Supplemental Information

Kinetically Controlled Synthesis of Rotaxane Geometric Isomers

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I. General Procedures

All chemical reagents were purchased from commercial sources. Triethylamine was distilled prior to each kinetics experiment and stored over KOH for no longer than one week. Removal of solvent was accomplished on a Büchi R-210 rotary evaporator, and further concentration was done under a Fisher Scientific Maxima C-Plus vacuum line.

Chromatography

Column chromatography was performed manually with Sorbent grade 60 silica with a mesh size between 230–400 using the forced flow of indicated solvents, or automatically with a Teledyne CombiFlash Rf+ chromatography system. The flow rate was typically no higher than 30 mL/min. Size Exclusion Chromatography (SEC) was performed on a Bio-Beads™ SX-1 Resin using CH_2Cl_2 or $CHCl_3$ as the eluent. All beads were allowed to swell for at least one hour before addition to the column. Beads were then washed with a minimum of three column volumes of solvent before each elution to ensure column was clean of any contaminants. A new fraction was collected every 2 minutes to ensure separation. A column length of at least 2 meters is recommended for SEC purification of pillar[5]arene-derivatives reported in this study.

Spectroscopy

High-resolution mass spectrometry data were obtained on a Waters XEVO G2-XS QTof in positive or negative ESI mode or on a LTQ Orbitrap in ESI mode. All ROESY, ^{1}H-NMR, and ^{13}C-NMR spectra were recorded at 298 K on a Bruker ARX 500 (500 MHz) spectrometer, on a Varian Unity Inova 500 (500 MHz) spectrometer, or on a Bruker Avance-III-800 (800 MHz) spectrometer. The spectra were referenced to the residual solvent peak ($CDCl_3$: 7.26 ppm for ^{1}H-NMR and 77.16 ppm for ^{13}C-NMR for both 1D and 2D experiments. Chemical shift values were recorded in parts per million (ppm), and 1,2,4,5–tetrabromobenzene (TBB, δ 7.87 ppm) was used as the internal standard for all kinetic measurements. Data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br = broad peak), coupling constants (Hz), and number of protons. For 2D experiments, MestReNova was used to process all FIDs.

II. Synthetic Procedures and Characterization Data
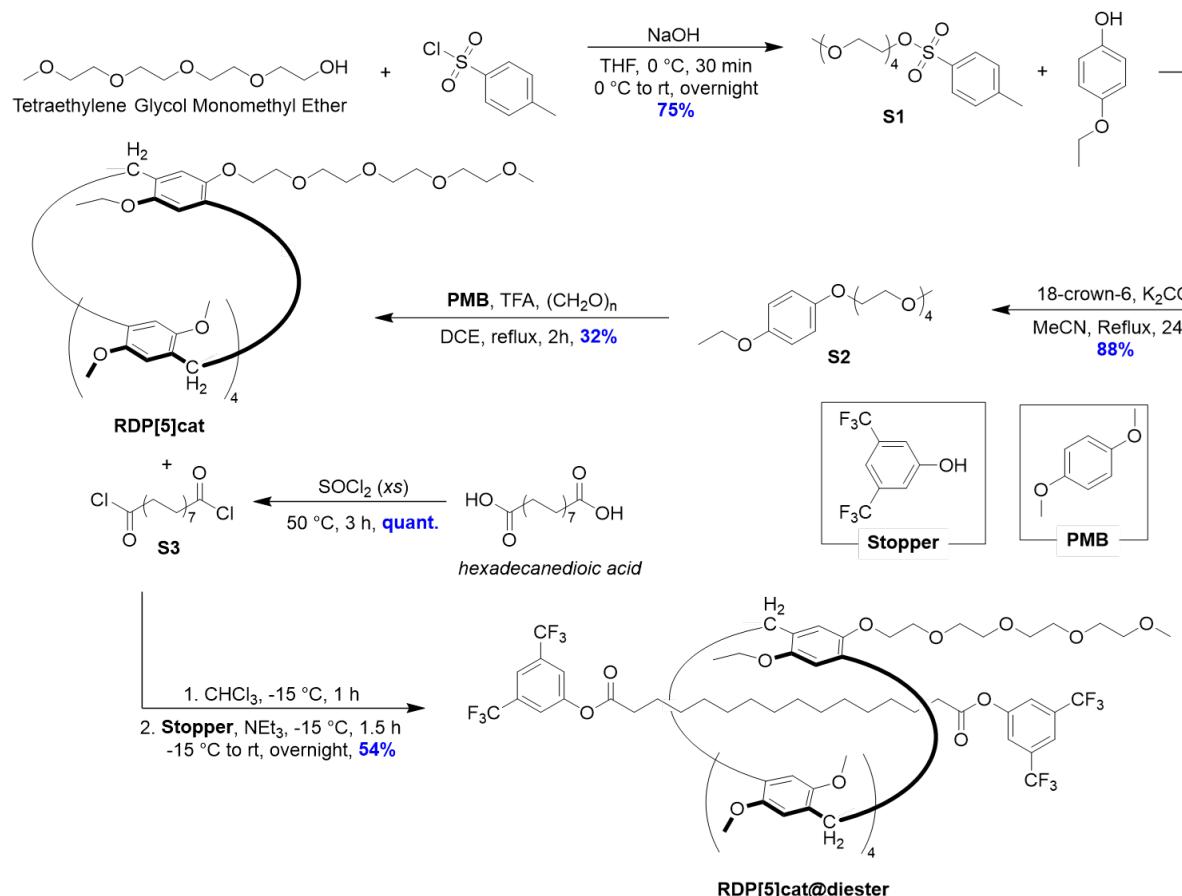
Scheme S1. Synthesis of the rim-differentiated pillar[5]arene rotaxane **RDP[5]cat@diester**. (**PMB** = 1,4-dimethoxybenzene)
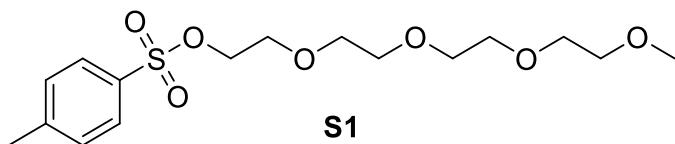
Synthesis of **2,5,8,11-tetraoxatridecan-13-yl 4-methylbenzenesulfonate** (**S1**). The synthesis for this compound was adapted from reference S1.[1] A round bottom flask containing sodium hydroxide (8.41 g, 210 mmol) in water (14.2 mL) was cooled to 0 °C in an ice-water bath. A solution of 2,5,8,11-tetraoxytridecan-13-ol (12.5 g, 60.1 mmol) in THF (31.2 mL) was then added dropwise the round bottom flask and allowed to stir at 0 °C for an additional 10 minutes. To complete the reaction setup, a solution of 4-toluenesulfonyl chloride (11.5 g, 60.1 mmol) in THF (34.1 mL) was added dropwise to the flask and the reaction mixture was allowed to warm to room temperature over 15 hours while stirring. Reaction progress was monitored by TLC (10% MeOH/DCM). For quenching, the solution was cooled to 0 °C in an ice-water bath for

1 hour, and the excess of NaOH was quenched with 1M HCl. Finally, the THF solvent was removed *in vacuo*. The product was extracted with DCM (3 x 100 mL), and the combined extracts were washed with saturated Na_2CO_3 (2 x 50 mL) and distilled water (2 x 50 mL). The organic phase was dried over sodium sulfate and concentrated *in vacuo*. Purification via flash chromatography over silica gel (0 – 20% MeOH/DCM over 20 min) afforded **S1** as a clear to light yellow oil (18.9 g, 52.2 mmol) in 87% yield.

¹H NMR (500 MHz, CDCl₃): δ 7.82 – 7.77 (m, 2H), 7.34 (d, *J* = 8.4 Hz, 2H), 4.18 – 4.13 (m, 2H), 3.71 – 3.65 (m, 2H), 3.66 – 3.60 (m, 6H), 3.58 (s, 4H), 3.57 – 3.51 (m, 2H), 3.37 (s, 3H), 2.44 (s, 3H).

¹³C NMR (125 MHz, CDCl₃): δ 144.91, 133.19, 129.95, 128.13, 72.08, 70.89, 70.75, 70.68, 69.37, 68.82, 59.17, 21.78.

HRMS (ESI+): Calcd. for $C_{16}H_{27}O_7S^+$ [M+H⁺] *m/z* = 363.1477, found 363.1467.

S2
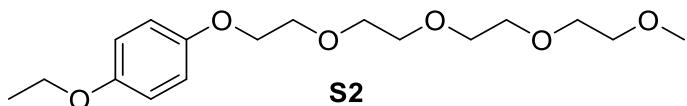
Synthesis of 13-(4-ethoxyphenoxy)-2,5,8,11-tetraoxatridecane (S2): The synthesis for this procedure was adapted from reference S2.[2] To a round bottom flask containing 4-ethoxyphenol (2.50 g, 18.1 mmol), potassium carbonate (7.50 g, 54.3 mmol), and 18-crown-6 (478 mg, 1.81 mmol) in acetonitrile (275 mL) was added **S1** (7.87 g, 21.7 mmol) and the reaction mixture was refluxed while stirring for 24 hours. Afterwards, the reaction was allowed to cool to room temperature, filtered over a small celite pad, and washed with DCM to ensure complete transfer of the product. The resulting solution was concentrated *in vacuo*, partitioned between DCM and distilled water, and extracted with DCM (3 x 100 mL). Finally, the combined organic layers were dried over sodium sulfate and concentrated *in vacuo*. The resulting crude material was purified via flash chromatography over silica gel (50 – 100% EtOAc/hexanes) to afford **S2** (5.3 g, 16.1 mmol) in 89% yield.

¹H NMR (500 MHz, CDCl₃): δ 6.86 – 6.77 (m, 4H), 4.07 (t, *J* = 5.0 Hz, 2H), 3.97 (q, *J* = 7.0 Hz, 2H), 3.82 (t, *J* = 5.0 Hz, 2H), 3.73 – 3.69 (m, 2H), 3.69 – 3.62 (m, 8H), 3.55 – 3.52 (m, 2H), 3.37 (s, 3H), 1.37 (t, *J* = 7.0 Hz, 3H).

¹³C NMR (125 MHz, CDCl₃): δ 153.34, 152.99, 115.71, 115.43, 72.04, 70.90, 70.74, 70.72, 70.63, 69.96, 68.19, 64.05, 59.13, 15.03.

HRMS (ESI+): Calcd. for $C_{17}H_{29}O_6^+$ [M+H$^+$] *m/z* = 329.1964; found 329.1959.
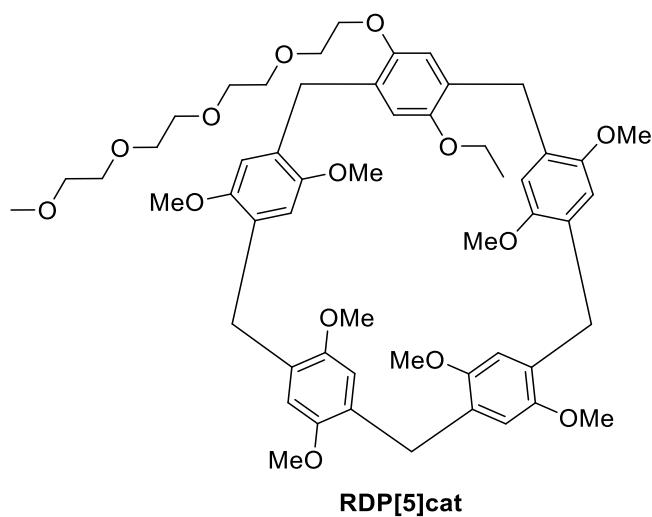
RDP[5]cat

Synthesis of RDP[5]cat: To a round-bottom flask containing **S2** (588 mg, 1.79 mmol) and finely ground paraformaldehyde (269 mg, 8.96 mmol) in 1,2-dichloroethane (80.3 mL) was added 1,4-dimethoxybenzene (**PMB**) (990 mg, 7.17 mmol). The solution was allowed to stir at room temperature until the **PMB** was fully dissolved. Trifluoroacetic acid (4.23 mL, 55.2 mmol, 5% v/v) was then added dropwise to the solution. The mixture was then refluxed with vigorous stirring for two hours and allowed to cool to room temperature. Finally, the solution was combined with distilled water (50 mL), and the aqueous layer was extracted with DCM (3 x 50 mL) and dried over anhydrous Na_2SO_4, filtered, and concentrated *in vacuo*. The crude product was purified using a combination of flash chromatography over silica gel (eluent: EtOAc/hexanes and/or DCM/MeOH) and size exclusion chromatography (SX-1 Biobeads, eluent: CHCl$_3$), affording **RDP[5]cat** as a light brown solid (534 mg, 0.57 mmol) in 32% yield.

^{1}H NMR (500 MHz, CDCl$_3$): δ 6.82 – 6.73 (m, 9H), 6.67 (s, 1H), 4.01 (t, *J* = 5.0 Hz, 2H), 3.83 (t, *J* = 5.1 Hz, 2H), 3.81 – 3.71 (m, 14H), 3.68 – 3.62 (m, 28H), 3.62 – 3.58 (m, 4H), 3.53 – 3.48 (m, 2H), 3.35 (s, 3H), 1.19 (t, *J* = 7.0 Hz, 3H).

^{13}C NMR (125 MHz, CDCl$_3$): δ 150.99, 150.93, 150.88, 150.84, 150.78, 150.30, 149.62, 128.91, 128.54, 128.37, 128.33, 128.32, 128.30, 128.24, 115.59, 114.62, 114.26, 114.12, 114.09, 113.96, 113.94, 72.04, 70.98, 70.82, 70.74, 70.69, 70.62, 70.35, 68.32, 63.53, 59.13, 55.98, 55.93, 55.85, 55.83, 55.80, 55.78, 30.12, 29.86, 29.70, 29.67, 29.34, 15.04.

HRMS (ESI+): Calcd. for $C_{54}H_{69}O_{14}^+$ [M+H$^+$] *m/z* = 941.4687, found 941.4683.

S3
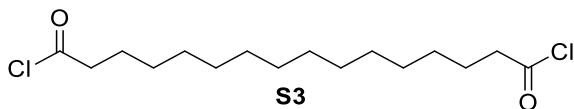
Synthesis of 1,16-hexadecanedioyl dichloride (S3): To a small pressure vial was added 1,16-hexadecanedioic acid (400 mg, 1.4 mmol) and thionyl chloride (3.0 mL). The vial was purged with argon, tightly capped, and stirred at 60 °C for 3 hours. The solution was then allowed to cool to room temperature, at which point a needle was carefully inserted through the cap's septum to allow for off gassing. The remaining thionyl chloride was then removed *in vacuo* to afford pure **S3** (450 mg, 1.4 mmol) in quantitative yields (>99%).

^{1}H NMR (500 MHz, CDCl$_3$): δ 2.88 (t, J = 7.3 Hz, 4H), 1.71 (p, J = 7.3 Hz, 4H), 1.42 – 1.19 (m, 20H).
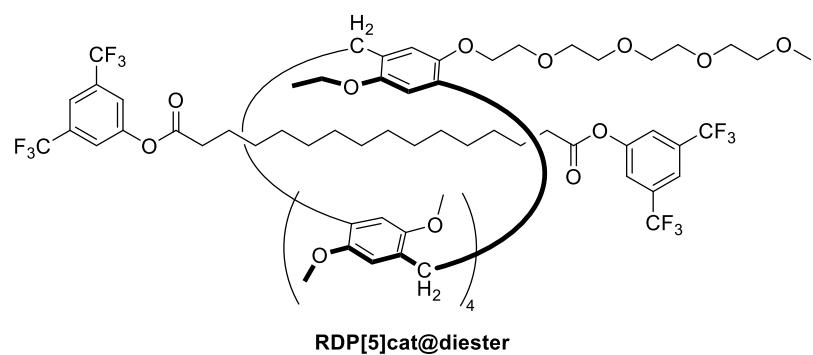
RDP[5]cat@diester

Synthesis of RDP[5]cat@diester: RDP[5]cat (263 mg, 0.28 mmol) and **S3** (271 mg, 0.839 mmol) were stirred in anhydrous CHCl$_3$ (1.97 mL) at −15 °C for 1 hour under an argon atmosphere. Next, a mixture of triethylamine (234 µL, 1.68 mmol) and 3,5-bis(trifluoromethyl)phenol (256 µL, 1.68 mmol) was added to the solution. The mixture was then stirred for 1 hour at −15 °C before being warmed to room temperature and stirred overnight. Finally, reaction mixture was then concentrated under reduced pressure and purified using flash column chromatography over silica (eluent: 25–100% EtOAc/hexanes) to afford **RDP[5]cat@diester** as a light red-brown oil (250 mg, 54%).

^{1}H NMR (500 MHz, CDCl$_3$): δ 7.77 (s, 2H), 7.62 (s, 2H), 7.61 (s, 2H), 6.96 – 6.84 (m, 10H), 4.07 – 3.96 (m, 2H), 3.97 – 3.66 (m, 42H), 3.63 (dtd, J = 16.8, 5.7, 3.1 Hz, 8H), 3.51 (dd, J = 5.7, 3.6 Hz, 2H), 3.36 (s, 3H), 1.68 – 1.62 (m, 2H), 1.40 (t, J = 6.9 Hz, 3H), 1.10 (d, J = 3.8 Hz, 4H), 1.05 – 0.93 (m, 4H), 0.75 (p, J = 7.7 Hz, 2H), 0.67 (p, J = 8.2 Hz, 2H), 0.46 (d, J = 7.9 Hz, 2H), 0.37 – 0.24 (m, 4H), 0.21 – 0.10 (m, 2H), 0.10 – -0.01 (m, 2H), -0.02 – -0.19 (m, 2H).

^{13}C NMR (125 MHz, CDCl$_3$): δ 171.15, 151.55, 150.42, 150.39, 150.35, 150.15, 149.35, 132.97, 132.92, 132.84 (q, J = 33.76), 132.80 (q, J = 34.16), 132.70, 132.65, 128.99, 128.41, 128.34,

128.31, 128.26, 128.23, 123.96, 123.95, 122.90 (q, J = 272.96), 122.88 (q, J = 272.96), 122.51, 122.47, 119.25, 115.12, 114.12, 113.70, 113.67, 113.59, 113.50, 113.47, 71.91, 70.76, 70.65, 70.61, 70.59, 70.52, 70.21, 68.04, 63.38, 59.01, 55.64, 55.54, 55.48, 55.46, 55.44, 55.43, 55.39, 33.40, 33.32, 30.59, 30.56, 30.27, 30.21, 30.18, 30.16, 29.07, 28.82, 28.76, 28.57, 28.53, 23.53, 23.42, 15.32.

HRMS (ESI+): Calcd. for $C_{86}H_{102}F_{12}NaO_{18}^+$ [M+Na$^+$] m/z = 1673.6772; found 1673.6776.
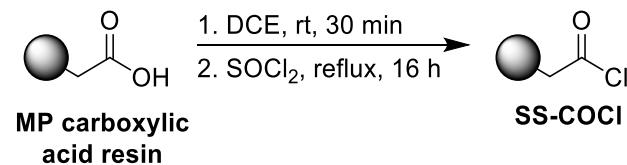
Synthesis of SS-COCl: MP carboxylic acid resin (1.31 g, 15-50 mesh, loading: 3.4-3.6 mmol/g) was added to 13.3 mL of dichloroethane in a round-bottom flask and stirred under bubbling argon for 30 minutes. To this flask was added 2.04 mL of thionyl chloride (3.32 g, 27.9 mmol). This solution was refluxed under an inert atmosphere for 16 hours before being cooled to room temperature. Finally, the solvent and residual thionyl chloride were removed *in vacuo* overnight, and the solid resin was used without further purification (1.31 g recovered).
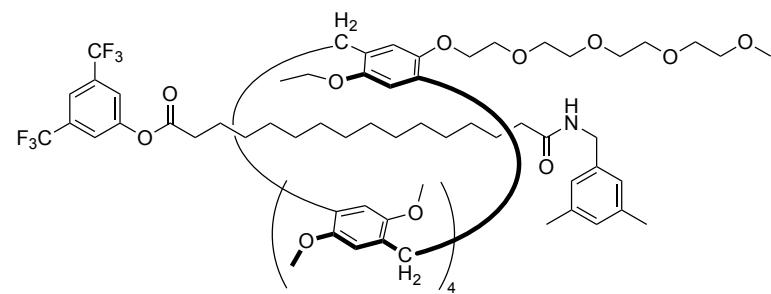
RDP[5]cat@MA$_{fav}$-1

Synthesis of RDP[5]cat@MA$_{fav}$-1: To a solution of **RDP[5]cat@diester** (66 mg, 0.04 mmol) in anhydrous CHCl$_3$ (40 mL) was added 3,5-dimethylbenzylamine (3,5-DMBA) (143 µL, 1 mmol) under an inert atmosphere of argon. The solution was then stirred for 60 hours at 30 °C, after which the reaction was cooled down to 0°C. In a separate round-bottom flask, **SS-COCl** was added to 40 mL of anhydrous CHCl$_3$ and cooled to 0°C. The vessel containing **RDP[5]cat@diester** was then cannulated over the course of two hours into the vessel containing **SS-COCl** under vigorous stirring. The reaction was allowed to stir and warm to room temperature overnight. The following day, the resin was filtered off and the resulting solution was concentrated and purified using flash chromatography over silica (5%–100% EtOAc in

hexanes) to afford **RDP[5]cat@MA$_{fav}$-1** as a light-yellow oil (25.8 mg, 57.5% based on recovered starting material).

^{1}H NMR (500 MHz, CDCl$_3$): δ 7.78 (s, 1H), 7.61 (s, 2H), 6.95 (s, 2H), 6.94 – 6.91 (m, *J* = 3.1 Hz, 3H), 6.91 – 6.84 (m, 8H), 6.12 (s, 1H), 4.39 (qd, *J* = 14.6, 5.5 Hz, 2H), 4.06 – 3.89 (m, 3H), 3.88 – 3.69 (m, 37H), 3.69 – 3.55 (m, 12H), 3.54 – 3.49 (m, 2H), 3.39 (s, 2H), 3.36 (s, 3H), 2.33 (s, 6H), 1.76 – 1.69 (m, 2H), 1.39 (t, *J* = 6.9 Hz, 3H), 0.99 (dt, *J* = 14.1, 6.6 Hz, 4H), 0.94 – 0.87 (m, 2H), 0.77 (s, 4H), 0.62 (s, 2H), 0.40 (s, 2H), 0.28 (s, 2H), 0.08 (d, *J* = 8.8 Hz, 2H), -0.12 (s, 4H).

^{13}C NMR (125 MHz, CDCl$_3$): δ 173.54, 171.27, 151.73, 150.56, 150.49, 150.41, 149.41, 138.87, 138.34, 132.96 (q, *J* = 34.08 Hz), 129.13, 128.47, 128.44, 128.42, 128.39, 128.35, 128.32, 125.80, 124.08, 123.17 (q, *J* = 273.17), 122.59, 122.57, 121.92, 119.36, 115.50, 114.28, 113.91, 113.80, 113.69, 113.66, 72.08, 72.02, 70.90, 70.74, 70.71, 70.61, 70.43, 68.45, 63.49, 59.19, 59.15, 55.94, 55.78, 55.69, 55.61, 55.52, 45.75, 43.56, 36.94, 33.46, 30.84, 30.76, 30.43, 30.39, 30.18, 30.05, 29.21, 29.15, 28.88, 28.68, 28.63, 25.62, 23.55, 21.42, 15.43, 8.65.

HRMS (ESI+): Calcd. for C$_{87}$H$_{112}$F$_6$NO$_{17}^+$ [M+H$^+$] *m/z* = 1556.7834; found 1556.7861.
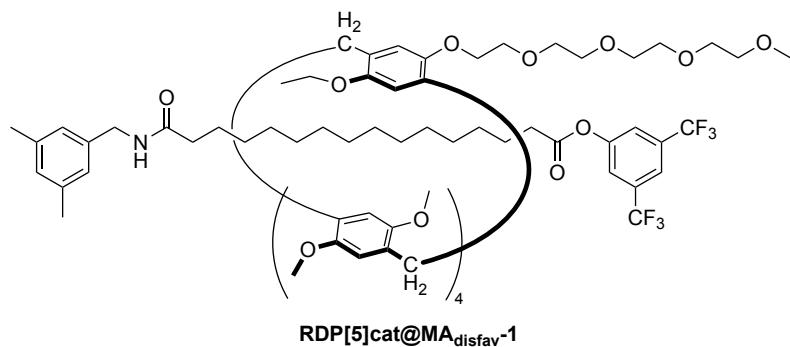
RDP[5]cat@MA$_{disfav}$-1

RDP[5]cat@MA$_{disfav}$-1 was isolated as a byproduct during the synthesis of **RDP[5]cat@MA$_{fav}$-1** as a light brown oil (2.1 mg, 4.5% based on recovered starting material).

^{1}H NMR (500 MHz, CDCl$_3$): δ 7.77 (s, 1H), 7.62 (s, 2H), 6.97 – 6.83 (m, 13H), 5.91 (s, 1H), 4.39 (t, J = 5.5 Hz, 2H), 4.03 – 3.92 (m, 3H), 3.91 – 3.57 (m, 51H), 3.51 (d, *J* = 4.6 Hz, 2H), 3.36 (s, 3H), 2.33 (s, 6H), 1.85 – 1.77 (m, 2H), 1.45 (t, *J* = 7.1 Hz, 3H), 1.03 (s, 2H), 0.97 – 0.82 (m, 6H), 0.64 (s, 2H), 0.54 – 0.42 (m, 2H), 0.19 (s, 4H), -0.02 (s, 2H), -0.09 – -0.20 (m, 2H), -0.47 (br s, 2H).

^{13}C NMR (125 MHz, CDCl$_3$): δ 173.30, 171.26, 151.85, 150.66, 150.60, 150.47, 150.26, 149.58, 138.76, 138.43, 132.92 (q, *J* = 34.75 Hz), 129.20, 129.11, 128.60, 128.56, 128.46, 128.43, 128.41, 128.37, 125.82, 124.13, 123.05 (q, *J* = 273.13 Hz), 122.67, 121.97, 115.30, 114.43,

113.98, 113.93, 113.84, 113.75, 113.70, 113.60, 72.06, 70.88, 70.79, 70.73, 70.66, 70.33, 68.19, 63.75, 59.15, 55.89, 55.83, 55.79, 55.72, 55.62, 43.64, 36.98, 33.29, 32.08, 30.88, 30.72, 30.54, 30.39, 30.22, 30.07, 29.86, 29.82, 29.52, 29.23, 28.87, 28.84, 28.74, 28.53, 25.66, 23.28, 22.85, 21.42, 15.60, 14.27.

HRMS (ESI+): Calcd. for $C_{87}H_{112}F_6NO_{17}^+$ [M+H$^+$] *m/z* = 1556.7834; found 1556.7847.
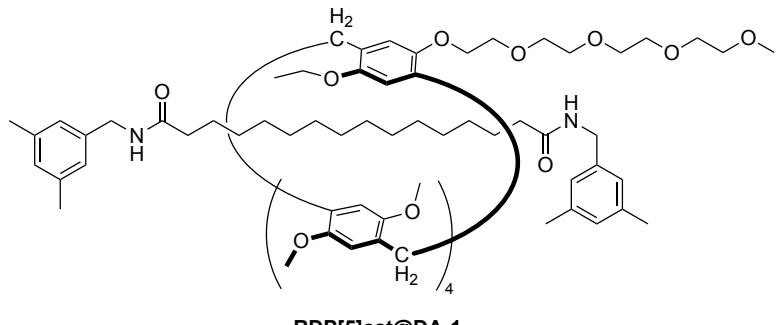
RDP[5]cat@DA-1

RDP[5]cat@DA-1 was isolated as a byproduct during the synthesis of **RDP[5]cat@MA$_{fav}$-1** as a brown solid (15.8 mg, 35% based on recovered starting material).

^{1}H NMR (500 MHz, CDCl$_3$): δ 6.96 (d, *J* = 5.7 Hz, 4H), 6.93 (s, 2H), 6.91 (s, 2H), 6.89 – 6.85 (m, 6H), 6.85 (s, 2H), 6.21 (t, *J* = 5.7 Hz, 1H), 5.98 (t, *J* = 5.8 Hz, 1H), 4.46 – 4.32 (m, 4H), 4.03 – 3.91 (m, 3H), 3.88 – 3.68 (m, 40H), 3.67 – 3.57 (m, 9H), 3.51 (dd, *J* = 5.7, 3.6 Hz, 2H), 3.36 (s, 3H), 2.34 (d, *J* = 2.8 Hz, 12H), 1.77 – 1.70 (m, 2H), 1.44 (t, *J* = 6.9 Hz, 3H), 1.00 – 0.71 (m, 8H), 0.67 – 0.41 (m, 6H), 0.14 (s, 2H), 0.05 – -0.14 (m, 4H), -0.50 – -0.56 (m, 4H).

^{13}C NMR (125 MHz, CDCl$_3$): δ 173.59, 173.38, 150.62, 150.59, 150.53, 150.49, 150.42, 149.51, 139.05, 138.81, 138.41, 138.31, 129.25, 129.19, 129.09, 128.62, 128.53, 128.43, 128.41, 128.40, 128.35, 128.33, 125.81, 115.68, 114.50, 114.12, 114.00, 113.86, 113.83, 113.81, 113.76, 113.68, 72.05, 70.90, 70.78, 70.74, 70.73, 70.65, 70.42, 68.56, 63.76, 59.16, 56.07, 55.95, 55.87, 55.84, 55.74, 55.66, 43.62, 43.50, 36.97, 36.96, 30.95, 30.91, 30.33, 30.24, 30.15, 30.13, 29.24, 28.74, 28.73, 28.48, 28.37, 25.63, 25.56, 21.44, 21.42, 15.58.

HRMS (ESI+): Calcd. for $C_{88}H_{121}N_2O_{16}^+$ [M+H$^+$] *m/z* = 1461.8716; found 1461.8704.
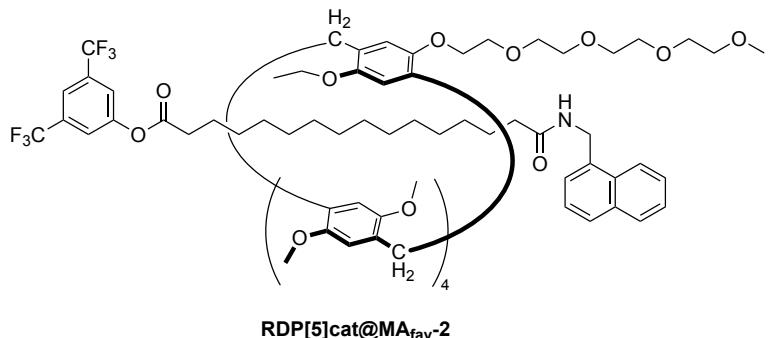
RDP[5]cat@MA_{fav}-2

An analytically pure sample of **RDP[5]cat@MA$_{fav}$-2** (43% yield based on NMR) was obtained from the NMR-scale reactions by (i) removal of the excess 1-naphthalenemethylamine by flushing through a silica plug with ethyl acetate, followed by (ii) purification with preparative TLC (eluent: 60% ethyl acetate in hexane).

^{1}H NMR (800 MHz, CDCl$_3$): δ 8.10 (d, *J* = 8.4 Hz, 1H), 7.90 (d, *J* = 8.1 Hz, 1H), 7.84 (d, *J* = 8.1 Hz, 1H), 7.77 (s, 1H), 7.62 – 7.58 (m, 3H), 7.56 – 7.53 (m, 1H), 7.51 (d, *J* = 6.9 Hz, 1H), 7.47 (t, *J* = 7.5 Hz, 1H), 6.92 (s, 1H), 6.90 (s, 1H), 6.89 – 6.86 (m, 6H), 6.85 (s, 1H), 6.83 (s, 1H), 6.16 (t, *J* = 5.4 Hz, 1H), 4.96 (dd, *J* = 14.5, 5.5 Hz, 1H), 4.89 (dd, *J* = 14.5, 5.3 Hz, 1H), 4.00 – 3.96 (m, 1H), 3.91 (ddt, *J* = 10.8, 7.1, 2.9 Hz, 2H), 3.84 (dd, *J* = 8.7, 6.9 Hz, 1H), 3.79 – 3.68 (m, 36H), 3.66 (s, 3H), 3.64 (dd, *J* = 7.0, 4.3 Hz, 2H), 3.62 – 3.56 (m, 9H), 3.49 (t, *J* = 4.7 Hz, 2H), 3.35 (s, 3H), 1.71 (td, *J* = 7.6, 3.3 Hz, 2H), 1.39 (t, *J* = 6.9 Hz, 3H), 0.99 (q, *J* = 7.4 Hz, 2H), 0.95 – 0.86 (m, 4H), 0.83 – 0.78 (m, 2H), 0.71 (t, *J* = 7.5 Hz, 2H), 0.62 (p, *J* = 7.9 Hz, 2H), 0.37 – 0.29 (m, 4H), 0.16 – 0.09 (m, 2H), -0.11 – -0.16 (m, 4H).

^{13}C NMR (200 MHz, CDCl$_3$): δ 173.34, 171.28, 151.72, 150.57, 150.53, 150.50, 150.40, 149.42, 134.34, 134.07, 132.97 (q, *J* = 34 Hz), 131.69, 129.18, 128.93, 128.67, 128.46, 128.42, 128.40, 128.36, 128.31, 126.74, 126.66, 126.19, 125.55, 123.89, 123.00 (q, *J* = 272 Hz), 122.58, 119.37, 115.47, 114.26, 113.96, 113.79, 113.67, 113.61, 72.03, 70.85, 70.75, 70.70, 70.63, 70.37, 68.37, 63.48, 59.14, 55.95, 55.73, 55.69, 55.61, 55.52, 41.81, 36.88, 33.48, 30.82, 30.75, 30.44, 30.40, 30.10, 30.04, 29.85, 29.26, 29.22, 29.18, 29.14, 28.90, 28.73, 28.65, 28.56, 25.62, 23.58, 15.43.

HRMS (ESI+): Calcd. For $C_{89}H_{110}F_6NO_{17}^+$ [M+H$^+$] *m/z* = 1578.7678; found 1578.7671.
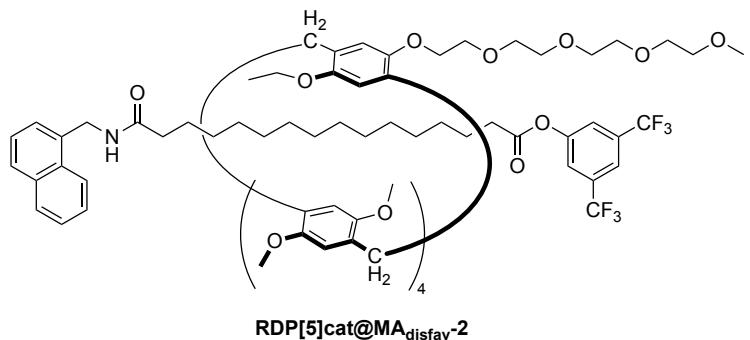
RDP[5]cat@MA$_{disfav}$-2

An analytically pure sample of **RDP[5]cat@MA$_{disfav}$-2** (6% yield based on NMR) was obtained from the NMR-scale reactions by (i) removal of the excess 1-naphthalenemethylamine by flushing through a silica plug with ethyl acetate, followed by (ii) purification with preparative TLC (eluent: 60% ethyl acetate in hexane).

^{1}H NMR (800 MHz, CDCl$_3$): δ 8.09 (d, *J* = 8.3 Hz, 1H), 7.92 (d, *J* = 8.0 Hz, 1H), 7.86 (d, *J* = 8.0 Hz, 1H), 7.79 (s, 1H), 7.63 (s, 2H), 7.59 (ddd, *J* = 8.4, 6.7, 1.4 Hz, 1H), 7.56 (t, *J* = 7.4 Hz, 1H), 7.49 (dt, *J* = 14.9, 7.0 Hz, 2H), 6.94 (d, *J* = 12.6 Hz, 2H), 6.90 (d, *J* = 4.8 Hz, 3H), 6.88 (d, *J* = 4.1 Hz, 2H), 6.86 (d, *J* = 9.0 Hz, 3H), 5.92 (s, 1H), 4.94 (qd, *J* = 14.5, 5.4 Hz, 2H), 4.04 – 3.99 (m, 2H), 3.98 – 3.94 (m, 1H), 3.88 – 3.84 (m, 1H), 3.83 – 3.60 (m, 48H), 3.52 (t, *J* = 4.7 Hz, 2H), 3.37 (s, 3H), 1.84 – 1.80 (m, 2H), 1.46 (t, *J* = 7.0 Hz, 3H), 1.06 – 1.00 (m, 6H), 0.87 – 0.83 (m, 4H), 0.65 (q, *J* = 7.9 Hz, 2H), 0.48 (p, *J* = 8.0 Hz, 2H), 0.21 (td, *J* = 15.3, 7.1 Hz, 4H), -0.00 – -0.06 (m, 2H), -0.12 – -0.19 (m, 2H), -0.48 (q, *J* = 7.4 Hz, 2H).

^{13}C NMR (200 MHz, CDCl$_3$): δ 173.18, 171.25, 150.59, 150.46, 149.55, 134.12, 131.65, 128.96, 128.78, 128.42, 128.35, 126.79, 126.70, 126.21, 125.56, 123.81, 122.67, 115.30, 114.39, 113.92, 113.85, 113.70, 72.05, 70.87, 70.78, 70.72, 70.65, 70.32, 68.18, 63.69, 59.15, 55.85, 55.77, 55.72, 55.61, 41.93, 36.91, 33.27, 30.86, 30.71, 30.54, 30.38, 30.16, 30.08, 29.86, 29.22, 28.84, 28.72, 28.51, 25.65, 23.26, 15.59, 14.27.

HRMS (ESI+): Calcd. For C$_{89}$H$_{110}$F$_6$NO$_{17}$$^+$ [M+H$^+$] *m/z* = 1578.7678; found 1578.7669.
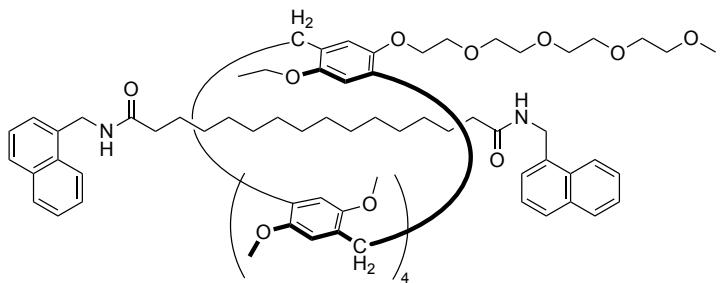
RDP[5]cat@DA-2

An analytically pure sample of **RDP[5]cat@DA-2** (19% yield based on NMR) was obtained from the NMR-scale reactions by (i) removal of the excess 1-naphthalenemethylamine by flushing through a silica plug with ethyl acetate, followed by (ii) purification with preparative TLC (eluent: 60% ethyl acetate in hexane).

^{1}H NMR (800 MHz, CDCl$_3$): δ 8.11 (d, *J* = 8.4 Hz, 1H), 8.08 (d, *J* = 8.3 Hz, 1H), 7.92 – 7.88 (m, 2H), 7.84 (t, *J* = 6.7 Hz, 2H), 7.59 (dddt, *J* = 17.0, 8.5, 6.6, 1.8 Hz, 2H), 7.56 – 7.46 (m, 6H), 6.90 (d, *J* = 1.9 Hz, 1H), 6.88 – 6.80 (m, 9H), 6.26 (d, *J* = 6.1 Hz, 1H), 5.95 (t, *J* = 5.5 Hz, 1H), 4.99 – 4.85 (m, 4H), 3.93 (tdd, *J* = 15.2, 6.5, 1.9 Hz, 2H), 3.86 (ddt, *J* = 10.7, 6.0, 2.8 Hz, 1H), 3.83 (ddd, *J* = 9.0, 6.9, 1.9 Hz, 1H), 3.78 – 3.55 (m, 50H), 3.49 (td, *J* = 4.8, 2.0 Hz, 2H), 3.34 (s, 3H), 1.77 – 1.71 (m, 2H), 1.42 (td, *J* = 7.0, 2.0 Hz, 3H), 0.92 – 0.86 (m, 4H), 0.83 – 0.75 (m, 4H), 0.58 – 0.47 (m, 6H), 0.00 (h, *J* = 7.4 Hz, 4H), -0.58 (qd, *J* = 15.3, 8.0 Hz, 4H).

^{13}C NMR (200 MHz, CDCl$_3$): δ 173.48, 173.23, 150.59, 150.51, 150.38, 149.48, 134.48, 134.18, 134.09, 131.72, 131.67, 129.17, 128.96, 128.93, 128.76, 128.63, 128.51, 128.46, 128.37, 128.34, 128.29, 126.74, 126.68, 126.66, 126.62, 126.20, 125.56, 123.92, 123.81, 115.60, 114.42, 114.15, 113.97, 113.87, 113.80, 113.72, 113.65, 72.03, 70.82, 70.74, 70.70, 70.63, 70.35, 68.44, 63.67, 59.15, 56.06, 55.88, 55.82, 55.76, 55.74, 55.62, 41.91, 41.77, 36.90, 36.87, 30.91, 30.88, 30.28, 30.17, 30.14, 30.09, 29.22, 29.15, 28.76, 28.70, 28.51, 28.26, 25.63, 25.55, 15.57.

HRMS (ESI+): Calcd. For $C_{92}H_{117}N_2O_{16}^+$ [M+H$^+$] *m/z* = 1505.8403; found 1505.8398.
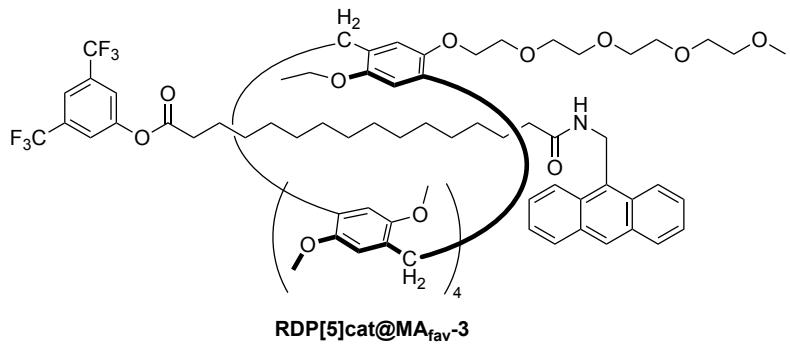
RDP[5]cat@MA_fav-3

An analytically pure sample of **RDP[5]cat@MA_fav-3** (51% yield based on NMR) was obtained from the NMR-scale reactions by (i) removal of the excess anthracene-9-methylamine by flushing through a silica plug with ethyl acetate, followed by (ii) purification with preparative TLC (eluent: 60% ethyl acetate in hexane).

^{1}H NMR (800 MHz, CDCl$_3$): δ 8.49 (s, 1H), 8.36 (d, J = 8.8 Hz, 2H), 8.06 (d, J = 8.4 Hz, 2H), 7.77 (s, 1H), 7.63 – 7.60 (m, 4H), 7.52 (dd, J = 8.4, 6.4 Hz, 2H), 6.92 (s, 1H), 6.87 – 6.85 (m, 7H), 6.83 (s, 1H), 6.80 (s, 1H), 6.11 (t, J = 4.9 Hz, 1H), 5.46 (dd, J = 4.9, 1.6 Hz, 2H), 3.92 – 3.86 (m, 2H), 3.82 (qd, J = 6.8, 2.9 Hz, 2H), 3.78 – 3.62 (m, 39H), 3.54 (td, J = 4.8, 2.6 Hz, 6H), 3.52 – 3.48 (m, 5H), 3.47 (t, J = 4.7 Hz, 2H), 3.33 (s, 3H), 1.79 (dt, J = 9.3, 6.3 Hz, 2H), 1.37 (t, J = 7.0 Hz, 3H), 1.09 – 0.99 (m, 2H), 0.93 (ddd, J = 11.2, 8.3, 4.3 Hz, 2H), 0.88 (t, J = 7.2 Hz, 2H), 0.82 (dd, J = 10.6, 6.2 Hz, 2H), 0.68 (ddt, J = 12.6, 8.7, 5.6 Hz, 2H), 0.52 (p, J = 7.9 Hz, 2H), 0.38 (p, J = 7.9 Hz, 2H), 0.12 (t, J = 7.6 Hz, 2H), 0.04 – -0.02 (m, 2H), -0.02 – -0.10 (m, 2H), -0.35 (qd, J = 9.7, 4.6 Hz, 2H).

^{13}C NMR (200 MHz, CDCl$_3$): δ 173.40, 171.25, 151.77, 150.52, 150.48, 150.45, 150.36, 149.42, 133.00 (q, J = 32 Hz), 131.69, 130.59, 129.39, 129.22, 129.11, 128.46, 128.40, 128.36, 128.29, 128.16, 126.76, 125.44, 124.15, 123.02 (q, J = 270 Hz), 122.58, 119.32, 115.38, 114.28, 113.84, 113.79, 113.74, 113.71, 113.54, 113.49, 72.01, 70.74, 70.70, 70.66, 70.61, 70.30, 68.26, 63.50, 59.12, 55.79, 55.72, 55.64, 55.59, 55.54, 36.72, 36.17, 33.37, 30.82, 30.66, 30.50, 30.40, 29.99, 29.96, 29.85, 29.25, 29.22, 29.18, 29.15, 29.12, 28.91, 28.80, 28.60, 28.56, 25.71, 23.41, 15.41.

HRMS (ESI+): Calcd. For C$_{93}$H$_{112}$F$_6$NO$_{17}^+$ [M+H$^+$] m/z = 1628.7834; found 1628.7833.
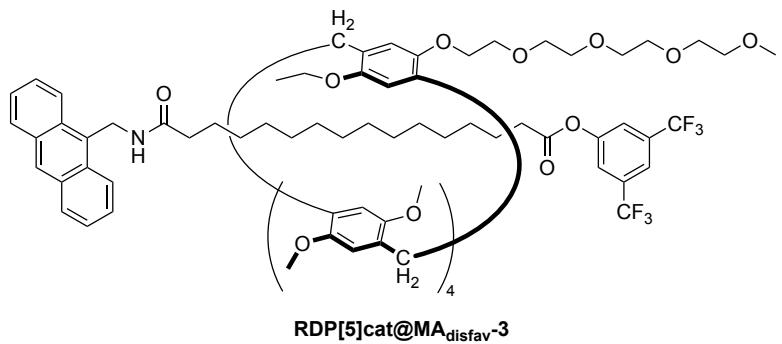
RDP[5]cat@MA_disfav-3

An analytically pure sample of **RDP[5]cat@MA_disfav-3** (3% yield based on NMR) was obtained from the NMR-scale reactions by removal of the excess anthracene-9-methylamine by (i) flushing through a silica plug with ethyl acetate, followed by (ii) purification with preparative TLC (eluent: 60% ethyl acetate in hexane).

^{1}H NMR (800 MHz, CDCl$_3$): δ 8.50 (s, 1H), 8.34 (d, J = 8.9 Hz, 2H), 8.06 (d, J = 8.5 Hz, 2H), 7.77 (s, 1H), 7.64 – 7.57 (m, 4H), 7.52 (t, J = 7.6 Hz, 2H), 6.93 (s, 1H), 6.90 (s, 1H), 6.88 (d, J = 3.8 Hz, 3H), 6.86 – 6.84 (m, 3H), 6.83 (d, J = 7.2 Hz, 2H), 5.80 (s, 1H), 5.46 (d, J = 4.9 Hz, 2H), 4.02 – 3.96 (m, 2H), 3.93 – 3.90 (m, 1H), 3.84 – 3.81 (m, 1H), 3.78 – 3.65 (m, 39H), 3.64 – 3.58 (m, 11H), 3.50 (t, J = 4.8 Hz, 2H), 3.35 (s, 3H), 1.88 (td, J = 7.4, 2.5 Hz, 2H), 1.42 (t, J = 6.9 Hz, 3H), 1.12 (td, J = 7.3, 2.5 Hz, 2H), 1.00 (d, J = 7.2 Hz, 2H), 0.98 – 0.95 (m, 2H), 0.92 – 0.90 (m, 2H), 0.88 (t, J = 7.1 Hz, 2H), 0.77 (s, 2H), 0.74 – 0.70 (m, 2H), 0.37 – 0.33 (m, 2H), -0.26 (d, J = 7.1 Hz, 2H), -0.31 – -0.41 (m, 2H), -0.73 (s, 2H).

^{13}C NMR (200 MHz, CDCl$_3$): δ 173.23, 171.23, 151.91, 150.58, 150.44, 149.51, 132.88 (q, J = 32 Hz), 131.69, 130.55, 129.43, 129.10, 128.97, 128.54, 128.46, 128.26, 126.82, 125.42, 124.01, 123.06 (q, J = 270 Hz), 122.67, 119.20, 115.34, 114.26, 114.04, 113.74, 113.45, 72.04, 70.85, 70.77, 70.71, 70.64, 70.30, 68.21, 63.54, 59.15, 55.87, 55.75, 55.70, 55.63, 55.48, 36.77, 36.23, 33.97, 33.14, 30.86, 30.63, 30.59, 30.37, 30.07, 30.02, 29.85, 29.20, 29.00, 28.86, 28.60, 28.41, 27.36, 27.06, 25.69, 23.07, 22.37, 15.57, 14.27, 13.80.

HRMS (ESI+): Calcd. For $C_{93}H_{112}F_6NO_{17}^+$ [M+H$^+$] m/z = 1628.7834; found 1628.7831.
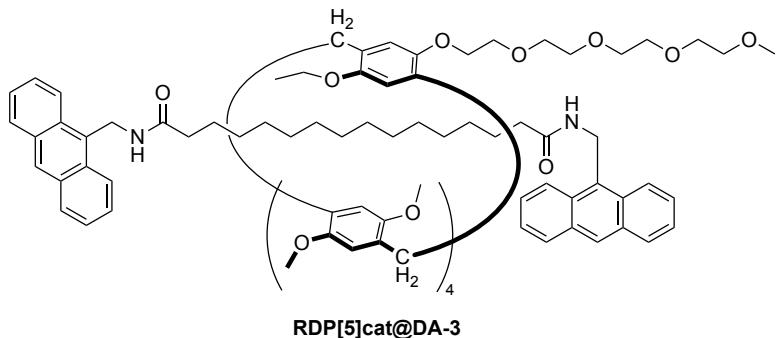
RDP[5]cat@DA-3

An analytically pure sample of **RDP[5]cat@DA-3** (18% yield based on NMR) was obtained from the NMR-scale reactions by (i) removal of the excess anthracene-9-methylamine by flushing through a silica plug with ethyl acetate, followed by (ii) purification with preparative TLC (eluent: 60% ethyl acetate in hexane).

^{1}H NMR (800 MHz, CDCl$_3$): δ 8.49 (d, J = 5.0 Hz, 2H), 8.40 – 8.37 (m, 2H), 8.36 – 8.33 (m, 2H), 8.07 – 8.05 (m, 4H), 7.65 – 7.59 (m, 4H), 7.55 – 7.51 (m, 4H), 6.87 (s, 1H), 6.83 (d, J = 5.2 Hz, 2H), 6.82 – 6.81 (m, 3H), 6.79 (s, 1H), 6.77 (s, 2H), 6.75 (s, 1H), 6.29 (t, J = 4.8 Hz, 1H), 5.88 (t, J = 4.9 Hz, 1H), 5.45 (dt, J = 8.4, 4.6 Hz, 4H), 3.89 – 3.85 (m, 1H), 3.78 (qd, J = 6.7, 3.3 Hz, 2H), 3.74 – 3.66 (m, 14H), 3.65 – 3.49 (m, 32H), 3.47 – 3.44 (m, 4H), 3.42 (ddd, J = 9.7, 5.5, 4.1 Hz, 1H), 3.39 – 3.36 (m, 1H), 3.33 (s, 3H), 3.30 (td, J = 9.9, 3.6 Hz, 1H), 1.75 (td, J = 7.9, 5.7 Hz, 2H), 1.38 (t, J = 6.9 Hz, 3H), 1.05 – 0.97 (m, 2H), 0.74 (q, J = 7.9 Hz, 2H), 0.68 – 0.61 (m, 4H), 0.43 (p, J = 8.2 Hz, 2H), 0.32 (h, J = 7.2 Hz, 2H), 0.08 (dtd, J = 9.8, 7.4, 3.0 Hz, 2H), 0.02 (ddd, J = 16.2, 7.1, 3.0 Hz, 2H), -0.13 (p, J = 8.4 Hz, 2H), -0.53 (ddt, J = 15.0, 9.6, 4.0 Hz, 2H), -0.70 (q, J = 9.4 Hz, 2H).

^{13}C NMR (200 MHz, CDCl$_3$): δ 173.64, 173.34, 150.54, 150.45, 150.42, 150.37, 150.35, 149.42, 131.70, 130.63, 130.57, 129.44, 129.39, 129.07, 129.05, 128.42, 128.34, 128.27, 128.24, 128.23, 128.20, 128.16, 128.10, 126.79, 126.73, 125.46, 125.43, 124.21, 124.02, 115.59, 114.29, 114.05, 113.94, 113.83, 113.76, 113.70, 113.64, 113.52, 72.01, 70.66, 70.64, 70.62, 70.60, 70.54, 70.23, 68.37, 63.52, 59.13, 55.93, 55.76, 55.69, 55.62, 55.56, 55.50, 36.73, 36.67, 36.22, 36.17, 30.83, 30.19, 30.17, 30.00, 29.95, 29.24, 29.20, 29.19, 29.08, 28.83, 28.59, 28.05, 25.62, 25.61, 15.53.

HRMS (ESI+): Calcd. For C$_{100}$H$_{121}$N$_2$O$_{16}^+$ [M+H$^+$] m/z = 1605.8716; found 1605.8720.

III. Kinetic Measurements and Analysis

For the kinetic experiments with quantitative ^{1}H NMR spectroscopy, we dissolved **RDP[5]cat@diester** (1 mM), 1,2,4,5-tetrabromobenzene (TBB, 1 mM, the internal standard), and 3,5-dimethylbenzylamine (25 mM), 1-naphthalenemethanamine (25 mM), or 9-anthracenemethanamine (25 mM) in anhydrous chloroform (1.0 mL) in a dry NMR tube. For all the kinetic experiments, the CDCl$_3$ solvent was dried using activated 3 Angstrom molecular sieves for 24 hours before use and stored over 3 Angstrom molecular sieves and K$_2$CO$_3$. After drying, the CDCl$_3$ was added via a syringe filter to the NMR tubes to remove any potential residual solids. To prevent solvent loss, all NMR tubes were sealed and checked for solvent level continuously throughout the experiment duration. The NMR tube was then heated to 30 ºC and the temperature was maintained at this temperature throughout the experiment, and reaction progress was then monitored by quantitative ^{1}H NMR spectroscopy. The chemical shifts of all the amide protons for the rotaxane products **RDP[5]cat@MA$_{fav}$-1**, **RDP[5]cat@MA$_{disfav}$-1**, and **RDP[5]cat@DA-1** (Figure 3b, S1), **RDP[5]cat@MA$_{fav}$-2**, **RDP[5]cat@MA$_{disfav}$-2**, and **RDP[5]cat@DA-2** (Figure S2), and **RDP[5]cat@MA$_{fav}$-3**, **RDP[5]cat@MA$_{disfav}$-3**, and **RDP[5]cat@DA-3** (Figure S4), were clearly distinct. Therefore, the integrals of these amide ^{1}H NMR resonances, relative to the resonance of the internal TBB standard, were used to calculate the concentrations of all possible rotaxane products in the NMR solutions over time. To maximize signal recovery and obtain more accurate integrals a 5.00 second d_1 delay was used for each time point. Finally, the rate constants (k_1, k_2, k_1', k_2') were determined by fitting the kinetic rate data obtained by quantitative ^{1}H NMR spectroscopy based on the kinetic model shown in Figure 3a with DynaFit. All reactions were treated as second order, using the standard differential equations implemented in the DynaFit software for this situation. Since the maximum concentrations of the minor products (**RDP[5]cat@MA$_{disfav}$**) were about an order of magnitude lower than the maximum concentrations of the major and difunctionalized products (**RDP[5]cat@MA$_{fav}$** and **RDP[5]cat@DA**), we increased the weights of [**RDP[5]cat@MA$_{disfav}$**](t) by a factor of 10 in all the fits to ensure that all the fitted curves accurately reproduced the experimental time-concentration curves.
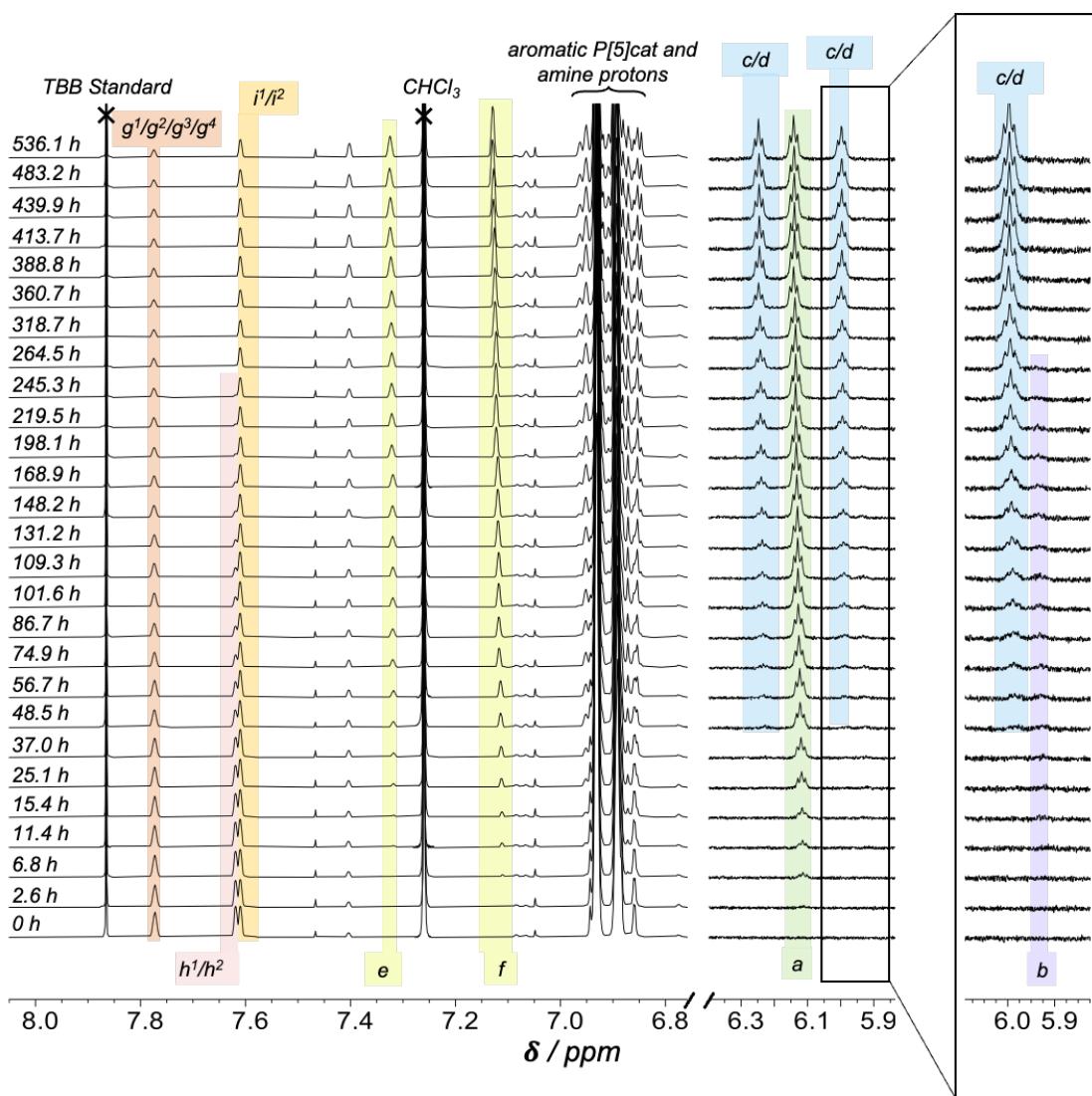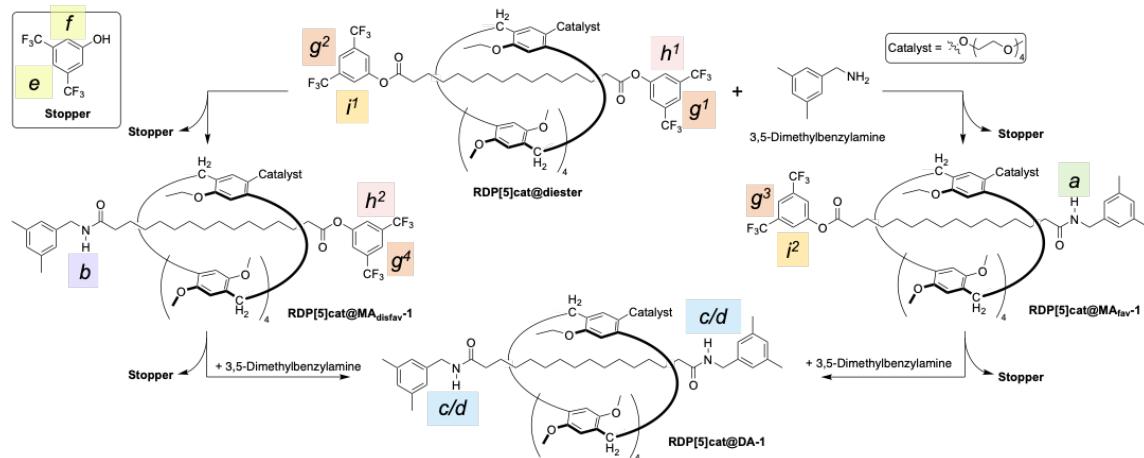
Figure S1. Stacked ¹H-NMR spectra (500 MHz, CDCl₃, 298K) for all recorded time points of the reaction with **RDP[5]cat@diester** and 3,5-dimethylbenzylamine. 256 Scans were recorded for each time point. Peaks for all rotaxane signals were assigned using the ¹H NMR spectra of the purified compounds (see Figures 3b, S15, S18, and S20).
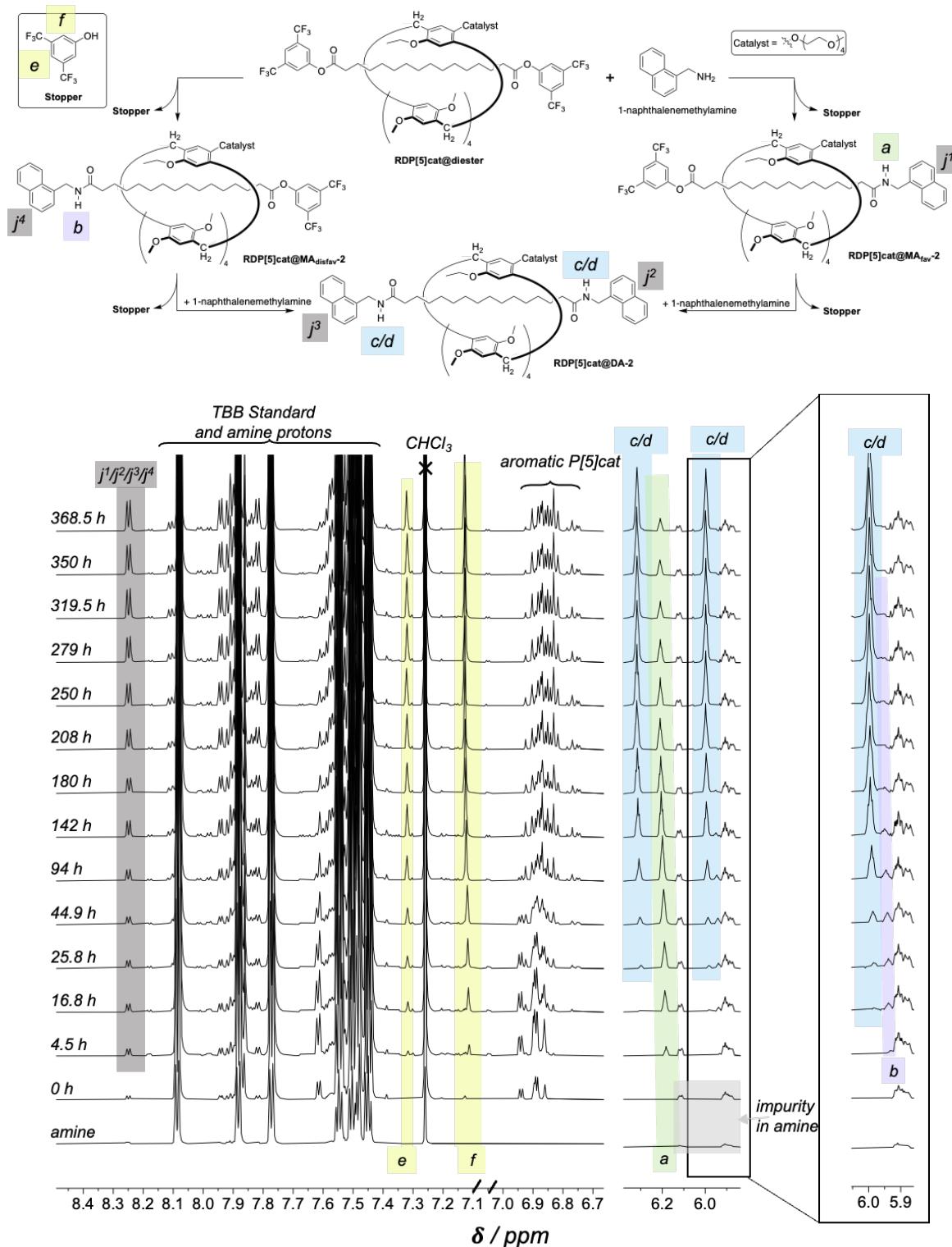
Figure S2. Stacked ^{1}H-NMR spectra (800 MHz, CDCl$_3$, 298K, recorded with a high-sensitivity cryoprobe) for all recorded time points of the reaction with **RDP[5]cat@diester** and 1-naphthalenemethanamine. 128 Scans were recorded for each time point. Peaks for all rotaxane signals were assigned using the ^{1}H NMR spectra of the purified compounds (see Figures S22, S24, and S26).
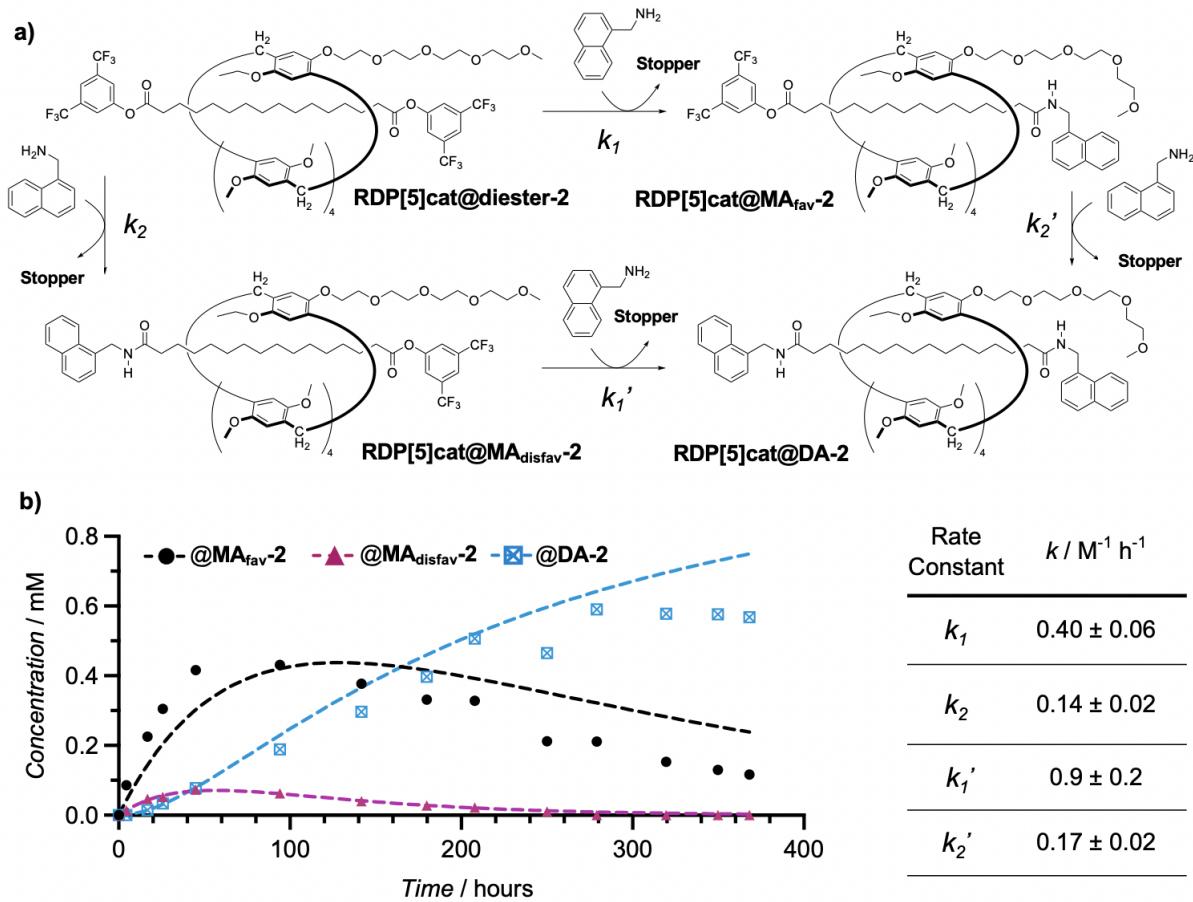
Figure S3. **a)** Complete kinetic pathway for through-space controlled stopper exchange with 1-naphthalenemethanamine as the nucleophile. Stopper = 3,5-bis(trifluoromethyl)phenol. Rate constants k_1 and k_1' denote substitution at the activated ester (proximal to the catalytic side-chain), while k_2 and k_2' denote substitution at the ester distal to the catalyst. **b)** Concentrations of all three reaction products measured by quantitative ^{1}H NMR spectroscopy with the TBB internal standard over the course of the reaction. Kinetics fits are shown as dashed lines. The kinetic fits were obtained using the Dynafit software package as detailed in the supplementary information. Derived rate constants with error bars (standard errors obtained from the Dynafit kinetic fits) are shown in the table on the right.

Figure S4. Stacked ^{1}H-NMR spectra (800 MHz, CDCl$_3$, 298K, recorded with a high-sensitivity cryoprobe) for all recorded time points of the reaction with **RDP[5]cat@diester** and anthracene-9-methanamine. 128 Scans were recorded for each time point. Peaks for all rotaxane signals were assigned using the ^{1}H NMR spectra of the purified compounds (see Figures S28, S30, and S32).
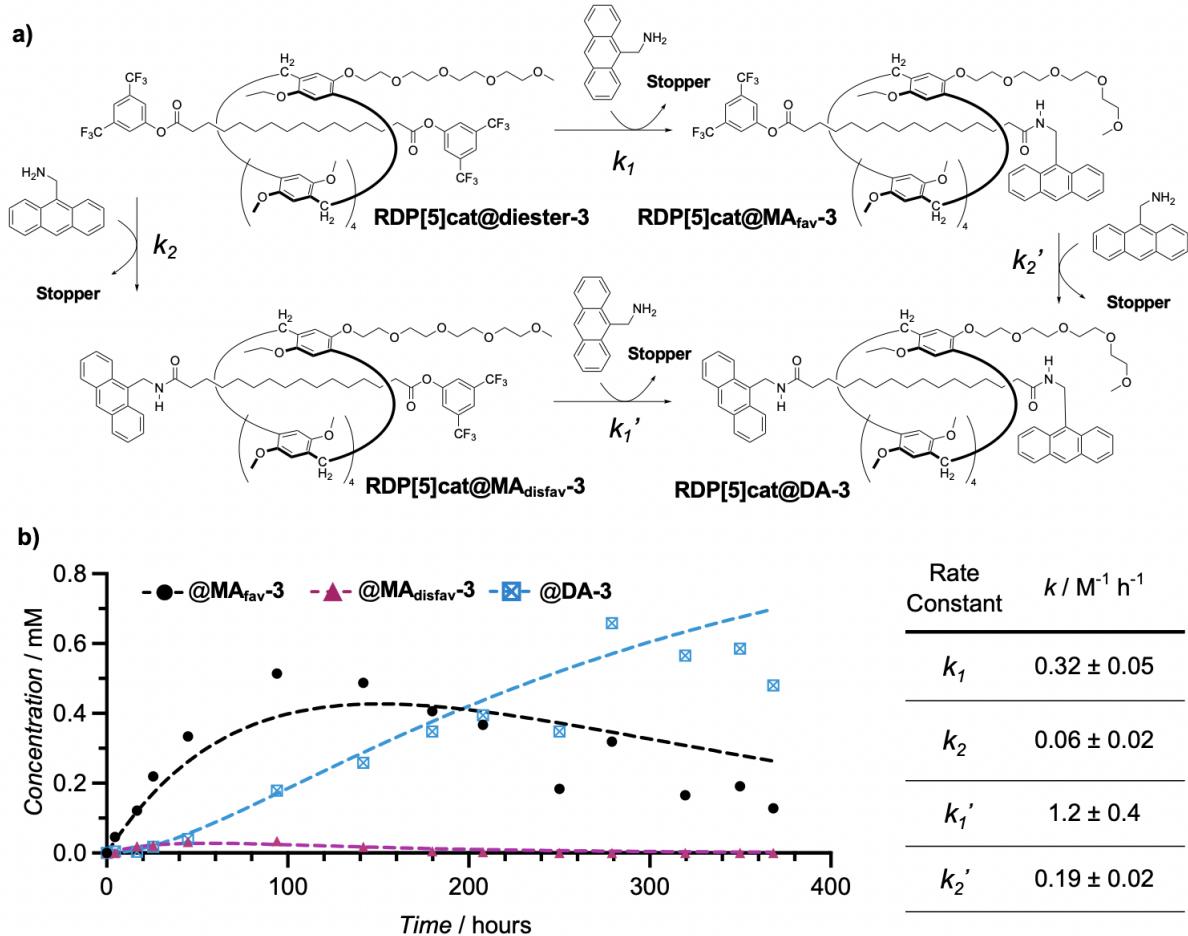
Figure S5. **a)** Complete kinetic pathway for through-space controlled stopper exchange with anthracene-9-methanamine as the nucleophile. Stopper = 3,5-bis(trifluoromethyl)phenol. Rate constants k_1 and $k_{1'}$ denote substitution at the activated ester (proximal to the catalytic side-chain), while k_2 and $k_{2'}$ denote substitution at the ester distal to the catalyst. **b)** Concentrations of all three reaction products measured by quantitative ^{1}H NMR spectroscopy with the TBB internal standard over the course of the reaction. Kinetics fits are shown as dashed lines. The kinetic fits were obtained using the Dynafit software package as detailed in the supplementary information. Derived rate constants with error bars (standard errors obtained from the Dynafit kinetic fits) are shown in the table on the right.

IV. Computational Details

Quantum Mechanical Calculations. We first obtained initial models for all structures by minimization and a conformational search (1,000 steps) at the molecular mechanics level with MacroModel (Schrödinger, Inc.) in vacuum with the OPLS4[3,4] force field. The minimized molecular mechanics models were then reoptimized at the DFT level at the B3LYP-MM/LACVP* level [5,6,7,8,10] of theory with the Jaguar software package (Schrödinger, Inc.). Next, the energies of the structures were refined by performing single-point calculations at the B3LYP-MM/aug-cc-pVDZ//B3LYP-MM/LACVP* level, and by adding zero-point energies, as well as harmonic Gibbs free energy corrections (both calculated at the B3LYP-MM/LACVP* level) to the B3LYP-MM/aug-cc-pVDZ//B3LYP-MM/LACVP* energies. Ultrafine pseudospectral grids and cutoffs (set with the iacc = 1 keyword in Jaguar) were used for all calculations with the larger aug-cc-pVDZ basis set to ensure proper convergence of the SCF. Finally, ring-to-axle binding free energies were calculated by subtracting the free energies of the ring and the axle from the free energy of the corresponding pseudorotaxane complexes shown in Figure 6 (which served as computationally accessible models for the corresponding rotaxanes).

To investigate the dominant attractive noncovalent interactions, which stabilize the conformation with the ring positioned over the active ester stopper for the favored rotaxane product **RDP[5]cat@MA$_{fav}$-1**, non-covalent interactions (NCI) calculations were also performed using a truncated version (see Figure 2b) of the rotaxane **RDP[5]cat@MA$_{fav}$-1**, with the ring positioned over the active ester stopper. The noncovalent interactions were obtained from the DFT-calculated electron density with the NCI method[9] at the B3LYP-MM/LACVP* level[10] of theory.

DFT-Optimized Coordinates (Lowest Free Energy Conformation Found for Each Structure)
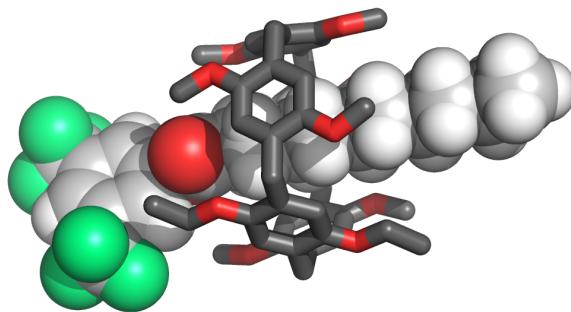
RDP[5]cat@MA$_{fav}$-1-Ring-over-Ester-Model

SCF energy (B3LYP-MM/LACVP*): -4063.722708 hartrees
Zero-point energy (B3LYP-MM/LACVP*): 848.082 kcal/mol
Gibbs free energy correction (B3LYP-MM/LACVP*): -66.813 kcal/mol

Angstroms

Atom	x	y	z
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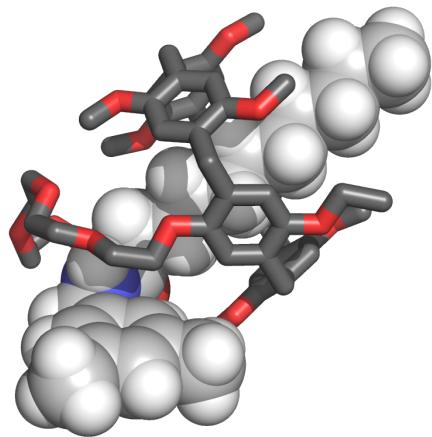
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SCF energy (B3LYP-MM/aug-cc-pVDZ//B3LYP-MM/LACVP*): -4064.289556 hartrees
Zero-point energy (B3LYP-MM/LACVP*): 1042.404 kcal/mol
Gibbs free energy correction (B3LYP-MM/LACVP*): -72.977 kcal/mol

	Angstroms		
Atom	x	y	z
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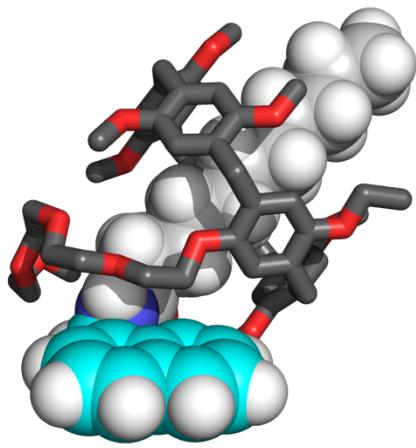
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Zero-point energy (B3LYP-MM/LACVP*): 1037.39 kcal/mol
Gibbs free energy correction (B3LYP-MM/LACVP*): -72.028 kcal/mol

	Angstroms		
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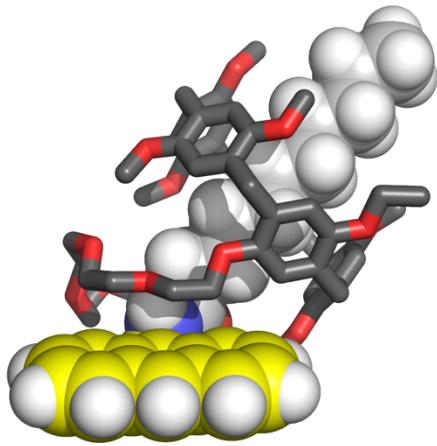
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SCF energy (B3LYP-MM/aug-cc-pVDZ//B3LYP-MM/LACVP*): -4292.962381 hartrees
Zero-point energy (B3LYP-MM/LACVP*): 1066.702 kcal/mol
Gibbs free energy correction (B3LYP-MM/LACVP*): -73.489 kcal/mol

		Angstroms	
Atom	x	y	z
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C9	-1.3841368450	-1.9497317890	-0.3497479249
C10	-2.4177761678	-2.6553063179	0.5381009400
C11	-3.8053634645	-1.9981263786	0.5394180578
C12	-4.8110315192	-2.7679778373	1.4040932653
C13	-6.1564838659	-2.0563580848	1.5729105765
C14	-7.1329817374	-2.8758329182	2.4246849511
C15	-8.3948518254	-2.0988401278	2.8138654274
C16	-9.3533558111	-2.9605114715	3.6552451679
C17	-10.5610414812	-2.1817066108	4.1489280664
O19	-10.4625913135	-1.1862889605	4.8782593153
H57	0.7298685485	-1.8927474885	-2.2470106221
H58	1.1886302585	-0.8714725125	-0.8768590998
H59	0.3596295316	-2.6511272751	0.7179726334
H60	-0.0985180927	-3.6634594581	-0.6418371294
H61	-1.7480515856	-1.9173164581	-1.3888685117
H62	-1.2853918329	-0.8990968143	-0.0348396942
H63	-2.0475938262	-2.6873980217	1.5717417565
H64	-2.5098823807	-3.7062576798	0.2252435525
H65	-4.1870672312	-1.9241755660	-0.4916272240
H66	-3.7160701816	-0.9689688318	0.9135327085
H67	-4.3727798010	-2.9310507437	2.3957523224
H68	-4.9727463405	-3.7641045726	0.9725329308
H69	-6.6044290596	-1.8550179461	0.5925013142
H70	-5.9917536796	-1.0807006978	2.0450722789
H71	-6.6239527669	-3.2025425167	3.3423376319
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H74	-8.1199294000	-1.2033476996	3.3825182638

H75	-9.6677358163	-3.8422321997	3.0836969253
H76	-8.8189201822	-3.3213775597	4.5440772232
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C86	-8.1222750420	-4.5206140752	-2.2393079812
C87	-7.3320093871	-0.7779061450	-2.1441150382
C88	-7.2887064533	-2.1405451031	-2.4422010862
C89	-8.1954796531	-3.0439277943	-1.8823799624
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C91	-9.2266570567	-1.1723628769	-0.7224581322
C92	-8.3064614407	-0.2732393630	-1.2666234853
C93	-5.2232113158	1.6641094302	1.3255264345
C94	-6.0597695424	1.5210440942	0.2174600432
C95	-7.4513747963	1.4625059644	0.3504275737
C96	-7.9961756821	1.5949144694	1.6372846383
C97	-7.1553976591	1.7335575185	2.7465452881
C98	-5.8490214911	-5.3486673404	-1.4370647285
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C109	-4.9523623624	-5.2203602395	4.6125313099
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C111	-4.4509280294	0.4495344805	4.3476912270
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C113	-2.8287985417	-1.3683363370	4.4476968511
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O123	-11.9584857209	-4.7411535195	1.5263643744
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C125	-12.8109887235	-5.8574997840	1.7629508734
C126	-12.6854999335	-6.3122424313	3.2017895018
O127	-11.3764390682	-6.8144317478	3.4110027840
C128	-11.0884823173	-7.2191018146	4.7394534342
C129	-10.8757178592	-6.0726347186	5.7212895637
O130	-12.1406383159	-5.5980107002	6.1743827317
C131	-12.0993935936	-4.3755378199	6.8981329687
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C138	-8.9513151457	-7.7722460017	1.6752763088
O139	-5.8424804163	-4.8171305827	5.5851580567
C140	-7.0523788333	-5.5446202318	5.7106211162
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O147	-3.8480829999	1.7125467878	1.2377398185
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H220         -13.4828068773          -2.4159918755           4.9390208007
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C226         -13.3315424771           0.6342103228          -0.4072461975
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H231         -15.0344017877          -0.2985379987          -1.3051123114
H232         -13.1595094455           1.3123283419          -1.2386296236
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C193         -15.0043708920          -2.9671667790           2.7986819164
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C196         -17.1209494875          -4.8652409836           2.5651680351
C197         -16.9069573020          -3.9707859076           1.5530146623
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H225         -16.4593536427          -5.5547733610           4.5194578954
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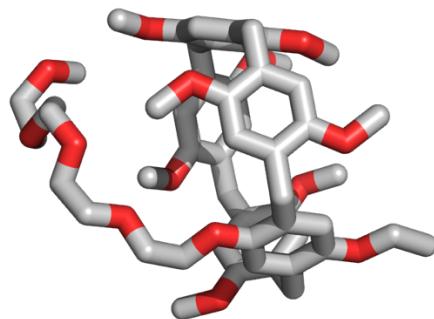
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SCF energy (B3LYP-MM/aug-cc-pVDZ//B3LYP-MM/LACVP*): -3152.083479 hartrees
Zero-point energy (B3LYP-MM/LACVP*): 725.914 kcal/mol
Gibbs free energy correction (B3LYP-MM/LACVP*): -57.52 kcal/mol

| | Angstroms | | |
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C86	-7.2600810619	-4.6378501656	-3.2447221412
C87	-6.4095417310	-0.9272512098	-2.8744283847
C88	-6.3517168554	-2.2787770236	-3.2239088803
C89	-7.3762769956	-3.1658729506	-2.8874263213
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C91	-8.5514679421	-1.3103103376	-1.8546992837
C92	-7.5271264494	-0.4230934715	-2.1944048116
C93	-5.7482618172	1.2385418634	1.5586773230
C94	-6.0232262274	1.1649779950	0.1915853241
C95	-7.3356736660	1.1925870793	-0.2874531009
C96	-8.3812491743	1.3059636636	0.6398075030
C97	-8.1049812985	1.3781887309	2.0079274167
C98	-5.1243994312	-5.5210482181	-2.1752429622
C99	-6.5240878345	-5.4197749083	-2.1708013542
C100	-7.2302981239	-6.0139528377	-1.1233827820
C101	-6.5682893218	-6.6905866776	-0.0961564069
C102	-5.1656764254	-6.7700157261	-0.0844733292
C103	-4.4618814964	-6.1855473731	-1.1394296061
C104	-4.6204164016	-4.9089313464	4.6109361810
C105	-3.7039966042	-4.6536937489	3.5852922173
C106	-3.6275461553	-5.4695525837	2.4569612424
C107	-4.4702957546	-6.5870497090	2.3320406787
C108	-5.3685757281	-6.8533991270	3.3648335437
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C111	-6.0476218212	-0.0188851564	4.4966521077
C112	-4.7273283858	-0.2270914776	4.8969056457
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C118        -6.5090748327        1.3353517230        3.9817561186
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O137        -7.2129150644       -7.3110178943        0.9403108891
C138        -8.6231188339       -7.1858384063        1.0235331947
O139        -6.3692854107       -6.2301217654        5.5068850337
C140        -7.2024205907       -7.3728647013        5.4323011496
O141        -2.7534929853       -5.2567429474        1.4173085197
C142        -2.0205993141       -4.0484507908        1.4064463643
O143        -2.9787616439       -1.7418616403        5.6913188781
C144        -2.0732680796       -0.6580179621        5.7449792482
O145        -8.2258308144       -0.8486654523        4.1561478459
C146        -9.0426921464       -1.9457256566        3.7974254331
O147        -4.4791598520        1.2303792864        2.0853273063
C148        -3.4017295480        0.9480783385        1.2157759563
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H152        -3.4073388646       -7.6359806807        0.7813061670
H153        -5.4068333151       -4.3617281273        6.5296771161
H154        -3.7329332034       -3.8795308151        6.2772765291
H155        -8.6048334929        1.4263292273       -2.0017943038
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H161        -5.2224185702        1.0689921480       -0.5335476656
H162        -8.9092993611        1.4363544572        2.7316060141
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H165        -3.0586115783       -3.7886868800        3.6883661909
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H168        -7.1657861158       -3.2104412341        4.9825692482
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H177           -3.9046703291           1.5144729434          -4.6783206945
H178           -3.0335208729           1.1212598952          -3.1832891671
H179           -2.5030477528           0.4218795532          -4.7289768321
H180          -12.4979431074          -6.6091269389          -0.2265563139
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H182          -13.4745326910          -6.5745834359           2.1366866708
H183          -12.4025371863          -5.2053869188           2.4905902055
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H192           -8.9097448582          -3.9231412462           6.6796619058
H193           -8.9789230176          -4.2655471176           8.4287334619
H194           -7.8429107828          -5.1604077248           7.3706282292
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H203           -7.8632442039          -7.3270496878           6.2992553488
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H207           -1.9186159395          -0.2038250715           4.7558925498
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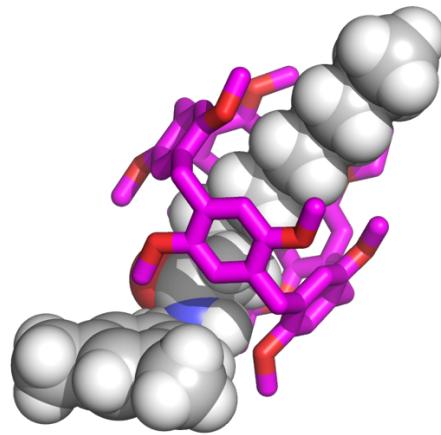
RDP[5]cat@MA_{disfav}-1-Model

SCF energy (B3LYP-MM/aug-cc-pVDZ//B3LYP-MM/LACVP*): -3488.190587 hartrees
Zero-point energy (B3LYP-MM/LACVP*): 903.453 kcal/mol
Gibbs free energy correction (B3LYP-MM/LACVP*): -65.64 kcal/mol

	Angstroms		
Atom	x	y	z
C1	4.7583113145	1.1637059928	0.9133578579
C2	3.3122797266	1.5900253652	0.6977221763
C3	2.4762443379	0.5627863932	-0.0623685070
C4	1.0523779379	1.0455919230	-0.3511838451
C5	0.1556692547	1.2510744407	0.8762602594
C6	-1.2962623697	1.4829030494	0.4390492122
C7	-2.2850209303	1.7675281830	1.5759638115
C8	-3.7191193113	1.9438341635	1.0565883353
C9	-4.7683894991	2.2367129384	2.1365409717
C10	-6.1892302335	2.3723535947	1.5693947477
C11	-7.2520487522	2.6592099594	2.6350210200
O12	5.1994107202	0.0499911795	0.6228029619
C13	6.9233583441	1.9077626969	1.8742958403
H27	3.3066954813	2.5495117123	0.1660260999
H28	2.8701132703	1.7933499282	1.6815387240
H29	2.4429669692	-0.3779574678	0.4977724683
H30	2.9690001501	0.3359658149	-1.0140459487
H31	0.5761612406	0.3115367664	-1.0040621972
H32	1.0958607946	1.9792587375	-0.9239813239
H33	0.5027652238	2.1041439455	1.4740412733
H34	0.2040192424	0.3705224054	1.5275284507
H35	-1.6392245750	0.5957435011	-0.1126182532
H36	-1.3226317745	2.3167006597	-0.2807538151
H37	-1.9731367690	2.6711010258	2.1213511812
H38	-2.2514463572	0.9503431205	2.3071471343

H39	-4.0131936325	1.0334838477	0.5111771083
H40	-3.7377044287	2.7537445086	0.3102747668
H41	-4.5003757943	3.1615508938	2.6703732130
H42	-4.7529097866	1.4358364289	2.8910015794
H43	-6.4508589144	1.4490555849	1.0323050342
H44	-6.2014786401	3.1729467804	0.8156061812
H45	-7.0397230177	3.5956573548	3.1661215414
H46	-7.2908960372	1.8572276503	3.3829727336
C50	-0.2963335494	-3.4281177350	-0.3856047462
C51	0.3245669114	-0.9021783468	4.8941210568
C52	2.1116926312	5.5490662639	-1.8281633995
C53	0.9443259580	0.4881973858	-4.5845469113
C54	2.8282212049	3.2989893257	-2.7876869019
C55	2.5394379324	2.1109674452	-3.4656720384
C56	1.2478894963	1.8174934296	-3.9089683463
C57	0.2348767728	2.7586639324	-3.6657860342
C58	0.5280431981	3.9569516318	-3.0089936761
C59	1.8175381282	4.2468950173	-2.5574756020
C60	3.3949243152	5.0795833315	1.7478274946
C61	3.3523859310	5.3047566780	0.3684752367
C62	2.1455151058	5.3868261154	-0.3187772888
C63	0.9563468959	5.2787635453	0.4276550979
C64	1.0008824706	5.0379055604	1.8010434241
C65	1.6253813228	-1.3766936840	-2.9895127390
C66	0.6142222019	-0.5914671970	-3.5664132013
C67	-0.6970143718	-0.7683256080	-3.1167212431
C68	-1.0021132901	-1.6752502610	-2.0975410076
C69	0.0091186873	-2.4590390003	-1.5180156900
C70	1.3147743523	-2.3034002463	-1.9913490244
C71	0.1442836095	-1.5871649905	3.5448479454
C72	1.2478821479	-2.1059976516	2.8583640001
C73	1.1152823307	-2.7064218626	1.6056713098
C74	-0.1467739514	-2.8005875345	0.9922365775
C75	-1.2508489601	-2.2968960720	1.6829269481
C76	-1.1174572887	-1.6986012123	2.9418488917
C77	0.3754256443	2.9103355833	4.5062649839
C78	1.7357909276	3.1763984395	4.2858676776
C79	2.6346729995	2.1021975789	4.3473320946
C80	2.1943626906	0.7963391382	4.5877841625
C81	0.8225701153	0.5281028681	4.7508497746
C82	-0.0661917078	1.6013133855	4.7270944389
O83	4.0786633618	3.6169179040	-2.3117018471
O84	-1.0264662830	2.4294383708	-4.1087056339
C85	2.2258057065	4.5859173794	3.9762925715
C86	2.2184356336	4.9128837762	2.4863738151
C87	-2.0891701351	3.3367640507	-3.8534867688
C88	5.1425301551	2.6934165972	-2.5284220287
C89	-3.3599535990	2.7276613721	-4.4205493371
C90	6.3999619073	3.2947351663	-1.9251955249

O91	2.9035004383	-1.1617623334	-3.4533105344
C92	3.9679862898	-1.8819288442	-2.8511457736
O93	-2.2723915287	-1.8516941934	-1.5908299025
C94	-3.3316357587	-1.1350295023	-2.1940647141
O95	-2.1836806610	-1.1784764378	3.6492805321
C96	-3.4886460269	-1.5110782357	3.2129731199
O97	2.1684643437	-3.2496648490	0.9112244785
C98	3.4762122397	-3.1212532903	1.4501038167
O99	3.0248001587	-0.2889968485	4.6913307394
C100	4.4161003608	-0.1194952505	4.4615056718
O101	-0.4798912423	3.9940607171	4.4711986446
C102	-1.7748775770	3.8346644300	5.0267473147
O103	4.6066712404	4.9581467088	2.4233619161
C104	5.7010663293	5.7220930669	1.9264721246
O105	-0.2080492589	5.4293279819	-0.2802118047
C106	-1.4291746021	5.4444348376	0.4374458592
H107	-1.3175105941	-3.8029188623	-0.4974418031
H108	0.3816917960	-4.2842358369	-0.4624507333
H109	-0.6291071556	-0.9018317691	5.4274431879
H110	1.0408020243	-1.4746733118	5.4917777115
H111	1.3448193108	6.2819221168	-2.0974718289
H112	3.0772810471	5.9425626239	-2.1618508146
H113	0.0999182417	0.6129963264	-5.2679972539
H114	1.8109106591	0.1799643291	-5.1762045321
H115	3.3098971492	1.3697168092	-3.6367010799
H116	-0.2490758360	4.6847656573	-2.8139298040
H117	4.2709057763	5.3826173181	-0.2015488956
H118	0.0890776235	4.9279588753	2.3748271065
H119	-1.4658635494	-0.1398204637	-3.5493746892
H120	2.0920578254	-2.8954035592	-1.5262786315
H121	2.2195799914	-2.0133075858	3.3242687835
H122	-2.2204214038	-2.3630775640	1.2024950868
H123	3.6916512842	2.3029538193	4.2054461972
H124	-1.1224398182	1.3900205166	4.8514975876
H125	3.2403502719	4.7096085239	4.3628275969
H126	1.5845932089	5.3036841541	4.4991796363
H127	-1.8802100277	4.3072467727	-4.3280404757
H128	-2.1856526238	3.5089163154	-2.7712268139
H129	5.2707297853	2.5202793014	-3.6069483083
H130	4.9092931806	1.7296387496	-2.0562406552
H131	-4.2077096359	3.4037377917	-4.2629086326
H132	-3.5835979247	1.7732396442	-3.9325307865
H133	6.2784479942	3.4229256812	-0.8452420868
H134	7.2538160095	2.6300614320	-2.0974981188
H135	6.6189172067	4.2672611663	-2.3792946408
H136	4.0757007079	-1.6329721546	-1.7880179538
H137	3.8353646388	-2.9665970115	-2.9643013521
H138	4.8716622373	-1.5775628520	-3.3847943520
H139	-3.2097117022	-0.0500680189	-2.0722428838

H140	−3.4196525319	−1.3667291856	−3.2646823102
H141	−4.2432440940	−1.4530176028	−1.6818470890
H142	−3.6216551264	−2.5990988192	3.1382080670
H143	−4.1710220584	−1.1130653805	3.9680658564
H144	−3.7260176338	−1.0562135455	2.2421525121
H145	3.5483780966	−3.5838588311	2.4438506041
H146	4.1331071757	−3.6573717710	0.7612430611
H147	3.7949889871	−2.0734389643	1.5004160230
H148	4.8636410947	−1.1028912081	4.6193168797
H149	4.6190658769	0.2043225950	3.4363743444
H150	4.8595272101	0.5929541598	5.1635836558
H151	−2.2142441455	4.8347971433	5.0592599507
H152	−2.4090702646	3.1848443258	4.4108085869
H153	−1.7242974336	3.4250685223	6.0444113638
H154	5.3984383580	6.7581656310	1.7333946376
H155	6.4678875788	5.7008438950	2.7043377118
H156	6.1177872134	5.2922749204	1.0067943554
H157	−2.2104939530	5.6296721850	−0.3031325931
H158	−1.6206254676	4.4860545581	0.9326850343
H159	−1.4431048138	6.2465880881	1.1876741450
H160	−8.2506949128	2.7480585497	2.1911692666
H161	−3.2535027000	2.5482212559	−5.4951314204
H162	5.0957155748	2.9881829413	1.7945104587
N163	5.5481630870	2.1452019083	1.4581398240
H163	7.5580428493	2.7149202651	1.4810175719
H164	7.2356449686	0.9792825890	1.3914635489
C150	7.4107883398	1.6008458344	6.1518305421
C151	7.9615087778	0.6136541459	5.3262702352
C152	7.7907541025	0.7273089592	3.9403790875
C153	7.0963032929	1.8043767315	3.3820439812
C154	6.5615756955	2.7805245689	4.2321753202
C155	6.7041724170	2.6871715642	5.6211887137
H165	7.5261037443	1.5166014612	7.2312356876
H166	8.1994435480	−0.0410988760	3.2865890239
H167	5.9980784040	3.6127207747	3.8184497814
C159	6.0611628774	3.7130932911	6.5270481259
H168	6.1425022710	4.7242281251	6.1123331934
H169	4.9912206647	3.5034177970	6.6602199580
H170	6.5209260850	3.7162399224	7.5208172485
C163	8.7332139314	−0.5452074801	5.9157246614
H171	9.7997944255	−0.3031489558	6.0146947056
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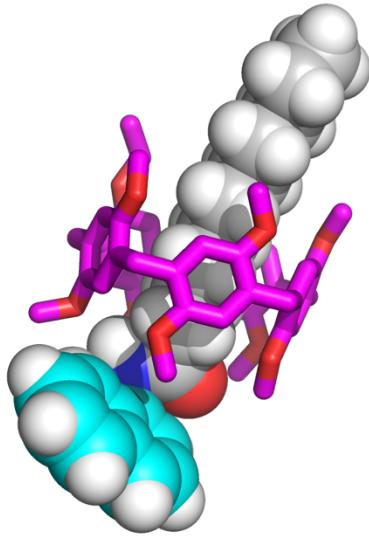
RDP[5]cat@MA_{disfav}-2-Model

SCF energy (B3LYP-MM/aug-cc-pVDZ//B3LYP-MM/LACVP*): -3563.20263 hartrees
Zero-point energy (B3LYP-MM/LACVP*): 898.002 kcal/mol
Gibbs free energy correction (B3LYP-MM/LACVP*): -65.048 kcal/mol

		Angstroms	
Atom	x	y	z
C1	3.6759354430	2.9072715469	2.4420899042
C2	2.8074028036	1.6641705418	2.4183457049
C3	1.3509822261	1.8994411720	1.9746072909
C4	0.5947410201	0.5658583996	1.9701763592
C5	-0.8993940328	0.6785301221	1.6553979377
C6	-1.5878667320	-0.6925514521	1.6943620838
C7	-3.1149172382	-0.6333049679	1.5601723210
C8	-3.7789712137	-2.0145812854	1.6449634942
C9	-5.3121571002	-1.9845607058	1.5911900188
C10	-5.9481952300	-3.3780700135	1.6977215892
C11	-7.4800558247	-3.3548017043	1.6630695508
O12	3.6044029983	3.7707045885	3.3237342361
C13	5.6737453094	3.9739014906	1.4845318764
H27	2.8032142531	1.2652148388	3.4381869145
H28	3.2626311685	0.9000766301	1.7782797095
H29	1.3304848552	2.3493444902	0.9746763187
H30	0.8722240018	2.6085060484	2.6581177574
H31	0.7092764981	0.0928347816	2.9529044892
H32	1.0706177798	-0.1110921731	1.2479573036
H33	-1.0454099203	1.1457304931	0.6710729752
H34	-1.3731118782	1.3426863553	2.3873856758
H35	-1.3350538956	-1.1878879419	2.6423094142
H36	-1.1736966407	-1.3319989302	0.8985018382
H37	-3.3886805440	-0.1541670108	0.6069058899

H38	−3.5137634225	0.0136020786	2.3550574411
H39	−3.4639884104	−2.5063546937	2.5782709996
H40	−3.4005301516	−2.6509722644	0.8299461035
H41	−5.6388582907	−1.5053810518	0.6557775608
H42	−5.6921883916	−1.3488022477	2.4054233865
H43	−5.6114788230	−3.8574654611	2.6284391065
H44	−5.5731333537	−4.0099447614	0.8796062725
H45	−7.8496835552	−2.9133356656	0.7289710257
H46	−7.8865038239	−2.7612622009	2.4916782497
C50	3.6992232604	−2.9952371905	0.8704175077
C51	1.2127473727	−1.5048713930	5.9746354930
C52	−1.3140516878	5.2142497168	−0.2812975698
C53	2.0621644130	1.1998048574	−2.9203526712
C54	0.9550959070	4.3482851379	−1.0529200398
C55	1.7406252334	3.3775161967	−1.6809458797
C56	1.1729370397	2.2408949581	−2.2604584862
C57	−0.2213506069	2.0900697775	−2.2058201535
C58	−1.0085503259	3.0663490691	−1.5869383530
C59	−0.4409496252	4.2007278591	−1.0032714515
C60	−0.7573307626	4.8070734655	3.4815575207
C61	−0.6155169829	5.2107162083	2.1518421318
C62	−1.5323309240	4.8242306317	1.1712454127
C63	−2.6229595053	4.0298701370	1.5553199802
C64	−2.7585162188	3.6135706794	2.8834323749
C65	3.7057000004	0.2103747033	−1.2271391007
C66	2.5236735559	0.1103264937	−1.9639436110
C67	1.7384055279	−1.0364764673	−1.7780769311
C68	2.1214216772	−2.0416181614	−0.8893247169
C69	3.3199428441	−1.9374265083	−0.1529309718
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O97       5.0042752583       -1.4055992688        2.7409187796
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C102     -3.7981056676       -0.3360519383        5.3488805747
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O105     -3.5101308948        3.6868892962        0.5569556649
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H107      3.3488590474       -3.9742563552        0.5313437558
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H109      0.5582450836       -2.3030621177        6.3371917130
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H150	4.0344271764	2.0606311238	6.5666639415
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N163	4.5791950772	3.0107813193	1.4217197753
H163	5.2660554014	4.9304352121	1.8192229208
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H170	8.2595925504	0.1105140508	-0.3259523210
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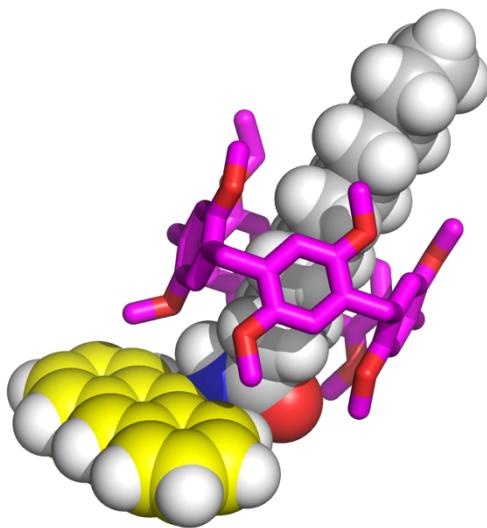
RDP[5]cat@MA_{disfav}-3-Model

SCF energy (B3LYP-MM/aug-cc-pVDZ//B3LYP-MM/LACVP*): -3716.854915 hartrees
Zero-point energy (B3LYP-MM/LACVP*): 927.595 kcal/mol
Gibbs free energy correction (B3LYP-MM/LACVP*): -65.964 kcal/mol

	Angstroms		
Atom	x	y	z
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C3	1.4935206486	1.7873048728	2.3861558502
C4	0.6879502949	0.4886840767	2.2806887712
C5	-0.7308845046	0.6801847734	1.7386906710
C6	-1.5061456657	-0.6428685309	1.6978081348
C7	-2.9870352725	-0.4836282102	1.3311773476
C8	-3.7513796963	-1.8143467541	1.3276194662
C9	-5.2480964528	-1.6833006547	1.0159591881
C10	-5.9920419858	-3.0262988384	1.0432877007
C11	-7.4890795037	-2.9018737826	0.7407117286
O12	3.6125580342	3.5462648239	4.2010058138
C13	5.5444931321	4.0767729316	2.2588246766
H27	2.6329272287	1.1705988565	4.1172148309
H28	3.3875678602	0.7468832473	2.5762444861
H29	1.6747377286	2.2010672679	1.3858097789
H30	0.9264647275	2.5380859911	2.9478929731
H31	0.6244742051	0.0302907330	3.2744747694
H32	1.2339656069	-0.2230817115	1.6487645410
H33	-0.6953726902	1.1261114322	0.7352140651
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H38	-3.4551575788	0.2057202067	2.0483276351
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H46	-7.9884896508	-2.2516217354	1.4699272388
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C61	-0.5502388295	5.0637185786	1.8927955434
C62	-1.4142523120	4.6964116060	0.8575202741
C63	-2.5854706024	3.9962780291	1.1837694084
C64	-2.8665347296	3.6758744196	2.5160146021
C65	3.8495885344	-0.1297567576	-0.3345853547
C66	2.8221926322	-0.2864640023	-1.2679618421
C67	2.0137849267	-1.4268514243	-1.1630485524
C68	2.2331109381	-2.3833641657	-0.1719659699
C69	3.2886197319	-2.2365236518	0.7514956205
C70	4.0820459097	-1.0956826942	0.6480999801
C71	1.1737144314	-2.0006209238	5.3196445842
C72	2.5190161937	-1.6445287116	5.1927735255
C73	3.2831063475	-2.0611326809	4.0994029570
C74	2.7131485952	-2.8745591984	3.1076581989
C75	1.3786938959	-3.2627679733	3.2532221334
C76	0.6105051116	-2.8300318150	4.3364997522
C77	-2.2913499466	1.0769643112	5.2434178988
C78	-1.6125005725	2.2995498781	5.3662644346
C79	-0.3035189875	2.2786240840	5.8579890867
C80	0.3239116398	1.0826423778	6.2161915556
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C102	-4.4019097527	-0.0034322118	4.9127566470
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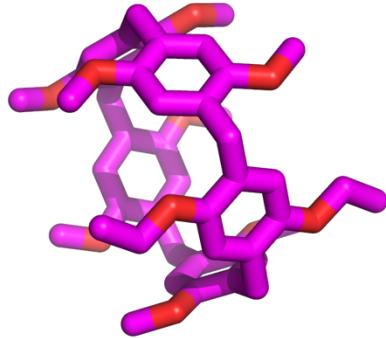
RDP[5]cat-Model

In this model of the ring (which was used for the disfavored rotaxane products where the tetra-glyme substituent is not directly interacting with the varying amide stoppers) the tetra-glyme-chains were replaced with ethyl groups to simplify the conformational space and speed up the calculations.

SCF energy (B3LYP-MM/aug-cc-pVDZ//B3LYP-MM/LACVP*): -2575.995623 hartrees
Zero-point energy (B3LYP-MM/LACVP*): 588.064 kcal/mol
Gibbs free energy correction (B3LYP-MM/LACVP*): -50.143 kcal/mol

```
                           Angstroms
   Atom            x                    y                    z
   C50        -0.1087617794         -3.5899343659         -0.4430214533
   C51         0.5565301043         -1.1121232740          4.8381973167
   C52         2.0372168058          5.5721656941         -1.7854327863
   C53         0.6160150904          0.5746433957         -4.5182231472
   C54         2.6704216802          3.3879755439         -2.9339122366
   C55         2.3154587101          2.2077907287         -3.5920306679
   C56         0.9801840081          1.8925433305         -3.8548761651
   C57        -0.0103594134          2.7988641797         -3.4460023821
   C58         0.3459995858          3.9881166820         -2.8055413887
   C59         1.6808061509          4.3006585882         -2.5378231212
   C60         3.1058853358          4.6535711117          1.7724778570
   C61         3.1346435145          4.9074344544          0.3992201281
   C62         2.0020662048          5.3620215904         -0.2808180730
   C63         0.8233489107          5.5660875960          0.4530247539
   C64         0.7975765522          5.3214499045          1.8280680519
   C65         1.5080652186         -1.3152836281         -3.0634526472
   C66         0.4247301252         -0.5369568937         -3.4997378328
   C67        -0.8317060618         -0.7785543720         -2.9389222811
   C68        -1.0171221167         -1.7635908862         -1.9659912901
   C69         0.0657285504         -2.5438932664         -1.5318338329
   C70         1.3209581704         -2.3051554394         -2.0958459038
   C71         0.3676922493         -1.8008549611          3.4968969079
   C72         1.4682621908         -2.3086085510          2.8009793604
   C73         1.3260850534         -2.8939360188          1.5409117200
   C74         0.0587815534         -2.9962742205          0.9458344794
   C75        -1.0413934361         -2.4923936715          1.6432509299
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C76	-0.8976157465	-1.8942000422	2.8978576682
C77	0.1897792135	2.6600237201	4.3136400511
C78	1.5246883591	3.0911749196	4.2566849246
C79	2.5343876932	2.1380944262	4.4061254024
C80	2.2376095202	0.7869318574	4.6017469067
C81	0.9034928127	0.3576810762	4.6684987661
C82	-0.1072927878	1.3113669060	4.5224676045
O83	3.9715963780	3.7280311259	-2.6346432822
O84	-1.3138262954	2.4416828612	-3.7131659389
C85	1.8664069425	4.5485052485	3.9930699205
C86	1.9277902138	4.8603904397	2.5069257119
C87	-2.3493760023	3.3372395912	-3.3344835210
C88	5.0085529474	2.8412161192	-3.0294953496
C89	-3.6726418284	2.7092705395	-3.7390187428
C90	6.3276556076	3.4432283399	-2.5746977271
O91	2.7277268147	-1.0398831232	-3.6433955532
C92	3.8447180804	-1.8025469816	-3.2330083859
O93	-2.2350889306	-2.0364988184	-1.3815052639
C94	-3.3521264340	-1.2728447703	-1.7888752374
O95	-1.9513871892	-1.3661642487	3.6136269026
C96	-3.2460699331	-1.4615609532	3.0544177223
O97	2.3812938706	-3.3994606091	0.8135894745
C98	3.6782193878	-3.2904278374	1.3650072983
O99	3.2004265751	-0.1910567337	4.7370567186
C100	4.5569035842	0.2045004968	4.6955915675
O101	-0.7705229013	3.6353184758	4.1577992976
C102	-2.1270374945	3.2385446079	4.1825731436
O103	4.1939879446	4.1996055417	2.4855742505
C104	5.4000353984	3.9759447925	1.7838871397
O105	-0.2694369111	6.0103479428	-0.2605014549
C106	-1.4766895015	6.2261934590	0.4423280389
H107	-1.1036248937	-4.0373351622	-0.5243189925
H108	0.6271618424	-4.3856803172	-0.5895089727
H109	-0.3618945383	-1.2009597102	5.4247314154
H110	1.3559664382	-1.6123075718	5.3917821253
H111	1.3315451449	6.3620721746	-2.0580833971
H112	3.0373447161	5.9012042646	-2.0803190529
H113	-0.3067797321	0.6986766512	-5.0917660021
H114	1.4087586602	0.2941340328	-5.2178845420
H115	3.0684782774	1.4903733279	-3.8929663911
H116	-0.4093368062	4.6898675677	-2.4745561080
H117	4.0324713820	4.7340967419	-0.1814404235
H118	-0.1111012150	5.4597750350	2.4006531548
H119	-1.6563378305	-0.1586637877	-3.2688037617
H120	2.1532280656	-2.8995858417	-1.7399573467
H121	2.4431482873	-2.2098584222	3.2631230462
H122	-2.0111491603	-2.5554434666	1.1653457762
H123	3.5603334974	2.4782324827	4.3394974424
H124	-1.1333123866	0.9644944579	4.5539465718
H125	2.8320238155	4.7777094618	4.4530975240
H126	1.1140082799	5.1892472774	4.4621455219
H127	-2.2105279594	4.3072232109	-3.8345350486
H128	-2.3167272242	3.5155801422	-2.2495378490
H129	4.9971236663	2.7099727252	-4.1217300408
H130	4.8530915079	1.8515401487	-2.5750887544

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H131        −4.5031605334          3.3760586284          −3.4816609220
H132        −3.8230764924          1.7551617043          −3.2224904029
H133         6.3497351141          3.5508130187          −1.4848537113
H134         7.1618618394          2.7995586741          −2.8753329898
H135         6.4737531998          4.4322562375          −3.0206564345
H136         4.0506396895         −1.6776861001          −2.1609005263
H137         3.7076314087         −2.8719389946          −3.4448159471
H138         4.6946018669         −1.4295960966          −3.8098623982
H139        −3.2135643527         −0.2039857531          −1.5736355153
H140        −3.5599930124         −1.3945446362          −2.8609623178
H141        −4.2025637100         −1.6489189816          −1.2147264084
H142        −3.5456070841         −2.5070251551           2.8975371500
H143        −3.9230006516         −0.9994701846           3.7771890961
H144        −3.3165616663         −0.9264075623           2.0971517983
H145         3.7648050009         −3.8368703722           2.3143647742
H146         4.3571740475         −3.7354456845           0.6334614721
H147         3.9613352248         −2.2421826369           1.5331957775
H148         5.1428894236         −0.7081184778           4.8291948292
H149         4.8171933664          0.6655846566           3.7326276180
H150         4.7999927604          0.9098621231           5.5021777251
H151        −2.7121010295          4.1491690480           4.0321969589
H152        −2.3554974815          2.5229966763           3.3807187500
H153        −2.4026142536          2.7895366839           5.1468319104
H154         5.7778994721          4.8972919635           1.3192765613
H155         6.1227776957          3.6271795541           2.5256767511
H156         5.2811838629          3.2093120328           1.0054506732
H157        −2.2014613971          6.5707159900          −0.2993313766
H158        −1.8458219805          5.3026285025           0.9095805219
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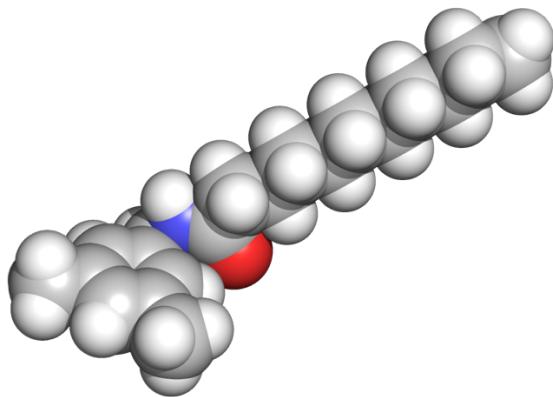

Amide-Stopper-1-Model

SCF energy (B3LYP-MM/aug-cc-pVDZ//B3LYP-MM/LACVP*): -912.126695 hartrees
Zero-point energy (B3LYP-MM/LACVP*): 313.216 kcal/mol
Gibbs free energy correction (B3LYP-MM/LACVP*): -33.639 kcal/mol

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                        Angstroms
 Atom             x                      y                      z
 C1          4.9005399027           0.3179977650           1.6047818226
 C2          3.3750116420           0.4017342299           1.6264763138
 C3          2.8532126669           1.2680753657           2.7789597036
 C4          1.3282444791           1.2093741058           2.9272789167
 C5          0.7978931323           2.0706574149           4.0813304960
 C6         -0.7246074305           1.9862057703           4.2525446297
 C7         -1.2624126056           2.8417334786           5.4073890459
 C8         -2.7831238254           2.7371141059           5.5846368516
 C9         -3.3292519554           3.5880588699           6.7387263831
 C10        -4.8490779455           3.4712875214           6.9172477697
 C11        -5.3905832774           4.3227595352           8.0705420905
 O12         5.5704320792           0.2861798956           2.6330379239
 C13         6.8795558070          -0.0234931021           0.1549756941
 H27         3.0007207140          -0.6264528018           1.7437813120
 H28         2.9916435098           0.7639861706           0.6631059065
 H29         3.1713153717           2.3082155752           2.6223367774
 H30         3.3395814130           0.9362166293           3.7031392456
 H31         1.0193642956           0.1646702122           3.0838619827
 H32         0.8512350281           1.5282938762           1.9880296719
 H33         1.0896536432           3.1186462794           3.9173185960
 H34         1.2873714737           1.7625921028           5.0169345612
 H35        -1.0125551185           0.9366901201           4.4151903767
 H36        -1.2138268568           2.2922337430           3.3155552236
 H37        -0.9861165204           3.8936275315           5.2407714846
 H38        -0.7660548698           2.5426736332           6.3426380328
 H39        -3.0564425070           1.6841536811           5.7503244103
 H40        -3.2791168754           3.0344237452           4.6484349344
 H41        -3.0634593983           4.6427861403           6.5718323863
 H42        -2.8309021044           3.2950588080           7.6750651015
 H43        -5.1131888407           2.4172687868           7.0850026360
 H44        -5.3467881194           3.7631967932           5.9813392546
 H45        -5.1734713391           5.3867644792           7.9135797830
 H46        -4.9362927168           4.0309922283           9.0257179141
 H160       -6.4769018595           4.2161734469           8.1723669880
 H162        4.8434203029           0.1321194505          -0.4318352926
 N163        5.4612060666           0.2751114519           0.3559505256
 H163        7.3921164511           0.3477601429           1.0457725960
 H164        7.2353919074           0.5506928447          -0.7076607199
 C150        7.5688847768          -4.2343723460          -0.4067742207
 C151        7.1853319517          -3.7621356451           0.8570263907
 C152        6.9758240558          -2.3920478370           1.0243590635
 C153        7.1487294928          -1.5031545219          -0.0461091609
 C154        7.5350076966          -2.0002906702          -1.2912398357
 C155        7.7479365795          -3.3716874759          -1.4903855495
 H165        7.7335854926          -5.3020743240          -0.5460427570
 H166        6.6798036691          -1.9987662201           1.9937995919
 H167        7.6745392071          -1.3120760562          -2.1242498261
 C159        8.1309567020          -3.9033055896          -2.8530793947
 H168        7.2435382260          -4.0835769072          -3.4748835684
 H169        8.7672448362          -3.1954750323          -3.3960184529
 H170        8.6709724663          -4.8529170550          -2.7755891045
 C163        7.0326170424          -4.7176422604           2.0186188607
 H171        6.4092562368          -4.2879760585           2.8092414980
 H172        8.0066530726          -4.9591032607           2.4644297635
 H173        6.5789565682          -5.6643536577           1.7032367730
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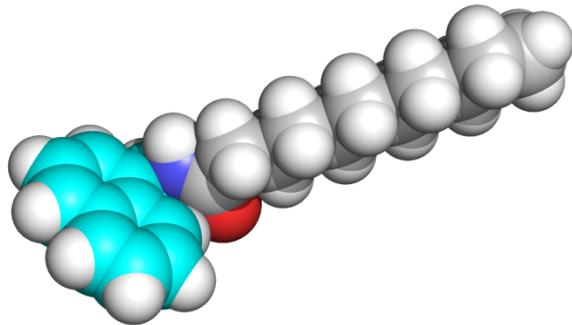
Amide-Stopper-2-Model

SCF energy (B3LYP-MM/aug-cc-pVDZ//B3LYP-MM/LACVP*): -987.145503 hartrees
Zero-point energy (B3LYP-MM/LACVP*): 308.2 kcal/mol
Gibbs free energy correction (B3LYP-MM/LACVP*): -32.779 kcal/mol

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                            Angstroms
Atom              x                    y                    z
C1          4.5152204022         4.1003154049         2.6289117701
C2          3.2907476862         3.2245755226         2.3785841831
C3          2.8884819379         3.1940783233         0.8977345450
C4          1.5690701995         2.4498927851         0.6600896873
C5          1.1645471027         2.3776659004        -0.8184295566
C6         -0.1676134612         1.6498027045        -1.0429381976
C7         -0.5767434076         1.5465494990        -2.5182920066
C8         -1.9169763915         0.8278488709        -2.7245990808
C9         -2.3338129832         0.7053712519        -4.1961199769
C10        -3.6791103683        -0.0075691963        -4.3903249523
C11        -4.0922207374        -0.1330399661        -5.8606452938
O12         4.6465737246         5.2042680714         2.1048017630
C13         6.5999903508         4.3233410155         3.9713398706
H27         2.4687196271         3.6518000803         2.9709161096
H28         3.4514790057         2.2052965527         2.7545324094
H29         3.6909457287         2.7212448355         0.3141057342
H30         2.8155659274         4.2274814427         0.5404066622
H31         0.7680558923         2.9419859644         1.2321451396
H32         1.6444409370         1.4283295285         1.0628562688
H33         1.9579870030         1.8714881462        -1.3881827234
H34         1.0987272255         3.3962219357        -1.2282480787
H35        -0.9608743906         2.1667016319        -0.4823189264
H36        -0.1045598859         0.6383268620        -0.6140003284
H37         0.2099985365         1.0191656842        -3.0782185269
H38        -0.6336857065         2.5557433534        -2.9526956562
H39        -2.7026251554         1.3613571378        -2.1687671582
H40        -1.8613092885        -0.1770156899        -2.2795078240
H41        -1.5531698788         0.1651813708        -4.7526869806
H42        -2.3867916784         1.7084763227        -4.6454100893
H43        -4.4585612730         0.5346808782        -3.8360159546
H44        -3.6263992883        -1.0084362644        -3.9382221703
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H45	−3.3499118167	−0.7026681280	−6.4336879005
H46	−4.1862680735	0.8534938675	−6.3315751778
H160	−5.0563918859	−0.6444432770	−5.9640637031
H162	5.2225424734	2.7073824952	3.9564227621
N163	5.4393287709	3.5768709009	3.4889138709
H163	6.5953471890	5.2698038298	3.4253838173
H164	7.5165286511	3.7883380907	3.6936935219
C150	6.5347553792	4.7437885988	8.2897016126
C153	6.5743343045	4.5201019055	5.4742117695
H165	6.5112794527	4.8321095682	9.3733958697
C161	7.4247662014	3.8969560636	7.6753364710
C162	7.4377583583	3.7887057422	6.2648667864
C167	5.6444114209	5.4211448783	6.0898717521
C168	5.6295052880	5.5244044930	7.5214351929
C169	4.7114604346	6.4111254497	8.1439606152
C170	3.8443790770	7.1711431158	7.3935164173
C171	3.8638208203	7.0781444185	5.9826235270
C172	4.7388048923	6.2265471997	5.3436807136
H175	4.7095002215	6.4800088499	9.2293872958
H176	3.1470154074	7.8471749017	7.8813155939
H177	3.1827315291	7.6879698686	5.3948000314
H178	4.7360450819	6.1793851971	4.2596827458
H166	8.1454206797	3.1107332437	5.7919455526
H167	8.1190567272	3.3052072599	8.2658074944
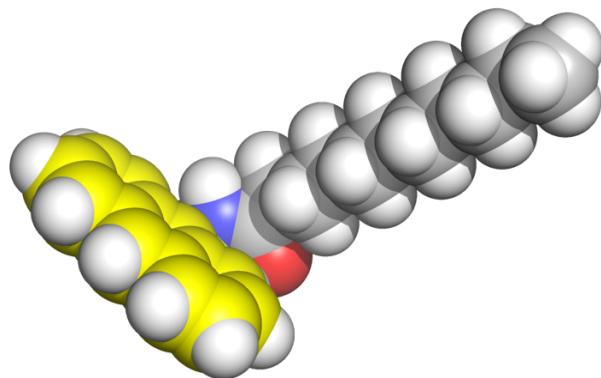
Amide-Stopper-3-Model

SCF energy (B3LYP-MM/aug-cc-pVDZ//B3LYP-MM/LACVP*): -1140.793815 hartrees
Zero-point energy (B3LYP-MM/LACVP*): 337.908 kcal/mol
Gibbs free energy correction (B3LYP-MM/LACVP*): -34.379 kcal/mol

	Angstroms		
Atom	x	y	z
C1	5.3874291674	1.6964897698	0.6907146803
C2	3.9008417290	2.0233105924	0.7743859345
C3	3.3450605532	1.7364462727	2.1807040629
C4	1.8648679409	2.1126508459	2.3183513687
C5	1.2940927140	1.8565071547	3.7199769918
C6	−0.1896113358	2.2302273662	3.8405576019

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C7       -0.7746427347      2.0108001399       5.2422883795
C8       -2.2582943352      2.3912906033       5.3420533517
C9       -2.8551870742      2.2017817142       6.7428411687
C10      -4.3383639199      2.5878783217       6.8286156307
C11      -4.9323082291      2.4088225251       8.2298491622
O12       6.2134168807      2.2526128729       1.4113605050
C13       7.0747301223      0.1837789357      -0.3285388577
H27       3.3262324138      1.4730093798       0.0173268519
H28       3.7879674773      3.0915614006       0.5502957430
H29       3.9496094882      2.2915981269       2.9075904924
H30       3.4789098614      0.6705305386       2.4139098367
H31       1.2740763619      1.5506908178       1.5791048860
H32       1.7361731525      3.1753828526       2.0640692603
H33       1.8764144396      2.4265273103       4.4587403752
H34       1.4265887852      0.7959687677       3.9807431058
H35      -0.7703601709      1.6470168478       3.1101076893
H36      -0.3204083305      3.2853012289       3.5568684676
H37      -0.1980006291      2.5974717270       5.9728933462
H38      -0.6475361710      0.9567726991       5.5311602687
H39      -2.8345429951      1.7948503405       4.6187905009
H40      -2.3833587904      3.4407192302       5.0355419800
H41      -2.2822771966      2.8001032968       7.4672026820
H42      -2.7343984241      1.1530424019       7.0534894150
H43      -4.9108628162      1.9857734055       6.1084842265
H44      -4.4580803980      3.6338706688       6.5116651009
H45      -4.4039300921      3.0271984418       8.9662548378
H46      -4.8587898758      1.3655725480       8.5616575686
H160     -5.9909851865      2.6924001083       8.2557375568
H162      4.9835018595      0.2460146216      -0.6992243025
N163      5.7272021224      0.7452009457      -0.2311254678
H163      7.7062618729      0.8078165137       0.3024436756
H164      7.4454054779      0.3019603215      -1.3507017809
C150      7.2119332163     -3.9932276507       0.8717650186
C153      7.1220499115     -1.2732470994       0.0936169588
H165      7.2570604590     -5.0389750366       1.1696320159
C50       7.3939594267     -3.0012633923       1.8393710020
C51       7.3330490632     -1.6097377879       1.4525545552
C52       7.4799387082     -0.6276734186       2.4875564893
C53       7.6950491456     -0.9991401607       3.7896090190
C54       7.7803728473     -2.3706651716       4.1584558628
C55       7.6297899011     -3.3419915968       3.2070793648
H58       7.3858187496      0.4263965912       2.2528457431
H59       7.7956675188     -0.2336518720       4.5544630253
H60       7.9566062410     -2.6403604694       5.1964145972
H61       7.6809673803     -4.3951807602       3.4734748799
C56       6.9088435346     -2.2891807909      -0.8684391626
C57       6.9584267908     -3.6769940022      -0.4649954713
C58       6.7410080440     -4.7017342304      -1.4373826229
C59       6.4737838568     -4.3938372238      -2.7431614454
C60       6.4113892641     -3.0312160925      -3.1489204697
C61       6.6224062548     -2.0197500881      -2.2484076416
H64       6.7884042034     -5.7377460801      -1.1099579392
H65       6.3058638627     -5.1819131898      -3.4721096882
H66       6.1928598406     -2.7925634357      -4.1865156262
H67       6.5615866122     -0.9940630863      -2.5961715727
```

V. ^{1}H, ^{13}C, and ^{1}H-^{1}H ROESY NMR Spectra
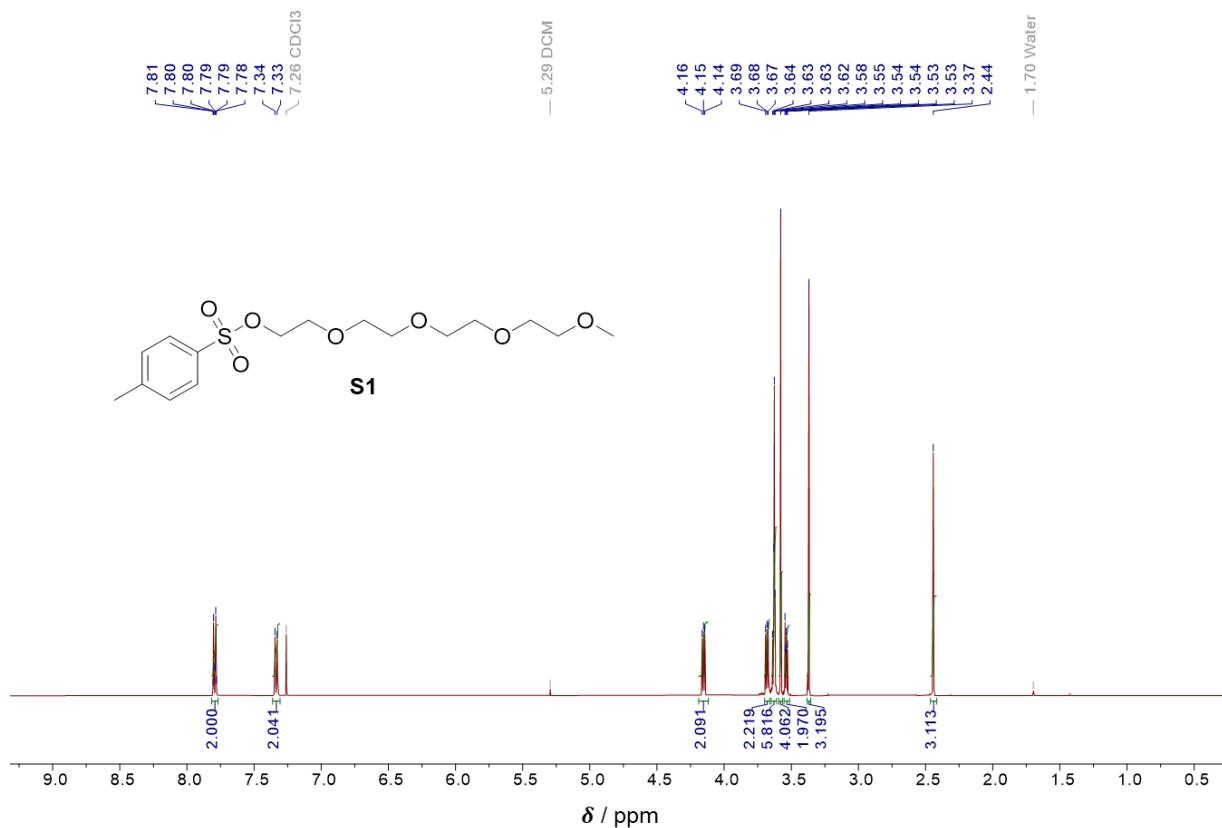
Figure S6. ^{1}H NMR (500 MHz, CDCl$_3$, 298 K) spectrum of **S1**.
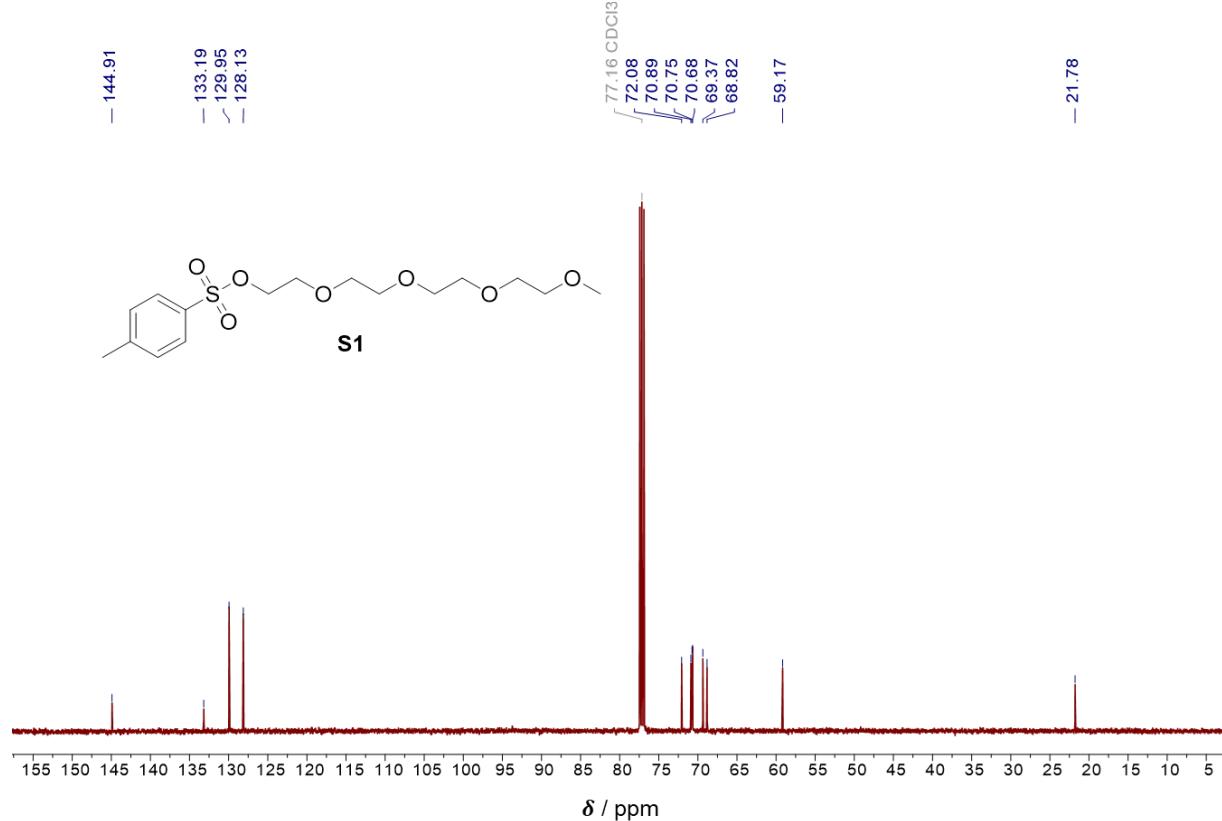
**Figure S7**. ^{13}C NMR (125 MHz, CDCl$_3$, 298 K) spectrum of **S1**.
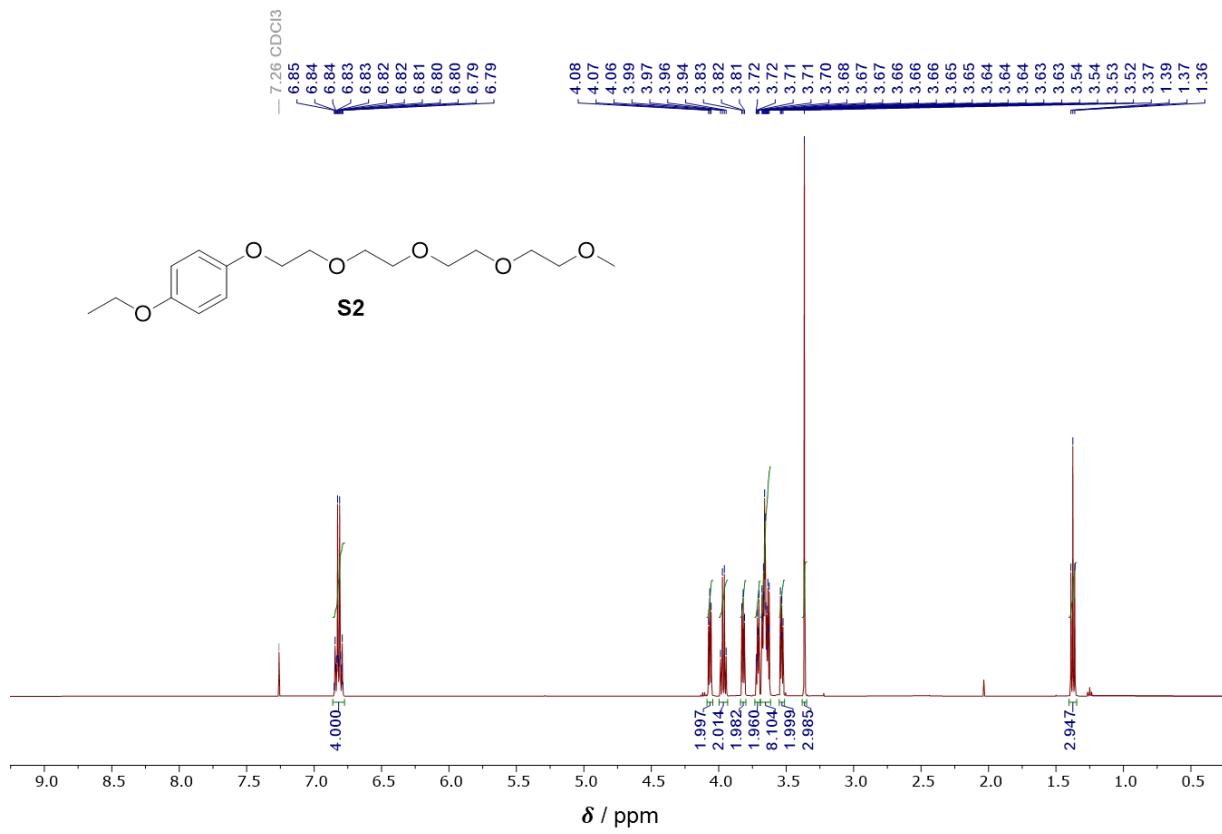
**Figure S8**. ^{1}H NMR (500 MHz, CDCl$_3$, 298 K) spectrum of **S2**.
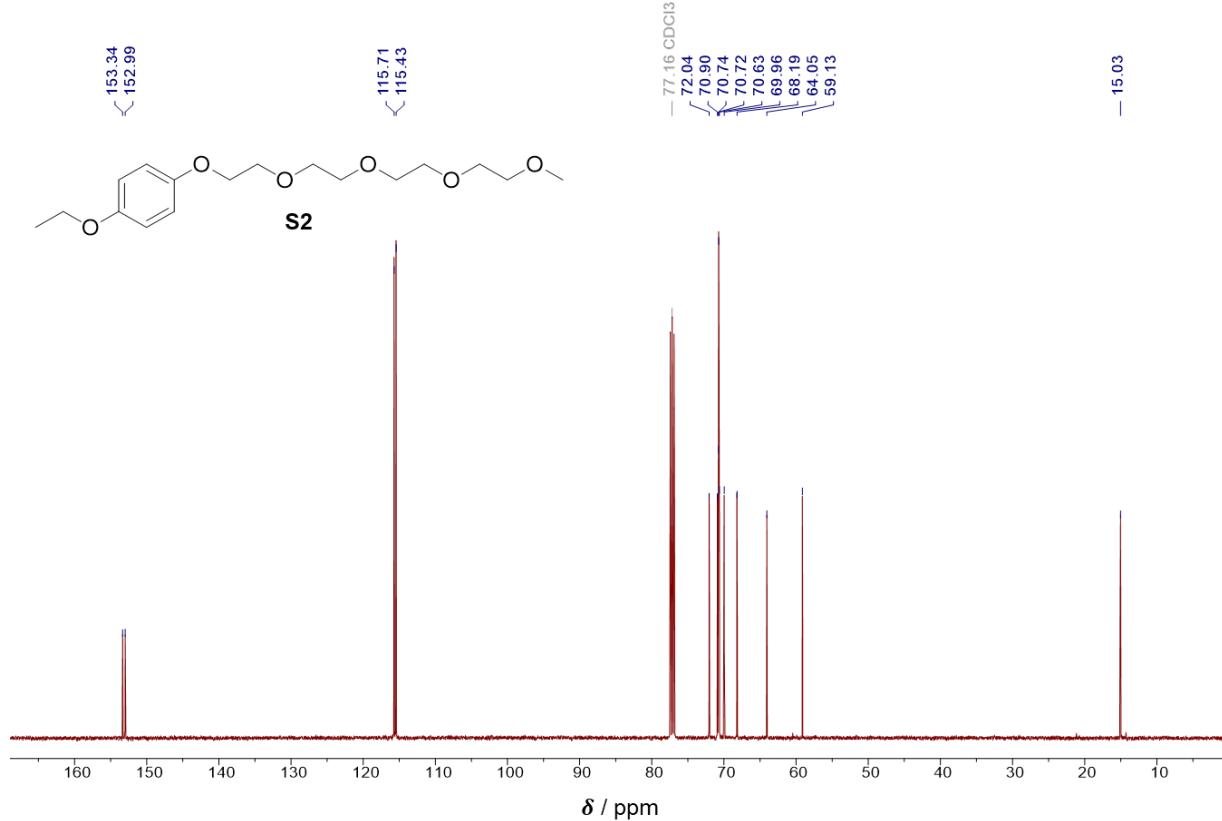

**Figure S9**. ^{13}C NMR (125 MHz, CDCl$_3$, 298 K) spectrum of **S2**.
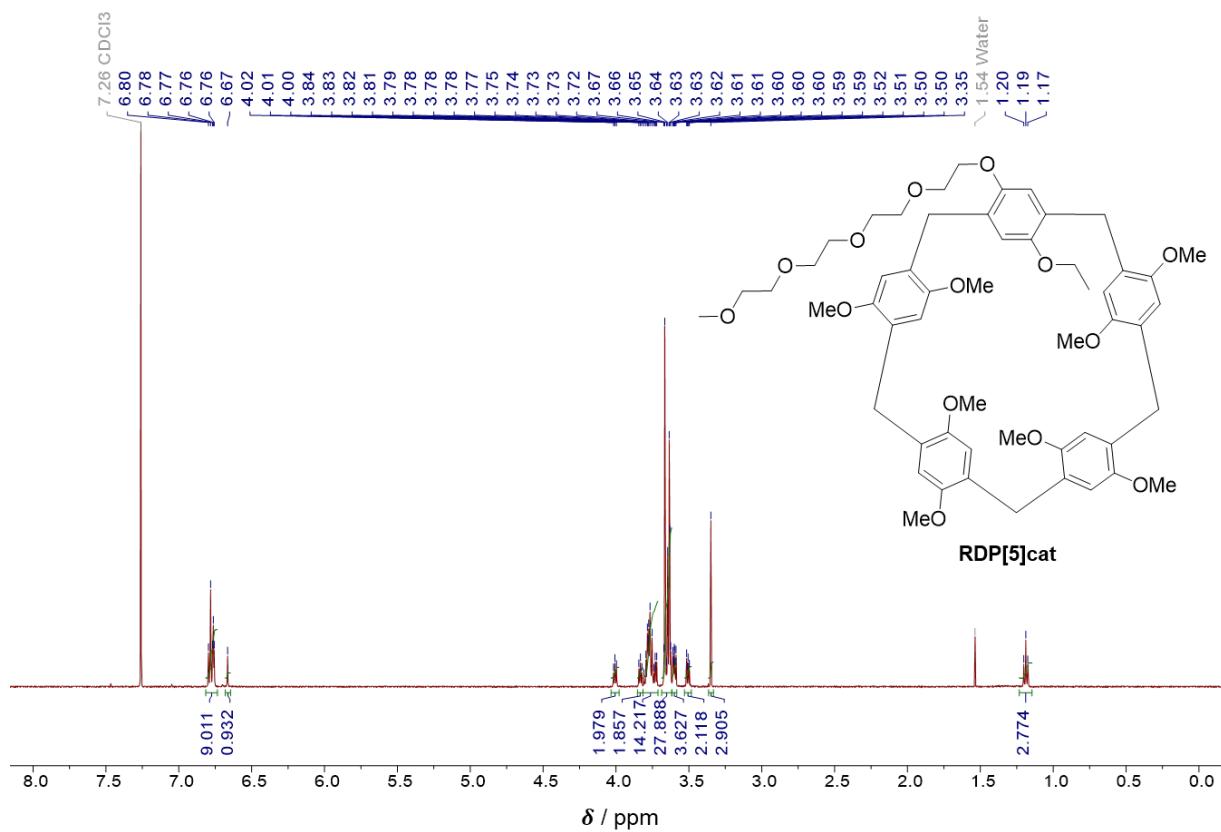
**Figure S10**. ^{1}H NMR (500 MHz, CDCl$_3$, 298 K) spectrum of **RDP[5]cat**.
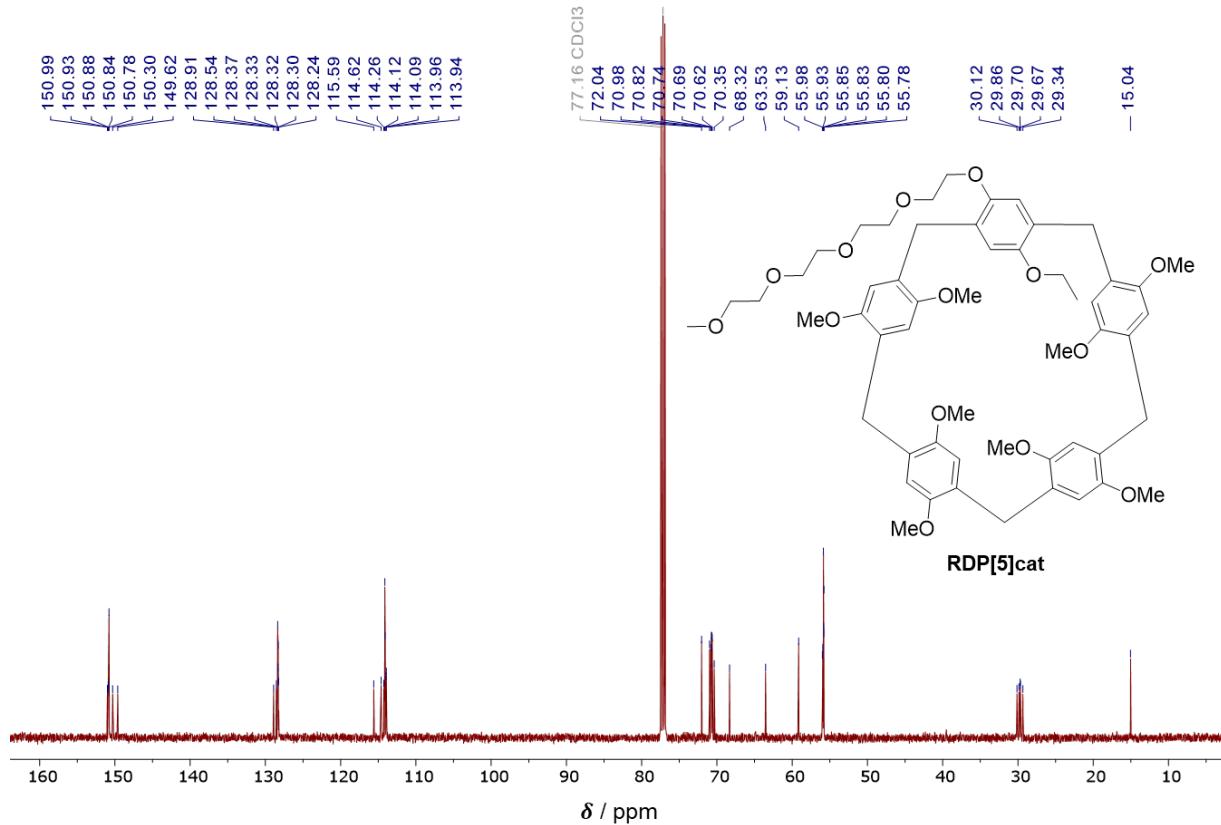
Figure S11. ^{13}C NMR (125 MHz, CDCl$_3$, 298 K) spectrum of **RDP[5]cat**.
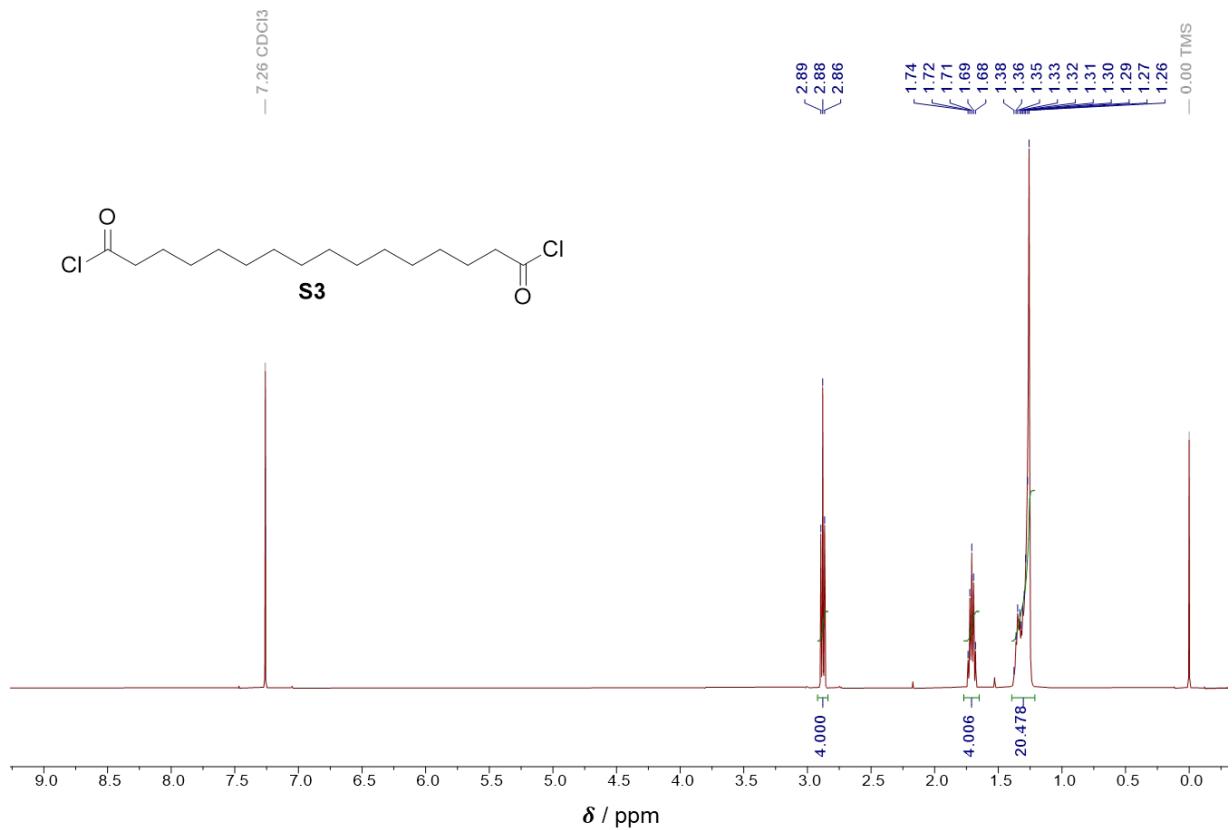
Figure S12. ^{1}H NMR (500 MHz, CDCl$_3$, 298 K) spectrum of **S3**.
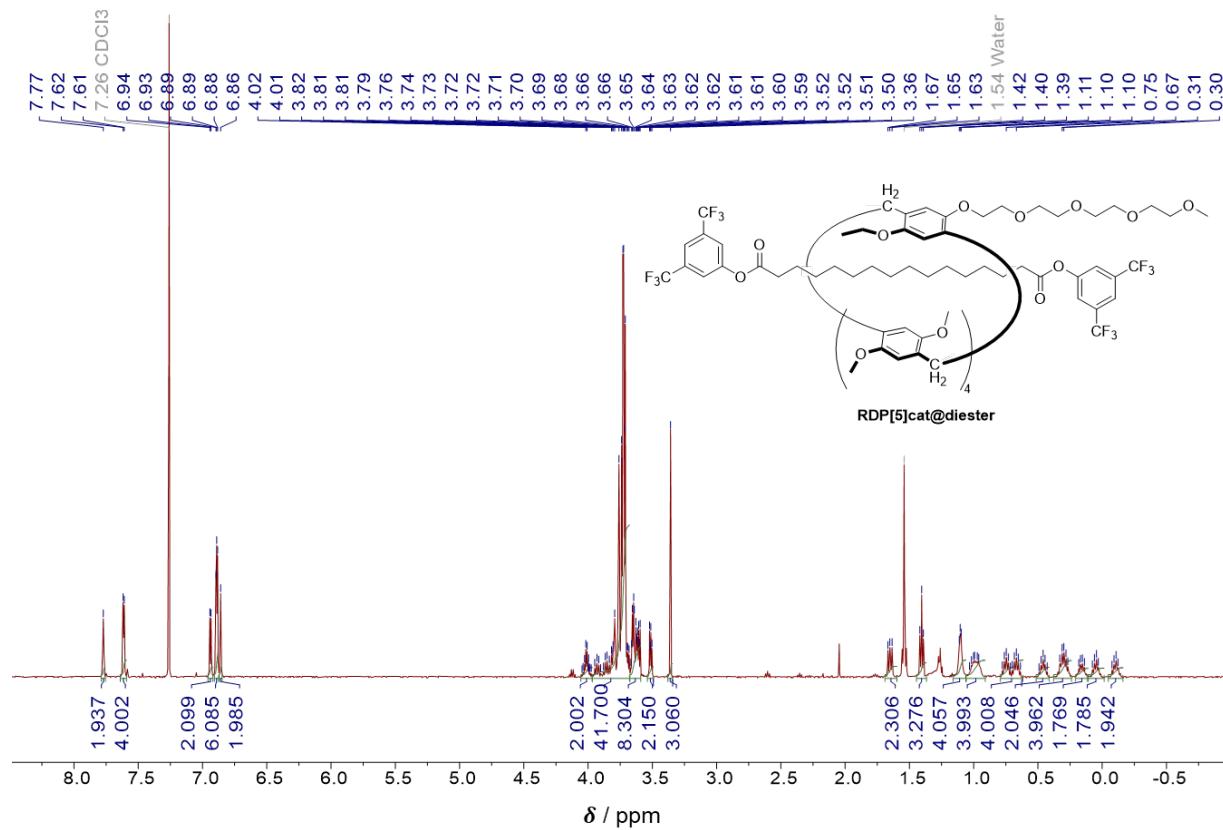
Figure S13. ^{1}H NMR (500 MHz, CDCl$_3$, 298 K) spectrum of **RDP[5]cat@diester.**
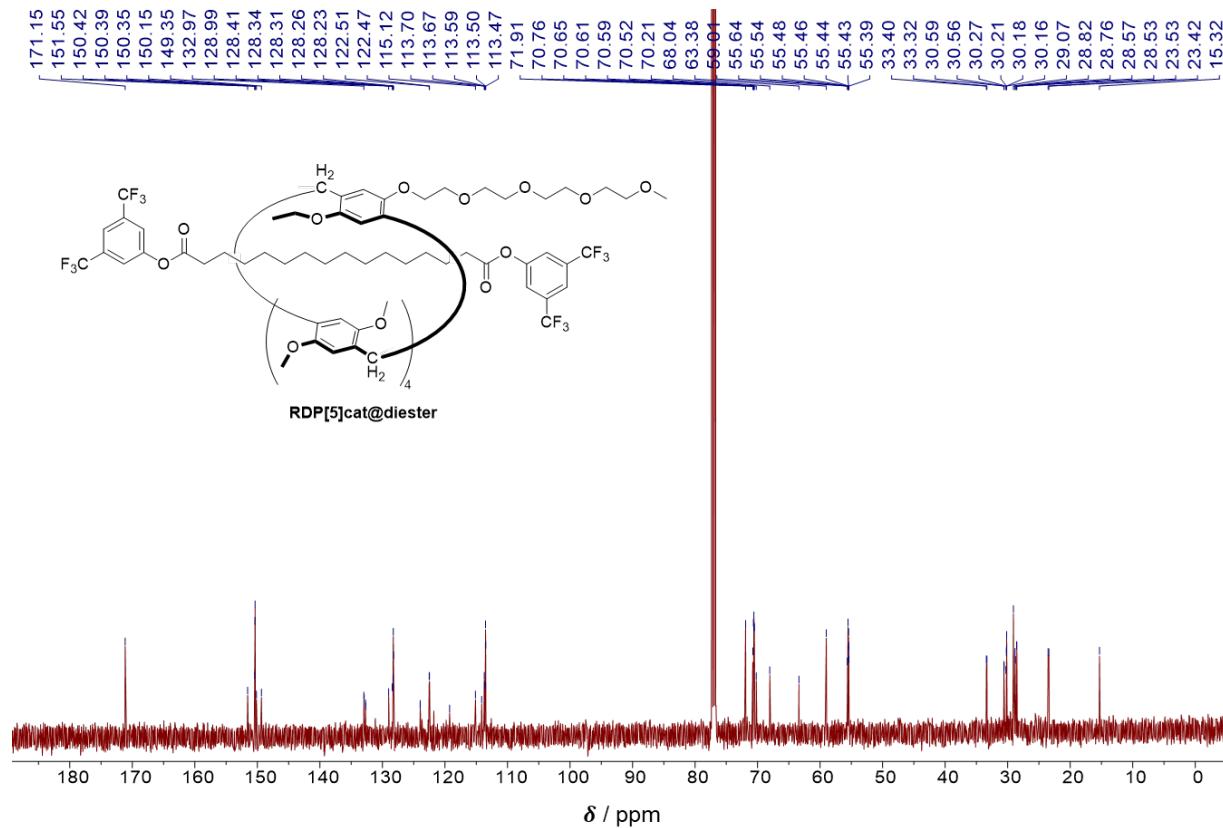
Figure S14. ^{13}C NMR (125 MHz, CDCl$_3$, 298 K) spectrum of **RDP[5]cat@diester.**
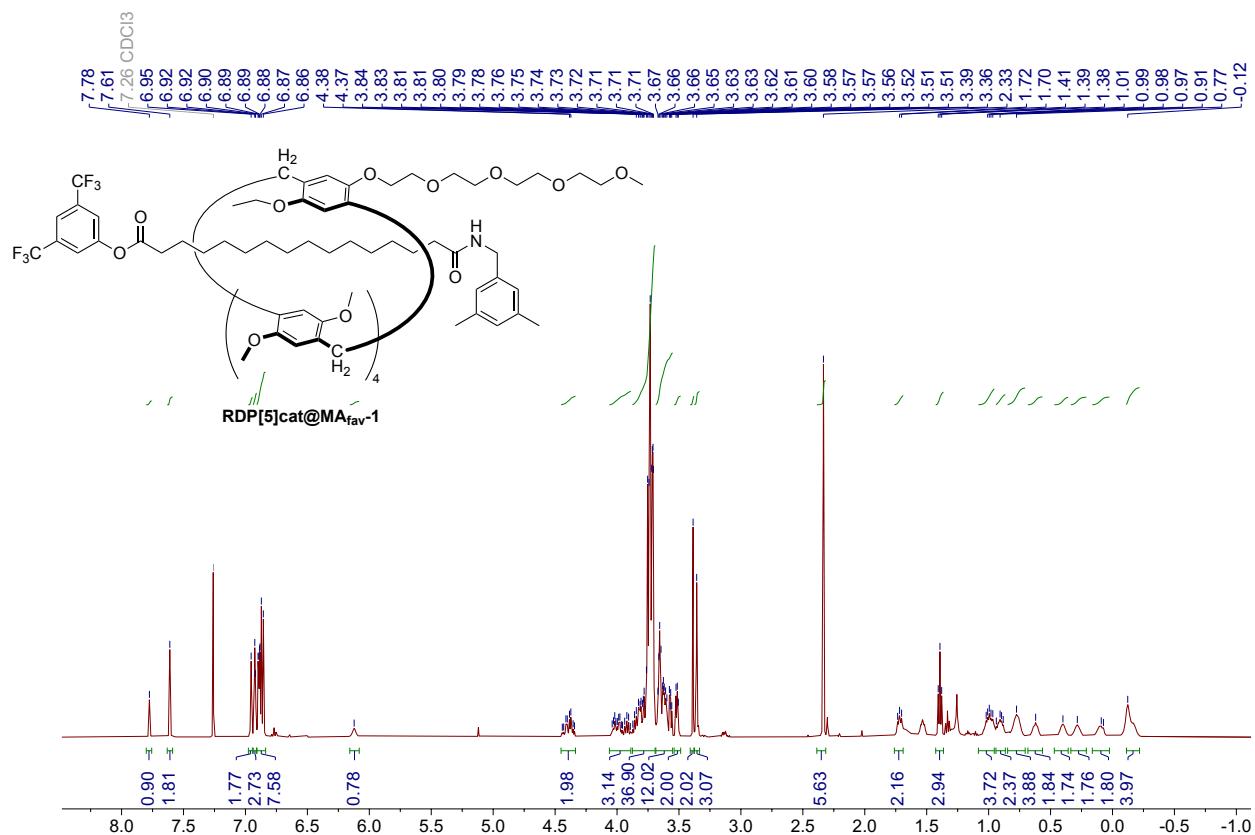
Figure S15. ^{1}H NMR (500 MHz, CDCl$_3$, 298 K) spectrum of **RDP[5]cat@MA$_{fav}$-1**.
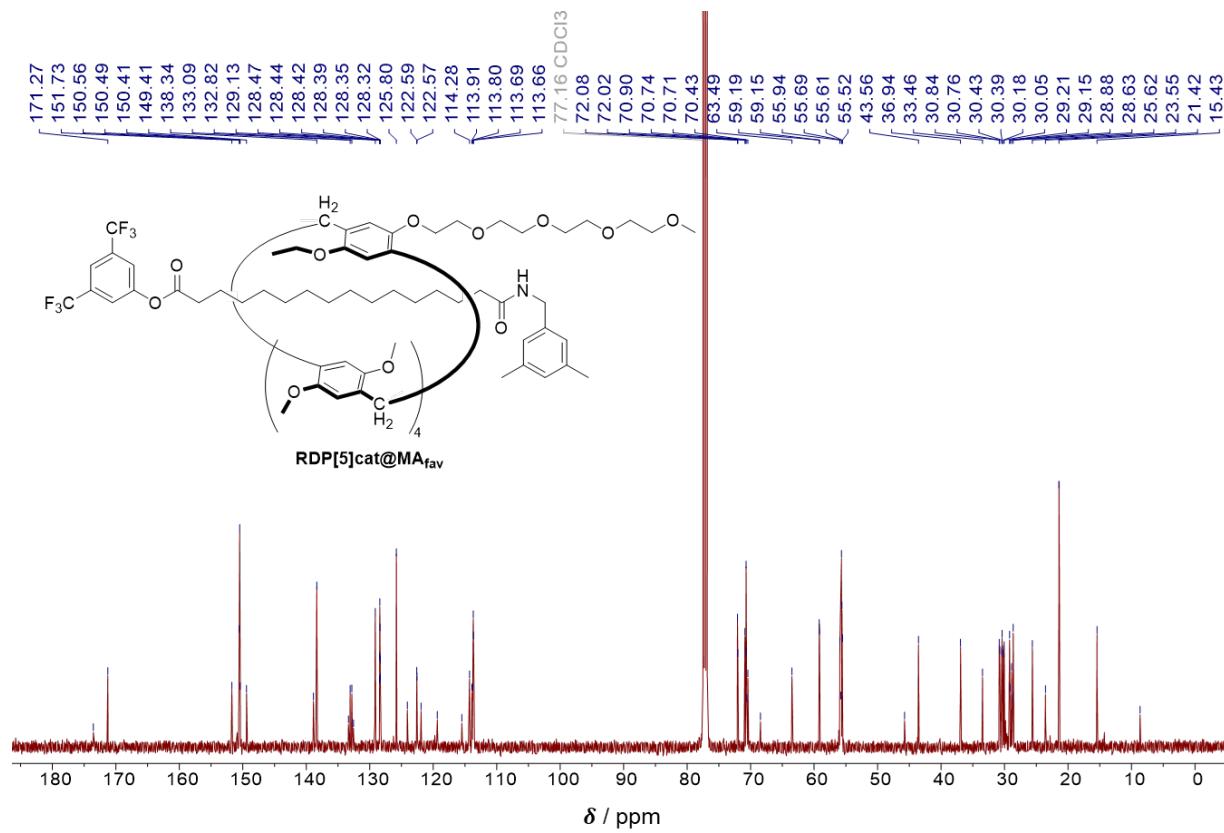
Figure S16. ^{13}C NMR (125 MHz, CDCl$_3$, 298 K) spectrum of **RDP[5]cat@MA$_{fav}$-1**.
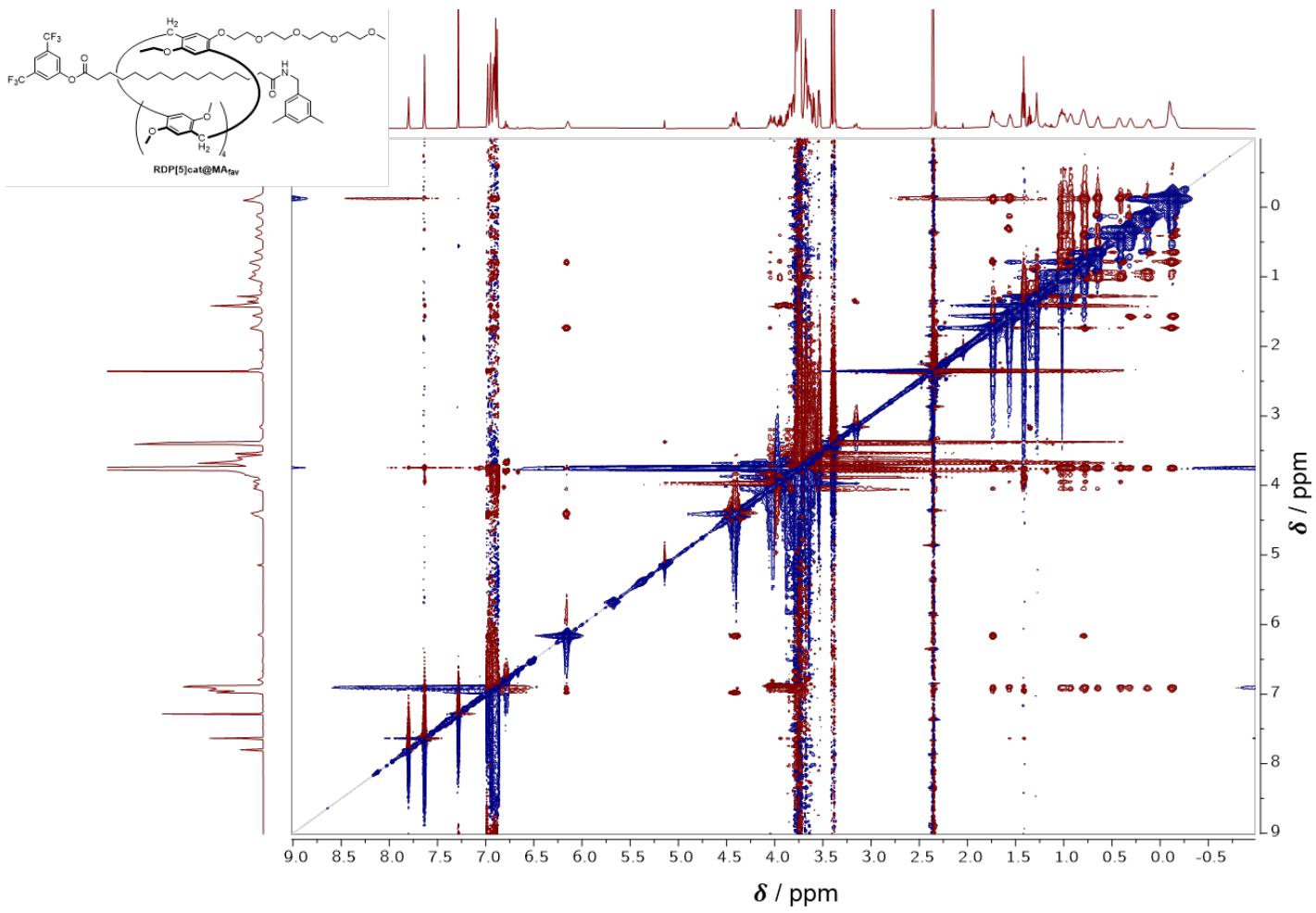
Figure S17. 2D {^{1}H – ^{1}H} ROESY NMR (500 MHz, CDCl$_3$, 298 K) spectrum of **RDP[5]cat@MA$_{fav}$-1**. The spectrum was acquired using a 2s relaxation delay, pulse width of 10.2250 (optimized to 90°) and 32 scans for each slice, apodization with a 90° sine square, manual phasing of f2 and reduction of t1 noise, and alignment to the CDCl$_3$ signal produced the final spectrum. Additional contour lines were added to increase visibility of all cross peaks.
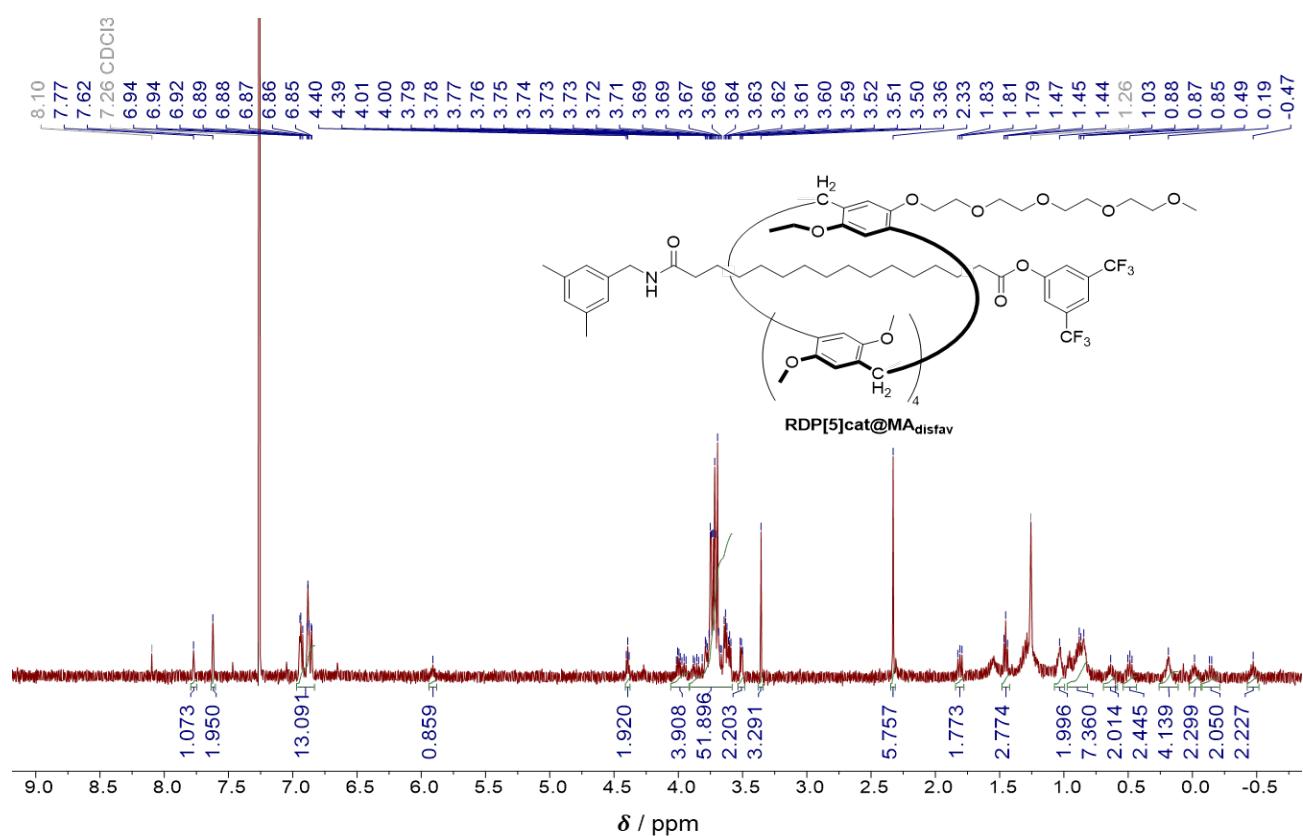
Figure S18. ^{1}H NMR (500 MHz, CDCl$_3$, 298 K) spectrum of **RDP[5]cat@MA$_{disfav}$-1**. The resonance at 8.10 ppm stems from an inseparable impurity arising from a small amount of benzylamine decomposition.
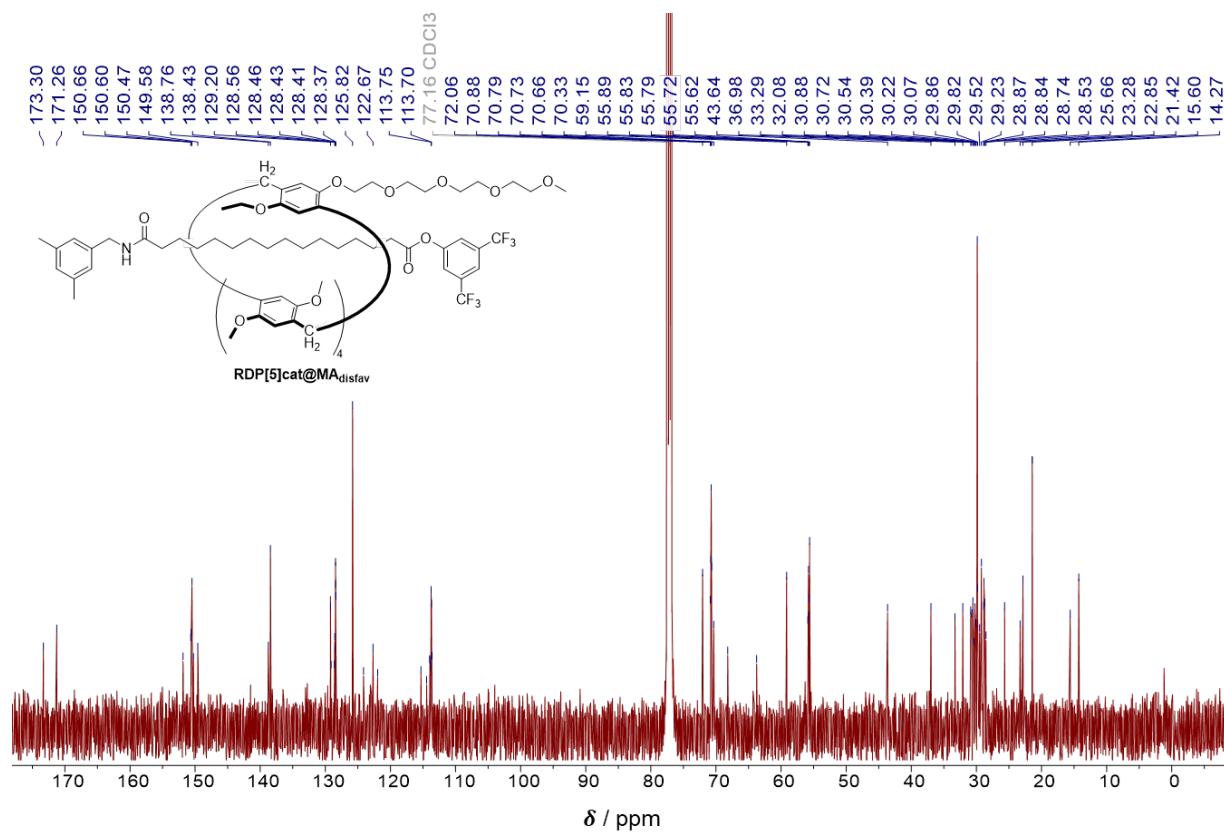
Figure S19. ^{13}C NMR (125 MHz, CDCl$_3$, 298 K) spectrum of **RDP[5]cat@MA$_{disfav}$-1**, recorded using a Shigemi NMR tube.
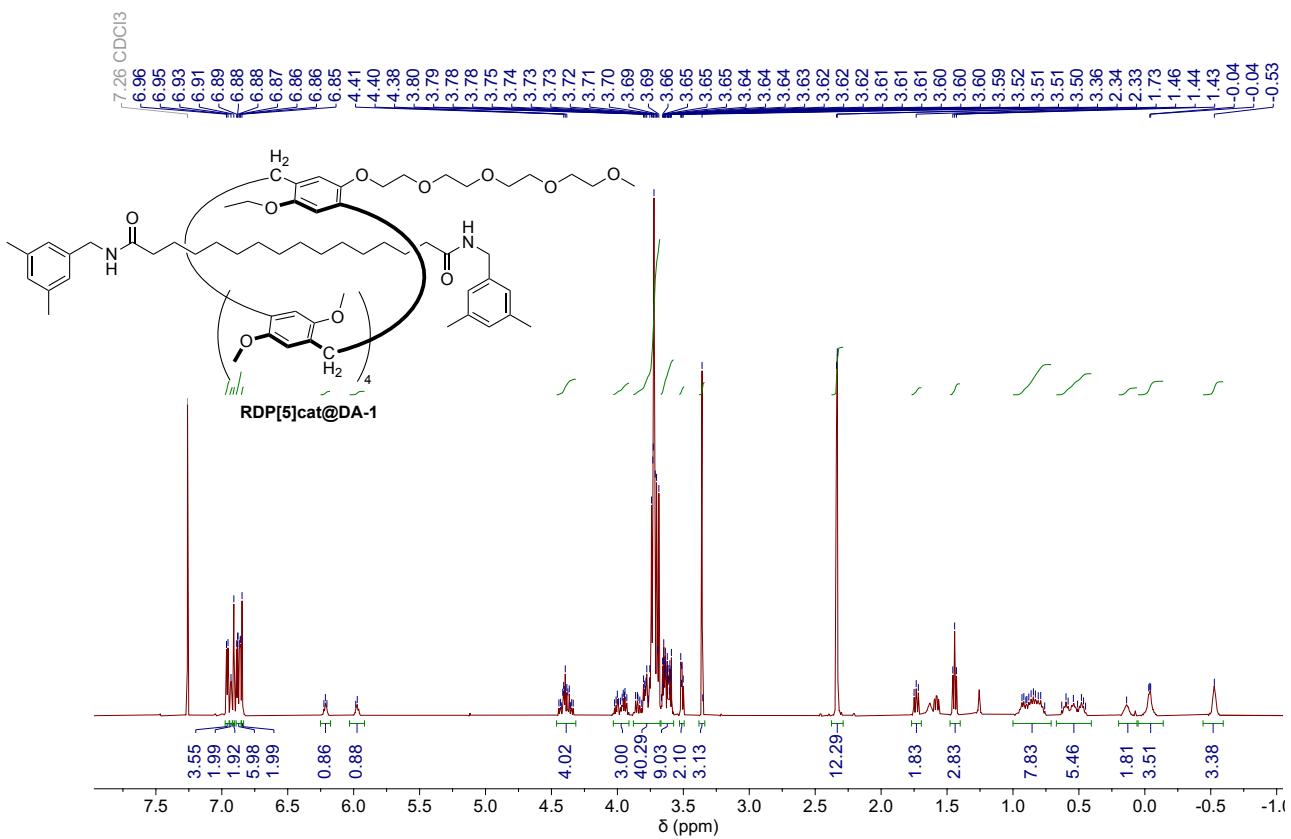
Figure S20. ^{1}H NMR (500 MHz, CDCl$_3$, 298 K) spectrum of **RDP[5]cat@DA-1**.
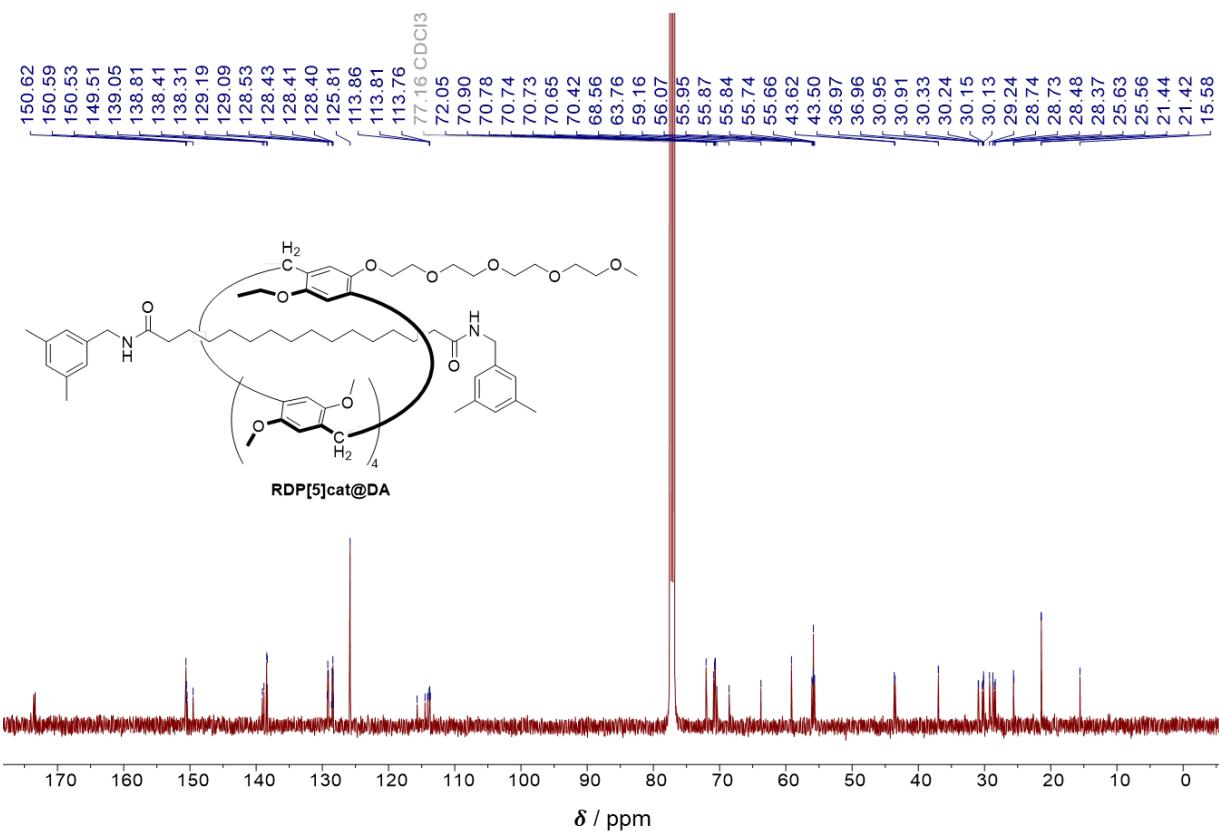
Figure S21. ^{13}C NMR (125 MHz, CDCl$_3$, 298 K) spectrum of **RDP[5]cat@DA-1**.
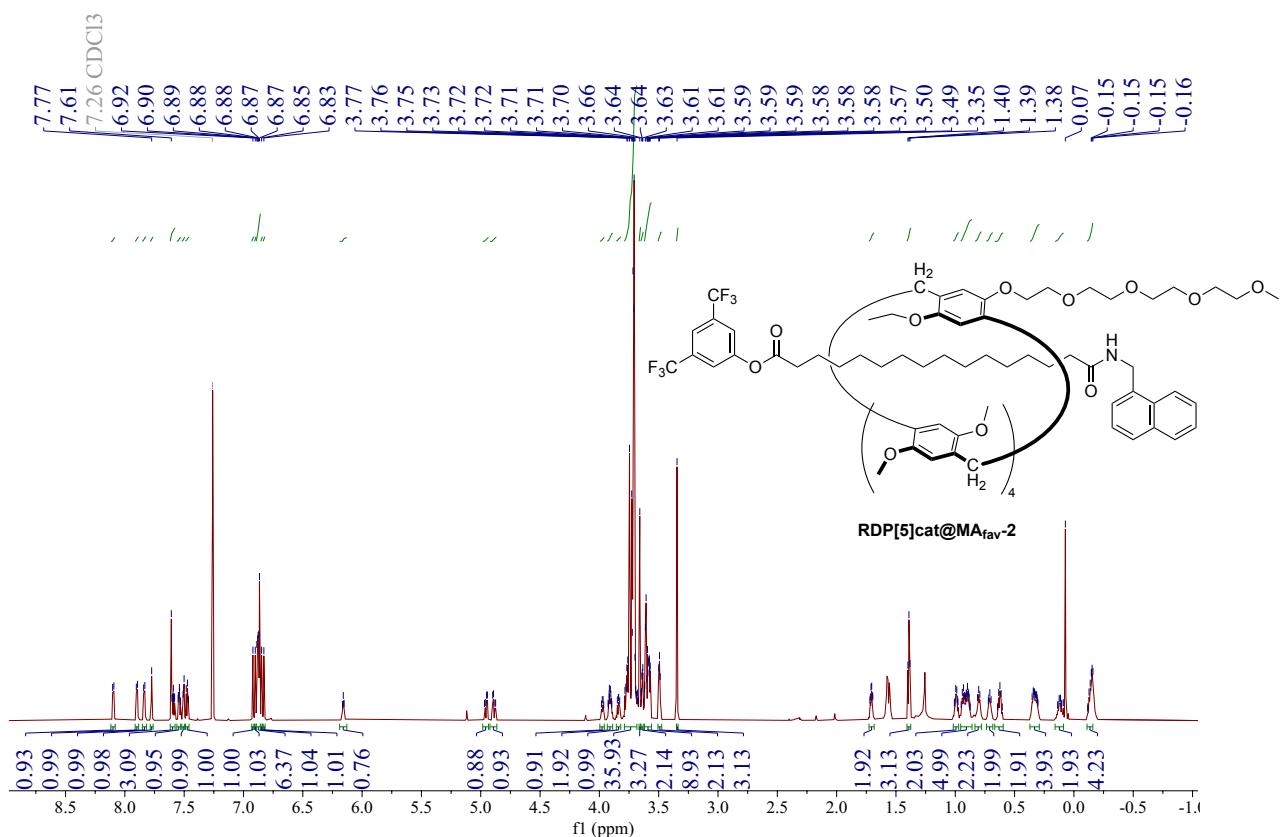
Figure S22. ^{1}H NMR (800 MHz, CDCl$_3$, 298 K) spectrum of **RDP[5]cat@MA$_{fav}$-2**.
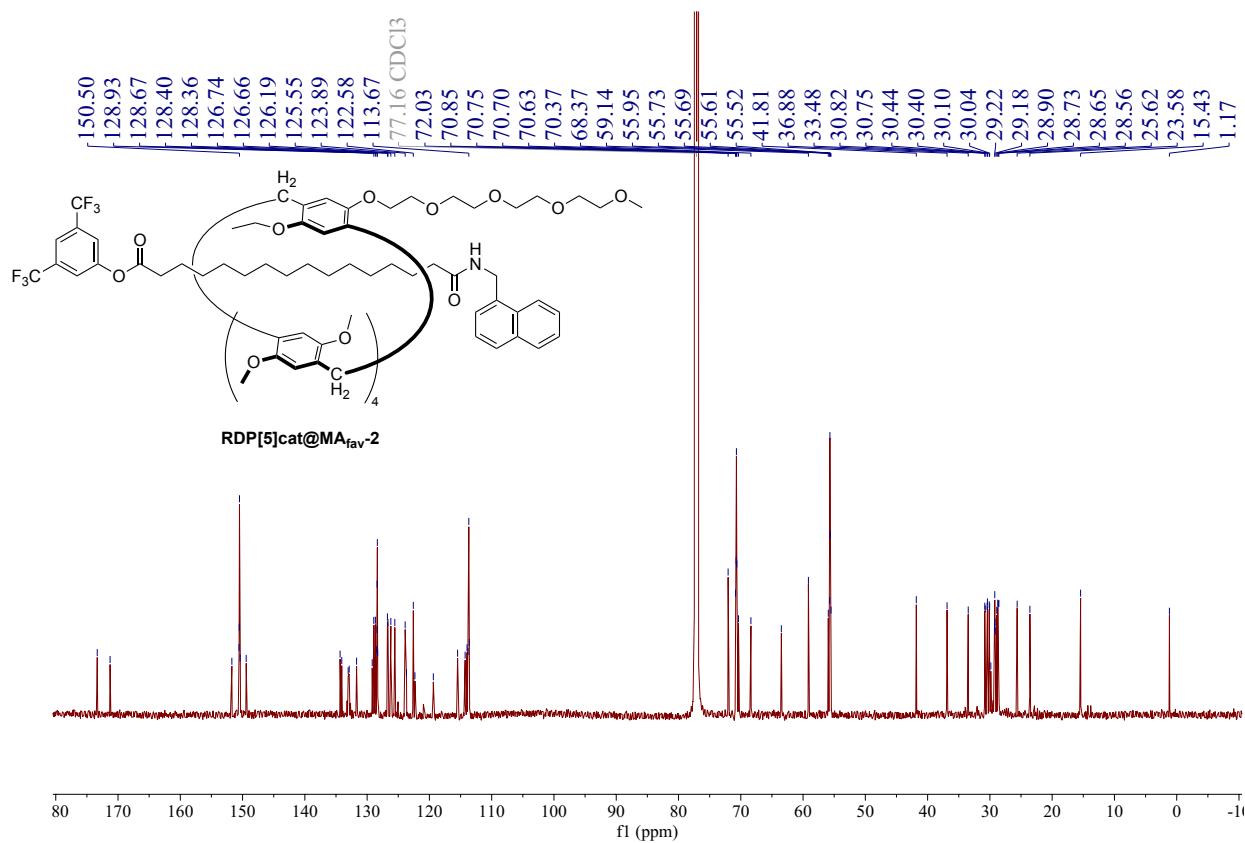
Figure S23. ^{13}C NMR (200 MHz, CDCl$_3$, 298 K) spectrum of **RDP[5]cat@MA$_{fav}$-2**.
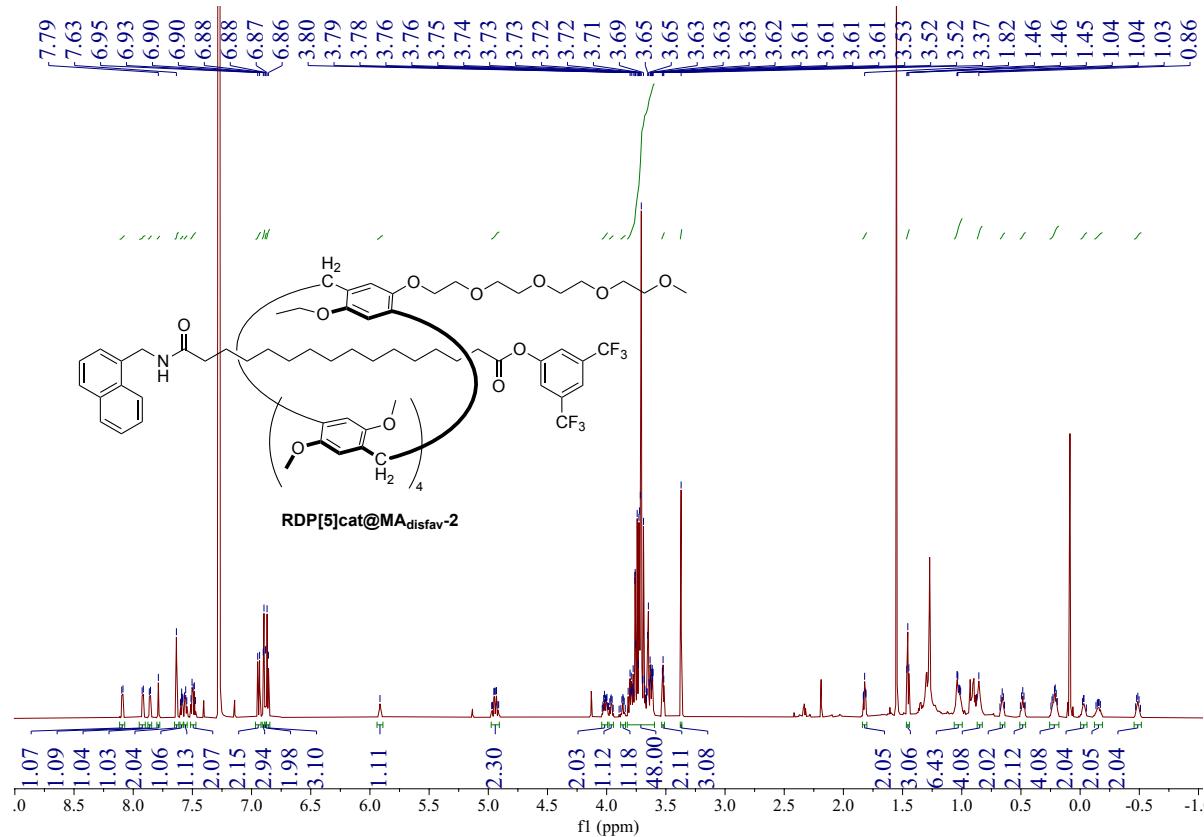
**Figure S24**. ^1H NMR (800 MHz, CDCl$_3$, 298 K) spectrum of **RDP[5]cat@MA$_{disfav}$-2**.
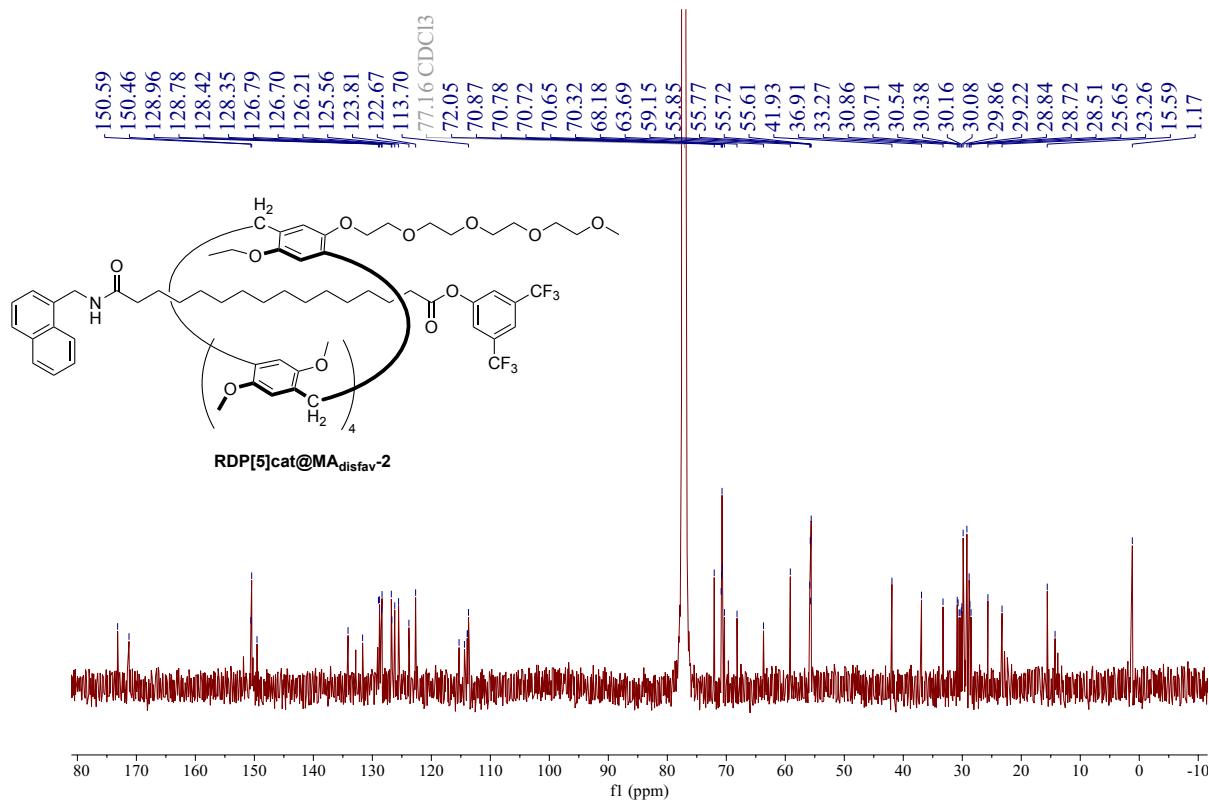
Figure S25. ^{13}C NMR (200 MHz, CDCl$_3$, 298 K) spectrum of **RDP[5]cat@MA$_{disfav}$-2**.
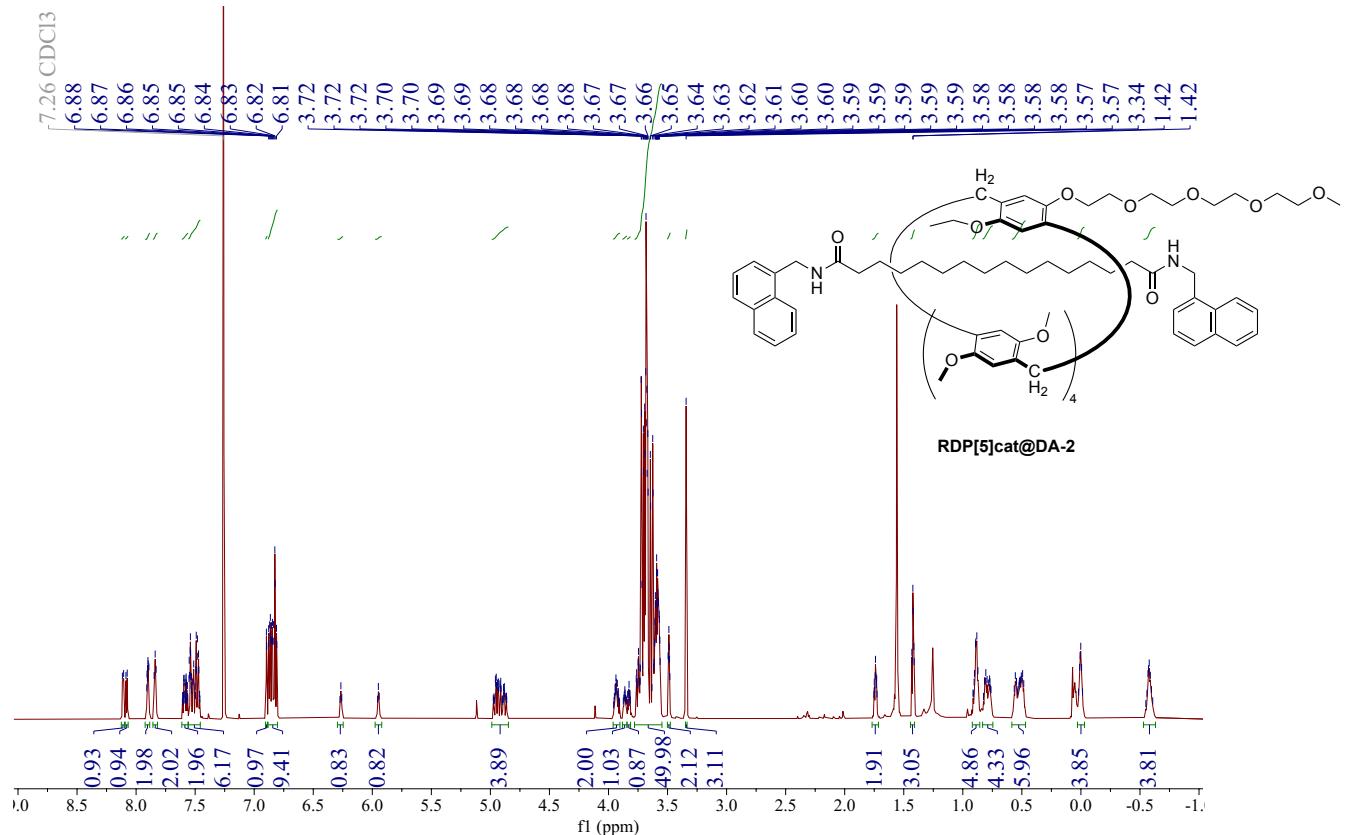
Figure S26. ^{1}H NMR (800 MHz, CDCl$_3$, 298 K) spectrum of **RDP[5]cat@DA-2**.
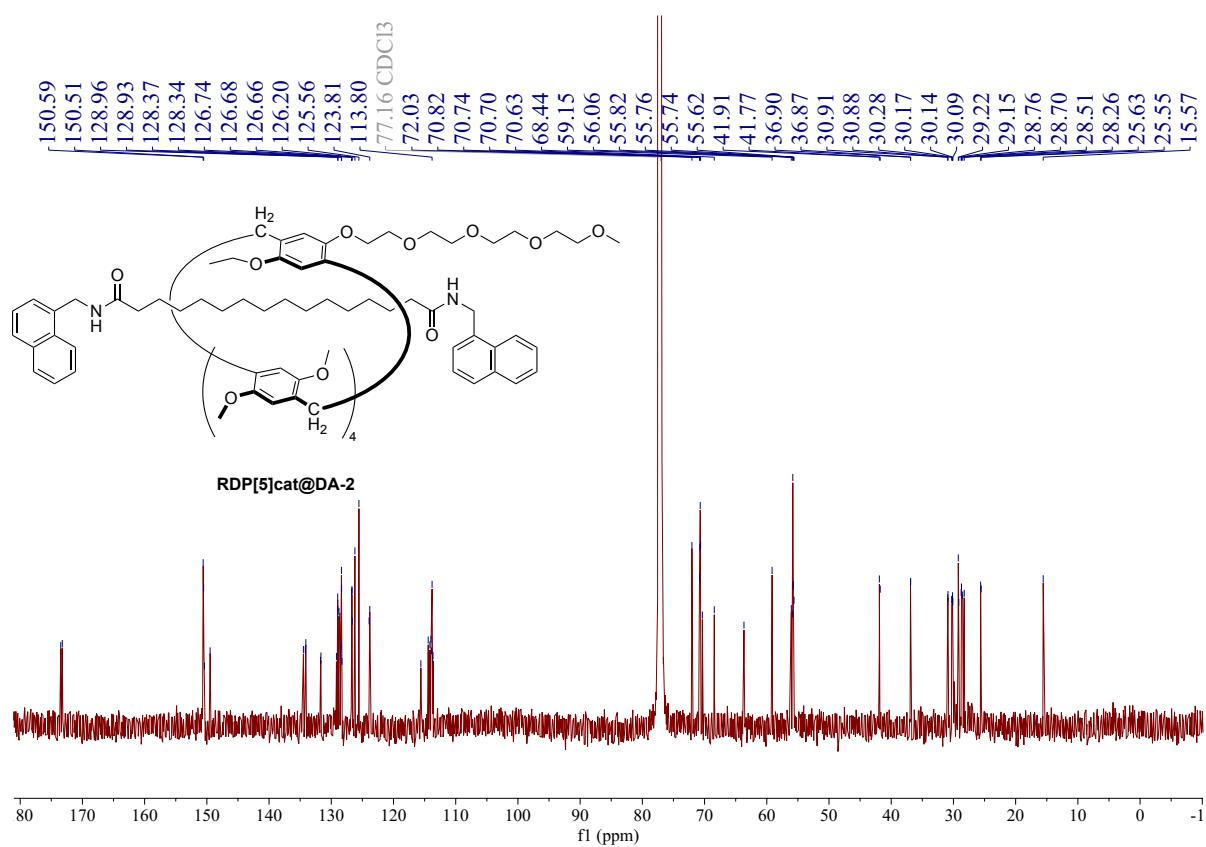
Figure S27. ^{13}C NMR (200 MHz, CDCl$_3$, 298 K) spectrum of **RDP[5]cat@DA-2**.
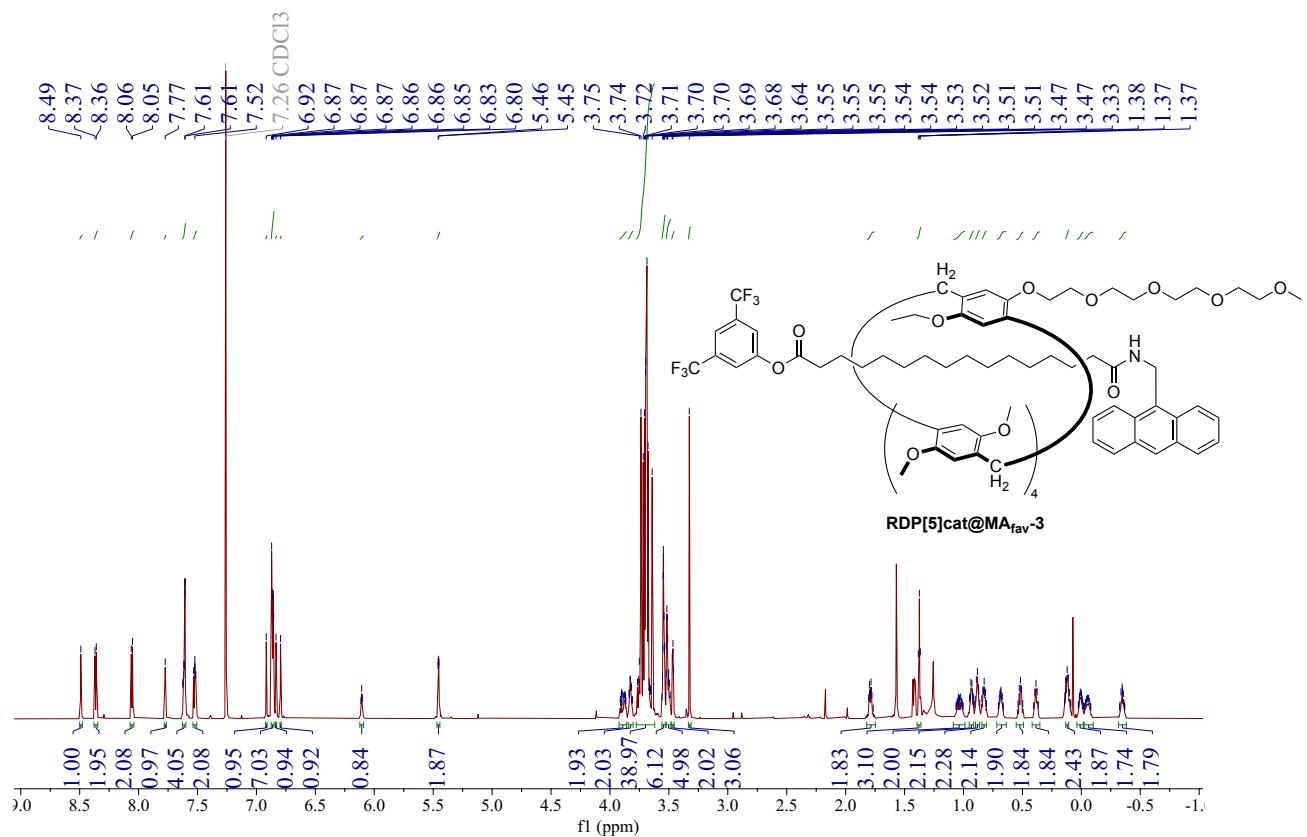
**Figure S28**. ^{1}H NMR (800 MHz, CDCl$_3$, 298 K) spectrum of **RDP[5]cat@MA$_{fav}$-3**.
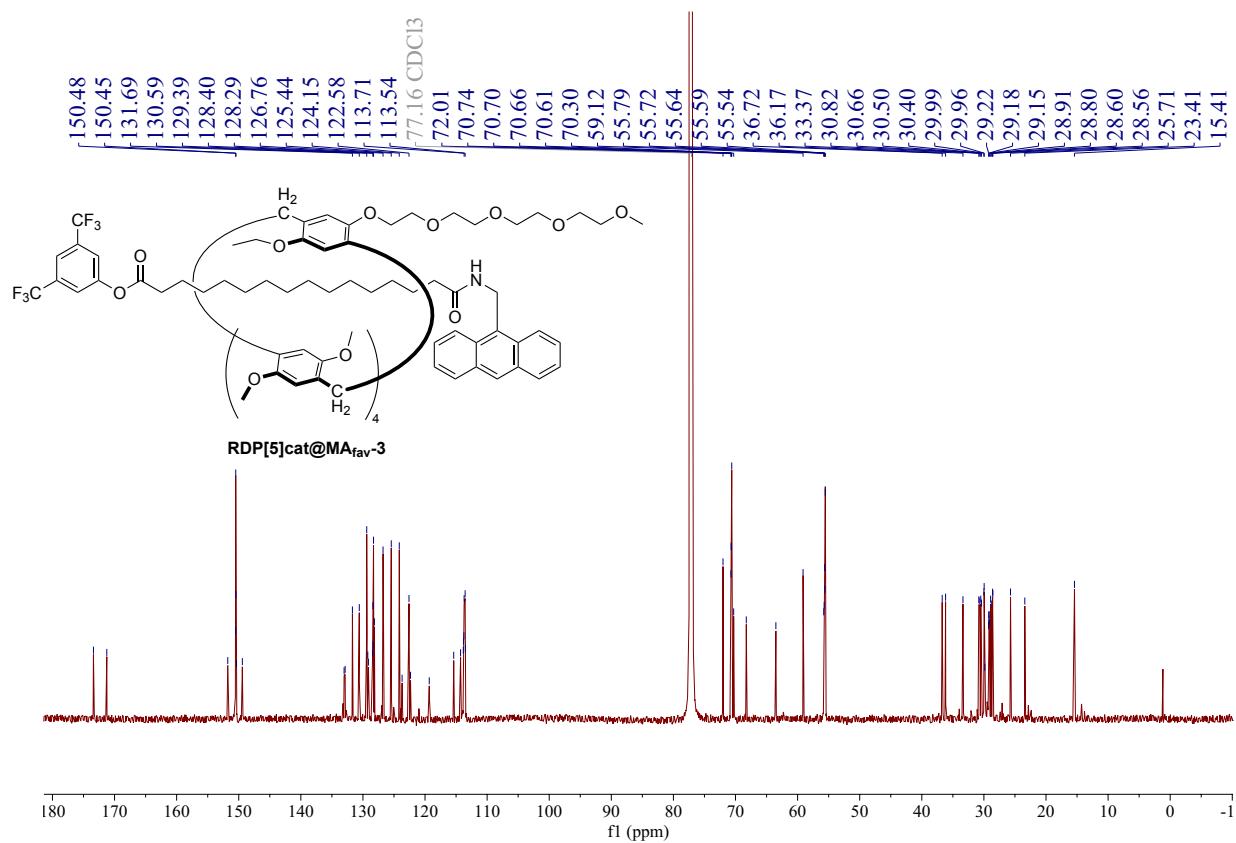
Figure S29. ^{13}C NMR (200 MHz, CDCl$_3$, 298 K) spectrum of **RDP[5]cat@MA$_{fav}$-3**.
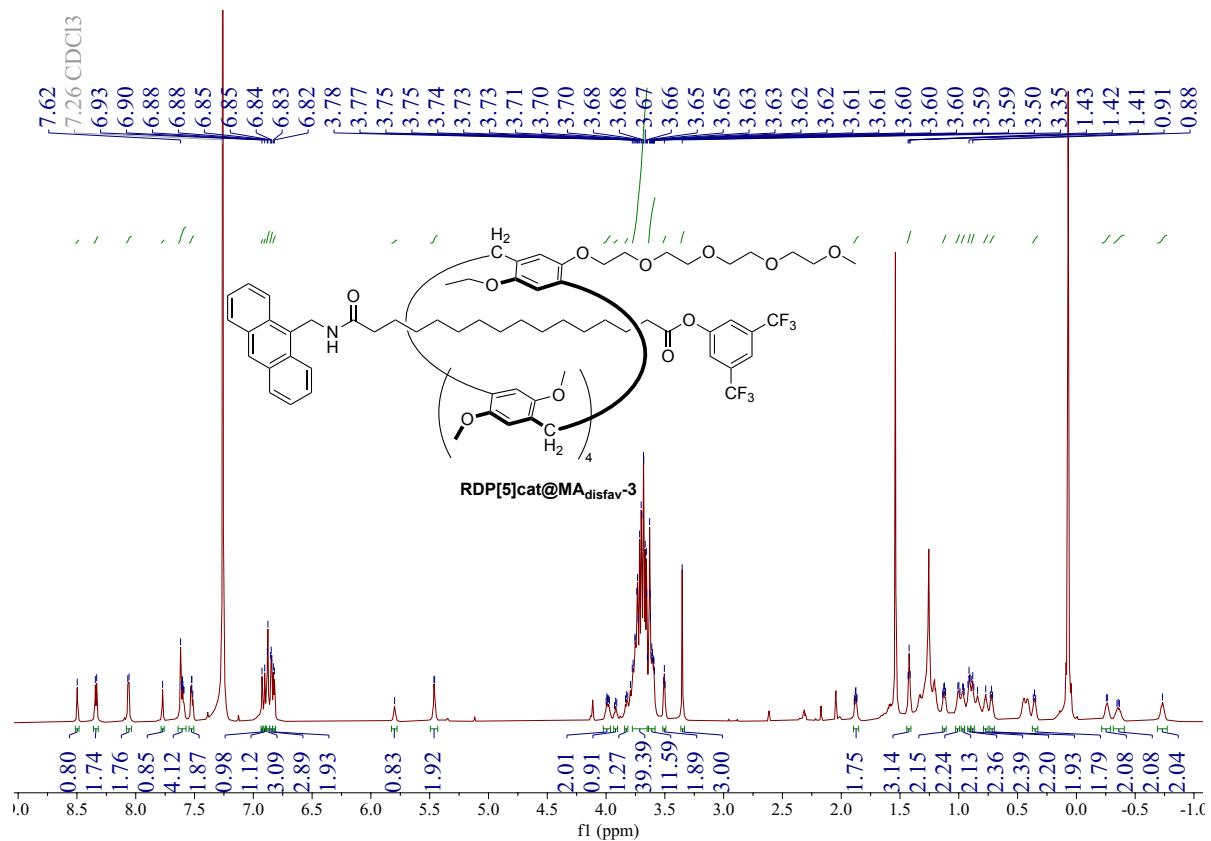
Figure S30. ^{1}H NMR (800 MHz, CDCl$_3$, 298 K) spectrum of **RDP[5]cat@MA$_{disfav}$-3**.
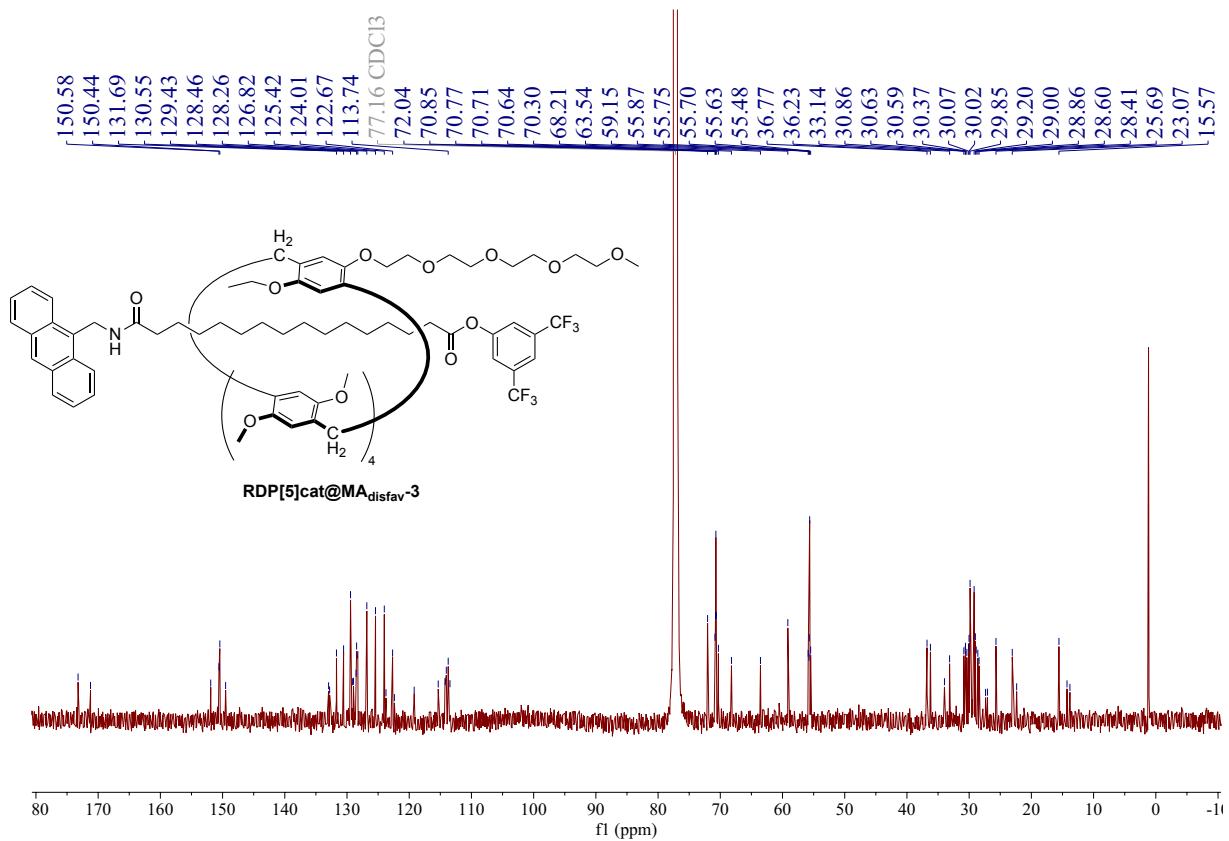
Figure S31. ^{13}C NMR (200 MHz, CDCl$_3$, 298 K) spectrum of **RDP[5]cat@MA$_{disfav}$-3**.
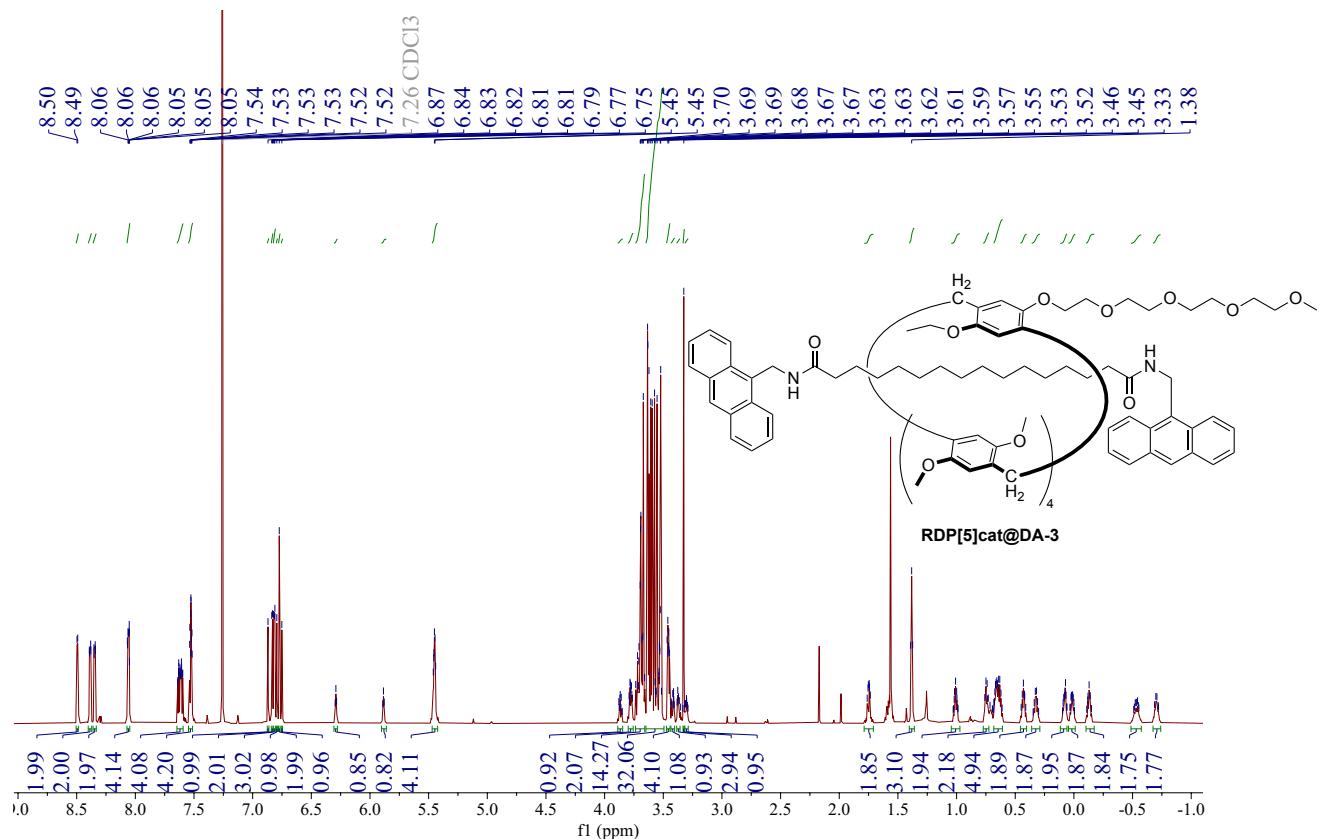
**Figure S32**. ^{1}H NMR (800 MHz, CDCl$_3$, 298 K) spectrum of **RDP[5]cat@DA-3**.
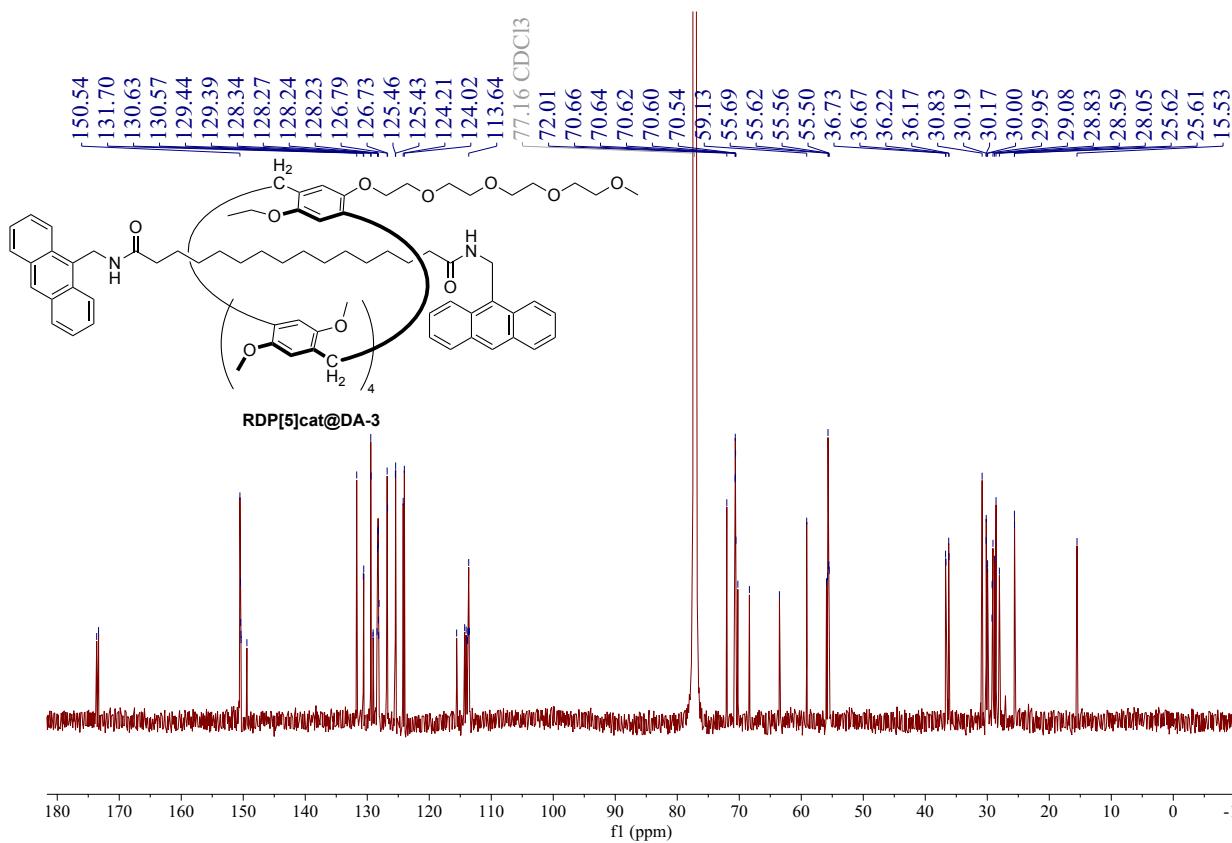
Figure S33. ^{13}C NMR (200 MHz, CDCl$_3$, 298 K) spectrum of **RDP[5]cat@DA-3**.

VI. Supplemental References

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