Electronic Supplementary Material (ESI) for Materials Chemistry Frontiers.

Electronic Supplementary Information

Ring-Opening Metathesis Polymerization of a Strained Stilbene-Based Macrocyclic Monomer

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Materials and Methods

Deuterated solvents were purchased from Cambridge Isotopes. Anhydrous tetrahydrofuran (THF), dimethylformamide (DMF), and pyridine were obtained from a solvent purification system. All other reagents were obtained from commercial sources and used as received. Moisture- and oxygen-sensitive reactions during monomer synthesis were carried out in flame-dried glassware and under an inert atmosphere of purified nitrogen using syringe/septa technique. Thin Layer Chromatography (TLC) was performed using Sorbent Technologies Silica Gel XHT TLC plates. Developed plates were visualized using UV light at wavelengths of 254 and 365 nm. Silica column chromatography was conducted with Zeochem Zeoprep 60 Eco 40-63 μm silica gel. ^{1}H and ^{13}C NMR spectroscopy was performed on a 300, 500, or 600 MHz Bruker NMR spectrometer. Spectra taken in $CDCl_3$ are reported in parts per million (ppm) referenced to TMS (δ 0.00 ppm) for ^{1}H NMR and residual $CHCl_3$ (δ 77.16 ppm) for ^{13}C NMR. Spectra taken in THF-d_8 are reported in parts per million (ppm) referenced to residual protio-solvent (^{1}H: 3.58, 1.72).

MALDI-TOF/MS was performed using a Bruker Daltonics AutoFlex II MALDI-TOF Mass spectrometer. The polymer matrix used was 1,8,9-anthracenetriol in THF, and data was obtained in linear (positive) mode.

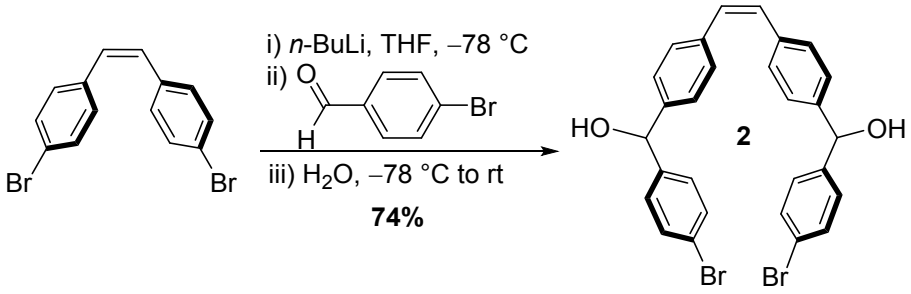
Gel permeation chromatography (GPC) was performed using an Agilent Technologies Infinity Series II pump, 3 in line columns (MZ Gel), Wyatt Technology light scattering and refractive index detectors with tetrahydrofuran (THF) as the mobile phase with an flow rate of 1 mL/min. Number average molecular weights (M_n) and weight-average molecular weights (M_w) were calculated from light scattering and refractive index data using Astra software from Wyatt Technology The absolute weight-average molecular weights were determined by a dn/dc value which was measured by assuming 100% mass recovery of the polymers after passing the columns. The dn/dc of **poly(1)** was found to be 0.246 (mL/g).

Thermogravimetric analysis was performed on a TA TGA Q50 under nitrogen from room temperature to 600 °C at 5 °C/min. Differential Scanning Calorimetry (DSC) was performed on a TA DSC Q250 calorimeter at a heating rate of 10 °C/min and cooling rate of 5 °C/min. The decomposition temperature of the polymer was determined at 2% weight loss. Heatflow in units of watts was recorded and is reported after normalizing by the mass of the sample (W/g).

Synthesis

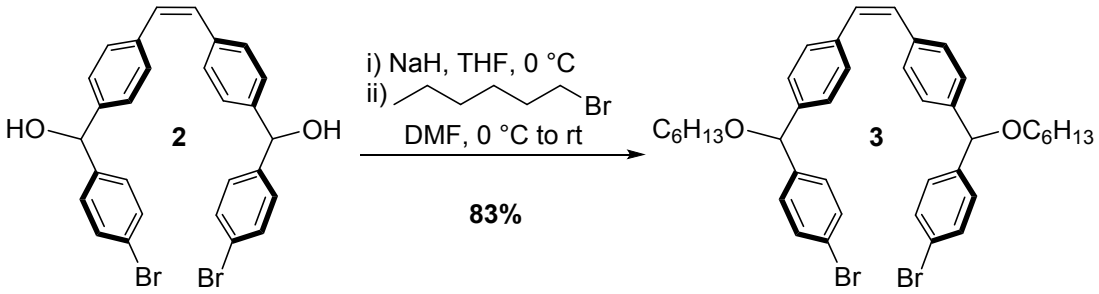
Cis-4,4'-dibromostilbene[1] and initiators **5a** and **5b**[2] were synthesized using previously reported procedures.

(Z)-(ethene-1,2-diylbis(4,1-phenylene))bis((4-bromophenyl)methanol) ***2***



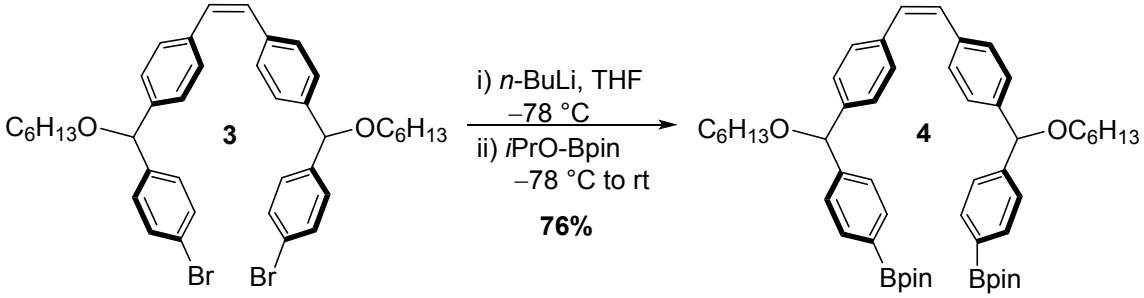
4,4'-dibromostilbene (12.0 g, 35.5 mmol, 1.00 equiv.) and THF (200 mL) were added to a 500 mL round bottom flask with a magnetic stir bar. The solution was cooled to -78 °C, then *n*-butyllithium (31.6 mL, 2.3 M in hexane, 2.05 equiv.) was added over the course of 20 min. After stirring at -78 °C for 3 min, 4-bromobenzaldehyde (13.1 g, 71.0 mmol, 2.00 equiv.) in THF (40 mL) was added in stream via cannula, during which the solution gradually became viscous with solid crashed out. The cold bath was removed and the mixture was kept stirring at room temperature for 2 hours. The reaction mixture was quenched with water (20 mL). The THF was removed under reduced pressure, then DCM (200 mL) was added to the mixture, which was washed with water (100 mL) and brine (100 mL) and dried over Na_2SO_4. Concentration under reduced pressure resulted in a yellow gel. The material was dissolved in DCM (80 mL) and stored in the freezer (-20 °C) overnight, resulting in powdered precipitate. The precipitate was collected by filtration and washed with DCM (10 mL) to give the product as a white powder (7.55 g). The filtrate was concentrated and the residue was purified by column chromatography (silica, 0% to 3% ethyl acetate in DCM) to yield more product (6.58 g). Overall, the product was obtained in a yield of 74%. ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.46 (d, *J* = 8.4 Hz, 4H, Ar-H), 7.25 (d, *J* = 8.4 Hz, 4H, Ar-H), 7.22 (d, *J* = 8.4 Hz, 4H, Ar-H), 7.19 (d, *J* = 8.4 Hz, 4H, Ar-H), 6.55 (s, 2H, C=C-H), 5.76 (d, *J* = 3.4 Hz, 2H, CH), 2.18 (d, *J* = 3.4 Hz, 2H, OH); ^{13}C NMR (150 MHz, $CDCl_3$): δ 142.74, 142.34, 136.90, 131.73, 130.11, 129.25, 128.34, 126.59, 121.63, 75.62. IR (neat): 3264.5, 1484.0, 1404.3, 1172.5, 1067.9, 1027.3, 1008.0, 819.5, 799.7 cm^{-1}. HRMS (TOF MS ASAP+) (m/z): $[M+H]^+$ calculated for $C_{28}H_{23}Br_2O_2$: 549.0065; found 549.0039.

*(Z)-1,2-bis(4-((4-bromophenyl)(n-hexyloxy)methyl)phenyl)ethene **3***



NaH (4.10 g, 60 wt% in mineral oil, 102.5 mmol, 4.00 equiv.) and THF (150 mL) were added to a 500 mL round bottom flask. The slurry was cooled to 0 °C at which point **X** (14.1 g, 25.6 mmol, 1.00 equiv.) in THF (30 mL) was added in stream. The mixture was stirred at 0 °C for 1 hour. Then 1-bromohexane (28.8 mL, 205 mmol, 8.00 equiv.) and DMF (30 mL) were added and the reaction was stirred at room temperature overnight. The reaction was carefully quenched with water. After THF was removed under vacuum, DCM (150 mL) was added. The solution was washed with water (100 mL), 5 wt% aqueous LiCl solution (3×100 mL), and brine (100 mL) and dried over Na_2SO_4. After concentration under reduced pressure, the crude solid was purified via column chromatography (silica, 0% to 8% ethyl acetate in hexanes) to yield a colorless oil (15.0 g, 83%). ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.44 (d, *J* = 8.4 Hz, 4H, Ar-H), 7.22 (d, *J* = 8.4 Hz, 4H, Ar-H), 7.20 (d, *J* = 8.1 Hz, 4H, Ar-H), 7.15 (d, *J* = 8.1 Hz, 4H, Ar-H), 6.52 (s, 2H, C=C-H), 5.24 (s, 2H, CH), 3.42 (td, *J* = 6.6, 3.1 Hz, 4H, OCH_2), 1.62 (dt, *J* = 15.0, 6.6 Hz, 4H, CH_2), 1.37 (p, *J* = 7.0 Hz, 4H, CH_2), 1.33-1.22 (overlap, 8H, CH_2), 0.88 (t, *J* = 7.0 Hz, 6H, CH_3); ^{13}C NMR (150 MHz, $CDCl_3$): δ 141.75, 141.14, 136.61, 131.58, 130.01, 129.03, 128.82, 126.89, 121.36, 82.87, 69.46, 31.79, 29.94, 26.04, 22.75, 14.21. IR (neat): 2927.3, 2855.3, 1484.3, 1395.0, 1088.7, 1069.8, 1009.8, 816.0, 799.2 cm^{-1}. HRMS (TOF MS ASAP+) (m/z): $[M+H]^+$ calculated for $C_{40}H_{47}Br_2O_2$: 717.1943; found 717.1893.

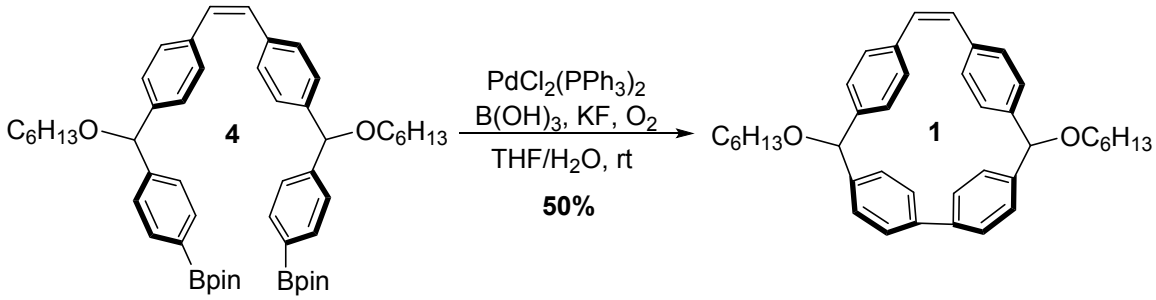
*(Z)-1,2-bis(4-((n-hexyloxy)(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)-methyl)phenyl)ethene **4***



3 (14.7 g, 20.5 mmol, 1.00 equiv.) was dissolved in THF and cooled to -78 °C. Then *n*-butyllithium (21.5 mL, 2.3 M in hexane, 2.40 equiv.) was added slowly via syringe. Isopropyl pinacol borate (16.7 mL, 81.8 mmol, 4.00 equiv.) was quickly added in stream. The mixture was stirred at -78 °C for 5 min. and allowed to warm to room temperature. After 2 hours, the reaction was carefully quenched with water. The mixture was extracted

with dichloromethane (3×), and the combined organic layers were washed with brine and dried over Na_2SO_4. The material was purified by column chromatography (silica, 0% to 8% ethyl acetate in hexanes), yielding a colorless oil (12.4 g, 76%). ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.77 (d, *J* = 8.0 Hz, 4H, Ar-H), 7.36 (d, *J* = 8.0 Hz, 4H, Ar-H), 7.22-7.13 (m, 8H, Ar-H), 6.48 (s, 2H, C=C-H), 5.29 (s, 2H, CH), 3.42 (t, *J* = 6.7 Hz, 4H, OCH_2), 1.63 (dt, *J* = 15.0, 6.7 Hz, 4H, CH_2), 1.42-1.20 (overlap, 36H, CH_2 and CH_3), 0.88 (t, *J* = 6.9 Hz, 6H, CH_3); ^{13}C NMR (150 MHz, $CDCl_3$): δ 145.76, 141.52, 136.38, 135.01, 129.91, 128.92, 126.94, 126.48, 83.86, 83.53, 69.43, 31.82, 29.97, 26.05, 25.01, 22.76, 14.22, ^{13}C-B signal not observed. IR (neat): 2929.0, 2856.5, 1610.9, 1511.2, 1397.2, 1357.4, 1319.2, 1270.6, 1142.6, 1085.9, 1019.6, 961.8, 858.2, 824.7, 798.9, 656.7 cm^{-1}. HRMS (TOF MS ASAP+) (m/z): $[M+H]^+$ calculated for $C_{52}H_{71}B_2O_6$: 813.5437; found 813.5327.

(Z)-3,8-bis(n-hexyloxy)-1,2,4,7(1,4)-tetrabenzenacyclooctanophan-5-ene ***1***



Bisboronate **4** (3.00 g, 3.76 mmol, 1.00 equiv.), $PdCl_2(PPh_3)_2$ (0.26 g, 0.38 mmol, 0.10 equiv.), and $B(OH)_3$ (1.16 g, 18.8 mmol, 5.00 equiv.) were dissolved in THF (450 mL) in a 500 mL round bottom flask equipped with a stir bar. The mixture was stirred open to air at room temperature for 10 min. until a clear yellow solution was achieved. Then KF (0.44 g, 7.52 mmol, 2.00 equiv.) was dissolved in water (45 mL) and added. The mixture was sonicated until orange color appeared, after which it was stirred overnight at room temperature. After THF was removed under vacuum, DCM was added. The solution was washed with water and brine and dried over Na_2SO_4. The material was purified by column chromatography (silica, 0% to 50% DCM in hexanes), yielding a colorless oil which solidified upon standing (1.05 g, 50%). ^{1}H NMR (600 MHz, $CDCl_3$): δ *trans* 7.45 (dd, *J* = 8.5, 2.0 Hz, 2H, Ar-H), 7.39 (dd, *J* = 8.5, 2.0 Hz, 2H, Ar-H), 7.35 (dd, *J* = 8.3, 2.0 Hz, 2H, Ar-H), 7.02 (dd, *J* = 8.3, 2.0 Hz, 2H, Ar-H), 6.65 (d, *J* = 8.3 Hz, 4H, Ar-H), 6.52 (d, *J* = 8.3 Hz, 4H, Ar-H), 6.45 (s, 2H, C=C-H), 5.28 (s, 2H, CH), 3.77 (dt, *J* = 9.0, 6.7 Hz, 2H, OCH_2), 3.61 (dt, *J* = 9.0, 6.7 Hz, 2H, OCH_2), 1.78-1.69 (m, 4H, CH_2), 1.50-1.41 (m, 4H, CH_2), 1.37-1.26 (overlap, 8H, CH_2), 0.90 (t, *J* = 6.9 Hz, 6H, CH_3); *cis* 7.46 (dd, *J* = 8.5, 2.0 Hz, 2H, Ar-H), 7.39 (dd, *J* = 8.5, 2.0 Hz, 2H, Ar-H), 7.34 (dd, *J* = 8.3, 2.0 Hz, 2H, Ar-H), 7.03 (dd, *J* = 8.3, 2.0 Hz, 2H, Ar-H), 6.65 (d, *J* = 8.3 Hz, 4H, Ar-H), 6.53 (d, *J* = 8.3 Hz, 4H, Ar-H), 6.46 (s, 2H, C=C-H), 5.27 (s, 2H, CH), 3.77 (dt, *J* = 9.0, 6.7 Hz, 2H, OCH_2), 3.61(dt, *J* = 9.0, 6.7 Hz, 2H, OCH_2), 1.78-1.69 (m, 4H, CH_2), 1.50-1.41 (m, 4H, CH_2), 1.37-1.26 (overlap, 8H, CH_2), 0.90 (t, J = 6.9 Hz, 6H, CH_3); ^{13}C NMR (150 MHz, $CDCl_3$): δ *trans* 144.48, 142.46, 140.92, 135.90, 130.71, 128.30, 128.03, 127.94, 127.36, 126.43, 125.87, 82.65, 69.59, 31.88, 30.06, 26.15, 22.81, 14.23; *cis* 144.50, 142.51, 140.96, 135.87, 130.70, 128.28, 127.91, 127.14, 126.58, 125.78, 82.60, 69.56, 31.89, 30.06, 25.15, 22.81,

14.24. IR (neat): 2950.6, 2925.6, 2851.0, 1450.0, 1414.2, 1332.9, 1186.3, 1094.1, 1015.2, 836.8, 805.2, 751.0, 735.1, 705.9 cm^{-1}. HRMS (TOF MS ASAP+) (m/z): $[M+H]^+$ calculated for $C_{40}H_{47}O_2$: 559.3576; found 559.3565.

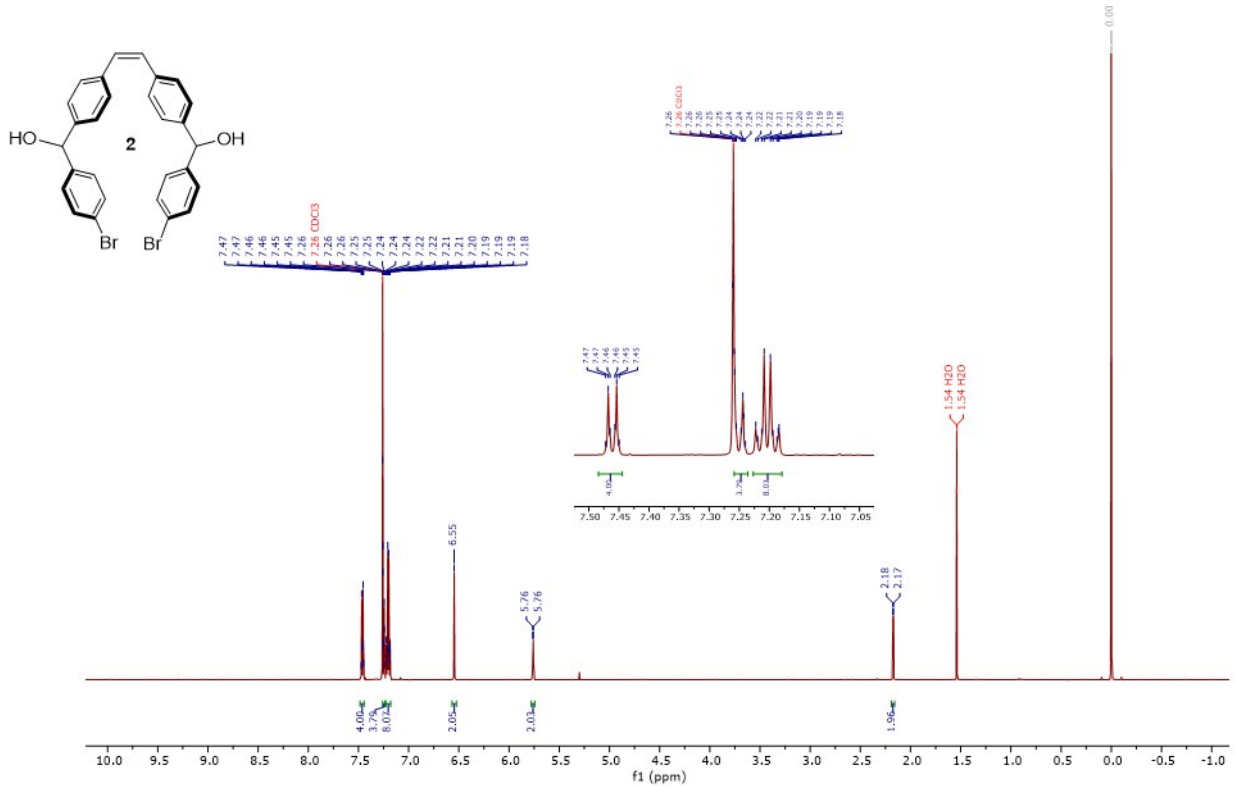


Fig. S1 *^{1}H NMR spectrum of **2** in $CDCl_3$.*

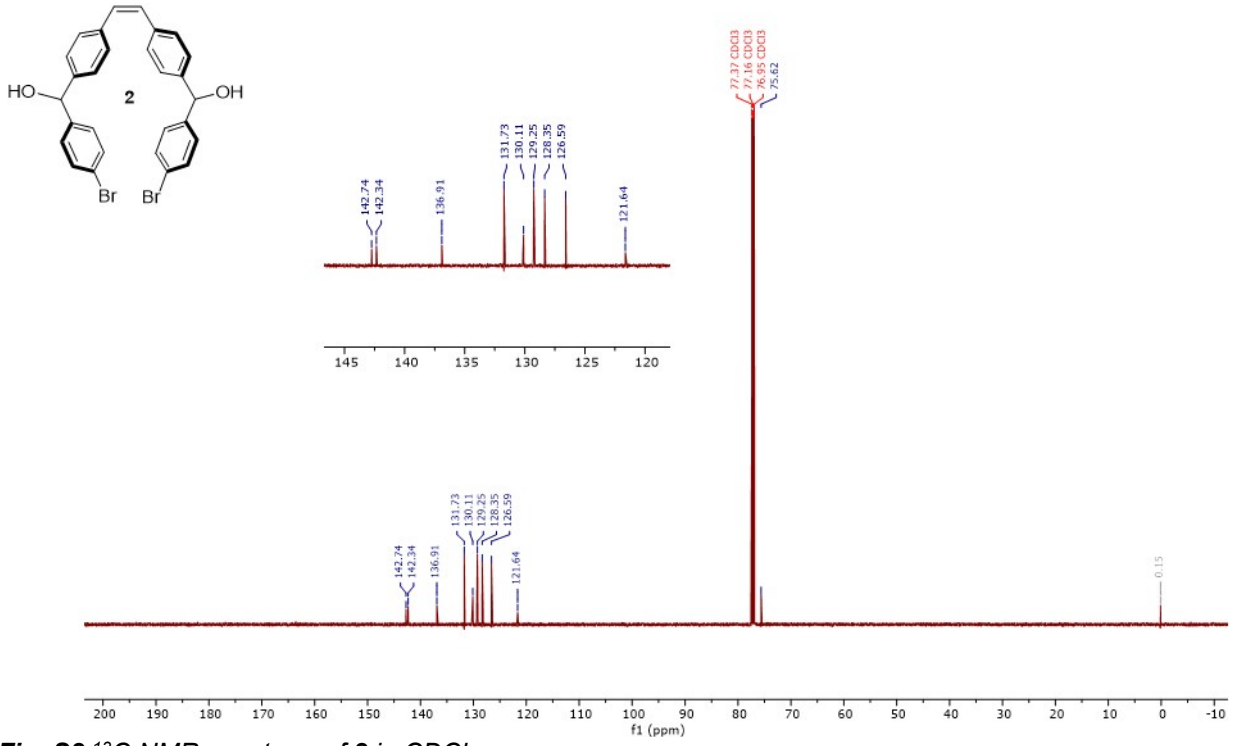


Fig. S2 *^{13}C NMR spectrum of **2** in $CDCl_3$.*

NMR Spectra

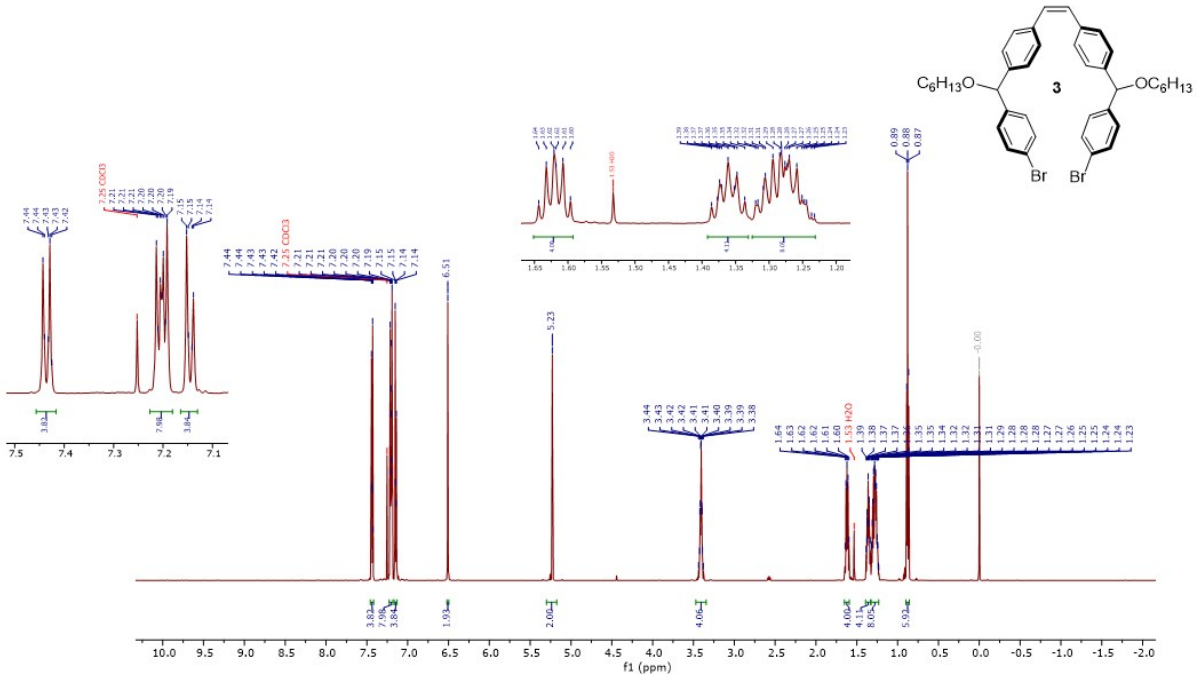


Fig. S3 *^{1}H NMR spectrum of **3** in $CDCl_3$.*

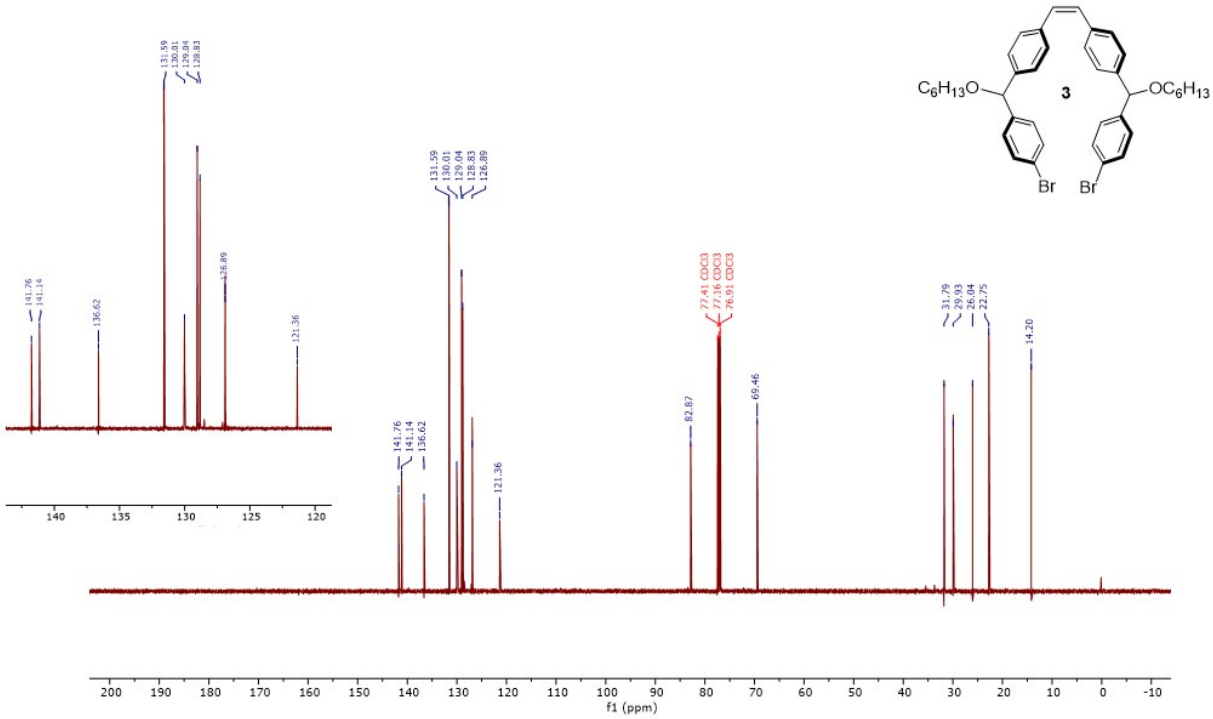


Fig. S4 *^{13}C NMR spectrum of **3** in $CDCl_3$.*

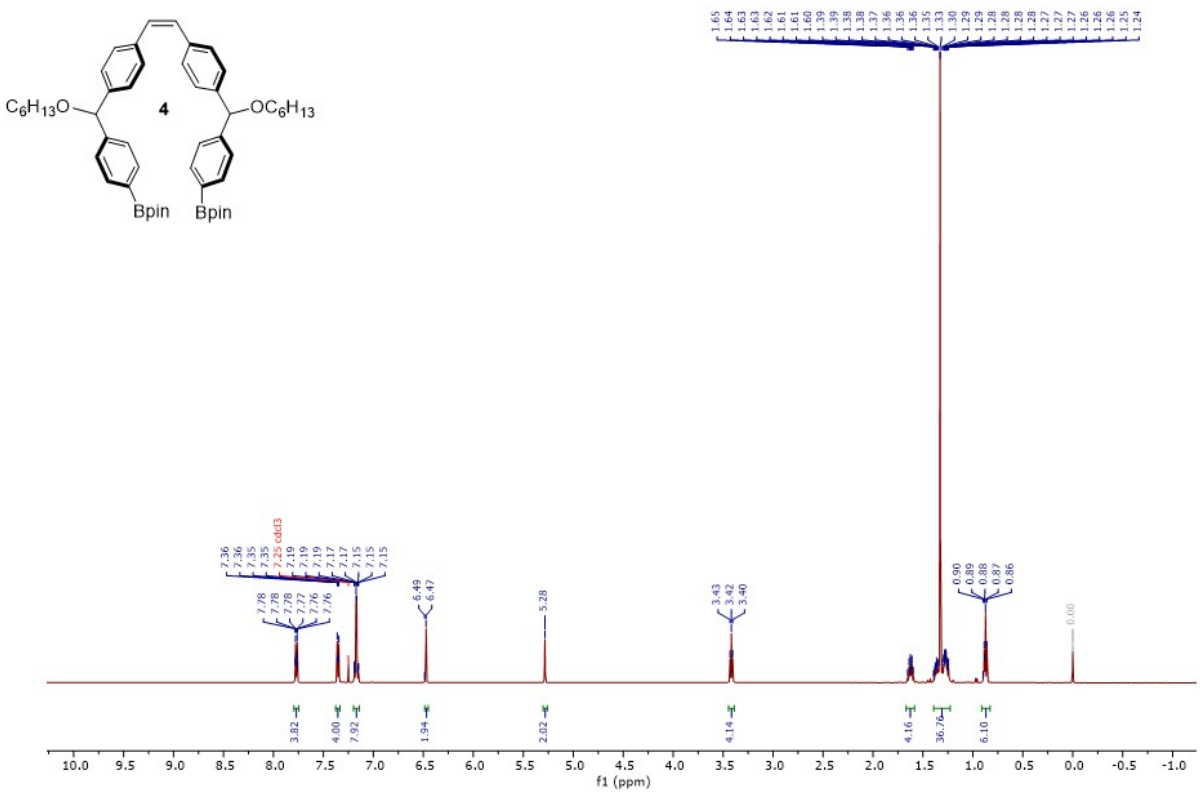


Fig. S5 *^{1}H NMR spectrum of **4** in $CDCl_3$.*

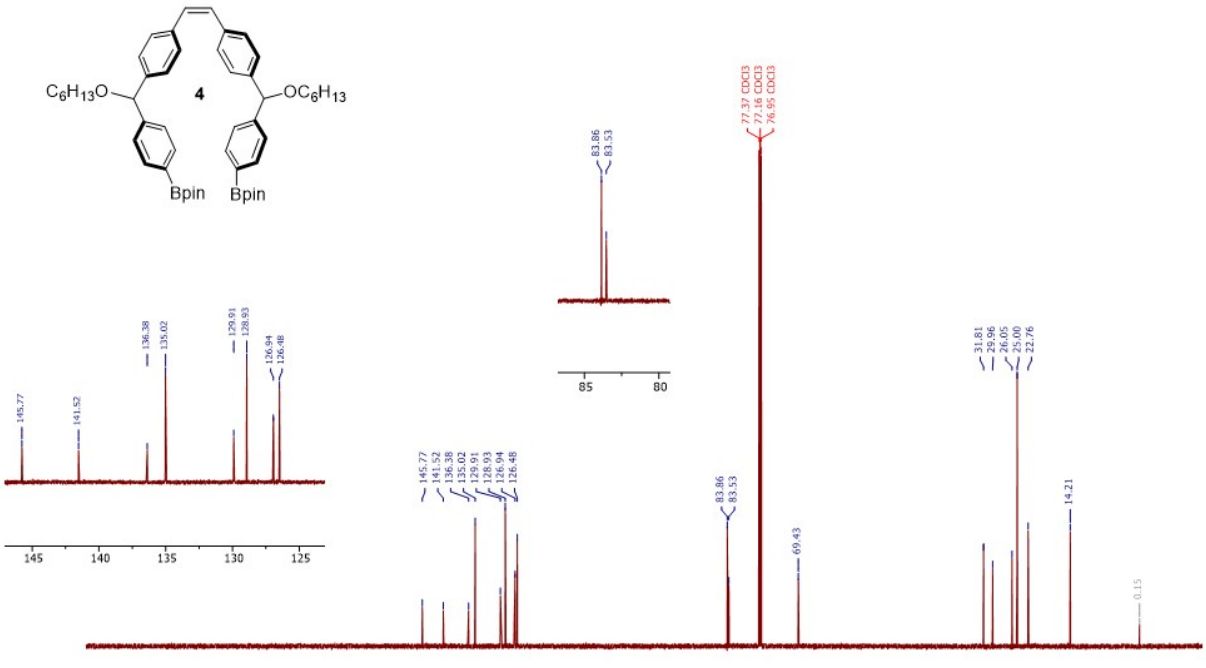


Fig. S6 *^{13}C NMR spectrum of **4** in $CDCl_3$.*

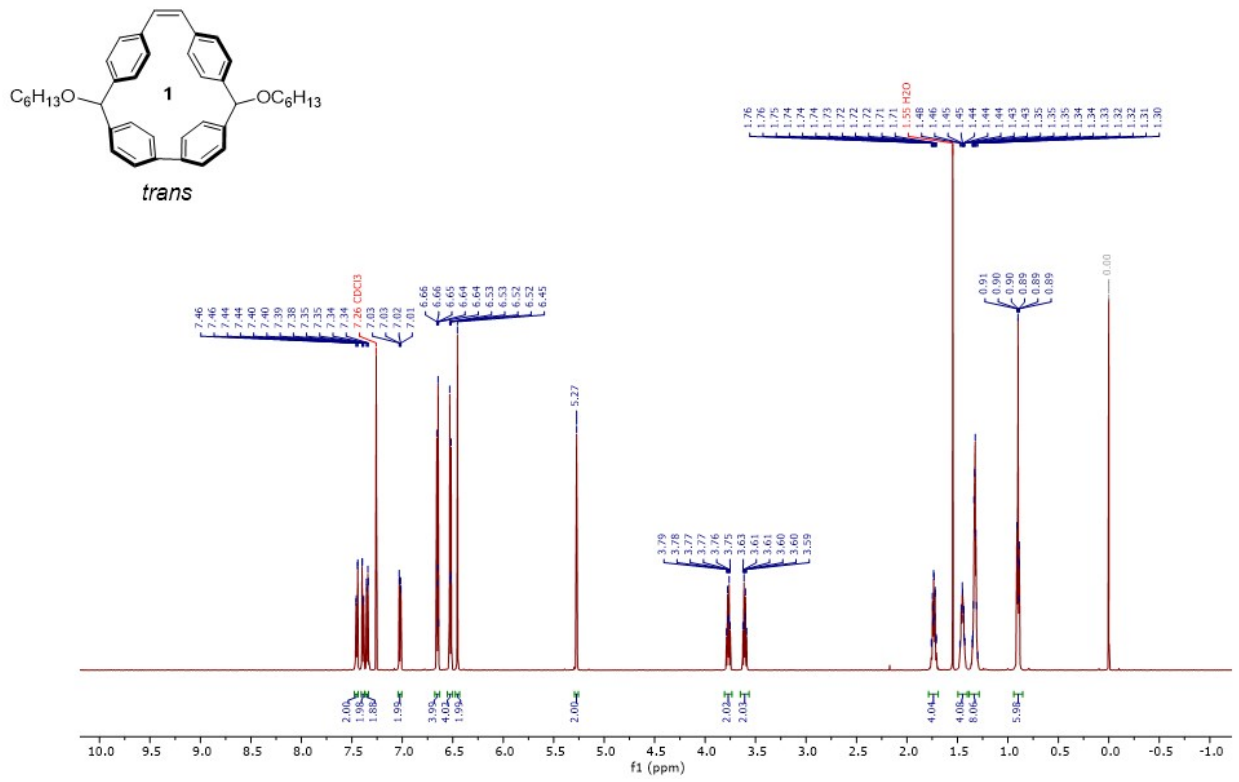


Fig. S7 *^{1}H NMR spectrum of **1** in $CDCl_3$.*

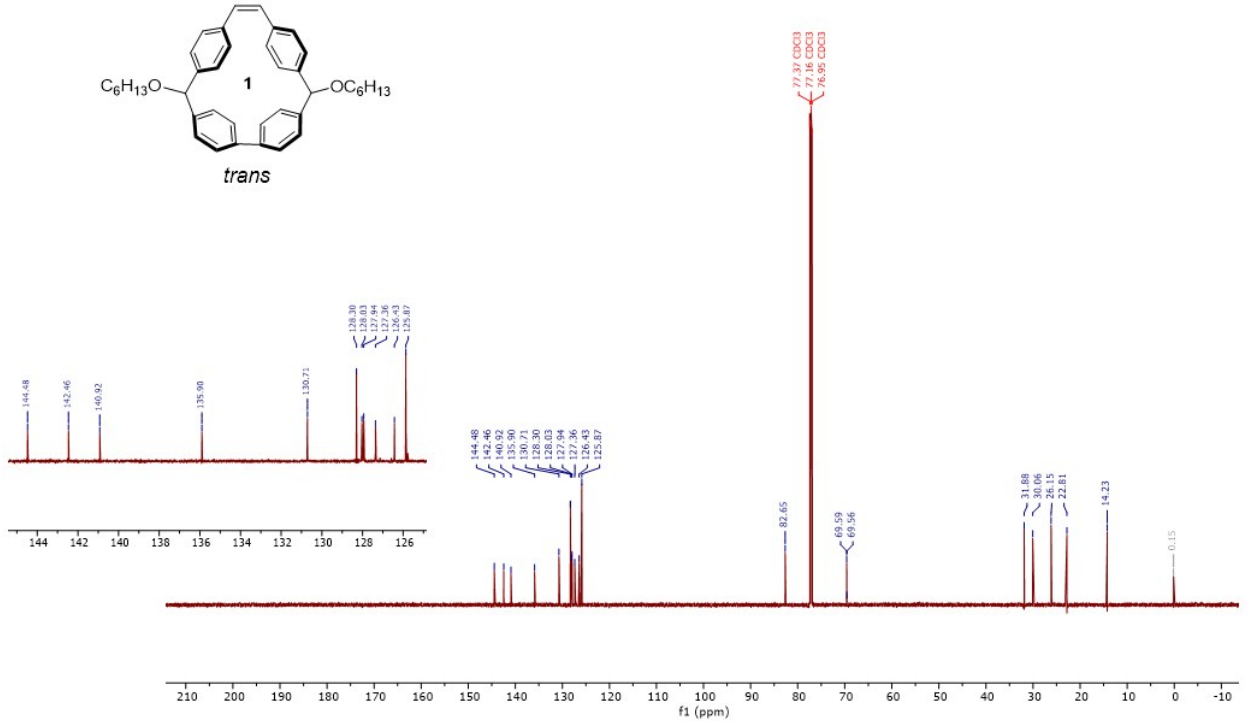


Fig. S8 *^{1}H NMR spectrum of **1** in $CDCl_3$.*

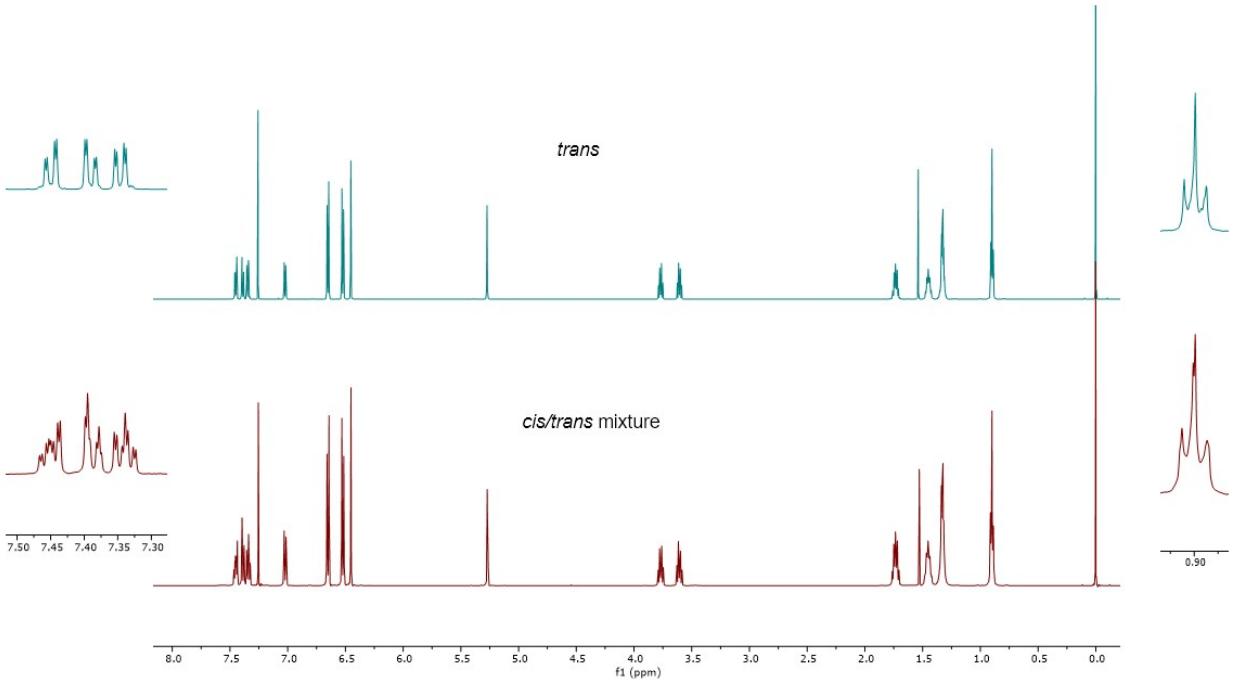


Fig. S9 *^{1}H NMR comparing trans isomer and a mixture of cis and trans isomers for the benzylether of* ***1****.*

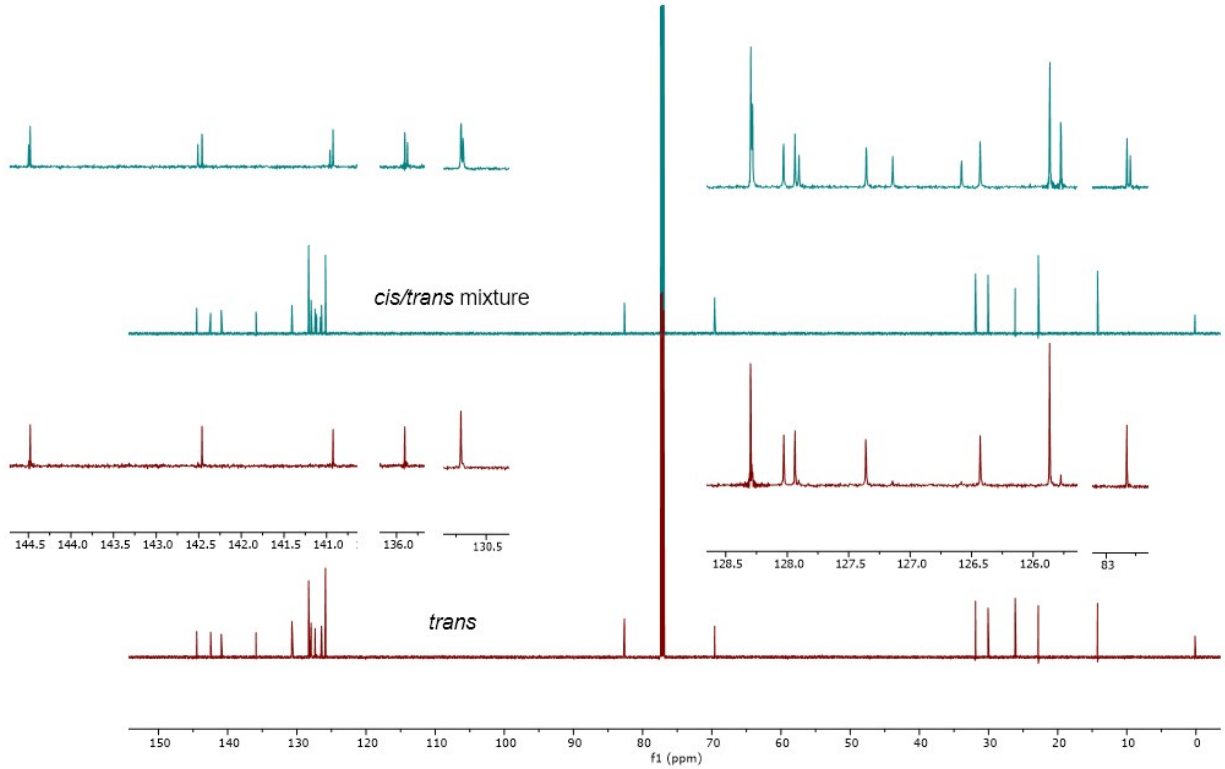


Fig. S10 *^{13}C NMR comparing trans isomer and a mixture of cis and trans isomers for the benzylether of* ***1****.*

Polymerization Studies

General Kinetics Procedure
In a dry box, **1** (0.110 g, 0.2 mmol) was added to a 7 mL vial. To the 7 ml vial **5b** (0.005 g, 0.002 mmol) in 0.2 mL of THF-d_8 was added, before being transferred and sealed in a screwcap NMR tube. After 10 minutes of equilibration time at room temperature the NMR tube was placed in a preheated NMR spectrometer. After 16 hours the polymerization was quenched via the addition 0.1 mL of ethyl vinyl ether in 1 mL of THF. Crude GPC was obtained before precipitation of the polymer into cold methanol. The polymer was isolated via vacuum filtration to provide **poly(1)** as a white solid (0.0825g, 75% yield, M_n:15.2 kDa, M_w: 23.4 kDa, $Đ$: 1.5).

Molecular Weight vs. Conversion
In a dry box, **1** (0.4965 g, 0.89 mmol) was charged into a flame-dried and N_2-purged 25 mL 3-neck flask with 7.9 mL of anhydrous THF and sealed, before being removed from the glovebox and being placed in a 34 °C oil bath. An oven-dried 7 mL vial was charged with **5b** (0.0228 g, 0.026 mmol) and 1 mL of anhydrous THF before being sealed and removed from the glovebox. The solution of **5b** was added to the 3-neck flask, followed by the immediate removal of a 0.2 mL aliquot of the reaction mixture which was quenched with 1 mL ethyl vinyl ether. The sample was split into 2 equal portions. GPC data was gathered on one portion and conversion was determined with the remaining.

Polymer-Polymer Molecular Weight Equilibrium
In a dry box, 71.5 kDa **poly(1)** (0.0788 g, 0.0011 mmol) and 15.2 kDa **poly(1)** (0.0167 g, 0.0011 mmol) were charged into a 2-dram vial followed by 0.512 mL of anhydrous THF. **5b** (0.00973 g, 0.0011 mmol) was added and the vial was removed from the dry box and placed into 40 °C oil bath. After 3.5 hours, the reaction was quenched with ethyl vinyl ether and diluted with THF before obtaining a crude GPC.

Polymer-trans-stilbene Molecular Weight Equilibrium
In a dry box, 41.5 kDa **poly(1)** (0.0748 g, 0.0018 mmol) was added to a 7 mL vial, followed by **5b** (0.0012 g, 0.002 mmol), *trans*-stilbene (0.024 g, 0.133 mmol) and 0.3 mL of anhydrous THF. The vial was placed in a 40 °C oil bath. After 3.5 hours the reaction was quenched with ethyl vinyl ether and diluted with THF before obtaining a crude GPC.

Polymer Characterization

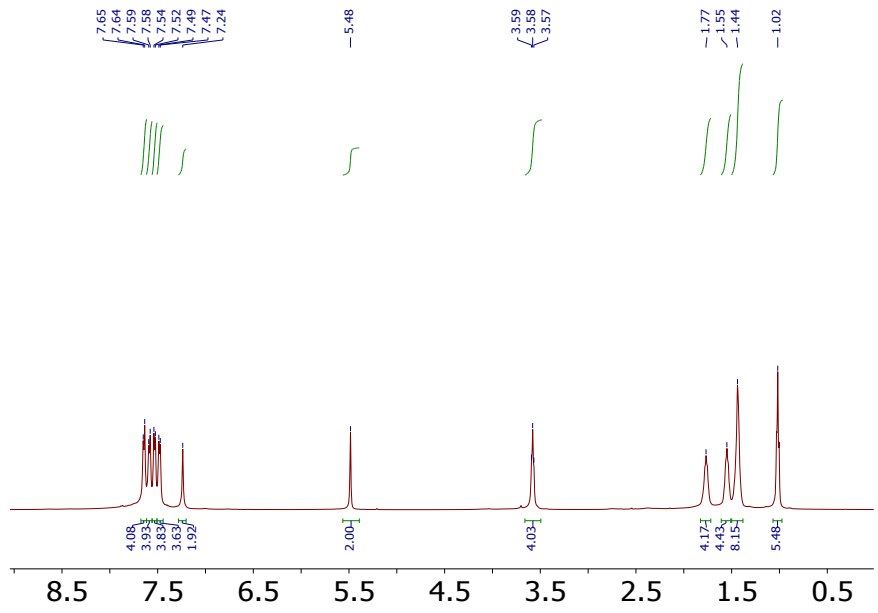


Fig. S11 *^{1}H NMR spectrum for* ***poly(1)*** *in THF-d_8.*

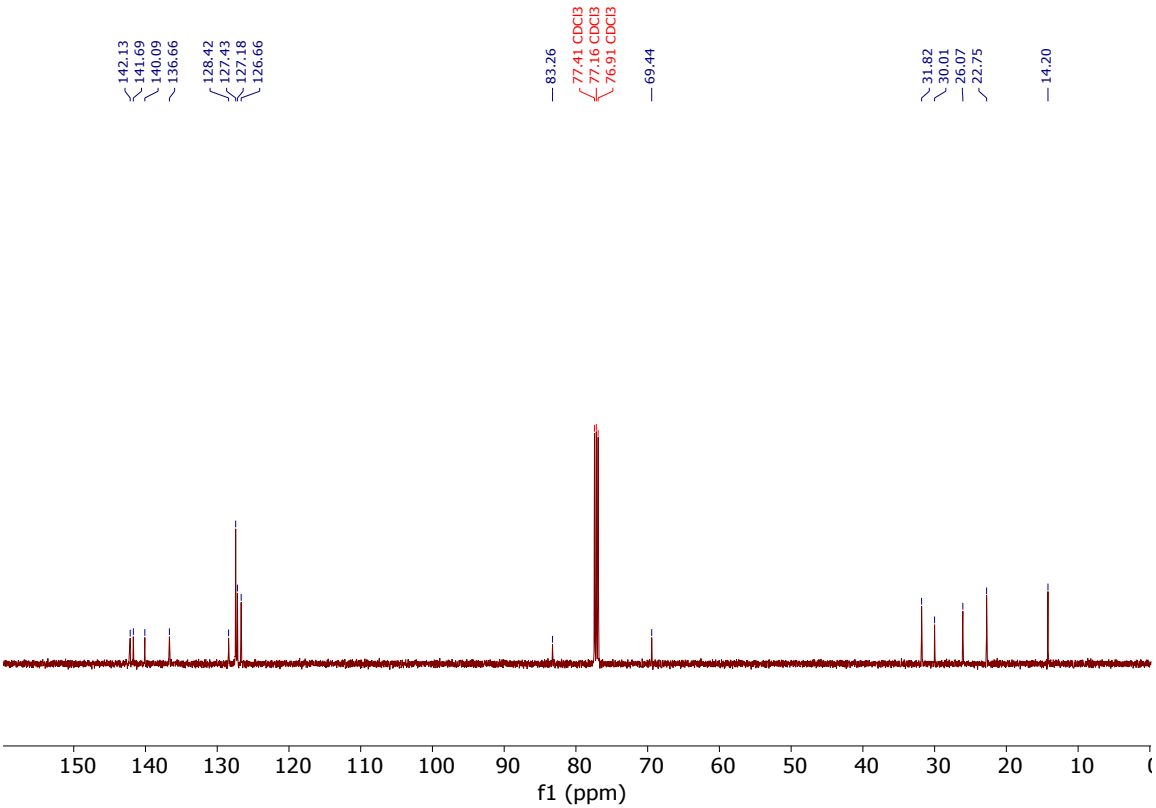


Fig. S12 *^{13}C NMR spectrum for* ***poly(1)*** *in $CDCl_3$.*

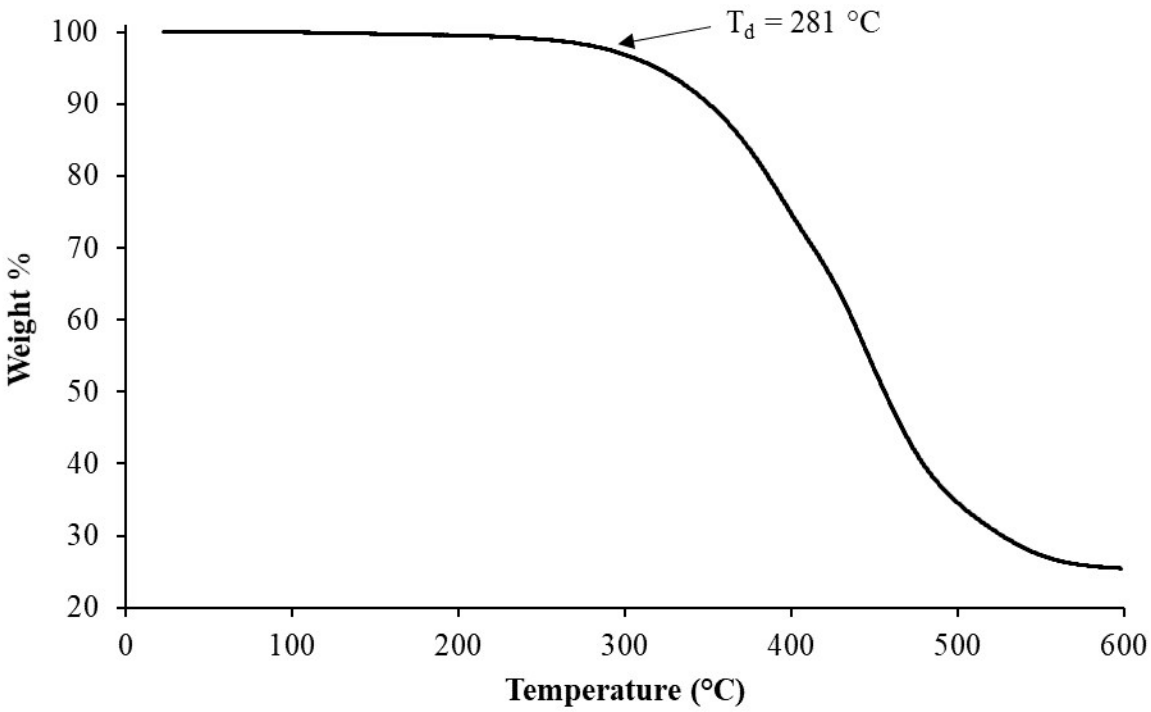


Fig. S13 *TGA trace for* ***poly(1)*** *under N_2 atmosphere.*

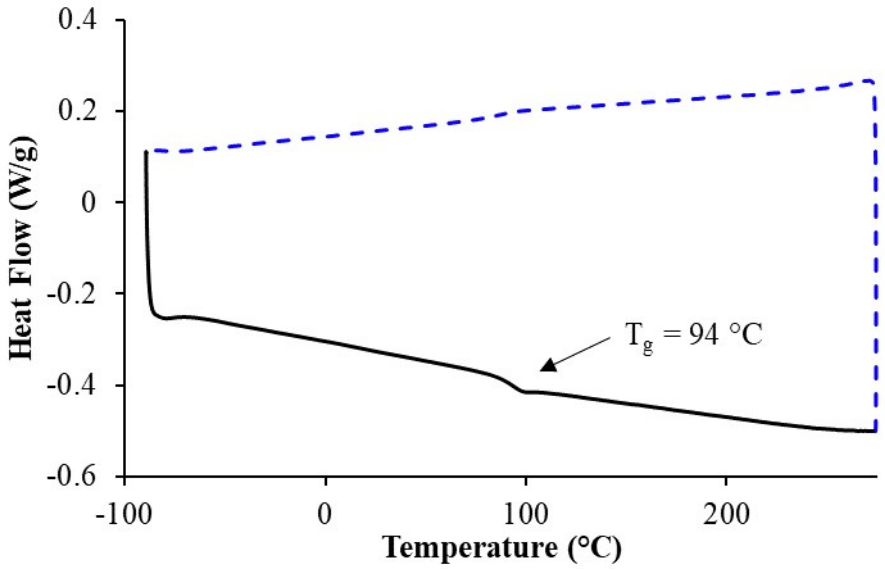


Fig. S14 *DSC trace for* ***poly(1)*** *showing the first cooling cycle (dashed blue) and second heating cycle (solid black).*

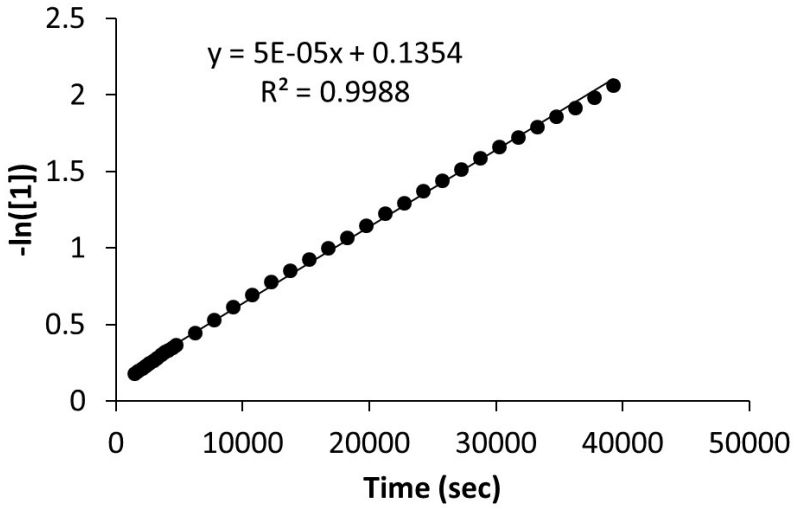
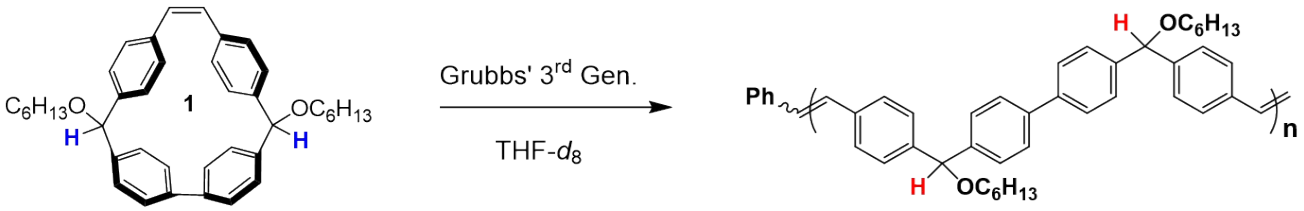


Fig. S15 *First order kinetics plot for the consumption of **1** over the course of the polymerization.*



poly(1)

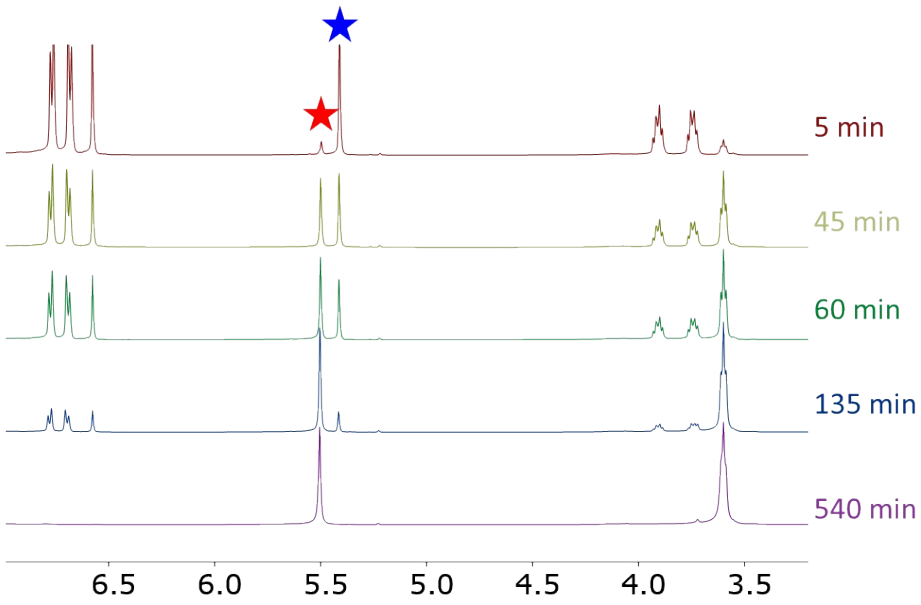


Fig. S16 *^{1}H NMR spectra showing the progression of the polymerization. Conversion was determined following the transformation of the benzylic ether hydrogen from monomer (blue star) to polymer (red star).*

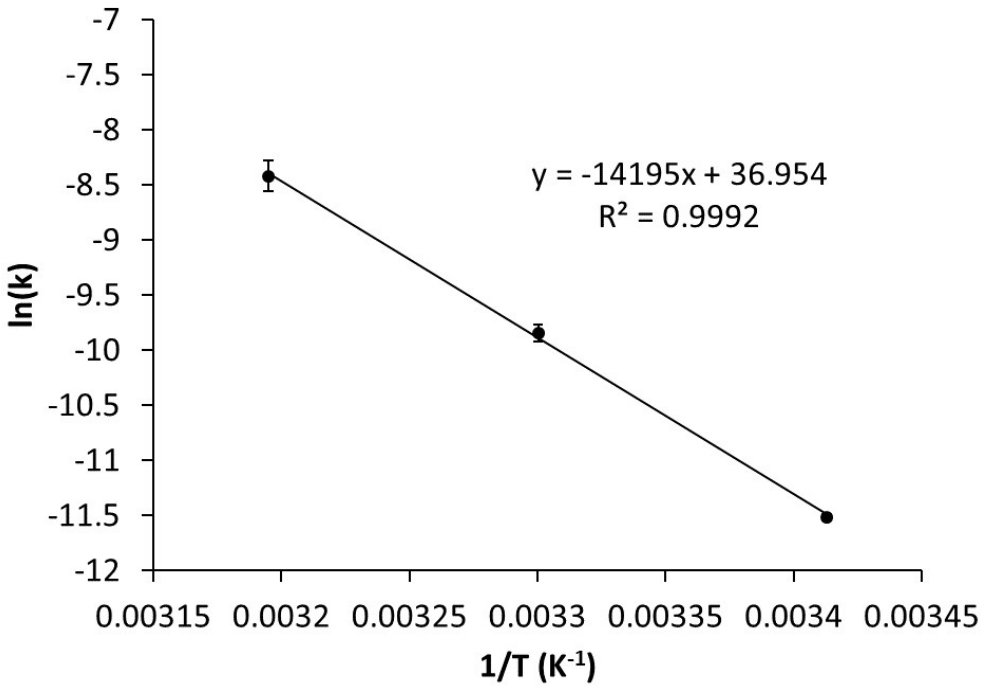


Fig. S17 *Arrhenius plot for the polymerization of* ***1*** *using* ***5b****.*

Strain Energy Analysis[3]

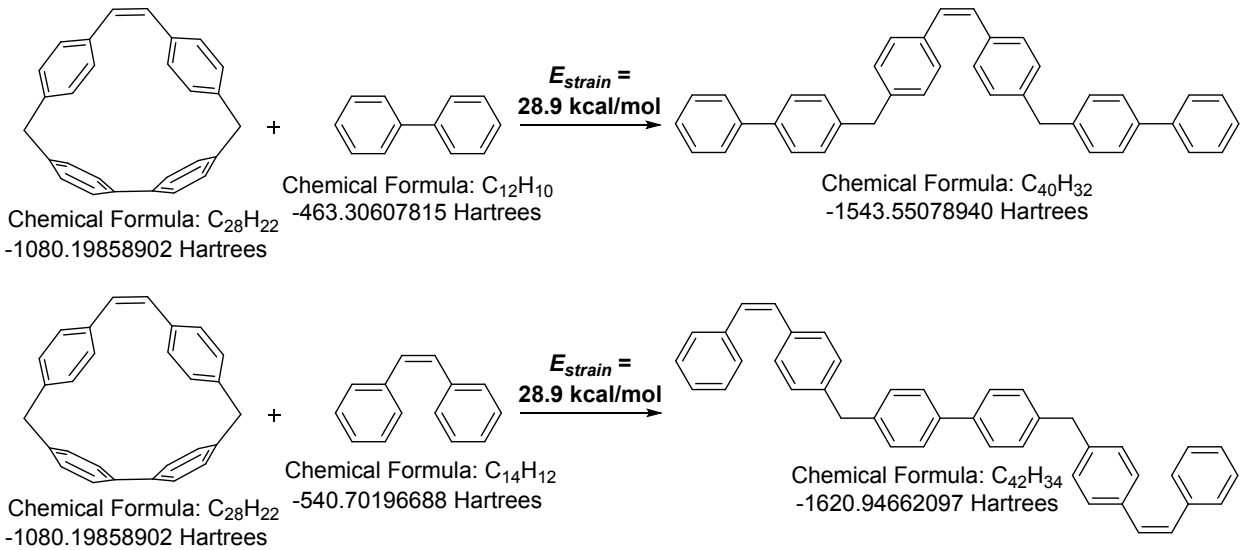


Fig. S18. *Homodesmotic reactions to estimate strain energy of model stilbene-based macrocycle (DFT at the B3LYP/6-31G* level of theory)*

Cartesian Coordinates of Selected Compounds

Model macrocycle, *B3LYP/6-31G** (Energy = -1080.19858902 Hartrees)

C 0.674124 4.084744 -0.022638
H 1.158173 5.060458 -0.081984
C -0.674138 4.084744 0.022674
H -1.158187 5.060457 0.082025
C -1.602165 2.932470 -0.044895
C -2.727402 2.850887 0.791136
C -1.427702 1.911694 -0.996191
C -3.593280 1.754108 0.735773
H -2.910445 3.637928 1.519504
C -2.305813 0.837367 -1.065855
H -0.588822 1.965508 -1.683239
C -3.388489 0.715678 -0.179790
H -4.429524 1.701635 1.430103
H -2.119246 0.053528 -1.794066
C 1.602152 2.932470 0.044906
C 2.727386 2.850907 -0.791131
C 1.427697 1.911675 0.996183
C 3.593271 1.754131 -0.735790
H 2.910424 3.637962 -1.519485
C 2.305814 0.837353 1.065826
H 0.588820 1.965473 1.683236
C 3.388489 0.715685 0.179757
H 4.429513 1.701676 -1.430124
H 2.119256 0.053499 1.794024
C 4.224271 -0.571312 0.154792
H 4.800790 -0.680054 1.082553
H 4.945468 -0.519954 -0.669832
C -4.224263 -0.571326 -0.154844
H -4.800757 -0.680079 -1.082621
H -4.945483 -0.519966 0.669759
C 3.260491 -1.735722 -0.006945
C 2.551442 -1.875186 -1.207237
C 2.816292 -2.476528 1.095733
C 1.313984 -2.505415 -1.229694
H 2.896286 -1.354709 -2.097999
C 1.578953 -3.122991 1.072869
H 3.388242 -2.458264 2.021464
C 0.742391 -3.026196 -0.052213
H 0.716192 -2.444596 -2.133843
H 1.216383 -3.602969 1.978265
C -3.260484 -1.735730 0.006935
C -2.551440 -1.875156 1.207233
C -2.816280 -2.476572 -1.095718

C -1.313979 -2.505379 1.229714
H -2.896288 -1.354650 2.097978
C -1.578941 -3.123032 -1.072829
H -3.388228 -2.458339 -2.021451
C -0.742381 -3.026197 0.052252
H -0.716189 -2.444528 2.133863
H -1.216367 -3.603038 -1.978209

Biphenyl, *B3LYP/6-31G** (Energy = -463.30607815 Hartrees)

C 2.859818 -1.138669 0.396129
C 1.465728 -1.138008 0.396512
C 0.742860 -0.000022 -0.000011
C 1.465705 1.137995 -0.396510
C 2.859788 1.138687 -0.396130
C 3.563714 0.000011 -0.000008
H 3.397098 -2.028241 0.714723
H 0.928274 -2.020474 0.732601
H 0.928222 2.020452 -0.732577
H 3.397058 2.028268 -0.714715
H 4.650390 0.000030 -0.000010
C -0.742860 -0.000022 0.000008
C -1.465704 1.137995 0.396508
C -1.465729 -1.138010 -0.396508
C -2.859787 1.138685 0.396135
H -0.928220 2.020453 0.732574
C -2.859819 -1.138668 -0.396130
H -0.928276 -2.020476 -0.732597
C -3.563713 0.000013 0.000005
H -3.397056 2.028268 0.714719
H -3.397099 -2.028240 -0.714726
H -4.650389 0.000034 0.000004

Cis-stilbene, *B3LYP/6-31G** (Energy = -540.70196688 Hartrees)

C 0.674910 1.824300 0.000588
C -0.674824 1.824402 -0.000276
C 1.646718 0.716745 -0.066921
C -1.646726 0.716889 0.066986
C -1.416888 -0.466736 0.792638
C -2.390029 -1.460780 0.863310
C -3.617421 -1.297825 0.215155
C -3.868259 -0.122302 -0.494226
C -2.897418 0.875936 -0.557095
C 1.416519 -0.467196 -0.791951

C 2.389648 -1.461241 -0.862731
C 3.617389 -1.298005 -0.215307
C 3.868596 -0.122171 0.493427
C 2.897768 0.876067 0.556393
H 1.142026 2.808617 0.042497
H -1.141815 2.808792 -0.041880
H -0.474145 -0.598368 1.313119
H -2.192613 -2.364109 1.434794
H -4.374418 -2.075379 0.272520
H -4.823000 0.021390 -0.993474
H -3.102906 1.793942 -1.103222
H 0.473525 -0.599085 -1.311901
H 2.191935 -2.364813 -1.433730
H 4.374359 -2.075579 -0.272747
H 4.823610 0.021762 0.992083
H 3.103544 1.794314 1.102007

Open adduct 1, *B3LYP/6-31G** (Energy = -1543.55078940 Hartrees)

C 0.653514 2.520168 -0.168802
H 1.093602 3.505364 -0.325722
C -0.653697 2.520207 0.169602
H -1.093747 3.505422 0.326507
C 1.614377 1.416684 -0.346839
C 2.682354 1.586056 -1.248807
C 1.576513 0.225023 0.396407
C 3.643737 0.597443 -1.428629
H 2.750858 2.509378 -1.819852
C 2.544647 -0.761171 0.217093
H 0.790317 0.075732 1.129004
C 3.589118 -0.599961 -0.701612
H 4.456057 0.759891 -2.133149
H 2.489670 -1.673229 0.807843
C -1.614570 1.416725 0.347682
C -1.576919 0.225273 -0.395894
C -2.682279 1.585880 1.250007
C -2.545013 -0.760969 -0.216576
H -0.790900 0.076180 -1.128724
C -3.643616 0.597225 1.429828
H -2.750586 2.509038 1.821340
C -3.589222 -0.599981 0.702455
H -2.490193 -1.672888 -0.807557
H -4.455725 0.759471 2.134638
C 4.631576 -1.686378 -0.906839
H 4.572817 -2.058306 -1.938380
H 4.380151 -2.540257 -0.263664

C -4.631729 -1.686348 0.907647
H -4.573269 -2.058039 1.939283
H -4.380169 -2.540373 0.264719
C -6.061361 -1.249927 0.629650
C -6.425779 -0.728875 -0.620030
C -7.057740 -1.369504 1.604111
C -7.737717 -0.349842 -0.884893
H -5.671009 -0.621994 -1.395533
C -8.373466 -0.987263 1.343160
H -6.801880 -1.762788 2.585770
C -8.742105 -0.470239 0.092161
H -7.995843 0.023245 -1.872213
H -9.118080 -1.066791 2.130497
C 6.061281 -1.249966 -0.629295
C 6.426064 -0.728986 0.620309
C 7.057367 -1.369434 -1.604069
C 7.738070 -0.349936 0.884811
H 5.671518 -0.622184 1.396044
C 8.373162 -0.987181 -1.343481
H 6.801220 -1.762644 -2.585683
C 8.742168 -0.470254 -0.092550
H 7.996474 0.023099 1.872078
H 9.117544 -1.066634 -2.131047
C -10.141882 -0.063247 -0.191117
C -11.226020 -0.799633 0.316345
C -10.421189 1.069364 -0.975010
C -12.540271 -0.418038 0.050574
H -11.034752 -1.694100 0.902834
C -11.735124 1.450667 -1.242767
H -9.599869 1.669921 -1.356231
C -12.801342 0.708936 -0.730991
H -13.362124 -1.008300 0.447681
H -11.925867 2.334934 -1.845449
H -13.825633 1.006131 -0.939211
C 10.142023 -0.063263 0.190352
C 11.226022 -0.799622 -0.317444
C 10.421536 1.069304 0.974232
C 12.540345 -0.418039 -0.052004
H 11.034593 -1.694054 -0.903932
C 11.735543 1.450595 1.241657
H 9.600315 1.669832 1.355713
C 12.801623 0.708892 0.729551
H 13.362090 -1.008281 -0.449363
H 11.926446 2.334828 1.844338
H 13.825970 1.006076 0.937514

Open adduct 2, *B3LYP/6-31G** (Energy = -1620.94662097 Hartrees)

C 1.842009 -1.149871 1.346883
C 0.613058 -0.553376 1.065627
C 0.386371 0.095444 -0.157695
C 1.442754 0.122751 -1.086016
C 2.666952 -0.473750 -0.802326
C 2.889130 -1.124487 0.419804
H 1.983383 -1.655123 2.300061
H -0.189055 -0.615118 1.795963
H 1.309277 0.641889 -2.031173
H 3.470380 -0.420920 -1.533218
C -0.921161 0.728585 -0.462192
C -1.465468 0.687828 -1.754740
C -1.661747 1.387329 0.535861
C -2.695970 1.280936 -2.036260
H -0.933957 0.162772 -2.543640
C -2.890675 1.974124 0.252386
H -1.255927 1.459534 1.541222
C -3.430400 1.934376 -1.041196
H -3.094059 1.228230 -3.047452
H -3.440951 2.474133 1.046011
C 4.220217 -1.795637 0.717128
H 4.361955 -2.643369 0.033582
H 4.177429 -2.226605 1.726407
C -4.763476 2.594554 -1.352488
H -4.676348 3.679553 -1.206889
H -4.984835 2.450882 -2.418687
C 5.428609 -0.880173 0.610093
C 5.510774 0.298489 1.364528
C 6.496304 -1.187719 -0.242315
C 6.622868 1.128500 1.272420
H 4.687434 0.574346 2.019072
C 7.615144 -0.362144 -0.332417
H 6.449591 -2.087352 -0.852588
C 7.710335 0.810010 0.436549
H 6.658513 2.042490 1.861258
H 8.416459 -0.621490 -1.016143
C -5.931176 2.086319 -0.522947
C -6.721362 2.962917 0.227433
C -6.254199 0.720513 -0.491438
C -7.800658 2.494913 0.975881
H -6.488558 4.025687 0.230666
C -7.336022 0.251635 0.244438
H -5.636471 0.014014 -1.040765
C -8.146159 1.133468 0.986128
H -8.391872 3.196970 1.559727

H -7.551026 -0.811639 0.260177
C 8.838100 1.754636 0.347413
H 8.546888 2.791741 0.516236
C -9.270276 0.690783 1.830394
H -9.410016 1.304949 2.720422
C -10.129743 -0.342496 1.702104
H -10.808597 -0.491618 2.542182
C 10.145764 1.560072 0.073998
H 10.741583 2.467550 -0.027636
C 10.929562 0.321779 -0.094898
C 12.032890 0.332049 -0.967518
C 10.677832 -0.853463 0.636859
C 12.832309 -0.797505 -1.134734
H 12.257452 1.238878 -1.524672
C 11.482018 -1.979571 0.477324
H 9.854291 -0.875195 1.342942
C 12.558536 -1.960785 -0.413611
H 13.673121 -0.766354 -1.822850
H 11.272530 -2.874263 1.058094
H 13.183859 -2.841149 -0.535503
C -10.334360 -1.307436 0.605663
C -10.793275 -2.599887 0.919155
C -10.171006 -0.976823 -0.752398
C -11.042794 -3.539993 -0.079152
H -10.948052 -2.867170 1.962131
C -10.428478 -1.913175 -1.751022
H -9.853434 0.024845 -1.022363
C -10.858731 -3.201040 -1.420582
H -11.387376 -4.534954 0.190581
H -10.301136 -1.633277 -2.793644
H -11.058890 -3.928937 -2.202263

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