHz.

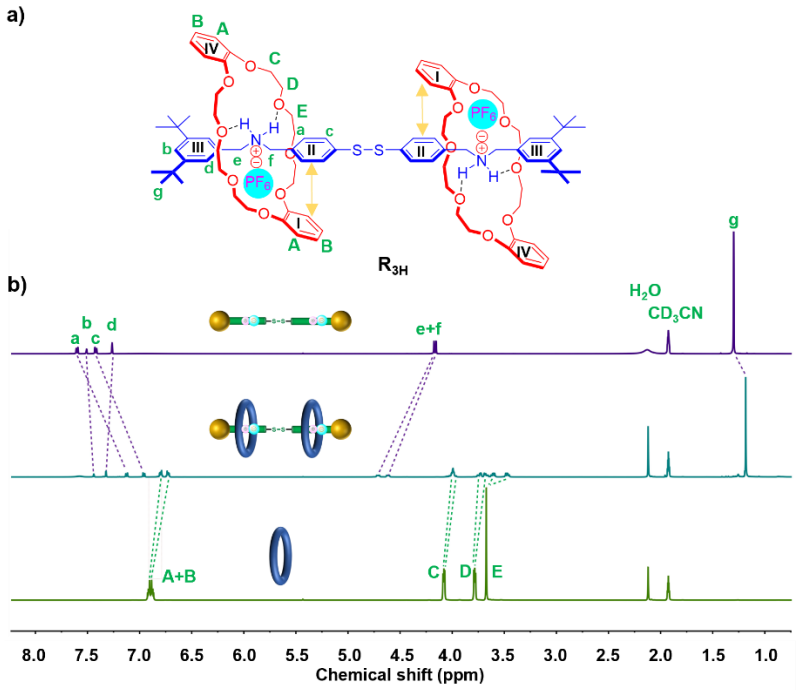


Figure S4 Proposed stable conformations of $\mathbf{R_{3H}}$ with labeled protons and benzene groups (a). Partial ^{1}H NMR spectra of **A**, $\mathbf{R_{3H}}$, and $\mathbf{W_F}$ (b). NMR conditions: 2.5 mM in $CDCl_3$ at 298 K, 500 MHz.

5. T_1 and T_2 determination

The pulse sequence for measuring T_1 was t1ir, T_1 values were extracted from a series of GRE images with recovery times 0.08, 0.2, 0.4, 0.8, 1.2, 1.6, 2.0, 2.6, 3.4, 4.2, 5.0, 6.0, 7.0, 9.0, 11.0, 15.0 s, and 16 averages. The pulse sequence for measuring T_2 was cpmg, T_2 values were extracted from a series of GRE images with recovery times 2000, 2200, 2400, 2800, 3200, 4000, 4800, 6000, 7200, 8600, 9400, 11000, 16000, 25000, 40000, 60000 s, and 16 averages.

6. Variable temperature ^{19}F MAS NMR

Variable temperature ^{19}F MAS NMR experiments were carried out on a Bruker Avance 400 MHz spectrometer with a 4.0 mm double-resonance MAS probe. The Larmor frequency is 375.7 MHz for ^{19}F. ^{19}F MAS NMR spectra were acquired with a $\pi/2$ pulse length of 5.0 μs and a recycle delay of 5 s. The T_1 relaxation time of various protons was measured using the inversion–recovery method. ^{19}F NMR chemical shift was externally referenced to trifluoroacetic acid.

Variable temperature ^{19}F MAS NMR experiments were further employed to extract the rotational correlation time of these three samples. To quantitatively evaluate the relaxation data, the

experimental R_1 data were fitted according to the Kubo-Tomita expression (equation 1) assuming exponential correlation functions and no correlations between the motions:

$$R_1 = \frac{1}{T_1} = \sum_{i \geq 1} C_i \left(\frac{\tau_{ci}}{1+4\omega_0{}^2\tau_{ci}{}^2} + \frac{4\tau_{ci}}{1+4\omega_0{}^2\tau_{ci}{}^2} \right) \quad (1)$$

where ω_0 is the ^{19}F Larmor frequency and τ_{ci} the rotational correlation time of the motion responsible for spin-lattice relaxation, given by:

$$\tau_{ci} = \tau_{0i}\, exp\left(\frac{E_{ai}}{RT}\right) \quad (2)$$

Here, τ_{0i} represents the pre-exponential factor corresponding to the rotational correlation time at infinite temperature, and E_{ai} denotes the activation energy. According to the fitted R_1 to Kubo-Tomita equation, its activation energy for a thermally activated process was estimated at 19.7 kJ/mol, and the correlation time was determined to be $\tau_0 = 3.3 \times 10^{-13}$ s^{-1}. In comparison, the rotational correlation times of the CF_3 group are determined to be 1.96×10^{-12} and 1.36×10^{-12} s^{-1} in $\mathbf{R_{3F}}$, and $\mathbf{R_{2F}}$, respectively.

7. Molecular dynamics simulations

The systems for MD simulations were built by placing each of the rotaxanes in the center of a cubic box with a volume of 60×60×60 $Å^3$ containing 4000 acetonitrile molecules. Here, the conformation of the wheel molecules on the rotexantes was adopted from X-ray structure published in our previous study[2]. And the axle conformation was generated by quantum chemical calculations with PM6 method performed on Gaussian09 software[3]. Then the modeling systems were built by PyMol and PackMol program[4].

MD simulations were performed by AMBER18 software package supported GPU computation with the CUDA version of pmemd program[5]. The topology parameters of the modeling systems were generated by quantum mechanical HF/6-31G* optimizations from Gaussian09 software[2] cooperated with RESP[6] approach and GAFF[7] force field from AMBER package. Each of the modeling systems was carried out 4 independent trajectories with conventional simulation steps of minimization, equilibration before MD production. During the equilibration processes, the systems were heated in constant volume (NVT ensemble) and equilibrated in constant pressure (NPT ensemble) conditions. After 10 ns of equilibration, the production MD simulations were performed for 100 ns under the constant pressure of 1.0 bar using Berendsen barostat at 300 K. Time step was

set to 1 fs and every 10 ps saved one snapshot. Analyses of the trajectories were applied CPPTRAJ program[8] and in-house scripts.

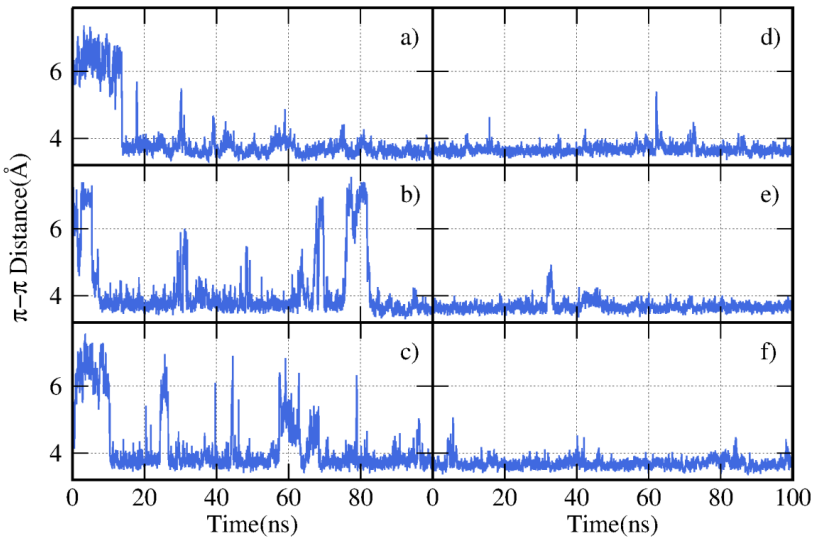
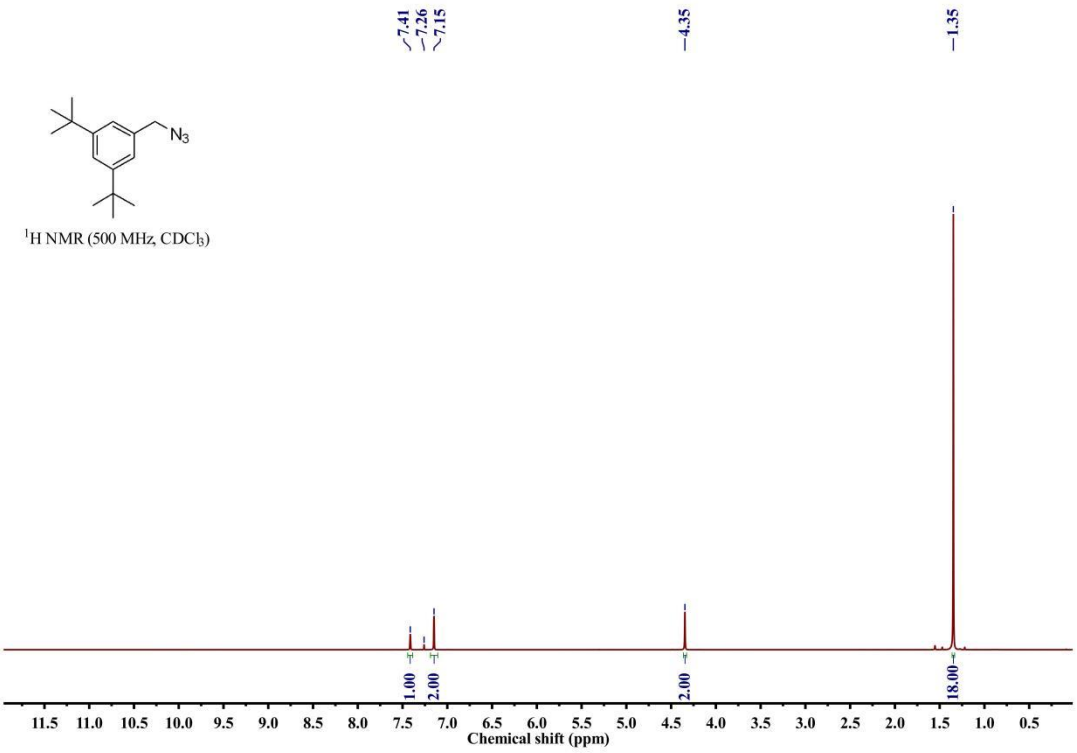


Figure S5. The other three of the simulated trajectories by the minimum π-π distance along the time, (a-c) rotaxane $\mathbf{R_{2F}}$ and (d-f) rotaxane $\mathbf{R_{3F}}$.

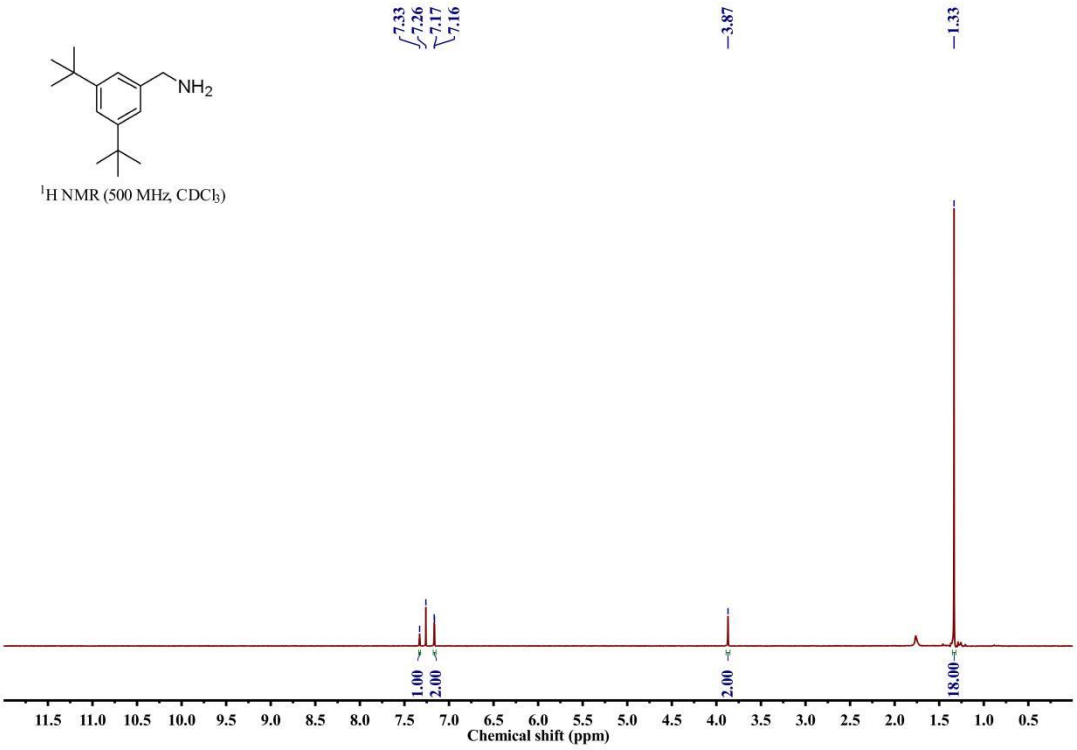
8. ^{19}F MRI phantom experiments of W_F, R_{2F}, and R_{3F}

^{19}F MRI phantom experiments were performed on a Bruker BioSpec 400 MHz MRI system. The temperature of the magnet room was maintained at 24 °C during the experiment. The ^{19}F phantom images were acquired using a RARE pulse sequence, RARE factor = 4, matrix size = 32 × 32, slice thickness = 20 mm, FOV = 3.0 cm × 3.0 cm, TR = 600 ms, TE = 17.5 ms, scan time = 307 s.

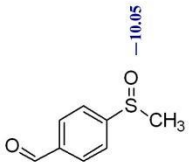
9. Copies of $^{1}H/^{13}C/^{19}F$ NMR and MS spectra of compounds



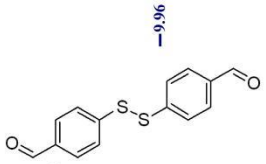
^{1}H NMR (500 MHz, $CDCl_3$)



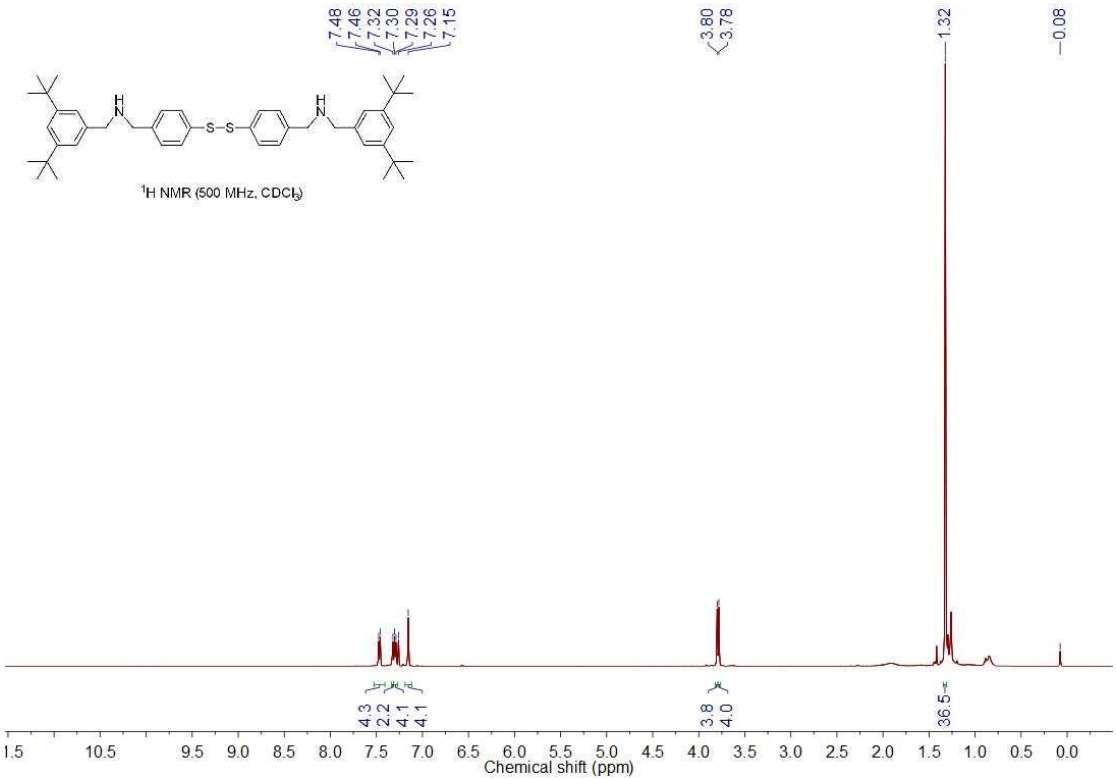
^{1}H NMR (500 MHz, $CDCl_3$)



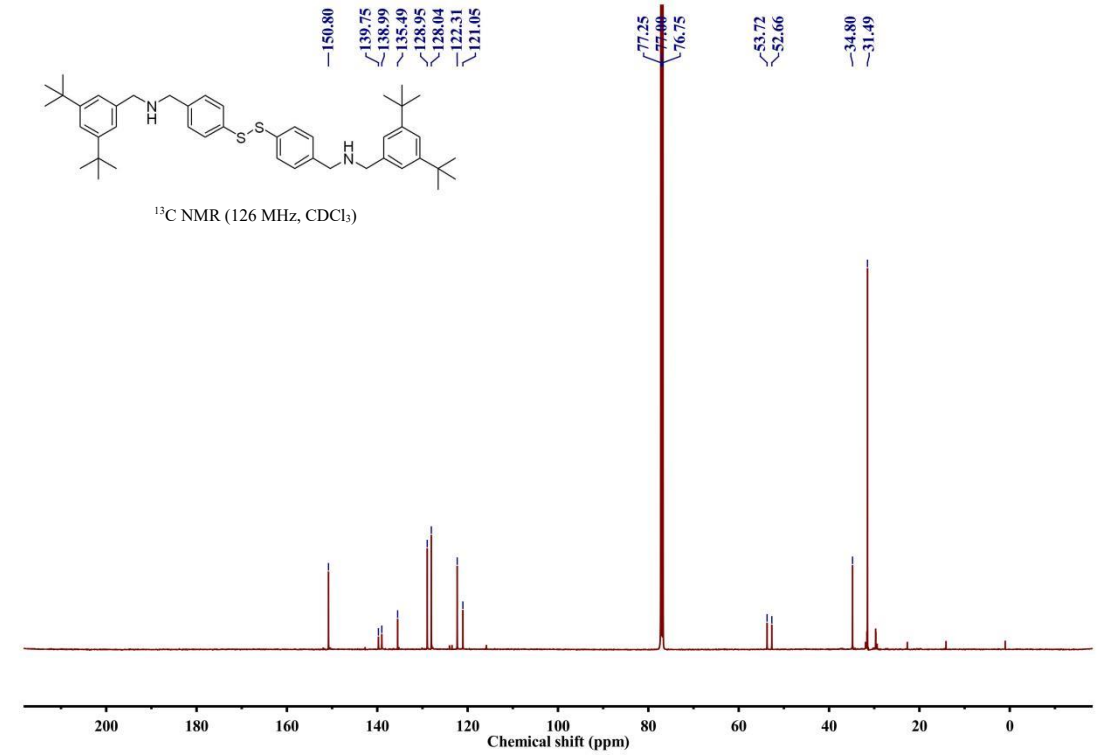
^{1}H NMR (600 MHz, $CDCl_3$)



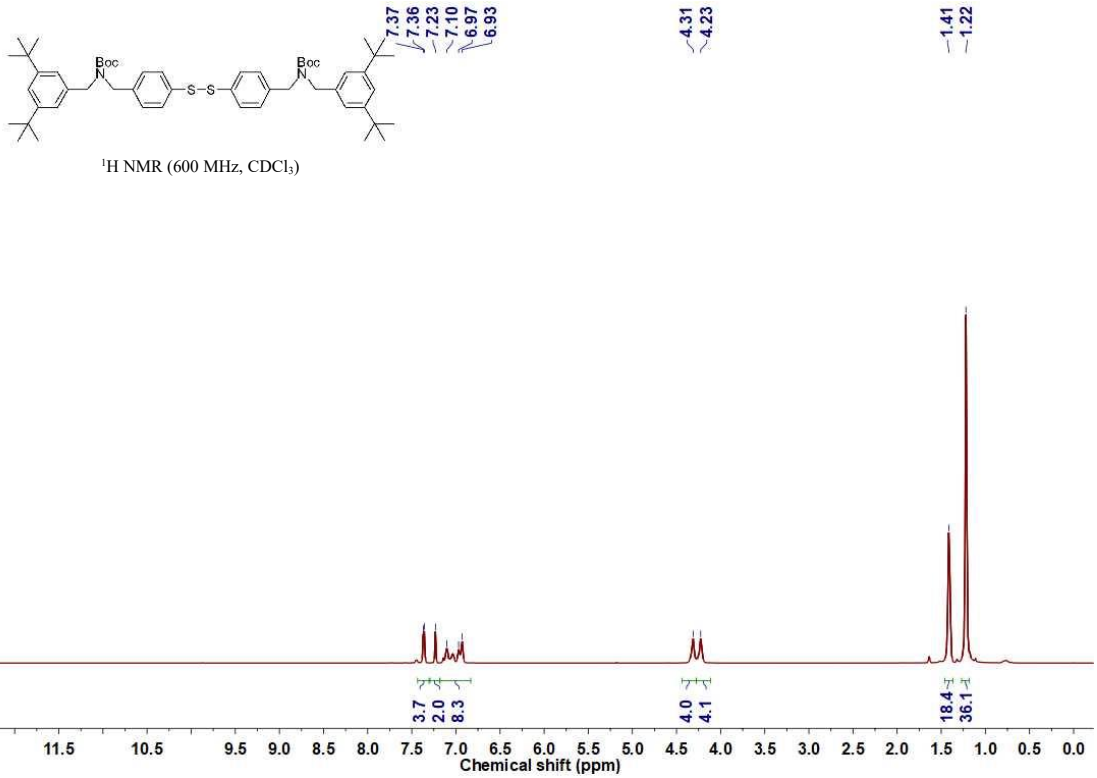
^{1}H NMR (500 MHz, $CDCl_3$)



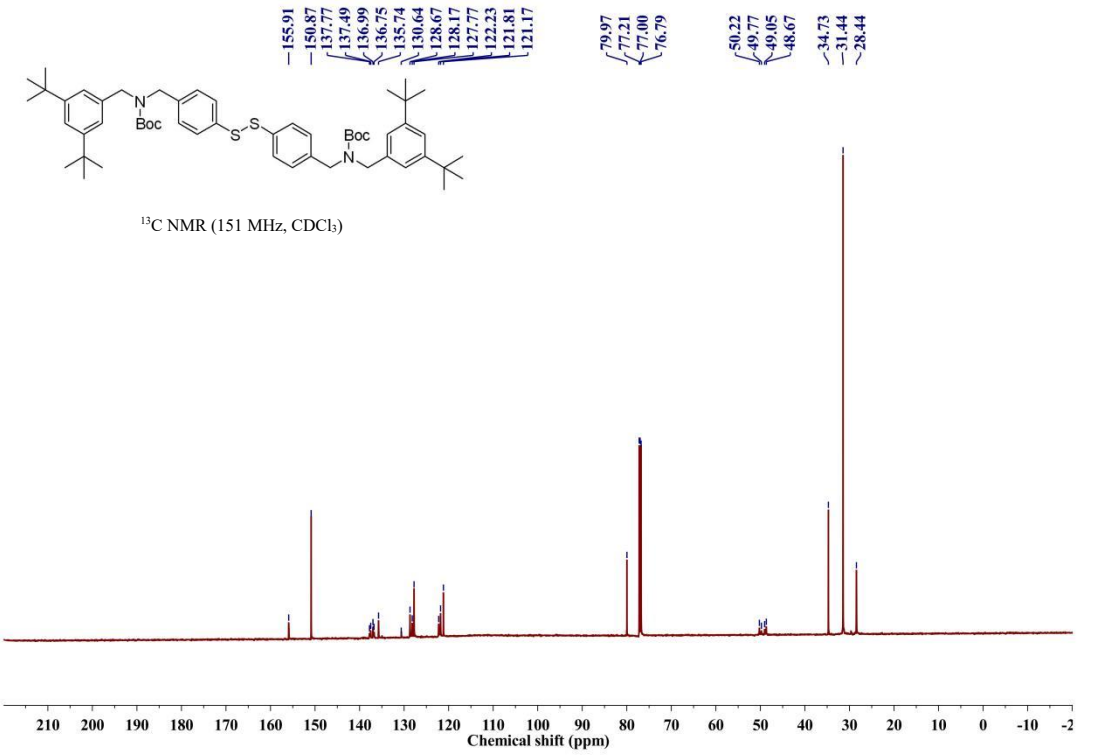
^{1}H NMR (500 MHz, $CDCl_3$)



^{13}C NMR (126 MHz, $CDCl_3$)

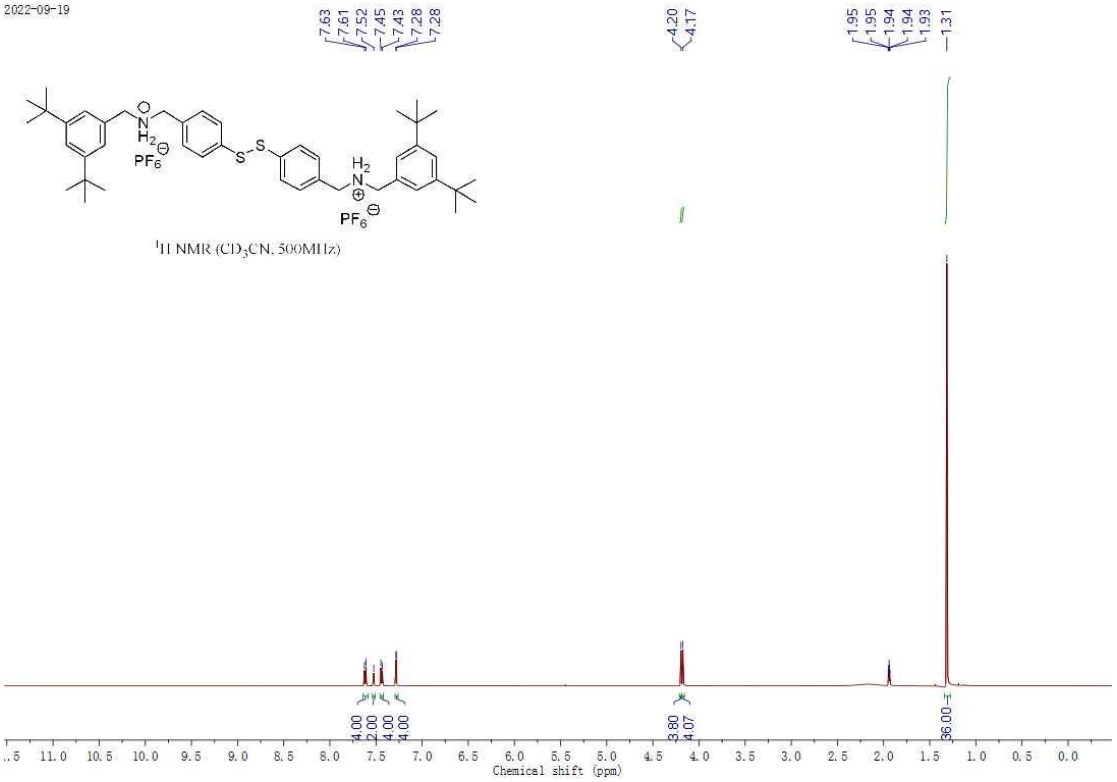


^{1}H NMR (600 MHz, $CDCl_3$)

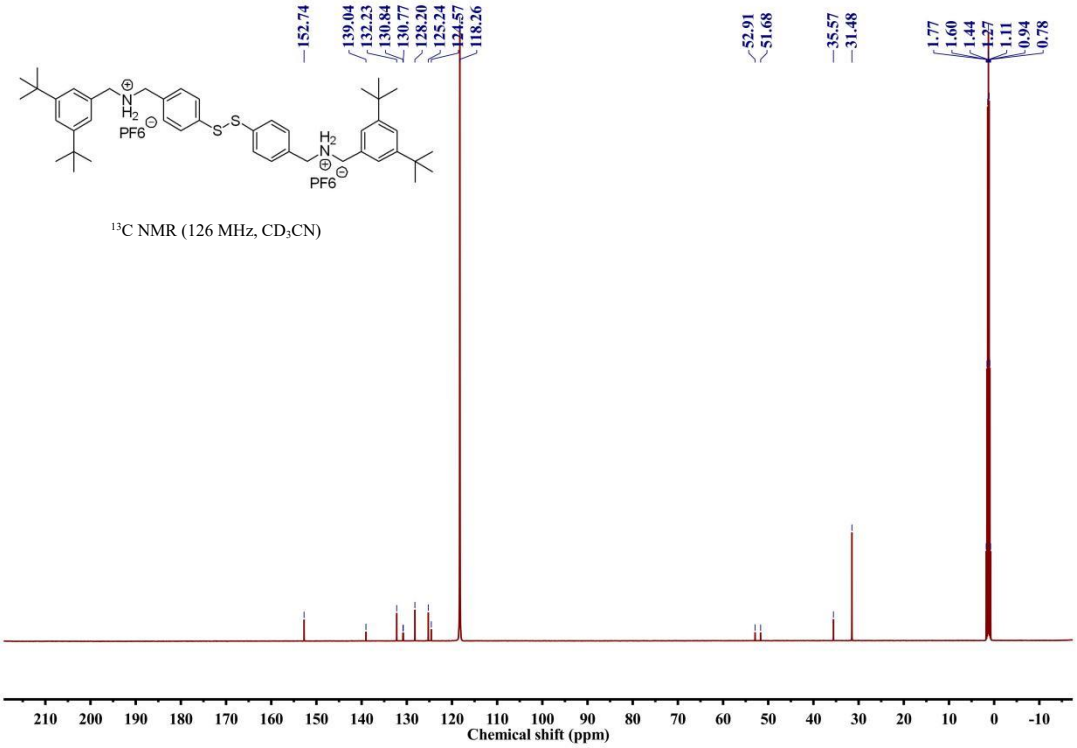


^{13}C NMR (151 MHz, $CDCl_3$)

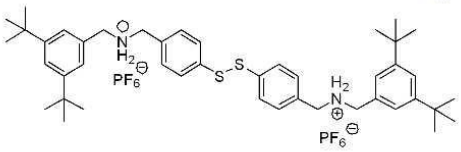
2022-09-19



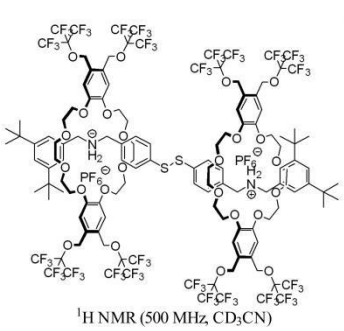
^{1}H NMR (CD_3CN, 500MHz)



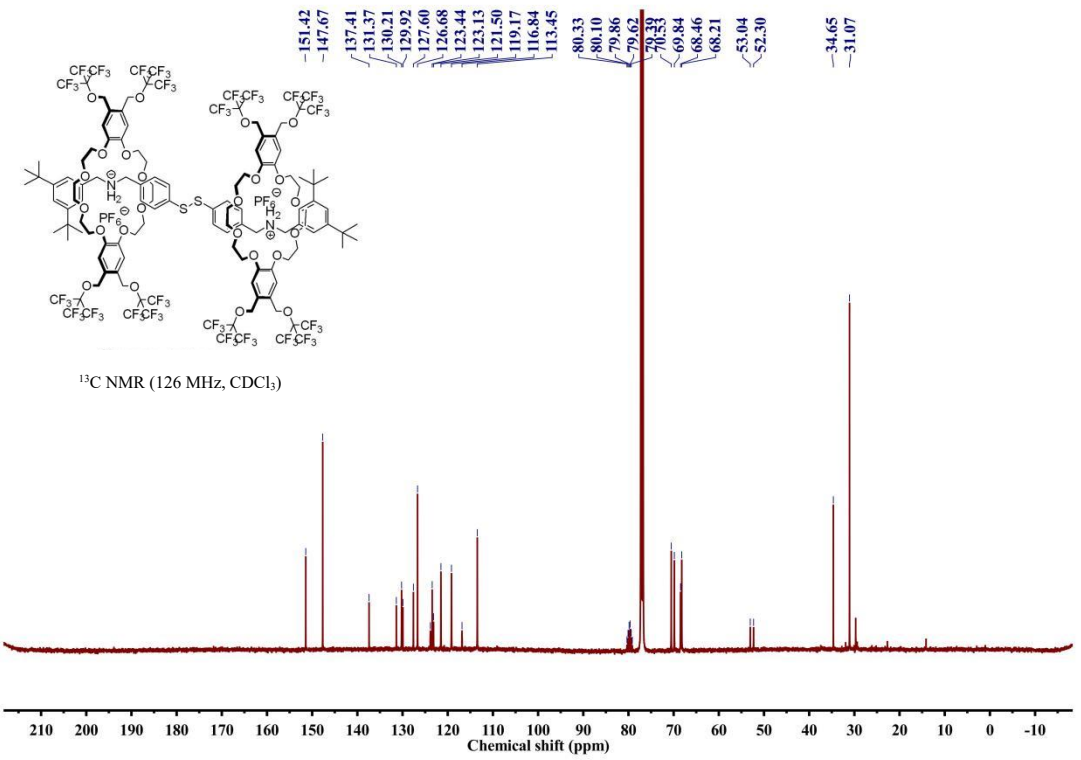
^{13}C NMR (126 MHz, CD_3CN)



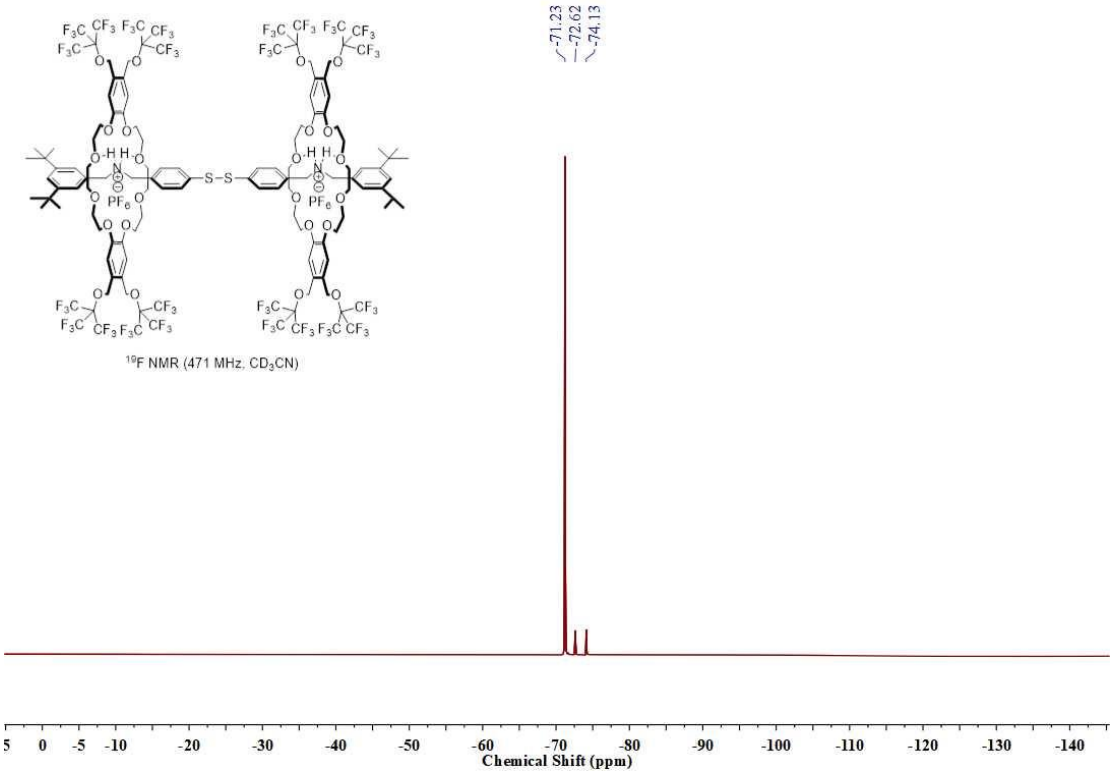
^{19}F NMR (CD_3CN, 471 MHz)



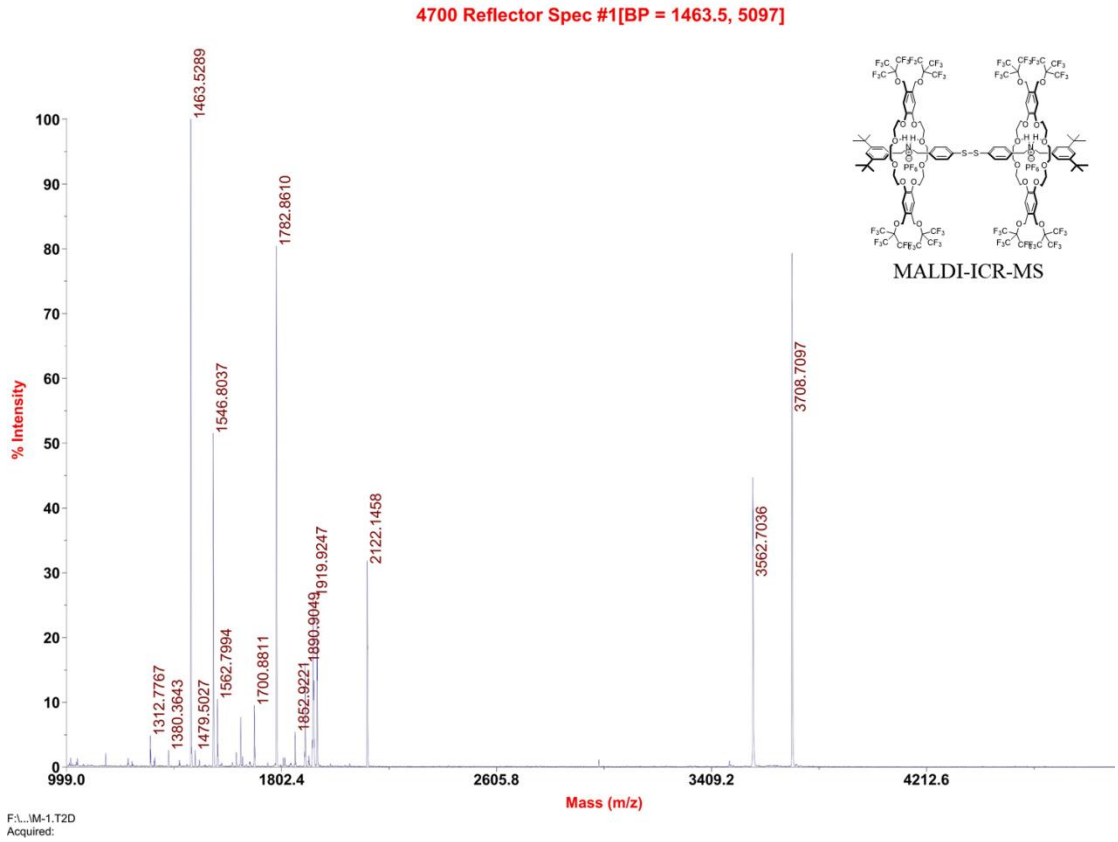
^{1}H NMR (500 MHz, CD_3CN)



^{13}C NMR (126 MHz, $CDCl_3$)



^{19}F NMR (471 MHz, CD_3CN)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MALDI-ICR-MS
% Intensity
Mass (m/z)
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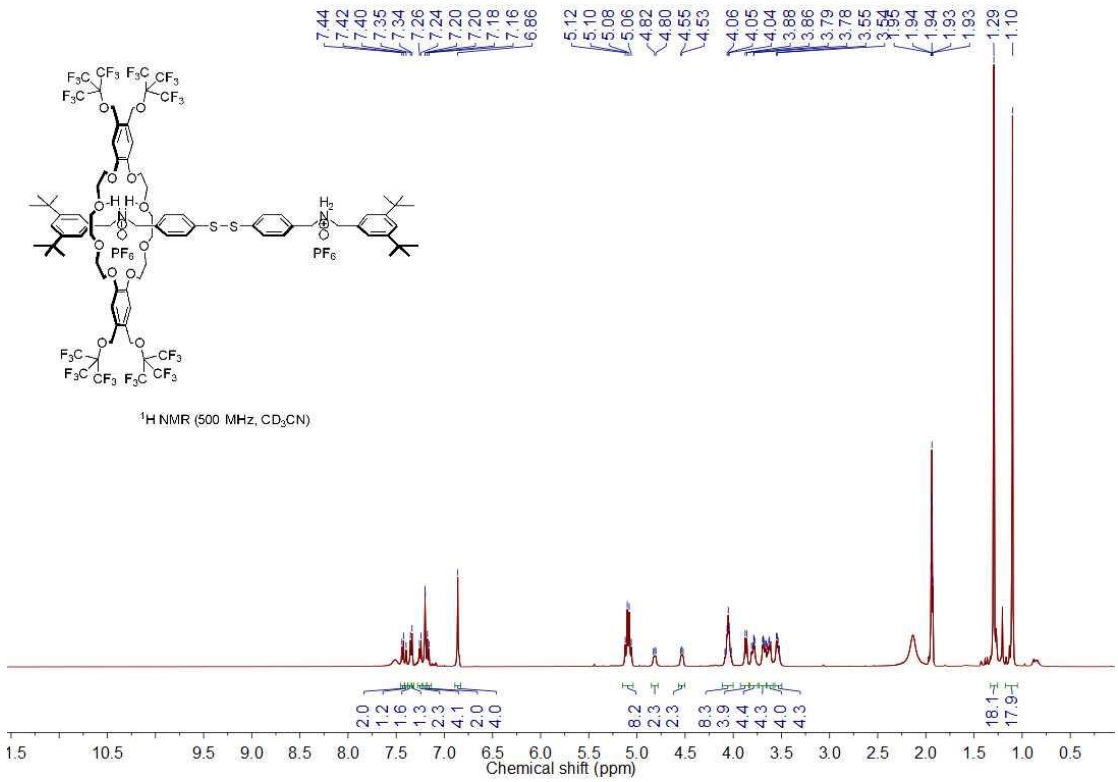
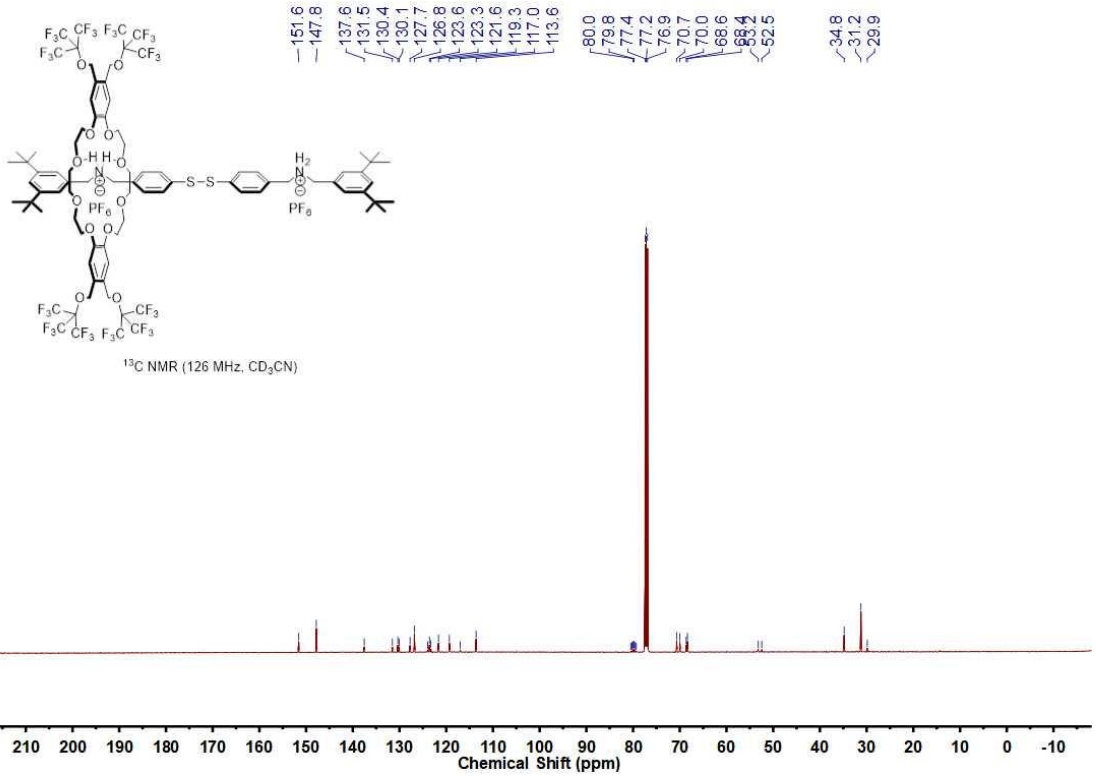
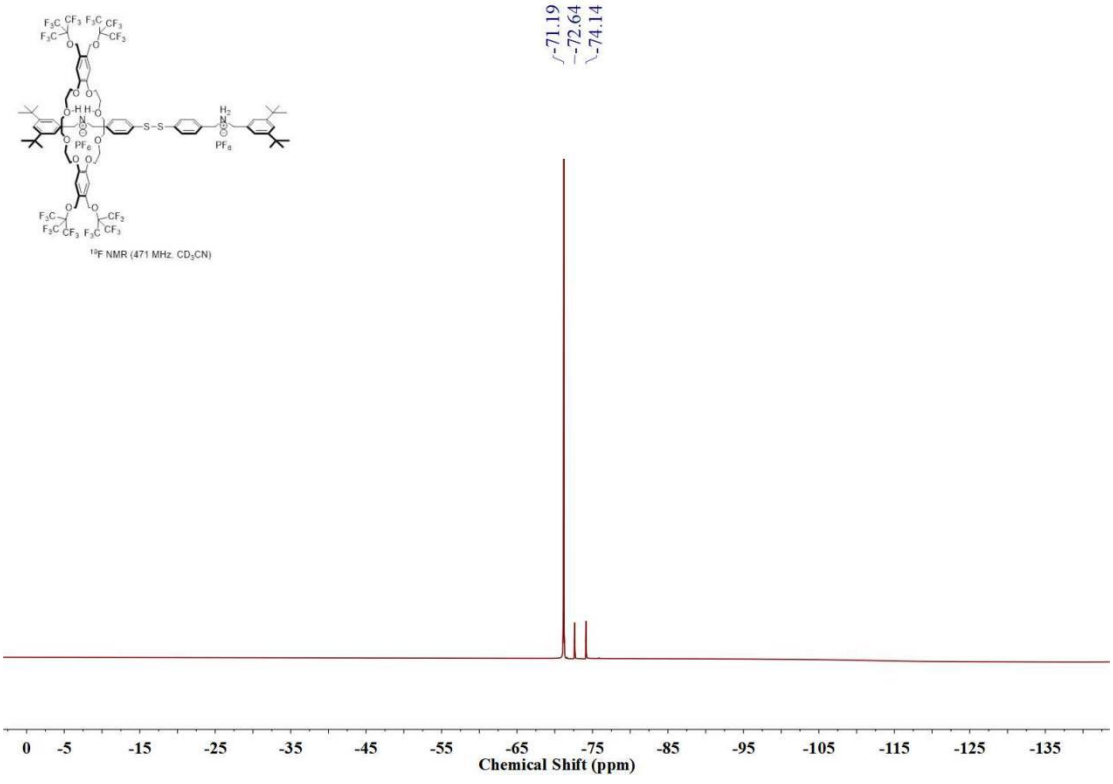
1546.8037
3708.7097
3562.7036
2122.1458
1919.9247
1890.9049
1852.9221
1700.8811
1562.7994
1479.5027
1380.3643
1312.7767
F:\...\M-1.T2D
Acquired:

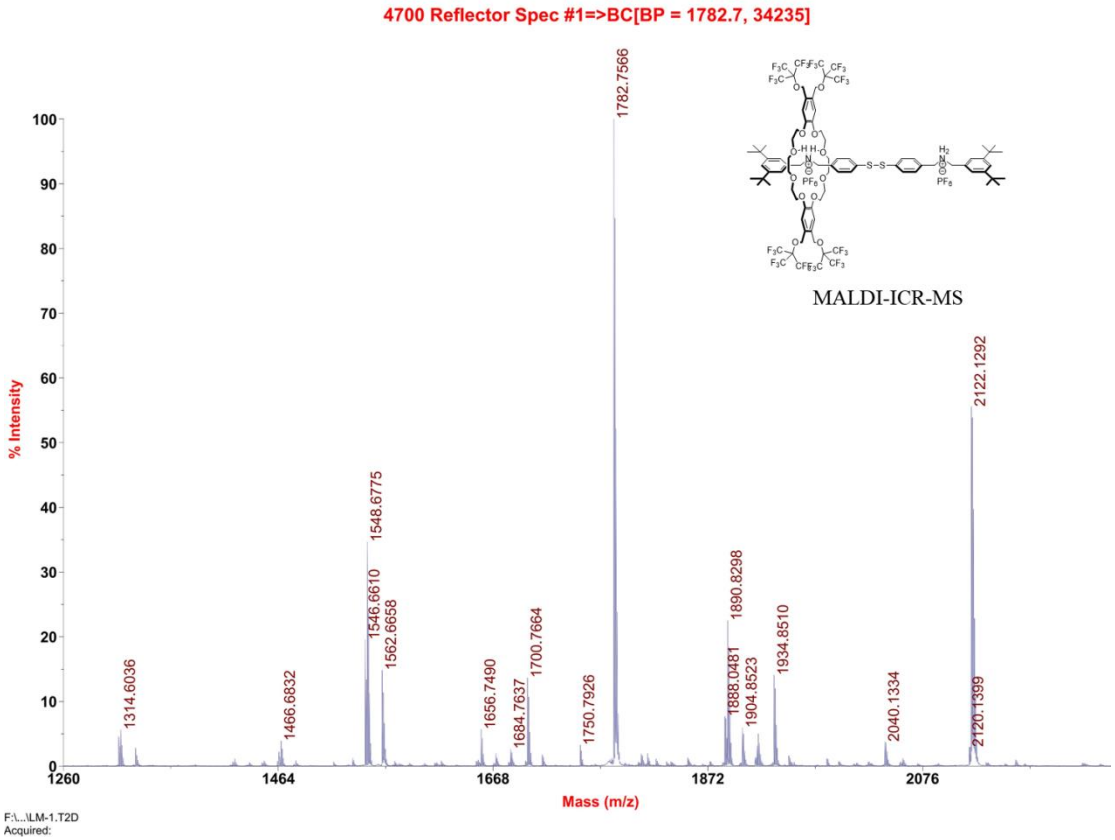

^{1}H NMR (500 MHz, CD$_3$CN)
Chemical shift (ppm)



^{13}C NMR (126 MHz, CD_3CN)



^{19}F NMR (471 MHz, CD_3CN)


4700 Reflector Spec #1=>BC[BP = 1782.7, 34235]
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1546.6610
1562.6658
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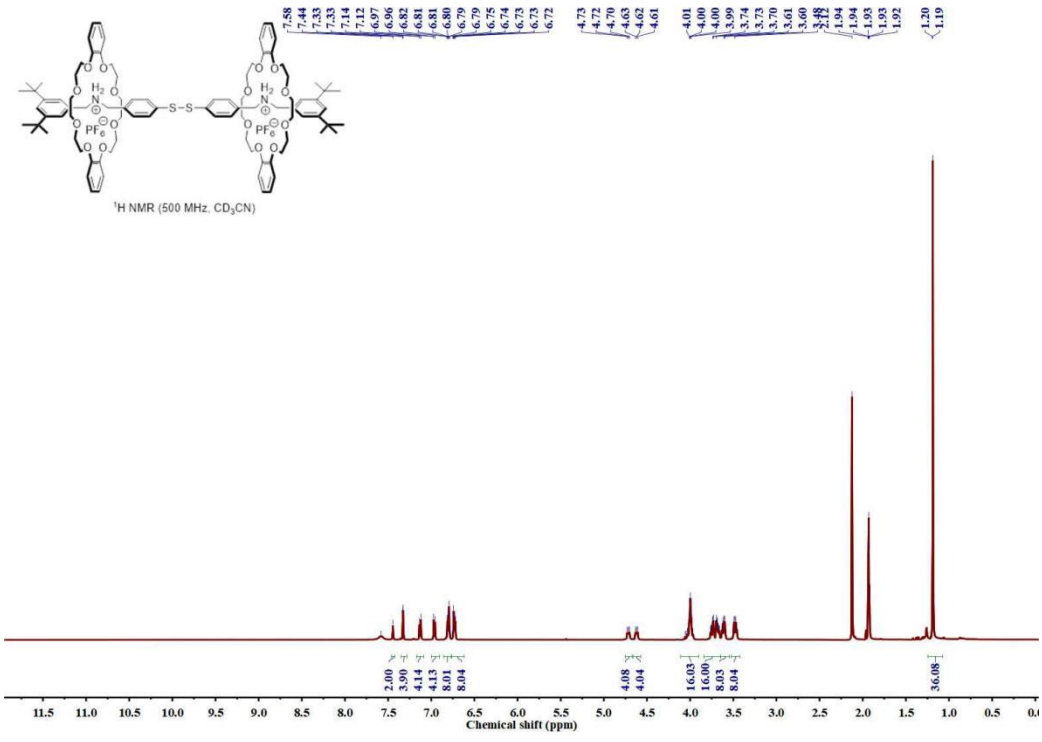
2122.1292
1934.8510
1700.7664
1314.6036
1466.6832
1656.7490
1684.7637
1750.7926
1888.0481
1904.8523
2040.1334
2120.1399
% Intensity
Mass (m/z)
MALDI-ICR-MS
F:\...\LM-1.T2D
Acquired:


^{1}H NMR (500 MHz, CD_3CN)
Chemical shift (ppm)

10. References

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