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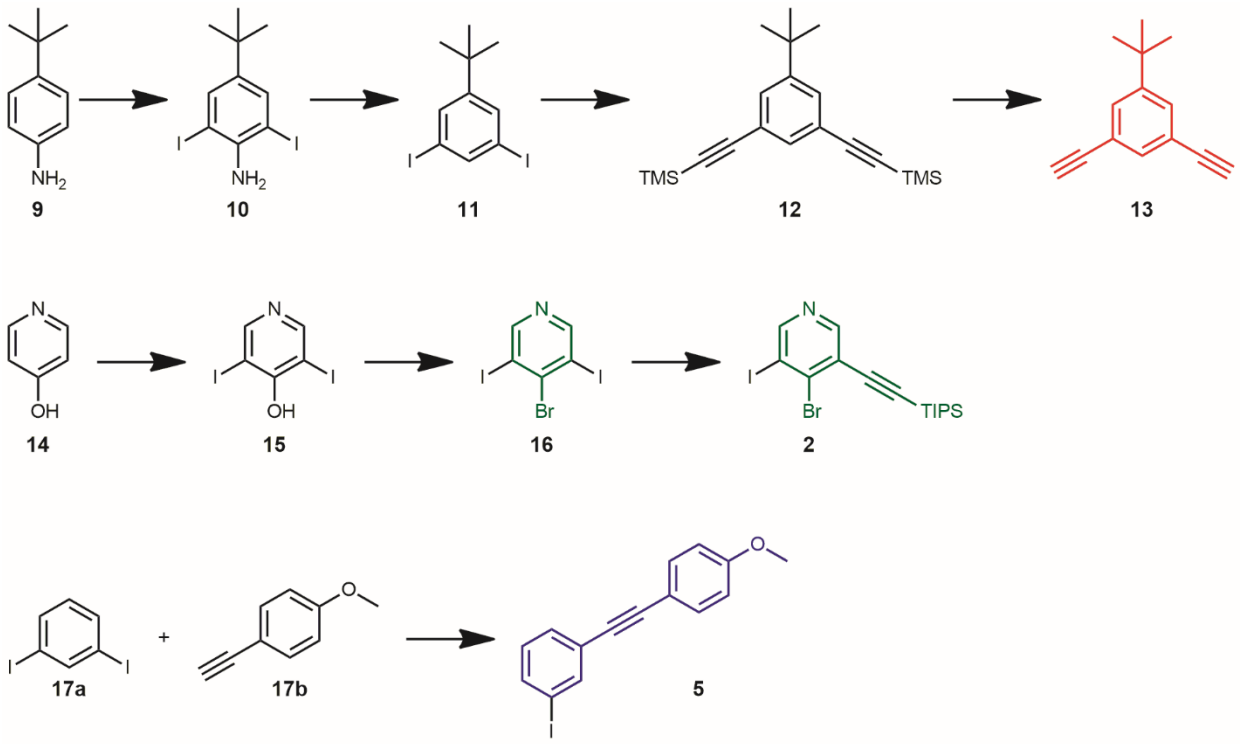
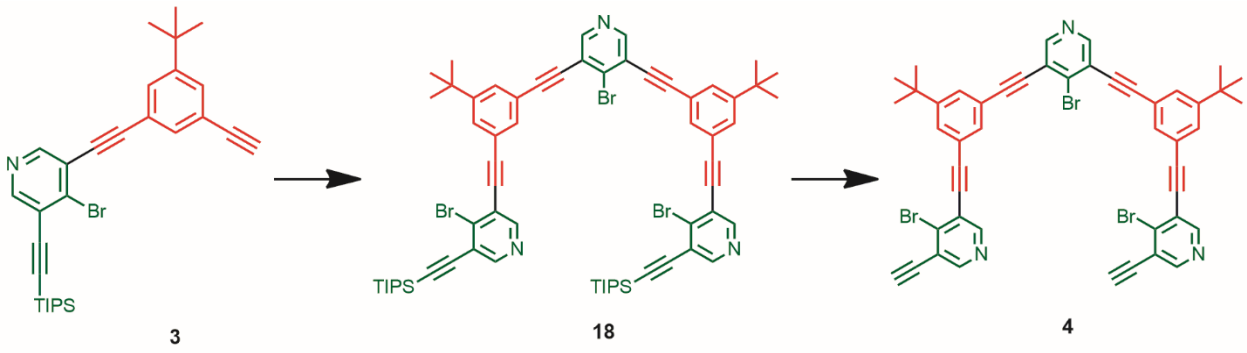
S1. General experimental procedures

All reagents were obtained from commercial sources and were used without further purification unless otherwise noted. Column chromatography was performed using normal phase silica gel (230–400 mesh, SiliaFlash® P60, SiliCycle). Thin layer chromatography was performed using normal phase silica gel glass backed plates (0.25 mm, F-254, SiliCycle) and observed under UV light. Activated Fischer Grade 514 molecular sieves were used when anhydrous solvents were required. For the synthesis of compounds **2**, **3**, **5**, **12**, **18**, and **19**, modified Sonogashira procedures were utilized.[1] Standard Schlenk line and air-free techniques were employed for these reactions. Preparatory HPLC separations were conducted with a Teledyne Isco CombiFlash RF+. A Teledyne Isco RediSep RF Gold Reversed-phase C18 column was utilized to carry out these separations. High-resolution masses for new compounds were obtained using an Agilent 6520 Accurate-Mass Q-TOF LC/MS. Due to their instability, compounds **6** and **8** were directly injected into a Bruker amaZon SL Ion Trap ESI-MS. X-ray crystallographic data were measured on a Bruker D8 Venture (for crystallographic collection and refinement details, see Section S4). The Gaussian 09 suite[2] was used to minimize the folded conformation of a single nonamer of **7** (for computational details, see Section S5). Nuclear magnetic resonance (NMR) spectra were recorded on a VNMRS Varian 500 MHz, Bruker Avance 400 MHz, or Agilent DD2 400 MHz spectrometer. Chemical shifts are reported in parts per million (ppm) from high to low frequency using the residual solvent peak as the internal reference ($CHCl_3$ = 7.26 ppm, DMF = 8.03 ppm). All proton (^1H) resonances are reported to the nearest 0.01 ppm. The multiplicity of the signals is designated as: s = singlet, d = doublet, t = triplet, m = multiplet, or some combination thereof. Coupling constants (*J*) are reported in to the nearest 0.01 Hertz (Hz). All carbon (^{13}C) resonances are reported to the nearest 0.01 ppm and are labeled relative to the center resonance of the residual solvent as the internal reference ($CDCl_3$ = 77.16 ppm, $(CD_3)_2SO$ = 39.52, $[D_7]$DMF = 163.15 ppm). For the ^{19}F NMR spectra, C_6F_6 (δ set to = 164.9 ppm) was used as an internal standard. NOESY and DOSY experiments were conducted to aid in structure determination of the triple helicate in solution. All 2D NOESY data, select ^1H NMR spectra for the characterization of compounds, and select ^1H NMR titration spectra were collected using a VNMRS Varian 600 MHz spectrometer. DOSY experiments were performed on a Bruker Avance III HD 600 MHz with a Prodigy BBO CryoProbe spectrometer. UV-Vis titration data were measured on an Agilent 8453 spectrophotometer. To setup ^1H and ^{13}C NMR samples of compound **6**, a Vigor Gas Separation Technologies Co., Ltd. Glovebox with a gas purification system (SG1200/750TS-F) was used.

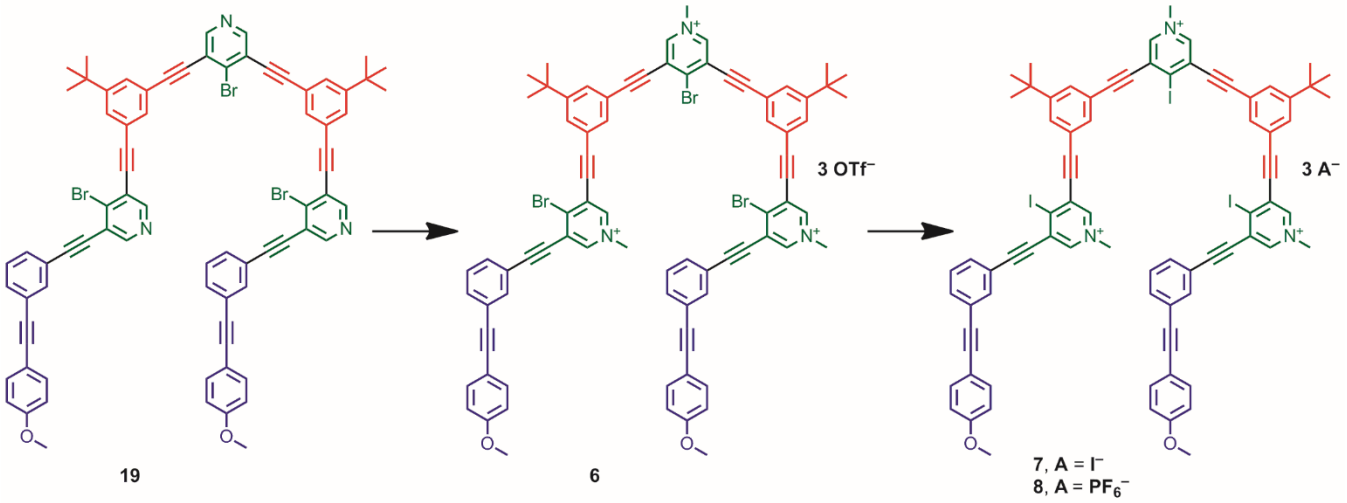
S2. Synthetic schemes



Scheme S1. Synthesis of monomeric and dimeric synthons.



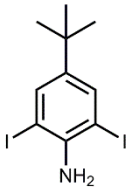
Scheme S2. Synthesis of dimeric and pentameric compounds.



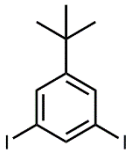
Scheme S3. Synthesis of neutral and alkylated nonamers and halogen and counteranion exchanges.

S3. Experimental procedures and characterization

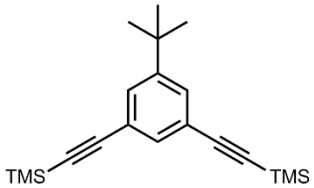
Known compounds



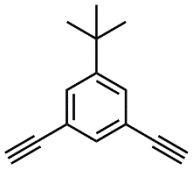
4-(tert-butyl)-2,5-diiodoaniline (**10**) A round bottom flask (2000 mL) was charged with 4-(*tert*-butyl)aniline (21.9 mL, 0.138 mol, 1.0 eq.), benzyl triethylammonium dichloroiodate (100.0 g, 0.287 mol, 2.0 eq.), calcium carbonate (55.46 g, 0.554 mol, 4.0 eq.), MeOH (513 mL), and DCM (1020 mL). The reaction was stirred at reflux for 12 h, open to the air. The reaction mixture was cooled to RT, filtered, and concentrated under reduced pressure. The residue was redissolved in DCM (250 mL), and the solution was washed with sodium thiosulfate (20% w/v, 150 mL), DI water (150 mL), and brine (150 mL). The DCM solution was then dried with anhydrous magnesium sulfate, filtered, and concentrated under reduced pressure. The product was purified by flash column chromatography (dry load, SiO_2, 1% EtOAc/hexanes, R_f = 0.3) to give a maroon oil (26.05 g, 47%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61 (s, 2H), 4.46 (s, 2H), 1.24 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.77, 143.88, 136.66, 81.84, 33.86, 31.46. Spectroscopic data are in accordance with published material.[3]



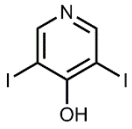
1-(tert-butyl)-3,5-diiodobenzene (**11**) A round bottom flask (2000 mL) was charged with **10** (36.70 g, 91.51 mmol, 1 eq.) and glacial acetic acid (1000 mL). A second round bottom flask (1000 mL) was charged with copper(I) oxide (37.44 g, 261.64 mmol, 2.86 eq.) and EtOH (600 mL). A third round bottom flask (2000 mL) was purged with nitrogen and charged with H_2SO_4 (52 mL). The flask containing H_2SO_4 was brought to 0 °C, and sodium nitrite (28.70 g, 415.97 mmol, 4.5 eq.) was added slowly, generating a slate blue, cloudy solution. The solution of **10** and acetic acid was slowly added to the H_2SO_4 and sodium nitrite mixture while still at 0 °C and under nitrogen, resulting in a yellow precipitate. The combined solutions were allowed to stir for 30 min under nitrogen. The combined solutions were removed from the ice bath, and the Cu_2O/EtOH was slowly added to them under nitrogen. Nitrogen gas bubbles evolved from the cloudy maroon solution. After the addition, the solution was slowly heated to 50 °C, returned to RT, and then allowed to sit for 24 h. The solution was concentrated under reduced pressure and redissolved in DCM (500 mL). Sodium carbonate was added to the solution until the gas evolution ceased. The sodium carbonate was filtered off, and the solution was washed with DI water (250 mL) and brine (150mL). The maroon organic layer was dried with brine and anhydrous magnesium sulfate and concentrated under reduced pressure. The product was separated from the maroon residue by flash column chromatography (dry load, SiO_2, hexanes, R_f = 0.5, top spot) to give a white powder (21.96 g, 62%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 (t, J = 1.49 Hz, 1H), 7.65 (d, J = 1.48 Hz, 2H), 1.27 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 155.63, 142.30, 134.19, 95.10, 34.96, 31.16. This procedure is similar to those employed recently.[4] Spectroscopic data are in accordance with published material.[5]



3,5-bis(trimethylsilylethynyl)-(tert-butyl)benzene (**12**) An oven dried Schlenk flask (500 mL) was charged with bis(triphenylphosphine)palladium(II) dichloride (0.660 g, 0.94mmol, 0.05 eq.) and copper(I) iodide (0.358 g, 1.88 mmol, 0.1 eq.). The Schlenk flask was then evacuated/backfilled with nitrogen three times. To this was added a nitrogen sparged solution of **11** (7.253 g, 18.8 mmol, 1 eq.), Et_3N (72 mL, 520 mmol, 27.7 eq.), ethynyltrimethylsilane (6.64 mL, 47 mmol, 2.5 eq.), and anhydrous THF (200 mL) via cannula. The reaction was allowed to stir under nitrogen overnight at 40 °C. The reaction was cloudy and yellow/orange in coloration then eventually turned black. The solution was removed from heat. Hexanes (150 mL) was added to the mixture, until a white precipitate formed. The solution was filtered, and the filtrate was concentrated under reduced pressure to give a cloudy yellow/orange oil. The product was purified by flash column chromatography (SiO_2, 0% → 10% EtOAc/hexanes, R_f = 0.38) to give a clear yellow oil (5.29 g, 86%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42 (s, 3H), 1.29 (s, 9H), 0.24 (s, 18H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 151.44, 132.91, 129.28, 123.08, 104.87, 94.18, 34.79, 31.22, 0.12. Spectroscopic data are in accordance with published material.[6]

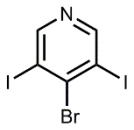


1-(tert-butyl)-3,5-diethynylbenzene (**13**) A round bottom flask (500 mL) was charged with **12** (5.29 g, 16.2 mmol, 1 eq.), K_2CO_3 (4.48 g, 32.4 mmol, 2 eq.), MeOH (160 mL), and THF (20 mL). The solution was allowed to stir under nitrogen for 2 h. The product was purified by flash column chromatography (SiO_2, hexanes, R_f = 0.6) to give a yellow oil (2.641 g, 89%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 (d, *J* = 1.48 Hz, 2H), 7.45 (t, *J* = 1.47 Hz, 1H), 3.06 (s, 2H), 1.30 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 151.72, 132.88, 129.87, 122.20, 83.32, 77.41, 34.75, 31.14. Spectroscopic data are in accordance with published material.[7]



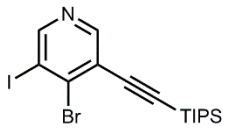
3,5-diiodopyridin-4-ol (**15**) A round bottom flask (2000 mL) was charged with 4-hydroxypyridine (18.00 g, 0.189 mol, 1 eq.), NaOH (47.69 g, 1.19 mol, 6.3 eq.), sodium acetate (144.4 g, 1.76 mol, 9.3 eq.), and DI water (600 mL). The solution was brought to reflux while stirring (using an overhead stirrer), and iodine (168 g, 0.662 mol, 3.5 eq.) was added in portions. To this stirring solution was added aqueous AcOH (50% v/v, 25 mL) causing a beige precipitate to form. This was followed by the addition of an aqueous NaOH solution (50% w/v, 25 mL), which caused the precipitate to disappear, leaving a clear yellow solution. This acidification/basification process was repeated twice with the same change in solution. After the final addition of the sodium NaOH, aqueous AcOH (50% v/v, 25 mL) was added until elemental iodine precipitated from solution. A beige precipitate also formed. The reaction was allowed to cool to RT and was filtered. The beige solid was washed with boiling DI water and was dried on vacuum (~1 Torr) overnight to give pure product (52.45 g, 80%). ^{1}H NMR (400 MHz, $(CD_3)_2SO$) δ 11.96 (s, 1H),

8.28 (s, 2H). ^{13}C NMR (101 MHz, $(CD_3)_2SO$) δ 170.43, 143.19, 86.58. Spectroscopic data are in accordance with published material.[8]



4-bromo-3,5-diiodopyridine (**16**) A flame dried, 3-neck round bottom flask (2000 mL) was charged with **15** (51.45 g, 0.148 mol, 1 eq.) and neat PBr_3 (~75 mL, "enough to cover the solids"). The mixture was allowed to stir at reflux under nitrogen for 4.5 h. The reaction was then allowed to cool to RT and was placed in an ice bath. The reaction mixture was quenched with an aqueous NaOH (50% w/v) solution until gas formation ceased **(WARNING: the gas formation was violent, pungent, and corrosive. Be sure to vent it to the top of the hood. Aqueous NaOH should be added in small portions and with great care.)** A gas inlet adapter was added to one neck (left), and compressed air was used to vent the forming gases out the top of the condenser (center), while a stopper was in the last neck (right). The solution was allowed to stir for 30 min to ensure that the quenching was complete and was brought to pH 9. The solution was extracted with DCM (2x 150 mL). The solids that formed between layers gradually dissolved in the DCM layer. The combined organic extractions were dried with brine (150 mL) and concentrated under reduced pressure to give a peach colored solid. The product was purified using flash column chromatography (SiO_2, dry load, DCM, R_f = 0.45) to give white needles (26.22 g, 43%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.81 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 156.63, 145.76, 100.68. Spectroscopic data are in accordance with published material.[8]

New compounds



4-bromo-3-iodo-5-((triisopropylsilyl)ethynyl)pyridine (**2**) An oven dried Schlenk flask (200 mL) was charged with **16** (8.63 g, 21.1 mmol, 1 eq.), bis(triphenylphosphine)palladium(II) dichloride (0.887 g, 1.26 mmol, 0.06 eq.), and copper(I) iodide (0.401 g, 2.11 mmol, 0.1 eq.). The reaction flask was evacuated/backfilled with nitrogen three times. A nitrogen sparged solution of ethynyltriisopropylsilane (5.0 mL, 22.3 mmol, 1.05 eq.), Et_3N (15 mL, 108 mmol, 5.1 eq.), and anhydrous DMF (150 mL) was transferred to the Schlenk flask via cannula, and the reaction was allowed to stir in a 55 °C oil bath under nitrogen for 12 h. The yellow solution was concentrated under reduced pressure, and the crude solid was purified by column chromatography (SiO_2, 5% EtOAc/hexanes, R_f = 0.38) to give a white powder (3.05 g, 31%). Mp = 60–64 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.79 (s, 1H), 8.52 (s, 1H), 1.19–1.13 (m, 21H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 156.20, 151.98, 142.10, 124.42, 102.09, 101.20, 101.12, 18.75, 11.34. HRMS ($C_{16}H_{24}BrINSi$ = $[M+H]^+$): calculated = 463.9906; found = 463.9918.

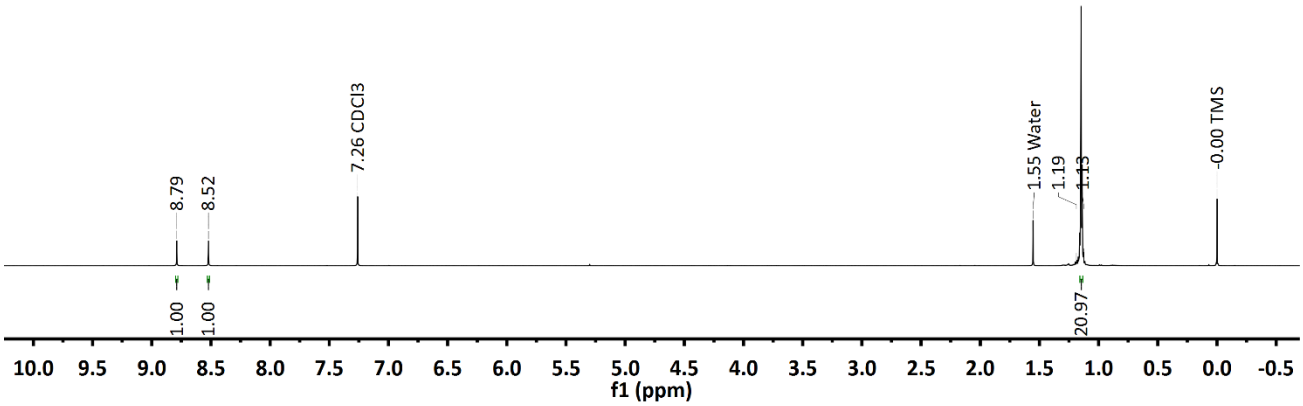


Figure S1. ^{1}H NMR spectrum of **2** (400 MHz, $CDCl_3$, 298 K).

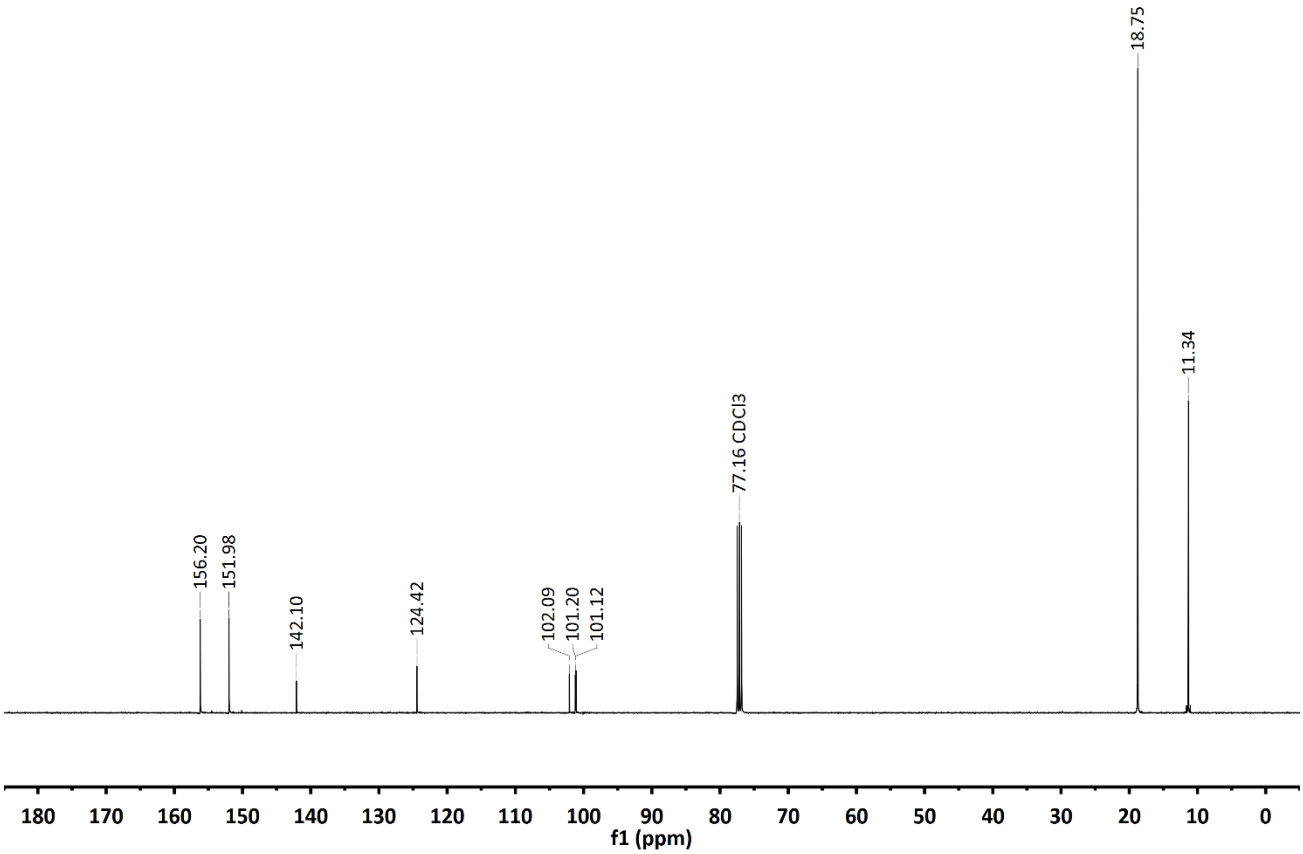
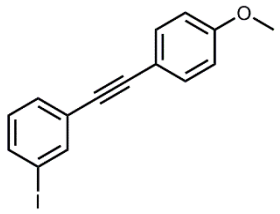


Figure S2. ^{13}C NMR spectrum of **2** (101 MHz, $CDCl_3$, 298 K).



1-iodo-3-((4-methoxyphenyl)ethynyl)benzene (**5**) An oven dried Schlenk flask (200 mL) was purged with nitrogen, and charged with 1,3-diiodobenzene (4.00 g, 12.1 mmol, 1 eq.), bis(triphenylphosphine)palladium(II) dichloride (0.426 g, 0.606 mmol, 0.05 eq.), and copper(I) iodide (0.231 g, 1.21 mmol, 0.1 eq.). The Schlenk flask was evacuated/backfilled with nitrogen three times. A nitrogen sparged solution of 1-ethynyl-4-methoxybenzene (1.57 mL, 12.1 mmol, 1 eq.), Et_3N (26 mL, 187 mmol, 15 eq.), and anhydrous THF (64 mL) was transferred to the Schlenk flask via cannula. The solution was allowed to stir under nitrogen in a 50 °C oil bath for 12 h. The solution was allowed to come to RT and was concentrated under reduced pressure. The crude material was purified by flash column chromatography (SiO_2, dry load, 10% EtOAc/hexanes, R_f = 0.39) to give a white powder (1.935 g, 48%). Mp = 99–101° C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 (t, *J* = 1.6 Hz, 1H), 7.64 (ddd, *J* = 7.96, 1.82, 1.05 Hz, 1H), 7.47–7.44 (m, 3H), 7.06 (t, *J* = 7.85 Hz, 1H), 6.88 (dt, *J* = 8.76, 2.80, 2.04 Hz, 2H), 3.83 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.01, 140.12, 137.01, 133.27, 130.65, 129.94, 125.86, 114.98, 114.20, 93.83, 90.94, 86.55, 55.47. HRMS ($C_{15}H_{12}IO$ = $[M+H]^+$): calculated = 334.9933; found = 334.9936.

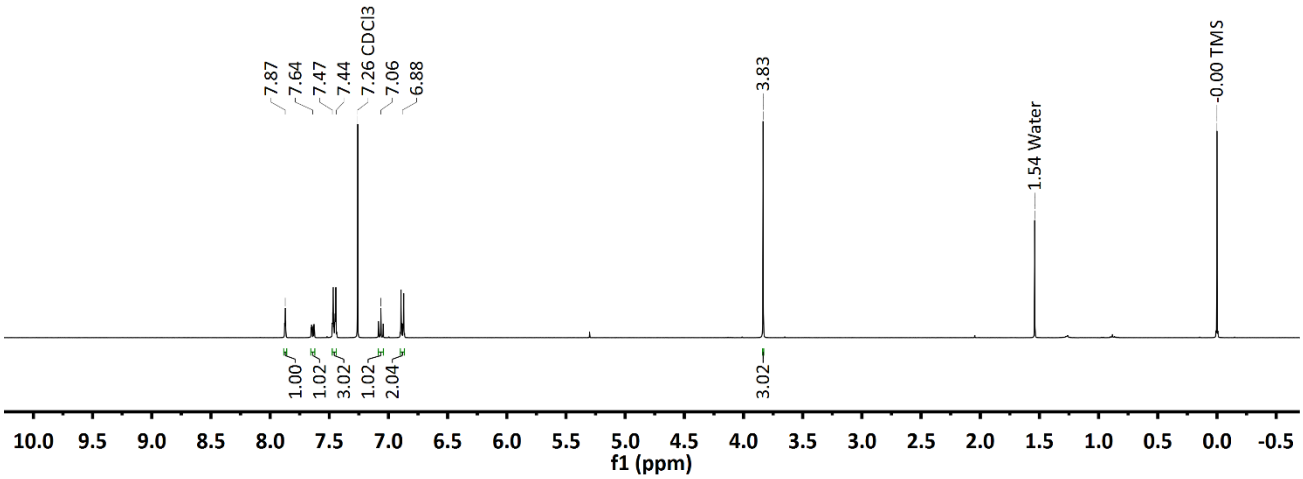


Figure S3. ^{1}H NMR spectrum of **5** (400 MHz, $CDCl_3$, 298 K).

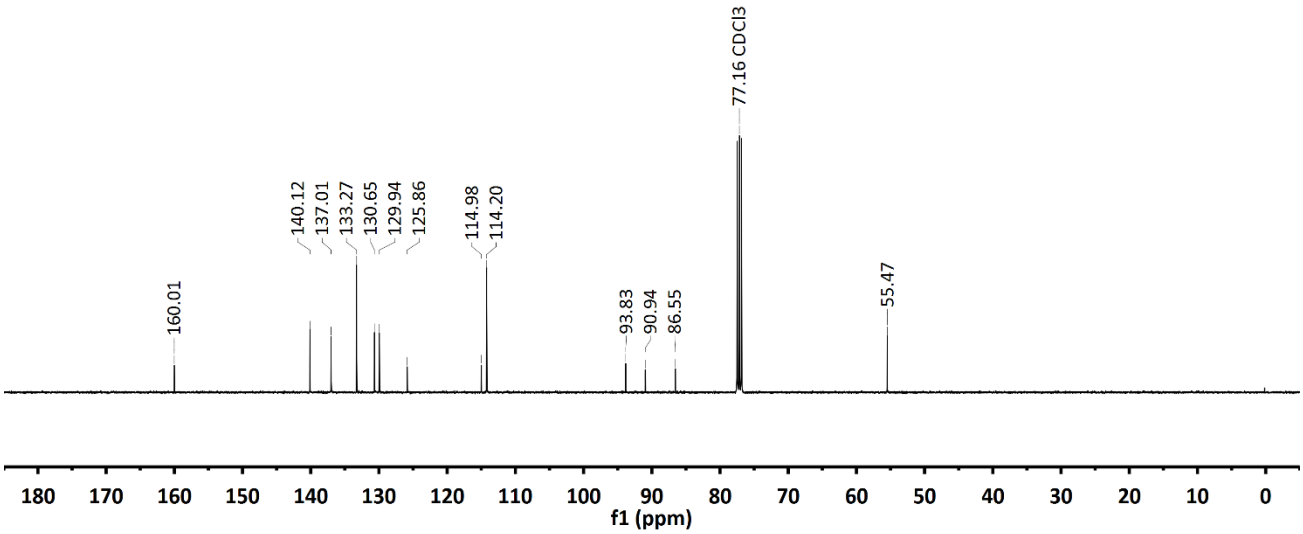
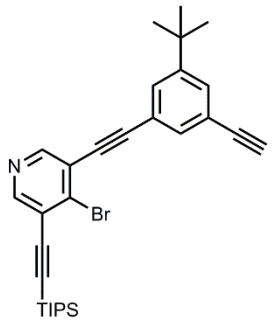


Figure S4. ^{13}C NMR spectrum of **5** (101 MHz, $CDCl_3$, 298 K).



4-bromo-3-((3-(tert-butyl)-5-ethynylphenyl)ethynyl)-5-((triisopropylsilyl)ethynyl)pyridine (dimer) (**3**) An oven dried Schlenk flask (500 mL) was charged with bis(triphenylphosphine)palladium(II) dichloride (0.231 g, 0.329 mmol, 0.5 eq.) and copper(I) iodide (0.125 g, 0.657 mmol, 0.1 eq.) and was evacuated/backfilled with nitrogen three times. A sonicated nitrogen sparged solution of **13** (3.590 g, 19.7 mmol, 3 eq.), Et_3N (115 mL, 131 mmol, 20 eq.), and anhydrous DMF (200 mL) was transferred to the Schlenk flask via cannula. A nitrogen sparged solution of **2** (3.052 g, 6.57 mmol, 1 eq.) and anhydrous DMF (100 mL) was loaded into a gas-tight syringe and added to the Schlenk flask over 10 h at RT. The reaction was allowed to stir under nitrogen for 12 h total. The solution was concentrated under reduced pressure, and the crude product was purified by flash column chromatography (SiO_2, 5% EtOAc/hexanes, R_f = 0.31) to give a yellow oil (0.710 g, 21%). We reason that the yield could be increased to ~33% if the reaction were monitored by TLC and a 1:1 ratio of starting materials were used. Even at room temperature, some product was consumed by a second cross-coupling at the bromine functionality (with excess **13** and via self-dimerization). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.57 (s, 1H), 8.53 (s, 1H), 7.57 (t, *J* = 1.74 Hz, 1H), 7.54 (d, *J* = 1.72 Hz, 2H), 3.09 (s, 1H), 1.34 (s, 9H), 1.19–1.13 (m, 21H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 152.01, 151.82, 151.12, 138.04, 132.64, 130.34, 129.42, 123.52, 123.13, 122.43, 122.28, 101.45, 101.04, 96.68, 84.96, 83.22, 77.61, 34.89, 31.21, 18.79, 11.37. HRMS ($C_{30}H_{37}BrNSi$ = $[M+H]^+$): calculated = 518.1879; found = 518.1861.

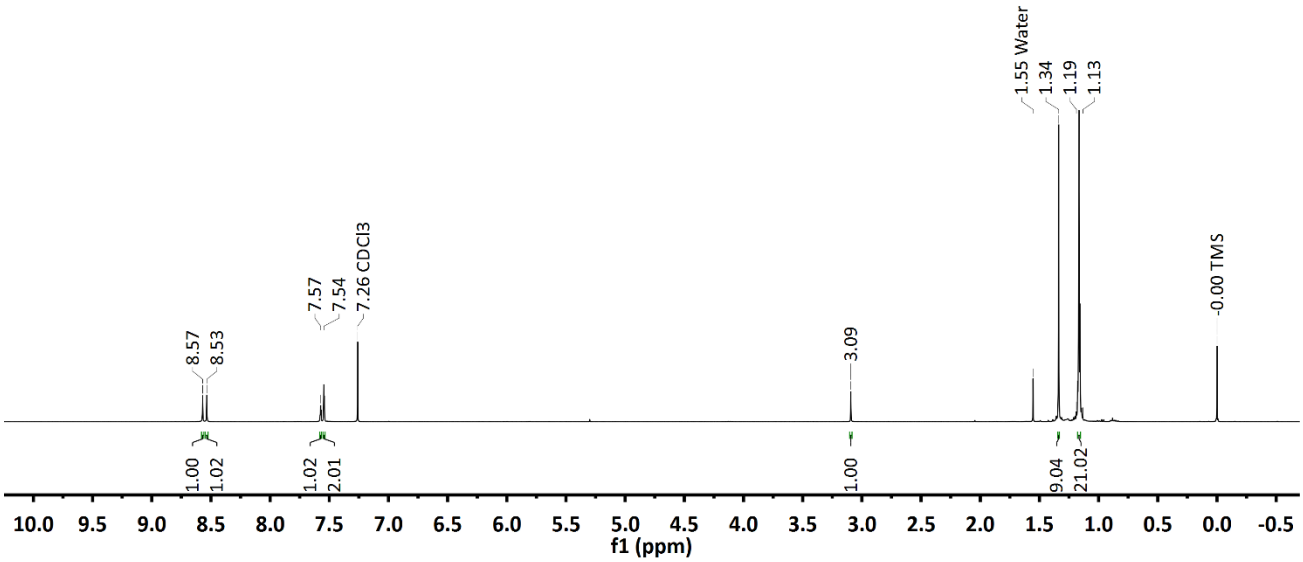


Figure S5. ^{1}H NMR spectrum of **3** (400 MHz, $CDCl_3$, 298 K).

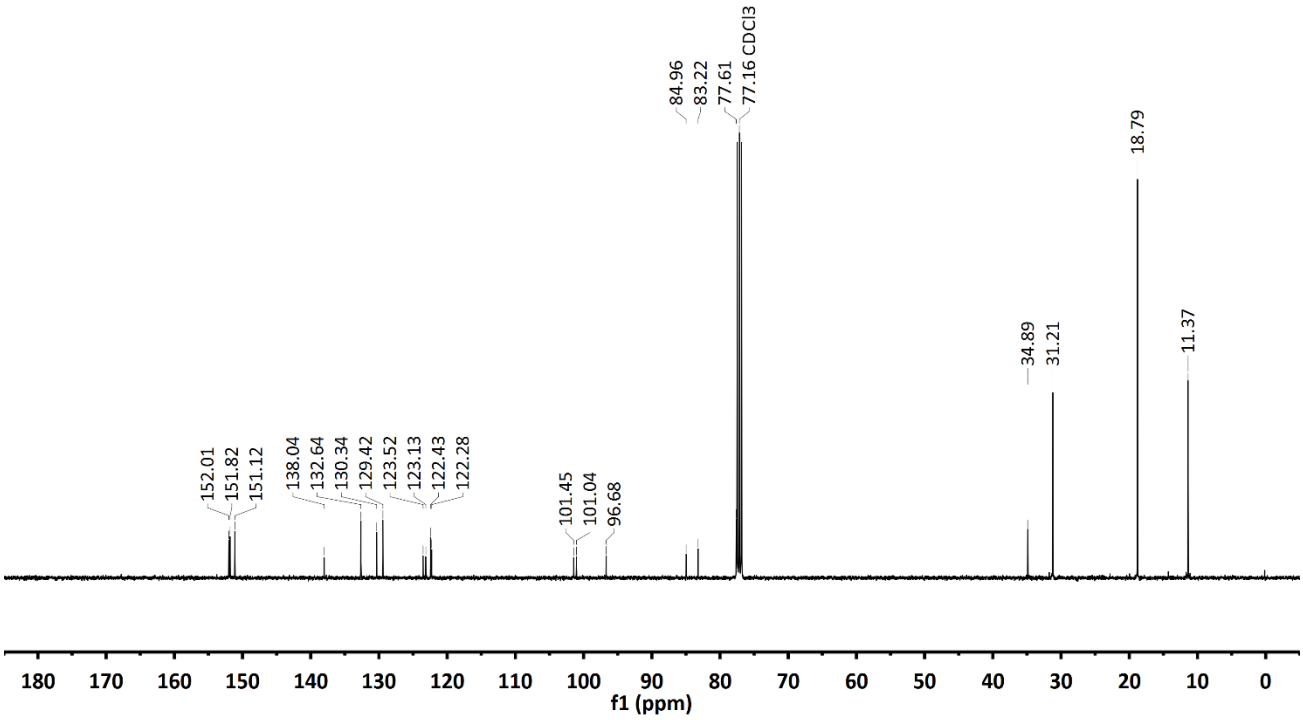
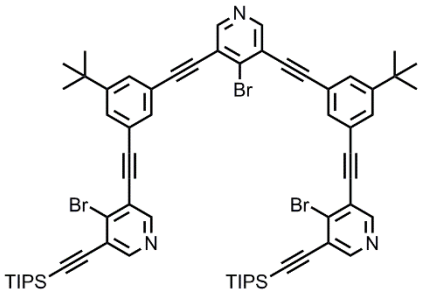


Figure S6. ^{13}C NMR spectrum of **3** (101 MHz, $CDCl_3$, 298 K).



5,5'-((((4-bromopyridine-3,5-diyl)bis(ethyne-2,1-diyl))bis(3-(tert-butyl)-5,1-phenylene))bis(ethyne-2,1-diyl))bis(4-bromo-3-((triisopropylsilyl)ethynyl)pyridine) (protected pentamer) (**18**) An oven dried Schlenk flask (100 mL) was charged with **16** (0.281 g, 0.685 mmol, 1 eq.), bis(triphenylphosphine)palladium(II) dichloride (0.0481g, 0.0685 mmol, 0.1 eq.), and copper(I) iodide (0.0261 g, 0.137 mmol, 0.2 eq.). The Schlenk flask was evacuated/backfilled with nitrogen three times. A nitrogen sparged solution of **3** (0.710 g, 1.37 mmol, 2 eq.), Et_3N (0.955 mL, 6.85 mmol, 10 eq.) and anhydrous DMF (31 mL) was transferred to the Schlenk flask via cannula. The reaction was allowed to stir under nitrogen in a 50 °C oil bath for 12 h. The solution was concentrated under reduced pressure and the crude product was purified by flash column chromatography (SiO_2, 7.5% → 25% EtOAc/hexanes, R_f = 0.1 with 7.5% EtOAc/hexanes) to give a yellow oil (0.375 g, 75%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.63 (s, 2H), 8.59 (s, 2H), 8.55 (s, 2H), 7.66 (t, *J* = 1.49 Hz, 2H), 7.65–7.63 (m, 4H), 1.38 (s, 18), 1.19–1.13 (m, 42H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 152.26, 151.88, 151.39, 151.15, 138.04, 137.71, 132.32, 129.94, 129.89, 123.53, 123.22, 123.06, 122.55, 122.45, 101.43, 101.09, 96.74, 96.52, 85.22, 85.09, 34.99, 31.24, 18.78, 11.37. HRMS ($C_{65}H_{73}Br_3N_3Si_2$ = $[M+H]^+$): calculated = 1188.2893; found = 1188.2926.

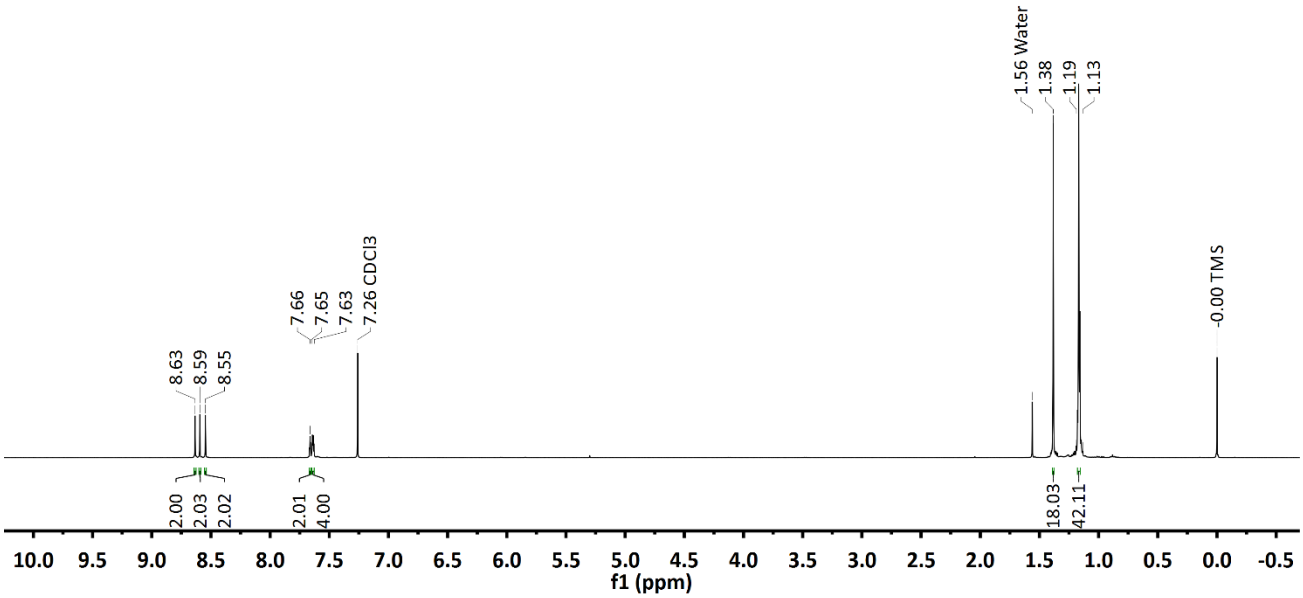


Figure S7. ^{1}H NMR spectrum of **18** (400 MHz, $CDCl_3$, 298 K).

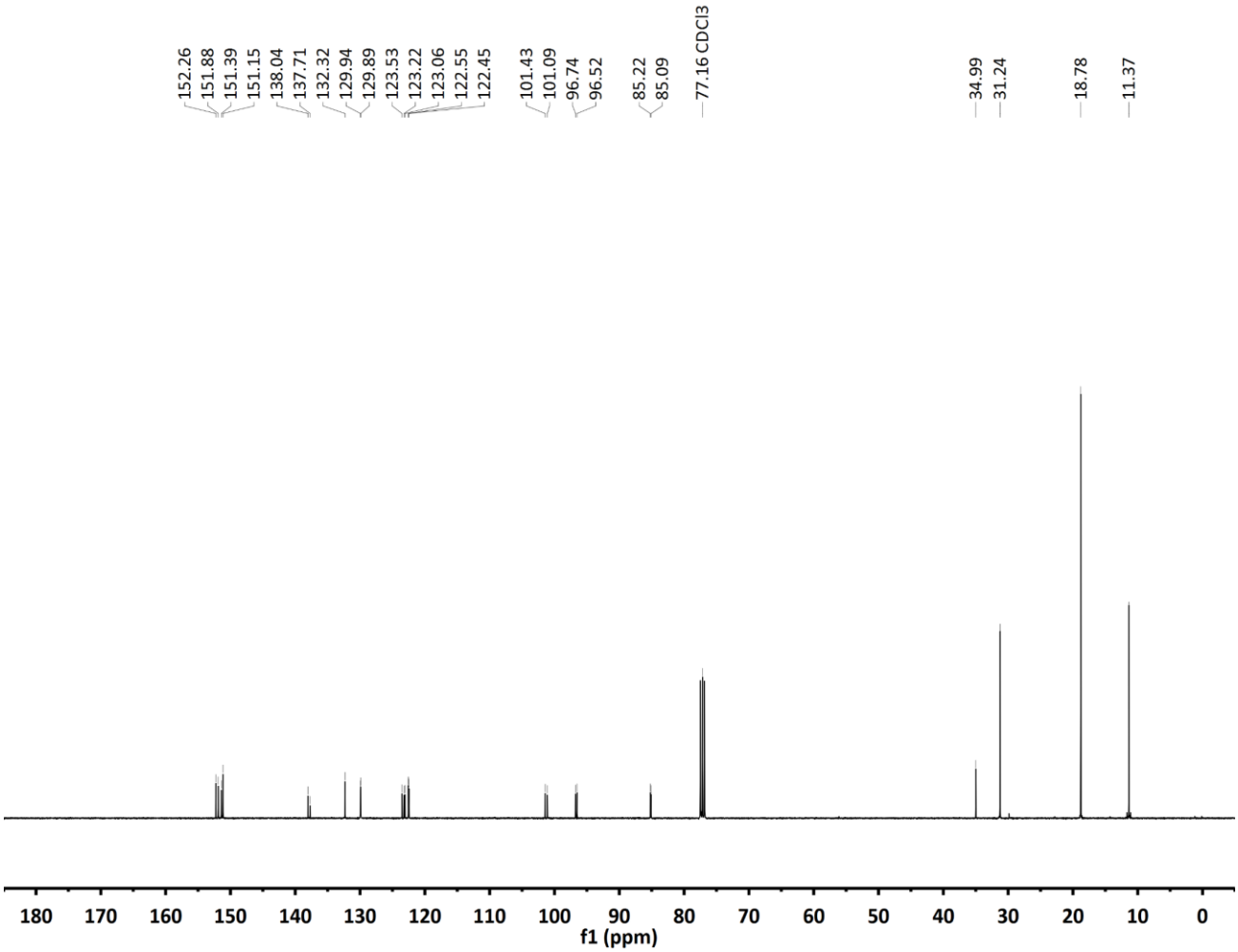
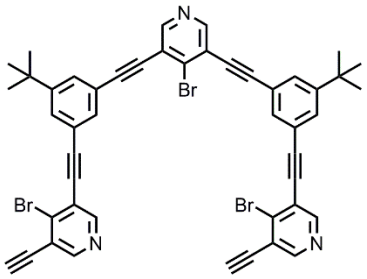


Figure S8. ^{13}C NMR spectrum of **18** (101 MHz, $CDCl_3$, 298 K).



5,5'-((((4-bromopyridine-3,5-diyl)bis(ethyne-2,1-diyl))bis(3-(tert-butyl)-5,1-phenylene))bis(ethyne-2,1-diyl))bis(4-bromo-3-ethynylpyridine) (deprotected pentamer) (**4**) A solution of **18** (2.192 g, 1.84 mmol, 1 eq.) was dissolved in anhydrous THF (92 mL) and sparged with nitrogen in an oven dried Schlenk flask (200 mL). The pale yellow solution was cooled to 0 °C. TBA fluoride (1 M in THF, 5.52 mL, 5.52 mmol, 3 eq.) was added dropwise over one min. The red solution was removed from the ice bath after the addition of the TBAF and allowed to stir for 10 min. The copper colored solution was diluted with DI water (200 mL), which caused the solution to become white and cloudy. The aqueous layer was extracted with DCM (3x 250 mL). The combined DCM extractions were dried with brine and anhydrous magnesium sulfate. The solution was concentrated under reduced pressure to give an off-white powder (1.60 g, quantitative). No further purification was necessary. TLC conditions 5% acetone/DCM, R_f = 0.37. Mp = 215 °C with decomposition. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.64 (s, 2H), 8.63 (s, 2H), 8.57 (s, 2H), 7.67 (t, *J* = 1.4 Hz, 2H), 7.64 (dt, *J* = 6.65, 1.70 Hz, 4H), 3.55 (s, 2H), 1.38 (s, 18H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 152.36, 152.10, 151.88, 151.40, 138.04, 137.75, 132.36, 130.00, 129.95, 123.28, 123.26, 122.53, 122.45, 122.37, 96.86, 96.76, 85.40, 85.15, 84.97, 78.96, 35.02, 31.25. HRMS ($C_{47}H_{33}Br_3N_3$ = $[M+H]^+$): calculated = 876.0225; found = 876.0264.

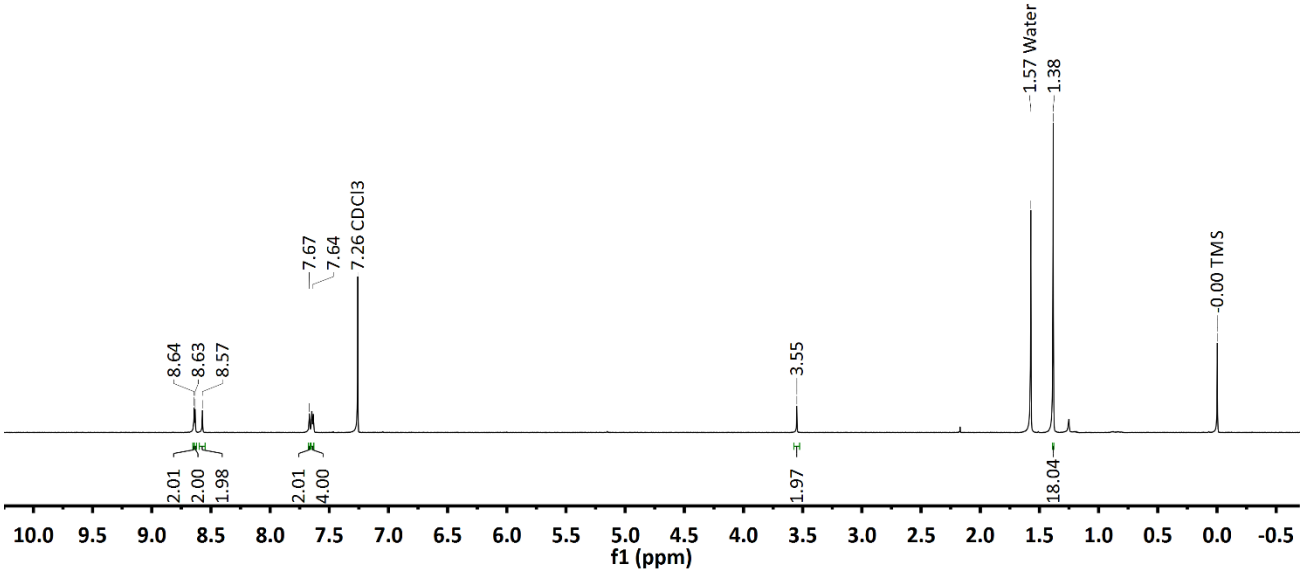


Figure S9. ^{1}H NMR spectrum of **4** (500 MHz, $CDCl_3$, 298 K).

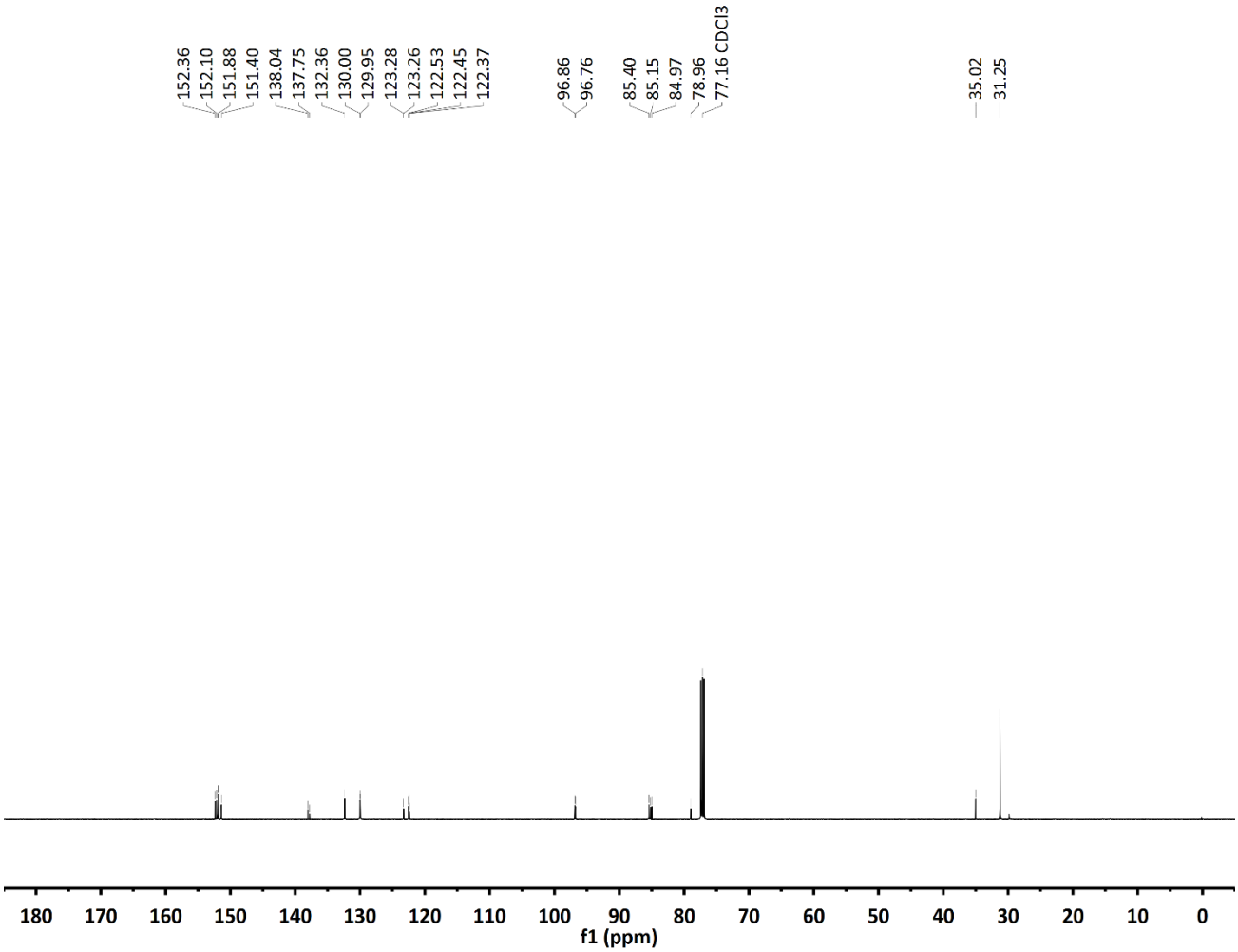
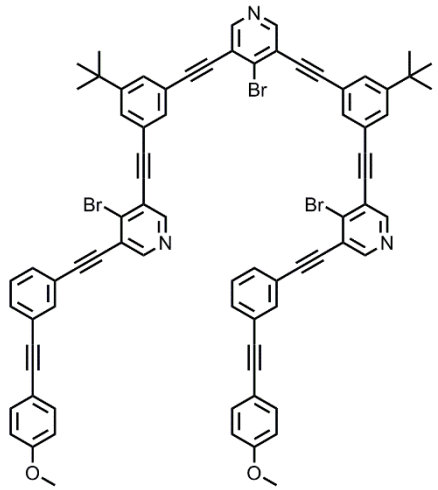


Figure S10. ^{13}C NMR spectrum of **4** (126 MHz, $CDCl_3$, 298 K).



5,5'-((((4-bromopyridine-3,5-diyl)bis(ethyne-2,1-diyl))bis(3-(tert-butyl)-5,1-phenylene))bis(ethyne-2,1-diyl))bis(4-bromo-3-((3-((4-methoxyphenyl)ethynyl)phenyl)ethynyl)pyridine) (neutral bromo-nonamer) (**19**) An oven dried Schlenk flask (100 mL) was charged with **4** (0.141 g, 0.161 mmol, 0.45 eq.), bis(triphenylphosphine)palladium(II) dichloride (0.0149g, 0.0212 mmol, 0.06 eq.), and copper(I) iodide (0.0067 g, 0.0351 mmol, 0.1 eq.). The Schlenk flask was evacuated/backfilled with nitrogen three times. A nitrogen sparged solution of **5** (0.118 g, 0.353 mmol, 1 eq.), Et_3N (1.0 mL, 7.06 mmol, 20 eq.), and THF (29 mL) was transferred to the Schlenk flask via cannula. The reaction was allowed to stir under nitrogen in a 50 °C oil bath for 24 h. The solution was concentrated under reduced pressure, and the residue was purified by flash column chromatography (SiO_2, 35% EtOAc/hexanes → 7.5% MeOH/EtOAc, R_f = 0.27 with 35% EtOAc/hexanes) to give a white solid (0.124 g, 61%). All efforts to remove traces of hydrocarbon grease from **19** were unsuccessful. Multiple flash chromatographic and reversed-phase preparatory HPLC separations were attempted. With either method, traces of hydrocarbon grease invariably coeluted with **19** due to its high retention and lipophilicity. Hexanes extractions only resulted in hexanes contamination. Recrystallizations also failed. However this contamination was removed in the subsequent step. Mp = 146–150 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.64 (s, 2H), 8.63 (s, 2H), 8.61 (s, 2H), 7.76 (t, *J* = 1.24 Hz, 2H), 7.69 (t, *J* = 1.44 Hz, 2H), 7.65 (d, *J* = 1.44 Hz, 4H), 7.56–7.52 (m, 4H), 7.48 (dt, *J* = 8.88, 2.08 Hz, 4H), 7.37 (t, *J* = 7.92 Hz, 2H), 6.89 (dt, *J* = 8.88, 2.04 Hz, 4H), 3.84 (s, 6H), 1.39 (s, 18H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.00, 152.30, 151.42, 151.36, 137.75, 134.76, 133.30, 132.36, 132.30, 131.26, 129.97, 128.75, 124.41, 123.34–123.19, 122.52, 122.50, 122.48, 115.07, 114.21, 96.76, 96.69, 96.66, 90.62, 87.14, 85.31, 85.16, 85.13, 55.47, 35.02, 31.26. HRMS ($C_{77}H_{53}Br_3N_3O_2$ = $[M+H]^+$): calculated = 1288.1688; found = 1288.1714.

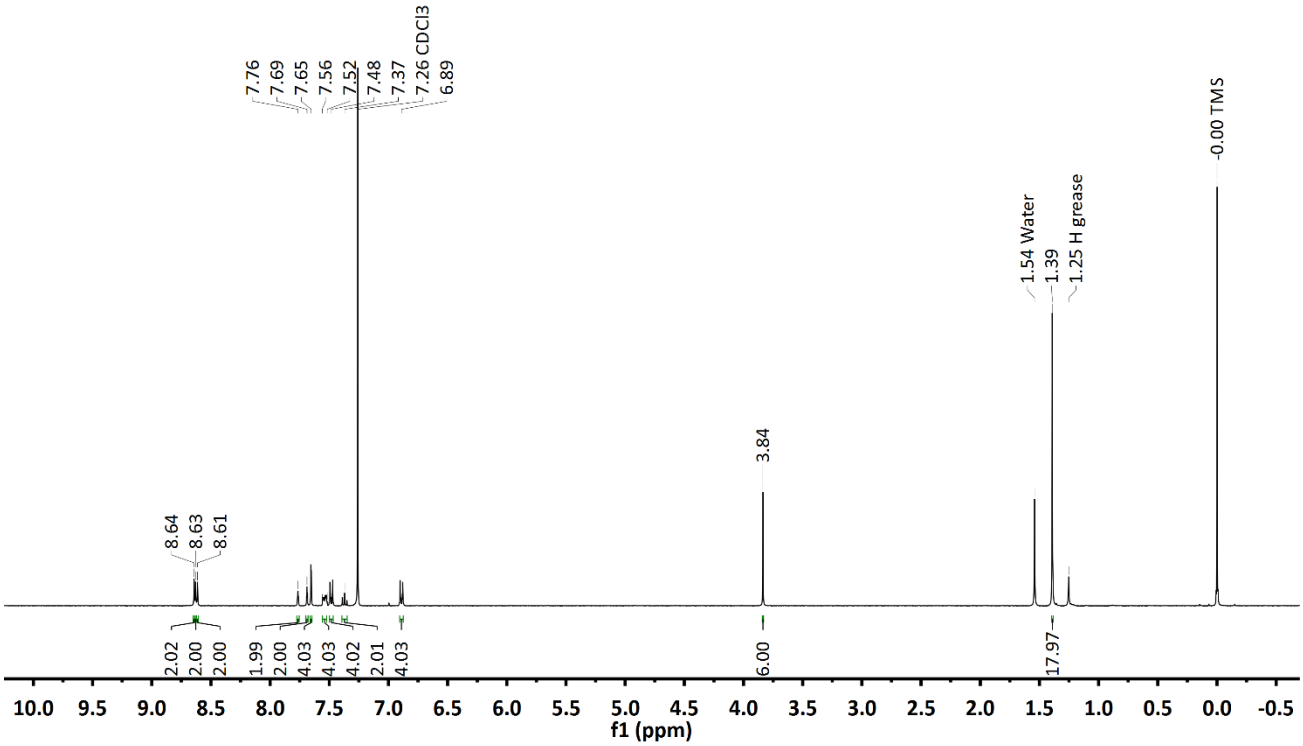


Figure S11. ^{1}H NMR spectrum of **19** (400 MHz, $CDCl_3$, 298 K).

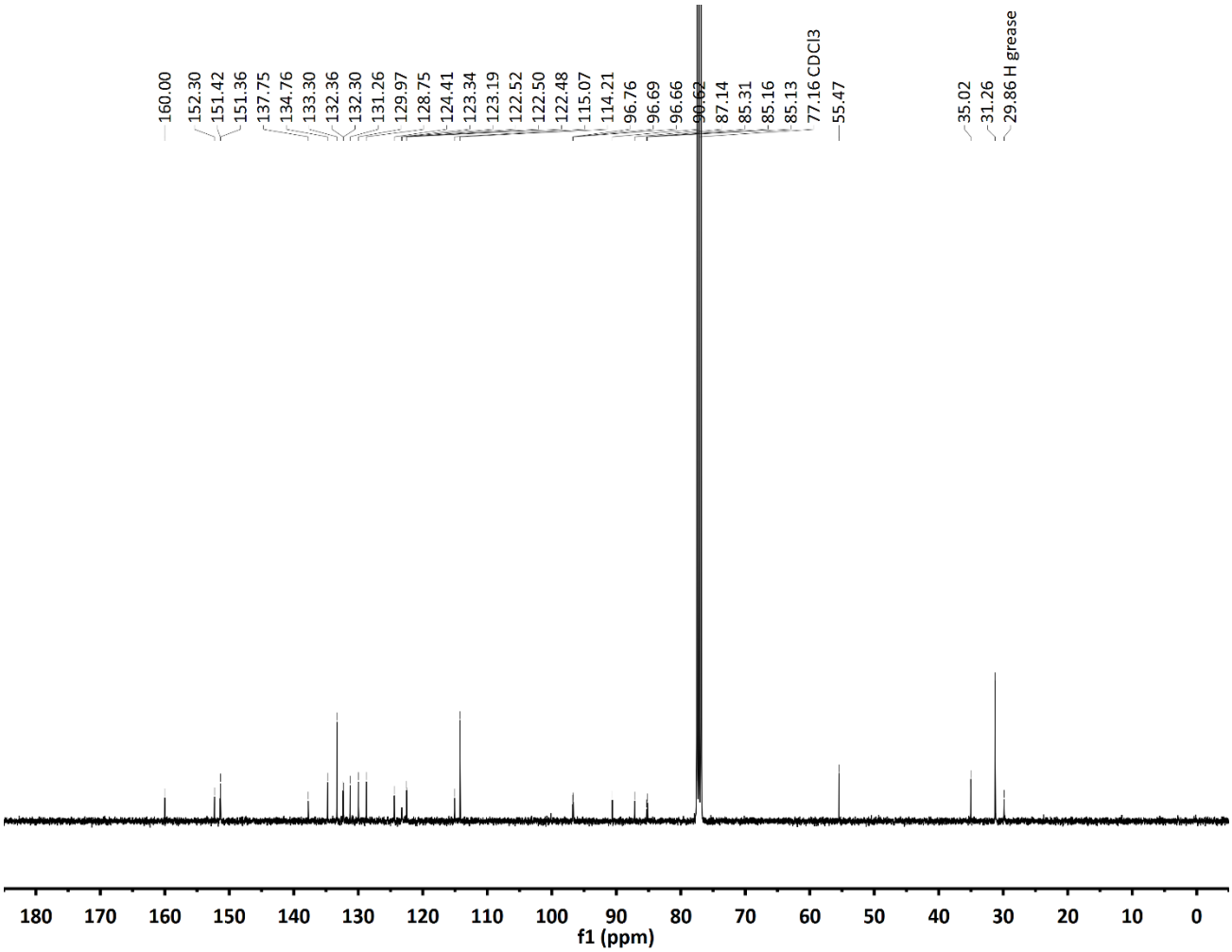
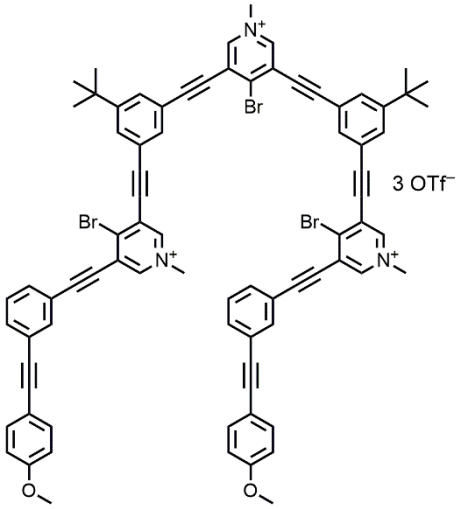


Figure S12. ^{13}C NMR spectrum of **19** (101 MHz, $CDCl_3$, 298 K).



5,5'-((((4-bromo-1-methylpyridine-1-ium-3,5-diyl)bis(ethyne-2,1-diyl))bis(3-(tert-butyl)-5,1-phenylene))bis(ethyne-2,1-diyl))bis(4-bromo-3-((3-((4-methoxyphenyl)ethynyl)phenyl)ethynyl)-1-methylpyridin-1-ium) trifluoromethanesulfonate (charged bromo-nonamer) (**6**) An oven dried round bottom flask was charged with **19** (0.300 g, 0.232 mmol, 1 eq.) and anhydrous DCM (60 mL). The headspace was purged with nitrogen, and methyl trifluoromethanesulfonate (0.105 mL, 0.930 mmol, 4 eq.) was added via syringe. The reaction was allowed to stir under nitrogen at RT for 12 h. The solution was filtered, and the solid was rinsed with anhydrous DCM to give a pale yellow powder (0.387 g, 93%). Due to the instability of **6** in solution, ^{1}H NMR samples were prepared in a nitrogen-filled glovebox (for glovebox details, see Section S1). ^{13}C NMR spectroscopic data could not be collected on account of peak broadening at high concentration (37 mM), consistent with nonspecific aggregation (see Figures S14–15). Furthermore, the instability of **6** precluded ^{13}C spectroscopic data collection at lower concentration. Mp = 210 °C with decomposition. ^{1}H NMR (400 MHz, 1:4 v/v [D_7]DMF-CD_3CN) δ 9.19 (s, 2H), 9.17 (s, 2H), 9.15 (s, 2H), 7.98 (d, *J* = 1.53 Hz, 4H), 7.92 (t, *J* = 1.48 Hz, 2H), 7.90 (t, *J* = 1.4 Hz, 2H), 7.79–7.73 (m, 4H), 7.65–7.59 (m, 6H), 7.07 (d, *J* = 8.92 Hz, 4H), 4.48 (s, 3H), 4.47 (s, 6H), 3.92 (s, 6H), 1.50 (s, 18H). ^{19}F NMR (376 MHz, 1:4 v/v [D_7]DMF-CD_3CN) δ -79.69. ESI-MS ($C_{80}H_{61}Br_3N_3O_2$ = $[M]^{3+}$): 444.10; ($C_{81}H_{61}Br_3F_3N_3O_5S$ = $[M+OTf^-]^{2+}$): 740.62.

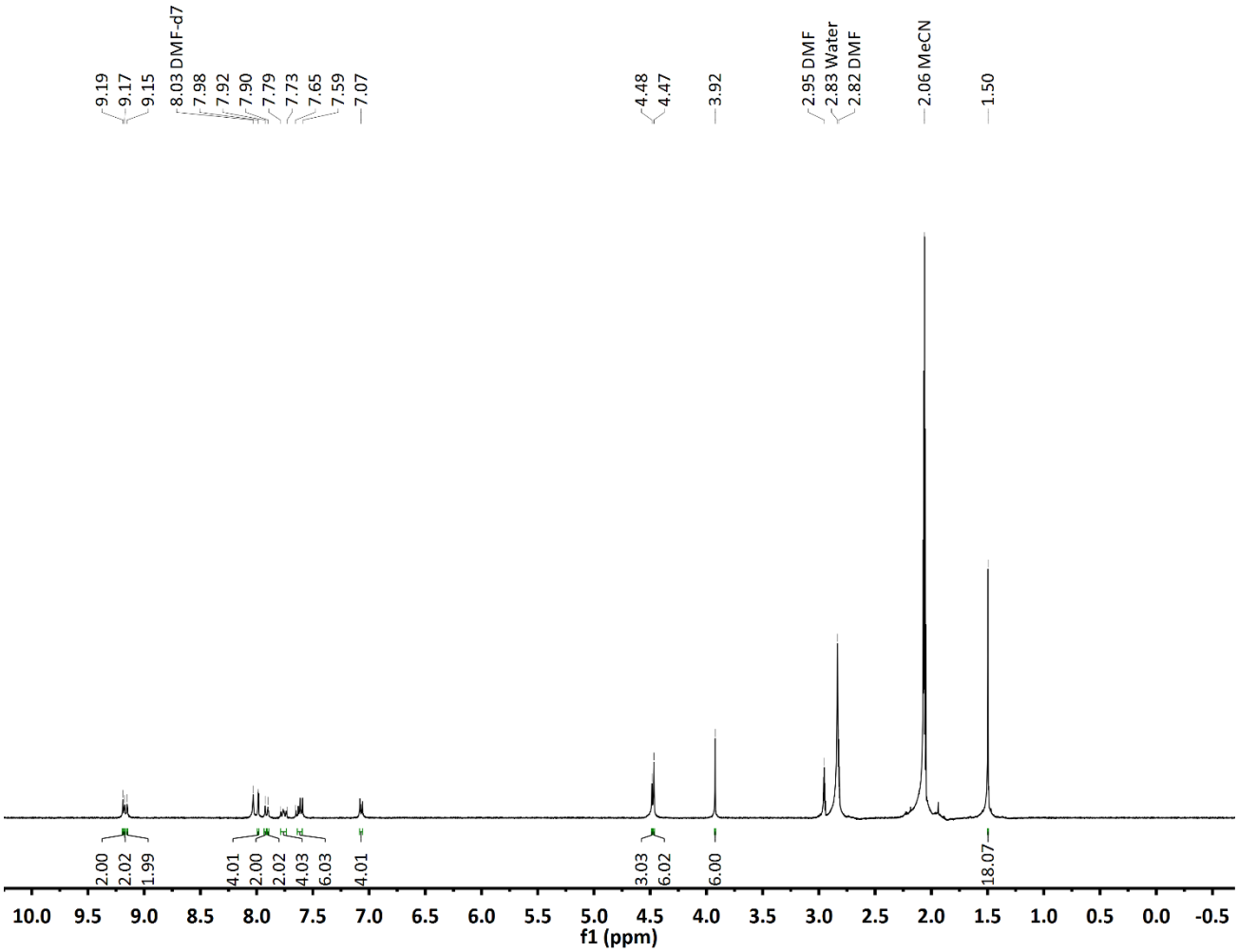


Figure S13. ^{1}H NMR spectrum of **6** (600 MHz, 1:4 v/v [D_7]DMF-CD_3CN, 298 K).

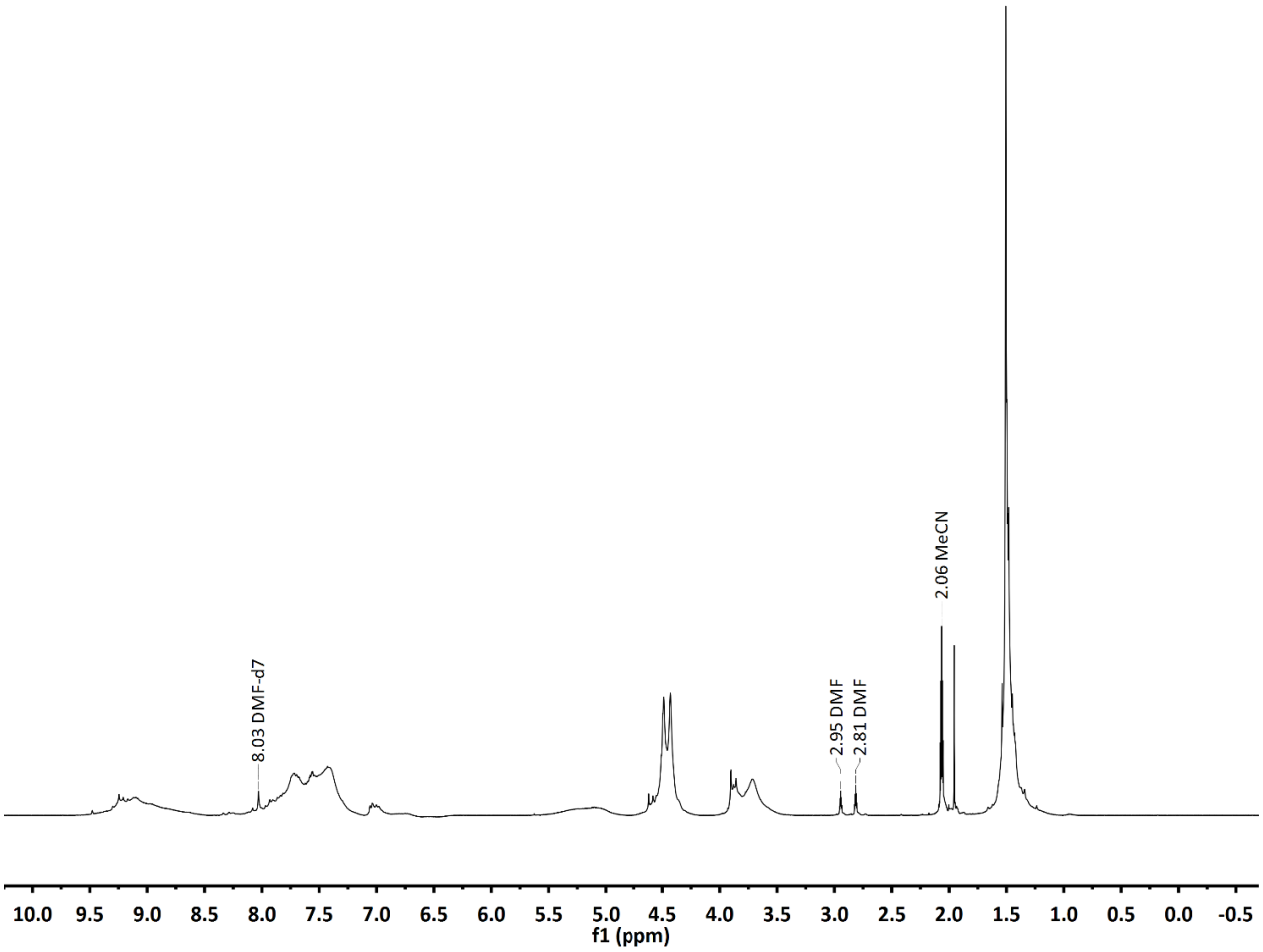


Figure S14. ^{1}H NMR spectrum of **6** at high concentration (37 mM, 400 MHz, 1:4 v/v [D_7]DMF-CD_3CN, 298 K).

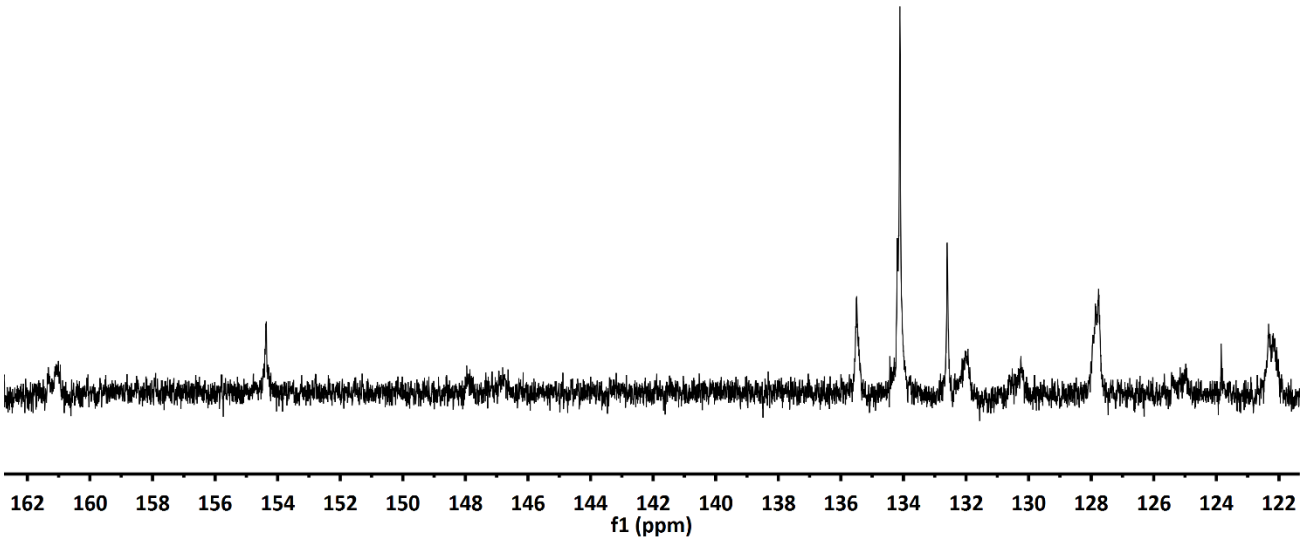


Figure S15. Portion of ^{13}C NMR spectrum of **6** (37 mM, 101 MHz, 1:4 v/v [D_7]DMF-CD_3CN, 298 K).

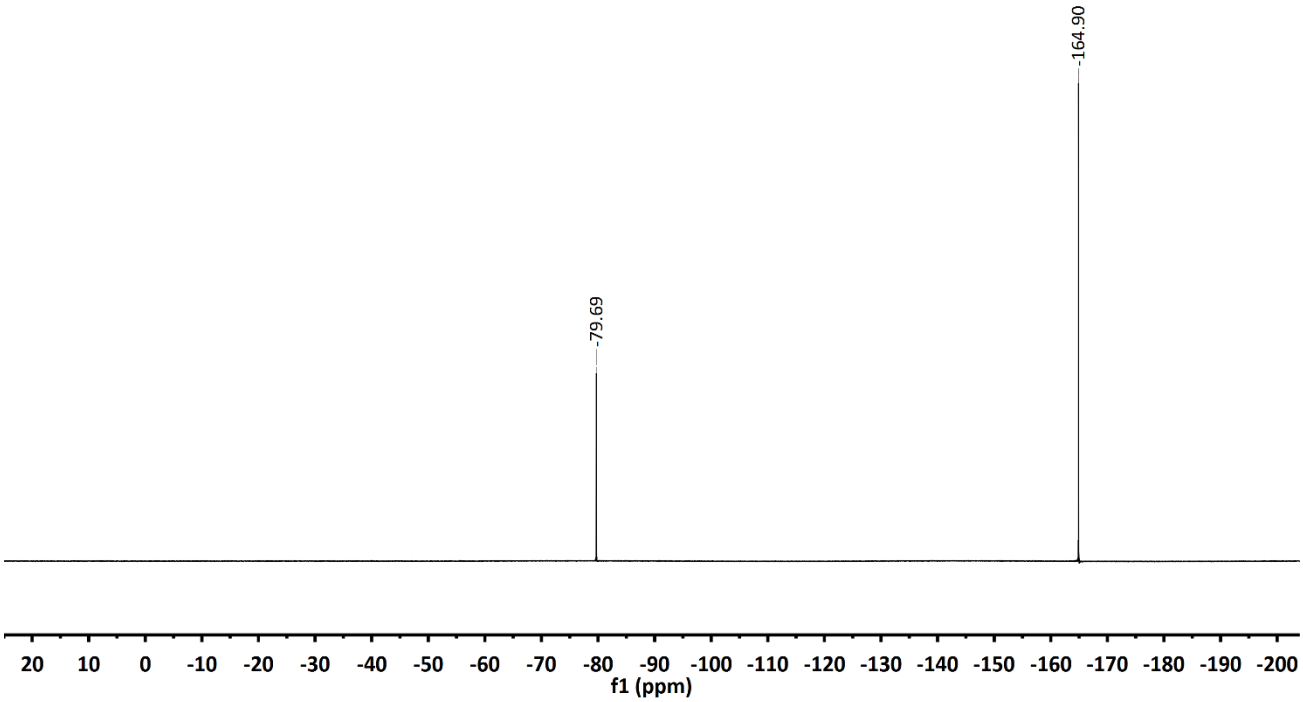
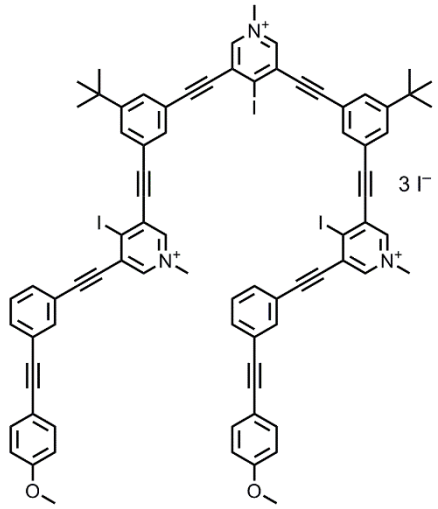


Figure S16. ^{19}F NMR spectrum of **6** (376 MHz, 1:4 v/v [D_7]DMF-CD_3CN, 298 K).



5,5'-((((4-iodo-1-methylpyridine-1-ium-3,5-diyl)bis(ethyne-2,1-diyl))bis(3-(tert-butyl)-5,1-phenylene))bis(ethyne-2,1-diyl))bis(4-iodo-3-((3-((4-methoxyphenyl)ethynyl)phenyl)ethynyl)-1-methylpyridin-1-ium) iodide (charged iodide iodo-nonamer) (**7**) A round bottom flask (100 mL) was charged with **6** (0.0530 g, 0.0297mmol, 1 eq.), sodium iodide (0.134 g, 0.892 mmol, 30 eq.), DMF (12.5 mL), and MeCN (37.5 mL). The solution was allowed to stir for 12 h under nitrogen. The solution was concentrated under reduced pressure. The residue was suspended in water (50 mL) with the help of sonication and was filtered. The solid was rinsed with water (50 mL) and diethyl ether (50 mL) and allowed to dry on vacuum to give a yellow solid (0.050 g, 90%). A ^{1}H NMR spectrum was collected at RT (298 K), but the best peak resolution was seen at 341 K. Therefore, the latter was integrated. Mp = 192 °C with decomposition. ^{1}H NMR (400 MHz, 1:3 v/v [D_7]DMF-CD_3CN) δ 9.55 (s), 9.44 (s), 9.41 (s), 9.21 (s), 9.02 (s), 8.23 (s), 8.19 (s), 8.08 (s), 8.02 (s), 7.97 (s), 7.92 (s), 7.75 (t, *J* = 1.48 Hz), 7.71 (s), 7.58 (t, *J* = 1.56 Hz), 7.56 (t, *J* = 1.80 Hz), 7.53 (s), 7.51 (t, *J* = 1.60 Hz), 7.50 (t, *J* = 1.40 Hz), 7.46–7.43 (m), 7.39–7.24 (m), 7.05 (dt, *J* = 3.88, 1.32 Hz), 6.99–6.94 (m), 6.59–6.52 (m), 4.48–4.41 (m), 4.36 (s), 3.59 (s), 3.54 (s), 3.52 (s), 1.60 (s), 1.56 (d, *J* = 2.56 Hz). ^{1}H NMR (500 MHz, 1:4 v/v [D_7]DMF-CD_3CN, 341 K) δ 9.56 (s, 2H), 9.46 (s, 2H), 9.39 (s, 2H), 9.26 (s, 2H), 9.06 (s, 2H), 8.09 (s, 2H), 8.00 (s, 2H), 7.95 (s, 2H), 7.91 (s, 2H), 7.88 (s, 2H), 7.76 (s, 2H), 7.73 (s, 2H), 7.70 (s, 2H), 7.61 (s, 2H), 7.57 (s, 4H), 7.54–7.49 (m, 6H), 7.45 (d, *J* = 7.73 Hz, 4H), 7.41–7.26 (m, 24H), 7.07 (d, *J* = 6.2 Hz, 2H), 6.98 (t, *J* = 7.65 Hz, 4H) , 6.57 (s, 12H), 4.48 (s, 3H), 4.43 (s, 12H), 4.40 (s, 6H), 4.34 (s, 6H), 3.61 (s, 6H), 3.57 (s, 6H), 3.53 (s, 6H), 1.61 (s, 18H), 1.57 (d, *J* = 4.8 H, 36H). ^{13}C NMR (101 MHz, 1:3 v/v [D_7]DMF-CD_3CN) δ 160.83, 160.79, 160.57, 154.42, 153.98, 153.55, 153.44, 145.62–145.36, 143.72–143.45, 134.35, 134.25, 134.22, 133.51–129.59, 124.39, 124.33, 124.05, 123.60, 123.57, 123.11, 123.03–122.31, 115.61–115.26, 115.04, 100.89–100.39, 100.06, 99.84, 99.65, 99.45, 99.22, 99.17, 99.09, 98.83, 92.57, 92.42, 91.92, 90.29–89.18, 88.70, 88.47, 88.15, 87.98, 87.78, 87.57, 87.30, 56.40–56.22, 55.91, 55.81, 55.79, 49.41–48.50, 32.52, 32.29, 32.04, 31.52. HRMS ($C_{80}H_{61}I_4N_3O_2$ = $[M+I^-]^{2+}$): calculated = 801.5466; found = 801.5433.

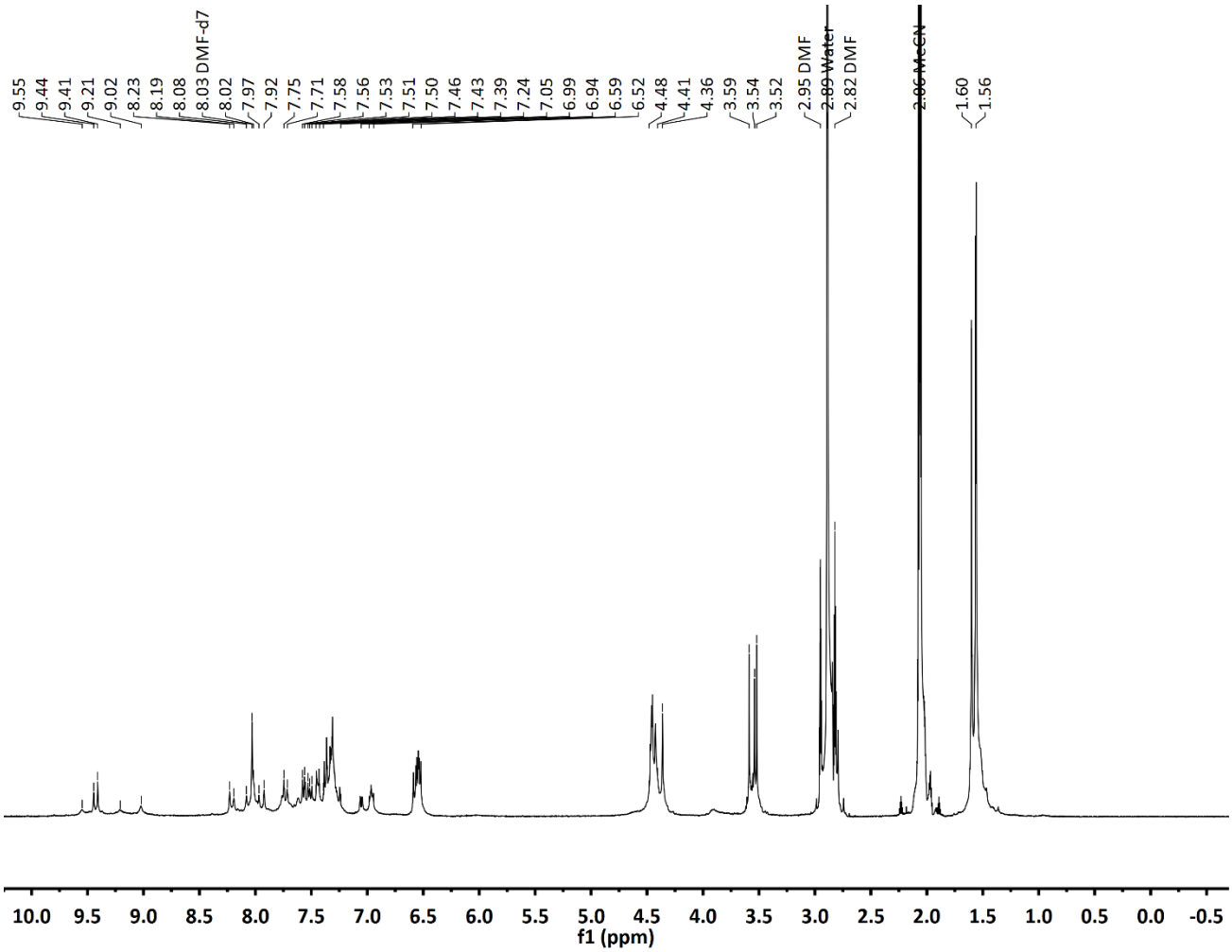


Figure S17. ^{1}H NMR spectrum of **7** (400 MHz, 1:3 v/v [D_7]DMF-CD_3CN, 298 K).

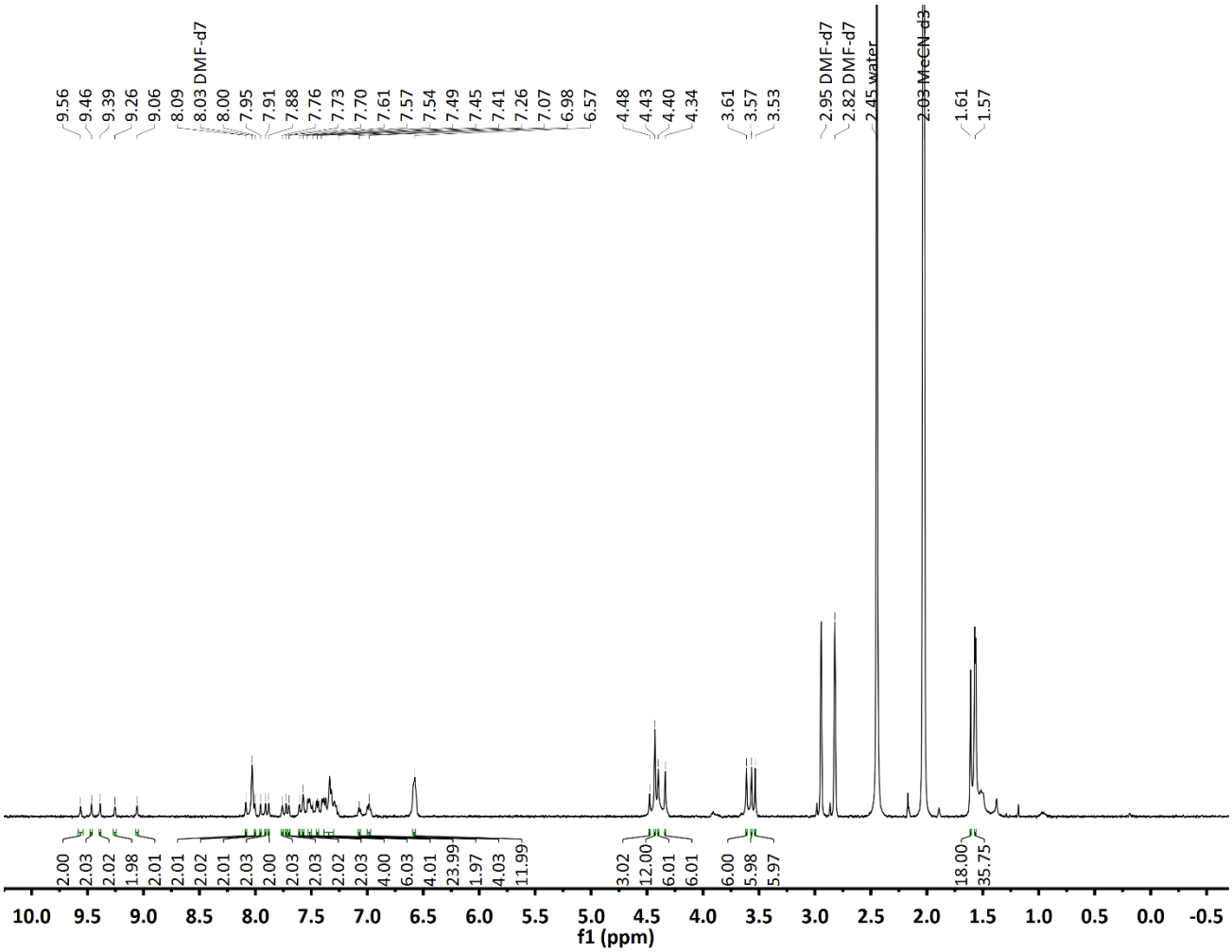


Figure S18. ^{1}H NMR spectrum of **7** (500 MHz, 1:4 v/v [D_7]DMF-CD_3CN, 341 K).

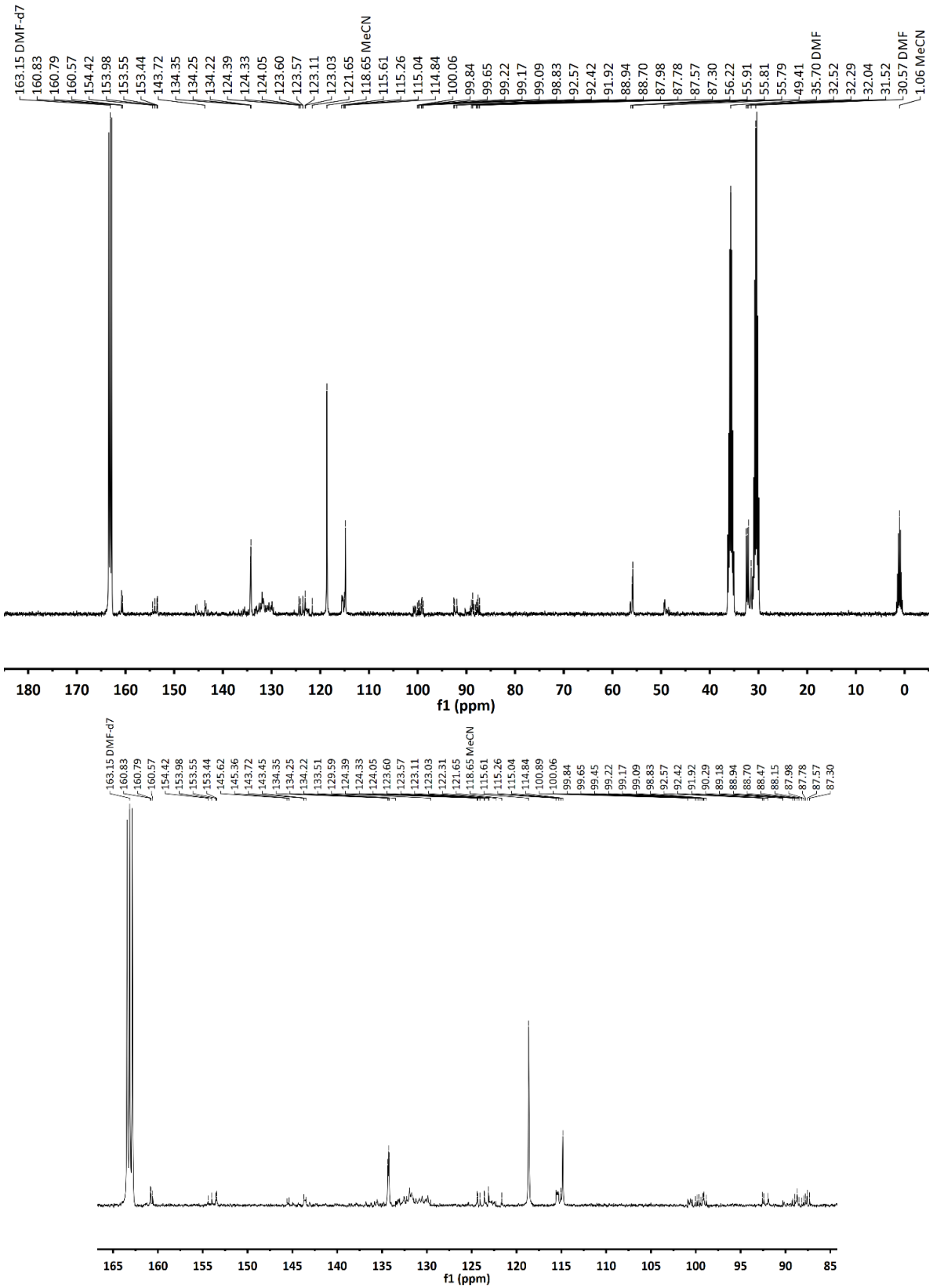
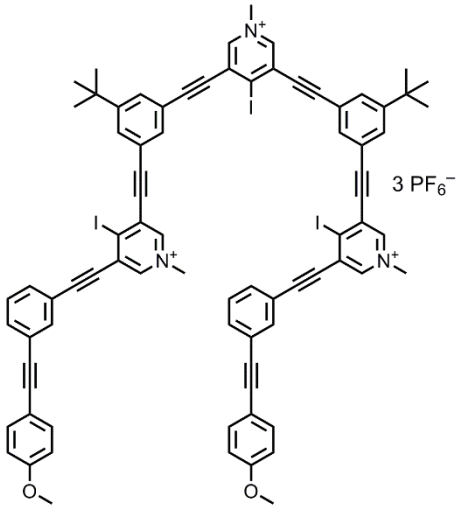


Figure S19. ^{13}C NMR spectrum of **7** with downfield portion of spectrum (101 MHz, 1:3 v/v $[D_7]$DMF-CD_3CN, 298 K).



5,5'-((((4-iodo-1-methylpyridine-1-ium-3,5-diyl)bis(ethyne-2,1-diyl))bis(3-(tert-butyl)-5,1-phenylene))bis(ethyne-2,1-diyl))bis(4-iodo-3-((3-((4-methoxyphenyl)ethynyl)phenyl)ethynyl)-1-methylpyridin-1-ium) hexafluorophosphate(V) (charged hexafluorophosphate iodo-nonamer) (**8**) A flame dried round bottom flask (25 mL) was charged with **7** (0.0150 g, 0.0081 mmol, 1 eq.), silver(I) hexafluorophosphate (0.0082 g, 0.0323 mmol), and an anhydrous mixture of 1:1 v/v DMF-EtOAc (5 mL). The solution was allowed to stir under nitrogen for 30 min. The cloudy mixture was filtered through a fine filter (0.2 μm), and the solid was rinsed with dry DMF (10 mL), diethyl ether (10 mL), and hexanes (10 mL). After rinsing, residual hexanes could not be removed from **8** even after drying *in vacuo* and recrystallizations. The filtrate was concentrated under reduced pressure, and the residue was recrystallized by the vapor diffusion of dry diethyl ether into a 1:1 v/v DMF-MeCN solution of **8**. The resulting beige powder was dried under vacuum to give the product (0.0152 g, 80%). ^{13}C NMR spectroscopic data could not be collected for the same reasons described for compound **6**. Mp = 112 °C with decomposition. ^{1}H NMR (600 MHz, 1:3 v/v [D_7]DMF-CD_3CN) δ 9.03 (s, 2H), 9.01 (s, 2H) 8.98 (s, 2H), 7.98 (d, *J* = 3.42 Hz, 4H), 7.93 (s, 2H), 7.89 (s, 2H), 7.76 (d, *J* = 7.62 Hz, 2H), 7.73 (d, *J* = 7.86 Hz, 2H), 7.62 (t, *J* = 7.92 Hz, 2H), 7.59 (d, *J* = 8.28 Hz, 4H), 7.06 (d, *J* = 8.28 Hz, 4H), 4.44 (s, 3H), 4.42 (s, 6H), 3.92 (s, 6H), 1.50 (s, 18H). ^{19}F NMR (376 MHz, 1:3 v/v [D_7]DMF-CD_3CN) δ -72.17, -74.05. ESI-MS ($C_{80}H_{61}I_3N_3O_2$ = $[M]^{3+}$): 492.34; ($C_{80}H_{61}F_6I_3N_3O_2P$ = $[M+PF_6^-]^{2+}$): 810.45.

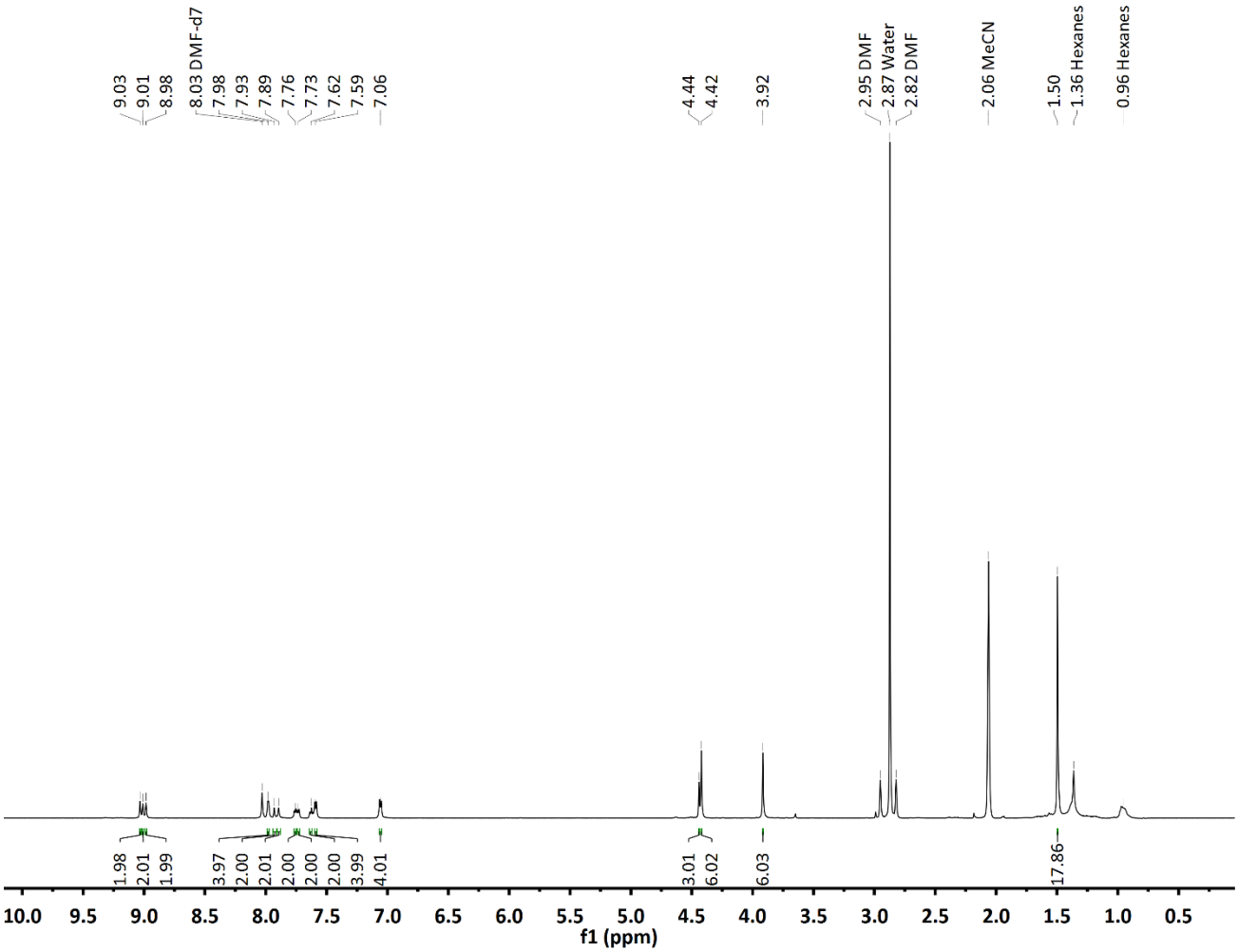


Figure S20. ^{1}H NMR spectrum of **8** (400 MHz, 1:3 v/v [D_7]DMF-CD_3CN, 298 K).

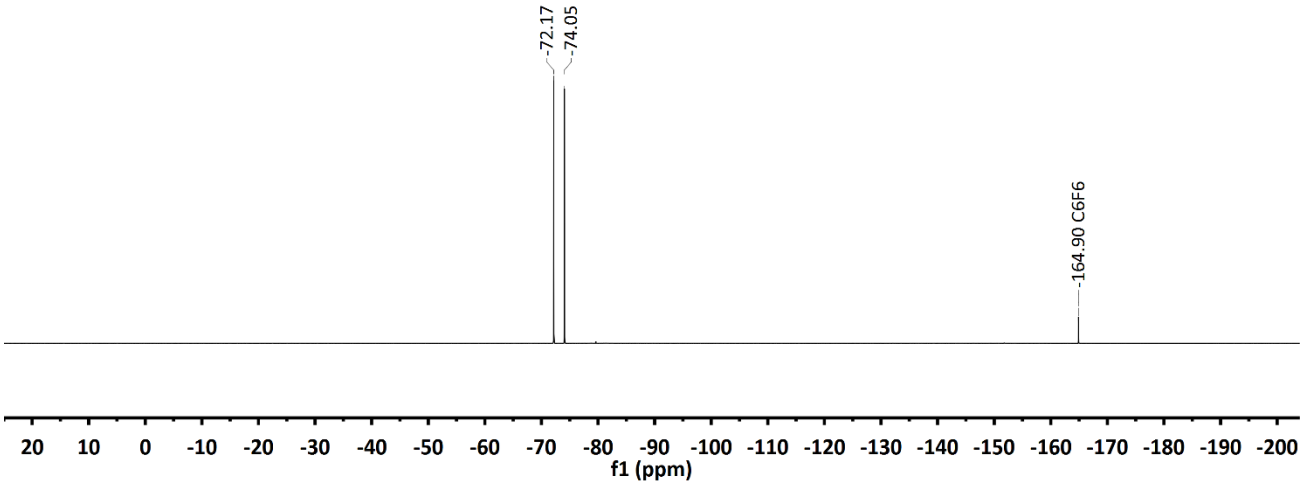


Figure S21. ^{19}F NMR spectrum of **8** (376 MHz, 1:3 v/v [D_7]DMF-CD_3CN, 298 K).

S4. Solid-state structure of the triple helicate

General refinement information

X-ray diffraction data for **7** were collected at 100 K on a Bruker D8 Venture using Cu$K\alpha$ (λ = 1.54178) radiation. Data have been corrected for absorption using SADABS[9] area detector absorption correction program. Using Olex2,[10] the structure was solved with the ShelXT[11] structure solution program using Direct Methods and refined with the ShelXL[12] refinement package using least squares minimization. Hydrogen atoms were placed in calculated positions using a ridged group model and refined with isotropic thermal parameters. The majority of non-hydrogen atoms were refined with anisotropic thermal displacement parameters (see below discussion for further details). The structure was found to contain indistinguishable solvent molecules within the lattice voids. Attempts at modeling this solvent were not able to produce a suitable model. The SQUEEZE[13] routine within PLATON[14] was utilized to account for the residual, diffuse electron density, and the model was refined against these data. A total of 4425 electrons per unit cell were corrected for. All calculations and refinements were carried out using APEX2,[15] SHELXTL,[16] Olex2, and PLATON.

Detailed refinement discussion

The initial solution had a significant resemblance to the predicted nonamer. After initial refinement the main chains were fully established and identification of the anisole rings and *tert*-butyl groups from the difference map were possible. The anisole rings required geometric restraints as refinement lacking these restraints led to chemically unreasonable rings. The use of displacement parameter restraints (RIGU, SIUM, ISOR) were employed as the locations of the anisole rings lend themselves to multiple positions or thermal motion, as illustrated by elongated ellipsoid shapes. The anisole methoxy groups required bond length and angle restraints (1,3-distances) (DFIX 1.37(2) for O-C(sp^2) and O-C(sp^3) 1.42(2) and DANG 2.39(4)). Additionally a few of these methoxy groups were refined isotropically, as the anisotropic displacement parameters were unreasonable even with the use of displacement restraints. A number of the *tert*-butyl groups were also refined isotropically. The difference map and the anisotropic displacement parameters indicate possible positional disorder of the *tert*-butyl carbons. Attempts at modeling the disorder over a number of positions were unsuccessful. Given these results it was decided to model a few of the more troublesome tert-butyl groups isotropically. Distance and angle restraints have also been placed on *tert*-butyl groups (DFIX 1.54(2) and DANG 2.68(4)). Upon initial refinement, the location of 7 of the 9 iodide atoms were located from the difference map. The other iodide atoms were subsequently identified, one of which was modeled as having disorder over two positions with site occupancy factors refined using a free variable. Use of displacement parameter restraints, RIGU and SIMU, for the main chain (not including the anisole rings, *tert*-butyl groups and the iodine atoms) were applied.

Crystallographic Data for **7** $C_{80}H_{61}I_6N_3O_2$, M = 1857.71, monoclinic, space group *C*2/*c* (no. 15), *a* = 54.1200(19), *b* = 36.8537(14), *c* = 35.419(2), β = 128.1810(10), *V* = 55530(5), *Z* = 24, *T* = 100 K, μ(Cu$K\alpha$) = 16.102 mm^{-1}, D_{calc} = 1.333 g ml^{-1}, $2\theta_{max}$ = 101.124, 291827 reflections collected, 29038 unique (R_{int} = 0.0668, R_{sigma} = 0.0322), R1 = 0.0837 ($I > 2\sigma(I)$), wR2 = 0.2858 (all data).

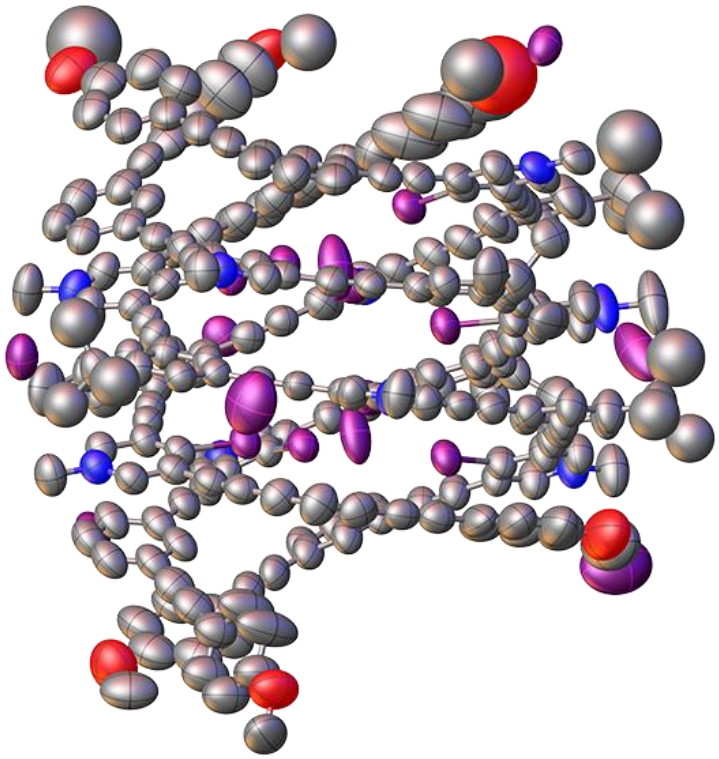


Figure S22. Thermal ellipsoidal representation of triple helicate **7** (at 50% probability; hydrogen atoms omitted for clarity).

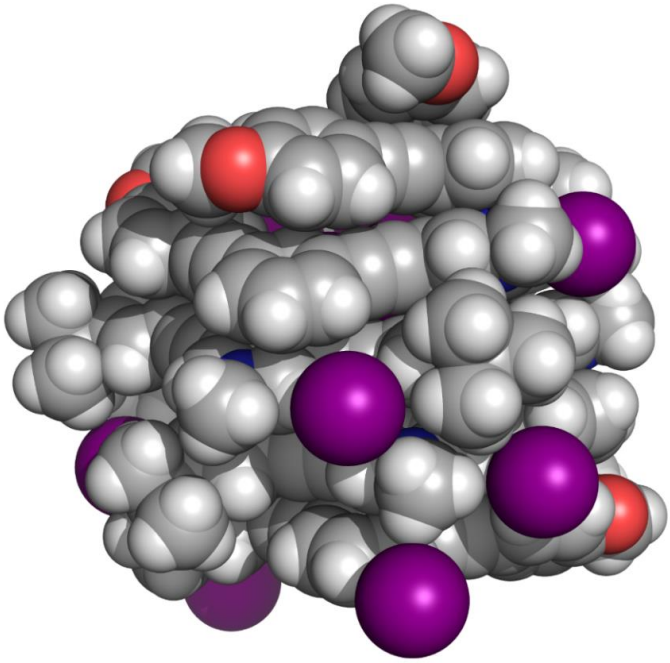


Figure S23. Solid-state space-filling representation of the extrachannel space of **7**. Six of the total of seven extrachannel iodide counteranions are visible.

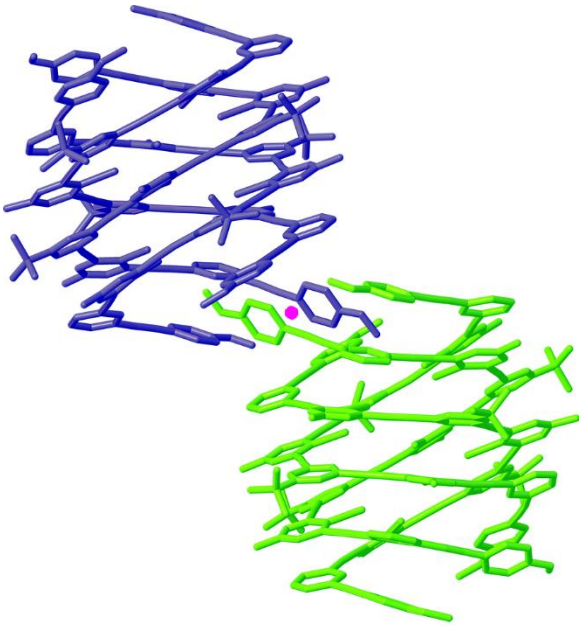


Figure S24. Solid-state stick representation of enantiomers of **7**. An intriguing inversion center (pink sphere) is sandwiched by two extra-channel anisole rings.

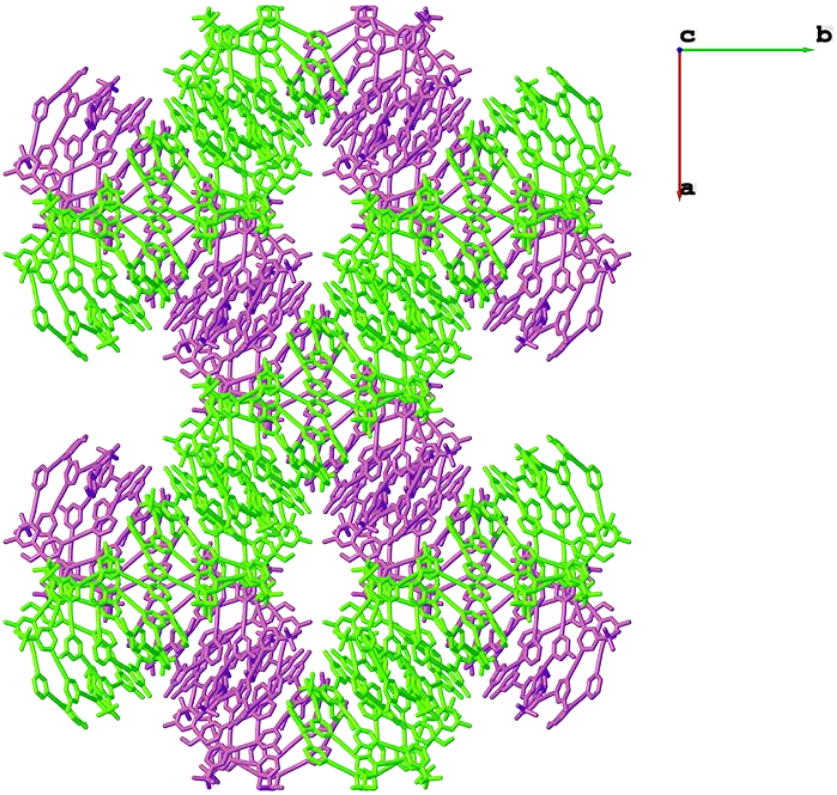


Figure S25. Crystal packing of **7** viewed down the crystallographic *c* axis. Triplex dimers proliferate end-on-end. A set of parallel columns (purple) stacks orthogonally to the other set (green).

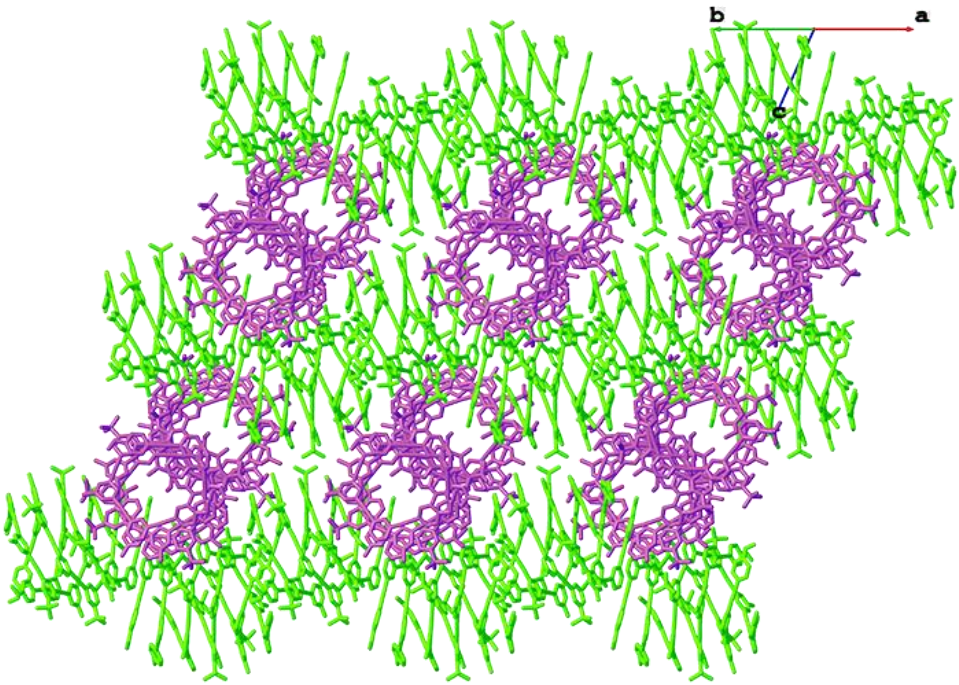


Figure S26. Crystal packing of **7** viewed along the [110] direction. Triplex dimers (green) proliferate end-on-end. Orthogonally stacked dimers (purple) are seen down their anion channels.

S5. DFT calculations of 1:1 binding

All DFT calculations were performed using the Gaussian 09 suite.[2] We performed a geometry optimization on the scaffold of **7** without iodide at the B98 level, using the LANL2DZ basis set for all atoms with effective core potential(ECP) for iodine. Single point energy calculations were carried out with iodide in two binding arrangements. In the first experiment, we calculated the energy of tridentate binding and in the second the energy of bidentate binding. These calculations were also at the B98 level, using the 6-31+G(d,p) basis set for non-halogen atoms C, O, N, H, and LANL2DZ with ECP for iodine and the iodide anion augmented with diffuse functions of p-symmetry and polarization functions of d-symmetry downloaded from the EMSL Basis Set Exchange.[17] This method takes into account the large polarizability of the covalently bonded iodines on the receptor and accurately models the "σ-hole". We began the conformational search from an MM2-minimized folded position. Due to long run times, an exhaustive conformational search was not conducted.

DFT minimization of a single strand of 7

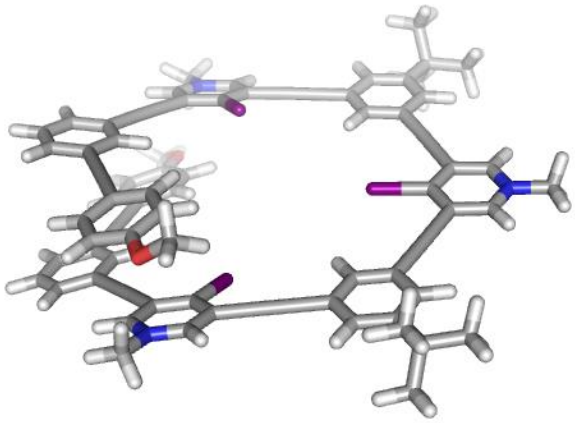


Figure S27. DFT-minimized single strand of **7** sans iodide.

SCF Done: E(RB98) = -3430.97540643 A.U. after 1 cycles
Convg = 0.2805D-08 -V/T = 2.0137

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	53	0.002231598	-0.000513591	-0.001695230
2	53	0.000574764	0.001018462	0.002422171
3	53	-0.002755753	-0.000651001	-0.000424034
4	6	0.003551069	0.002688850	0.000913389
5	6	-0.002891622	0.001236914	0.003690681
6	6	-0.003449003	-0.002243652	-0.000790780
7	6	0.000392625	-0.000292203	-0.000710834
8	6	-0.000516788	-0.000992563	-0.001258051
9	1	-0.001089783	-0.001705827	-0.002243033
10	6	-0.000946375	-0.000347659	-0.000014014
11	6	-0.001293536	0.000436684	0.001544661
12	1	-0.001662456	0.000789678	0.002226635

13	6	0.000834506	0.001305689	0.001668341
14	1	0.001042274	0.001706468	0.002225410
15	6	0.001998422	0.000539407	-0.000145961
16	1	0.002678445	0.000901423	-0.000065255
17	6	-0.000748329	-0.000432332	-0.000430776
18	6	-0.000354099	-0.000737012	-0.001741051
19	1	-0.000684182	-0.001421862	-0.002385681
20	6	0.003281445	-0.001457506	-0.001315806
21	6	0.001390973	0.000782616	0.000025171
22	1	0.002585017	0.001257901	0.000409527
23	6	0.000264879	0.000638866	0.000785872
24	6	-0.001052125	0.000001165	0.001278126
25	1	-0.001927763	0.000001178	0.002187748
26	6	-0.004986429	-0.001589950	0.000301582
27	6	-0.003194573	-0.000057936	0.002574530
28	6	0.000191901	-0.000025633	-0.000017057
29	1	0.000604760	-0.000200266	0.002714823
30	1	-0.001055982	0.002659965	-0.000390010
31	1	-0.002337055	-0.001902814	-0.000352411
32	6	0.000549266	0.000011014	-0.000718181
33	6	0.001567728	0.000711350	0.000305338
34	1	0.002542309	0.001284564	0.000587733
35	6	0.000101522	0.000061186	0.001019898
36	6	-0.000868717	-0.000063403	0.001107889
37	1	-0.001769826	-0.000194130	0.002153258
38	6	0.000066000	-0.000191242	-0.000131293
39	6	0.014196873	-0.005103961	-0.001460636
40	6	-0.000071978	-0.000500873	-0.001526773
41	1	-0.000244741	-0.000762075	-0.002415710
42	6	0.000441703	0.000627747	0.001773396
43	1	0.000336882	0.001063927	0.002589882
44	7	-0.001605880	0.000227800	0.001512069
45	6	-0.001609782	-0.000455510	-0.000737689
46	1	-0.002804830	-0.000610956	-0.000859471
47	6	0.000079780	-0.000255934	-0.000470879
48	6	0.001854579	-0.000332027	-0.001319607
49	6	0.000688896	-0.000013335	-0.000080786
50	6	0.000455928	0.000814638	0.002061351
51	6	0.000498070	0.000290654	0.000250077
52	6	0.001224080	0.000210004	-0.001186522
53	1	0.001873969	0.000284769	-0.002220456
54	7	-0.000381146	-0.000887109	-0.001159071
55	6	-0.001583086	-0.000801692	-0.000057941
56	1	-0.002490015	-0.001402029	-0.000494248
57	6	-0.000251064	0.000043954	0.000563092
58	6	-0.002984019	-0.000756475	0.003103417
59	6	0.002721210	0.000653536	-0.002930903
60	6	0.012507234	-0.005585446	-0.001516623
61	6	0.000026617	0.000963394	0.001534315
62	1	0.000110299	0.001465384	0.002598019
63	6	-0.000657169	0.000100564	0.000622735

64	6	-0.001475054	-0.001063011	-0.000628052
65	1	-0.002298837	-0.001592613	-0.000686468
66	6	-0.000236570	-0.001011623	-0.001591414
67	1	-0.000053636	-0.001530362	-0.002487655
68	6	0.001259977	-0.000335534	-0.001117558
69	8	0.004146743	-0.002051822	-0.004127166
70	6	0.001262572	0.001132978	0.000716864
71	1	0.002445195	0.001440836	0.000669443
72	6	-0.000495745	0.000022207	0.000295922
73	6	-0.002097497	-0.000667218	-0.000265309
74	6	-0.000468074	-0.000271268	-0.000566932
75	6	0.001210366	-0.000527009	-0.001533854
76	1	0.002025354	-0.000596097	-0.001916200
77	7	0.001906173	0.000852735	0.000491903
78	6	0.000326751	0.000777207	0.001373103
79	1	0.000938177	0.001382436	0.002491576
80	6	-0.004498761	-0.001351789	-0.001359005
81	6	0.003167851	0.000032630	-0.002558591
82	6	0.001281784	0.000434284	-0.000051970
83	6	0.008789560	-0.005313595	-0.011442466
84	6	-0.000347192	-0.001455922	-0.002129045
85	1	-0.001430490	-0.001692382	-0.001990596
86	6	-0.001911518	-0.000799208	-0.000220986
87	6	-0.000917940	0.000803118	0.001616272
88	1	-0.001406048	0.001140154	0.002395872
89	6	0.000715825	0.001227159	0.001264874
90	1	0.001283180	0.001771609	0.002037446
91	6	0.004670380	0.001387437	0.001808306
92	8	0.001679162	-0.004083864	-0.003996075
93	6	-0.000276237	-0.000529828	-0.001557958
94	1	-0.000356913	-0.000854941	-0.002708716
95	6	-0.000860128	-0.000301183	-0.000264077
96	6	-0.001544257	-0.000023469	0.001173313
97	1	-0.002200075	-0.000014823	0.001813191
98	6	0.000320201	0.000644289	0.002029040
99	1	0.000386428	0.000836164	0.002738343
100	6	0.001691594	0.000554797	0.000544637
101	1	0.002595059	0.000842001	0.000917203
102	6	0.000756662	0.000027525	-0.000488982
103	6	0.002553415	-0.001145389	-0.003573262
104	6	0.004846259	0.001262064	-0.000489571
105	6	-0.000208915	0.000281305	-0.000095792
106	1	0.000504411	0.001469503	0.002460939
107	1	0.001926636	-0.002611166	0.000267380
108	1	0.001159438	0.001641325	-0.002190746
109	6	-0.000674705	-0.000699834	-0.004288766
110	6	0.000664997	0.000890655	0.003840767
111	6	0.000906013	0.002089657	0.003767648
112	6	-0.000962714	-0.002382649	-0.004000553
113	6	0.005290268	0.000164688	-0.001443328
114	1	-0.000576419	-0.003030832	0.000239283

115	1	-0.002358307	0.001614410	-0.002775889
116	1	-0.003122612	0.000009421	0.000065346
117	6	-0.001923138	0.003847546	0.002775872
118	6	-0.002125158	0.001005351	0.000638874
119	6	-0.000187756	-0.000089942	0.000010355
120	6	0.000270567	0.000092494	-0.000283241
121	6	-0.000772224	-0.000035630	0.000726382
122	1	0.002329190	0.000042810	-0.002533858
123	1	-0.000663254	-0.003323118	0.000512046
124	1	-0.002753919	0.001309829	-0.001448273
125	1	0.001265547	0.001883904	0.002484302
126	1	0.002366113	0.000324720	-0.002508238
127	1	-0.002740584	0.001713165	-0.001167925
128	1	0.001474311	0.001536430	0.002756016
129	1	-0.000385648	-0.003273576	0.000912907
130	1	0.002301100	0.000043267	-0.002438919
131	6	-0.003473107	0.000780464	0.000165361
132	6	-0.007080307	0.001986745	0.000680153
133	6	-0.003837623	0.000614205	0.000230798
134	1	0.000087907	0.000606012	0.003288634
135	1	0.002547111	-0.001323098	-0.001358851
136	1	-0.003103968	-0.002540965	0.000287841
137	1	-0.000077151	0.002783175	-0.001846649
138	1	-0.000265894	0.001089005	0.002951227
139	1	-0.004100110	-0.000170594	-0.000117554
140	1	-0.000034545	0.002440349	-0.002386777
141	1	-0.003120900	-0.001793500	-0.001665952
142	1	0.002392224	-0.001959886	0.000255077
143	1	-0.006477279	0.003608074	0.008222531
144	1	-0.000041934	-0.002478169	0.002160198
145	1	-0.002104600	-0.000061133	-0.002478069
146	1	0.003086462	0.001092013	-0.000791461
147	1	-0.002959181	0.009586803	0.000224506
148	1	-0.002207628	0.001024778	0.006192030
149	1	-0.012813928	-0.001448436	-0.000405397

Single point energy calculation of tridentate XBing

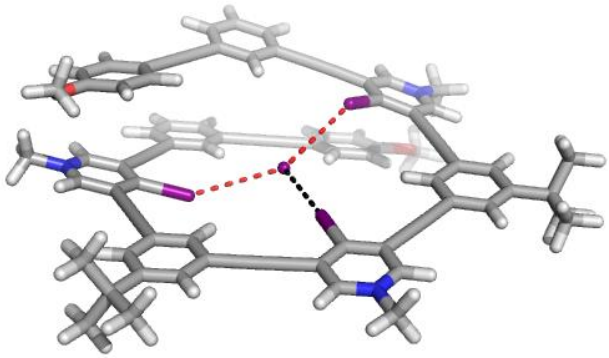


Figure S28. Single point energy calculation of a single strand of **7** with iodide. The DFT-minimized conformation of a single strand of **7** was used in this calculation. Black dashes represent an energetically favorable XB. Red dashes represent a nonbonding or repulsive interaction. The C–I···I⁻ angles are 179° (black dashes), 141°, and 146° (red dashes).

SCF Done: E(RB98) = -3443.27471508 A.U. after 50 cycles
Convg = 0.4787D-08 -V/T = 2.0179

I	-3.3793	-0.2712	1.7721
I	0.5474	4.2413	-0.0793
I	3.1079	-1.3837	-1.5052
C	4.3441	5.3114	-0.5362
C	2.597	-5.3765	-1.5734
C	3.3415	6.0255	-0.4549
C	1.4303	-6.1838	-1.8082
C	0.1432	-5.5812	-1.8829
H	0.0412	-4.5019	-1.7612
C	-1.0091	-6.3772	-2.1224
C	-0.8543	-7.7888	-2.2856
H	-1.7361	-8.4024	-2.4763
C	0.423	-8.3855	-2.2105
H	0.5254	-9.4634	-2.3434
C	1.567	-7.5955	-1.9721
H	2.5553	-8.0547	-1.9206
C	5.5081	4.4686	-0.616
C	6.8133	5.0482	-0.6564
H	6.8998	6.1338	-0.6313
C	7.9777	4.2452	-0.727
C	7.8024	2.8346	-0.7556
H	8.6736	2.1801	-0.8134
C	6.5104	2.2372	-0.7183
C	5.3541	3.0592	-0.6492
H	4.3601	2.6115	-0.6232
C	-3.4578	-5.3206	-2.3104
C	0.9606	-5.4186	2.4942
C	-9.2964	-2.3324	0.3675
H	-9.5132	-3.2459	0.9349
H	-9.3203	-2.5382	-0.7142

H	-10.0323	-1.5637	0.6347
C	-4.125	5.8994	0.3388
C	-4.3497	4.5054	0.4708
H	-3.512	3.8073	0.4648
C	-5.6805	4.0284	0.6054
C	-6.7662	4.9493	0.6112
H	-7.7784	4.5566	0.7179
C	-6.5612	6.3507	0.4855
C	-7.7822	7.3119	0.5016
C	-5.2275	6.8076	0.3487
H	-5.0227	7.8722	0.246
C	-6.9504	-2.7526	1.0504
H	-7.2305	-3.8031	1.0613
N	-7.9193	-1.8449	0.7338
C	-7.6439	-0.5071	0.669
H	-8.4587	0.16	0.3969
C	-6.3448	-0.0078	0.9429
C	-5.3166	-0.9446	1.2981
C	-5.6204	-2.3483	1.3407
C	0.8512	6.318	-0.1964
C	2.1766	6.8467	-0.3608
C	2.3313	8.2572	-0.4343
H	3.3133	8.7075	-0.5591
N	1.2555	9.0958	-0.3523
C	-0.0146	8.6103	-0.1962
H	-0.8235	9.3357	-0.1384
C	-0.2686	7.2174	-0.113
C	-2.7799	6.388	0.1867
C	-1.6162	6.7728	0.048
C	-9.8095	-4.0072	-3.4749
C	4.5572	-5.7364	2.4813
H	4.2662	-6.7806	2.3541
C	3.5431	-4.7396	2.6198
C	3.9437	-3.3895	2.8366
H	3.1793	-2.622	2.9708
C	5.3086	-3.033	2.8948
H	5.5877	-1.994	3.0763
C	6.2991	-4.035	2.7317
O	7.6777	-3.7695	2.7107
C	5.9198	-5.3886	2.535
H	6.6996	-6.1498	2.4722
C	4.7892	-3.9383	-1.1267
C	4.8444	-2.504	-1.1092
C	6.0919	-1.846	-0.8393
C	7.2374	-2.6464	-0.6055
H	8.2063	-2.2018	-0.3914
N	7.1697	-4.0118	-0.638
C	5.9925	-4.6545	-0.8834
H	6.0036	-5.7415	-0.8853
C	-4.6521	-3.35	1.6403
C	2.1491	-5.0977	2.5539

C	-4.8003	-4.8161	-2.4437
C	-5.0863	-3.4261	-2.2814
C	-6.3998	-2.9411	-2.4167
H	-6.6203	-1.8741	-2.3409
C	-7.4615	-3.8364	-2.7143
C	-7.1971	-5.2187	-2.8941
H	-7.9965	-5.9173	-3.1433
C	-5.876	-5.6968	-2.7585
H	-5.6717	-6.7591	-2.9025
C	-3.8104	-4.2237	1.8676
O	-8.7389	-3.2641	-2.7857
C	-1.4361	-4.8331	2.1956
H	-1.1602	-3.7843	2.0771
C	-2.8037	-5.2187	2.1172
C	-3.1662	-6.5893	2.2779
H	-4.2151	-6.8836	2.2217
C	-2.1636	-7.5533	2.5136
H	-2.4392	-8.6005	2.6449
C	-0.8057	-7.1728	2.5856
H	-0.0344	-7.9218	2.771
C	-0.4263	-5.805	2.4253
C	3.6002	-4.6855	-1.3741
C	-2.3198	-5.7857	-2.2119
C	8.4141	-4.8014	-0.3326
H	8.2202	-5.8642	-0.5178
H	8.668	-4.6444	0.726
H	9.2266	-4.4627	-0.9891
C	-5.9243	2.6139	0.7304
C	-6.1194	1.402	0.842
C	6.2343	-0.4217	-0.7921
C	6.3709	0.8029	-0.7545
C	1.4513	10.5872	-0.4283
H	1.1352	11.0429	0.5196
H	0.8589	10.9927	-1.2611
H	2.4992	10.8134	-0.616
C	8.1791	-2.6298	3.4763
C	9.4059	4.8466	-0.7887
C	9.3964	6.406	-0.7462
C	10.1091	4.3927	-2.116
C	10.2245	4.3238	0.4437
H	10.4342	6.7747	-0.7834
H	8.9437	6.7921	0.1844
H	8.8632	6.8394	-1.6108
H	10.1909	3.2947	-2.1875
H	11.131	4.8055	-2.1544
H	9.5596	4.7545	-3.0019
H	10.3145	3.2239	0.4445
H	9.7552	4.632	1.3938
H	11.2452	4.7403	0.4149
C	-8.5614	7.1589	1.8537
C	-8.7664	6.9443	-0.693

C	-7.3824	8.8092	0.3283
H	-8.9274	6.1296	2.0087
H	-7.9092	7.4229	2.7038
H	-9.4368	7.8294	1.8724
H	-8.2597	7.0496	-1.6678
H	-9.1437	5.9107	-0.6112
H	-9.6397	7.6178	-0.6864
H	-6.8716	8.9937	-0.6335
H	-8.2833	9.4434	0.3477
H	-6.7274	9.1448	1.1518
H	-4.2855	-2.7405	-2.0863
H	7.7745	-2.6496	4.5012
H	7.9265	-1.6721	2.9879
H	9.2684	-2.7568	3.5049
H	-9.497	-4.3374	-4.49
H	-10.1554	-4.8865	-2.8978
H	-10.662	-3.3029	-3.5902
I	0.0723	0.639	0.0673

Single point energy calculation of bidentate XBing

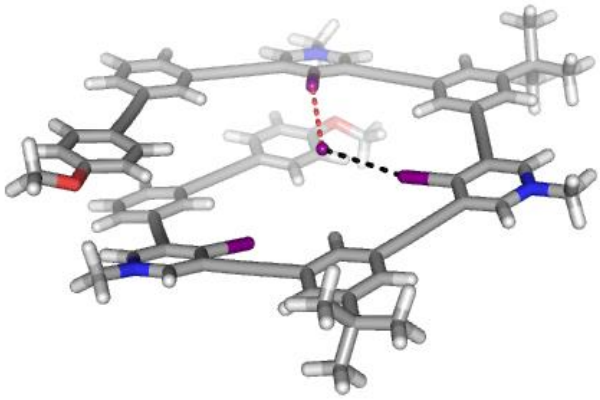


Figure S29. Single point energy calculation of a single strand of **7** with iodide. The DFT-minimized conformation of a single strand of **7** was used in this calculation. Black dashes represent an energetically favorable XB. Red dashes represent a suboptimal interaction. The I···I⁻ distance between the nonbonding XB donor and iodide is 4.6 Å, 113% of ΣvdW radii. The C–I···I⁻ angles are 168° (black dashes), and 152° (red dashes). The I···I⁻ distances were set to 3.5 and 3.6 Å to closely match an unpublished crystal structure of **1** with iodide (Scheme 1). When the C–I···I⁻ angles were set to 160°, the calculation failed to converge.

SCF Done: E(RB98) = -3443.27304780 A.U. after 31 cycles
Convg = 0.6310D-08 -V/T = 2.0179

I	-3.3793	-0.2712	1.7721
I	0.5474	4.2413	-0.0793
I	3.1079	-1.3837	-1.5052
C	4.3441	5.3114	-0.5362
C	2.597	-5.3765	-1.5734
C	3.3415	6.0255	-0.4549
C	1.4303	-6.1838	-1.8082
C	0.1432	-5.5812	-1.8829
H	0.0412	-4.5019	-1.7612
C	-1.0091	-6.3772	-2.1224
C	-0.8543	-7.7888	-2.2856
H	-1.7361	-8.4024	-2.4763
C	0.423	-8.3855	-2.2105
H	0.5254	-9.4634	-2.3434
C	1.567	-7.5955	-1.9721
H	2.5553	-8.0547	-1.9206
C	5.5081	4.4686	-0.616
C	6.8133	5.0482	-0.6564
H	6.8998	6.1338	-0.6313
C	7.9777	4.2452	-0.727
C	7.8024	2.8346	-0.7556
H	8.6736	2.1801	-0.8134
C	6.5104	2.2372	-0.7183
C	5.3541	3.0592	-0.6492
H	4.3601	2.6115	-0.6232

C	-3.4578	-5.3206	-2.3104
C	0.9606	-5.4186	2.4942
C	-9.2964	-2.3324	0.3675
H	-9.5132	-3.2459	0.9349
H	-9.3203	-2.5382	-0.7142
H	-10.0323	-1.5637	0.6347
C	-4.125	5.8994	0.3388
C	-4.3497	4.5054	0.4708
H	-3.512	3.8073	0.4648
C	-5.6805	4.0284	0.6054
C	-6.7662	4.9493	0.6112
H	-7.7784	4.5566	0.7179
C	-6.5612	6.3507	0.4855
C	-7.7822	7.3119	0.5016
C	-5.2275	6.8076	0.3487
H	-5.0227	7.8722	0.246
C	-6.9504	-2.7526	1.0504
H	-7.2305	-3.8031	1.0613
N	-7.9193	-1.8449	0.7338
C	-7.6439	-0.5071	0.669
H	-8.4587	0.16	0.3969
C	-6.3448	-0.0078	0.9429
C	-5.3166	-0.9446	1.2981
C	-5.6204	-2.3483	1.3407
C	0.8512	6.318	-0.1964
C	2.1766	6.8467	-0.3608
C	2.3313	8.2572	-0.4343
H	3.3133	8.7075	-0.5591
N	1.2555	9.0958	-0.3523
C	-0.0146	8.6103	-0.1962
H	-0.8235	9.3357	-0.1384
C	-0.2686	7.2174	-0.113
C	-2.7799	6.388	0.1867
C	-1.6162	6.7728	0.048
C	-9.8095	-4.0072	-3.4749
C	4.5572	-5.7364	2.4813
H	4.2662	-6.7806	2.3541
C	3.5431	-4.7396	2.6198
C	3.9437	-3.3895	2.8366
H	3.1793	-2.622	2.9708
C	5.3086	-3.033	2.8948
H	5.5877	-1.994	3.0763
C	6.2991	-4.035	2.7317
O	7.6777	-3.7695	2.7107
C	5.9198	-5.3886	2.535
H	6.6996	-6.1498	2.4722
C	4.7892	-3.9383	-1.1267
C	4.8444	-2.504	-1.1092
C	6.0919	-1.846	-0.8393
C	7.2374	-2.6464	-0.6055
H	8.2063	-2.2018	-0.3914

N	7.1697	-4.0118	-0.638
C	5.9925	-4.6545	-0.8834
H	6.0036	-5.7415	-0.8853
C	-4.6521	-3.35	1.6403
C	2.1491	-5.0977	2.5539
C	-4.8003	-4.8161	-2.4437
C	-5.0863	-3.4261	-2.2814
C	-6.3998	-2.9411	-2.4167
H	-6.6203	-1.8741	-2.3409
C	-7.4615	-3.8364	-2.7143
C	-7.1971	-5.2187	-2.8941
H	-7.9965	-5.9173	-3.1433
C	-5.876	-5.6968	-2.7585
H	-5.6717	-6.7591	-2.9025
C	-3.8104	-4.2237	1.8676
O	-8.7389	-3.2641	-2.7857
C	-1.4361	-4.8331	2.1956
H	-1.1602	-3.7843	2.0771
C	-2.8037	-5.2187	2.1172
C	-3.1662	-6.5893	2.2779
H	-4.2151	-6.8836	2.2217
C	-2.1636	-7.5533	2.5136
H	-2.4392	-8.6005	2.6449
C	-0.8057	-7.1728	2.5856
H	-0.0344	-7.9218	2.771
C	-0.4263	-5.805	2.4253
C	3.6002	-4.6855	-1.3741
C	-2.3198	-5.7857	-2.2119
C	8.4141	-4.8014	-0.3326
H	8.2202	-5.8642	-0.5178
H	8.668	-4.6444	0.726
H	9.2266	-4.4627	-0.9891
C	-5.9243	2.6139	0.7304
C	-6.1194	1.402	0.842
C	6.2343	-0.4217	-0.7921
C	6.3709	0.8029	-0.7545
C	1.4513	10.5872	-0.4283
H	1.1352	11.0429	0.5196
H	0.8589	10.9927	-1.2611
H	2.4992	10.8134	-0.616
C	8.1791	-2.6298	3.4763
C	9.4059	4.8466	-0.7887
C	9.3964	6.406	-0.7462
C	10.1091	4.3927	-2.116
C	10.2245	4.3238	0.4437
H	10.4342	6.7747	-0.7834
H	8.9437	6.7921	0.1844
H	8.8632	6.8394	-1.6108
H	10.1909	3.2947	-2.1875
H	11.131	4.8055	-2.1544
H	9.5596	4.7545	-3.0019

H	10.3145	3.2239	0.4445
H	9.7552	4.632	1.3938
H	11.2452	4.7403	0.4149
C	-8.5614	7.1589	1.8537
C	-8.7664	6.9443	-0.693
C	-7.3824	8.8092	0.3283
H	-8.9274	6.1296	2.0087
H	-7.9092	7.4229	2.7038
H	-9.4368	7.8294	1.8724
H	-8.2597	7.0496	-1.6678
H	-9.1437	5.9107	-0.6112
H	-9.6397	7.6178	-0.6864
H	-6.8716	8.9937	-0.6335
H	-8.2833	9.4434	0.3477
H	-6.7274	9.1448	1.1518
H	-4.2855	-2.7405	-2.0863
H	7.7745	-2.6496	4.5012
H	7.9265	-1.6721	2.9879
H	9.2684	-2.7568	3.5049
H	-9.497	-4.3374	-4.49
H	-10.1554	-4.8865	-2.8978
H	-10.662	-3.3029	-3.5902
I	0.4466	0.7509	-0.5232

S6. Anion-dependent formation and denaturing of the triple helicate

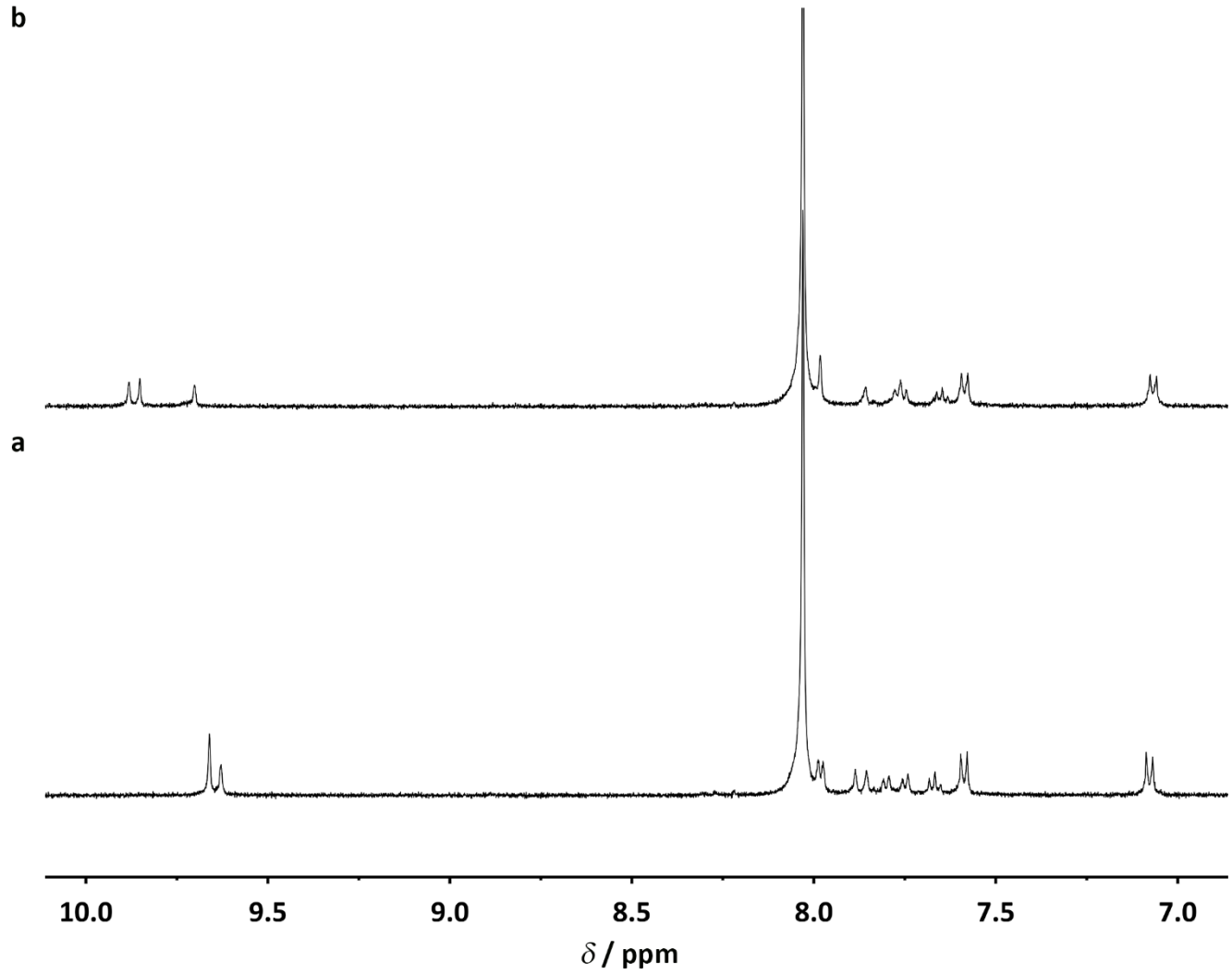


Figure S30. ^{1}H NMR spectroscopic titration. a) ^{1}H NMR spectrum of **6**. b) ^{1}H NMR spectrum of **6** with excess TBA bromide. Conditions for figures (a)–(b): 500 MHz, [D_7]DMF, 298 K.

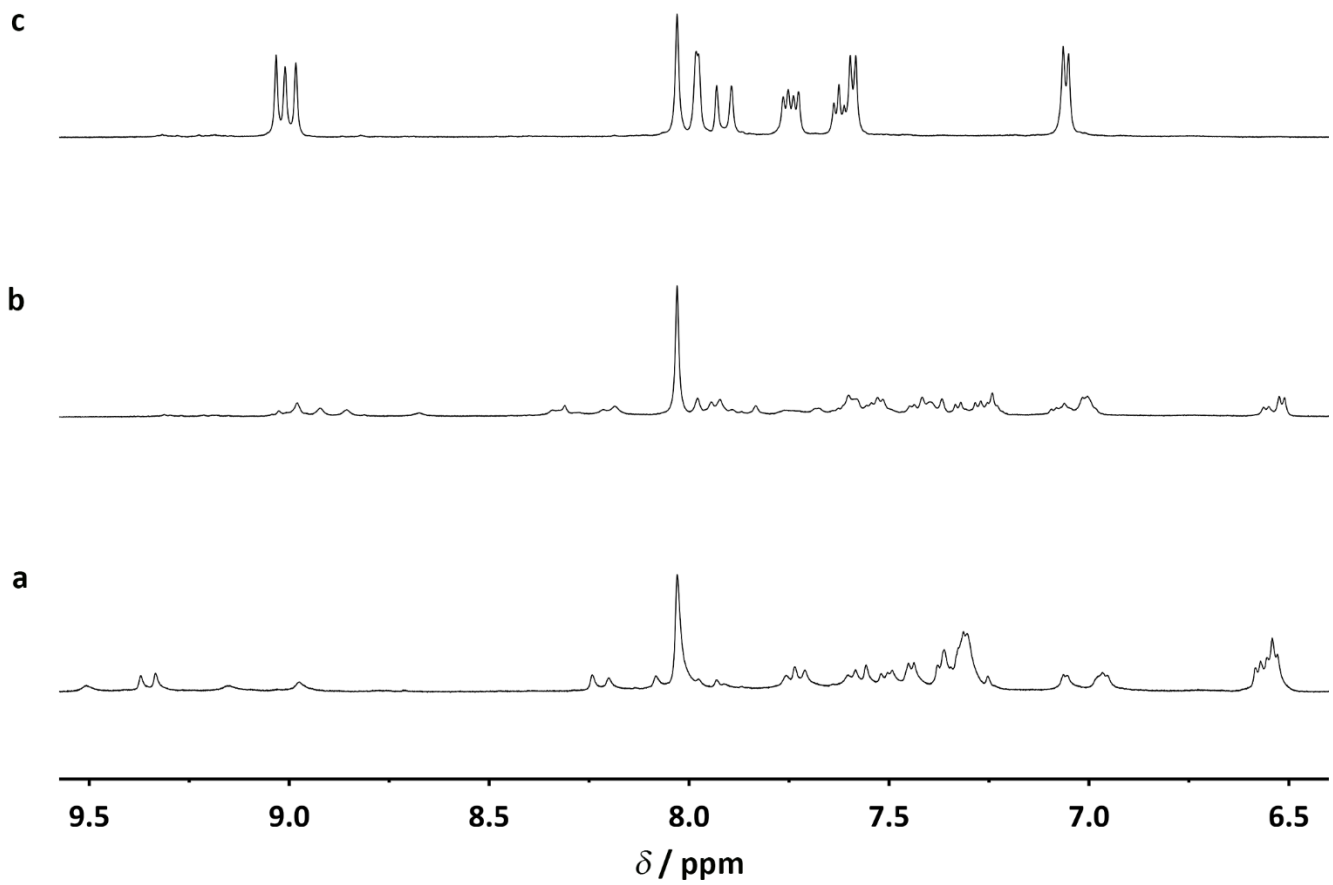


Figure S31. ^{1}H NMR spectroscopic titration. a) ^{1}H NMR spectrum of **7**. b) ^{1}H NMR spectrum of **7** with roughly 1.5 eq. of $AgPF_6$. c) ^{1}H NMR spectrum of **7** with excess $AgPF_6$. Conditions for figures (a)–(c): 600 MHz, 1:3 v/v [D_7]DMF-CD_3CN, 298 K.

S7. Triple helicate proton assignments

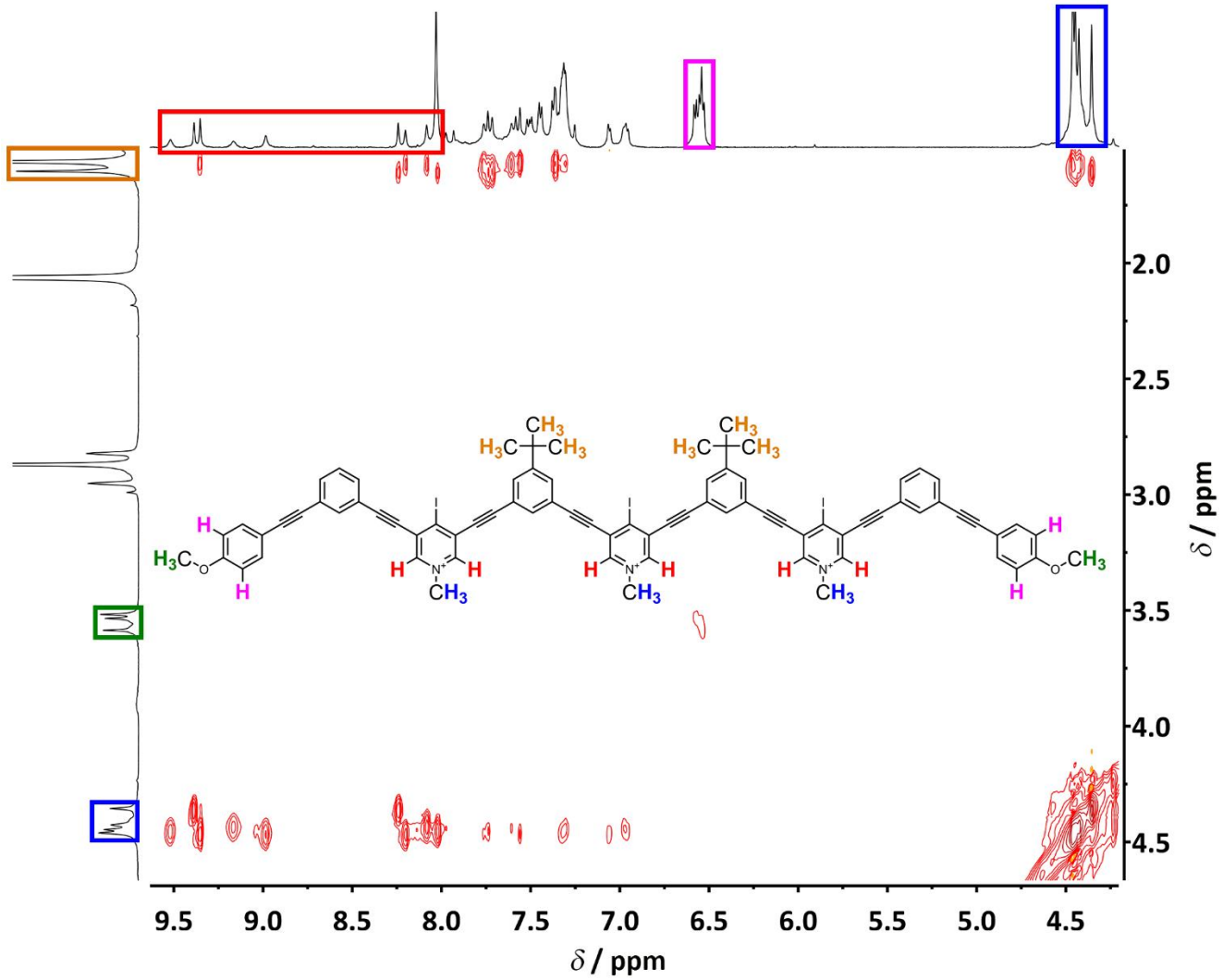


Figure S32. Proton assignments of **7** deduced from chemical shifts and NOEs (600 MHz, 1:3 v/v [D_7]DMF-CD_3CN, 298 K).

S8. 2D NOESY evidence of higher-order helication in solution

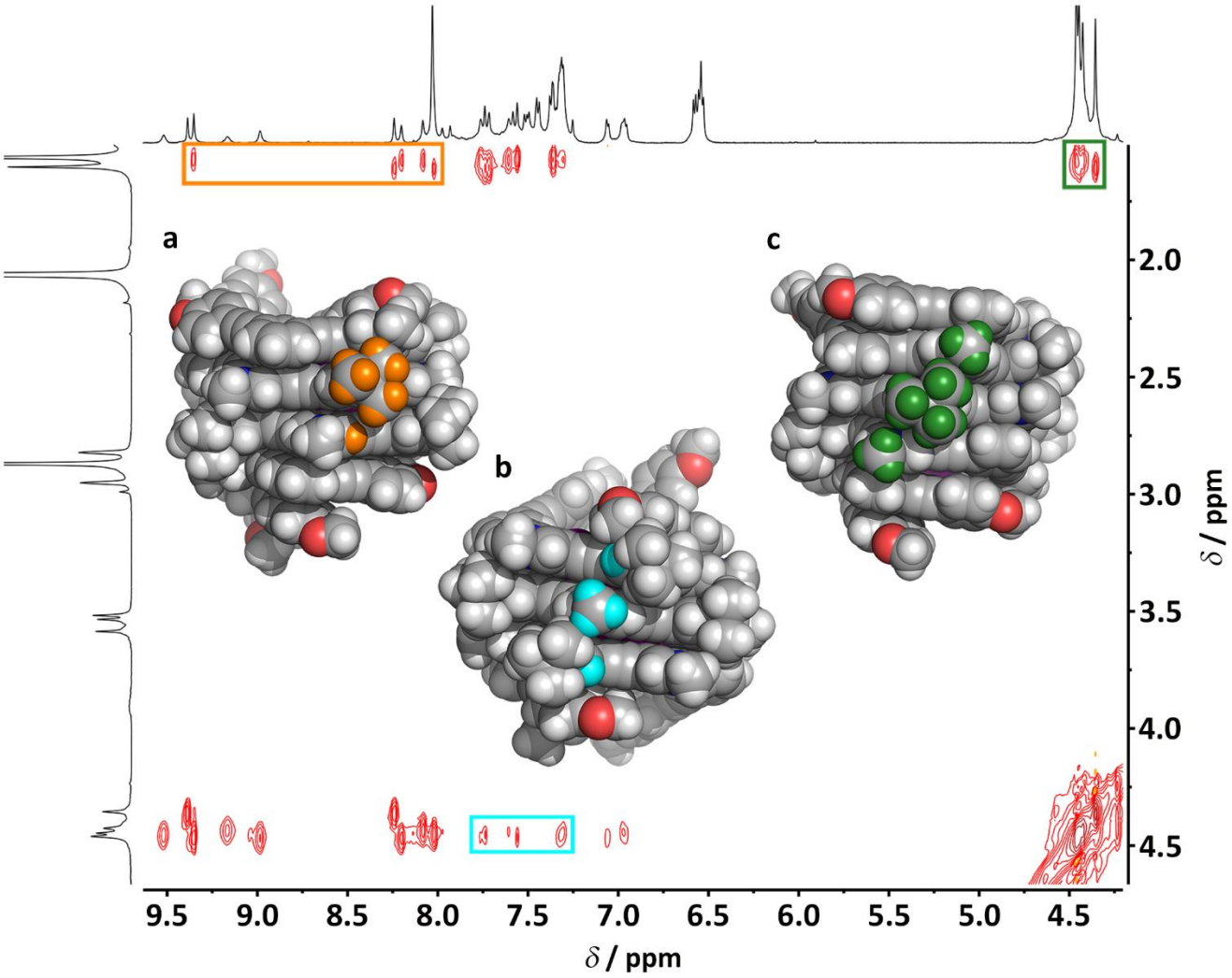


Figure S33. 2D NOESY spectrum of triple helicate **7**. a) *tert*-Butyl and pyridinium cross peaks. b) *tert*-Butylbenzene and pyridinium methyl cross peaks. **c**) Pyridinium methyl and *tert*-butyl cross peaks. Conditions for figures (a)–(c): 600 MHz, 1:3 v/v [D_7]DMF-CD_3CN, 298 K. Not all colors are representative of atom identity.

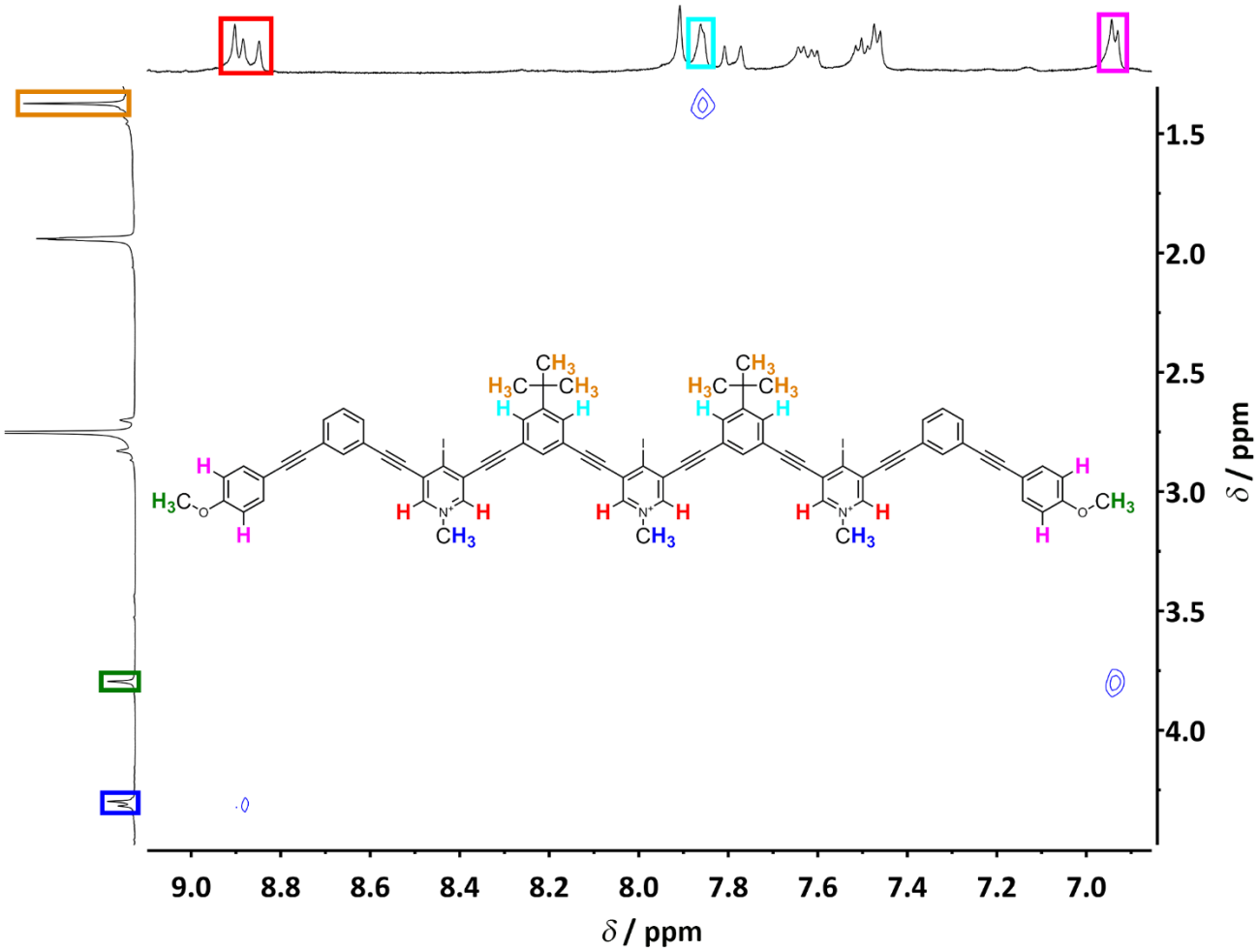


Figure S34. 2D NOESY experiment conducted on **8** (600 MHz, 1:3 v/v [D_7]DMF-CD_3CN, 298 K).

S9. Solution and crystallographic structure analysis

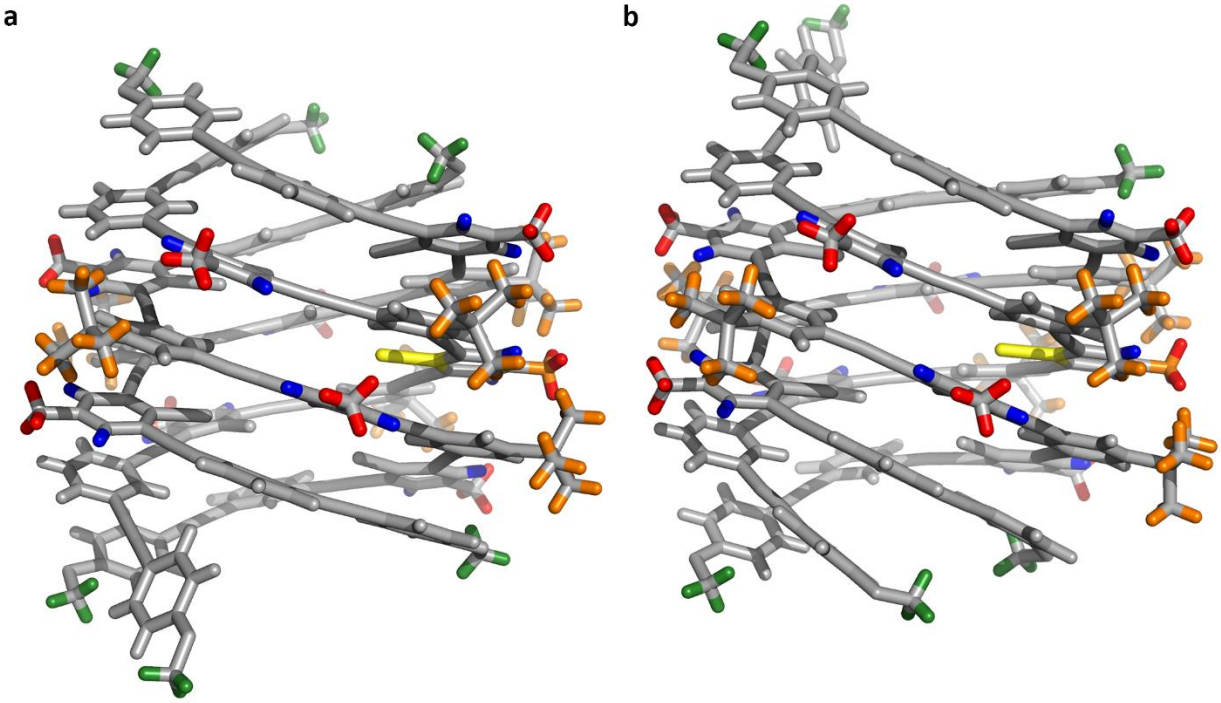


Figure S35. a) Solid-state representation of triple helicate **7** in starting position. b) Triple helicate **7** from Figure (a) after a C_2 operation has been conducted. Figures (a)–(b): yellow sticks represent the C–X bond of the nonbonding iodopyridinium and aligns with the complex's axis of molecular C_2 symmetry. Not all colors are representative of atom identity.

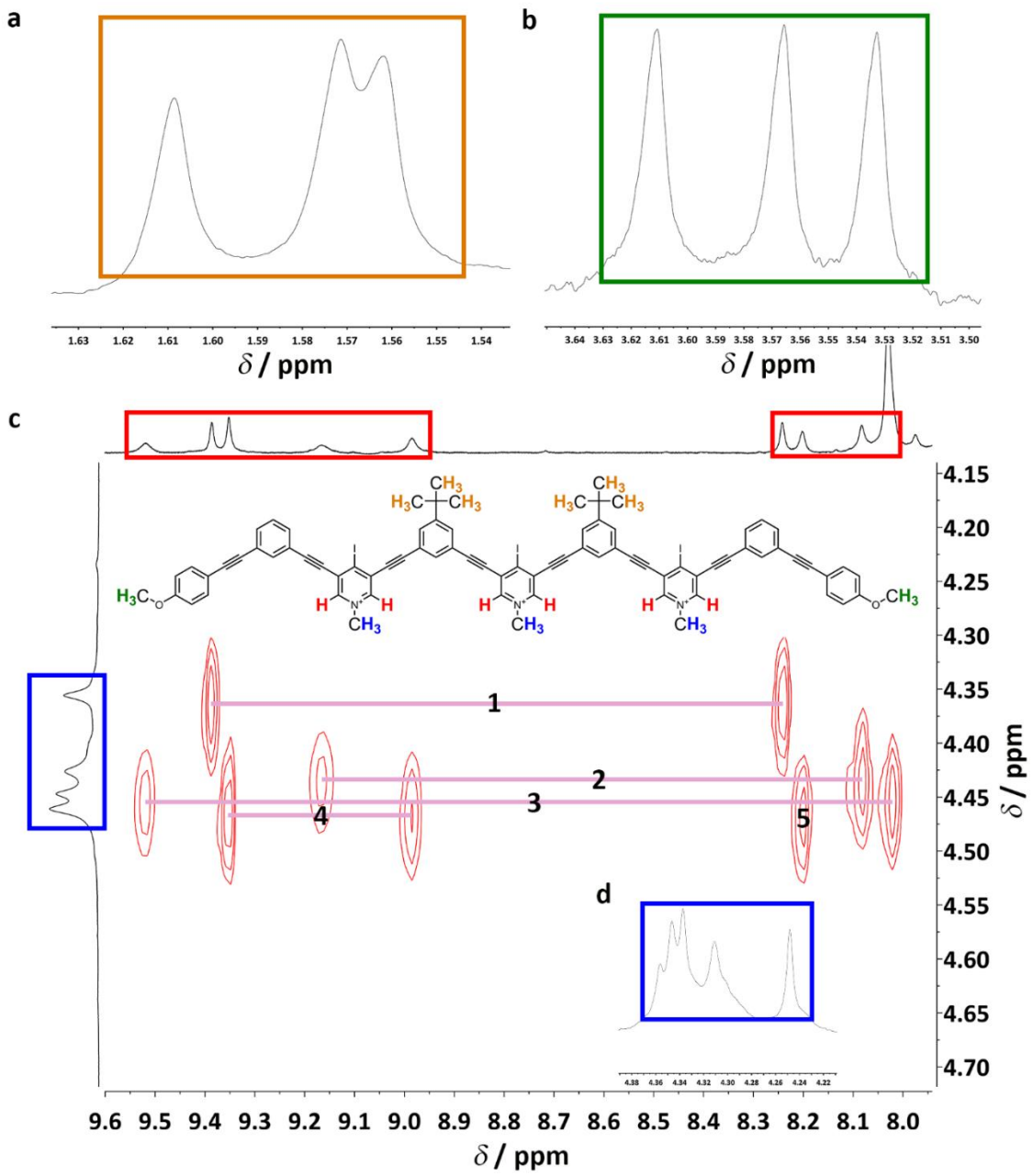


Figure S36. ^{1}H NMR and 2D NOESY spectroscopic analysis of the numbers and relative intensities of key resonances of **7**. a) ^{1}H NMR spectrum of three *tert*-butyl peaks of equal intensity. b) ^{1}H NMR spectrum of three methoxy methyl peaks of equal intensity. c) Nine pyridinium protons along the f2 axis are present with their NOEs (one is obscured by the DMF residual solvent peak). ^{1}H NMR spectrum of three resolved pyridinium methyl peaks of equal intensity (corresponding to the horizontal mauve lines 1–3) and one peak of 1.5x intensity (4–5). NOEs between pyridinium methyl and pyridinium resonances elucidate the overlapped components of this peak. Pyridinium methyl peaks corresponding to 1–4 each correlate with one relatively upfield pyridinium peak and one downfield. The buried pyridinium methyl peak corresponding to 5 likely belongs to the nonbonding pyridinium proton (600 MHz, 298 K). d) A better resolved ^{1}H NMR spectrum displaying four equal pyridinium methyl signals and one of half intensity (400 MHz, 298 K). Conditions for figures (a)–(b): 500 MHz, 1:4 v/v [D_7]DMF-CD_3CN, 336 K. Conditions for figures (c)–(d) 1:3 v/v [D_7]DMF-CD_3CN.

Solution and crystallographic structure analysis of the pyridinium aromatics

Analysis of the electronics, symmetries, and steric environments of the nine pyridinium aromatics provided a more nuanced comparison between the solution and crystallographic data. The nonbonding pyridinium ring—whose own axis of C_2 symmetry defines that of the entire triplex—contributes a single ^{1}H NMR signal (see Figure S37, orange). The two terminally exposed pyridinium rings (a symmetrical pair) contribute two signals (see Figure S37, cyan and red). The final six signals are produced by the six remaining and buried pyridiniums, which constitute three symmetrical pairs (see Figure S37, black, magenta, green, brown, blue, and yellow; see Table S1 for a summary). Of the nine pyridinium signals, five are shifted downfield and four upfield in organic solvents (see Figure S36 c). We hypothesize that the five downfield pyridinium protons are deshielded on account of HBing with extrachannel iodides (see Figure S23). Adding TBA iodide to **7** shifted these five pyridinium resonances downfield (up to 0.55 ppm, see Figure 2 b), while the chemical shifts of all other signals were unaffected. The downfield migration of the five pyridinium protons was largely suppressed in an aqueous environment (see Figure S38). In addition, NOEs between the upfield pyridinium and *tert*-butyl protons suggest steric shielding (see Figures S39 a and c). One *tert*-butyl cross peak correlates with a downfield pyridinium resonance (see Figure S32), likely belonging to the exposed terminal pyridinium pair (see Figure S39 e). These distinctive ^{1}H NMR spectroscopic and crystallographic features find unity in a common supramolecular structure (see Table S2 for a summary).

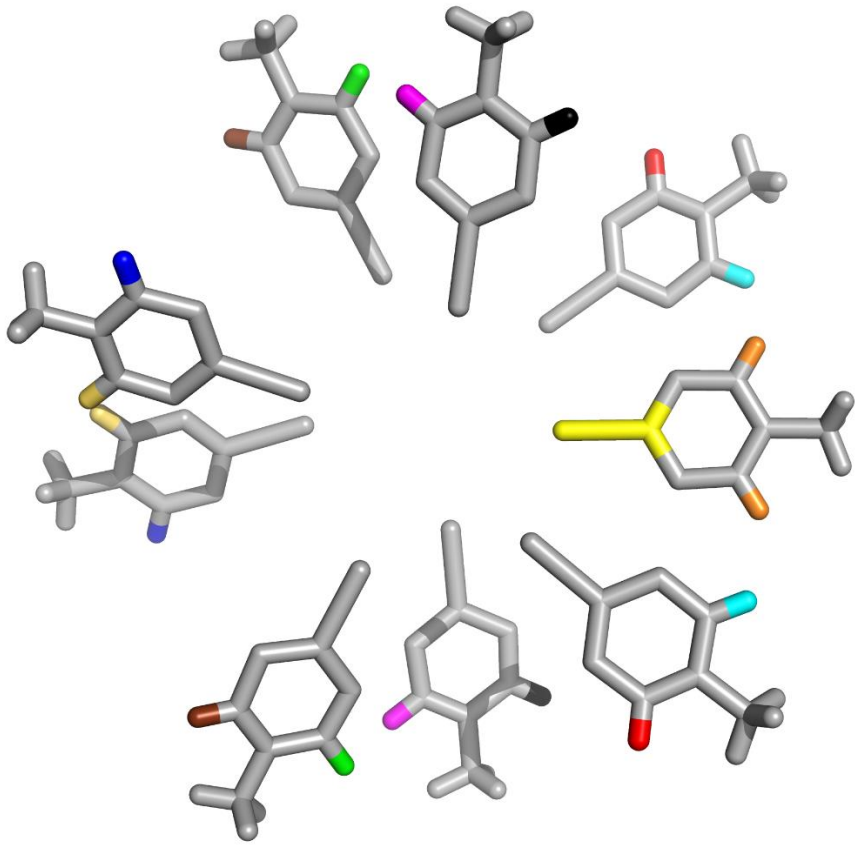


Figure S37. Top view of X-ray crystallographic configuration of pyridinium XB donors (scaffolding removed for clarity). The yellow stick aligns with the complex's axis of molecular C_2 symmetry. The pyridiniums with the cyan and red protons are likely terminal aromatic rings. The orange, black, magenta, green, brown, blue, and yellow protons likely belong to the pyridiniums buried within the cylindrical wall of the complex.

Color code	Pyridinium location	Protons (#)	^{1}H NMR Signals based on symmetry (#)
Orange	Buried (nonbonding)	2	1
Cyan	Terminal	2	1
Red	Terminal	2	1
Black	Buried	2	1
Magenta	Buried	2	1
Green	Buried	2	1
Brown	Buried	2	1
Blue	Buried	2	1
Yellow	Buried	2	1

Table S1. The origins of each pyridinium proton due to the complex's molecular C_2 symmetry (500 MHz, 1:3 v/v [D_7]DMF-CD_3CN, 341 K; for color code, see Figure S37).

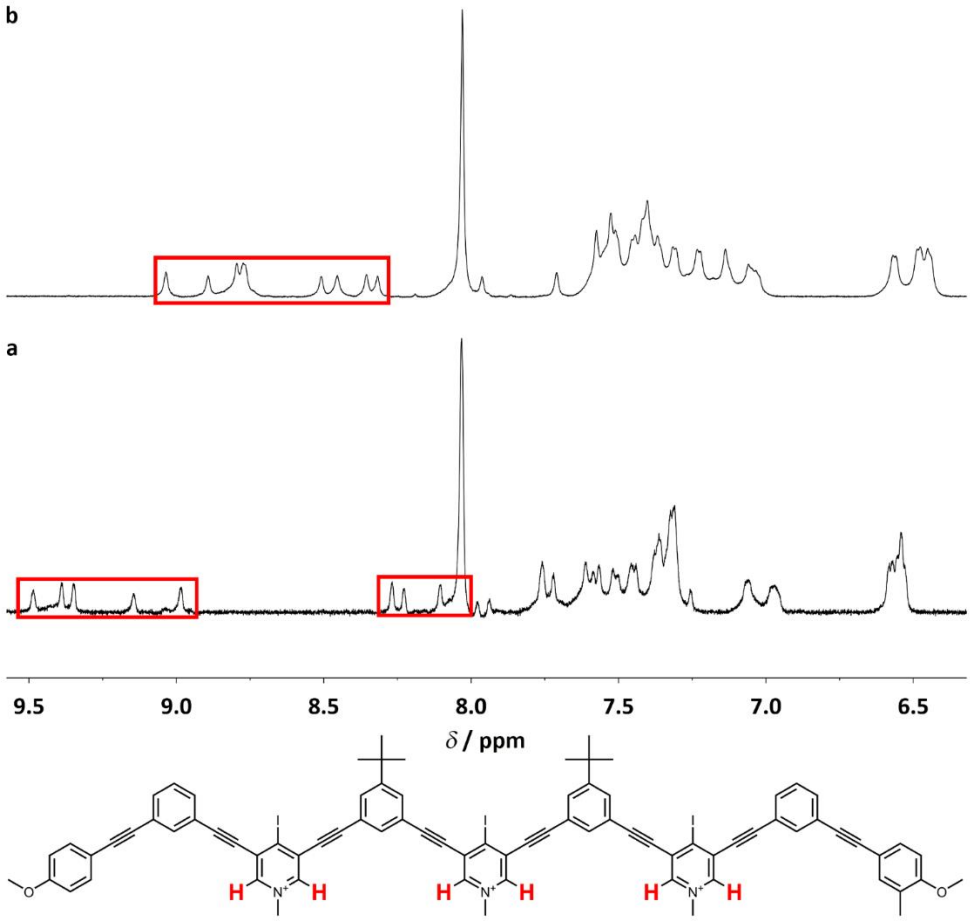


Figure S38. Pyridinium resonances in organic and aqueous media of triple helicate **7**. a) Triplex **7** in organic solvents (3 eq. of iodide; 1:3 v/v [D_7]DMF-CD_3CN). b) Triplex **7** in an aqueous environment (3 eq. of iodide; 1:1 v/v D_2O-[D_7]DMF). The five downfield pyridinium resonances (2 are overlapped) are shifted upfield relative to the corresponding peaks in Figure (a) (up to 0.45 ppm). Conditions for figures (a)–(b): 600 MHz, 298 K.

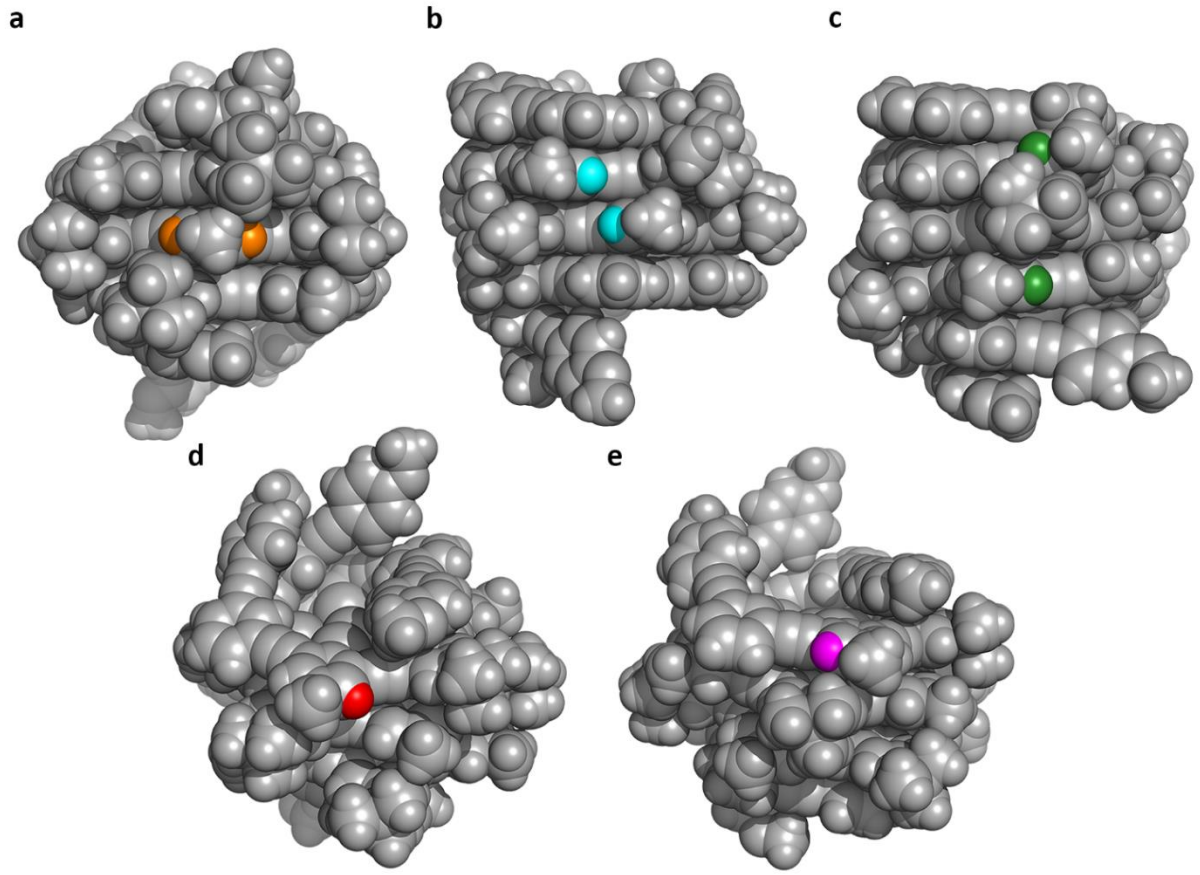


Figure S39. Crystallographic and steric environments of the pyridinium protons of **7**. a) Protons belonging to the nonbonding pyridinium donor. Both are sterically shielded by *tert*-butyl groups. b) Examples of pyridinium protons that are buried within the cylindrical wall of the complex. These protons are buried but not sterically shielded by *tert*-butyl groups. c) Examples of buried pyridinium protons that are also sterically shielded by *tert*-butyl groups. d) An example of a pyridinium proton that is terminally exposed but not in close proximity to a *tert*-butyl group. e) Example of a pyridinium proton that is terminally exposed and also in close proximity to a *tert*-butyl group.

Type	**Figure S39 color code**	**^{1}H NMR Signals (#)**	**Triple helicate protons (#)**	**Relative shift**	**Crystallographic environment**
Non-bonding	Orange (a)	1	2	Upfield	Shielded
Terminal shielded	Magenta (e)	1	2	Downfield	Shielded; terminally exposed
Terminal exposed	Red (d)	1	2	Downfield	Terminally exposed
Buried shielded	Green (c)	3	6	Upfield	Shielded
Buried exposed	Cyan (b)	3	6	Downfield	Exposed

Table S2. A summary of the solution and crystallographic environments of the pyridinium protons of **7** (500 MHz, 1:4 v/v [D_7]DMF-CD_3CN, 336 K).

S10. 2D DOSY verification of monodispersity and size

To calculate the hydrodynamic radii (r_H) of **7**, **8**, and an internal standard (dichloromethane), the Einstein-Stokes equation was used:[18]

$$D_t = \frac{kT}{6\pi\eta r_H} \quad (1)$$

where D_t is the diffusion coefficient of the analyte, k the Boltzmann constant, T the temperature, η the solvent viscosity, and r_H the hydrodynamic radius of the analyte. The reported D_t values are an average of all peaks corresponding a given species. Ratios of r_H values was used to compare the relative sizes of **8** and **7**, as well as **7** and the internal standard (DCM r_{solv} = 2.49 Å). The latter ratio was used to establish a rough estimate of the radius of the triple helicate (8.2 Å). The triplex's heightwise crystallographic radius was determined by averaging 20 evenly spaced measurements taken parallel to the screw axis of **7** (6.4 Å).The widthwise crystallographic radius of the triple helicate was estimated by calculating the length of the line drawn orthogonally from the screw axis of **7** to the methyl carbon of the nonbonding pyridinium (9.5 Å).

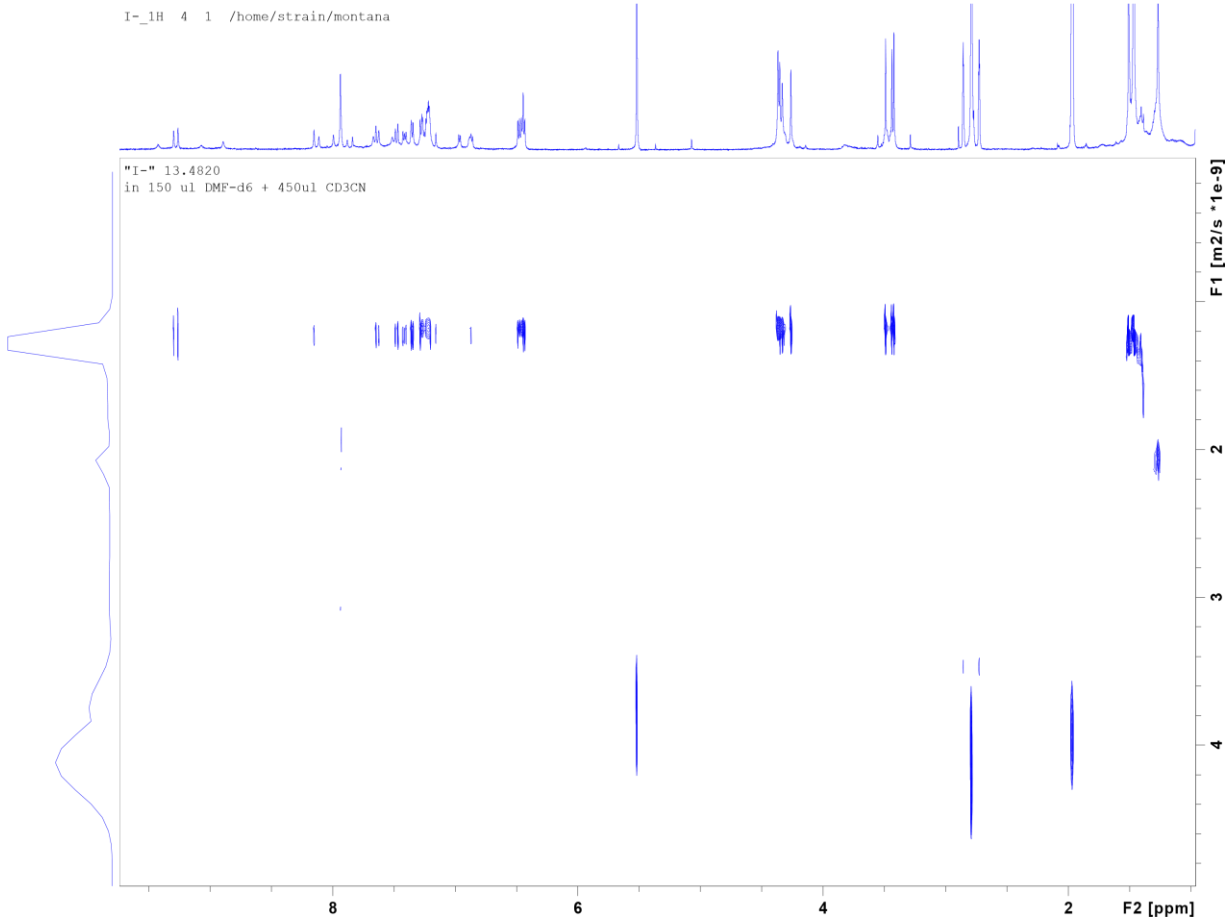


Figure S40. 2D DOSY spectrum of the triple helicate **7**. The average diffusion coefficient is 1.12 × 10^{-9} m^2 s^{-1} (600 MHz, 1:3 v/v [D_7]DMF-CD_3CN, 298 K).

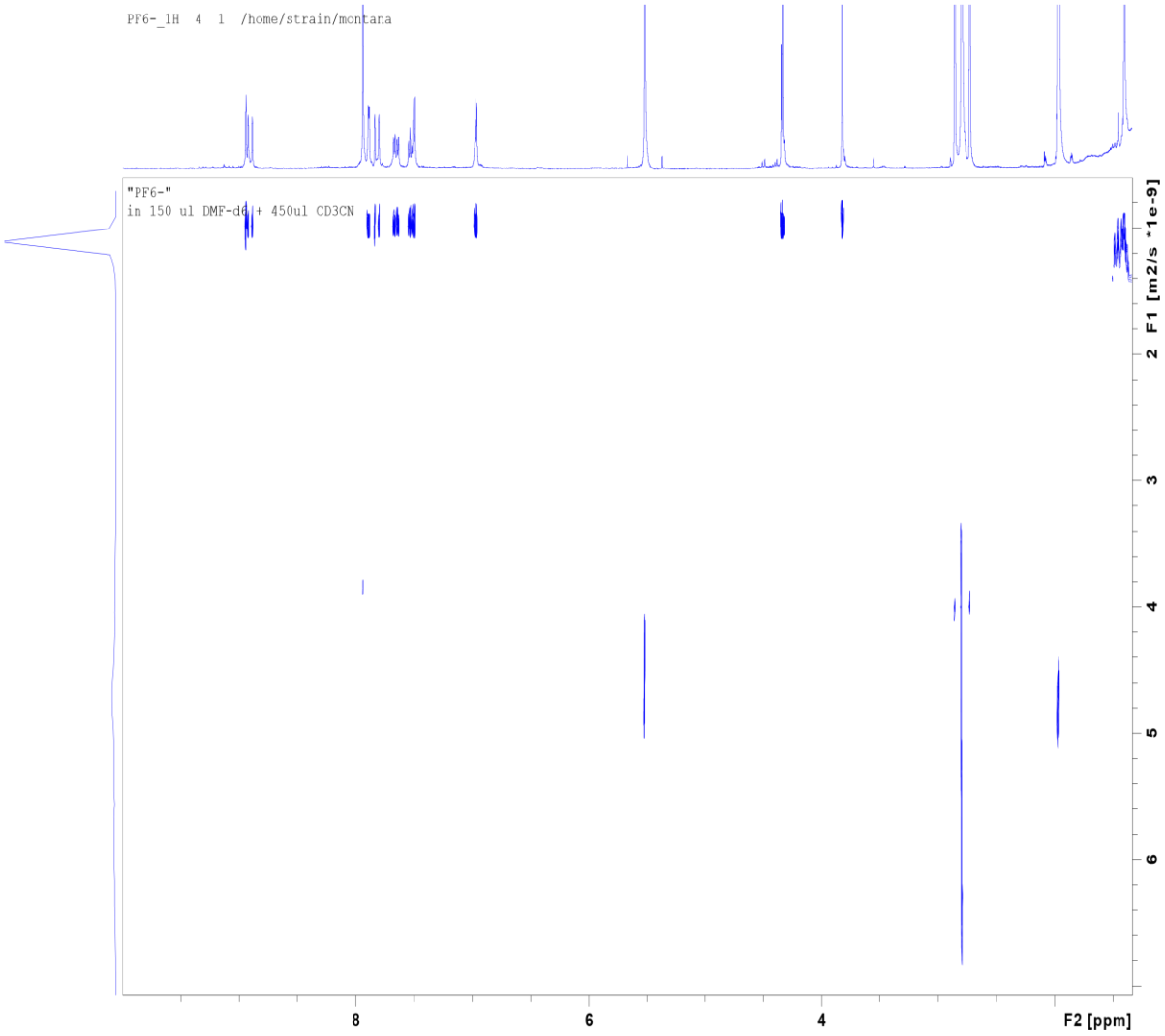


Figure S41. 2D DOSY spectrum of PF_6^- salt **8**. The average diffusion coefficient is 8.56×10^{-10} m^2 s^{-1} (600 MHz, 1:3 v/v [D_7]DMF-CD_3CN, 298 K).

DOSY data and refinements for the triple helicate 7

SIMFIT RESULTS
==========

Dataset : /home/strain/montana/I-_1H/4/pdata/1/ct1t2.txt

AREA fit : Diffusion : Variable Gradient :

I=I[0]*exp(-D*SQR(2*PI*gamma*Gi*LD)*(BD-LD/3)*1e4)

40 points for Integral 1, Integral Region from 9.330 to 9.230 ppm

Converged after 63 iterations!

Results Comp. 1

I[0] = 3.220e-02
Diff Con. = 1.125e-09 m2/s
Gamma = 4.258e+03 Hz/G
Little Delta = 3.400m
Big Delta = 49.900m

RSS = 2.305e-05
SD = 7.591e-04

Point	Gradient	Expt	Calc	Difference
1	0.000e+00	2.994e-02	3.220e-02	2.259e-03
2	0.000e+00	2.930e-02	3.220e-02	2.901e-03
3	5.803e+00	2.900e-02	2.764e-02	-1.360e-03
4	6.297e+00	2.804e-02	2.690e-02	-1.144e-03
5	6.790e+00	2.695e-02	2.612e-02	-8.313e-04
6	7.284e+00	2.634e-02	2.531e-02	-1.030e-03
7	7.778e+00	2.522e-02	2.447e-02	-7.513e-04
8	8.272e+00	2.429e-02	2.361e-02	-6.849e-04
9	8.766e+00	2.328e-02	2.272e-02	-5.565e-04
10	9.260e+00	2.200e-02	2.182e-02	-1.756e-04
11	9.753e+00	2.159e-02	2.091e-02	-6.813e-04
12	1.025e+01	2.035e-02	2.000e-02	-3.515e-04
13	1.074e+01	1.928e-02	1.908e-02	-2.003e-04
14	1.123e+01	1.825e-02	1.816e-02	-9.406e-05
15	1.173e+01	1.742e-02	1.725e-02	-1.732e-04
16	1.222e+01	1.620e-02	1.635e-02	1.495e-04
17	1.272e+01	1.567e-02	1.546e-02	-2.105e-04
18	1.321e+01	1.499e-02	1.459e-02	-4.064e-04
19	1.370e+01	1.391e-02	1.373e-02	-1.771e-04
20	1.420e+01	1.286e-02	1.290e-02	3.995e-05
21	1.469e+01	1.210e-02	1.209e-02	-3.353e-06
22	1.519e+01	1.094e-02	1.131e-02	3.710e-04
23	1.568e+01	1.028e-02	1.055e-02	2.762e-04

24	1.617e+01	9.304e-03	9.827e-03	5.232e-04
25	1.667e+01	8.821e-03	9.129e-03	3.082e-04
26	1.716e+01	7.883e-03	8.463e-03	5.794e-04
27	1.766e+01	7.525e-03	7.827e-03	3.021e-04
28	1.815e+01	6.762e-03	7.224e-03	4.618e-04
29	1.864e+01	6.399e-03	6.652e-03	2.526e-04
30	1.914e+01	6.017e-03	6.112e-03	9.533e-05
31	1.963e+01	5.359e-03	5.604e-03	2.452e-04
32	2.012e+01	4.480e-03	5.126e-03	6.466e-04
33	2.062e+01	4.345e-03	4.679e-03	3.340e-04
34	2.111e+01	4.129e-03	4.261e-03	1.316e-04
35	2.161e+01	3.641e-03	3.872e-03	2.314e-04
36	2.210e+01	3.139e-03	3.511e-03	3.716e-04
37	2.259e+01	2.854e-03	3.177e-03	3.231e-04
38	2.309e+01	2.662e-03	2.868e-03	2.053e-04
39	2.358e+01	2.384e-03	2.583e-03	1.984e-04
40	2.408e+01	2.129e-03	2.321e-03	1.921e-04

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40 points for Integral 2, Integral Region from 8.183 to 8.082 ppm

Converged after 54 iterations!

Results Comp. 1

I[0] = 3.219e-02
Diff Con. = 1.179e-09 m2/s
Gamma = 4.258e+03 Hz/G
Little Delta = 3.400m
Big Delta = 49.900m

RSS = 2.356e-05
SD = 7.675e-04

Point	Gradient	Expt	Calc	Difference
1	0.000e+00	2.996e-02	3.219e-02	2.224e-03
2	0.000e+00	2.930e-02	3.219e-02	2.884e-03
3	5.803e+00	2.872e-02	2.742e-02	-1.297e-03
4	6.297e+00	2.726e-02	2.666e-02	-6.050e-04
5	6.790e+00	2.713e-02	2.585e-02	-1.279e-03
6	7.284e+00	2.618e-02	2.501e-02	-1.167e-03
7	7.778e+00	2.459e-02	2.414e-02	-4.494e-04
8	8.272e+00	2.366e-02	2.325e-02	-4.127e-04
9	8.766e+00	2.307e-02	2.233e-02	-7.366e-04
10	9.260e+00	2.200e-02	2.141e-02	-5.939e-04
11	9.753e+00	2.128e-02	2.047e-02	-8.082e-04
12	1.025e+01	1.991e-02	1.953e-02	-3.715e-04
13	1.074e+01	1.892e-02	1.860e-02	-3.280e-04
14	1.123e+01	1.757e-02	1.766e-02	8.962e-05

15	1.173e+01	1.700e-02	1.673e-02	-2.674e-04
16	1.222e+01	1.594e-02	1.582e-02	-1.215e-04
17	1.272e+01	1.479e-02	1.492e-02	1.244e-04
18	1.321e+01	1.427e-02	1.404e-02	-2.323e-04
19	1.370e+01	1.324e-02	1.318e-02	-6.315e-05
20	1.420e+01	1.228e-02	1.234e-02	6.282e-05
21	1.469e+01	1.148e-02	1.153e-02	5.420e-05
22	1.519e+01	1.057e-02	1.075e-02	1.745e-04
23	1.568e+01	9.893e-03	9.997e-03	1.035e-04
24	1.617e+01	8.659e-03	9.277e-03	6.187e-04
25	1.667e+01	8.323e-03	8.588e-03	2.652e-04
26	1.716e+01	7.639e-03	7.932e-03	2.929e-04
27	1.766e+01	7.048e-03	7.309e-03	2.608e-04
28	1.815e+01	6.520e-03	6.720e-03	2.000e-04
29	1.864e+01	5.641e-03	6.163e-03	5.219e-04
30	1.914e+01	5.317e-03	5.640e-03	3.225e-04
31	1.963e+01	4.647e-03	5.150e-03	5.025e-04
32	2.012e+01	4.477e-03	4.690e-03	2.131e-04
33	2.062e+01	4.162e-03	4.262e-03	9.976e-05
34	2.111e+01	3.236e-03	3.864e-03	6.279e-04
35	2.161e+01	2.779e-03	3.495e-03	7.166e-04
36	2.210e+01	2.847e-03	3.154e-03	3.067e-04
37	2.259e+01	2.650e-03	2.840e-03	1.898e-04
38	2.309e+01	2.170e-03	2.551e-03	3.811e-04
39	2.358e+01	1.831e-03	2.286e-03	4.557e-04
40	2.408e+01	1.658e-03	2.044e-03	3.857e-04

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40 points for Integral 4, Integral Region from 7.706 to 7.571 ppm

Converged after 54 iterations!

Results Comp. 1

I[0] = 7.521e-02
Diff Con. = 1.157e-09 m2/s
Gamma = 4.258e+03 Hz/G
Little Delta = 3.400m
Big Delta = 49.900m

RSS = 1.216e-04
SD = 1.743e-03

Point	Gradient	Expt	Calc	Difference
1	0.000e+00	7.017e-02	7.521e-02	5.039e-03
2	0.000e+00	6.838e-02	7.521e-02	6.828e-03
3	5.803e+00	6.675e-02	6.427e-02	-2.479e-03
4	6.297e+00	6.475e-02	6.250e-02	-2.256e-03
5	6.790e+00	6.249e-02	6.064e-02	-1.847e-03

6	7.284e+00	6.101e-02	5.871e-02	-2.304e-03
7	7.778e+00	5.794e-02	5.670e-02	-1.235e-03
8	8.272e+00	5.605e-02	5.464e-02	-1.406e-03
9	8.766e+00	5.437e-02	5.254e-02	-1.830e-03
10	9.260e+00	5.191e-02	5.040e-02	-1.512e-03
11	9.753e+00	4.972e-02	4.824e-02	-1.481e-03
12	1.025e+01	4.702e-02	4.607e-02	-9.564e-04
13	1.074e+01	4.481e-02	4.389e-02	-9.205e-04
14	1.123e+01	4.256e-02	4.172e-02	-8.426e-04
15	1.173e+01	4.028e-02	3.957e-02	-7.162e-04
16	1.222e+01	3.767e-02	3.744e-02	-2.289e-04
17	1.272e+01	3.575e-02	3.535e-02	-3.985e-04
18	1.321e+01	3.352e-02	3.330e-02	-2.152e-04
19	1.370e+01	3.139e-02	3.130e-02	-9.044e-05
20	1.420e+01	2.934e-02	2.935e-02	1.068e-05
21	1.469e+01	2.693e-02	2.746e-02	5.270e-04
22	1.519e+01	2.476e-02	2.563e-02	8.699e-04
23	1.568e+01	2.351e-02	2.387e-02	3.566e-04
24	1.617e+01	2.140e-02	2.218e-02	7.825e-04
25	1.667e+01	1.925e-02	2.056e-02	1.307e-03
26	1.716e+01	1.796e-02	1.902e-02	1.058e-03
27	1.766e+01	1.649e-02	1.755e-02	1.059e-03
28	1.815e+01	1.548e-02	1.616e-02	6.776e-04
29	1.864e+01	1.398e-02	1.485e-02	8.652e-04
30	1.914e+01	1.297e-02	1.361e-02	6.361e-04
31	1.963e+01	1.190e-02	1.245e-02	5.495e-04
32	2.012e+01	1.055e-02	1.136e-02	8.081e-04
33	2.062e+01	9.846e-03	1.034e-02	4.912e-04
34	2.111e+01	8.543e-03	9.389e-03	8.453e-04
35	2.161e+01	7.786e-03	8.508e-03	7.218e-04
36	2.210e+01	7.224e-03	7.692e-03	4.678e-04
37	2.259e+01	5.763e-03	6.940e-03	1.177e-03
38	2.309e+01	5.110e-03	6.246e-03	1.136e-03
39	2.358e+01	4.665e-03	5.609e-03	9.438e-04
40	2.408e+01	3.813e-03	5.025e-03	1.212e-03

==========

40 points for Integral 5, Integral Region from 7.546 to 7.320 ppm

Converged after 54 iterations!

Results Comp. 1

I[0] = 1.759e-01
Diff Con. = 1.136e-09 m2/s
Gamma = 4.258e+03 Hz/G
Little Delta = 3.400m
Big Delta = 49.900m

RSS = 5.896e-04

SD = 3.839e-03

Point	Gradient	Expt	Calc	Difference
1	0.000e+00	1.643e-01	1.759e-01	1.152e-02
2	0.000e+00	1.609e-01	1.759e-01	1.501e-02
3	5.803e+00	1.564e-01	1.507e-01	-5.732e-03
4	6.297e+00	1.521e-01	1.466e-01	-5.481e-03
5	6.790e+00	1.475e-01	1.424e-01	-5.140e-03
6	7.284e+00	1.426e-01	1.379e-01	-4.675e-03
7	7.778e+00	1.370e-01	1.333e-01	-3.675e-03
8	8.272e+00	1.324e-01	1.285e-01	-3.880e-03
9	8.766e+00	1.269e-01	1.237e-01	-3.274e-03
10	9.260e+00	1.215e-01	1.187e-01	-2.800e-03
11	9.753e+00	1.163e-01	1.137e-01	-2.605e-03
12	1.025e+01	1.107e-01	1.087e-01	-2.048e-03
13	1.074e+01	1.055e-01	1.036e-01	-1.860e-03
14	1.123e+01	1.005e-01	9.860e-02	-1.861e-03
15	1.173e+01	9.422e-02	9.361e-02	-6.156e-04
16	1.222e+01	8.882e-02	8.867e-02	-1.500e-04
17	1.272e+01	8.345e-02	8.380e-02	3.441e-04
18	1.321e+01	7.929e-02	7.903e-02	-2.627e-04
19	1.370e+01	7.403e-02	7.435e-02	3.263e-04
20	1.420e+01	6.993e-02	6.980e-02	-1.272e-04
21	1.469e+01	6.420e-02	6.538e-02	1.180e-03
22	1.519e+01	6.051e-02	6.110e-02	5.970e-04
23	1.568e+01	5.607e-02	5.698e-02	9.079e-04
24	1.617e+01	5.180e-02	5.302e-02	1.226e-03
25	1.667e+01	4.722e-02	4.922e-02	2.001e-03
26	1.716e+01	4.268e-02	4.559e-02	2.912e-03
27	1.766e+01	4.007e-02	4.213e-02	2.067e-03
28	1.815e+01	3.673e-02	3.885e-02	2.119e-03
29	1.864e+01	3.415e-02	3.575e-02	1.594e-03
30	1.914e+01	3.155e-02	3.282e-02	1.267e-03
31	1.963e+01	2.854e-02	3.006e-02	1.519e-03
32	2.012e+01	2.541e-02	2.748e-02	2.065e-03
33	2.062e+01	2.411e-02	2.505e-02	9.436e-04
34	2.111e+01	2.080e-02	2.279e-02	1.993e-03
35	2.161e+01	1.903e-02	2.069e-02	1.662e-03
36	2.210e+01	1.783e-02	1.874e-02	9.125e-04
37	2.259e+01	1.512e-02	1.694e-02	1.820e-03
38	2.309e+01	1.358e-02	1.528e-02	1.698e-03
39	2.358e+01	1.207e-02	1.374e-02	1.674e-03
40	2.408e+01	1.130e-02	1.234e-02	1.038e-03

==========

40 points for Integral 6, Integral Region from 7.320 to 7.136 ppm

Converged after 51 iterations!

Results Comp. 1

I[0] = 2.356e-01
Diff Con. = 1.117e-09 m2/s
Gamma = 4.258e+03 Hz/G
Little Delta = 3.400m
Big Delta = 49.900m

RSS = 1.006e-03
SD = 5.014e-03

Point	Gradient	Expt	Calc	Difference
1	0.000e+00	2.207e-01	2.356e-01	1.487e-02
2	0.000e+00	2.156e-01	2.356e-01	1.999e-02
3	5.803e+00	2.096e-01	2.024e-01	-7.205e-03
4	6.297e+00	2.041e-01	1.970e-01	-7.052e-03
5	6.790e+00	1.979e-01	1.914e-01	-6.488e-03
6	7.284e+00	1.919e-01	1.855e-01	-6.414e-03
7	7.778e+00	1.847e-01	1.794e-01	-5.313e-03
8	8.272e+00	1.777e-01	1.731e-01	-4.652e-03
9	8.766e+00	1.712e-01	1.666e-01	-4.557e-03
10	9.260e+00	1.635e-01	1.601e-01	-3.383e-03
11	9.753e+00	1.568e-01	1.535e-01	-3.353e-03
12	1.025e+01	1.498e-01	1.468e-01	-3.006e-03
13	1.074e+01	1.421e-01	1.401e-01	-2.019e-03
14	1.123e+01	1.354e-01	1.334e-01	-2.012e-03
15	1.173e+01	1.276e-01	1.268e-01	-8.626e-04
16	1.222e+01	1.211e-01	1.202e-01	-9.533e-04
17	1.272e+01	1.139e-01	1.137e-01	-1.735e-04
18	1.321e+01	1.077e-01	1.073e-01	-3.823e-04
19	1.370e+01	1.010e-01	1.011e-01	4.176e-05
20	1.420e+01	9.448e-02	9.500e-02	5.181e-04
21	1.469e+01	8.759e-02	8.908e-02	1.494e-03
22	1.519e+01	8.247e-02	8.335e-02	8.763e-04
23	1.568e+01	7.698e-02	7.782e-02	8.364e-04
24	1.617e+01	6.998e-02	7.250e-02	2.517e-03
25	1.667e+01	6.445e-02	6.739e-02	2.940e-03
26	1.716e+01	5.997e-02	6.250e-02	2.537e-03
27	1.766e+01	5.570e-02	5.784e-02	2.139e-03
28	1.815e+01	5.100e-02	5.341e-02	2.415e-03
29	1.864e+01	4.673e-02	4.921e-02	2.487e-03
30	1.914e+01	4.292e-02	4.524e-02	2.326e-03
31	1.963e+01	3.949e-02	4.151e-02	2.024e-03
32	2.012e+01	3.546e-02	3.800e-02	2.534e-03
33	2.062e+01	3.287e-02	3.470e-02	1.833e-03
34	2.111e+01	2.940e-02	3.162e-02	2.226e-03
35	2.161e+01	2.697e-02	2.876e-02	1.783e-03
36	2.210e+01	2.406e-02	2.609e-02	2.034e-03
37	2.259e+01	2.197e-02	2.363e-02	1.659e-03
38	2.309e+01	1.916e-02	2.134e-02	2.186e-03

39	2.358e+01	1.744e-02	1.924e-02	1.798e-03
40	2.408e+01	1.548e-02	1.730e-02	1.823e-03

==========

40 points for Integral 7, Integral Region from 6.550 to 6.382 ppm

Converged after 54 iterations!

Results Comp. 1

I[0] = 1.267e-01
Diff Con. = 1.117e-09 m2/s
Gamma = 4.258e+03 Hz/G
Little Delta = 3.400m
Big Delta = 49.900m

RSS = 3.000e-04
SD = 2.738e-03

Point	Gradient	Expt	Calc	Difference
1	0.000e+00	1.185e-01	1.267e-01	8.203e-03
2	0.000e+00	1.160e-01	1.267e-01	1.080e-02
3	5.803e+00	1.125e-01	1.089e-01	-3.561e-03
4	6.297e+00	1.100e-01	1.060e-01	-3.938e-03
5	6.790e+00	1.064e-01	1.030e-01	-3.406e-03
6	7.284e+00	1.031e-01	9.980e-02	-3.256e-03
7	7.778e+00	9.948e-02	9.651e-02	-2.965e-03
8	8.272e+00	9.579e-02	9.313e-02	-2.666e-03
9	8.766e+00	9.271e-02	8.966e-02	-3.047e-03
10	9.260e+00	8.810e-02	8.614e-02	-1.964e-03
11	9.753e+00	8.459e-02	8.258e-02	-2.017e-03
12	1.025e+01	8.067e-02	7.898e-02	-1.687e-03
13	1.074e+01	7.662e-02	7.538e-02	-1.246e-03
14	1.123e+01	7.244e-02	7.178e-02	-6.635e-04
15	1.173e+01	6.902e-02	6.820e-02	-8.163e-04
16	1.222e+01	6.465e-02	6.466e-02	1.787e-05
17	1.272e+01	6.157e-02	6.117e-02	-3.946e-04
18	1.321e+01	5.769e-02	5.775e-02	5.939e-05
19	1.370e+01	5.433e-02	5.439e-02	6.292e-05
20	1.420e+01	5.106e-02	5.112e-02	5.646e-05
21	1.469e+01	4.710e-02	4.794e-02	8.393e-04
22	1.519e+01	4.456e-02	4.485e-02	2.938e-04
23	1.568e+01	4.114e-02	4.187e-02	7.372e-04
24	1.617e+01	3.774e-02	3.902e-02	1.279e-03
25	1.667e+01	3.459e-02	3.627e-02	1.679e-03
26	1.716e+01	3.224e-02	3.364e-02	1.395e-03
27	1.766e+01	2.958e-02	3.113e-02	1.553e-03
28	1.815e+01	2.737e-02	2.874e-02	1.376e-03
29	1.864e+01	2.475e-02	2.648e-02	1.731e-03

30	1.914e+01	2.344e-02	2.435e-02	9.121e-04
31	1.963e+01	2.135e-02	2.234e-02	9.910e-04
32	2.012e+01	1.904e-02	2.045e-02	1.411e-03
33	2.062e+01	1.771e-02	1.868e-02	9.648e-04
34	2.111e+01	1.585e-02	1.702e-02	1.175e-03
35	2.161e+01	1.457e-02	1.548e-02	9.085e-04
36	2.210e+01	1.293e-02	1.404e-02	1.113e-03
37	2.259e+01	1.199e-02	1.272e-02	7.273e-04
38	2.309e+01	1.047e-02	1.149e-02	1.019e-03
39	2.358e+01	9.343e-03	1.035e-02	1.010e-03
40	2.408e+01	8.259e-03	9.312e-03	1.053e-03

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40 points for Integral 9, Integral Region from 4.431 to 4.288 ppm

Converged after 44 iterations!

Results Comp. 1

I[0] = 2.767e-01
Diff Con. = 1.101e-09 m2/s
Gamma = 4.258e+03 Hz/G
Little Delta = 3.400m
Big Delta = 49.900m

RSS = 1.283e-03
SD = 5.664e-03

Point	Gradient	Expt	Calc	Difference
1	0.000e+00	2.598e-01	2.767e-01	1.682e-02
2	0.000e+00	2.540e-01	2.767e-01	2.267e-02
3	5.803e+00	2.474e-01	2.382e-01	-9.145e-03
4	6.297e+00	2.406e-01	2.320e-01	-8.632e-03
5	6.790e+00	2.331e-01	2.254e-01	-7.735e-03
6	7.284e+00	2.253e-01	2.186e-01	-6.786e-03
7	7.778e+00	2.174e-01	2.114e-01	-5.904e-03
8	8.272e+00	2.097e-01	2.041e-01	-5.619e-03
9	8.766e+00	2.017e-01	1.966e-01	-5.060e-03
10	9.260e+00	1.929e-01	1.890e-01	-3.854e-03
11	9.753e+00	1.847e-01	1.813e-01	-3.361e-03
12	1.025e+01	1.761e-01	1.735e-01	-2.601e-03
13	1.074e+01	1.678e-01	1.657e-01	-2.078e-03
14	1.123e+01	1.594e-01	1.579e-01	-1.544e-03
15	1.173e+01	1.512e-01	1.501e-01	-1.040e-03
16	1.222e+01	1.426e-01	1.424e-01	-1.885e-04
17	1.272e+01	1.349e-01	1.349e-01	-8.164e-05
18	1.321e+01	1.271e-01	1.274e-01	2.739e-04
19	1.370e+01	1.197e-01	1.201e-01	4.443e-04
20	1.420e+01	1.119e-01	1.130e-01	1.073e-03

21	1.469e+01	1.049e-01	1.060e-01	1.077e-03
22	1.519e+01	9.789e-02	9.929e-02	1.408e-03
23	1.568e+01	9.169e-02	9.279e-02	1.101e-03
24	1.617e+01	8.454e-02	8.653e-02	1.993e-03
25	1.667e+01	7.795e-02	8.052e-02	2.566e-03
26	1.716e+01	7.213e-02	7.475e-02	2.625e-03
27	1.766e+01	6.723e-02	6.925e-02	2.021e-03
28	1.815e+01	6.134e-02	6.402e-02	2.678e-03
29	1.864e+01	5.682e-02	5.905e-02	2.232e-03
30	1.914e+01	5.136e-02	5.435e-02	2.996e-03
31	1.963e+01	4.736e-02	4.993e-02	2.569e-03
32	2.012e+01	4.310e-02	4.576e-02	2.651e-03
33	2.062e+01	3.978e-02	4.184e-02	2.066e-03
34	2.111e+01	3.613e-02	3.818e-02	2.053e-03
35	2.161e+01	3.273e-02	3.476e-02	2.030e-03
36	2.210e+01	3.017e-02	3.158e-02	1.415e-03
37	2.259e+01	2.684e-02	2.864e-02	1.794e-03
38	2.309e+01	2.383e-02	2.590e-02	2.071e-03
39	2.358e+01	2.157e-02	2.338e-02	1.815e-03
40	2.408e+01	1.961e-02	2.106e-02	1.448e-03

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40 points for Integral 10, Integral Region from 4.288 to 4.205 ppm

Converged after 58 iterations!

Results Comp. 1

I[0] = 7.831e-02
Diff Con. = 1.098e-09 m2/s
Gamma = 4.258e+03 Hz/G
Little Delta = 3.400m
Big Delta = 49.900m

RSS = 1.022e-04
SD = 1.598e-03

Point	Gradient	Expt	Calc	Difference
1	0.000e+00	7.346e-02	7.831e-02	4.850e-03
2	0.000e+00	7.206e-02	7.831e-02	6.251e-03
3	5.803e+00	6.983e-02	6.745e-02	-2.376e-03
4	6.297e+00	6.810e-02	6.569e-02	-2.412e-03
5	6.790e+00	6.627e-02	6.384e-02	-2.428e-03
6	7.284e+00	6.390e-02	6.190e-02	-2.003e-03
7	7.778e+00	6.173e-02	5.989e-02	-1.837e-03
8	8.272e+00	5.949e-02	5.783e-02	-1.666e-03
9	8.766e+00	5.707e-02	5.571e-02	-1.359e-03
10	9.260e+00	5.455e-02	5.355e-02	-9.943e-04
11	9.753e+00	5.244e-02	5.137e-02	-1.065e-03

12	1.025e+01	4.971e-02	4.917e-02	-5.348e-04
13	1.074e+01	4.743e-02	4.696e-02	-4.687e-04
14	1.123e+01	4.518e-02	4.476e-02	-4.212e-04
15	1.173e+01	4.284e-02	4.256e-02	-2.761e-04
16	1.222e+01	4.029e-02	4.039e-02	1.017e-04
17	1.272e+01	3.836e-02	3.824e-02	-1.126e-04
18	1.321e+01	3.585e-02	3.614e-02	2.832e-04
19	1.370e+01	3.390e-02	3.407e-02	1.719e-04
20	1.420e+01	3.173e-02	3.205e-02	3.170e-04
21	1.469e+01	2.994e-02	3.009e-02	1.488e-04
22	1.519e+01	2.800e-02	2.818e-02	1.817e-04
23	1.568e+01	2.604e-02	2.634e-02	3.033e-04
24	1.617e+01	2.347e-02	2.457e-02	1.098e-03
25	1.667e+01	2.221e-02	2.286e-02	6.569e-04
26	1.716e+01	2.064e-02	2.123e-02	5.911e-04
27	1.766e+01	1.914e-02	1.967e-02	5.387e-04
28	1.815e+01	1.759e-02	1.819e-02	6.002e-04
29	1.864e+01	1.595e-02	1.678e-02	8.308e-04
30	1.914e+01	1.467e-02	1.545e-02	7.845e-04
31	1.963e+01	1.374e-02	1.420e-02	4.559e-04
32	2.012e+01	1.229e-02	1.301e-02	7.266e-04
33	2.062e+01	1.096e-02	1.190e-02	9.381e-04
34	2.111e+01	1.010e-02	1.086e-02	7.584e-04
35	2.161e+01	9.678e-03	9.893e-03	2.150e-04
36	2.210e+01	8.532e-03	8.991e-03	4.581e-04
37	2.259e+01	7.810e-03	8.154e-03	3.438e-04
38	2.309e+01	7.013e-03	7.378e-03	3.655e-04
39	2.358e+01	6.196e-03	6.662e-03	4.656e-04
40	2.408e+01	5.664e-03	6.002e-03	3.376e-04

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40 points for Integral 11, Integral Region from 3.526 to 3.459 ppm

Converged after 47 iterations!

Results Comp. 1

I[0] = 9.545e-02
Diff Con. = 1.099e-09 m2/s
Gamma = 4.258e+03 Hz/G
Little Delta = 3.400m
Big Delta = 49.900m

RSS = 1.559e-04
SD = 1.974e-03

Point	Gradient	Expt	Calc	Difference
1	0.000e+00	8.951e-02	9.545e-02	5.937e-03
2	0.000e+00	8.765e-02	9.545e-02	7.804e-03

3	5.803e+00	8.549e-02	8.221e-02	-3.277e-03
4	6.297e+00	8.316e-02	8.006e-02	-3.096e-03
5	6.790e+00	8.010e-02	7.780e-02	-2.298e-03
6	7.284e+00	7.810e-02	7.544e-02	-2.660e-03
7	7.778e+00	7.511e-02	7.300e-02	-2.115e-03
8	8.272e+00	7.236e-02	7.047e-02	-1.886e-03
9	8.766e+00	6.950e-02	6.789e-02	-1.606e-03
10	9.260e+00	6.659e-02	6.526e-02	-1.324e-03
11	9.753e+00	6.382e-02	6.261e-02	-1.214e-03
12	1.025e+01	6.085e-02	5.993e-02	-9.219e-04
13	1.074e+01	5.787e-02	5.723e-02	-6.380e-04
14	1.123e+01	5.530e-02	5.454e-02	-7.593e-04
15	1.173e+01	5.221e-02	5.187e-02	-3.461e-04
16	1.222e+01	4.919e-02	4.922e-02	2.536e-05
17	1.272e+01	4.684e-02	4.660e-02	-2.401e-04
18	1.321e+01	4.395e-02	4.403e-02	8.134e-05
19	1.370e+01	4.129e-02	4.151e-02	2.230e-04
20	1.420e+01	3.847e-02	3.905e-02	5.853e-04
21	1.469e+01	3.617e-02	3.666e-02	4.869e-04
22	1.519e+01	3.415e-02	3.434e-02	1.904e-04
23	1.568e+01	3.152e-02	3.209e-02	5.684e-04
24	1.617e+01	2.928e-02	2.993e-02	6.493e-04
25	1.667e+01	2.691e-02	2.786e-02	9.452e-04
26	1.716e+01	2.486e-02	2.587e-02	1.004e-03
27	1.766e+01	2.336e-02	2.397e-02	6.051e-04
28	1.815e+01	2.133e-02	2.216e-02	8.360e-04
29	1.864e+01	1.925e-02	2.045e-02	1.193e-03
30	1.914e+01	1.786e-02	1.882e-02	9.660e-04
31	1.963e+01	1.654e-02	1.729e-02	7.513e-04
32	2.012e+01	1.507e-02	1.585e-02	7.769e-04
33	2.062e+01	1.367e-02	1.450e-02	8.327e-04
34	2.111e+01	1.250e-02	1.323e-02	7.345e-04
35	2.161e+01	1.179e-02	1.205e-02	2.646e-04
36	2.210e+01	1.021e-02	1.095e-02	7.432e-04
37	2.259e+01	9.349e-03	9.931e-03	5.818e-04
38	2.309e+01	8.350e-03	8.986e-03	6.359e-04
39	2.358e+01	7.434e-03	8.113e-03	6.789e-04
40	2.408e+01	6.844e-03	7.309e-03	4.648e-04

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40 points for Integral 12, Integral Region from 3.459 to 3.367 ppm

Converged after 46 iterations!

Results Comp. 1

I[0] = 1.412e-01
Diff Con. = 1.100e-09 m2/s
Gamma = 4.258e+03 Hz/G
Little Delta = 3.400m

Big Delta = 49.900m

RSS = 3.316e-04
SD = 2.879e-03

Point	Gradient	Expt	Calc	Difference
1	0.000e+00	1.328e-01	1.412e-01	8.425e-03
2	0.000e+00	1.297e-01	1.412e-01	1.157e-02
3	5.803e+00	1.257e-01	1.216e-01	-4.091e-03
4	6.297e+00	1.231e-01	1.184e-01	-4.648e-03
5	6.790e+00	1.189e-01	1.151e-01	-3.836e-03
6	7.284e+00	1.152e-01	1.116e-01	-3.634e-03
7	7.778e+00	1.111e-01	1.080e-01	-3.109e-03
8	8.272e+00	1.070e-01	1.042e-01	-2.806e-03
9	8.766e+00	1.032e-01	1.004e-01	-2.832e-03
10	9.260e+00	9.853e-02	9.652e-02	-2.008e-03
11	9.753e+00	9.434e-02	9.259e-02	-1.758e-03
12	1.025e+01	9.006e-02	8.861e-02	-1.447e-03
13	1.074e+01	8.584e-02	8.463e-02	-1.215e-03
14	1.123e+01	8.110e-02	8.064e-02	-4.614e-04
15	1.173e+01	7.715e-02	7.668e-02	-4.640e-04
16	1.222e+01	7.275e-02	7.276e-02	9.036e-06
17	1.272e+01	6.916e-02	6.888e-02	-2.787e-04
18	1.321e+01	6.491e-02	6.508e-02	1.706e-04
19	1.370e+01	6.133e-02	6.135e-02	2.050e-05
20	1.420e+01	5.702e-02	5.771e-02	6.890e-04
21	1.469e+01	5.332e-02	5.417e-02	8.453e-04
22	1.519e+01	5.011e-02	5.073e-02	6.194e-04
23	1.568e+01	4.670e-02	4.741e-02	7.081e-04
24	1.617e+01	4.254e-02	4.422e-02	1.674e-03
25	1.667e+01	3.955e-02	4.114e-02	1.594e-03
26	1.716e+01	3.728e-02	3.820e-02	9.243e-04
27	1.766e+01	3.430e-02	3.539e-02	1.097e-03
28	1.815e+01	3.132e-02	3.272e-02	1.404e-03
29	1.864e+01	2.881e-02	3.018e-02	1.369e-03
30	1.914e+01	2.633e-02	2.778e-02	1.456e-03
31	1.963e+01	2.425e-02	2.552e-02	1.271e-03
32	2.012e+01	2.220e-02	2.339e-02	1.189e-03
33	2.062e+01	2.033e-02	2.139e-02	1.058e-03
34	2.111e+01	1.859e-02	1.952e-02	9.295e-04
35	2.161e+01	1.707e-02	1.778e-02	7.036e-04
36	2.210e+01	1.513e-02	1.615e-02	1.023e-03
37	2.259e+01	1.398e-02	1.465e-02	6.617e-04
38	2.309e+01	1.250e-02	1.325e-02	7.530e-04
39	2.358e+01	1.110e-02	1.196e-02	8.598e-04
40	2.408e+01	1.044e-02	1.077e-02	3.286e-04

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40 points for Integral 15, Integral Region from 1.558 to 1.432 ppm

Converged after 33 iterations!

Results Comp. 1

I[0] = 7.972e-01
Diff Con. = 1.139e-09 m2/s
Gamma = 4.258e+03 Hz/G
Little Delta = 3.400m
Big Delta = 49.900m

RSS = 1.056e-02
SD = 1.624e-02

Point	Gradient	Expt	Calc	Difference
1	0.000e+00	7.512e-01	7.972e-01	4.601e-02
2	0.000e+00	7.318e-01	7.972e-01	6.533e-02
3	5.803e+00	7.120e-01	6.829e-01	-2.912e-02
4	6.297e+00	6.913e-01	6.643e-01	-2.697e-02
5	6.790e+00	6.689e-01	6.449e-01	-2.398e-02
6	7.284e+00	6.457e-01	6.246e-01	-2.108e-02
7	7.778e+00	6.210e-01	6.036e-01	-1.738e-02
8	8.272e+00	5.976e-01	5.820e-01	-1.558e-02
9	8.766e+00	5.732e-01	5.600e-01	-1.320e-02
10	9.260e+00	5.469e-01	5.375e-01	-9.365e-03
11	9.753e+00	5.239e-01	5.148e-01	-9.075e-03
12	1.025e+01	4.982e-01	4.920e-01	-6.271e-03
13	1.074e+01	4.740e-01	4.691e-01	-4.879e-03
14	1.123e+01	4.489e-01	4.462e-01	-2.690e-03
15	1.173e+01	4.251e-01	4.236e-01	-1.533e-03
16	1.222e+01	3.999e-01	4.012e-01	1.277e-03
17	1.272e+01	3.770e-01	3.791e-01	2.049e-03
18	1.321e+01	3.549e-01	3.574e-01	2.548e-03
19	1.370e+01	3.337e-01	3.362e-01	2.522e-03
20	1.420e+01	3.116e-01	3.156e-01	4.028e-03
21	1.469e+01	2.903e-01	2.956e-01	5.267e-03
22	1.519e+01	2.719e-01	2.762e-01	4.309e-03
23	1.568e+01	2.522e-01	2.575e-01	5.269e-03
24	1.617e+01	2.330e-01	2.396e-01	6.569e-03
25	1.667e+01	2.144e-01	2.223e-01	7.939e-03
26	1.716e+01	1.986e-01	2.059e-01	7.266e-03
27	1.766e+01	1.832e-01	1.903e-01	7.037e-03
28	1.815e+01	1.689e-01	1.754e-01	6.454e-03
29	1.864e+01	1.548e-01	1.613e-01	6.492e-03
30	1.914e+01	1.418e-01	1.481e-01	6.325e-03
31	1.963e+01	1.301e-01	1.356e-01	5.490e-03
32	2.012e+01	1.186e-01	1.239e-01	5.303e-03
33	2.062e+01	1.079e-01	1.130e-01	5.087e-03
34	2.111e+01	9.799e-02	1.028e-01	4.769e-03
35	2.161e+01	9.011e-02	9.326e-02	3.144e-03

36	2.210e+01	8.102e-02	8.445e-02	3.429e-03
37	2.259e+01	7.247e-02	7.631e-02	3.846e-03
38	2.309e+01	6.530e-02	6.879e-02	3.491e-03
39	2.358e+01	5.845e-02	6.188e-02	3.424e-03
40	2.408e+01	5.321e-02	5.553e-02	2.326e-03

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DOSY data and refinements for PF_6^- salt 8

SIMFIT RESULTS
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Dataset : /home/strain/montana/PF6-_1H/4/pdata/1/ct1t2.txt

AREA fit : Diffusion : Variable Gradient :

I=I[0]*exp(-D*SQR(2*PI*gamma*Gi*LD)*(BD-LD/3)*1e4)

40 points for Integral 1, Integral Region from 8.995 to 8.865 ppm

Converged after 57 iterations!

Results Comp. 1

I[0] = 1.426e-01
Diff Con. = 8.521e-10 m2/s
Gamma = 4.258e+03 Hz/G
Little Delta = 3.400m
Big Delta = 49.900m

RSS = 2.876e-05
SD = 8.480e-04

Point	Gradient	Expt	Calc	Difference
1	0.000e+00	1.404e-01	1.426e-01	2.207e-03
2	0.000e+00	1.389e-01	1.426e-01	3.746e-03
3	3.519e+00	1.372e-01	1.367e-01	-5.195e-04
4	4.074e+00	1.351e-01	1.347e-01	-4.433e-04
5	4.630e+00	1.330e-01	1.325e-01	-5.079e-04
6	5.185e+00	1.303e-01	1.300e-01	-3.131e-04
7	5.741e+00	1.278e-01	1.273e-01	-4.257e-04
8	6.297e+00	1.253e-01	1.244e-01	-8.832e-04
9	6.852e+00	1.217e-01	1.214e-01	-3.581e-04
10	7.408e+00	1.182e-01	1.181e-01	-1.095e-04
11	7.963e+00	1.153e-01	1.147e-01	-6.024e-04
12	8.519e+00	1.114e-01	1.111e-01	-2.771e-04
13	9.074e+00	1.082e-01	1.075e-01	-7.459e-04
14	9.630e+00	1.043e-01	1.037e-01	-6.047e-04
15	1.019e+01	1.004e-01	9.983e-02	-5.696e-04
16	1.074e+01	9.647e-02	9.592e-02	-5.553e-04
17	1.130e+01	9.266e-02	9.196e-02	-6.938e-04
18	1.185e+01	8.834e-02	8.799e-02	-3.525e-04
19	1.241e+01	8.406e-02	8.400e-02	-6.189e-05
20	1.296e+01	8.018e-02	8.003e-02	-1.447e-04
21	1.352e+01	7.715e-02	7.608e-02	-1.070e-03
22	1.407e+01	7.225e-02	7.217e-02	-7.623e-05
23	1.463e+01	6.827e-02	6.833e-02	5.745e-05

24	1.519e+01	6.485e-02	6.454e-02	-3.053e-04
25	1.574e+01	6.091e-02	6.084e-02	-7.126e-05
26	1.630e+01	5.711e-02	5.723e-02	1.167e-04
27	1.685e+01	5.376e-02	5.372e-02	-4.325e-05
28	1.741e+01	5.027e-02	5.032e-02	4.610e-05
29	1.796e+01	4.678e-02	4.703e-02	2.419e-04
30	1.852e+01	4.345e-02	4.386e-02	4.166e-04
31	1.908e+01	4.063e-02	4.082e-02	1.908e-04
32	1.963e+01	3.775e-02	3.792e-02	1.630e-04
33	2.019e+01	3.452e-02	3.514e-02	6.214e-04
34	2.074e+01	3.215e-02	3.249e-02	3.438e-04
35	2.130e+01	2.970e-02	2.999e-02	2.869e-04
36	2.185e+01	2.660e-02	2.762e-02	1.015e-03
37	2.241e+01	2.508e-02	2.538e-02	2.951e-04
38	2.296e+01	2.227e-02	2.327e-02	9.983e-04
39	2.352e+01	2.047e-02	2.130e-02	8.283e-04
40	2.408e+01	1.884e-02	1.944e-02	6.003e-04

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40 points for Integral 3, Integral Region from 7.856 to 7.784 ppm

Converged after 52 iterations!

Results Comp. 1

I[0] = 7.483e-02
Diff Con. = 8.470e-10 m2/s
Gamma = 4.258e+03 Hz/G
Little Delta = 3.400m
Big Delta = 49.900m

RSS = 1.325e-05
SD = 5.755e-04

Point	Gradient	Expt	Calc	Difference
1	0.000e+00	7.348e-02	7.483e-02	1.350e-03
2	0.000e+00	7.239e-02	7.483e-02	2.439e-03
3	3.519e+00	7.201e-02	7.173e-02	-2.775e-04
4	4.074e+00	7.078e-02	7.070e-02	-7.197e-05
5	4.630e+00	6.957e-02	6.954e-02	-2.601e-05
6	5.185e+00	6.850e-02	6.826e-02	-2.335e-04
7	5.741e+00	6.722e-02	6.686e-02	-3.575e-04
8	6.297e+00	6.548e-02	6.535e-02	-1.313e-04
9	6.852e+00	6.370e-02	6.374e-02	4.062e-05
10	7.408e+00	6.243e-02	6.203e-02	-3.976e-04
11	7.963e+00	6.064e-02	6.025e-02	-3.885e-04
12	8.519e+00	5.888e-02	5.839e-02	-4.827e-04
13	9.074e+00	5.701e-02	5.648e-02	-5.324e-04
14	9.630e+00	5.514e-02	5.451e-02	-6.342e-04

15	1.019e+01	5.274e-02	5.249e-02	-2.511e-04
16	1.074e+01	5.101e-02	5.045e-02	-5.621e-04
17	1.130e+01	4.901e-02	4.838e-02	-6.272e-04
18	1.185e+01	4.675e-02	4.630e-02	-4.444e-04
19	1.241e+01	4.462e-02	4.422e-02	-4.039e-04
20	1.296e+01	4.232e-02	4.214e-02	-1.820e-04
21	1.352e+01	4.081e-02	4.007e-02	-7.383e-04
22	1.407e+01	3.828e-02	3.802e-02	-2.592e-04
23	1.463e+01	3.609e-02	3.601e-02	-8.217e-05
24	1.519e+01	3.417e-02	3.403e-02	-1.405e-04
25	1.574e+01	3.155e-02	3.209e-02	5.334e-04
26	1.630e+01	3.003e-02	3.019e-02	1.632e-04
27	1.685e+01	2.831e-02	2.835e-02	4.003e-05
28	1.741e+01	2.640e-02	2.657e-02	1.665e-04
29	1.796e+01	2.459e-02	2.484e-02	2.518e-04
30	1.852e+01	2.297e-02	2.318e-02	2.082e-04
31	1.908e+01	2.114e-02	2.158e-02	4.414e-04
32	1.963e+01	1.988e-02	2.005e-02	1.688e-04
33	2.019e+01	1.819e-02	1.859e-02	4.061e-04
34	2.074e+01	1.692e-02	1.720e-02	2.761e-04
35	2.130e+01	1.562e-02	1.588e-02	2.612e-04
36	2.185e+01	1.435e-02	1.463e-02	2.853e-04
37	2.241e+01	1.329e-02	1.345e-02	1.660e-04
38	2.296e+01	1.161e-02	1.234e-02	7.321e-04
39	2.352e+01	1.080e-02	1.130e-02	4.996e-04
40	2.408e+01	9.789e-03	1.032e-02	5.356e-04

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40 points for Integral 4, Integral Region from 7.704 to 7.610 ppm

Converged after 53 iterations!

Results Comp. 1

I[0] = 1.146e-01
Diff Con. = 8.531e-10 m2/s
Gamma = 4.258e+03 Hz/G
Little Delta = 3.400m
Big Delta = 49.900m

RSS = 2.073e-05
SD = 7.199e-04

Point	Gradient	Expt	Calc	Difference
1	0.000e+00	1.126e-01	1.146e-01	1.935e-03
2	0.000e+00	1.114e-01	1.146e-01	3.156e-03
3	3.519e+00	1.100e-01	1.098e-01	-1.812e-04
4	4.074e+00	1.083e-01	1.082e-01	-1.426e-04
5	4.630e+00	1.067e-01	1.064e-01	-3.184e-04

6	5.185e+00	1.048e-01	1.044e-01	-3.235e-04
7	5.741e+00	1.027e-01	1.023e-01	-4.055e-04
8	6.297e+00	1.006e-01	9.995e-02	-6.400e-04
9	6.852e+00	9.806e-02	9.747e-02	-5.916e-04
10	7.408e+00	9.514e-02	9.484e-02	-2.916e-04
11	7.963e+00	9.277e-02	9.210e-02	-6.670e-04
12	8.519e+00	8.988e-02	8.924e-02	-6.367e-04
13	9.074e+00	8.697e-02	8.629e-02	-6.823e-04
14	9.630e+00	8.404e-02	8.326e-02	-7.857e-04
15	1.019e+01	8.056e-02	8.016e-02	-3.991e-04
16	1.074e+01	7.738e-02	7.702e-02	-3.573e-04
17	1.130e+01	7.415e-02	7.384e-02	-3.119e-04
18	1.185e+01	7.106e-02	7.064e-02	-4.131e-04
19	1.241e+01	6.783e-02	6.744e-02	-3.871e-04
20	1.296e+01	6.455e-02	6.425e-02	-3.015e-04
21	1.352e+01	6.151e-02	6.107e-02	-4.390e-04
22	1.407e+01	5.820e-02	5.793e-02	-2.618e-04
23	1.463e+01	5.483e-02	5.484e-02	1.139e-05
24	1.519e+01	5.187e-02	5.180e-02	-7.211e-05
25	1.574e+01	4.833e-02	4.883e-02	4.995e-04
26	1.630e+01	4.576e-02	4.593e-02	1.637e-04
27	1.685e+01	4.259e-02	4.311e-02	5.190e-04
28	1.741e+01	4.050e-02	4.037e-02	-1.325e-04
29	1.796e+01	3.737e-02	3.773e-02	3.622e-04
30	1.852e+01	3.524e-02	3.519e-02	-4.500e-05
31	1.908e+01	3.217e-02	3.275e-02	5.775e-04
32	1.963e+01	3.041e-02	3.041e-02	6.517e-06
33	2.019e+01	2.780e-02	2.818e-02	3.799e-04
34	2.074e+01	2.570e-02	2.606e-02	3.624e-04
35	2.130e+01	2.348e-02	2.405e-02	5.713e-04
36	2.185e+01	2.144e-02	2.214e-02	7.075e-04
37	2.241e+01	2.009e-02	2.035e-02	2.613e-04
38	2.296e+01	1.845e-02	1.866e-02	2.016e-04
39	2.352e+01	1.638e-02	1.707e-02	6.954e-04
40	2.408e+01	1.540e-02	1.558e-02	1.875e-04

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40 points for Integral 5, Integral Region from 7.581 to 7.479 ppm

Converged after 58 iterations!

Results Comp. 1

I[0] = 1.723e-01
Diff Con. = 8.480e-10 m2/s
Gamma = 4.258e+03 Hz/G
Little Delta = 3.400m
Big Delta = 49.900m

RSS = 3.978e-05

SD = 9.972e-04

Point	Gradient	Expt	Calc	Difference
1	0.000e+00	1.691e-01	1.723e-01	3.131e-03
2	0.000e+00	1.680e-01	1.723e-01	4.227e-03
3	3.519e+00	1.658e-01	1.651e-01	-6.603e-04
4	4.074e+00	1.635e-01	1.627e-01	-7.814e-04
5	4.630e+00	1.606e-01	1.601e-01	-4.915e-04
6	5.185e+00	1.583e-01	1.571e-01	-1.137e-03
7	5.741e+00	1.546e-01	1.539e-01	-7.035e-04
8	6.297e+00	1.509e-01	1.504e-01	-5.435e-04
9	6.852e+00	1.470e-01	1.467e-01	-3.350e-04
10	7.408e+00	1.432e-01	1.428e-01	-4.574e-04
11	7.963e+00	1.394e-01	1.387e-01	-7.165e-04
12	8.519e+00	1.346e-01	1.344e-01	-2.693e-04
13	9.074e+00	1.308e-01	1.300e-01	-8.229e-04
14	9.630e+00	1.260e-01	1.254e-01	-5.350e-04
15	1.019e+01	1.213e-01	1.208e-01	-5.294e-04
16	1.074e+01	1.167e-01	1.161e-01	-6.537e-04
17	1.130e+01	1.121e-01	1.113e-01	-7.405e-04
18	1.185e+01	1.066e-01	1.065e-01	-5.628e-05
19	1.241e+01	1.020e-01	1.017e-01	-2.708e-04
20	1.296e+01	9.701e-02	9.694e-02	-7.671e-05
21	1.352e+01	9.322e-02	9.217e-02	-1.049e-03
22	1.407e+01	8.782e-02	8.746e-02	-3.573e-04
23	1.463e+01	8.282e-02	8.282e-02	-6.546e-07
24	1.519e+01	7.852e-02	7.826e-02	-2.623e-04
25	1.574e+01	7.361e-02	7.379e-02	1.839e-04
26	1.630e+01	6.942e-02	6.943e-02	8.211e-06
27	1.685e+01	6.475e-02	6.519e-02	4.478e-04
28	1.741e+01	6.112e-02	6.108e-02	-3.502e-05
29	1.796e+01	5.685e-02	5.711e-02	2.541e-04
30	1.852e+01	5.330e-02	5.328e-02	-1.730e-05
31	1.908e+01	4.909e-02	4.961e-02	5.140e-04
32	1.963e+01	4.591e-02	4.609e-02	1.819e-04
33	2.019e+01	4.231e-02	4.273e-02	4.185e-04
34	2.074e+01	3.875e-02	3.953e-02	7.843e-04
35	2.130e+01	3.564e-02	3.650e-02	8.607e-04
36	2.185e+01	3.340e-02	3.362e-02	2.178e-04
37	2.241e+01	3.027e-02	3.091e-02	6.444e-04
38	2.296e+01	2.736e-02	2.836e-02	9.927e-04
39	2.352e+01	2.534e-02	2.596e-02	6.217e-04
40	2.408e+01	2.320e-02	2.371e-02	5.176e-04

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40 points for Integral 6, Integral Region from 7.022 to 6.913 ppm

Converged after 59 iterations!

Results Comp. 1

I[0] = 1.280e-01
Diff Con. = 8.735e-10 m2/s
Gamma = 4.258e+03 Hz/G
Little Delta = 3.400m
Big Delta = 49.900m

RSS = 2.303e-05
SD = 7.588e-04

Point	Gradient	Expt	Calc	Difference
1	0.000e+00	1.261e-01	1.280e-01	1.867e-03
2	0.000e+00	1.244e-01	1.280e-01	3.608e-03
3	3.519e+00	1.232e-01	1.225e-01	-7.304e-04
4	4.074e+00	1.216e-01	1.207e-01	-8.525e-04
5	4.630e+00	1.190e-01	1.187e-01	-3.612e-04
6	5.185e+00	1.169e-01	1.164e-01	-5.019e-04
7	5.741e+00	1.148e-01	1.139e-01	-8.166e-04
8	6.297e+00	1.117e-01	1.113e-01	-4.433e-04
9	6.852e+00	1.086e-01	1.085e-01	-1.554e-04
10	7.408e+00	1.059e-01	1.055e-01	-3.802e-04
11	7.963e+00	1.028e-01	1.024e-01	-4.371e-04
12	8.519e+00	9.950e-02	9.910e-02	-4.027e-04
13	9.074e+00	9.628e-02	9.575e-02	-5.345e-04
14	9.630e+00	9.274e-02	9.230e-02	-4.345e-04
15	1.019e+01	8.918e-02	8.879e-02	-3.908e-04
16	1.074e+01	8.578e-02	8.522e-02	-5.584e-04
17	1.130e+01	8.176e-02	8.162e-02	-1.366e-04
18	1.185e+01	7.826e-02	7.801e-02	-2.483e-04
19	1.241e+01	7.462e-02	7.439e-02	-2.306e-04
20	1.296e+01	7.070e-02	7.079e-02	8.398e-05
21	1.352e+01	6.795e-02	6.721e-02	-7.415e-04
22	1.407e+01	6.352e-02	6.367e-02	1.525e-04
23	1.463e+01	5.972e-02	6.019e-02	4.739e-04
24	1.519e+01	5.717e-02	5.678e-02	-3.911e-04
25	1.574e+01	5.327e-02	5.344e-02	1.698e-04
26	1.630e+01	5.002e-02	5.019e-02	1.764e-04
27	1.685e+01	4.684e-02	4.704e-02	2.065e-04
28	1.741e+01	4.362e-02	4.399e-02	3.698e-04
29	1.796e+01	4.076e-02	4.104e-02	2.837e-04
30	1.852e+01	3.811e-02	3.822e-02	1.054e-04
31	1.908e+01	3.542e-02	3.550e-02	8.420e-05
32	1.963e+01	3.286e-02	3.291e-02	4.902e-05
33	2.019e+01	2.992e-02	3.044e-02	5.224e-04
34	2.074e+01	2.738e-02	2.810e-02	7.147e-04
35	2.130e+01	2.576e-02	2.588e-02	1.143e-04
36	2.185e+01	2.359e-02	2.378e-02	1.949e-04
37	2.241e+01	2.144e-02	2.181e-02	3.716e-04
38	2.296e+01	1.962e-02	1.995e-02	3.315e-04

39	2.352e+01	1.802e-02	1.822e-02	1.998e-04
40	2.408e+01	1.652e-02	1.660e-02	7.253e-05

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40 points for Integral 8, Integral Region from 4.360 to 4.287 ppm

Converged after 46 iterations!

Results Comp. 1

I[0] = 2.876e-01
Diff Con. = 8.399e-10 m2/s
Gamma = 4.258e+03 Hz/G
Little Delta = 3.400m
Big Delta = 49.900m

RSS = 9.584e-05
SD = 1.548e-03

Point	Gradient	Expt	Calc	Difference
1	0.000e+00	2.832e-01	2.876e-01	4.366e-03
2	0.000e+00	2.805e-01	2.876e-01	7.124e-03
3	3.519e+00	2.764e-01	2.758e-01	-6.644e-04
4	4.074e+00	2.731e-01	2.719e-01	-1.253e-03
5	4.630e+00	2.684e-01	2.674e-01	-9.904e-04
6	5.185e+00	2.637e-01	2.625e-01	-1.134e-03
7	5.741e+00	2.585e-01	2.572e-01	-1.307e-03
8	6.297e+00	2.525e-01	2.514e-01	-1.096e-03
9	6.852e+00	2.463e-01	2.453e-01	-9.910e-04
10	7.408e+00	2.400e-01	2.388e-01	-1.184e-03
11	7.963e+00	2.330e-01	2.320e-01	-9.959e-04
12	8.519e+00	2.258e-01	2.249e-01	-9.070e-04
13	9.074e+00	2.185e-01	2.176e-01	-9.164e-04
14	9.630e+00	2.112e-01	2.100e-01	-1.169e-03
15	1.019e+01	2.031e-01	2.023e-01	-7.197e-04
16	1.074e+01	1.952e-01	1.945e-01	-6.796e-04
17	1.130e+01	1.871e-01	1.866e-01	-4.324e-04
18	1.185e+01	1.792e-01	1.787e-01	-5.761e-04
19	1.241e+01	1.714e-01	1.707e-01	-6.647e-04
20	1.296e+01	1.631e-01	1.627e-01	-3.919e-04
21	1.352e+01	1.566e-01	1.548e-01	-1.762e-03
22	1.407e+01	1.466e-01	1.470e-01	4.014e-04
23	1.463e+01	1.388e-01	1.392e-01	4.475e-04
24	1.519e+01	1.320e-01	1.316e-01	-3.516e-04
25	1.574e+01	1.239e-01	1.242e-01	2.681e-04
26	1.630e+01	1.167e-01	1.169e-01	2.213e-04
27	1.685e+01	1.097e-01	1.099e-01	1.537e-04
28	1.741e+01	1.024e-01	1.030e-01	6.027e-04
29	1.796e+01	9.604e-02	9.635e-02	3.138e-04

30	1.852e+01	8.974e-02	8.996e-02	2.222e-04
31	1.908e+01	8.302e-02	8.381e-02	7.862e-04
32	1.963e+01	7.745e-02	7.793e-02	4.808e-04
33	2.019e+01	7.178e-02	7.229e-02	5.151e-04
34	2.074e+01	6.609e-02	6.693e-02	8.397e-04
35	2.130e+01	6.105e-02	6.184e-02	7.865e-04
36	2.185e+01	5.667e-02	5.701e-02	3.473e-04
37	2.241e+01	5.141e-02	5.246e-02	1.045e-03
38	2.296e+01	4.733e-02	4.816e-02	8.345e-04
39	2.352e+01	4.329e-02	4.413e-02	8.351e-04
40	2.408e+01	3.932e-02	4.034e-02	1.024e-03

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40 points for Integral 9, Integral Region from 3.859 to 3.780 ppm

Converged after 51 iterations!

Results Comp. 1

I[0] = 2.049e-01
Diff Con. = 8.391e-10 m2/s
Gamma = 4.258e+03 Hz/G
Little Delta = 3.400m
Big Delta = 49.900m

RSS = 4.794e-05
SD = 1.095e-03

Point	Gradient	Expt	Calc	Difference
1	0.000e+00	2.017e-01	2.049e-01	3.204e-03
2	0.000e+00	2.000e-01	2.049e-01	4.986e-03
3	3.519e+00	1.974e-01	1.965e-01	-8.736e-04
4	4.074e+00	1.950e-01	1.937e-01	-1.215e-03
5	4.630e+00	1.915e-01	1.906e-01	-8.788e-04
6	5.185e+00	1.879e-01	1.871e-01	-7.843e-04
7	5.741e+00	1.842e-01	1.833e-01	-9.091e-04
8	6.297e+00	1.801e-01	1.792e-01	-8.848e-04
9	6.852e+00	1.753e-01	1.748e-01	-4.595e-04
10	7.408e+00	1.707e-01	1.702e-01	-5.165e-04
11	7.963e+00	1.659e-01	1.653e-01	-5.414e-04
12	8.519e+00	1.610e-01	1.603e-01	-7.390e-04
13	9.074e+00	1.555e-01	1.551e-01	-4.330e-04
14	9.630e+00	1.504e-01	1.497e-01	-6.334e-04
15	1.019e+01	1.447e-01	1.442e-01	-4.313e-04
16	1.074e+01	1.391e-01	1.387e-01	-4.002e-04
17	1.130e+01	1.334e-01	1.330e-01	-3.917e-04
18	1.185e+01	1.277e-01	1.274e-01	-3.085e-04
19	1.241e+01	1.217e-01	1.217e-01	2.199e-05
20	1.296e+01	1.161e-01	1.160e-01	-9.973e-05

21	1.352e+01	1.116e-01	1.104e-01	-1.166e-03
22	1.407e+01	1.049e-01	1.048e-01	-1.172e-04
23	1.463e+01	9.909e-02	9.929e-02	2.058e-04
24	1.519e+01	9.365e-02	9.388e-02	2.230e-04
25	1.574e+01	8.858e-02	8.858e-02	-6.030e-06
26	1.630e+01	8.361e-02	8.339e-02	-2.159e-04
27	1.685e+01	7.826e-02	7.836e-02	9.323e-05
28	1.741e+01	7.351e-02	7.346e-02	-4.746e-05
29	1.796e+01	6.871e-02	6.873e-02	2.428e-05
30	1.852e+01	6.363e-02	6.418e-02	5.501e-04
31	1.908e+01	5.925e-02	5.979e-02	5.407e-04
32	1.963e+01	5.535e-02	5.560e-02	2.439e-04
33	2.019e+01	5.146e-02	5.158e-02	1.208e-04
34	2.074e+01	4.730e-02	4.776e-02	4.575e-04
35	2.130e+01	4.385e-02	4.413e-02	2.819e-04
36	2.185e+01	4.019e-02	4.069e-02	4.974e-04
37	2.241e+01	3.652e-02	3.744e-02	9.261e-04
38	2.296e+01	3.380e-02	3.438e-02	5.722e-04
39	2.352e+01	3.063e-02	3.150e-02	8.741e-04
40	2.408e+01	2.818e-02	2.880e-02	6.270e-04

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40 points for Integral 12, Integral Region from 1.436 to 1.386 ppm

Converged after 37 iterations!

Results Comp. 1

I[0] = 7.228e-01
Diff Con. = 8.993e-10 m2/s
Gamma = 4.258e+03 Hz/G
Little Delta = 3.400m
Big Delta = 49.900m

RSS = 6.218e-04
SD = 3.943e-03

Point	Gradient	Expt	Calc	Difference
1	0.000e+00	7.171e-01	7.228e-01	5.712e-03
2	0.000e+00	7.099e-01	7.228e-01	1.295e-02
3	3.519e+00	6.999e-01	6.910e-01	-8.839e-03
4	4.074e+00	6.872e-01	6.806e-01	-6.599e-03
5	4.630e+00	6.754e-01	6.687e-01	-6.647e-03
6	5.185e+00	6.612e-01	6.556e-01	-5.537e-03
7	5.741e+00	6.455e-01	6.413e-01	-4.211e-03
8	6.297e+00	6.286e-01	6.259e-01	-2.702e-03
9	6.852e+00	6.106e-01	6.096e-01	-9.878e-04
10	7.408e+00	5.930e-01	5.923e-01	-6.898e-04
11	7.963e+00	5.750e-01	5.743e-01	-7.650e-04

12	8.519e+00	5.548e-01	5.555e-01	6.463e-04
13	9.074e+00	5.349e-01	5.361e-01	1.195e-03
14	9.630e+00	5.141e-01	5.163e-01	2.137e-03
15	1.019e+01	4.931e-01	4.961e-01	2.916e-03
16	1.074e+01	4.733e-01	4.756e-01	2.266e-03
17	1.130e+01	4.517e-01	4.549e-01	3.174e-03
18	1.185e+01	4.313e-01	4.342e-01	2.908e-03
19	1.241e+01	4.102e-01	4.134e-01	3.271e-03
20	1.296e+01	3.899e-01	3.929e-01	2.951e-03
21	1.352e+01	3.726e-01	3.724e-01	-1.880e-04
22	1.407e+01	3.486e-01	3.523e-01	3.607e-03
23	1.463e+01	3.287e-01	3.325e-01	3.773e-03
24	1.519e+01	3.106e-01	3.131e-01	2.447e-03
25	1.574e+01	2.920e-01	2.942e-01	2.156e-03
26	1.630e+01	2.739e-01	2.757e-01	1.825e-03
27	1.685e+01	2.569e-01	2.579e-01	1.006e-03
28	1.741e+01	2.401e-01	2.407e-01	6.317e-04
29	1.796e+01	2.241e-01	2.241e-01	5.887e-05
30	1.852e+01	2.088e-01	2.083e-01	-5.601e-04
31	1.908e+01	1.938e-01	1.931e-01	-7.303e-04
32	1.963e+01	1.799e-01	1.786e-01	-1.331e-03
33	2.019e+01	1.671e-01	1.648e-01	-2.321e-03
34	2.074e+01	1.539e-01	1.517e-01	-2.178e-03
35	2.130e+01	1.422e-01	1.394e-01	-2.806e-03
36	2.185e+01	1.308e-01	1.278e-01	-3.040e-03
37	2.241e+01	1.205e-01	1.169e-01	-3.646e-03
38	2.296e+01	1.108e-01	1.067e-01	-4.146e-03
39	2.352e+01	1.010e-01	9.714e-02	-3.858e-03
40	2.408e+01	9.295e-02	8.825e-02	-4.700e-03

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DOSY data and refinement for the internal standard, dichloromethane

40 points for Integral 8, Integral Region from 5.561 to 5.486 ppm

Converged after 52 iterations!

Results Comp. 1

I[0] = 2.797e-01
Diff Con. = 3.718e-09 m2/s
Gamma = 4.258e+03 Hz/G
Little Delta = 3.400m
Big Delta = 49.900m

RSS = 7.459e-03
SD = 1.366e-02

Point	Gradient	Expt	Calc	Difference
1	0.000e+00	2.711e-01	2.797e-01	8.564e-03
2	0.000e+00	2.429e-01	2.797e-01	3.680e-02
3	5.803e+00	2.152e-01	1.688e-01	-4.642e-02
4	6.297e+00	1.885e-01	1.543e-01	-3.417e-02
5	6.790e+00	1.635e-01	1.401e-01	-2.348e-02
6	7.284e+00	1.405e-01	1.262e-01	-1.427e-02
7	7.778e+00	1.188e-01	1.129e-01	-5.974e-03
8	8.272e+00	9.948e-02	1.002e-01	7.228e-04
9	8.766e+00	8.291e-02	8.832e-02	5.413e-03
10	9.260e+00	6.785e-02	7.728e-02	9.427e-03
11	9.753e+00	5.502e-02	6.714e-02	1.212e-02
12	1.025e+01	4.445e-02	5.789e-02	1.345e-02
13	1.074e+01	3.531e-02	4.956e-02	1.425e-02
14	1.123e+01	2.769e-02	4.211e-02	1.442e-02
15	1.173e+01	2.117e-02	3.552e-02	1.435e-02
16	1.222e+01	1.615e-02	2.974e-02	1.359e-02
17	1.272e+01	1.243e-02	2.472e-02	1.230e-02
18	1.321e+01	9.044e-03	2.041e-02	1.137e-02
19	1.370e+01	6.414e-03	1.672e-02	1.031e-02
20	1.420e+01	4.648e-03	1.360e-02	8.950e-03
21	1.469e+01	3.421e-03	1.098e-02	7.557e-03
22	1.519e+01	2.181e-03	8.797e-03	6.616e-03
23	1.568e+01	1.282e-03	6.999e-03	5.716e-03
24	1.617e+01	7.923e-04	5.530e-03	4.738e-03
25	1.667e+01	4.374e-04	4.335e-03	3.898e-03
26	1.716e+01	3.249e-05	3.374e-03	3.342e-03
27	1.766e+01	2.937e-05	2.607e-03	2.578e-03
28	1.815e+01	-2.249e-04	1.999e-03	2.224e-03
29	1.864e+01	-9.501e-05	1.522e-03	1.617e-03
30	1.914e+01	-3.932e-04	1.151e-03	1.544e-03
31	1.963e+01	-3.852e-04	8.638e-04	1.249e-03
32	2.012e+01	-4.265e-04	6.434e-04	1.070e-03

33	2.062e+01	-2.851e-04	4.757e-04	7.608e-04
34	2.111e+01	-4.428e-04	3.492e-04	7.920e-04
35	2.161e+01	-4.025e-04	2.545e-04	6.570e-04
36	2.210e+01	-3.278e-04	1.841e-04	5.118e-04
37	2.259e+01	-4.406e-04	1.323e-04	5.729e-04
38	2.309e+01	-1.505e-04	9.428e-05	2.448e-04
39	2.358e+01	-3.196e-04	6.672e-05	3.863e-04
40	2.408e+01	-3.161e-04	4.687e-05	3.630e-04

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S11. Triple helicate UV-Vis titrations

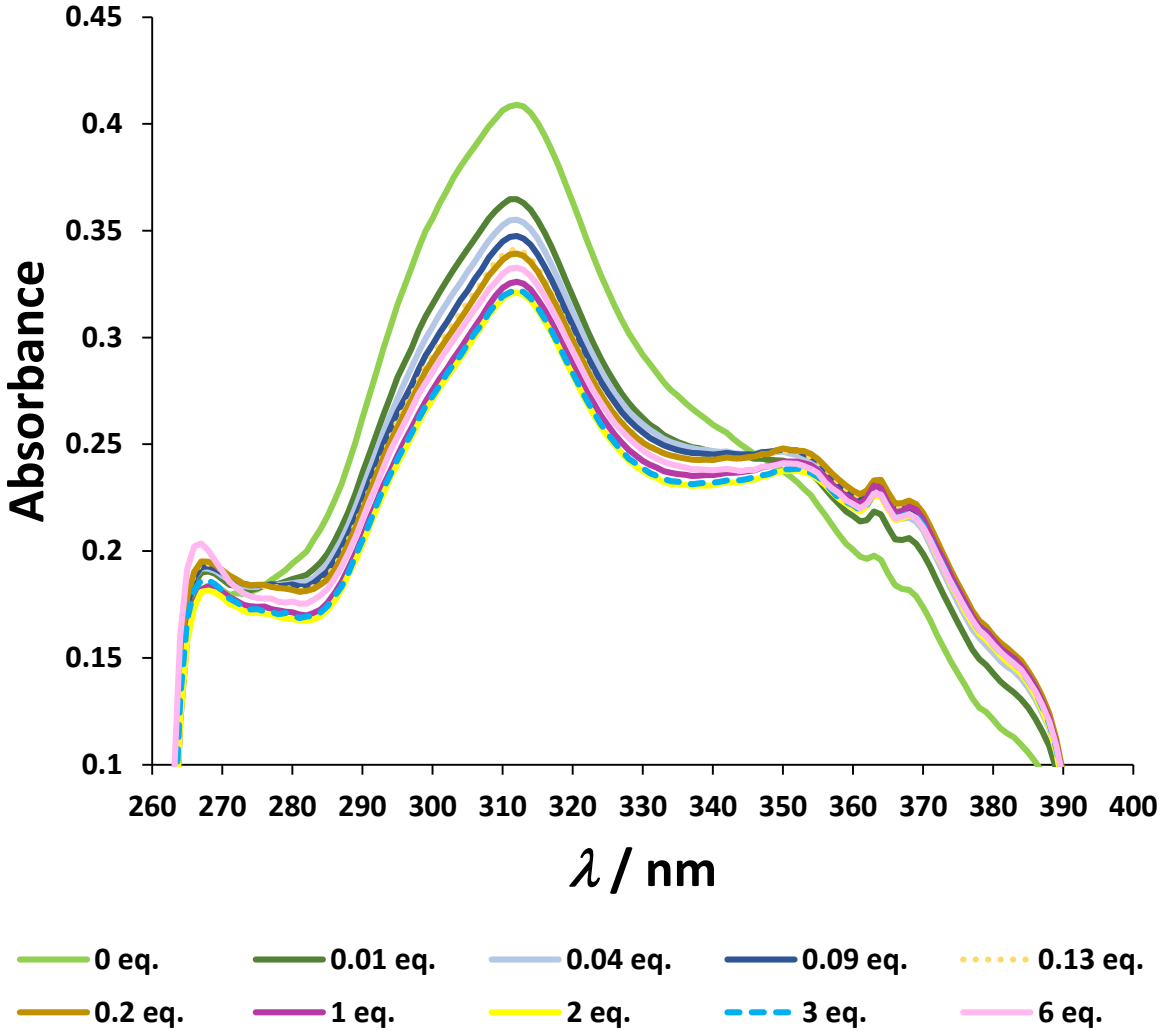

Figure S42. UV-Vis difference spectrum of **8** (5 μM) with additions of TBA iodide (colors represent eq. of guest added; 1:3 v/v DMF-MeCN, 298 K).

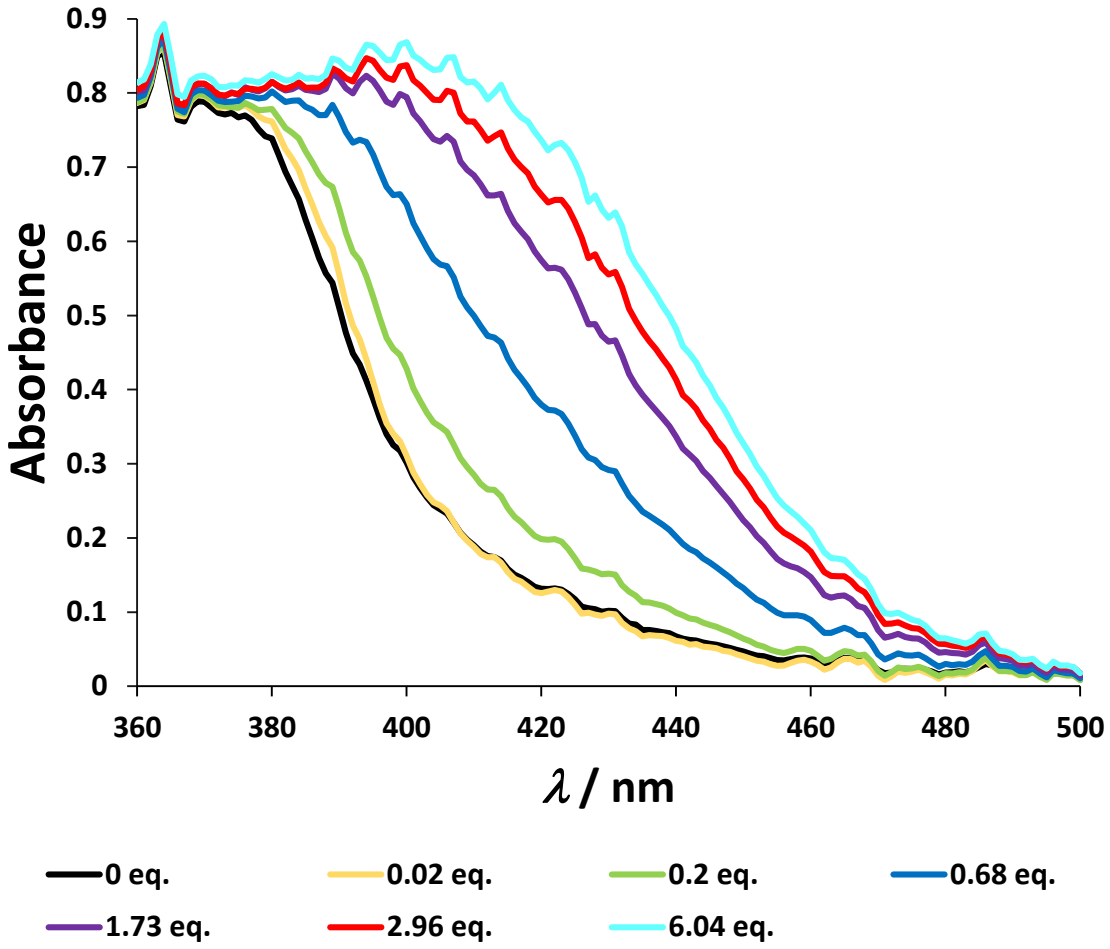

Figure S43. UV-Vis difference spectrum of **8** (0.3 mM) with additions of TBA iodide (colors represent eq. of guest added; 1:3 v/v DMF-MeCN, 298 K).

S12. Triple helicate fidelity and stability in aqueous phase

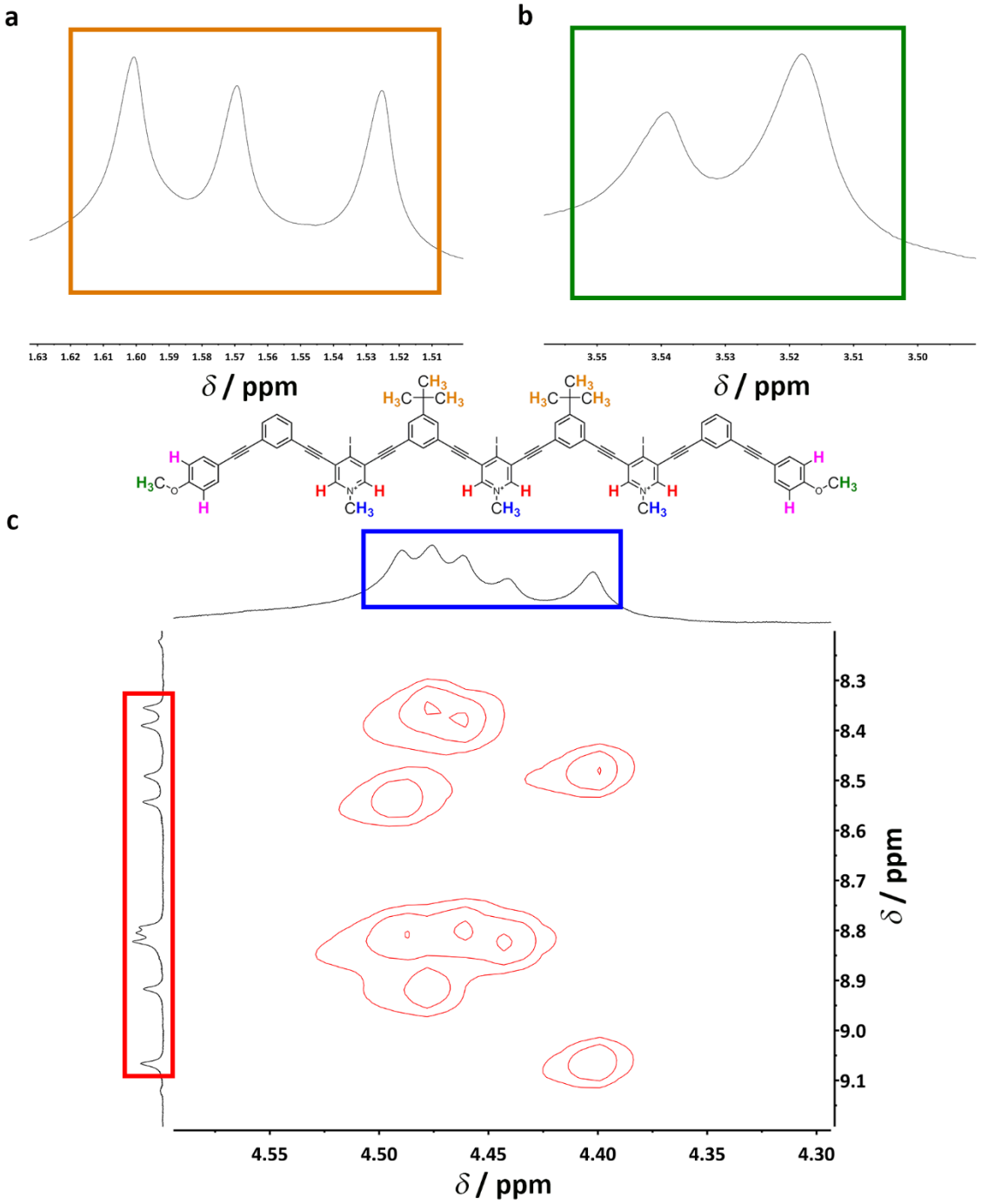

Figure S44. ^{1}H NMR and 2D NOESY spectroscopic analysis of the numbers and relative intensities of key resonances of **7**. a) ^{1}H NMR spectrum of three *tert*-butyl peaks of equal intensity. b) ^{1}H NMR spectrum of two methoxy methyl peaks. One is twice the intensity of the other and likely two overlapping peaks. c) ^{1}H NMR spectrum of four pyridinium methyl peaks of equal intensity and one of half intensity. Nine pyridinium protons are clearly seen with their NOEs. Conditions for figures (a)–(c): 600 MHz, 1:1 v/v D_2O-[D_7]DMF, 298 K.

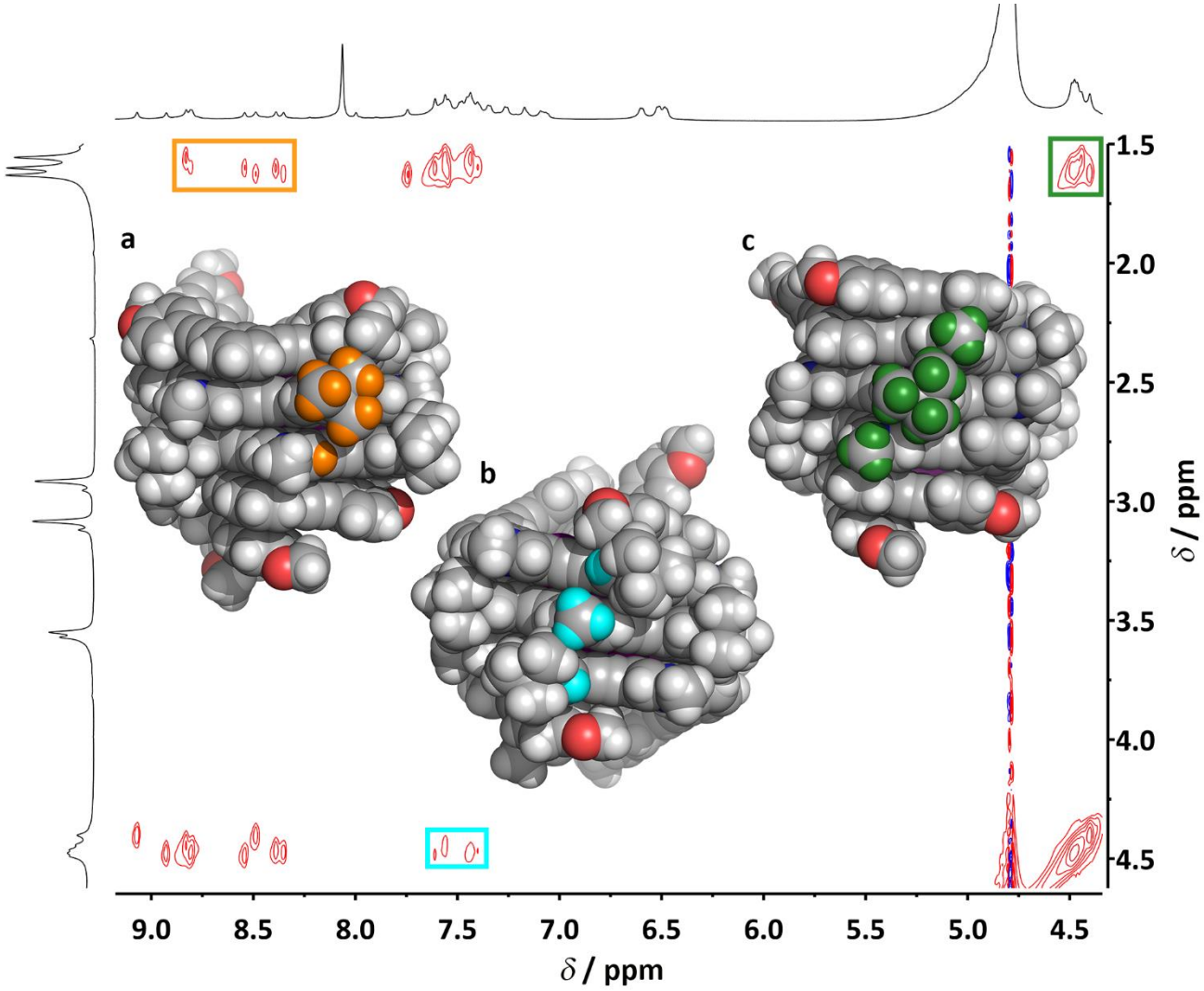

Figure S45. 2D NOESY spectrum of triple helicate **7** in an aqueous environment. a) *tert*-Butyl and pyridinium cross peaks. b) *tert*-Butylbenzene and pyridinium methyl cross peaks. **c**) Pyridinium methyl and *tert*-butyl cross peaks. Conditions for figures (a)–(c): 600 MHz, 1:1 v/v D_2O-[D_7]DMF, 298 K. Not all colors are representative of atom identity.

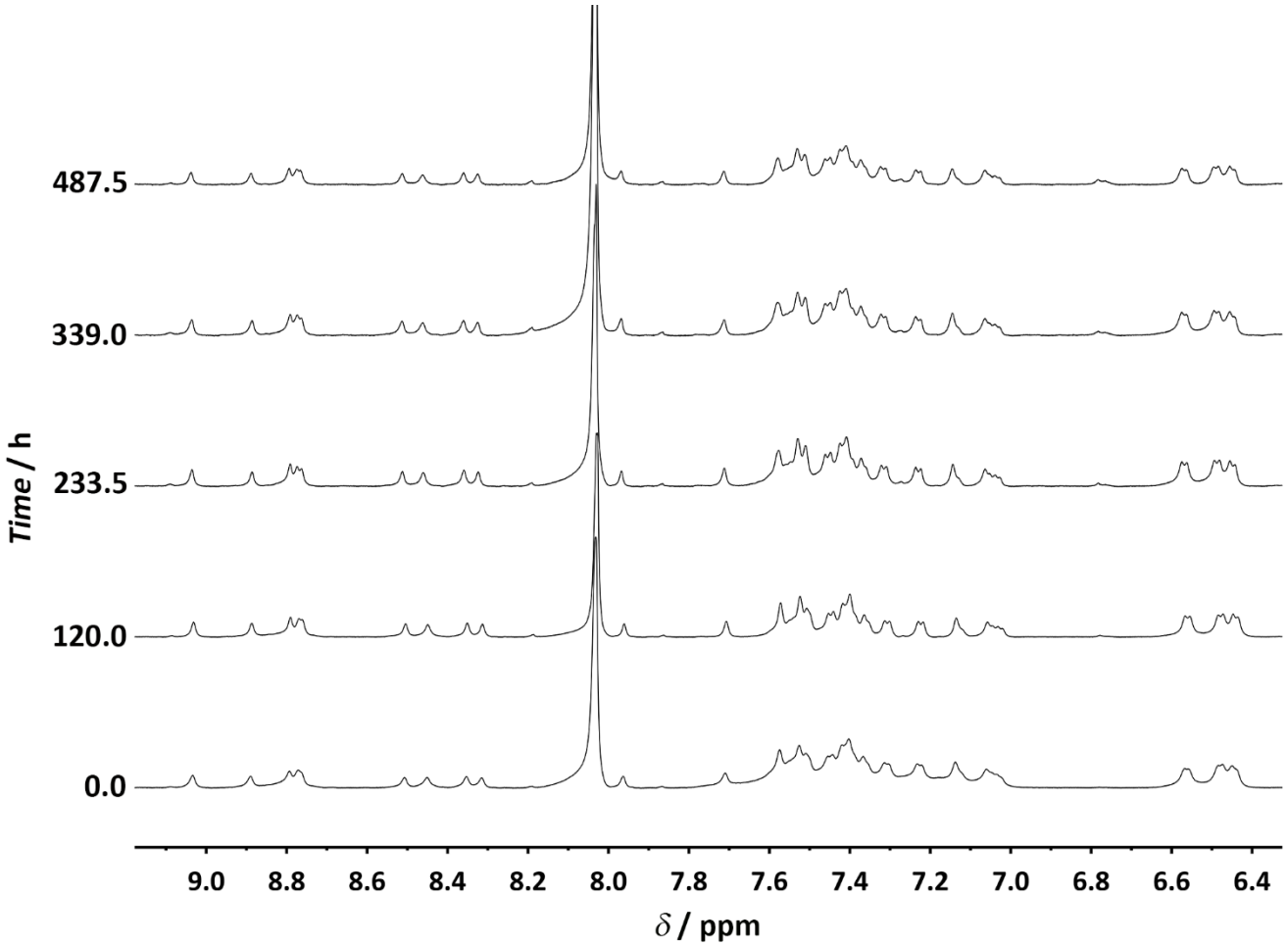

Figure S46. ^{1}H NMR spectra of triple helicate **7** in an aqueous environment. After 487.5 h (approximately 20 days), **7** showed only minimal signs of decomposition (600 MHz, 1:1 v/v D_2O-[D_7]DMF, 298 K).

S13. References

[1] K. Sonogashira, Y. Tohda, N. Hagihara, *Tetrahedron Lett.* **1975**, *16*, 4467-4470.

[2] Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato,M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.;Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.;Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian 09, Revision B.01; Gaussian, Inc.: Wallingford, CT, 2009.

[3] W. B. Wan, M. M. Haley, *J. Org. Chem.* **2001**, *66*, 3893-3901.

[4] S. Z. Vatsadze, I. D. Titanyuk, A. V. Chernikov, N. V. Zyk, *Russ. Chem. Bull.*, *53*, 471-473.

[5] A. J. Martínez-Martínez, A. R. Kennedy, R. E. Mulvey, C. T. O'Hara, *Science* **2014**, *346*, 834-837.

[6] D. A. Shultz, H. Lee, R. K. Kumar, K. P. Gwaltney, *J. Org. Chem.* **1999**, *64*, 9124-9136.

[7] Y. Tobe, J.-y. Kishi, I. Ohki, M. Sonoda, *J. Org. Chem.* **2003**, *68*, 3330-3332.

[8] T. Usuki, H. Yamada, T. Hayashi, H. Yanuma, Y. Koseki, N. Suzuki, Y. Masuyama, Y. Y. Lin, *Chem. Commun.* **2012**, *48*, 3233-3235.

[9] G. M. Sheldrick, SADABS: Area Detector Absorption Correction; University of Göttingen: Göttingen, Germany, 2001.

[10] O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard, H. Puschmann, *J. Appl. Crystallogr.* **2009**, *42*, 339-341.

[11] G. Sheldrick, *Acta Crystallogr. Sect. A* **2015**, *71*, 3-8.

[12] G. Sheldrick, *Acta Crystallogr. Sect. C* **2015**, *71*, 3-8.

[13] A. Spek, *Acta Crystallogr. Sect. C* **2015**, *71*, 9-18.

[14] A. Spek, *Acta Crystallogr. Sect. D* **2009**, *65*, 148-155.

[15] Bruker (2007). APEX2. Bruker AXS Inc., Madison, Wisconsin, USA.

[16] G. Sheldrick, *Acta Crystallogr. Sect. A* **2008**, *64*, 112-122.

[17] aD. Feller, *J. Comput. Chem.* **1996**, *17*, 1571-1586; bK. L. Schuchardt, B. T. Didier, T. Elsethagen, L. Sun, V. Gurumoorthi, J. Chase, J. Li, T. L. Windus, *J. Chem. Inf. Model.* **2007**, *47*, 1045-1052.

[18] A. Macchioni, G. Ciancaleoni, C. Zuccaccia, D. Zuccaccia, *Chem. Soc. Rev.* **2008**, *37*, 479-489.