Synthesis of Substituted [8]Cycloparaphenylenes by [2+2+2] Cycloaddition.

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Supporting Information

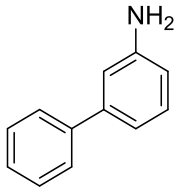
Contents:

General information:

All reactions dealing with air and moisture sensitive compounds were carried out under an inert atmosphere of argon using septum techniques. The solvents and starting material were purchased and used without further purification. Dry solvents were obtained from a solvent purification system (Pure-Solv^{TM}). Dry solvent for small scale reactions was purchased from Aldrich (crown cap over molecular sieves). Flash column chromatography was performed with silica gel 60 (40 – 63 μm) from Fluka, Sigma-Aldrich, Merck, SiliCycle Inc.
$Pd(PPh_3)_4$ was prepared according to a literature procedure.[1]
Microwave reactions were performed in an *Initiator 8* (400 W) from *Biotage*.
Nuclear magnetic resonance (NMR) spectra were recorded on a Bruker DPX-NMR (^{1}H 400 MHz, ^{13}C 101 MHz) or a Bruker Avance 500 (^{1}H 500MHz, ^{13}C 126 MHz).
Chemical shifts are reported in parts per million (ppm) relative to tetramethylsilane or residual solvent peak. Coupling constants (J) are reported in Hertz (Hz). The measurements were performed at room temperature unless otherwise stated. The carbon shifts marked with * were determined from 2D HMQC and HMBC data with increments in the indirect dimension. The multiplicities are written as: s=singlet, d=doublet, t=triplet, q=quartet, quin=quintet and m=multiplet. NMR-solvents were obtained from Cambridge Isotope Laboratories, Inc. (Andover, MA, USA).
Electron spray mass spectrometry was measured on a Bruker esquire 3000 plus, and fast atom bombardment (FAB) mass spectrometry was measured on a MAR 312. High-resolution mass (HR-ESI MS) spectra were recorded using a Bruker maXis 4G QTOF-ESI Spectrometer, or Bruker's solariX (ESI/MALDI-FTICR-MS) for Accurate Mass Measurement.
Melting points were measured on a SRS EZ-Melt MPA 120 or a Büchi 530 instrument.
UV-Vis absorption was measured on a Agilent UV-Vis single beam Spectrophotometer Emission spectra were measured on a Shimadzu RF-5301PC Spectrofluorophotometer.
Quantum yield measurements were done on a Hamamatsu Absolute PL Quantum Yield Spectrometer C11347, and Fluorescence lifetimes were measured using a Hamamatsu Compact Fluorescence Lifetime Spectrometer C11367-11.

[1] Tellier, F.; Sauvêtre, R.; Normant, J.-F. *Journal of Organometallic Chemistry* **1985**, *292*, 19.

Experimental procedures

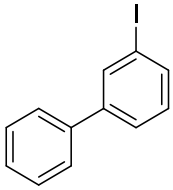


Synthesis of [1,1'-biphenyl]-3-amine:

A three-necked flask was charged with phenylboronic pinacol ester (639 mg, 3.13 mmol, 1.10 equiv), 3-bromoaniline (316 μL, 2.85 mmol, 1.00 equiv), and $Pd(PPh_3)_4$ (165 mg, 0.142 mmol, 5 mol %) and flushed with nitrogen. THF (70 mL) and aqueous K_2CO_3 (2 M, 20 mL) were added to the reaction mixture, which was degassed with a nitrogen stream for 20 min and stirred at 80 °C overnight. The reaction was allowed to cool to rt, and the organic layer was separated and washed with water and brine (100 mL). After drying over Na_2SO_4 and removal of the solvent under reduced pressure, the residue was purified by column chromatography on silica gel (EtOAc/hexane: 6/4) to yield the product as a yellow oil (372 mg, 77%).

^{1}H NMR (400 MHz, $CDCl_3$, δ/ppm): 7.57 (m, 2H), 7.42 (m, 2H), 7.33 (m, 1H), 7.23 (m, 1H) 7.00 (m, 1H), 6.92 (m, 1H), 6.68 (m, 1H), 3.74 (bs, 2H).

Analytical data are in accordance with the literature.[2]



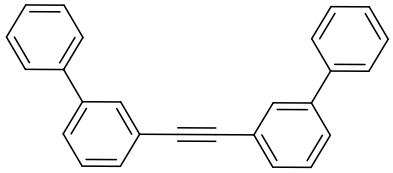
Synthesis of 3-iodo-1,1'-biphenyl:

To a solution of p-TsOH·H_2O (9.54 g, 50.2 mmol, 3.00 equiv) in MeCN (60 mL) was added (1,1'-biphenyl)-3-amine (2.83 g, 16.7 mmol, 1.00 equiv). The resulting suspension was cooled to 10–15 °C and a solution of $NaNO_2$ (2.35 mg, 33.4 mmol, 2.00 equiv) and KI (7.01 g, 41.8 mmol, 2.50 equiv) in H_2O (11 mL) was gradually added. The reaction mixture was stirred for 10 min then allowed to warm to 20 °C and stirred for 4 h. To the reaction mixture was then added H_2O (50 mL), $NaHCO_3$ (1 M; until pH = 9–10) and $Na_2S_2O_3$ (2 M, 40 mL). The aromatic iodide was extracted with EtOAc dried over Na_2SO_4 and concentrated under reduced pressure. The residue was purified by flash chromatography (cyclohexane) to give 3.98 g of product (85%).

^{1}H NMR (400 MHz, $CDCl_3$, δ/ppm): 7.94 (m, 1H), 7.67 (m, 1H), 7.55 (m, 1H), 7.53 (m, 2H) 7.44 (m, 2H), 7.36 (m, 1H), 7.17 (m, 1H).
^{13}C NMR (101 MHz, $CDCl_3$, δ/ppm): 143.4, 139.6, 136.3, 136.3, 130.6, 129.0, 127.9, 127.3, 126.5, 94.9.

Analytical data are in accordance with the literature.[3]

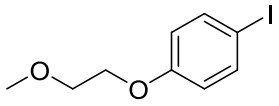
[2] Komáromi, A.; Szabó, F.; Novák, Z. *Tetrahedron Lett.* **2010,** 51, 5411-5414.



Synthesis of 1,2-di[(1,1'-biphenyl)-3-yl]ethyne:

To a 250 mL flask under argon was added 3-iodobiphenyl (3.89 g, 13.9 mmol, 1.00 equiv) in THF (125 mL). The mixture was degassed by bubbling argon through for 30 min. Then, CuI (265 mg, 1.39 mmol, 10 mol %), $Pd(PPh_3)_4$ (963 mg, 0.834 mmol, 6 mol %), DBU (13 mL, 6.00 equiv), water (81.9 µL, 5.56 mmol, 40 mol %) and TMS acetylene (989 µL, 6.95 mmol, 0.500 equiv) were added. The mixture was stirred at rt for 30 min and then at reflux for 4 days. The mixture was then washed with aq NH_4Cl (2x). The organic phase was then dried over Na_2SO_4 and concentrated under reduced pressure. The residue was purified by flash chromatography (cyclohexane) to obtain 2.02 g of product as a white solid (88%).

^{1}H NMR (400 MHz, CD_2Cl_2, δ/ppm): 7.82 (m, 2H), 7.63 (m, 6H), 7.55 (m, 2H), 7.51 – 7.43 (m, 6H), 7.42 – 7.36 (m, 2H).
^{13}C NMR (101 MHz, $CDCl_3$, δ/ppm): 141.6 (2C), 140.5 (2C), 130.5 (4C), 129.0 (6C), 127.8 (2C), 127.3 (2C), 127.3 (4C), 123.8 (2C), 89.6 (2C).
HR-MS (EI): calc. for $[C_{26}H_{18}]^+$: $[M]^+$ 330.1409; found: 330.1387.
Mp: 142.3-144.8°C



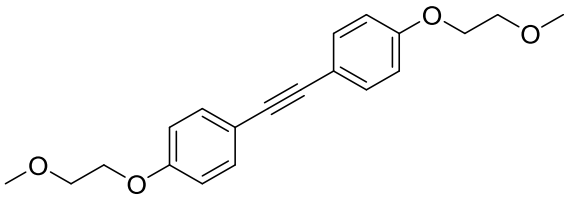
Synthesis of 1-Iodo-4-(2-methoxyethoxy)benzene

A suspension of NaH (60% in mineral oil, 1.08 g, 27.0 mmol, 2.00 equiv) in 100 mL dry THF was prepared. Then, 4-iodophenol (3.00 g, 13.5 mmol, 1.00 equiv) in 10 mL THF was added dropwise at 0 °C. The resulting mixture was stirred at rt for 4 h. Then, 2-bromomethylether (1.29 mL, 13.5 mmol, 1.00 equiv) was added dropwise at 0 °C and the mixture was stirred at 50 °C overnight. After that, 2-bromomethylether (2 mL) were added and the mixture was stirred 24 h. The mixture was quenched with sat. NaCl and extracted with EtOAc. The residue was purified by column chromatography to yield the title product as a transparent liquid (2.00 g, 46%)

^{1}H NMR (400 MHz, $CDCl_3$, δ/ppm): 7.54 (m, 2H), 6.70 (m, 2H), 4.07 (m, 2H), 3.73 (m, 2H), 3.44 (s, 3H).

Analytical data are in accordance with the literature.[4]

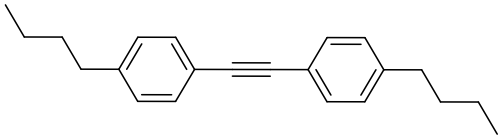
[3] Dektar, J. L.; Hacker, N. P. *J. Org. Chem*. **1990**, *55*, 639.
[4] patent: WO2006/22442 A1, **2006**



Synthesis of 1,2-bis [4-(2-methoxyethoxy)phenyl]ethyne

To a 20 mL vial under nitrogen was added CuI (62.3 mg, 327 µmol, 10 mol %), $Pd(PPh_3)_4$ (227 mg, 196 µmol, 6 mol %), 1-Iodo-4-(2-methoxyethoxy)benzene (1.00 g, 3.60 mmol, 1.00 equiv) in dry THF (10 mL). Nitrogen was bubbled through the solution for 10 min. Then, DBU (2.93 mL, 19.6 mmol, 6.00 equiv), water (23.6 µL, 1.31 mmol, 40 mol %) and TMS-acetylene (237 µL, 1.63 mmol, 0.500 equiv) were added. The mixture was stirred at reflux overnight. The cooled mixture was poured on NH_4Cl and the water phase was extracted with EtOAc (3x50 mL). The combined organic layers were washed with sat. NH_4Cl sat, brine, dried over Na_2SO_4 and concentrated under reduced pressure. The residue was purified by flash chromatography (cyclohexane) to give 376.6 mg, 70%, as colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$, δ/ppm): 7.43 (m, 4H), 6.89 (m, 4H), 4.13 (m, 4H), 3.76 (m, 4H), 3.46 (s, 6H).
^{13}C NMR (101 MHz, $CDCl_3$, δ/ppm): 158.5 (2C), 132.9 (4C), 115.9 (2C), 114.6 (4C), 87.9 (2C), 70.9 (2C), 67.3 (2C), 59.3(2C).
GCMS (m/z): 326, 210
HR-MS (EI): calc. for $[C_{20}H_{22}O_4]^+$: $[M]^+$ 326.1518; found: 326.1507.



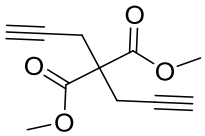
Synthesis of 1,2-Bis 4-(*n*-butyl)phenylethyne

To a 250 mL flask under argon was added CuI (894 mg, 4.69 mmol, 10 mol %), $Pd(PPh_3)_4$ (3.25 g, 2.82 mmol, 6 mol %), 1-bromo-4-*n*-butylbenzene (10.0 g, 46.9 mmol, 1.00 equiv) in dry THF (100 mL). Argon was bubbled through the solution for 10 min. Then DBU (38.0 mL, 251 mmol, 5.35 equiv), water (338 µL, 18.8 mmol, 40 mol %) and TMS-acetylene (3.34 mL, 23.5 mmol, 0.500 equiv) were added. The mixture was stirred at reflux overnight. The mixture was allowed to cool to rt, poured on NH_4Cl, and the water phase was extracted with EtOAc (3x100 mL). The combined organic layers were washed with sat. NH_4Cl, brine, dried over Na_2SO_4 and concentrated under reduced pressure. The residue was purified by flash chromatography (cyclohexane) and recrystalized (ethanol/DCM) to give 2.66 g of the title compound as white solid (39%).

^{1}H NMR (400 MHz, $CDCl_3$, δ/ppm): 7.43 (m, 4H), 7.15 (m, 4H), 2.61 (t, *J* = 7.6 Hz, 4H), 1.60 (m, 4 H), 1.35 (m, 4H), 0.93 (t, *J* = 7.3 Hz, 6H).

Analytical data are in accordance with the literature.[5]

[5] Weifeng, C.; Kebin, L.; Ziqiang, H.; Liliang, W.; Guoqiao, L.; Zhifang, L. *Organometallics* **2011** *30*, 2026-2030.

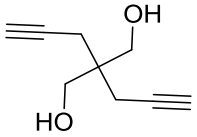


Synthesis of dipropargyl methylmalonate[6]

Under an inert atmosphere of argon NaH (2.86 g, 71.5 mmol, 1.10 equiv, 60 wt % in mineral oil) was added portion wise at 0 °C to a solution of dimethyl malonate (109, 7.43 mL, 65.0 mmol, 1.00 equiv) in 150 mL anhydrous THF. The mixture was allowed to warm to rt (over 30 min), whereas the mixture became cloudy. Then, propargyl bromide (7.70 mL, 71.5 mmol, 1.10 equiv) was slowly added and the mixture turned brown. The mixture was stirred for 2.5 h at rt. Then, the solution was cooled down to 0 °C and NaH (2.86 g, 71.5 mmol, 1.10 equiv, 60 wt % in mineral oil) was added portion wise. The mixture was warmed and propargyl bromide (7.70 mL, 71.5 mmol, 1.10 equiv) was slowly added. The mixture was stirred for 5 h, quenched with water and extracted twice with TBME. The combined organic layers were washed with brine and the combined aqueous layers were reextracted with TBME. The organic layers were dried over MgSO4, filtered and concentrated under reduced pressure. The crude product was recrystallized from hexane and to obtain the dipropargylester as a yellowish solid (9.65 g, 46.3 mmol, 71%).

^{1}H NMR (400 MHz, $CDCl_3$, δ/ppm): 3.74 (s, 6H); 2.97 (d, *J* = 2.6 Hz, 4H); 2.01 (t, *J* = 2.6 Hz, 2H).
^{13}C NMR (101 MHz, $CDCl_3$) δ: 169.3 (2C), 78.6 (2C), 72.0 (2C), 56.6, 53.5, (2C), 23.0 (2C)

Analytical data are in accordance with the literature.

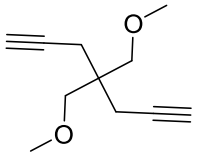


Synthesis of bis(homopropargyl)dialcohol

Dipropargylester (3.00 g, 14.4 mmol, 0.95 equiv) was dissolved in 60 mL dry THF and cooled to –10 °C - –20 °C (gas bubbler attached). Then, $LiAlH_4$ (1.76 g, 45.0 mmol, 3.00 equiv) was added over 1 h at this temperature. The mixture was allowed to warm to rt and stirred overnight. Afterwards, it was carefully quenched with water and 6% NaOH was added. Then, the suspension was acidified with 1 M HCl, extracted three times with TBME, and the organic layer was dried over $MgSO_4$ and evaporated. Recrystallization from hexane and ethyl acetate yielded the title compound as white needles. (1.83 g, 12.0 mmol, 84%)

^{1}H NMR (400 MHz, $CDCl_3$, δ/ppm): 3.77 (d, *J* = 5.7 Hz, 4H), 2.40 (d, *J* = 2.7 Hz, 4H), 2.13 (t, *J* = 5.7 Hz, 2H), 2.07 (t, *J* = 2.7 Hz, 2H).
^{13}C NMR(101 MHz, $CDCl_3$, δ/ppm): 80.4, 71.4, 66.7, 42.2, 21.9.
MS (FBA) m/z (%): 153 (100%) [$M+H^+$], 137, 91, 43.
EA (%): calc.: C, 71.03; H, 7.95; found: C, 70.96; H, 8.04.
IR (υ /cm^{-1}): 3333, 3277, 3264, 3257, 3245, 3243, 3211, 3207, 3203, 3200, 3194, 3187, 3133, 2938, 2886, 2885, 1467, 1460, 1428, 1372, 1367, 1313, 1127, 1106, 1024, 1003
Mp: 61-62°C

[6] Llerena, D.; Buisine, O.; Aubert, C.; Malacria, M. *Tetrahedron*, **1998.** *54*. 9373-9392.

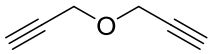


Synthesis of 4,4-bis(methoxymethyl)hepta-1,6-diyne 3b[7]

A solution of bis(homopropargyl)dialcohol (4.90 g, 32.2 mmol. 0.976 equiv) and iodomethane (8.1 mL, 129 mmol, 3.90 equiv) in dry THF (100 mL) was added dropwise at 0 °C to a suspension of sodium hydride (60% in oil, 3.63 g, 90.8 mmol) in THF (100 mL). The mixture was stirred for 1 h at rt, diluted with Et_2O and slowly quenched with water. Then, a few milliliters of a saturated solution of NH_4Cl were added, the organic layer was washed twice with NH_4Cl solution and brine, dried over $MgSO_4$, filtered and concentrated. The crude mixture was purified by distillation under reduced pressure (85 °C, 5 mbar) to furnish the title compound as a colorless liquid (4.84 g, 26.9 mmol, 78%).

^{1}H NMR (400 MHz, $CDCl_3$, δ/ppm): 3.35 (d, *J* = 3.4 Hz, 4H), 3.34 (s,6H), 2.35 (d, *J* = 2.7 Hz, 4H), 1.98 (t, *J* = 2.7 Hz, 2H).

Analytical data are in accordance with the literature.



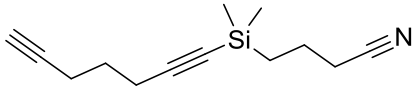
Propargylether 3c[8]

Propargylic alcohol (34.4 mL, 585 mmol, 1.40 equiv) and propargylbromide (36.0 mL, 418 mmol, 1.00 equiv) were placed in a flask. Freshly powdered NaOH (25 g, 625 mmol, 1.50 equiv) were added in small portions with vigorous stirring. The temperature was kept between 60 and 70 °C. 5 mL of THF were added to facilitate stirring. When, the reaction subsided, the mixture was heated for an additional 1 h in a bath at 70-80 °C. Again 15 mL of THF were added. After colling to 30 °C, 50 mL of icewater was added with vigorous stirring. The product is isolated by extraction with Et_2O (2x) and the extracts washed with water. After drying the organic solution over $MgSO_4$, most of the ether is distilled off at normal pressure. The remaining liquid was purified by distillation to give 40.1 g (95%) dipropargyl ether as coloreless liquid, bp. 40-60 °C/100 mbar.

^{1}H NMR (400 MHz, $CDCl_3$, δ/ppm): 4.24 (d, *J* = 1.0Hz, 4H), 2.45 (t, *J* = 1.0 Hz, 2H).
^{13}C NMR (126 MHz, $CDCl_3$, δ/ppm): 79.1, 75.5, 56.8.

Analytical data are in accordance with the literature

[7] X. Wang, H. Chakrapani, J. W. Madine, M. A. Keyerleber, R. A. Widenhoefer, *J. Org. Chem.*, **2002,** 67, 2778.
[8] Geiger, R. E.; Lalonde, M.; Stoller, H.; Schleich, K. *Helvetica Chimica Acta*. **1984.** 67. 1274 - 1282

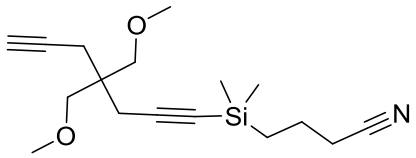


CPDMS-hepta-1,6-diyne 4a[9]

1,6-Heptadiyne **3a** (8.70 mL, 76.0 mmol, 1.30 equiv) was dissolved in 180 mL dry THF and ethylmagnesium bromide (1 M in THF 40.0 mL and 3 M in Et_2O (8.50 mL, 65.5 mmol, 1.10 equiv) was added dropwise at 0 °C. The mixture was stirred for 30 min at 0 °C and 1h at rt, then CPDMS-Cl (9.50 mL, 57.9 mmol, 1.00 equiv) was added dropwise at 0 °C. After 1d at rt the solution was slowly quenched with water and diluted with EtOAc. After work up, the crude oil was purified by column chromatography on silica gel (ethyl acetate/hexane 1:15 to 1:1) to yield 7.60 g (60%) of the title compound as colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$, δ/ppm): 2.39 (t, *J* = 7.0 Hz, 2H), 2.35 (t, *J* = 7.1 Hz, 2H), 2.29 (td, *J* = 7.1 Hz, *J* = 2.4 Hz, 2H), 1.96 (td, *J* = 2.6 Hz, *J* = 0.6 Hz, 1H), 1.74 (m, 4H), 0.73 (m, 2H), 0.14 (s, 6H).
^{13}C NMR (101 MHz, $CDCl_3$, δ/ppm): 119.9, 107.8, 83.5, 83.4, 69.1, 27.6, 20.8, 20.6, 19.1, 17.7, 16.0, –1.5.

Analytical data are in accordance with the literature

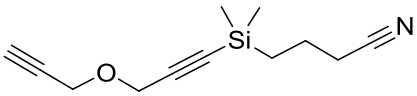


CPDMS-4,4-bis(methoxymethyl)hepta-1,6-diyne 4b

4,4-Bis(methoxymethyl)hepta-1,6-diyne **3b** (3.72 g, 20.0 mmol, 1.00 equiv) was dissolved in 100 mL dry THF and ethylmagnesium bromide (3 M in Et_2O, 5.87 mL, 17.6 mmol, 0.880 equiv) was added dropwise at 0 °C. The mixture was stirred for 30 min at 0 °C and 1 h at rt, then CPDMS-Cl (2.71 g, 16.6 mmol, 0.830 equiv) was added dropwise at 0 °C. After 2 d at rt the solution was diluted with ether and slowly quenched with water. The organic layer was washed twice with NH_4Cl, the aqueous layer was re-extracted with TBME and the combined organic phases were washed with brine, dried over $MgSO_4$, filtered and evaporated. The crude mixture was purified by column chromatography (SiO_2, hexane/ethyl acetate, 6:1) to obtain the monoprotected alkyne as a colorless liquid (2.94 g, 9.62 mmol, 58%).

^{1}H NMR (500 MHz, $CDCl_3$, δ/ppm): 3.17 (s, 10H), 2.25 (t, *J* = 7.0 Hz, 2H), 2.21 (s, 2H), 2.16 (d, *J* = 2.7 Hz, 2H), 1.82 (t, *J* = 2.6 Hz, 1H), 1.62 (ddd, *J* = 19.0 Hz, 9.5 Hz, 6.3 Hz, 2H), 0.64 – 0.55 (m, 2H), 0.16 (s, 6H).
^{13}C NMR (126 MHz, $CDCl_3$, δ/ppm): 121.4, 106.7, 86.5, 82.2, 75.2, 72.1, 61.1, 43.4, 24.9, 23.6, 22.3, 22.1, 17.5, 1.6 (2C).
MS (FAB) m/z: 306 (100%) [$M+H^+$], 126, 98, 45.
EA (%): calc.: C, 66.84; H, 8.91; N, 4.59; found: C, 66.00; H, 8.78; N, 4.49.
IR (υ /cm^{-1}): 3291, 2926, 2887, 2812, 2177, 1733, 1477, 1455, 1428, 1250, 1195, 1174, 1101, 1031

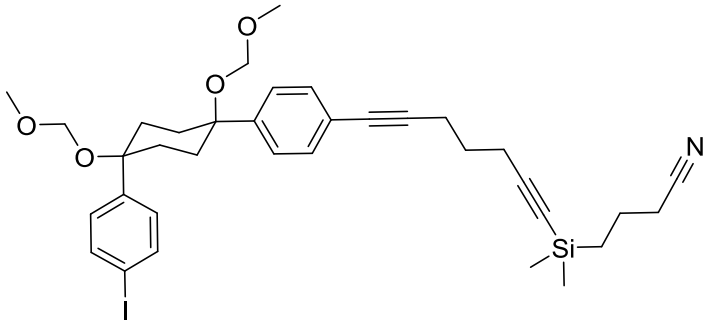
[9] S. López, F. Fernández-Trillo, P. Midón, L. Castedo, C. Saá, *J. Org. Chem.* **2005,** *70*, 6346–6352.



CPDMS-dipropargylether 4c

To a solution of 1,1,1,3,3,3-hexamethyldisilazane (18.8 mL, 88.6 mmol, 1.00 equiv) in THF (8 mL) cooled to -78 °C was added n-butyllithium (2.5 M in hexane. 35.5 mL, 477 mmol, 5.00 equiv) under nitrogen dropwise. After stirring for 15 min at that temperature, the cooling bath was removed and the pale yellow solution was stirred for an additional 15 min. Then it was added via syringe to a solution of CPDMSCl (15.2 mL, 92.8 mmol, 1.05 equiv) in THF -78 °C. The mixture was stirred for 1h, then dipropargylether **3c** (9.20 g, 97.8 mmol, 1.10 equiv) was added and stirring was continued for 2 h. Saturated ammonium chloride was then added to the reaction, extracted with ether, dried over $MgSO_4$, and the solvent removed in vacuo. The crude product was purified by distillation (142 °C/0.7 mbar) to give 14.9 g, 77%.

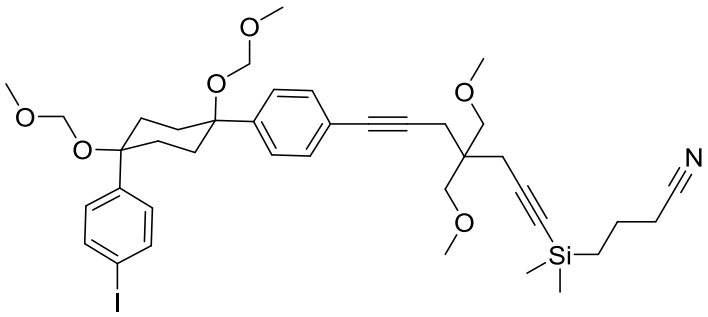
^{1}H NMR (400 MHz, $CDCl_3$, δ/ppm): 4.23 (m, 4H), 2.45 (t, *J* = 2.4 Hz 1H), 2.39 (t, *J* = 7.0 Hz, 2H), 1.75 (m, 2H), 0.77 (m, 2H), 0.17 (s, 6H).
^{13}C NMR (126 MHz, $CDCl_3$, δ/ppm): 120.1, 102.3, 90.6, 79.2, 75.6, 57.7, 57.0, 20.9, 20.9, 15.9, -1.69.
HR-MS (ESI): calc. for $[C_{12}H_{17}NNaOSi]^+$: $[M+Na]^+$ 242.0972; found 242.0972.



Synthesis of 5a

To an oven-dried flask was added *cis*-1,4-bis(4-iodophenyl)-1,4-bis(methoxymethoxy)cyclohexane **2** (12.0 g, 19.7 mmol, 1.00 equiv), 200 mL dry THF and the protected alkyne **4a** (4.29 g, 19.7 mmol, 1.00 equiv). Argon was bubbled through the solution for 15 min. Then, $Pd(PPh_3)_4$ (1.14 g, 0.986 mmol, 5 mol %), CuI (376 mg, 1.97 mmol, 10.0 mol %) were added with argon counterflow followed by 100 mL di*iso*propylamine. The reaction mixture was stirred overnight at rt. Afterwards, it was poured on sat. NH_4Cl, and extracted with EtOAc (3x). The combined organic layers were washed with sat. NH_4Cl, brine, dried over Na_2SO_4 and concentrated under reduced pressure. The crude product was purified on column chromatography to give 8.32 g (61%) of the title compound as colorless oil.

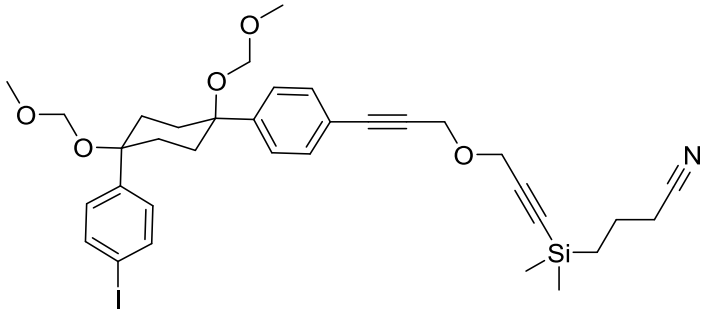
^{1}H NMR (400 MHz, $CDCl_3$, δ/ppm): 7.64 (m, 2H), 7.35 (s, 4H), 7.15 (m, 2H), 4.44 – 4.38 (m, 4H), 3.42 – 3.35 (m, 6H), 2.51 (t, *J* = 7.0 Hz, 2H), 2.40 (t, *J* = 7.0 Hz, 4H), 2.27 (s, 4H), 2.04 (d, *J* = 4.3 Hz, 4H), 1.86 – 1.76 (m, 2H), 1.77 – 1.71 (m, 2H), 0.79 – 0.70 (m, 2H), 0.18 – 0.12 (m, 6H).
^{13}C NMR (101 MHz, $CDCl_3$, δ/ppm)*: 142.3, 141.6, 137.5 (2C), 131.6 (2C), 128.8 (2C), 126.8 (2C), 123.1, 119.8, 107.8, 93.4, 92.2 (2C), 89.5, 83.2, 80.9, 77.9 (2C), 56.1 (2C), 32.8 (4C), 27.7, 20.7, 20.3, 19.1, 18.6, 15.8, -1.5 (2C).
FAB MS m/z (%): 697 (M^+, 6%), 126 (100), 574 (82).
HR-MS (ESI): calc. for $[C_{35}H_{44}INaO_4Si]^+$: $[M+Na]^+$ 720.1976; found 720.1990.



Synthesis of 5b

To a 250 mL oven-dried flask filled with 80 mL THF was added $Pd(PPh_3)_4$ (227 mg, 191 µmol, 10mol %), CuI (72.6, 381 µmol, 20mol %). Then, nitrogen was bubbled through the solution for 10 min, after which the diiodide **2** (1.19 g, 1.96 mmol, 1.00 equiv), the protected alkyne **4b** (582 mg 1.91 mmol, 1.00 equiv) and 10 mL di*iso*propylamine were added. The mixture was stirred at rt overnight. The mixture was then poured on NH_4Cl and the aqueous phase was extracted with EtOAc (3 x). The combined organic extracts were washed with sat. NH_4Cl and brine before drying over Na_2SO_4 and concentration under reduced pressure. The residue was purified by column chromatography on silica (cyclohexane/EtOAc, 8/2) to yield 560 mg of the product as yellow oil (37%).

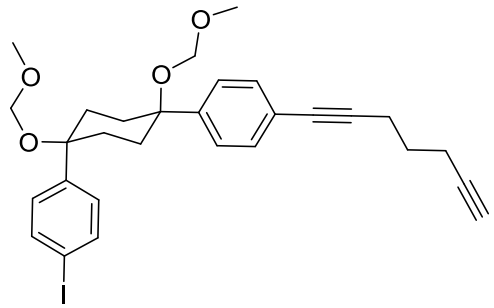
^{1}H NMR (400 MHz, $CDCl_3$, δ/ppm): 7.67 – 7.60 (m, 2H), 7.35 (s, 4H), 7.16 (m, 2H), 4.41 (d, *J* = 5.2 Hz, 4H), 3.39 (d, *J* = 3.1 Hz, 6H), 3.38 (s, 4H), 3.35 (s, 6H), 2.52 (s, 2H), 2.41 (s, 2H), 2.39 (t, *J* = 7.0 Hz, 2H), 2.28 (bs, 4H), 2.01 (bs, 4H), 1.81 – 1.71 (m, 2H), 0.78 – 0.70 (m, 2H), 0.16 (s, 6H).
^{13}C NMR (150Hz, $C_2D_2Cl_4$, 358K, δ/ppm)*: 142.9, 142.2, 137.5 (2C), 131.6 (2C), 128.7 (2C), 126.6 (2C), 123.2, 119.2, 105.4, 93.1, 91.9 (2C), 87.5, 84.9, 82.4, 77.7 (2C), 74.3, 74.2 (2C), 59.5 (2C), 55.8 (2C), 32.8 (4C), 23.8, 23.6, 20.6, 20.3, 16.0, -1.9 (2C).
HR-MS (ESI): calc. for $[C_{39}H_{52}INNaO_6Si]^+$: $[M+Na]^+$ 808.2501; found 808.2510.



Synthesis of 5c

To a 250 mL oven dried flask filled with 160 mL THF was added $Pd(PPh_3)_4$ (380 mg, 329 µmol, 10 mol %), CuI (125 mg, 658 µmol, 20 mol %) then nitrogen was bubbled through for 10 min after which the diiodide **2** (2.00 g, 3.29 mmol, 1.00 equiv) and the protected alkyne **4c** (721 mg 3.29 mmol, 1.00 equiv) and 12 mL di*iso*propylamine were added. The mixture was stirred at rt overnight. The mixture was then poured on NH_4Cl and the aqueous phase was extracted with EtOAc (3x) The combined organic extracts were washed with sat. NH_4Cl and brine before drying over Na_2SO_4 and concentration under reduced pressure. The residue was purified by column chromatography on silica (cyclohexane/EtOAc, 8/2) to yield 1.01 g of the product as a yellow oil (44%).

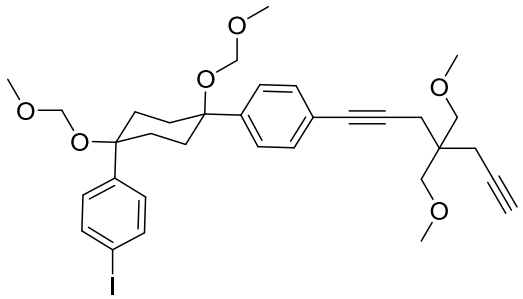
^{1}H NMR (400 MHz, $CDCl_3$, δ/ppm): 7.65 (m, 2H), 7.39 (m, 4H), 7.16 (m, 2H), 4.45 (s, 2H), 4.41 (s, 4H), 4.29 (s, 2H), 3.39 (s, 6H), 2.39 (m, 2H), 2.29 (m, 4H), 2.26 (m, 4H), 1.77 (m, 2H), 0.78 (m, 2H), 0.19 (s, 6H).
^{13}C NMR (150Hz, $C_2D_2Cl_4$, 358K, δ/ppm)*: 143.2, 142.6, 137.4 (2C), 131.8 (2C), 128.6 (2C), 126.6 (2C), 121.6, 119.4, 102.3, 93.1, 92.1 (2C), 90.3, 86.5, 85.0, 77.7 (2C), 57.6 (4C), 57.5 (2C), 55.8 (2C), 15.7, 20.7, 20.3, -2.0 (2C).
HR-MS (ESI): calc. for $[C_{34}H_{42}INaO_5Si]^+$: $[M+Na]^+$ 722.1769; found 722.1777.



Synthesis of 6a

5a (8.00 g, 11.5 mmol, 1.00 equiv) was dissolved in dry THF (100 mL). The mixture was degassed with argon for 30 min and a 1 M solution of TBAF in THF (23 mL, 22.9 mmol, 2.00 equiv) was added. The reaction mixture was stirred for 30 min at rt and diluted with EtOAc and brine. The aqueous phase was extracted three times with EtOAc and the combined organic layers were dried over Na_2SO_4. After removal of the solvent under reduced pressure the crude product was purified by column chromatography (cyclohexane/EtOAc, 8/2). to give 5.43 g of the product as a yellow oil (83%).

^{1}H NMR (500 MHz, $CDCl_3$, δ/ppm): 7.65 (d, *J* = 8.3 Hz, 2H), 7.35 (s, 4H), 7.15 (d, *J* = 8.3 Hz, 2H), 4.43 (m, 4H), 3.41 (m, 6H), 2.55 (t, *J* = 7.0 Hz, 2H), 2.38 (m, 2H), 2.36 (bm, 4H), 2.06 (bm, 4H), 1.99 (m, 1H), 1.83 (m, 2H).
^{13}C NMR (126Hz, $CDCl_3$, δ/ppm)*: 142.5, 141.6, 137.9 (2C), 131.5 (2C), 128.6 (2C), 126.5 (2C), 123.0, 93.3, 92.0 (2C), 89.5, 83.3, 80.5, 77.9 (2C), 68.7, 55.6 (2C), 32.8 (4C), 27.7, 18.1, 17.4.
FAB MS m/z (%): 572 (M^+16%), 45 (100), 449 (96%).
HR-MS (ESI): calc. for $[C_{29}H_{33}INaO_4]^+$: $[M+Na]^+$ 595.1316; found 595.1313.

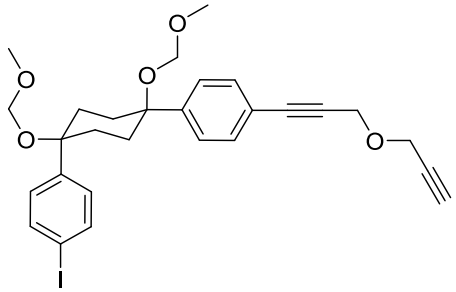


Synthesis of 6b

To a 20 mL vial the protected alkyne **5b** (560 mg, 713 umol, 1.00 equiv) was introduced with dry THF (15 mL). Then nitrogen was bubbled through the solution for 20 min, after which TBAF (1.5 mL, 1 M solution in THF, 2.00 equiv) was added drop-wise. After stirring 30 min at rt, the mixture

was quenched with brine. The aqueous phase was extracted with EtOAc (3 x) and the organic extracts were dried over Na_2SO_4 and concentrated. The residue was purified by column chromatography on silica (cyclohexane/EtOAc: 8/2) to give 386 mg of a yellow oil (82%).

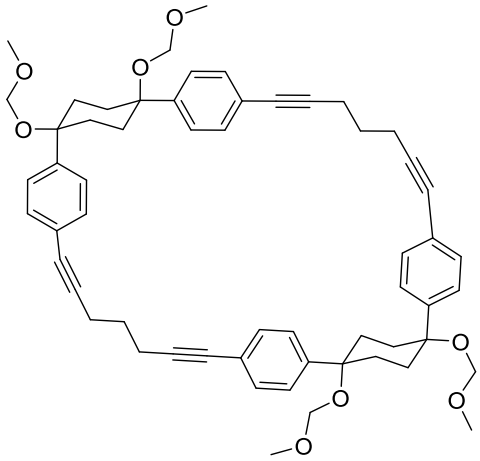
^{1}H NMR (500 MHz, $CDCl_3$, δ/ppm): 7.64 (m, 2H), 7.35 (s, 4H), 7.16 (d, 2H), 4.40 (d, 4H), 3.40 (s, 6H), 3.39 (d, 4H), 3.36 (s, 6H), 2.54 (s, 2H), 2.39 (m, 2H), 2.28 (bm, 4H), 2.00 (bm, 4H), 1.99 (m, 1H).
^{13}C NMR (150Hz, $C_2D_2Cl_4$, 358K, δ/ppm)*: 142.8, 142.3, 137.5 (2C), 131.5 (2C), 128.8 (2C), 126.6 (2C), 123.0, 93.3, 92.1 (2C), 86.9, 82.1, 80.7, 77.8 (2C), 73.7 (2C), 70.4, 59.2 (2C), 55.9 (2C), 42.0, 32.8 (4C), 22.8, 21.9.
HR-MS (ESI): calc. for $[C_{33}H_{41}INaO_6]^+$: $[M+Na]^+$ 683.1840; found 683.1850.



Synthesis of 6c

To a vial the protected alkyne **5c** (1.00 g, 1.43 mmol, 1.00 equiv) was introduced with dry THF 15 mL. Then, nitrogen was bubbled through the solution for 20 min, after which TBAF (2.86 mL, 1 M solution in THF, 2.86 mmol, 2.00 equiv) was added drop-wise. After stirring for 30 min at rt, the mixture was quenched with brine. The aqueous phase was extracted with EtOAc (3 x) the organic extracts were dried over Na_2SO_4 and concentrated. The residue was purified by column chromatography on silica (cyclohexane/EtOAc: 8/2) to give 428 mg of yellow oil (52%).

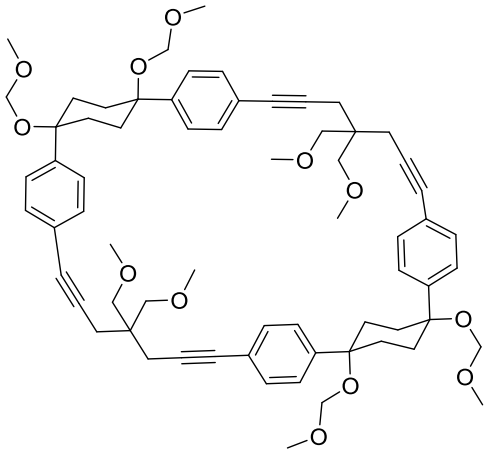
^{1}H NMR (500 MHz, $CDCl_3$, δ/ppm): 7.65 (m, 2H), 7.45 – 7.36 (m, 4H), 7.15 (m, 2H), 4.48 (s, 2H), 4.41 (d, *J* = 3.7 Hz, 4H), 4.31 (d, *J* = 2.3 Hz, 2H), 3.39 (d, *J* = 4.5 Hz, 6H), 2.47 (t, *J* = 2.3 Hz, 1H), 2.31 (s, 4H), 2.11 – 1.97 (m, 4H).
^{13}C NMR (150Hz, $C_2D_2Cl_4$, 358K, δ/ppm)*: 143.2, 142.7, 137.5 (2C), 131.8 (2C), 128.8 (2C), 126.8 (2C), 121.7, 93.2, 92.1 (2C), 86.3, 84.4, 79.0, 77.8 (2C), 75.0, 57.1, 56.4, 56.0 (2C), 32.6 (4C).
HR-MS (ESI): calc. for $[C_{28}H_{31}INaO_5]^+$: $[M+Na]^+$ 597.1108; found 597.1114.



Synthesis of macrocycle 7a

To an oven-dried Schlenck-flask compound **6a** (5.43 g, 9.49 mmol, 1.00 equiv) and 250 mL dry THF were added. Argon was bubbled through the solution for 15 min. Then, $Pd(PPh_3)_4$ (1.10 g, 949 µmol, 10.0 mol %) and CuI (362 mg, 1.90 µmol, 20.0 mol %) were added with argon counterflow followed by 34 mL of di*iso*propylamine. The reaction mixture was stirred overnight at rt. Afterwards, the mixture was poured on sat. NH_4Cl, and extracted with ethyl acetate (3x). The combined organic layers were washed with sat. NH_4Cl, brine, dried over Na_2SO_4 and concentrated under reduced pressure. The crude product was purified on column chromatography (cyclohexane/EtOAc, 7/3), the residue was then suspended in cyclohexane/EtOAc and filtrated to give 488 mg of product as a white solid (11%).

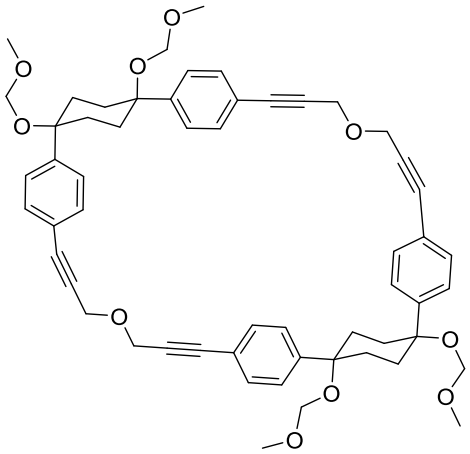
^{1}H NMR (400 MHz, $CDCl_3$, δ/ppm): 7.33 (s, 16H), 4.44 (s, 8H), 3.39 (s, 12H), 2.57 (t, *J* = 7.0 Hz, 8H), 2.38-2.16 (m, 8H), 2.04 (s, 8H), 1.93-1.78 (m, 4H)
^{13}C NMR (126 MHz, $CDCl_3$, δ/ppm) *: 141.1 (4C), 131.4 (8C), 126.7 (8C), 122.8 (4C), 92.0 (4C), 89.5 (4C), 80.8 (4C), 78.0 (4C), 55.7 (4C), 32.8 (8C), 27.7 (2C), 18.4 (4C).
HR-MS (ESI): calc. for $[C_{58}H_{64}NaO_8]^+$: $[M+Na]^+$ 911.4493; found 911.4506.
Mp: >350°C



Synthesis of 7b

To a 50 mL oven-dried flask the building block **6b** (386 mg, 58.4 µmol, 1.00 equiv) was transferred with THF (20 mL). $Pd(PPh_3)_4$ (67.5 mg, 58.4 µmol, 10 mol %) and CuI (22.3 mg, 11.7 µmol, 20 mol %) were added. Then, nitrogen was bubbled through the solution for 10 min after which 2 mL di*iso*propylamine were added. The mixture was stirred at rt overnight. The mixture was then poured on NH_4Cl and the aqueous phase was extracted with EtOAc (3 x). The combined organic extracts were washed with sat. NH_4Cl and brine before drying over Na_2SO_4 and concentration under reduced pressure. The residue was purified by column chromatography on silica (cyclohexane/EtOAc: 7/3) to yield 90.0 mg of yellow wet solid. The solid was suspended in few mL cyclohexane and filtrated to give 19 mg of a white solid (6%).

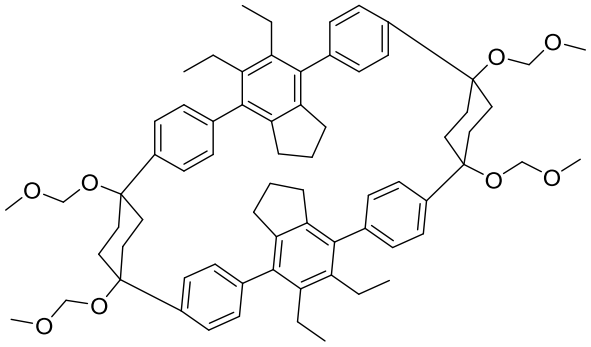
^{1}H NMR (400 MHz, $CDCl_3$, δ/ppm): 7.33 (m, 16H), 4.44 (s, 8H), 3.44 (s, 8H), 3.40 (s, 12 H), 3.37 (s, 12H), 2.59 (s, 8H), 2.27 (bs, 8H), 2.08 (bs, 8H).
^{13}C NMR (150Hz, $C_2D_2Cl_4$, 353K, δ/ppm)*: 141.9 (4C), 131.0 (8C), 126.0 (8C), 122.5 (4C), 91.6 (4C), 86.9 (4C), 82.1 (4C), 77.4 (4C), 73.9 (4C), 59.0 (4C), 55.3 (4C), 42.4 (2C), 32.6 (8C), 22.6 (4C).
HR-MS (ESI): calc. for $[C_{66}H_{80}NaO_{12}]^+$: $[M+Na]^+$ 1087.5542; found 1087.5556.
Mp: 230°C (decomposition)



Shot gun synthesis of macrocycle 7c

To a 50 mL oven-dried flask the building block **6c** (386 mg, 58.4 µmol, 1.00 equiv) was transferred with THF (20 mL). $Pd(PPh_3)_4$ (84.1 mg, 72.8 µmol, 10 mol %)and CuI (27.7 mg, 146 µmol, 20 mol %) were added. Then, nitrogen was bubbled through the solution for 10 min after which 3 mL di*iso*propylamine were added. The mixture was stirred at rt overnight. The mixture was then poured on NH_4Cl and the aqueous phase was extracted with EtOAc (3 x). The combined organic extracts were washed with sat. NH_4Cl and brine before drying over Na_2SO_4 and concentration under reduced pressure. The residue was purified by column chromatography on silica (cyclohexane/EtOAc: 6/4) to yield 13 mg of pale yellow solid (4%)

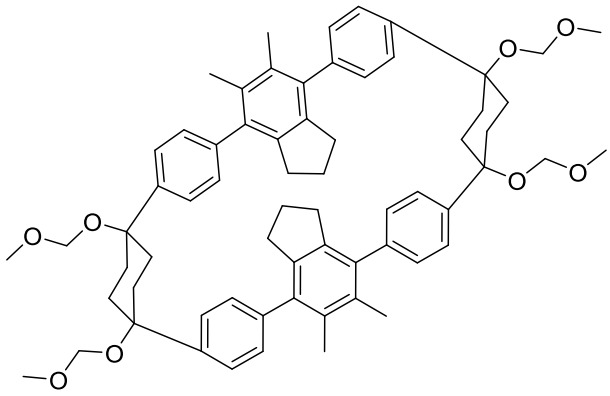
^{1}H NMR (400 MHz, $CDCl_3$, δ/ppm): 7.43 – 7.30 (m, 16H), 4.52 (s, 8H), 4.46 (s, 8H), 3.40 (s, 12H), 2.27 (bs, 8H), 2.04 (bs, 8H).
^{13}C NMR (150Hz, $C_2D_2Cl_4$, 353K, δ/ppm)*: 142.8 (4C), 131.0 (8C), 126.1 (8C), 121.3 (4C), 91.6 (4C), 86.5 (4C), 84.4 (4C), 77.4 (4C), 56.5 (4C), 55.4.0 (4C), 32.4 (8C).
HR-MS (ESI): calc. for $[C_{56}H_{60}NaO_{10}]^+$: $[M+Na]^+$ 915.4079; found 915.4085.
Mp: >350°C



Synthesis of 8a

Macrocycle **7a** (115 mg, 129 µmol, 1.00 equiv), anhydrous 2-propanol (10 mL), and anhydrous THF (10 mL) were placed in a 20 mL microwave flask equipped with a stir bar. The reaction mixture was degassed by bubbling N_2 through the solution for 15 min. Then, $RhCl(PPh_3)_3$ (24.1 mg, 25.8 µmol, 20 mol %.) and 3-hexyne (147 µL, 1.29 mmol, 10.0 equiv) were added and the reaction flask was irradiated with microwave at 100 °C for 6 h. The reaction mixture was filtrated and washed with cyclohexane to give 71.0 mg of pure product as an off-white solid (52%).

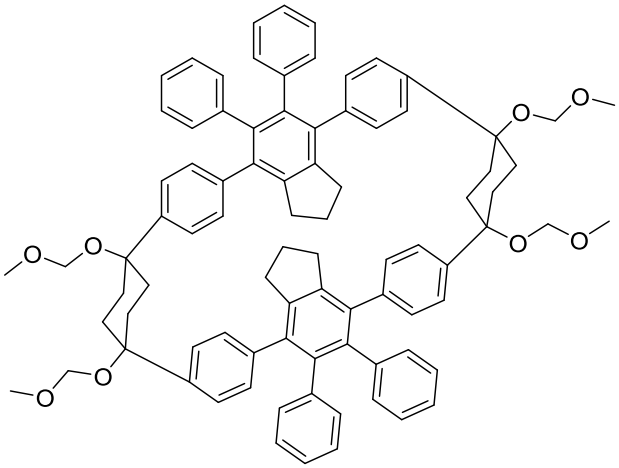
^{1}H NMR (400 MHz $CDCl_3$, δ/ppm): 7.35 (m, 8H), 7.04 (m, 8H), 4.75 (s, 8H), 3.50 (s, 12H), 2.74 (q, *J* = 7.4 Hz, 8H), 2.27 (m, 8H), 2.15 – 1.95 (m, 8H), 1.80 (t, *J* = 7.5 Hz, 8H), 1.09 (m, 16H).
^{13}C NMR (101 MHz, $CDCl_3$, δ/ppm): 141.2 (4C), 141.1 (4C), 139.6 (4C), 138.1 (4C), 137.7 (4C), 129.4 (8C), 127.1 (8C), 92.9 (4C), 78.4 (4C), 56.0 (4C), 34.1 (8C), 32.9 (4C), 23.5 (4C), 23.3 (2C), 16.7 (4C).
HR-MS (ESI): calc. for $[C_{70}H_{84}NaO_8]^+$: $[M+Na]^+$ 1075.6058; found 1075.6071.
Mp: 278-284°C



Synthesis of 8b

Macrocycle **7a** (57.0 mg, 64.1 μmol, 1.00 equiv), anhydrous 2-propanol (2 mL), and anhydrous THF (2 mL) were placed in a 5 mL microwave flask equipped with a stir bar. The reaction mixture was degassed by bubbling N_2 through the solution for 5 min. Then, $RhCl(PPh_3)_3$ (12.0 mg, 10 μmol, 20 mol %) and 2-butyne (50 μL, 641 μmol, 10.0 equiv) were added and the reaction flask was irradiated with microwave at 100 °C for 6 h. The reaction mixture was filtrated to give 38 mg of pure product as a white solid (81%).

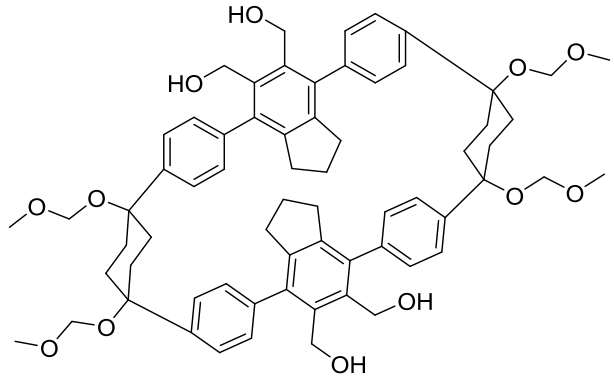
^{1}H NMR (400 MHz, $CDCl_3$, δ/ppm): 7.36 (m, 8H), 7.03 (m, 8H), 4.74 (s, 8H), 3.49 (s, 12H), 2.29 (m, 8H), 2.24 (s, 12H), 2.02 (m, 8H), 1.87 (t, *J* = 7.5 Hz, 8H), 1.08 (m, 4H).
^{13}C NMR (101 MHz, $CDCl_3$, δ/ppm): 140.8 (8C), 139.7 (4C), 137.8 (4C), 132.1 (4C), 129.5 (8C), 127.3 (8C), 92.9 (4C), 78.2 (4C), 56.1 (4C), 34.2 (8C), 33.1 (4C), 23.8 (2C), 18.1 (4C).
FAB MS m/z (%): 996.5.
HR-MS (ESI): calc. for $[C_{66}H_{76}NaO_8]^+$: $[M+Na]^+$ 1019.5432; found 1019.5448.
Mp: 283-288°C



Synthesis of 8c

Macrocycle **7a** (203 mg, 228 μmol, 1.00 equiv), diphenylacetylene (411 mg, 2.28 mmol, 10.0 equiv), anhydrous 2-propanol (10 mL), and anhydrous THF (10 mL) were placed in a 20 mL microwave flask equipped with a stir bar. The reaction mixture was degassed by bubbling Ar through the solution for 15 min. Then, $RhCl(PPh_3)_3$ (42.7 mg, 45.7 μmol, 20 mol %.) was added and the reaction flask was placed in the microwave reactor at 100 °C for 6 h. The reaction mixture was allowed to cool to rt and was filtrated and washed with hexane and EtOAc to give 191 mg of product as white solid (67%).

^{1}H NMR (400 MHz, $CDCl_3$, δ/ppm): 7.12 (m, 8H), 6.92 (m Hz, 8H), 6.86 (m, 12H), 6.80 (m, 8H), 4.61 (s, 8H), 3.37 (s, 12H), 2.43 (t, *J* = 7.5 Hz, 8H), 2.15 – 2.05 (m, 8H), 1.94 (m, 8H), 1.59 (m, 4H).
^{13}C NMR (126 MHz $CDCl_3$, δ/ppm): 142.4 (4C), 140.0 (4C), 139.9 (4C), 139.6 (4C), 138.5 (4C) 137.3 (4C), 131.4 (8C), 129.9 (8C), 126.7 (8C), 126.3 (8C), 125.4 (4C), 92.6 (4C), 78.4 (4C), 55.7 (4C), 33.9 (8C), 33.3 (4C), 24.2 (2C).
HR-MS (ESI): calc. for $[C_{86}H_{84}NaO_8]^+$: $[M+Na]^+$ 1267.6058; found 1267.6062
Mp: >350°C decomposition

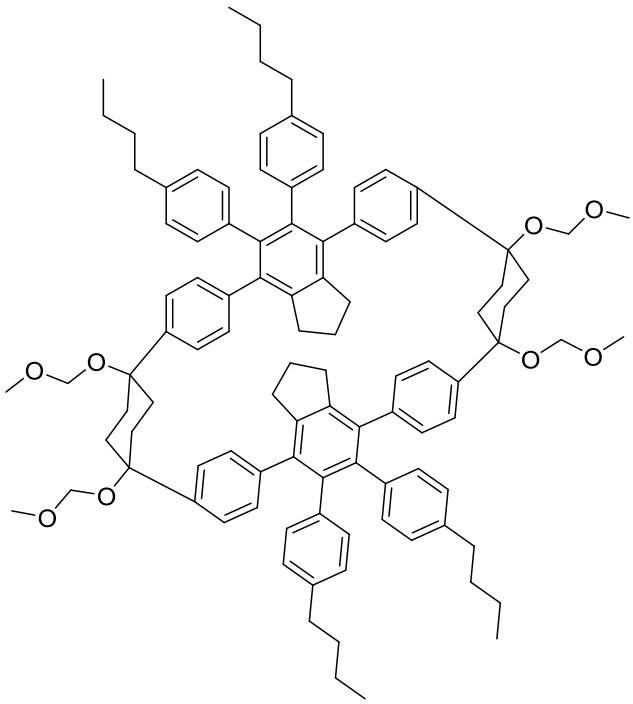


Synthesis of 8d

Macrocycle **7a** (100 mg, 112 mmol, 1.00 equiv), anhydrous 2-propanol (5 mL), and anhydrous THF (5 mL) were placed in a 10 mL microwave flask equipped with a stir bar. The reaction mixture was degassed by bubbling N_2 through the solution for 15 min. Then, $RhCl(PPh_3)_3$ (21.0 mg, 22.4 μmol,

20 mol %.) and 2-butyne-1,4-diol (96.8 mg, 1.12 mmol, 10.0 equiv) were added and the reaction flask was irradiated with microwave at 100 °C for 6 h. The reaction mixture was filtrated to give 73 mg of product as a white solid (61%).

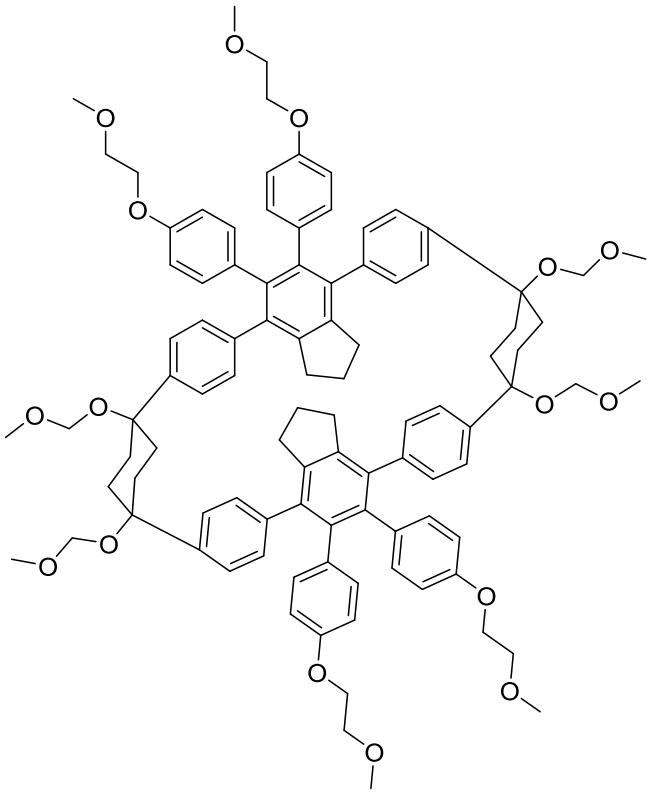
^{1}H NMR (400 MHz, $CDCl_3$) δ: broad signals (insoluble material)
HR-MS (ESI): calc. for $[C_{66}H_{76}NaO_{12}]^+$: $[M+Na]^+$ 1083.5229; found 1083.5242.
Mp: 262-273°C



Synthesis of 8e

To a microwave vial was added THF (5 mL) isopropanol (5 mL). Then argon was bubbled through the solvent for 15 min. The macrocycle **7a** (100 mg, 112 μmol, 1.00 equiv), 1,2-bis[4-(n-butyl)phenyl]ethyne (326 mg, 1.12 mmol, 10.0 equiv) and and $RhCl(PPh_3)_3$ (20.0 mg, 22.4 μmol, 20 mol %) was added. The vial was sealed and irradiated by microwave at 100 °C for 6 h. The product was chromatographed on column (cyclohexane/EtOAc, gradient) to afford 89.0 mg of product as white solid (54%).

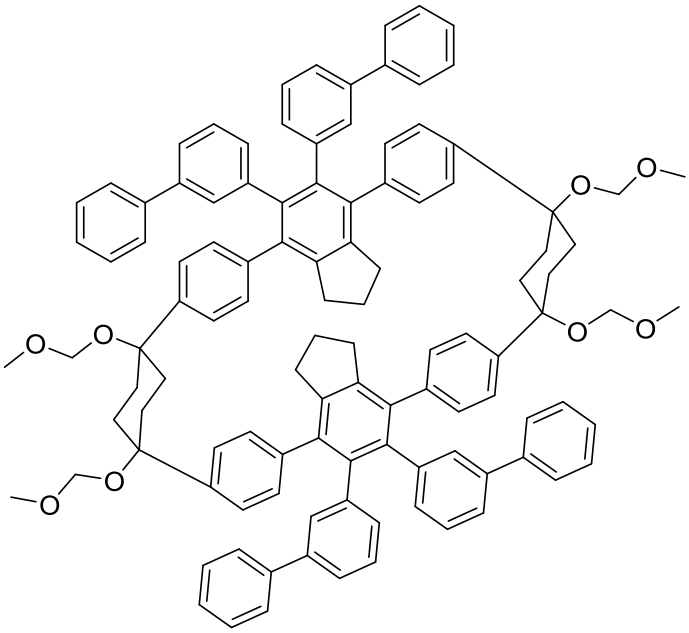
^{1}H NMR (400 MHz, $CDCl_3$, δ/ppm): 7.11 (m, 8H), 6.91 (m, 8H), 6.64 (s, 16H), 4.61 (s, 8H), 3.35 (s, 12H), 2.46 (t, *J* = 7.5 Hz, 8H), 2.35 (t, *J* = 7.5 Hz, 8H), 2.05 (m, 8H), 1.93 (m, 8H), 1.59 (m, 4H), 1.37 (m, 8H), 1.16 (m, 8H), 0.83 (t, *J* = 7.3 Hz, 12H).
^{13}C NMR (126 MHz, $CDCl_3$, δ/ppm): 142.0 (4C), 140.1 (4C), 139.5 (4C), 139.4 (4C), 138.5 (4C), 137.3 (4C), 137.1 (4C), 131.1 (8C), 129.9 (8C), 126.5 (8C), 126.3 (8C), 92.5 (4C), 78.3 (4C), 55.6 (4C), 34.9 (4C), 33.8 (8C), 33.3 (4C), 24.3 (2C), 21.9 (4C), 13.9 (4C).
HR-MS (ESI): calc. for $[C_{102}H_{120}NO_8]^+$: $[M+NH_4]^+$ 1486.9008; found 1486.9004.
Mp: 272-274°C



Synthesis of 8f

To a microwave vial was added THF (3 mL) and *iso*propanol (3 mL). Then argon was bubbled through the solvent for 15 min. The macrocycle **7a** (60 mg, 57.5 µmol, 1.00 equiv), 1,2-bis [4-(2-methoxyethoxy)phenyl]ethyne (220 mg, 675 µmol, 10.0 equiv) and $RhCl(PPh_3)_3$ (12.6 mg, 13.5 µmol, 20 mol %) was added. The vial was sealed and irradiated by microwave at 100 °C for 6 h. The solid was filtrated and recrystalization in cyclohexane/DCM afforded 15 mg of pure product as an off-white solid. The rest was chromatographed on column (cyclohexane/EtOAc, gradient) to afford 34 mg of product (47%).

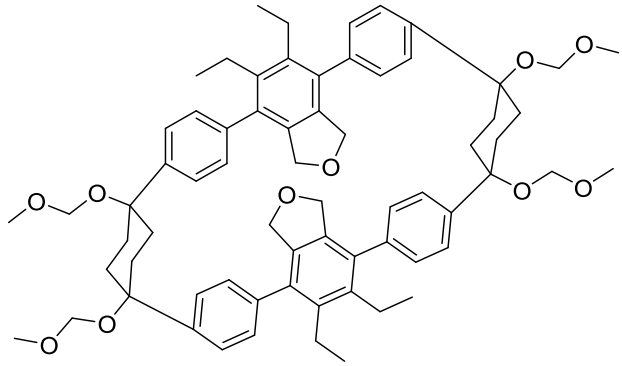
^{1}H NMR (400 MHz, $CDCl_3$, δ/ppm): 7.12 (m, 8H), 6.90 (m, 8H), 6.72 (m, 8H), 6.45 (m, 8H), 4.63 (s, 8H), 3.92 (m, 8H), 3.65 (m, 8H), 3.40 (s, 12H), 3.39 (s, 12H), 2.33 (t, *J* = 7.5 Hz, 8H), 2.11 (m, 8H), 1.93 (m, 8H), 1.50 (p, *J* = 7.5 Hz, 4H).
^{13}C NMR (126 MHz, $CDCl_3$, δ/ppm): 156.3 (4C), 142.2 (4C), 140.1 (4C), 139.3 (4C), 138.2 (4C), 137.8 (4C), 132.6 (4C), 132.4 (8C), 130.1 (8C), 126.2 (8C), 112.9 (8C), 92.7 (4C), 78.3 (4C), 71.1 (4C), 66.7 (4C), 59.2 (4C), 55.7 (4C), 34.0 (8C), 33.3 (4C), 24.1 (2C).
HR-MS (ESI): calc. for $[C_{98}H_{108}NaO_{16}]^+$: $[M+Na]^+$ 1563.7530; found 1563.7527.
Mp: 270-272°C



Synthesis of 8g

To a microwave vial was added THF (10 mL) and isopropanol (10 mL). Then argon was bubbled through the solvent for 15 min, the macrocycle **7a** (200 mg, 225 μmol, 1.00 equiv), 1,2-di[(1,1'-biphenyl)-3-yl]ethyne (743 mg, 2.25 mmol, 10.0 equiv) and $Rh(PPh_3)_3Cl$ (41.6 mg, 45 μmol, 20 mol %) were added. The vial was sealed and irradiated by microwave at 100 °C for 6 h. The product was chromatographed on column (CH/EtOAc, gradient) to afford 258 mg of product as white solid (74%).

^{1}H NMR (400 MHz $CDCl_3$ δ/ppm): 7.20 (m, 12H), 7.13 (m, 12H), 7.07 (m, 12H), 6.94 (m, 12H), 6.86 (m, 4H), 4.63 (s, 8H), 3.37 (s, 12H), 2.46 (m, 8H), 2.03 (m, 8H), 1.92 (m, 8H), 1.62 (s, 4H).
^{13}C NMR (150Hz, $C_2D_2Cl_4$, 348K, δ/ppm): 143.0, 141.2, 140.4, 139.8, 139.5, 138.2, 137.3, 131.4, 131.0, 130.8, 130.4, 130.1, 126.9, 126.3, 125.2, 124.5, 122.3, 92.6, 78.6, 55.6, 34.1, 33.1, 24.3
HR-MS (ESI): calc. for $[C_{110}H_{100}NaO_8]^+$: $[M+Na]^+$ 1571.7310; found 1571.7317.
Mp: 274-276°C

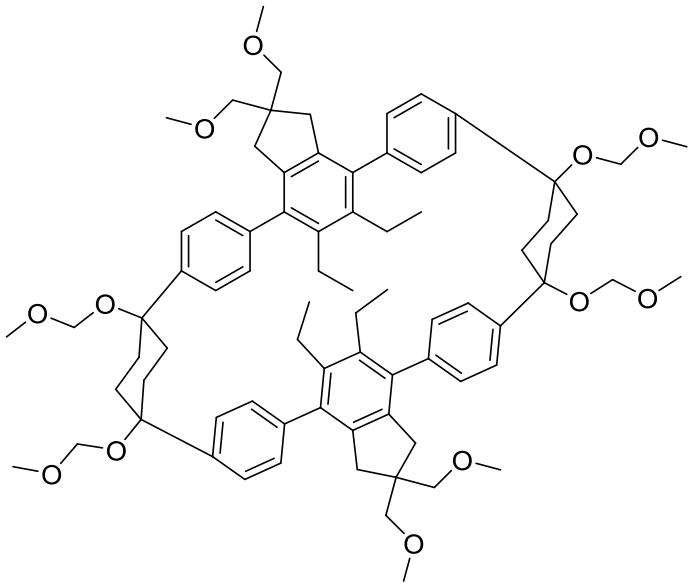


Synthesis of 8h

To a 20 mL microwave vial was introduced THF (5 mL) and *i*PrOH (5 mL) Argon was bubbled through the solvent for 15 min. Then, **7c** (60 mg, 67.2 μmol, 1.00 equiv), 3-hexyne (100 μL, 896 μmol, 13.0 equiv) and $RhCl(PPh_3)_3$ (16.6 mg, 17.9 μmol, 27 mol %) were added and the vial was

sealed and irradiated in the microvawe reactor at 100 °C for 6 h. The crude mixture was concentrated, suspended in cyclohexane/EtOAc (1/1) and filtrated to give 33 mg of a grey solid (46%).

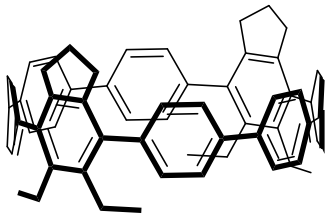
^{1}H NMR (400 MHz, $CDCl_3$, δ/ppm): 7.38 (m, 8H), 7.11 (m, 8H), 4.71 (s, 8H), 3.93 (s, 8H), 3.48 (s, 12H), 2.79 (m, 8H), 2.31 (m, 8H), 1.95 (m, 8H), 1.11 (t, *J* = 7.4 Hz, 12H).
^{13}C NMR (101 MHz, $CDCl_3$, δ/ppm): 140.0 (4C), 138.8 (4C), 137.0 (4C), 135.2 (8C), 128.9 (8C), 127.5 (8C), 92.8 (4C), 77.8 (4C), 74.1 (4C), 56.0 (4C), 33.9 (8C), 23.2 (4C), 16.6 (4C).
HR-MS (ESI): calc. for $[C_{68}H_{80}NaO_{10}]^+$: $[M+Na]^+$ 1079.5644; found 1079.5658.
Mp: >350°C decomposition.



Synthesis of 8i

To a microwave vial was added THF (10 mL) and *iso*propanol (10 mL). Then, argon was bubbled through the solvent for 15 min. The macrocycle **7b** (100 mg, 93.9 μmol, 1.00 equiv), 3-hexyne (107 μL, 939 μmol, 10.0 equiv) and $Rh(PPh_3)_3Cl$ (17.5 mg, 18.8 μmol, 20 mol %) were added. The vial was sealed and irradiated by microwave at 100 °C for 6 h. The mixture was concentrated, suspended in cyclohexane/EtOAc (1/1) and filtrated to give 78.5 mg of product as a grey solid (68%).

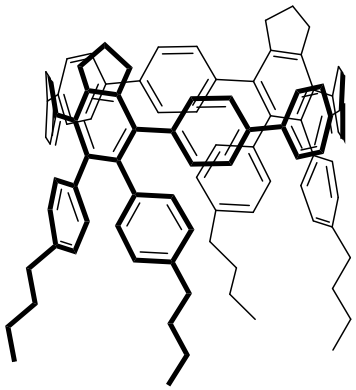
^{1}H NMR (600 MHz, $C_2D_2Cl_4$, 158 K, δ/ppm): 7.27 (m, 8H), 6.98 (m, 8H), 4.67 (s, 8H), 3.38 (s, 12H), 3.06 (s, 12H), 2.83 (s, 8H), 2.52 (q, *J* = 7.4 Hz, 8H), 2.29 (m, 8H), 1.95 (m, 8H), 1.89 (bs, 8H), 0.96 (t, *J* = 7.4 Hz, 12H).
^{13}C NMR (150Hz, $C_2D_2Cl_4$, 358K, δ/ppm): 140.5 (4C), 140.0 (4C), 138.8 (4C), 138.5 (4C), 138.0 (4C), 129.2 (8C), 126.9 (8C), 92.5 (4C), 77.8 (4C), 75.9 (4C), 59.0 (4C), 55.4 (4C), 46.8 (2C), 38.8 (4C), 33.9 (8C), 23.3 (4C), 16.3 (4C).
HR-MS (ESI): calc. for $[C_{78}H_{100}NaO_{12}]^+$: $[M+Na]^+$ 1251.7107; found 1251.7092.
Mp: 272-279°C



Synthesis of 9a

In a 20 mL vial **8a** (120 mg, 114 μmol, 1.00 equiv) and $NaHSO_4/H_2O$ (274 mg, 2.28 mmol, 20.0 equiv) were placed in 5 mL *m*-xylene and 5 mL DMSO. The mixture was stirred under air at 130 °C for 24 h. The mixture was cooled to rt and extracted with water and EtOAc. The organic phase was washed again with water and dried over Na_2SO_4 and concentrated under reduced pressure. The residue was chromatographed on TLC (hexane/DCM: 1/1) to give 6.0 mg of **9a** as a pale yellow solid (7%).

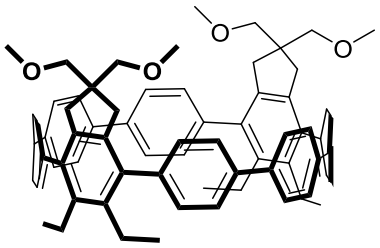
^{1}H NMR (500 MHz, CD_2Cl_2, δ/ppm): 7.35 (s, 8H), 7.30 – 7.25 (m, 8H), 7.04 – 6.93 (m, 8H), 2.98 (q, *J* = 7.5 Hz, 8H), 1.90 (t, *J* = 7.7 Hz, 8H), 1.28 – 1.20 (m, 4H), 1.14 (t, *J* = 7.4 Hz, 12H).
^{13}C NMR (126 MHz, CD_2Cl_2, δ/ppm)*: 141.9, 139.3, 138.4, 137.9, 137.8, 137.3, 131.1, 127.2, 126.3, 32.4, 23.1, 21.8, 16.2.
HR-MS (MALDI): calc. for $[C_{62}H_{56}]^+$: $[M]^+$ 800.4377; found 800.4378. (DCTB matrix)



Synthesis of 9b

In a 20 mL vial **8e** (80.0 mg, 54.4 μmol, 1.00 equiv) and $NaHSO_4/H_2O$ (150 mg, 1.08 mmol, 20.0 equiv) were placed in 7.5 mL *m*-xylene and 7.5 mL DMSO. The mixture was stirred under air at 130 °C for 48 h. The mixture was cooled to rt and extracted with water and EtOAc. The organic phase was washed again with water and dried over Na_2SO_4 and concentrated under reduced pressure. The residue was chromatographed on TLC (Hexane/DCM: 1/1 +1% MeOH) to give 3.00 mg of **9b** as a pale yellow solid (5%).

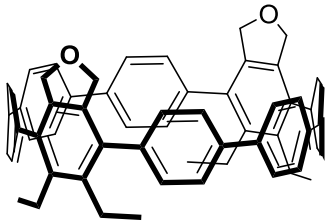
^{1}H NMR (500 MHz, CD_2Cl_2, δ/ppm): 7.35 (s, 8H), 7.22 (m, 8H), 7.01 (m, 8H), 6.89 (m, 8H), 6.76 (m, 8H), 2.50 – 2.43 (m, 8H), 2.29 (t, *J* = 7.6 Hz, 8H), 1.53 (m, 4H), 1.47 (m, 8H), 1.22 (m, 8H), 0.93 – 0.86 (m, 12H).
^{13}C NMR (126 MHz, CD_2Cl_2, δ/ppm)*: 143.5 (4C), 140.3 (4C), 139.5 (4C), 139.0 (8C), 138.7 (4C), 138.3 (4C), 138.2 (4C), 132.2 (8C), 131.8 (8C), 128.2 (8C), 126.9 (8C), 126.7 (8C), 35.1 (4C), 33.4 (4C), 33.3 (4C), 23.7 (2C), 22.4 (4C), 13.8 (4C).
HR-MS (MALDI): calc. for $[C_{94}H_{88}]^+$: $[M]^+$ 1216.6881; found 1216.6884. (DCTB matrix)



Synthesis of 9c

In a 20 mL vial **8i** (33 mg, 26.8 μmol, 1.00 equiv) and $NaHSO_4/H_2O$ (64.0 mg, 0.537 mmol, 20.0 equiv) were placed in 5 mL *m*-xylene and 5 mL DMSO. The mixture was stirred under air at 130 °C for 24 h. The mixture was cooled to rt and extracted with water and EtOAc. The organic phase was washed again with water and dried over Na_2SO_4 and concentrated under reduced pressure. The residue was chromatographed on TLC (Hexane/DCM: 1/1 +1%MeOH) to give 1.9 mg of **9c** as white solid (4%).

^{1}H NMR (500 MHz, CD_2Cl_2, δ/ppm)*: 7.45 (s, 8H), 7.37 – 7.30 (m, 8H), 7.09 – 7.02 (m, 8H), 3.06 (q, *J* = 7.4 Hz, 8H), 2.87 (s, 12H), 2.73 (s, 8H), 1.98 (s, 8H), 1.21 (t, *J* = 7.4 Hz, 12H).
^{13}C NMR (126 MHz, CD_2Cl_2, δ/ppm): 141.0, 140.1, 139.3, 139.0, 138.9, 138.5, 132.1, 128.1, 127.1, 75.9, 59.0, 45.9, 24.4, 17.1.
HR-MS (ESI): calc. for $[C_{70}H_{72}NaO_4]^+$: $[M+Na]^+$ 999.5323; found 999.5340.

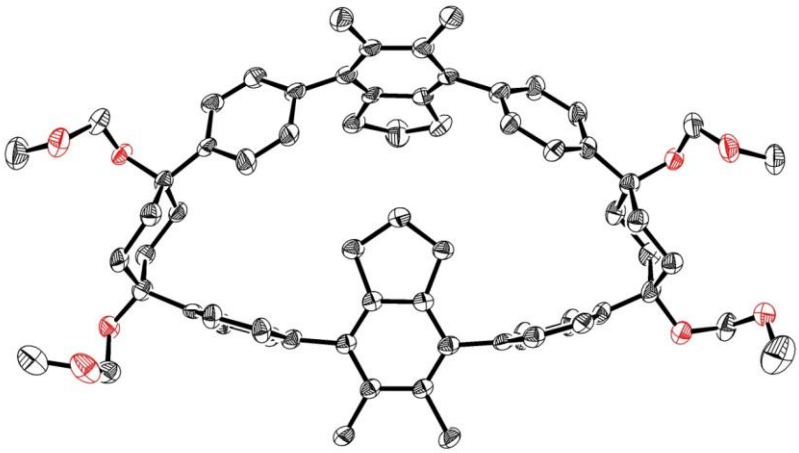


Synthesis of 9d

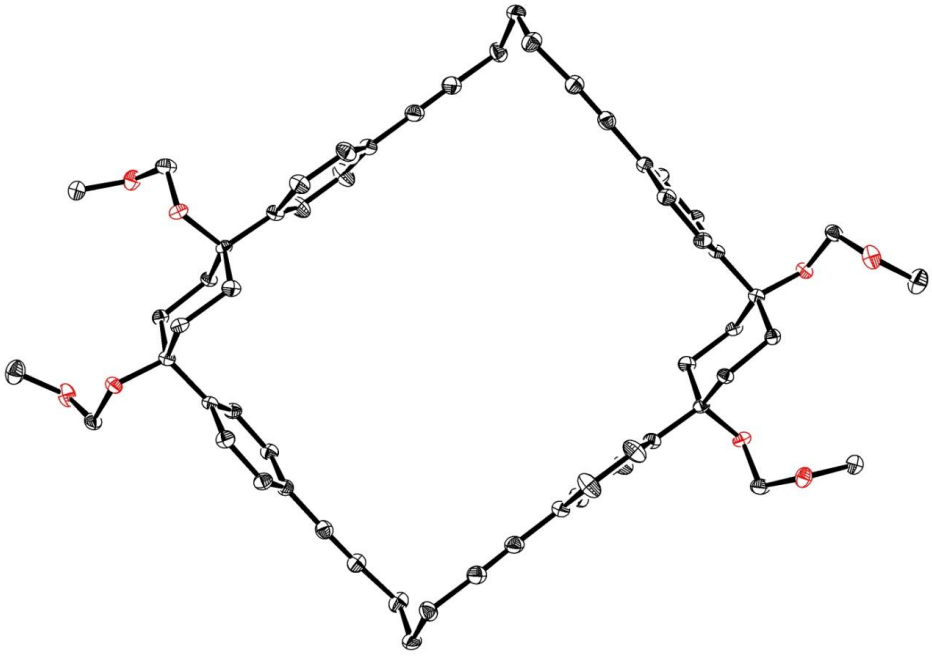
In a 20 mL vial **8h** (30.0 mg, 28.4 μmol, 1.00 equiv) and $NaHSO_4/H_2O$ (78.0 mg, 567 μmol, 20.0 equiv) were placed in 5 mL *m*-xylene and 5 mL DMSO. The mixture was stirred under air at 130 °C for 48 h. The mixture was cooled to rt and extracted with water and EtOAc. The organic phase was washed again with water and dried over Na_2SO_4 and concentrated under reduced pressure. The residue was chromatographed on TLC (hexane/DCM: 1/1 +1% MeOH)) to give 0.6 mg of **9d** as a pale yellow solid 3%.

^{1}H NMR (500 MHz, CD_2Cl_2, δ/ppm): 7.44 (s, 8H), 7.39 (m, 8H), 7.06 (m, 8H), 4.07 (s, 8H), 3.11 (q, *J* = 7.5 Hz, 8H), 1.26 (m, 12H).
^{13}C NMR (126 MHz, CD_2Cl_2, δ/ppm)*: 139.4 (8C), 139.1 (4C), 138.9 (4C), 138.7 (4C), 135.8 (4C), 131.0 (8C), 128.2 (8C), 127.5 (8C), 74.7 (4C), 23.9 (4C), 17.1 (4C).
HR-MS (MALDI): calc. for $[C_{60}H_{52}O_2]^+$: $[M]^+$ 804.3962; found 804.3964. (DCTB matrix)

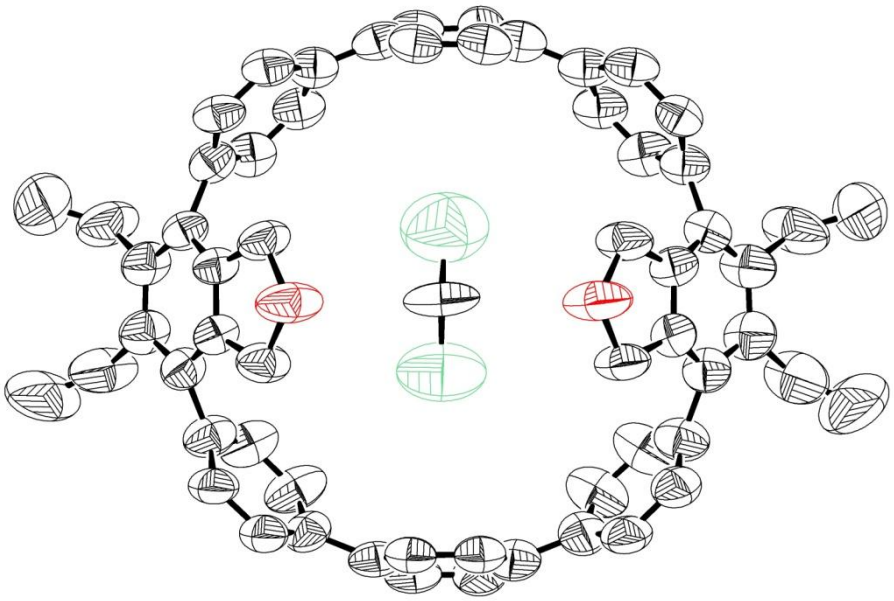
Crystallographic data:



Crystal data for **8b**: formula $C_{68}H_{78}Cl_6O_8$, M = 1236.08, F(000) = 2608, colourless plate, size 0.010 · 0.070 · 0.220 mm^3, monoclinic, space group P 21/c, Z = 4, a = 20.300(2) Å, b = 13.4605(14) Å, c = 23.478(3) Å, α = 90°, β = 99.477(5)°, γ = 90°, V = 6327.9(12) $Å^3$, Dcalc. = 1.297 Mg · m^{-3}. The crystal was measured on a Bruker Kappa Apex2 diffractometer at 123K using graphite-monochromated Mo K_α-radiation with λ = 0.71073 Å, Θmax = 26.376°. Minimal/maximal transmission 0.98/1.00, μ = 0.326 mm^{-1}. The Apex2 suite has been used for data collection and integration. From a total of 47114 reflections, 12921 were independent (merging r = 0.364). From these, 12870 were considered as observed (I>2.0σ(I)) and were used to refine 739 parameters. The structure was solved by Direct methods using the program SIR92. Least-squares refinement against Fsqd was carried out on all non-hydrogen atoms using the program CRYSTALS. R = 0.1001 (observed data), wR = 0.2828 (all data), GOF = 1.0315. Minimal/maximal residual electron density = -2.62/2.87 e $Å^{-3}$. Chebychev polynomial weights were used to complete the refinement. Plots were produced using Ortep 3v2



Crystal data for **7a**: formula $C_{62}H_{68}Cl_{12}O_8$, M = 1366.65, F(000) = 708, yellow needle, size 0.020 · 0.060 · 0.220 mm^3, triclinic, space group P -1, Z = 1, a = 6.1849(4) Å, b = 15.7299(11) Å, c = 16.9383(11) Å, α = 97.464(4)°, β = 94.271(4)°, γ = 96.956(4)°, V = 1615.07(19) $Å^3$, Dcalc. = 1.405 Mg · m^{-3}. The crystal was measured on a Bruker Kappa Apex2 diffractometer at 123K using graphite-monochromated Mo K_α-radiation with λ = 0.71073 Å, Θmax = 30.089°. Minimal/maximal transmission 0.97/0.99, μ = 0.567 mm^{-1}. The Apex2 suite has been used for data collection and integration. From a total of 32270 reflections, 9430 were independent (merging r = 0.065). From these, 4577 were considered as observed (I>2.0σ(I)) and were used to refine 370 parameters. The structure was solved by Other methods using the program Superflip. Least-squares refinement against F was carried out on all non-hydrogen atoms using the program CRYSTALS. R = 0.0526 (observed data), wR = 0.0960 (all data), GOF = 1.1104. Minimal/maximal residual electron density = -0.70/0.63 e $Å^{-3}$. Chebychev polynomial weights were used to complete the refinement. Plots were produced using Ortep 3v2



Crystal data for **9d**: formula $C_{121}H_{108}Cl_2O_4$, M = 1697.09, F(000) = 1800, colourless plate, size 0.020 · 0.170 · 0.260 mm^3, monoclinic, space group P 21/c, Z = 2, a = 19.4814(18) Å, b = 18.4101(14) Å, c = 18.5749(15) Å, α = 90°, β = 99.456(6)°, γ = 90°, V = 6571.4(10) $Å^3$, Dcalc. = 0.858 Mg · m-3. The crystal was measured on a Bruker Kappa Apex2 diffractometer at 123K using graphite-monochromated Cu K_α-radiation with λ = 1.54180 Å, Θmax = 68.290°. Minimal/maximal transmission 0.88/0.99, μ = 0.750 mm^{-1}. The Apex2 suite has been used for data collection and integration. From a total of 11798 reflections, 11798 were independent (merging r = 0.075). From these, 5987 were considered as observed (I>2.0σ(I)) and were used to refine 586 parameters. The structure was solved by Other methods using the program Superflip. Least-squares refinement against F was carried out on all non-hydrogen atoms using the program CRYSTALS. R = 0.0912 (observed data), wR = 0.2421 (all data), GOF = 1.1016. Minimal/maximal residual electron density = -0.23/0.44 e $Å^{-3}$. Chebychev polynomial weights were used to complete the refinement. Plots were produced using Ortep 3v2

The structure contains large cavities occupied by disordered solvent molecules. As the data quality was not optimal, and as the solvent molecules appear heavily disordered, it was not possible to identify more than the DCM molecule in the centre of the structure. For this reason SQUEEZE (A.L.Spek, Acta Cryst. 2009, D65, 148-155.) was used in order to finish the refinement.

Computational study

We performed density functional theory (DFT) calculations under the generalized gradient approximation as implemented in the AIMPRO code[10] The exchange-correlation energy contribution is evaluated using the formula described by Perdew, Burke and Ernzerhof[11]. Atom-centred Gaussian basis functions are used to construct the many-electron wavefunction. In all cases, spin-average calculations have been used. The calculations were carried out using supercells, fitting the charge density to plane waves within an energy cut-off of 150 Ha (Ha=Hartree energy). Electronic level occupation was obtained using the Fermi occupation with kT=0.01eV. Core electrons are replaced by norm-conserving pseudopotentials based on the Hartwigsen-Goedecker-Hutter (HGH) scheme[12] using 22 independent Gaussian functions per carbon and oxygen atom, 12 per hydrogen. Calculations are performed with Brillouin zone sampling k-points within the Monkhorst-Pack scheme[13]

For the ring relaxation, we have used the molecule in a vacuum box method with a single k-point and box-size chosen so there is always over 8Å between neighbouring molecules. The Poly(p-phenylene) (PPP) and the other related chains were optimized using an infinite structure in the z direction and converged k-point grids of 1x1x*n* along the chain direction. Supercell sizes have been checked and chosen to be sufficiently large so there are no interactions between either the rings or chains. Energies have converged to better than 10^{-7} Ha. Atomic positions and lattice parameters (only for the chains) were geometrically optimized until the maximum atomic position change in a given iteration dropped below 10^{-5} a_0 (a_0: Bohr radius).

Previous theoretical studies have calculated the structures and strain energies of cycloparaphenylenes (CPPs) using DFT at the B3LYP/6-31G(d) theory level. The strain energy was estimated on the basis of the homodesmotic reaction using CPP_n and *n* biphenyls giving *n* p-terphenyls. We compared their results with ours for two different CPPs using their approach to calculate the strain energy. This is summarized in the table below:

Table 1: Strain energy of CPP using different approaches

	Strain energy (kcal.mol^{-1})	
n in [n]CPP	Segawa 2010[14]	This work
6	96.0	89.9
8	72.2	68.3

This shows sufficiently good agreement in the strain energy between the two, given the difference in basis sets and exchange-correlation functional used. However, we decided to take a different approach to calculate the strain energy, which to us seems more appropriate due to the fact that only the two relevant structures are used. In this case the strain energy was calculated as the difference in total energy between the ring and the infinite chain (in the case of standard CPPs this gives the

[10] Briddon-Accurate Kohn-Sham DFT with the speed of tight binding: Current techniques and future directions in materials modelling-:Physica status solidi B-248-1309-1318 (2011).
[11] Perdew, Burke and Ernzerhof Phys. Rev. Lett. 77, 3865 (1996).
[12] Hartwigsen C, Goedecker S, Hutter J. Relativistic separable dual-space Gaussian pseudopotentials from H to Rn. Phys Rev B 1998;58:3641.
[13] Monkhorst HJ, Pack JD. Special points for Brillouin-zone integrations. Phys Rev B 1976;13:5188.
[14] Segawa, Y.; Omachi, H.; Itami, K. *Organic Letters* **2010**, *12*, 2262.

infinite conjugated polymer chain PPP). This is achieved by breaking a bond in the CPP and straightening the fragment, and then placing this in a repeating supercell such that the broken bonds connect to each other across opposite sides of the cell. This approach avoids any additional energetic terms due to changes in conjugation that may be present in the hypothetical homodesmotic reaction approach.

The structural properties of the 8 poly-(p-phenylene) are in very good agreement with other theoretical work on biphenyl[15]. For example, the C-C bond length between two rings is 1.48Å compared to 1.46Å in this previous work. The torsion angle is identical between the two calculations.

The following table summarizes the resultant calculated strain energies for the structures relevant to this work.

Table 2: Diameters, dihedral angles and strain energies of the related structures.

	Diameter (nm)	Dihedral angle (°)	Strain Energy (kcal.mol$^{-1)}$
[8]CPP	1.116	29.5	62.87
8a	1.116	49.9	63.69
8b	1.130	45.8	51.06
8c	1.121	51.8	73.61
8d	1.115	45.1	62.39

We note that the small difference in strain energy determined by this method as compared to the homodesmotic method shows that additional energy terms due to conjugation change in the homodesmotic case are small (5.43 kcal/mol).

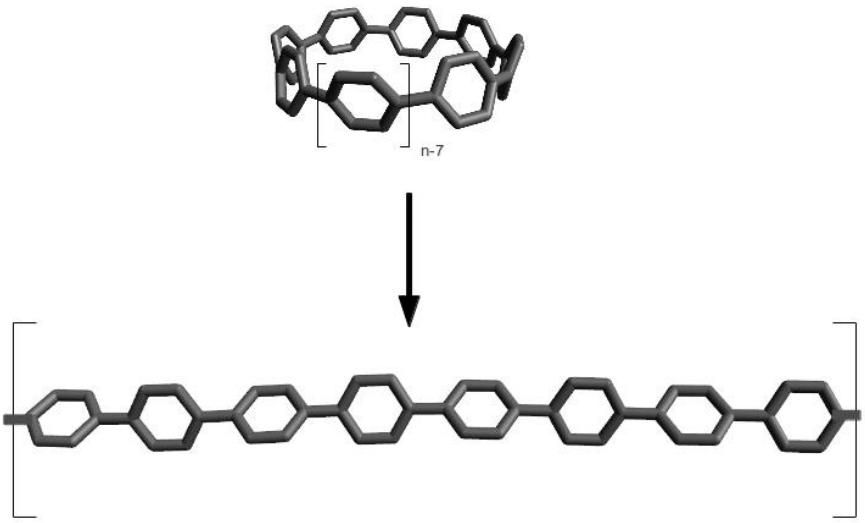


Figure 1: Reaction used for the calculation of the strain energies of the investigated structure

[15] Rabias-Synthetic Metals-108-223-230 (2000)

The results show that ring strain is largely independent of the side-group functionalization. This seems reasonable since the benzenoid rings are not conjugated and hence ring strain is primarily simply a function of ring curvature. In table 2, ring diameter is defined as the average C-C distance for equatorial carbon atoms 11.20Å (+/- 0.15Å).

For each structure, isomers can be found and they all lie in the range of 150 meV (94 kcal/mol). Aside from the isomers described[12] depending on tilt orientation of the ideal benzenoid rings, further isomer options exist in these cases depending on the tilt angle of the functionalised rings.

In summary, we present a new approach for the calculation of the ring strain energy. This approach provides several advantages listed below:

- The two calculations (ring and linear-chain) feature identical numbers of atoms, in identical bonding configurations, with no additional molecular species required (such as H_2 or biphenyl).
- There is no bond-cleavage point in the chain, since both ring and linear chain structures are infinite.
- There is no change in neighbour map / z-matrix between the two systems. Thus this approach does not incorporate any change in energetic stability due to, e.g. increased electronic confinement, change in conjugation, etc.
- The approach is applicable to any ring structure regardless of its chemical composition.
- The system correctly interpolates to zero energy difference between the two calculations as the chain length / ring circumference tends to infinity.

Cartesian coordinates of linear chains:

9a chain

C	-1.31674294316	2.29162052355	5.97276309631
C	-0.58957438387	1.21617878912	5.18483389771
C	-0.70124456991	1.20887770546	3.77065543361
C	0.01677001843	0.26001394459	3.00811172840
C	0.83414181591	-0.66792036419	3.67309437221
C	1.75763914073	-1.68828281280	3.04609480884
C	0.91031558744	-0.69029855033	5.06568010504
C	1.88781929034	-1.74138877973	5.54609422018
C	0.19451569460	0.23716145422	5.84286399354
H	1.09907539841	1.88554280695	10.14367916055
C	0.69386164524	1.07597220520	9.53495330822
C	0.74961193473	1.15914768319	8.14492115452
H	1.20828655137	2.02979358749	7.67766851174
C	0.23434060380	0.13625164677	7.33225756753
C	-0.28752303364	-1.00187363361	7.97372638422
H	-0.71186460037	-1.80229729638	7.36609673216
C	-0.31398592062	-1.10272492078	9.36438726142
H	-0.75118022055	-1.98420275222	9.83645370296
C	0.15823537885	-0.05520698082	10.17287941486
H	-0.95368168026	1.69243782267	14.35255862292
C	-0.47744387635	0.88632448320	13.79133822712
C	-0.46233194768	0.92412970952	12.39876677606
H	-0.92609659140	1.76069296715	11.87297872191
C	0.10331688961	-0.12483775621	11.65317606342
C	0.63432717071	-1.22071417365	12.35313411777
H	1.10867253890	-2.02856719993	11.79279695812
C	0.62016539046	-1.25888278696	13.74680266928
H	1.08396968250	-2.09536049500	14.27212088535
C	0.07199722176	-0.20140195505	14.49244260726
H	0.92615780039	1.75019697696	18.63535423618
C	0.51494936508	0.89759467474	18.09445135527
C	0.54411253954	0.88929139279	16.70101052050
H	0.96526670216	1.74001678507	16.16236172953
C	0.07135504435	-0.21668144988	15.97453777009
C	-0.41438881364	-1.31882709794	16.69827501327
H	-0.79637521712	-2.18523867793	16.15492041295
C	-0.47585620666	-1.29210940328	18.09171341786
H	-0.91526564737	-2.13597490905	18.62723694274
C	-0.02741049553	-0.17645926825	18.82231927287
C	-1.04073611187	0.82897539771	22.38695629265
C	-0.92435276140	0.84514036385	20.97239499411
C	-0.14399227534	-0.13705254421	20.31041059643
C	0.51800336211	-1.10803211306	21.08327700296
C	0.46195408080	-1.07661811180	22.47848293465
C	-0.30456254761	-0.10951188469	23.15064309233
H	0.70696333381	1.96776891725	27.21138585156
C	0.29445349179	1.08888939723	26.71159261272
C	0.23144034196	1.05307968254	25.32017359248
H	0.59322583913	1.90211417389	24.73652430803
C	-0.27189028892	-0.07274365791	24.64075716020
C	-0.68691137856	-1.16986874000	25.41406719807
H	-1.10058843633	-2.04762029200	24.91359981577
C	-0.60553629983	-1.14344782579	26.80500980614
H	-0.95960022180	-1.99837608770	27.38424134059
C	-0.12393237180	-0.01020708563	27.48279879770
H	-0.84517767120	2.09397064079	31.57617029903
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C	-0.48665087947	1.17789097008	29.66113125912
H	-0.84624652574	2.04364738990	29.10153832278
C	-0.08694373698	0.02702444438	28.95998213247
C	0.32034617895	-1.09261900941	29.70791343323
H	0.68144519123	-1.97893648070	29.18417519567
C	0.31594322137	-1.06503806200	31.09994957690
H	0.67219651932	-1.93211522903	31.65989667699
C	-0.08874224306	0.08388631685	31.80008882874
H	0.90743756263	2.14438377563	1.25754205013
C	0.46727621041	1.28570140268	0.74931327291
C	0.43626837052	1.24287243589	-0.64235861688
H	0.85555567229	2.06669832464	-1.22064804806
C	-0.08060909414	0.12510291978	-1.32015590854
C	-0.57932027986	-0.94028835719	-0.55190012731
H	-1.01507011812	-1.80407552845	-1.05817959343
C	-0.56729895353	-0.88592808740	0.84020395976
H	-0.99174809363	-1.70804271936	1.41903050397
C	-0.03996596380	0.22487631445	1.51938814518
C	2.47465483073	-2.36764824444	4.24734437878
H	2.46485254124	-1.19943323107	2.35791983420
H	1.20648586510	-2.41572365539	2.43219860643
H	3.55860435145	-2.20756726959	4.19335402179
H	2.32030366824	-3.45373667307	4.23110592502
H	1.39828490408	-2.49661196864	6.17839145441
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C	1.97811097693	-2.88330091648	21.88522921659
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H	1.70937461615	-3.94807688137	21.91624194232
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H	0.88453555484	-2.93738378429	19.96651981802
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C	-0.56528104485	3.63832289735	5.98937599081
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H	-4.19808293894	1.83337622232	23.48151050163
H	-3.50877735051	0.19654702463	23.59574379930
H	-2.66642637918	2.04908388223	20.57283786250
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H	-0.71684946874	3.60255302441	21.26675869035
H	-1.54875642890	4.07722719275	19.76899290424
H	0.02738348245	3.26649560685	19.70345656421
H	-3.26774818807	0.87562074079	3.88553747596
H	-3.57310377304	1.45833914572	2.24560459956
H	-3.77869245305	2.55103705961	3.62273687050
H	-1.47366805963	1.95659458393	7.00660038057
H	-2.31791569725	2.44750380689	5.54772293341
H	0.36601507462	3.56770172313	6.56583541838
H	-1.17854240933	4.42981001586	6.44122916495
H	-0.28743406859	3.96099805312	4.97693706108
H	-1.41192931573	2.24948295869	2.02966725496
H	-1.53639108457	3.17696439546	3.50430051983

9b chain

C	-0.45353832031	1.00061200493	5.06367672204
C	-0.52883815756	0.98755084546	3.64655801775
C	0.15024397247	0.00692906394	2.88792392859
C	0.90955716839	-0.94051035269	3.60182265431
C	1.83456794406	-1.98556453776	3.02297980841
C	0.95754416753	-0.94434185024	5.00298002051
C	1.92077611285	-1.98833082447	5.52196363016
C	0.26346457720	0.01077982788	5.76612127523
H	0.93674491730	1.92625449854	9.99467192410
C	0.61967188692	1.05423024541	9.41955660142
C	0.66331531480	1.09534967361	8.02864080242
H	0.99839018032	2.00665627732	7.53563782605
C	0.28478053297	-0.01767408381	7.25589053523
C	-0.12319080174	-1.17666728803	7.94070798666
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C	-0.15910684894	-1.22151012541	9.33153056717
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C	0.15653197495	-0.14467063148	11.57389064054
C	0.55638212088	-1.29188054536	12.28201559039
H	0.94304696875	-2.14943062706	11.72894770869
C	0.52358534596	-1.32633699682	13.67299077478
H	0.88382272472	-2.21020744396	14.20241228766
C	0.09114416658	-0.21134499944	14.40989930968
H	0.79859749372	1.89406091218	18.47091572236
C	0.44704595471	0.99695874930	17.96942934131
C	0.48692229406	0.94327056122	16.58123912656
H	0.86476122389	1.79856657205	16.01904164681
C	0.08075389185	-0.20583728882	15.88509222666
C	-0.34232579009	-1.31322318595	16.63931082307
H	-0.66949212894	-2.21887106122	16.12502444215
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H	-0.79695651417	-2.10042327268	18.58563842942
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H	-0.97719854188	-2.05281847360	24.79476268056
C	-0.52953331089	-1.15429911272	26.69630508529
H	-0.79499045173	-2.05689994480	27.24832882048
C	-0.13276979267	-0.00161624279	27.40046380134
H	-0.69645664824	2.07082975931	31.53861128735
C	-0.39281640475	1.16575249444	31.00856303858
C	-0.40559717088	1.16033708868	29.61526039677
H	-0.72646530465	2.05474229347	29.08030895078
C	-0.06963359270	0.00534179800	28.88192321610
C	0.29615972547	-1.13570150788	29.61902467902
H	0.61454412212	-2.03571627355	29.08770585398
C	0.30256402206	-1.13261583358	31.01410386808
H	0.63102168563	-2.02576649024	31.54749460425
C	-0.05487550578	0.01773169206	31.74789659755
H	1.02552224006	1.94943151444	1.13186443909
C	0.56868806345	1.09986323682	0.62750138791
C	0.48400127665	1.11404693084	-0.76409513026
H	0.87842315247	1.97299077963	-1.31048943443
C	-0.05132163980	0.02706126566	-1.47908975253
C	-0.54341888607	-1.05280007293	-0.72148409650
H	-1.02003432029	-1.89052915883	-1.23374160211
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C	0.09164141201	0.01482240318	1.38818847502
C	2.56797778658	-2.59955055378	4.24903644577
H	2.53127924790	-1.52456876966	2.30598471675
H	1.27762235641	-2.74474653428	2.45343673327
H	3.63930093070	-2.36331808828	4.21399880450
H	2.48848759313	-3.69406060656	4.25276997309
H	1.41287092099	-2.75194471258	6.12981230814
H	2.66326595682	-1.52685972519	6.19250677168
C	1.28222617863	-2.07206621625	22.99819449082
C	1.92838051878	-2.80885985089	21.79257680944
C	1.38590681672	-2.13441220604	20.50394095683
H	0.71316637705	-2.77083338518	23.62626064633
H	2.03272961981	-1.62085799587	23.66615866792
H	1.67115111841	-3.87662487396	21.80934553077
H	3.02370752095	-2.75562946891	21.83630663175
H	0.84267802757	-2.85658881030	19.87741891482
H	2.18685039867	-1.73564693782	19.86203772084
C	-2.06490226842	1.91851313900	22.89197233570

C	-3.41396112600	1.56087454876	23.07017209531
C	-4.40803190057	2.49739175977	23.41896822956
C	-4.08830719337	3.84713481718	23.62402001545
C	-2.72869043484	4.18923248241	23.47623532609
C	-1.74695884935	3.26883636206	23.11928677044
H	-3.70334069955	0.52342092974	22.89114625144
H	-5.43972103153	2.14974176825	23.50936808649
H	-2.43854877493	5.22914235277	23.64589384882
H	-0.72326013981	3.61963829028	22.97914636447
C	-4.96755419729	5.01764671937	24.08425468410
C	-6.50803133075	5.17054067169	24.09377414328
C	-6.77689337862	6.50736998375	24.83806068249
C	-8.18607803565	7.11649246789	24.83095172056
H	-8.98263058803	6.37471857370	24.97931078288
H	-8.39677021886	7.65849412395	23.89828390531
H	-8.27190188253	7.85142128783	25.64670811007
H	-6.08481084480	7.26536952996	24.43280247044
H	-6.45855114216	6.36497729702	25.88367183947
H	-7.01979404304	4.34744459353	24.61905065156
H	-6.92374364309	5.20211045639	23.07312358666
H	-4.60180641138	5.89174177896	23.51996475681
H	-4.64890578041	5.22052610396	25.12253826868
C	-1.07945938471	2.18020915868	5.72582522090
C	-1.24458382317	2.11875062104	2.98201553339
C	-1.52737823793	2.11486901728	20.16751126509
C	-0.77175255689	3.25301612840	19.85755626122
C	-2.91549412380	2.17606700016	19.97928321454
C	-3.52549695975	3.35481073178	19.56492080574
C	-2.77279540879	4.50572781539	19.28109970208
C	-1.38104315735	4.42217046048	19.40094841098
C	-3.48111216640	5.78880833418	18.90408303654
C	-2.57594108237	6.98146449619	18.59704284722
C	-3.35145553825	8.23224179824	18.17721377591
C	-2.43039779093	9.41792862334	17.88213308238
H	-3.52022272806	1.30329785317	20.22700819421
H	-4.61501763849	3.39609455037	19.49663960149
H	-0.75816836333	5.28731227474	19.17149864534
H	0.30710266304	3.24039253453	20.02478852961
H	-4.06867687171	8.50164022885	18.97040041448
H	-3.95907571490	7.99804633822	17.28736444005
H	-1.86306007748	9.71008287450	18.77801659657
H	-2.99048194683	10.29841021064	17.53950026095
H	-1.69914380112	9.16277398483	17.10109038787
H	-4.16513941956	6.05737713265	19.72910999728
H	-4.13686142501	5.59473632982	18.03771574102
H	-1.86809812297	6.71162736823	17.79484991181
H	-1.95810555047	7.21532104432	19.48120689714
C	-2.42729777069	2.22195899992	6.09261791423
C	-0.34841290445	3.38107371678	5.73646153348
C	-0.97237136453	4.59020797937	5.98344184979
C	-3.05510058585	3.44329597948	6.34106347297
C	-2.35083510771	4.65048547716	6.23455402746
C	-3.00281008283	6.00845981202	6.30217568757
C	-4.51637006671	6.01395362491	6.46213561982
C	-5.08634172049	7.43110748334	6.50149830243
C	-6.59600414485	7.43326404606	6.73004725673
H	0.70680727421	3.35459587565	5.45626315197
H	-3.00406300141	1.29432122952	6.11189428013
H	-4.12372552703	3.45260740289	6.56175744094
H	-0.40498846591	5.52216912773	5.90910185434
H	-2.74096206456	6.55124735910	5.37523298679
H	-2.54371161282	6.59482810943	7.11702074935
H	-4.79540820567	5.48153495227	7.38710567276
H	-4.97863152767	5.45017300833	5.63311182041
H	-4.83963421754	7.94902425293	5.55902642896
H	-4.57981291637	8.00033275050	7.29892272581
H	-7.11370102404	6.89849810067	5.92047358703
H	-7.00598338072	8.45016291754	6.78127273830
H	-6.84249103322	6.92054530643	7.67125739113
C	-0.50427338855	3.26497676329	2.67793108143
C	-2.62701993665	2.14993604367	2.74951229432
C	-1.10884926448	4.40591638847	2.16789324461
C	-2.49164127670	4.45726457730	1.95564620190
C	-3.23704591548	3.30246360569	2.24706998510
C	-3.15240553927	5.72955871456	1.45612585678
C	-2.16755690278	6.88584807191	1.26734579393
C	-2.75990967014	8.21842006569	0.81104947795
C	-1.64961721612	9.25524307318	0.60837275359
H	-3.23296093684	1.27549075272	2.99542975252
H	-4.31957144567	3.30965644628	2.09615035468
H	0.56520397997	3.26987692006	2.89132516615
H	-0.48496793722	5.27334438222	1.96267583063
H	-3.94425116813	6.02490878768	2.16666639923
H	-3.67355893090	5.52294420761	0.50519374130
H	-1.39727312412	6.58141053230	0.53820205186
H	-1.62928305596	7.05443592228	2.21617488086
H	-2.03525315942	10.23135564926	0.28640693147
H	-0.93196866977	8.91099108404	-0.15120729398
H	-1.08378523621	9.40872665786	1.53970618634
H	-3.32425972494	8.07988974623	-0.12540012305
H	-3.48431536551	8.58069920406	1.55878944757

9c chain

C	-1.37202811423	1.81137078812	5.93557222859
C	-0.58700865116	0.91498772507	5.00168490984
C	-0.76383259080	0.99110179778	3.59853204112
C	0.09067741806	0.24207406094	2.75246138353
C	1.11630173157	-0.52106449096	3.32149152973
C	2.20615733910	-1.28416717216	2.61479707433
C	1.28745536219	-0.59513895648	4.70464842340
C	2.52837086642	-1.38793946102	5.04440979719
C	0.41803119711	0.08415169998	5.56399309671
H	1.69139439491	1.36287905392	9.90592050213
C	1.17080810057	0.64170368255	9.27448940957
C	1.19156762583	0.79479015125	7.88924918082
H	1.73462855517	1.63260644908	7.45246198054
C	0.51891144114	-0.10659201525	7.04840851050
C	-0.10839222765	-1.21290869298	7.65178521983
H	-0.63604167856	-1.92858314507	7.01844025885
C	-0.10067820995	-1.38515542554	9.03748357374

H	-0.62247518417	-2.23559496109	9.47890809686	C	-0.46739338712	-0.91000325238	0.58922937773
C	0.51380071281	-0.44326371854	9.87839969600	H	-0.79144389406	-1.77377521210	1.17255138677
H	-0.20303701522	1.35718628928	14.10671085406	C	-0.02889432550	0.24191067648	1.26500576775
C	0.11846764379	0.49180967680	13.52630545398	C	2.90429421802	-2.13737250589	3.72077350337
C	0.11745843279	0.55795725411	12.13666290988	H	2.92704863890	-0.57892043743	2.16311226334
H	-0.19708492132	1.47649821641	11.63803619075	H	1.83841570063	-1.90990091632	1.78785041946
C	0.47288418114	-0.55474842661	11.35549123250	H	2.38416679879	-2.04270590773	5.90898525164
C	0.80441698078	-1.74540352208	12.02536721072	H	3.33978822321	-0.69376318667	5.32781088457
H	1.10807860364	-2.61576526287	11.44240803608	C	2.22382016729	-1.93204381646	22.94786309783
C	0.81637147226	-1.80742226854	13.41851103164	C	2.78898342531	-2.89368801956	21.86818645320
H	1.13423995278	-2.72740126868	13.91198434004	C	2.31591380606	-2.29129848715	20.50396953628
C	0.48783185081	-0.68734398396	14.20100624331	H	1.89677873355	-2.47208011376	23.85051805990
H	1.36901442955	1.30254086174	18.31512886543	H	3.00254785375	-1.22405149415	23.28712638101
C	0.99629561477	0.42418565224	17.78721948459	H	1.99931700103	-3.10784685180	19.83566378492
C	1.00381348112	0.40198901774	16.39512927721	H	3.13312619255	-1.76159583847	19.98669036306
H	1.39540975987	1.25905000936	15.84525617286	C	-0.59246931710	3.11994194382	6.16990971448
C	0.53411530619	-0.71466725996	15.68075500266	C	-1.90862546119	1.77740612179	2.97516508943
C	0.10059441640	-1.82567886832	16.42495331831	C	-1.50834412886	1.12957313232	19.71529343627
H	-0.28116056895	-2.70325090351	15.90044795537	C	-1.88382652327	1.13774862988	22.62050172156
C	0.08537617879	-1.79852259064	17.82086535124	C	-3.16194467539	0.90207653931	2.77788406731
H	-0.30438526247	-2.65510944815	18.37345132680	C	-3.14658955754	0.26517884738	22.74591027078
C	0.50496800496	-0.66146188644	18.53203889144	C	-1.12126892532	2.61812476139	19.59492920124
C	-0.73173678878	0.36801877659	22.00410110879	H	-2.10837904786	2.03311229819	22.02596773908
C	-0.59366057132	0.29624496820	20.59682239375	H	-1.60322838995	1.49533535439	23.62115253857
C	0.37364385113	-0.57009738744	20.01786060340	H	-3.44900158585	-0.14403567443	21.77073624360
C	1.20075021435	-1.32968087336	20.86398720481	H	-3.99190631610	0.84134867767	23.15060220061
C	1.11522956465	-1.18280436726	22.25227380296	H	-2.96575017627	-0.58585762731	23.41774282675
C	0.14761254341	-0.35773696327	22.83823271238	H	-2.54296111237	1.05670361954	20.08549134104
H	0.81227100200	1.84247077899	26.90623481051	H	-1.52152185224	0.69532798750	18.70656705595
C	0.45144450933	0.94802759384	26.39477440081	H	-1.30286101858	3.23049190890	20.49355259633
C	0.49841098727	0.88068361038	25.00437295049	H	-1.70550122801	3.08798657721	18.79009341499
H	0.88345130894	1.72412148456	24.42817641701	H	-0.05950665758	2.72114943920	19.33269116652
C	0.07783053016	-0.27295918829	24.32294502771	H	-2.94600089395	0.05588264148	2.11025105301
C	-0.38106450298	-1.36138379940	25.08303969916	H	-3.98211352455	1.48291010719	2.33273171219
H	-0.72219487760	-2.26132952500	24.56710408080	H	-3.51222440104	0.48850402757	3.73444293579
C	-0.42307444882	-1.29776178494	26.47426131086	H	-1.52665882053	1.30103878700	6.89644058121
H	-0.81426219570	-2.14323070063	27.04366858192	H	-2.37081736628	2.03254515043	5.53329004833
C	-0.00901854907	-0.14054031424	27.15700016109	H	0.45177259548	2.90368568887	6.42281099091
H	-0.78124512597	2.08364131979	31.18124141917	H	-1.01825997812	3.71116441483	6.99151890866
C	-0.44101699204	1.17164417746	30.68778783191	H	-0.58380151600	3.74097723673	5.26443934022
C	-0.42674092902	1.10454974444	29.29796643443	H	-1.59321958381	2.14873978574	1.98977101226
H	-0.75636139668	1.96478601178	28.71210715148	H	-2.18502117744	2.67376914831	3.55094662909
C	-0.04277019396	-0.07230108328	28.63215879406	C	2.12845419748	-4.26120469779	22.08672602314
C	0.32148062267	-1.18286550967	29.41476261361	C	4.31567128166	-3.00660165875	22.04574403800
H	0.66293682923	-2.09374740416	28.92049900075	O	4.96249561144	-4.06149487388	21.35561602536
C	0.30889498790	-1.11575295091	30.80392740459	O	2.42133742055	-5.13503955281	20.99123663556
H	0.64260679086	-1.97565654045	31.38827209306	C	1.52284743730	-6.23774945093	20.93310963888
C	-0.07053180187	0.06276463990	31.47058938033	C	5.13260310537	-3.84116308931	19.95976638774
H	0.74429777403	2.23827246429	1.00021760194	H	5.92384385257	-4.52960996957	19.63789094322
C	0.37298473265	1.34538075198	0.49374320551	H	5.45119458376	-2.80374318938	19.74358000245
C	0.34127094399	1.29731918609	-0.89881698433	H	4.20684054283	-4.06457337374	19.40408851498
H	0.69612602544	2.15266078019	-1.47626425427	H	4.52973769711	-3.21718823674	23.10672969074
C	-0.08559337024	0.14074030621	-1.57532208593	H	4.78328960896	-2.03026911939	21.79490065685
C	-0.49460459482	-0.96069499876	-0.80261266229	H	1.03158802955	-4.11941845701	22.17318498637
H	-0.86238033699	-1.85725553977	-1.30458951300	H	2.48478963640	-4.70205096412	23.04150933117

H	0.47157389999	-5.90193054233	20.86393714384
H	1.61455415477	-6.90471225168	21.81148093356
H	1.78464296268	-6.80566010254	20.03325985995
C	4.42047815131	-2.14330986638	3.41238610465
C	2.27553610965	-3.55329557456	3.66138778979
O	2.92793814053	-4.60744683071	4.36716355350
O	5.21808513984	-3.10505529245	4.09742385077
C	5.63515921857	-4.20634360722	3.29434529573
C	3.00797156924	-4.41981198697	5.77987420527
H	2.26987134892	-3.90234245428	2.61854301632
H	1.21983584147	-3.47786590924	3.99695515892
H	3.84539276937	-3.73741600814	6.00660748329
H	3.20595959403	-5.40061050171	6.22000307483
H	2.06069572321	-4.03539916657	6.19941774522
H	4.83184476749	-1.15881313444	3.69948285273
H	4.55962500101	-2.24926960259	2.32050995884
H	6.52528921804	-4.62401531133	3.78238582146
H	5.91043907646	-3.88182788031	2.27402316089
H	4.84611907255	-4.97354372209	3.23777912611

9d chain

C	-1.31781143469	2.30094723013	5.97033634017
C	-0.59333011552	1.22509110267	5.18311363771
C	-0.70370689081	1.21932486275	3.76724263121
C	0.00963186219	0.26780840019	3.00157022390
C	0.81554759426	-0.65803415113	3.67499462776
C	1.75460185108	-1.69314914507	3.11868921551
C	0.89162279720	-0.67949230240	5.06305240547
C	1.87871663965	-1.73991186548	5.47263885932
C	0.18626130658	0.24400713965	5.84596678188
H	1.09316133959	1.88797243079	10.14533931409
C	0.68942661764	1.07835647178	9.53546301038
C	0.74517462367	1.16265560029	8.14582652473
H	1.20196159965	2.03357737443	7.67641412770
C	0.23242945147	0.13747406365	7.33409646564
C	-0.28372418851	-1.00529640388	7.97280557999
H	-0.70265406031	-1.80811123978	7.36388693999
C	-0.31397871156	-1.10397183899	9.36417764151
H	-0.75108079407	-1.98550562982	9.83697612448
C	0.15353166478	-0.05404770575	10.17183575432
H	-0.96754886974	1.68670623067	14.35270354908
C	-0.48749873823	0.88423923007	13.79024945238
C	-0.47392809539	0.92200056968	12.39793456256
H	-0.94332985139	1.75537836095	11.87156615262
C	0.09736800861	-0.12254407624	11.65187840373
C	0.63753430042	-1.21608855863	12.35037987501
H	1.11646606637	-2.01890402605	11.78831212806
C	0.62483648500	-1.25321475206	13.74384983176
H	1.09561615421	-2.08603163329	14.26981797702
C	0.07034094245	-0.20109110471	14.49014958352
H	0.91853372370	1.75366832588	18.63266309777
C	0.51205178950	0.90045873066	18.08979115445
C	0.54265330761	0.89045849343	16.69738990400
H	0.96131865037	1.74189012945	16.15777202392
C	0.07238390240	-0.21714086935	15.97212432668
C	-0.40545615953	-1.32308263054	16.69550500274
H	-0.78496519815	-2.18987922398	16.15156364797
C	-0.46352390353	-1.29849937069	18.08935331785
H	-0.89353038904	-2.14553654759	18.62735789431
C	-0.02558212546	-0.17680705074	18.81552876896
C	-1.04280406558	0.83702995545	22.37995011669
C	-0.92769997690	0.85216158539	20.96501835927
C	-0.15049523028	-0.13129474156	20.30036890796
C	0.50335649801	-1.09784788121	21.07763842450
C	0.44902440295	-1.06775058041	22.46737485186
C	-0.30784526057	-0.10310546276	23.14578123832
H	0.70586483159	1.96973425486	27.20343194411
C	0.29616139430	1.09077146748	26.70269711639
C	0.22986396402	1.05641631973	25.31240509354
H	0.58542675029	1.90727423639	24.72826900946
C	-0.26688327139	-0.07191288274	24.63417307911
C	-0.66944498746	-1.17584531725	25.40416337981
H	-1.07406446838	-2.05654227291	24.90268899390
C	-0.59032836627	-1.14730291616	26.79538575163
H	-0.94077587929	-2.00257516873	27.37581473280
C	-0.11636666574	-0.01159763101	27.47281054994
H	-0.85282051151	2.08751386086	31.56634126273
C	-0.49175038328	1.20263970532	31.04160147860
C	-0.48663035287	1.17443172774	29.65048031004
H	-0.84696116717	2.04007952531	29.09044553886
C	-0.08173199742	0.02696315575	28.94981015010
C	0.32824479030	-1.09260518698	29.69809509054
H	0.69473183283	-1.97615681235	29.17464518596
C	0.31940296382	-1.06608075771	31.08981564766
H	0.67738440227	-1.93151234468	31.65150558878
C	-0.09092734449	0.07969484652	31.78895855795
H	0.90180085307	2.14581782670	1.25101353090
C	0.46356017951	1.28612187288	0.74246519244
C	0.43281944440	1.23988488275	-0.64801853328
H	0.85100978189	2.06369395691	-1.22866825479
C	-0.08335767885	0.12112637033	-1.32367866677
C	-0.57666029183	-0.94683170303	-0.55476112699
H	-1.01170690112	-1.81115338639	-1.05948492420
C	-0.56092617236	-0.89266950901	0.83862736702
H	-0.98003736396	-1.71600751027	1.41937778489
C	-0.04026056394	0.22415229543	1.51344218623
O	2.39698632863	-2.29572153226	4.25301421001
H	2.52735288686	-1.24676880172	2.46539691448
H	1.24162770808	-2.48282774961	2.54066898518
H	1.42363174618	-2.55389458891	6.06619922126
H	2.71982671808	-1.32428134104	6.05734730900
C	1.36185053942	-2.13603325293	23.01024552319
O	1.93897131551	-2.79031108092	21.86563849749
C	1.42281826013	-2.21215451754	20.65570620037
H	0.83410207656	-2.89435529659	23.61584011068
H	2.17259790546	-1.71352613018	23.63317418372
H	0.90325195675	-3.00569007716	20.08830306842
H	2.26880509365	-1.85185785643	20.04229862725
C	-0.56464926223	3.64652872910	5.97952709502
C	-1.66602383381	2.17881224555	3.08718212676

C	-1.64516257935	1.93611158782	20.17941793244
C	-2.05015610563	1.74711869811	23.06310117286
C	-3.15527078792	1.75118495535	3.22040706578
C	-3.47035208959	1.15012958518	23.02397889012
C	-0.93588545645	3.30334949200	20.23685989572
H	-2.06479149144	2.74494085084	22.60273755552
H	-1.76975895315	1.89918955764	24.11303097948
H	-3.79146969571	0.93547226246	21.99486469916
H	-4.19799575410	1.84486244554	23.46662917898
H	-3.51432905210	0.20577479040	23.58425179990
H	-2.66807111747	2.05405213760	20.56508735899
H	-1.75063899800	1.62632960500	19.13073285115
H	-0.71050383013	3.59919608955	21.27009301814
H	-1.55837688483	4.09369358779	19.79442932360
H	0.01897180570	3.28148092064	19.69483843093
H	-3.26563773820	0.87512100275	3.87293822552
H	-3.58071531138	1.48428332658	2.24444275470
H	-3.77132760700	2.55716909984	3.64012906834
H	-1.47194994013	1.96553723289	7.00476617683
H	-2.31933909655	2.45465266666	5.54587576735
H	0.36032606633	3.58020529329	6.56749295186
H	-1.18271185341	4.44633232372	6.40937452298
H	-0.27669472596	3.95647565294	4.96623258252
H	-1.41287036972	2.25248601110	2.02404403951
H	-1.53976971226	3.19102200811	3.49326125286

Cartesian coordinates of substituted CPPs:

9a ring

C	-2.73066	6.01112	0.55341
C	-3.62608	4.96899	0.35653
C	-4.46550	4.52090	1.39594
C	-4.96280	3.12869	1.30089
C	-5.31056	2.54732	0.06468
C	-5.20297	1.17423	-0.13426
C	-4.74519	0.32677	0.89501
C	-4.02557	-0.93541	0.60235
C	0.71634	8.25423	1.07143
C	-0.69363	8.19063	1.12355
C	-3.13164	-0.90838	-0.48536
C	-2.07305	-1.80137	-0.56811
C	-1.85563	-2.78242	0.41927
C	6.00495	1.04377	0.91652
C	6.30327	1.92501	-0.14313
C	6.16766	3.30134	0.01253
C	5.74245	3.85106	1.23842
C	4.99148	5.12927	1.29641
C	3.99035	5.29581	0.32055
C	2.93980	6.18286	0.51294
C	2.85005	6.97532	1.67368
C	1.48890	7.49558	1.99399
C	-1.33684	7.35076	2.07855
C	-2.63610	6.67523	1.79472
C	-3.62241	6.36844	2.75203
C	-4.51041	5.30512	2.56303
C	-4.75647	2.25462	2.38465
C	-4.65043	0.87935	2.18608
C	-3.92821	-2.02955	1.48260
C	-2.87162	-2.94033	1.38480
C	5.83346	1.61174	2.19313
C	5.70769	2.99130	2.35180
C	4.98853	6.02398	2.38214
C	3.94549	6.93973	2.55791
C	0.83585	6.93466	3.10221
C	-0.56570	6.86339	3.14841
H	-1.98484	6.22413	-0.21436
H	-3.56718	4.38810	-0.56515
H	-5.58774	3.19155	-0.77164
H	-5.39539	0.75800	-1.12494
C	1.41869	9.13454	0.04590
C	-1.55559	9.05261	0.21823
H	-3.17847	-0.07589	-1.18893
H	-1.31439	-1.64461	-1.33292
H	6.55665	1.51805	-1.12375
H	6.30855	3.95839	-0.84763
H	3.95903	4.60653	-0.52459
H	2.09249	6.16167	-0.17223
H	-3.65650	6.92694	3.68760
H	-5.20988	5.04573	3.36010
H	-4.50779	2.66954	3.36306
H	-4.32102	0.24666	3.01277
H	-4.65505	-2.13861	2.28998
H	-2.80016	-3.75112	2.11116
H	5.62602	0.95915	3.04353
H	5.40605	3.39075	3.32171
H	5.78641	5.97080	3.12552
H	3.95268	7.59458	3.43036
C	1.43999	6.10462	4.21969
C	-1.00629	6.00247	4.31843
C	-0.47249	-3.32395	0.54188
C	0.20237	-3.11941	1.75975
C	-0.37506	-2.76405	3.11539
C	2.07363	-2.64048	3.18013
C	1.60542	-3.05276	1.79954
C	2.36274	-3.22024	0.62775
C	1.70107	-3.74331	-0.52332
C	2.55402	-4.32904	-1.63518
C	-0.44627	-4.23778	-1.82929
C	0.29138	-3.76011	-0.58345
C	4.66043	-2.45504	1.51960
C	3.66633	-2.50597	0.52190
H	4.69261	-3.23004	2.28619
H	6.26622	-1.34019	2.42546
C	5.55822	-1.38431	1.59543
C	5.50890	-0.32996	0.66470

C	4.66000	-0.49937	-0.44752
H	3.01327	-1.56395	-1.30897
C	3.76234	-1.55401	-0.51530
H	4.59515	0.29664	-1.19039
C	2.69777	-5.85651	-1.49591
C	-0.29923	-3.39461	-3.11683
H	3.55783	-3.88491	-1.59545
H	2.15038	-4.08750	-2.62629
H	3.15367	-6.11439	-0.53033
H	3.33192	-6.26594	-2.29518
H	1.72440	-6.36326	-1.54456
H	-1.51285	-4.30338	-1.57586
H	-0.13580	-5.27129	-2.05295
H	-0.21408	-2.32143	-2.90082
H	-1.17457	-3.53220	-3.76678
H	0.58343	-3.67165	-3.70702
C	0.79995	-2.09979	3.86286
H	-0.70722	-3.68252	3.63132
H	-1.25482	-2.11083	3.04807
H	2.88702	-1.90269	3.15443
H	2.46955	-3.52212	3.71510
H	0.74920	-1.01031	3.71964
H	0.78047	-2.28955	4.94433
C	0.26154	5.90908	5.19365
H	-1.33572	5.01210	3.95876
H	-1.85290	6.42583	4.87392
H	2.30393	6.57833	4.70195
H	1.80108	5.14315	3.81423
H	0.25692	6.73483	5.92062
H	0.32302	4.97150	5.76153
C	-1.94669	10.37033	0.91331
H	-2.47612	8.51303	-0.04414
H	-1.04547	9.27720	-0.72735
H	-2.52148	10.16609	1.82717
H	-2.56323	10.99850	0.25511
H	-1.05812	10.94834	1.20428
C	1.46230	8.61469	-1.40557
H	2.44973	9.31088	0.38565
H	0.93000	10.12175	0.05223
H	2.20745	7.81728	-1.51878
H	1.73785	9.42189	-2.09923
H	0.49291	8.21069	-1.72866

9b ring

C	-3.06843831192	5.90583274391	0.30595912128
C	-3.96483126686	4.85243741917	0.27341189444
C	-4.76173400574	4.52354393649	1.38781030247
C	-5.23427025406	3.11916760372	1.43546738760
C	-5.62977575806	2.45491045939	0.25676329271
C	-5.40997789209	1.08953441207	0.10430531836
C	-4.81227457915	0.33706403918	1.13407765481
C	-3.94871349756	-0.82724376565	0.79505381052
C	-2.92511736717	-0.52217370612	-0.12348169658
C	-1.86054407287	-1.38557425855	-0.32496520651
C	-1.78163300999	-2.62638388302	0.33670340770
C	6.06333297210	0.96305153990	0.56577422042
C	6.18189602207	2.00959863835	-0.37222526324
C	5.95036899393	3.33385208352	-0.00212450966
C	5.61078488885	3.65771557549	1.32418295220
C	4.72421609847	4.81169729835	1.61294210631
C	3.54149386872	4.48588954971	2.30549014159
C	2.47767595984	5.36777294708	2.36619788405
C	2.53210039602	6.64429582105	1.77012775971
C	-2.92342637521	6.72490112971	1.44698120364
C	-3.87684885391	6.52501810592	2.47158752452
C	-4.75961564809	5.43941976539	2.45321735579
C	-4.90207974701	2.31815555256	2.54420226145
C	-4.69596060771	0.94497054951	2.39597415217
C	-3.90679645535	-2.08203262012	1.42275380433
C	-2.84775804332	-2.97275580568	1.18403881450
C	6.01540817359	1.33114290973	1.92512118861
C	5.79720407810	2.65393430374	2.29593169084
C	4.81843262630	6.10993127010	1.08005858439
C	3.75023722289	7.01358801055	1.16721792757
H	-2.38495626521	6.02316488805	-0.53159534641
H	-3.94004183099	4.17119548876	-0.57794730707
H	-6.00443794707	3.03829921267	-0.58641799052
H	-5.60230226381	0.61417552664	-0.85911564423
H	-2.91999332470	0.46105063352	-0.59600808543
H	-1.01261112715	-1.06095562851	-0.92957996277
H	6.33073354443	1.77138999399	-1.42697914890
H	5.88068873162	4.10105833450	-0.77604641220
H	3.41872014782	3.47408569268	2.69342077237
H	1.53583423125	5.02827607702	2.79767307174
H	-3.90253881994	7.19271633949	3.33000744823
H	-5.42439010700	5.28236752270	3.30517201664
H	-4.62299679837	2.79975543036	3.48355060441
H	-4.26821009545	0.37709389645	3.22492658784
H	-4.69667709386	-2.36244128893	2.12171189373
H	-2.83665451375	-3.93665341477	1.69537990830
H	5.98605815196	0.55343032966	2.69037126793
H	5.64024143273	2.89662725068	3.34872054838
H	5.73169842743	6.41615791787	0.56665598956
H	3.85170481252	8.00159176091	0.71780325128
C	4.77150558455	-2.58368320256	0.87128373923
C	3.70037099982	-2.52315835673	-0.04361803536
H	4.85479871077	-3.43366687893	1.54954295421
H	6.46316588428	-1.58569831110	1.75308451223
C	5.69206360268	-1.53473099938	0.98183709232
C	5.58040663748	-0.38367999123	0.17842107007
C	4.65153768047	-0.43929083387	-0.88000414839
H	2.95760074154	-1.41069254229	-1.74239720388
C	3.73887743925	-1.47577080650	-0.98690365341
H	4.53830871294	0.42456282113	-1.53536856514
H	2.97894400337	7.53122607180	-8.08352915150
H	-1.90113489645	6.31832848259	4.44421848556
H	2.03060678272	6.04987469376	-1.09328123190
H	-0.46789936627	7.11362383452	-2.22463427188
H	-1.85636738650	7.76937489641	-4.12930410217
C	3.13831413705	8.61931594069	-8.07305913467

H	2.15420408208	9.09593466434	-8.19002724817	H	4.79832339864	-7.49692390914	-8.66084986962
H	-3.46274381414	8.02293616019	-5.65883224192	H	-0.42906798596	-4.00707536432	3.27633534691
C	-1.29634140483	7.80171019607	-2.05958090449	H	3.76511146547	-5.17910680306	-1.39927355191
C	-2.09257876072	8.17450561935	-3.14476404976	H	0.37606679694	-6.00221072242	-2.14559470698
H	3.35879179747	6.64969096202	-3.09280013670	H	-0.75757828620	-6.83486594703	-4.17741060486
H	2.80089118796	7.63380696157	-5.50506924026	C	4.74010529078	-6.49838597925	-9.11789845421
H	1.18302475258	6.20717634643	4.57230240569	H	3.69766938598	-6.34033389103	-9.43080606758
H	3.73984957685	8.87597332457	-8.95584564351	H	-0.82964055535	-5.02933860067	-7.08688196842
H	-5.08310633123	8.89621664614	-3.95911046201	C	-0.34455609331	-5.36465055211	-2.65974673019
C	-1.52675410468	7.33980987547	4.25035543608	C	-0.98373664159	-5.83191245817	-3.80829706797
C	2.08002613764	7.09022605915	-1.41804177013	H	5.15473193202	-5.45278658291	-3.43004496502
H	-3.99126657080	8.20941268023	-8.19351200731	H	4.34321366186	-6.33520441789	-6.36348182578
C	-1.62742662105	7.44651151048	1.60337493175	H	2.75777563868	-3.93630724361	3.11582788700
C	-0.96206755418	7.44452642724	2.84552258198	H	5.36147576652	-6.50976894644	-10.02395818228
H	-5.60249439946	9.07382895180	-6.43543038469	H	-2.43240844293	-6.55632092828	-5.92957166160
C	2.82887116215	7.43262225615	-2.54389588104	C	-0.10789063189	-3.03951784230	2.85305240041
C	-0.84083328000	7.82628404348	0.46249968770	C	3.48394769024	-4.66757195736	-2.32151019263
C	-1.56902084972	8.26854979144	-0.76168862003	H	-0.92820708318	-4.59289145821	-9.66991733792
C	0.43823383483	7.38297656462	2.89675621347	C	-0.43933935559	-3.27829460245	0.26669850388
C	-3.63428263697	9.10611540097	-5.54125742333	C	0.35090082943	-3.24247985495	1.42377797044
C	3.00567996985	8.71766931466	-5.52528676732	H	-2.58744778285	-6.13526948677	-8.53582174588
C	-3.18669426098	9.03639167290	-2.98684108510	C	4.26541348075	-4.81918091695	-3.46640881968
C	-4.11798244494	9.40985223587	-4.12162138607	C	0.19855738775	-3.61845239984	-0.96453934444
H	2.01866520616	9.20828539525	-5.56935512125	C	-0.59187110392	-4.07499704455	-2.15368117909
C	0.91371360859	7.24824435691	4.33113820547	C	1.75470946908	-3.22395965130	1.34843821445
H	-2.36905652121	8.02282869994	4.42498139775	C	-1.89511989139	-4.75161855169	-7.01871009398
C	3.81864254983	9.06372306684	-6.77625866504	C	4.33520187818	-5.35524410755	-6.86935464507
C	0.57299078702	7.74549913082	0.51952135471	C	-1.90048983495	-5.03190669489	-4.50375159915
C	1.21480866764	7.34569960505	1.72702678080	C	-2.52693677334	-5.46596662543	-5.80742401503
H	-0.37017561551	7.22291476537	6.13585005540	H	3.28266797825	-5.16423555210	-7.13797217028
C	-4.63191503883	9.56855760910	-6.60874525377	C	2.34488186556	-2.98990788322	2.72433226865
C	-0.31778629251	7.69083664958	5.14403112857	H	-0.96960282837	-2.36345026241	2.93339810002
C	-4.15571148980	9.28552363230	-8.03509024304	C	5.19242056668	-5.41446829831	-8.13756267079
C	1.39175761968	8.07381423820	-0.68737280794	C	1.61486023051	-3.59657353821	-1.04385064353
H	4.81500307049	8.59622204458	-6.70086727139	C	2.39876162960	-3.23941425669	0.09848199176
C	-2.64833632367	9.16152420748	-0.61298486701	H	1.21108173389	-2.83221726657	4.62104355082
H	-4.88701620053	9.62386850001	-8.78215033009	C	-2.60300700865	-5.04964476930	-8.34398219074
C	-3.43287140759	9.53715399858	-1.69858261427	C	1.14855283025	-2.50622886751	3.57451335886
C	2.92420150641	8.76391702185	-2.98048427506	C	-1.97961167189	-4.30440658027	-9.52722288719
H	-2.65782861831	9.59047275377	-5.71239322696	C	2.34323182119	-3.84514874049	-2.32143965107
C	3.71254261260	9.12071690852	-4.21780410572	H	6.24548858569	-5.58252725770	-7.85623449654
H	1.81241633752	7.84997358434	4.52932764329	C	-1.54395371844	-3.29278021328	-2.83079781769
H	-4.35323943232	10.48522391173	-4.04296300415	H	-2.51243416789	-4.51165277440	-10.46525069778
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H	-2.87010654701	9.55611992065	0.38023162334	C	4.81226803428	-4.27272328086	-5.88525415024
H	4.70029057736	8.63092708917	-4.18281920042	H	3.17462827024	-2.27064482926	2.71487479717
H	-4.26485318027	10.22798765368	-1.54435366266	H	-3.60748255037	-5.24452447140	-5.78971436660
H	-0.28646661268	8.78048342432	5.29296912033	H	-2.00203875518	-3.21683227557	-9.36519659932
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C	2.24020403574	9.74125103669	-2.24521813352	H	-3.66718110522	-4.77485919738	-8.25245451073
H	3.90629792032	10.20527005414	-4.22969756056	H	-1.78643289218	-2.29508315765	-2.47665064875
H	0.95824087059	10.18097873227	-0.56326977894	H	5.84993449629	-4.49190179510	-5.58511430416
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H	4.84031507872	-3.30332135573	-6.40998853018
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H	2.52126027960	-2.81280971748	-5.57648836901

9c ring

C	-2.75093072704	6.30366603419	0.59974008858
C	-3.62999357074	5.25441856559	0.37186038207
C	-4.41109861110	4.71524825377	1.41369252578
C	-4.85672975687	3.30819720866	1.27872518555
C	-5.11550497719	2.72352260804	0.02116687210
C	-4.96196227311	1.35411850414	-0.17713637140
C	-4.55994483851	0.50888043349	0.87638658939
C	-3.83837645371	-0.76305135190	0.63287439013
C	0.76927154417	8.36406675592	1.08668967218
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H	2.51324865057	9.40703245565	0.41652539133
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C	-0.22104540687	7.68337919352	8.14380876862
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O	1.76058375566	4.28780441920	6.34942818600
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C	0.88957002082	-3.81890330936	4.96519401944
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9d ring

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C	-0.69782912286	8.18529022251	1.13242182920
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H	2.12432786674	-4.19850292024	-2.61900139544
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H	1.74786970991	-6.42731390324	-1.41215156093
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H	-0.25422654864	-2.37841719390	-2.91969846766
H	-1.17280190998	-3.62479252252	-3.78155752445
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H	-0.98513458936	-1.77537629713	2.98563457395
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H	2.64725407670	-3.23872640587	3.67987881381
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H	-2.49429232434	8.54933282094	-0.00492639150
H	-1.05815961249	9.28153331684	-0.71146903136
H	-2.46916063381	10.19235862226	1.87233226063
H	-2.51968022849	11.03249621295	0.30340099531
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C	1.44758847777	8.67716582913	-1.39576133275
H	2.45080506619	9.30339076156	0.41242235279
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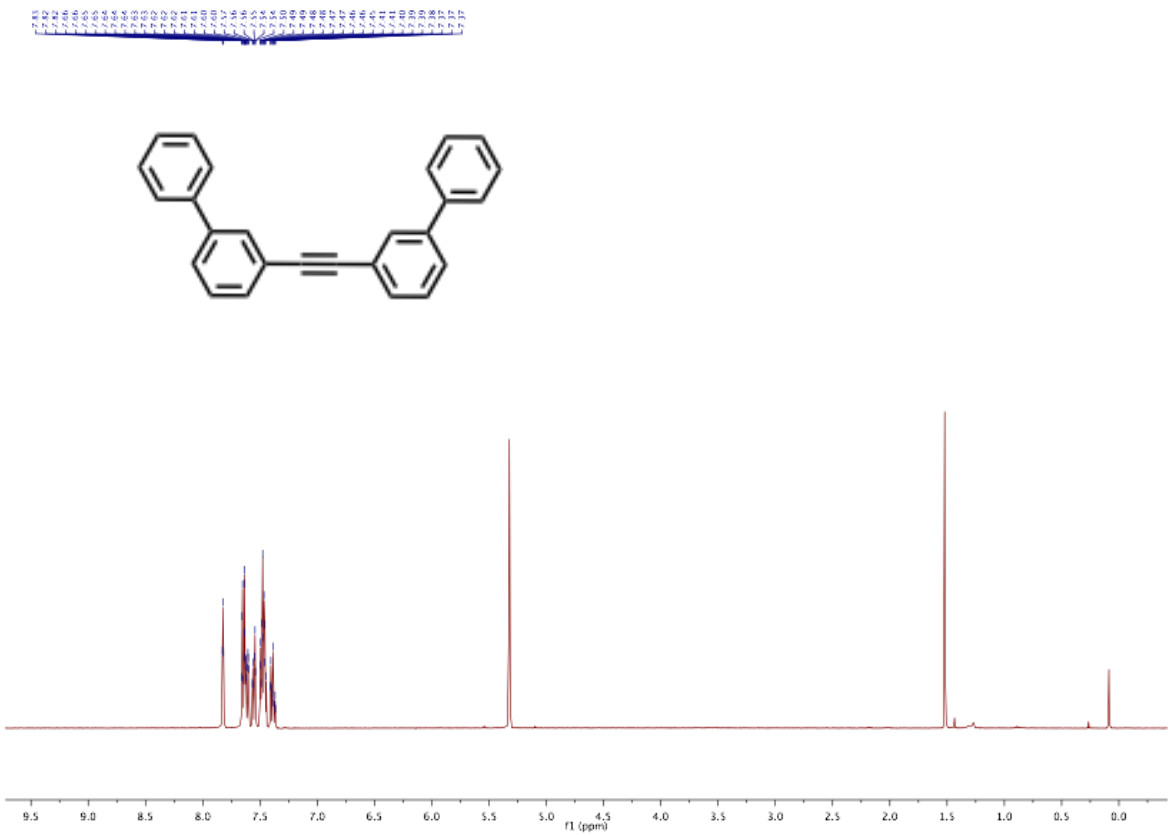
H	2.18667556923	7.88069915684	-1.54605449749
H	1.72605203740	9.50830188352	-2.05872547570
H	0.47447167066	8.29367838348	-1.73098444596

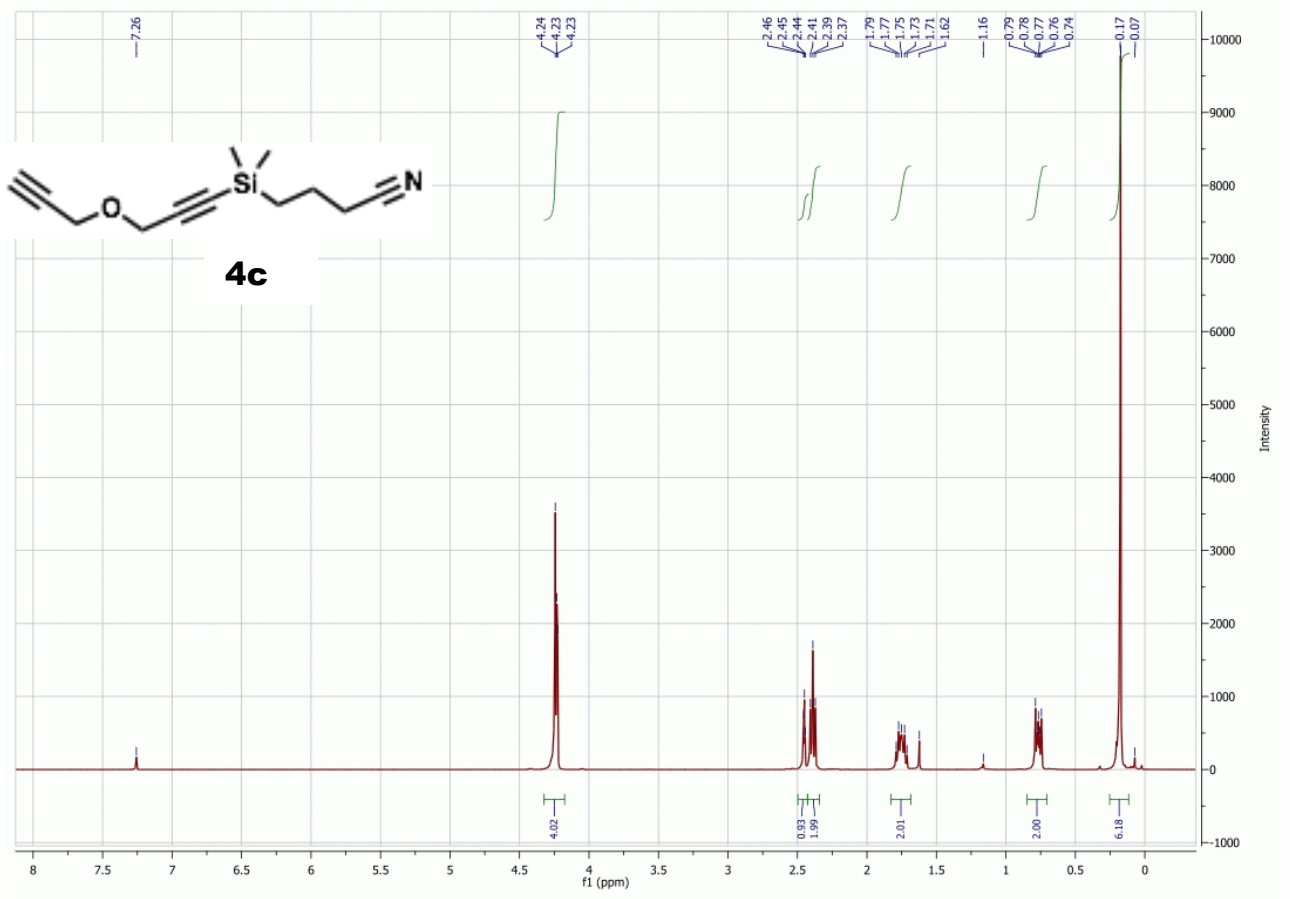
^{1}H-NMR spectra of products

^{1}H-NMR spectrum of 1,2-bis [4-(2-methoxyethoxy)phenyl]ethyne ($CDCl_3$)

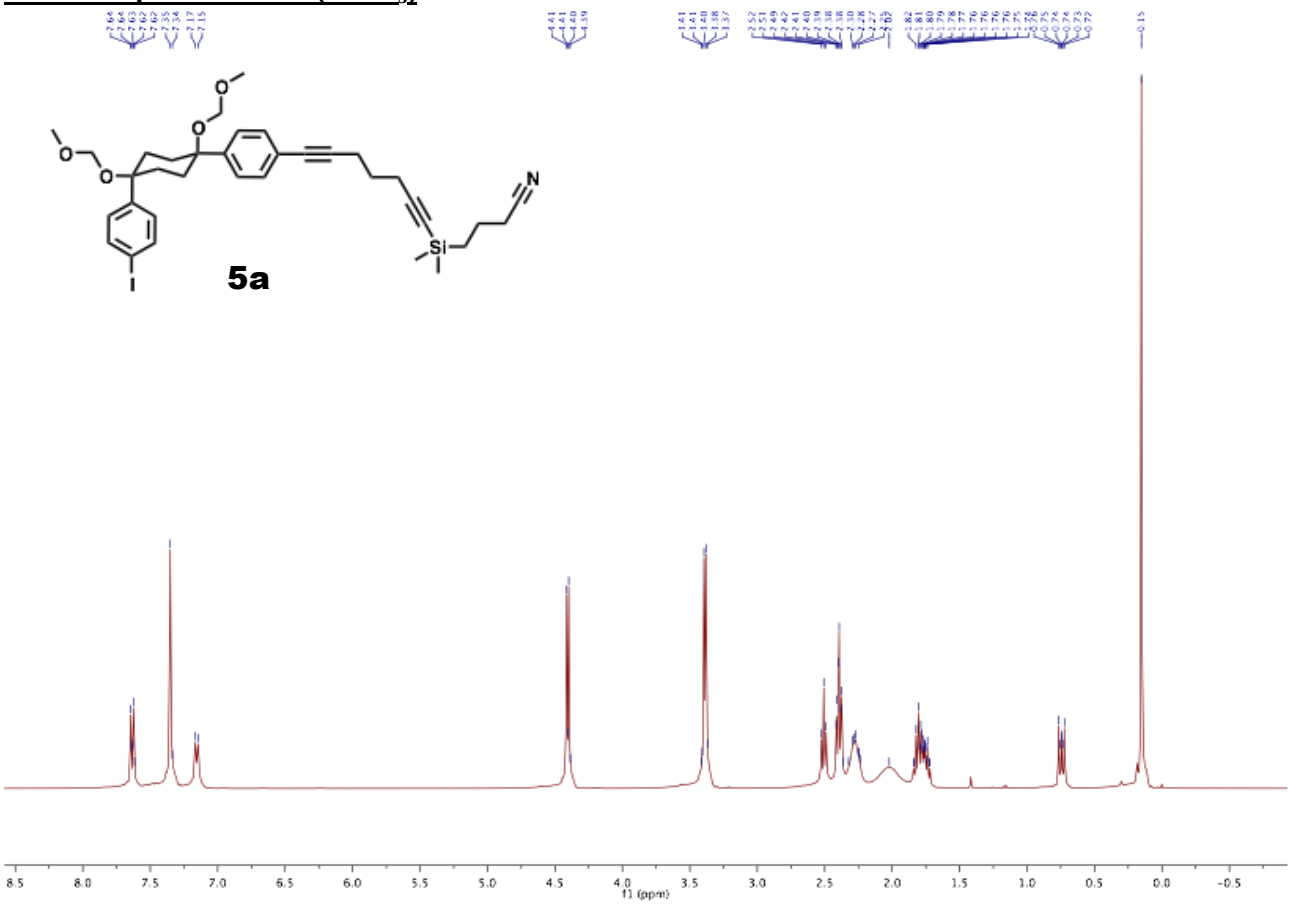
^{1}H-NMR spectrum of 1,2-di[(1,1'-biphenyl)-3-yl]ethyne (CD_2Cl_2)



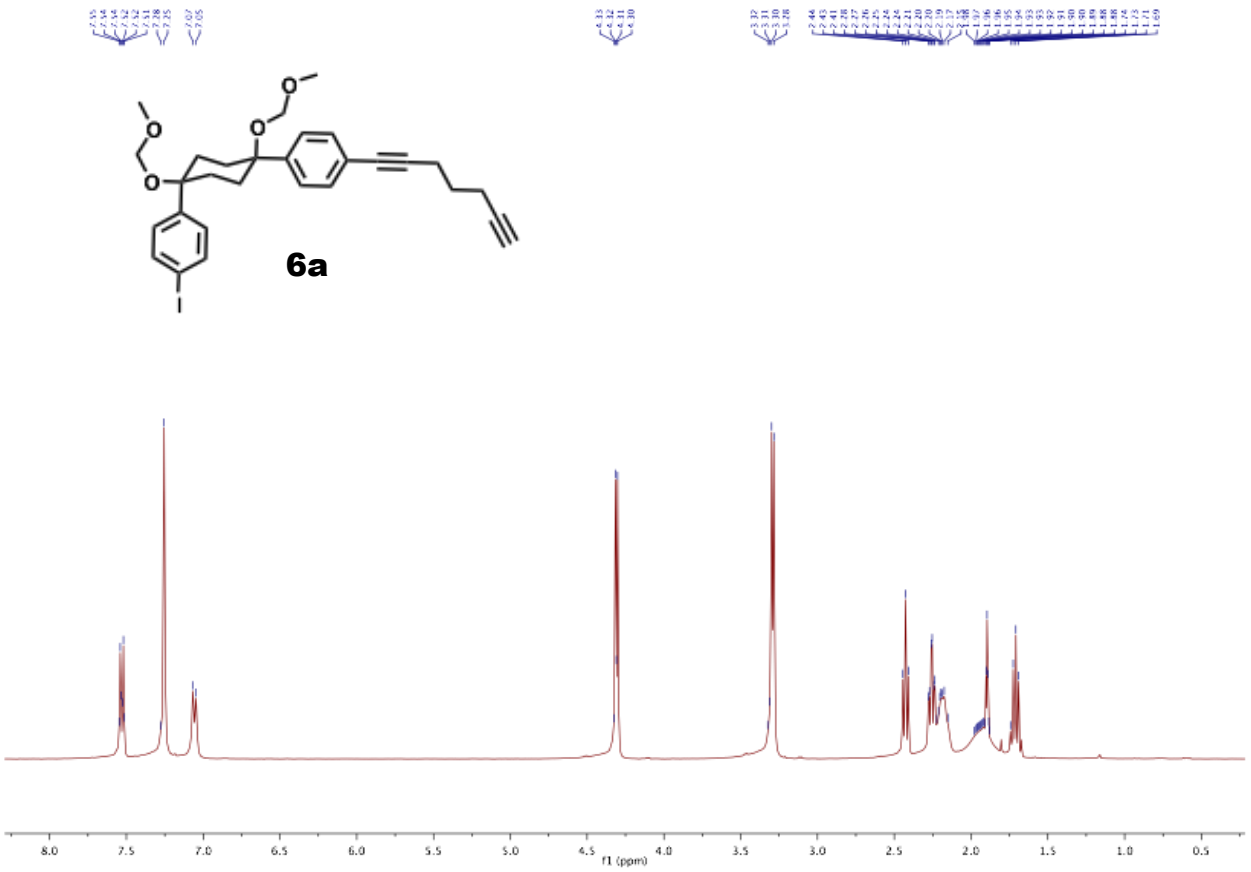
^{1}H-NMR spectrum of 4c ($CDCl_3$)



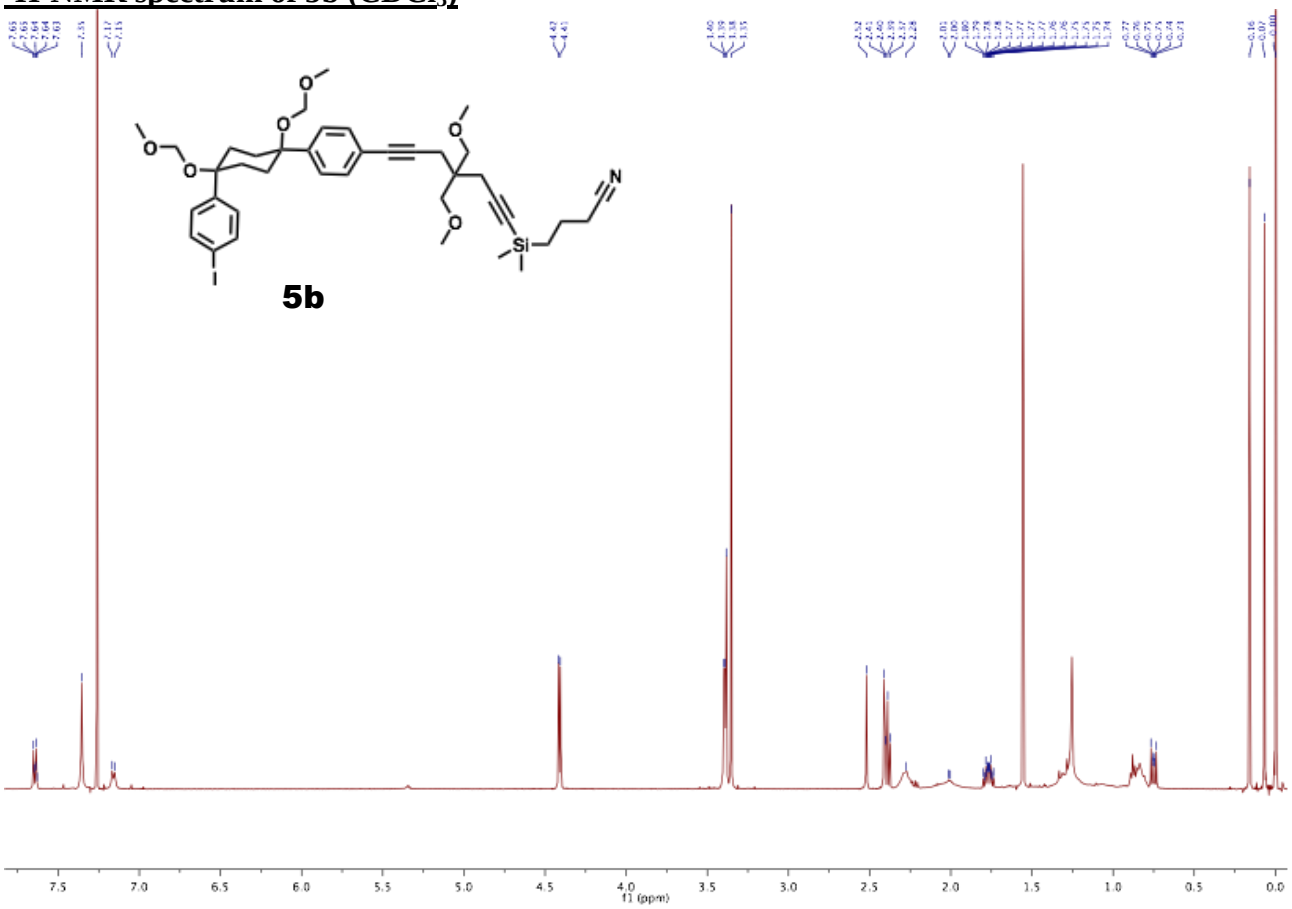
^{1}H-NMR spectrum of 5a ($CDCl_3$)



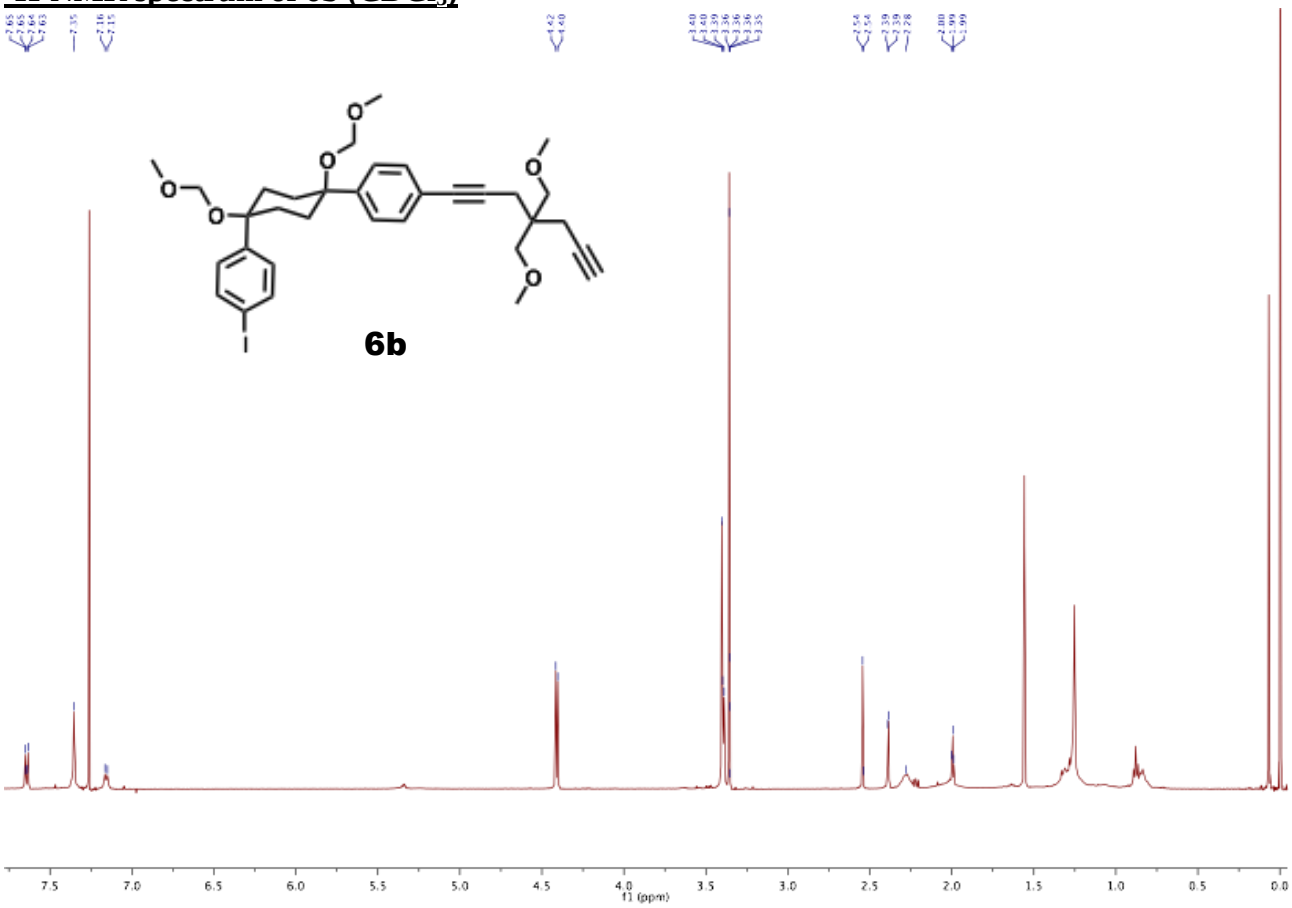
^{1}H-NMR spectrum of 6a ($CDCl_3$)



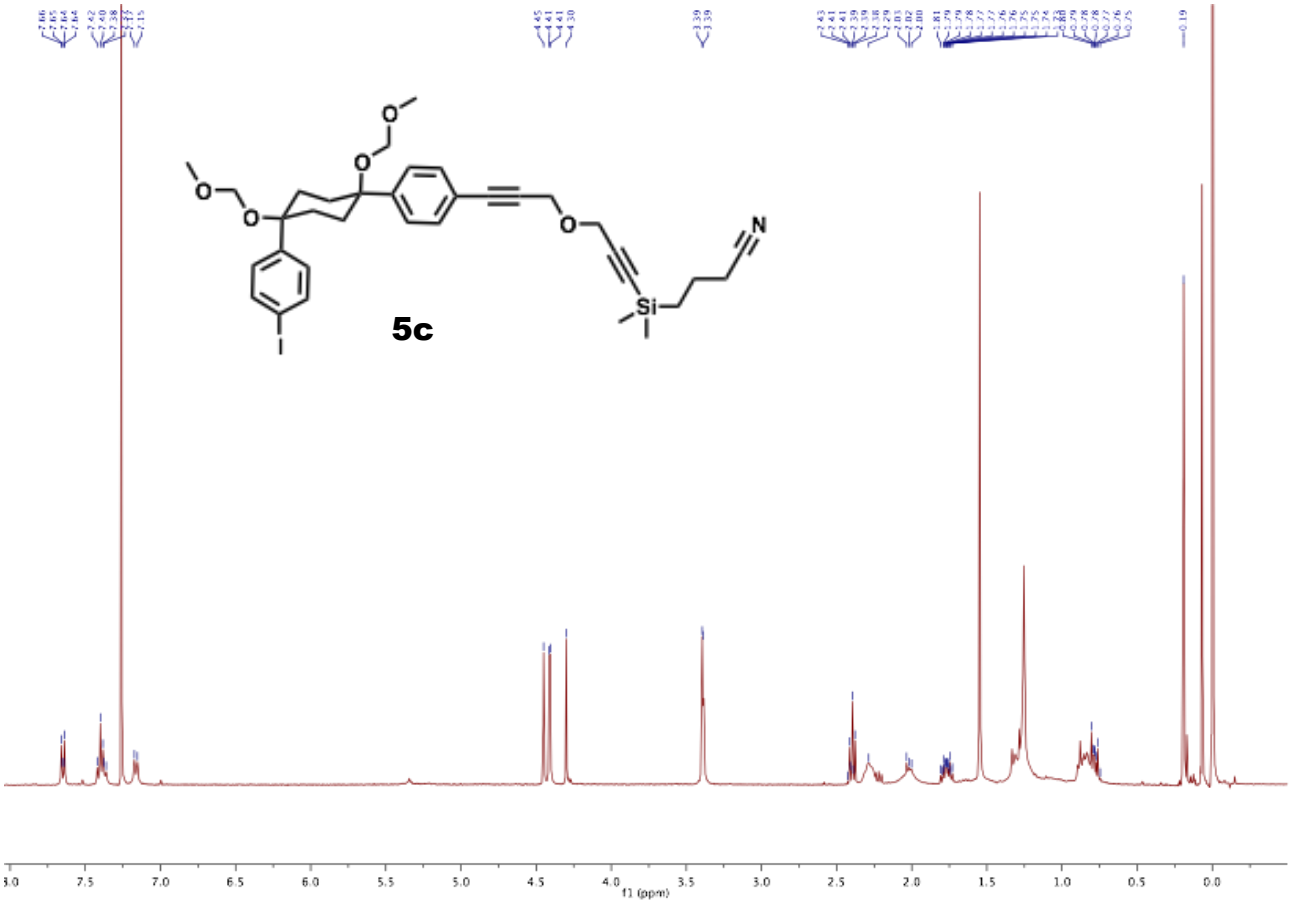
^{1}H-NMR spectrum of 5b ($CDCl_3$)



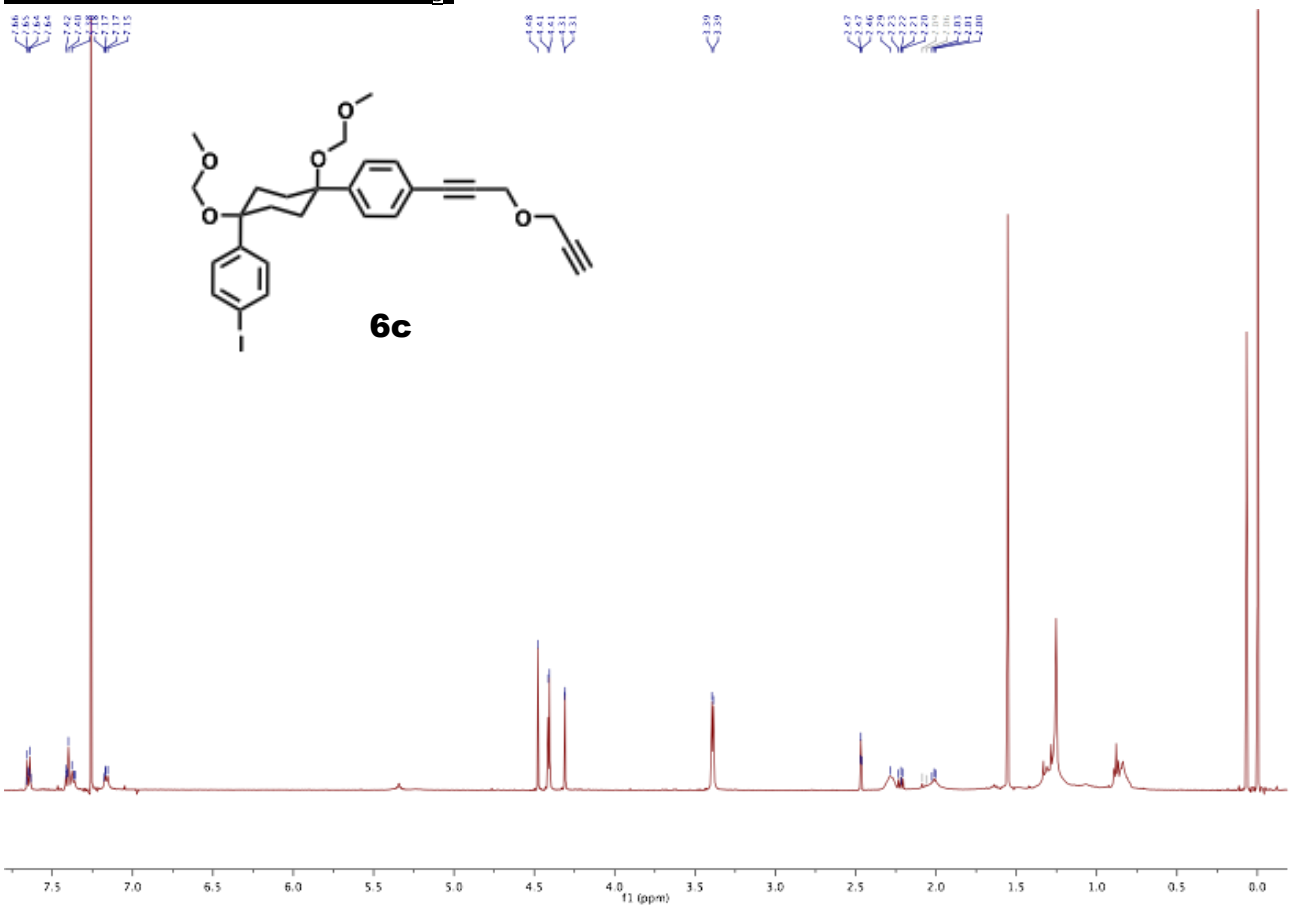
^{1}H-NMR spectrum of 6b ($CDCl_3$)



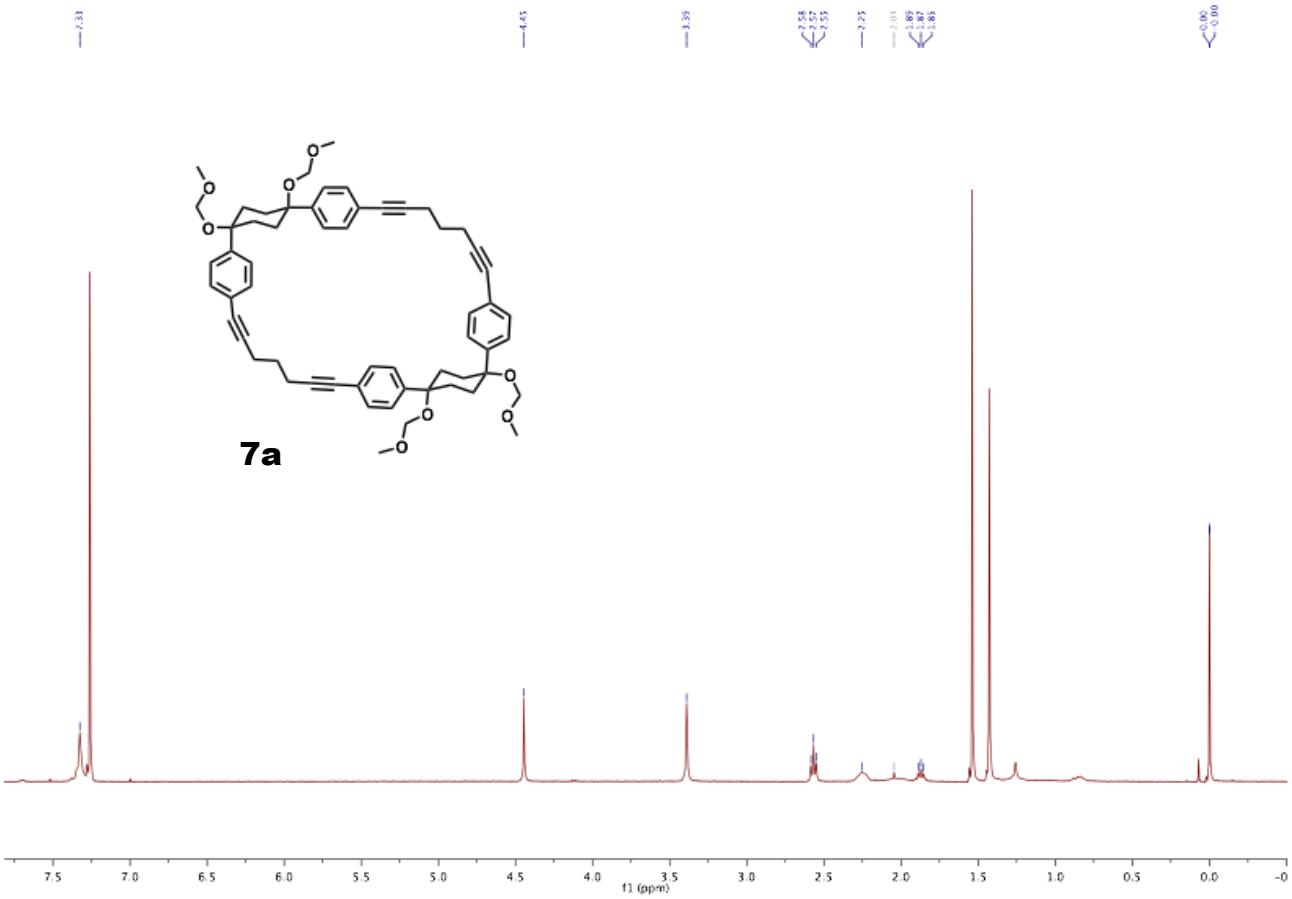
^{1}H-NMR spectrum of 5c ($CDCl_3$)



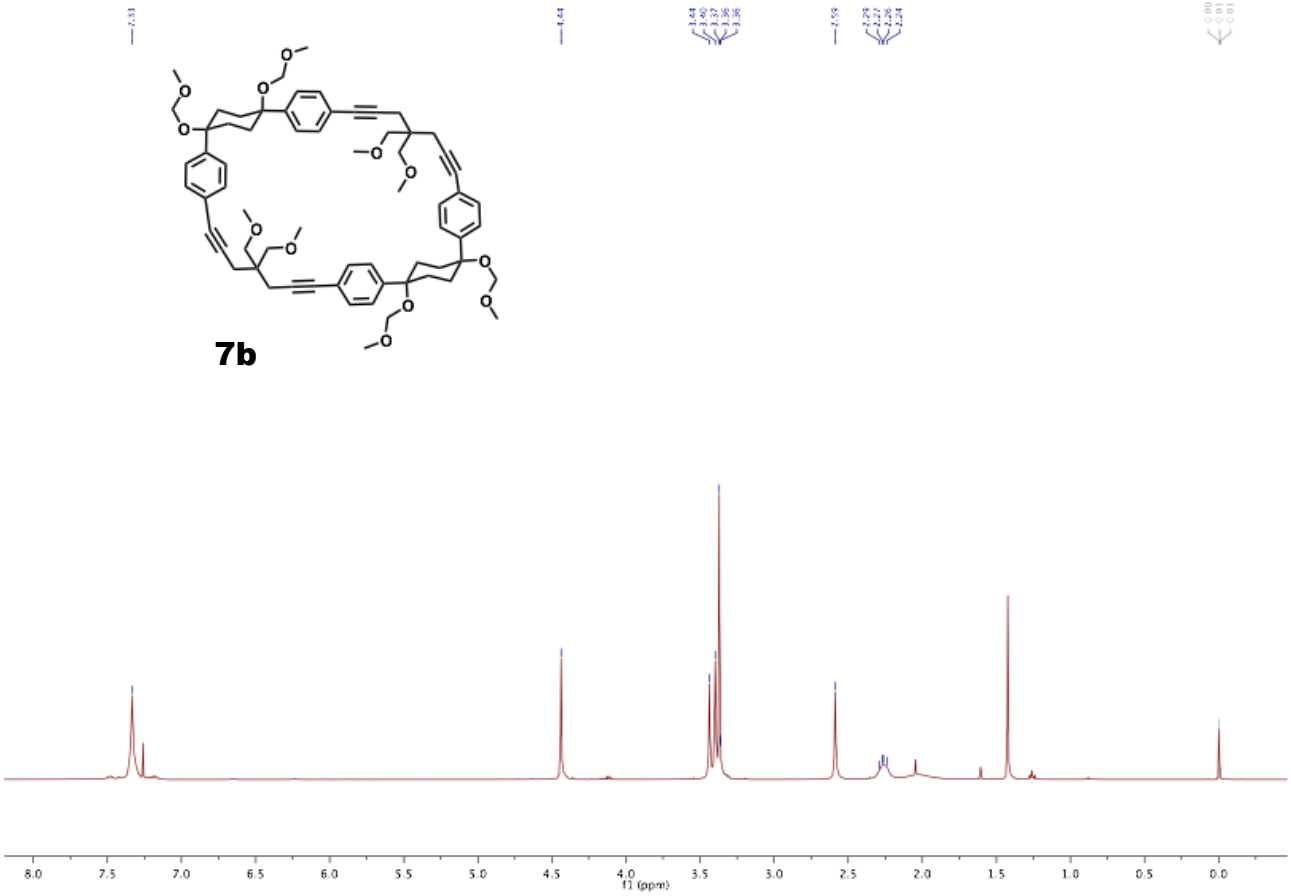
^{1}H-NMR spectrum of 6c ($CDCl_3$)



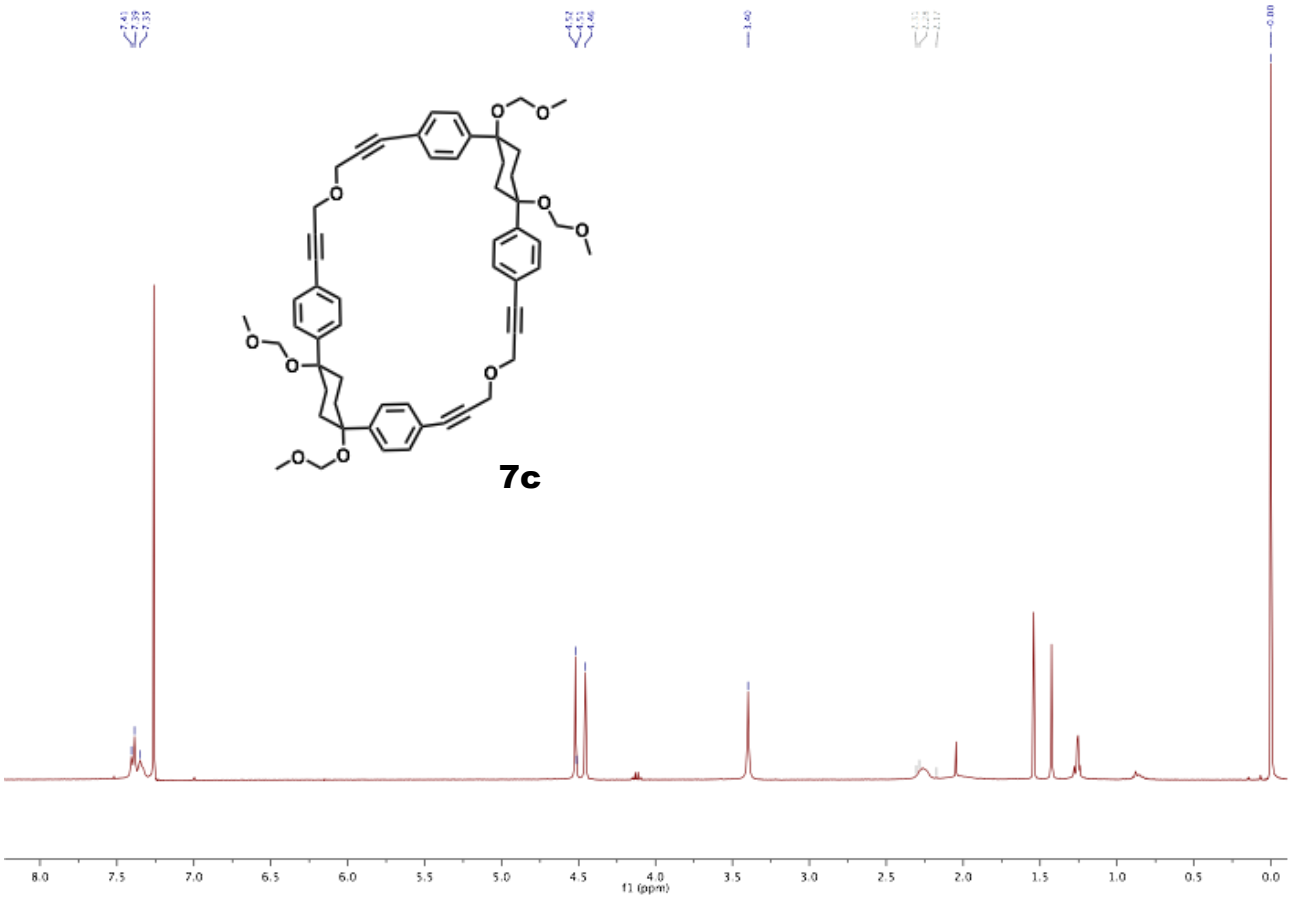
^{1}HNMR spectrum of 7a ($CDCl_3$)



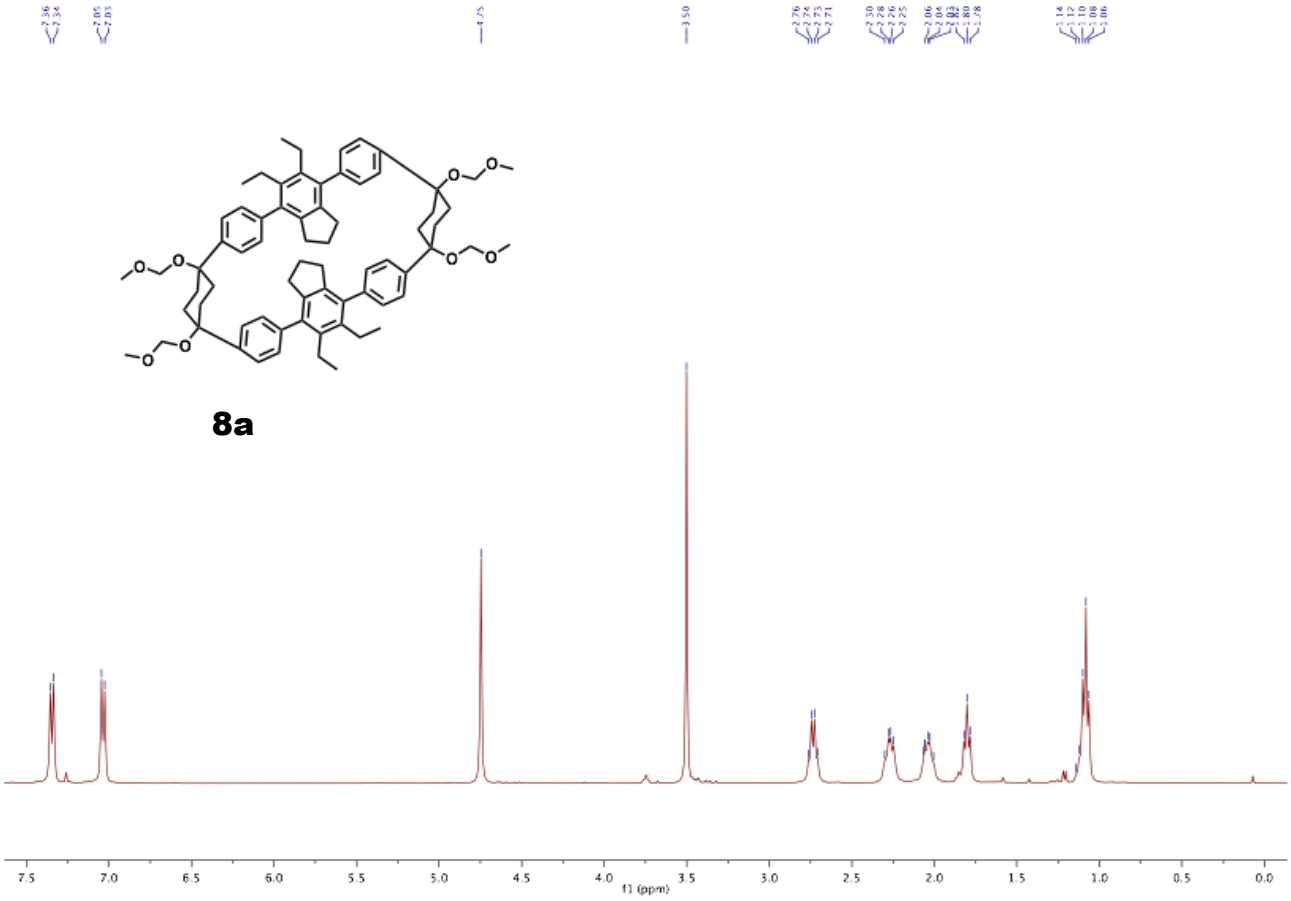
^{1}H-NMR spectrum of 7b ($CDCl_3$)



^{1}H-NMR spectrum of 7c ($CDCl_3$)

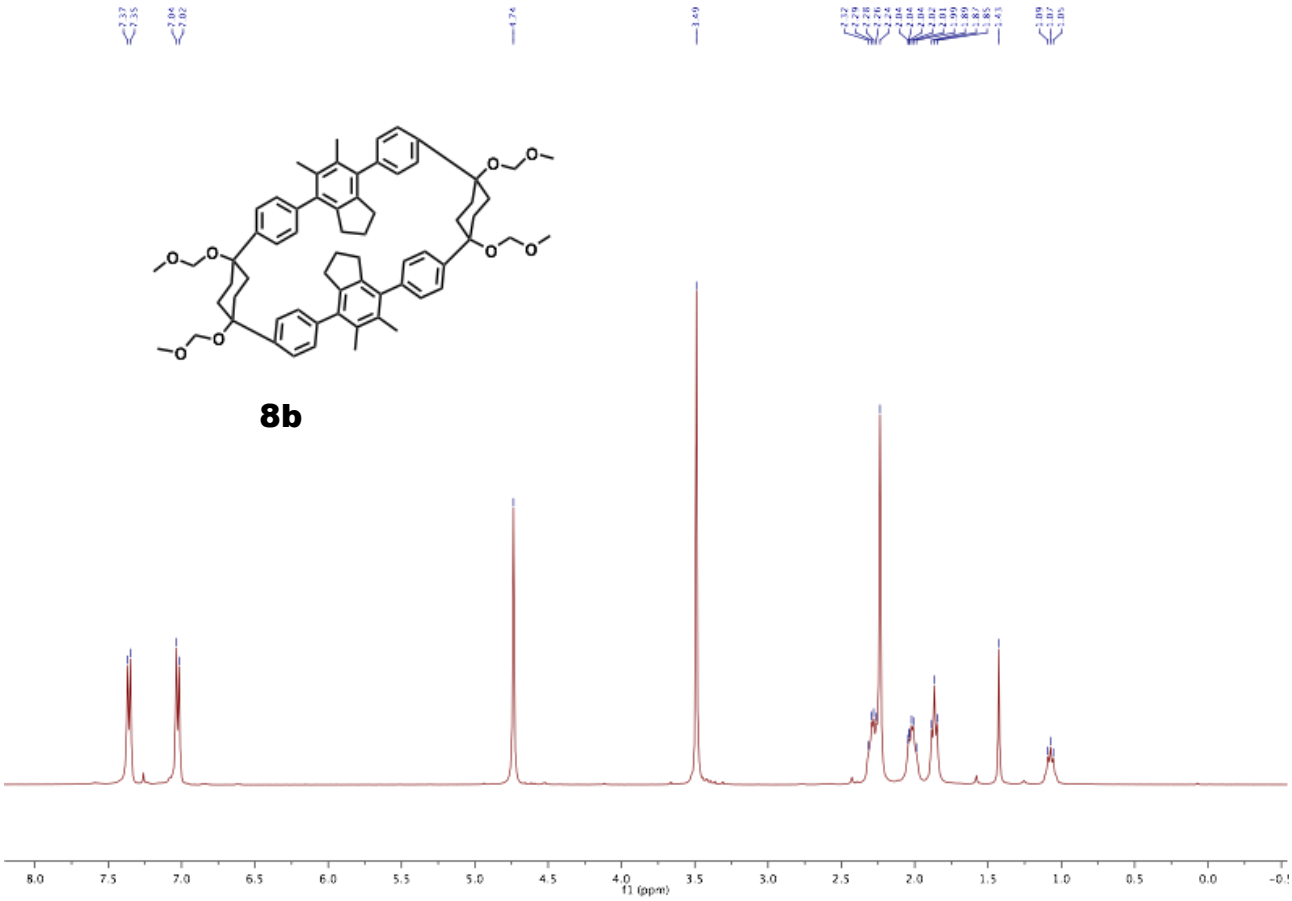


^{1}H-NMR spectrum of 8a ($CDCl_3$)



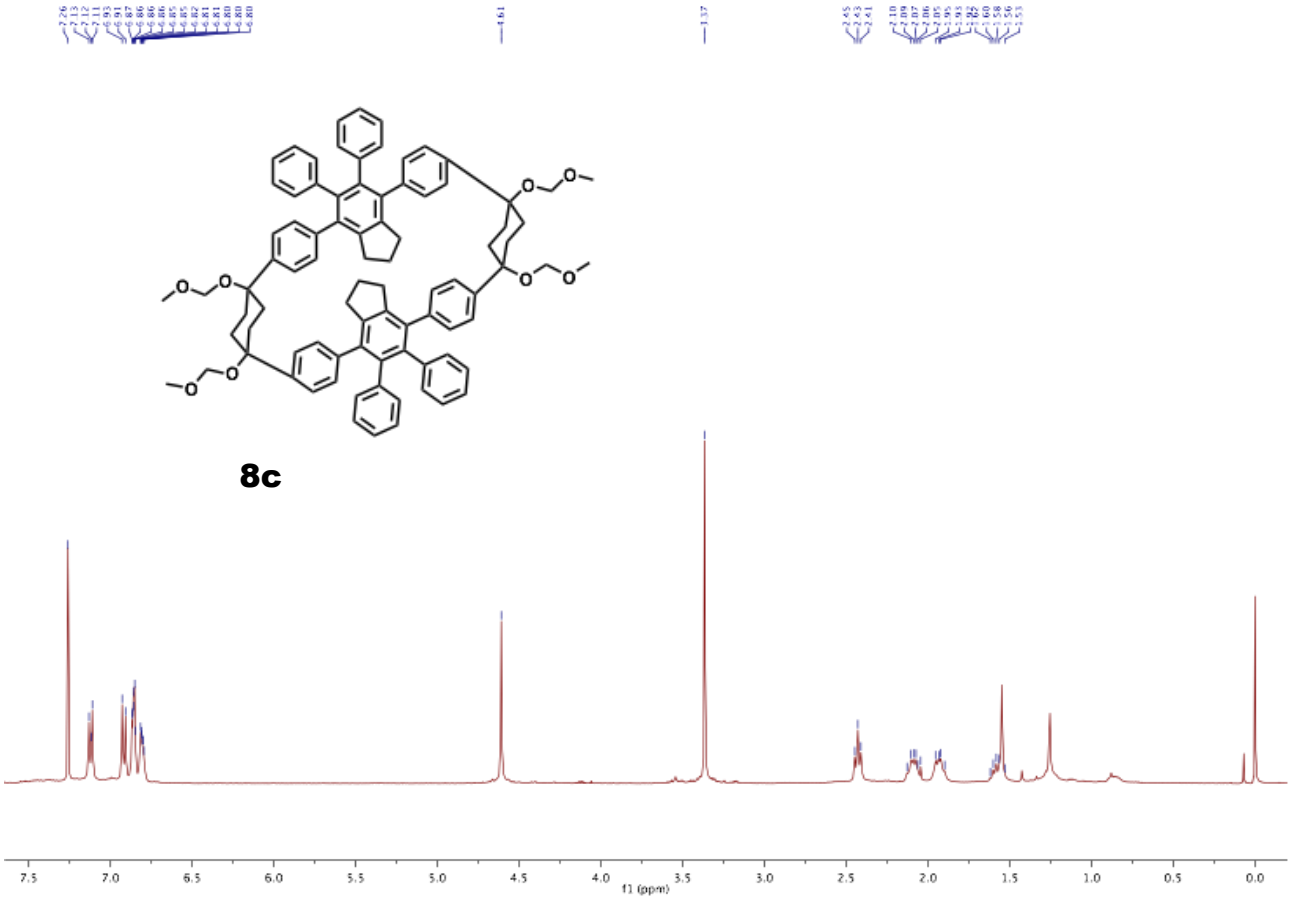
8a

^{1}H-NMR spectrum of 8b ($CDCl_3$)

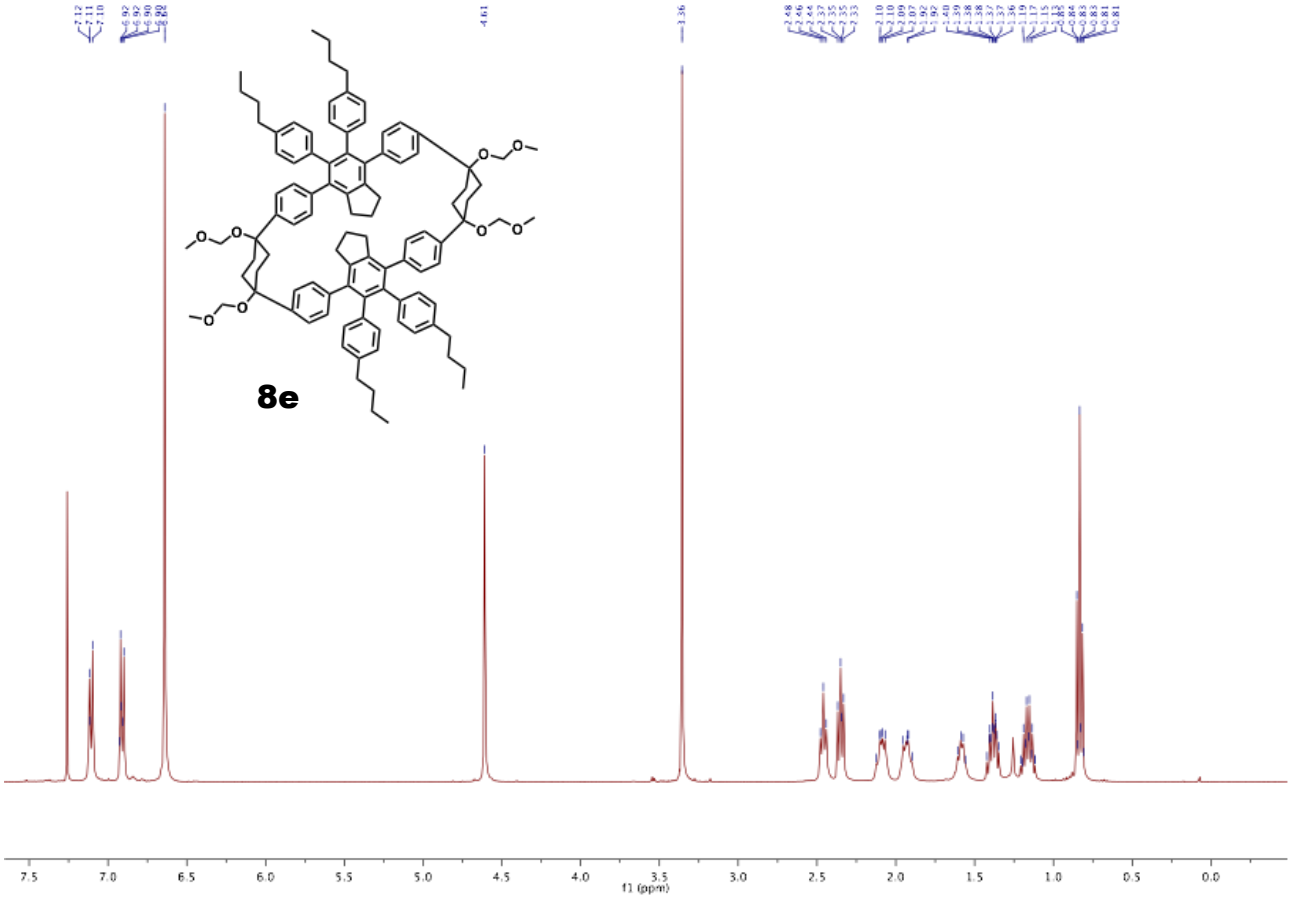


8b

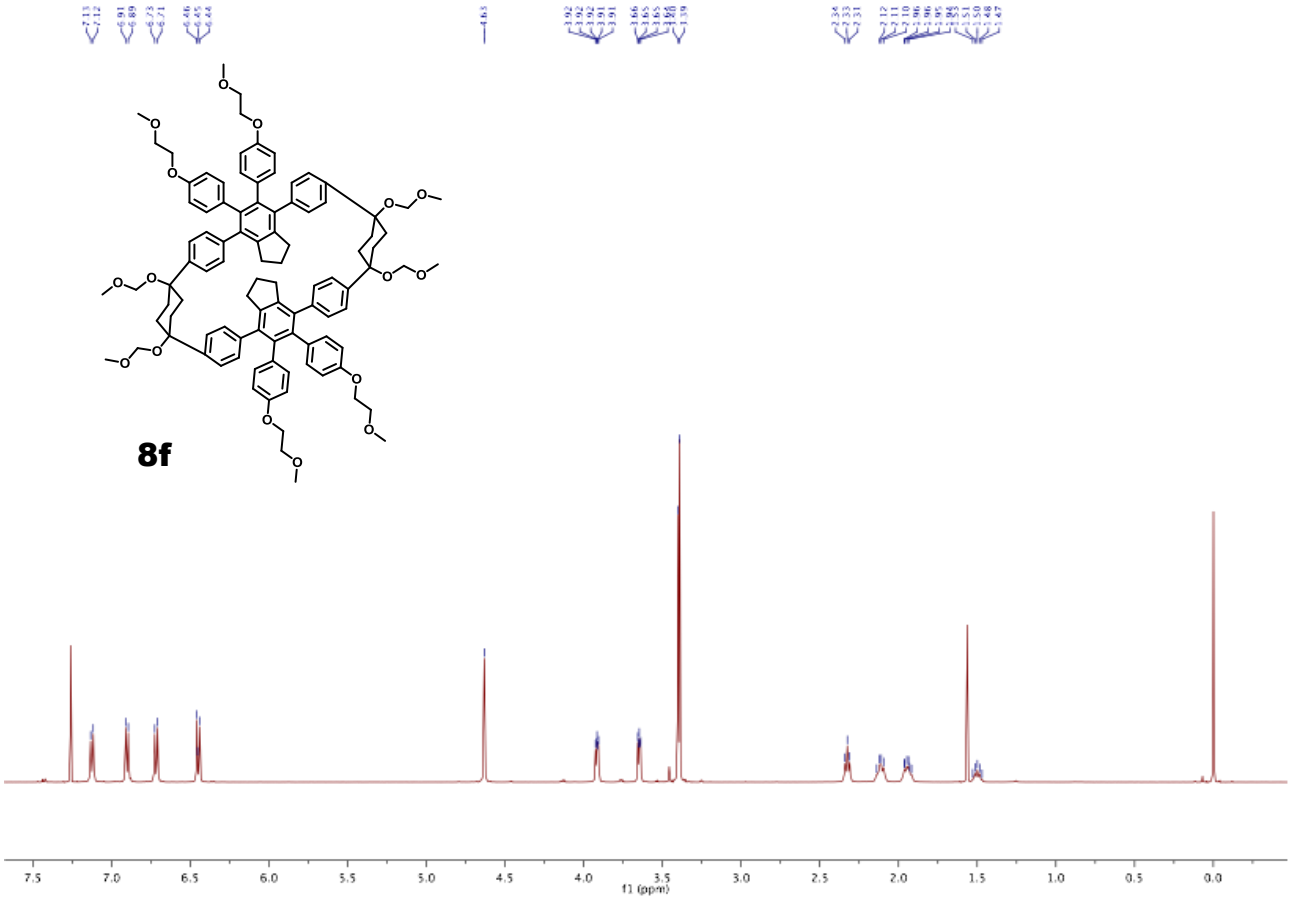
^{1}H-NMR spectrum of 8c ($CDCl_3$)



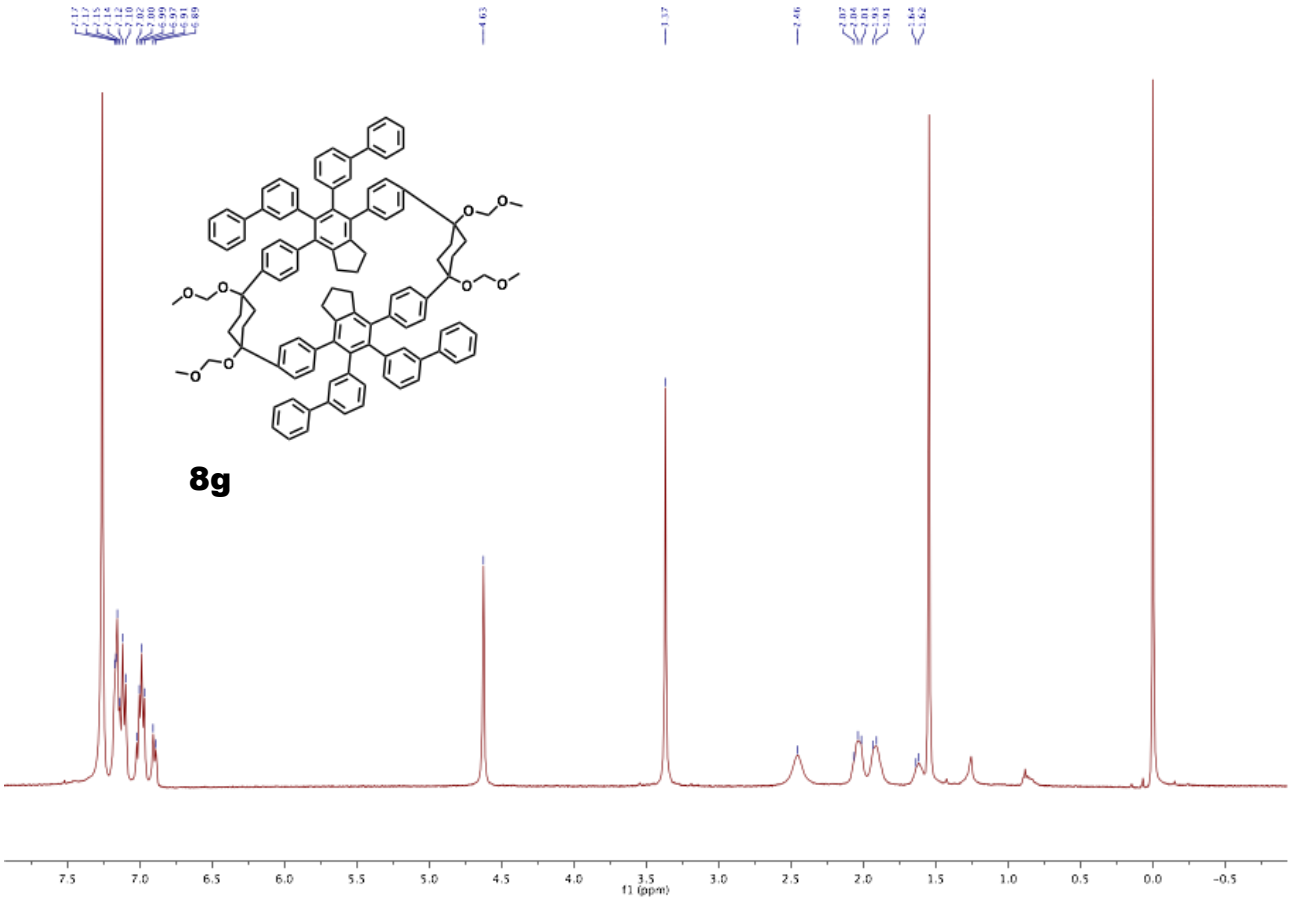
^{1}H-NMR spectrum of 8e ($CDCl_3$)



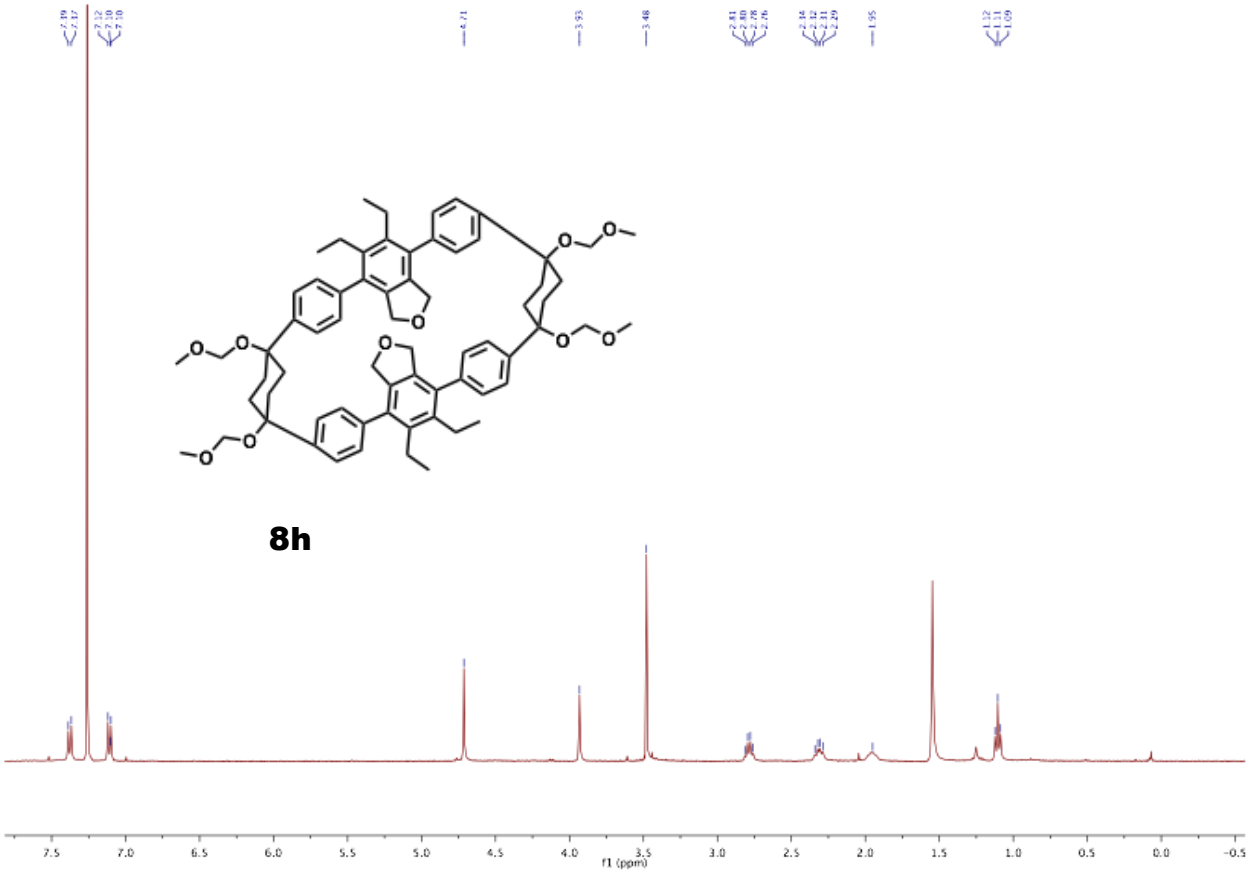
^{1}H-NMR spectrum of 8f ($CDCl_3$)



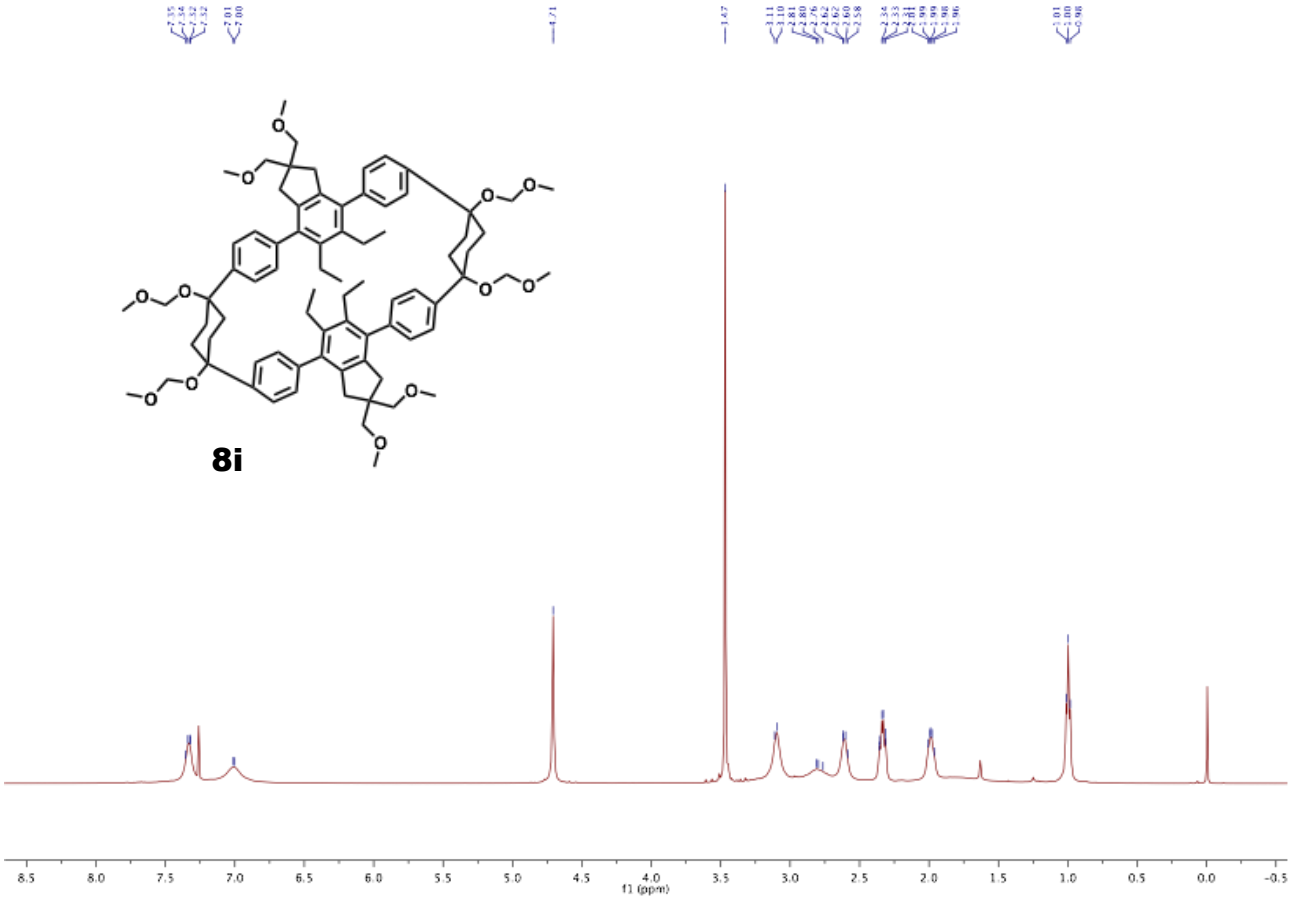
^{1}H-NMR spectrum of 8g ($CDCl_3$)



^{1}H-NMR spectrum of 8h ($CDCl_3$)

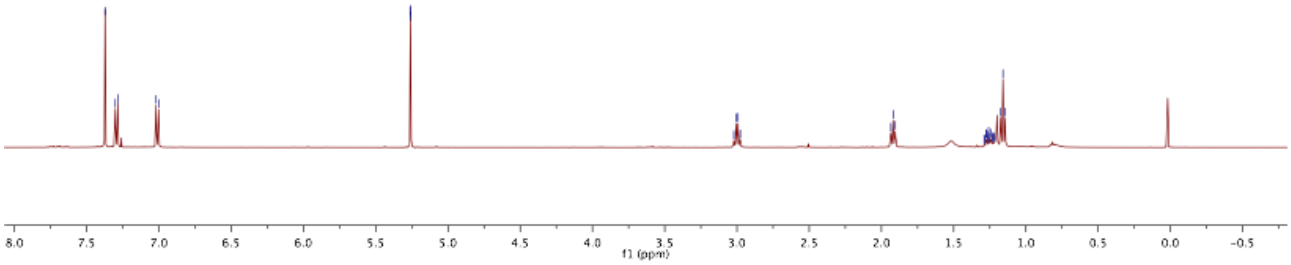


^{1}H-NMR spectrum of 8i ($CDCl_3$)



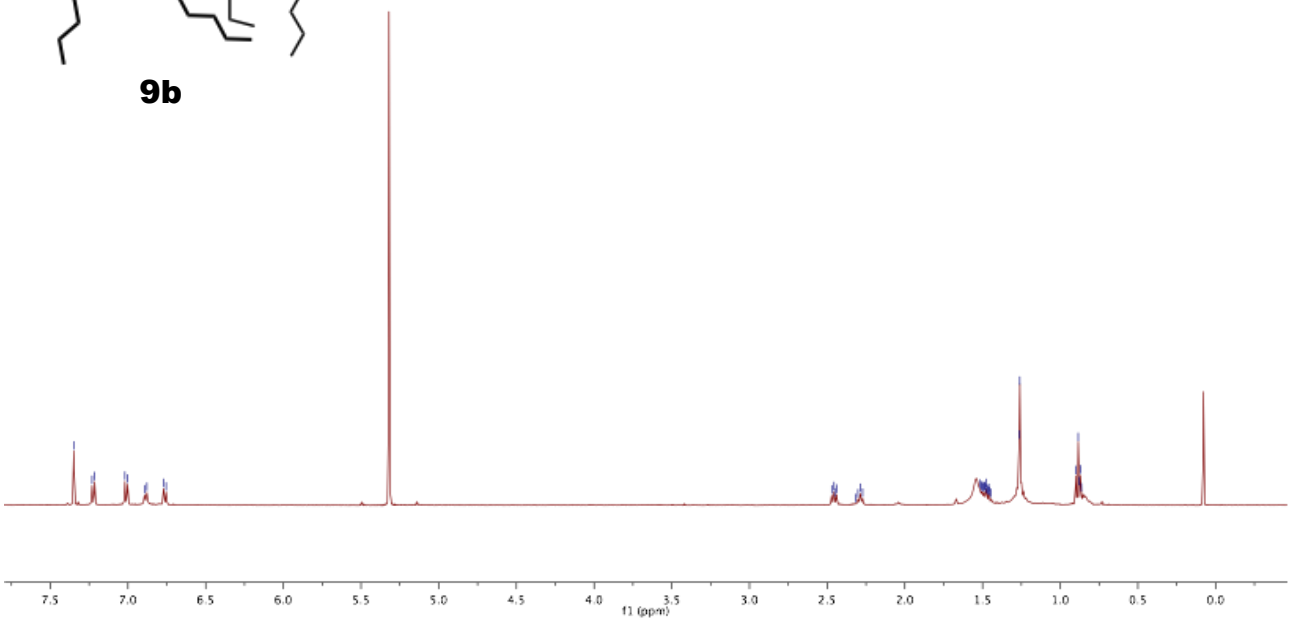
^{1}H-NMR spectrum of 9a (CD_2Cl_2)

9a

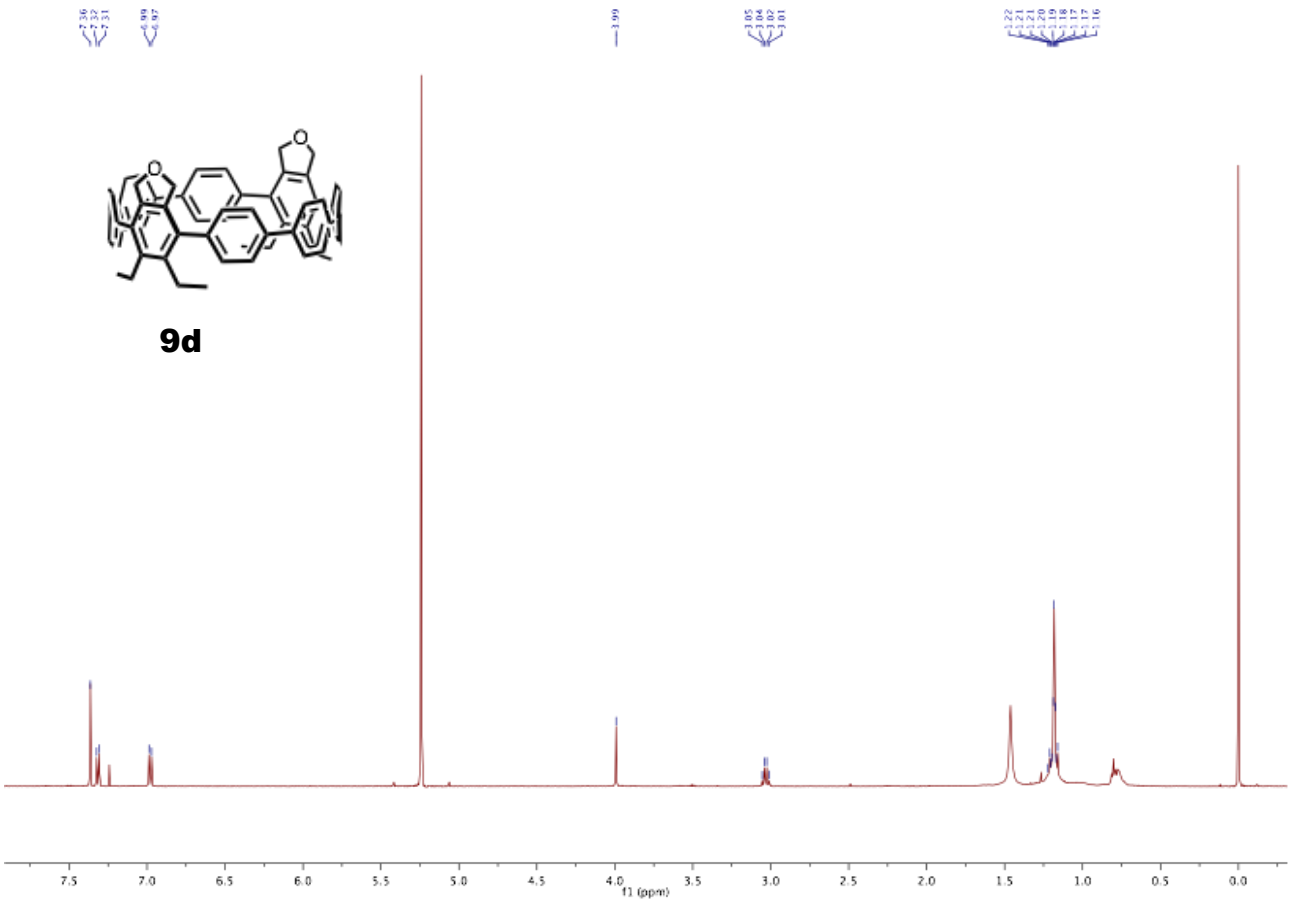


^{1}H-NMR spectrum of 9b (CD_2Cl_2)

9b

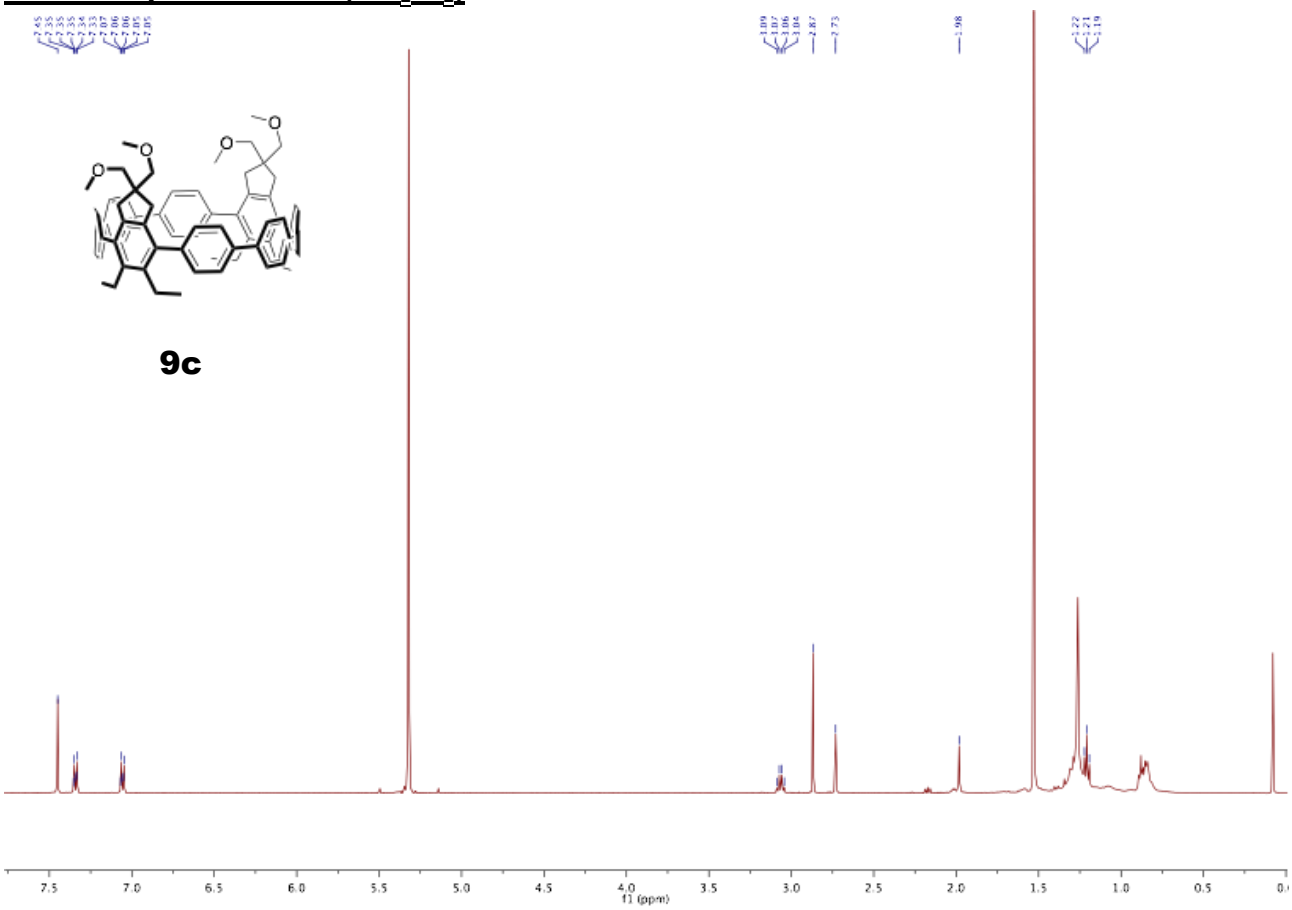


^{1}H-NMR spectrum of 9d (CD_2Cl_2)



9d

^{1}H-NMR spectrum of 9c (CD_2Cl_2)



9c