Supplementary Information for:

Programmable Assembly of Multistranded Helices in Water

Dimitri Delcourt,[a] Reguram Arumugaperumal,[a] Prachi Verma,[a] Perttu Permi,[a,b] Rosa M. Gomila,[c] Antonio Frontera,[c] and Fabien B. L. Cougnon[a*]

[a] Department of Chemistry, Nanoscience Center, University of Jyväskylä, P.O. Box 35, FI-40014 JYU, Finland

[b] Department of Biological and Environmental Science, Nanoscience Center, University of Jyväskylä, P.O. Box 35, FI-40014 JYU, Finland

[c] Department de Química, Universitat de les Illes Balears, Carretera de Valldemossa km 7.5, 07122 Palma de Mallorca, Baleares, Spain

Corresponding Author

* fabien.b.l.cougnon@jyu.fi

Table of Contents

1. Methods and General Information

All reagents and solvents were purchased from commercial sources and used without further purification – except triethylamine, which was distilled on potassium hydroxide under inert atmosphere before being used. Reagents were purchased from Sigma-Aldrich [(triisopropylsilyl)acetylene, trimethylsilylacetylene, triethylamine, bis(triphenylphosphine)palladium(II) dichloride, tetrakis(triphenylphosphine)palladium(0) , methyl trifluoromethanesulfonate, potassium perfluorobutanesulfonate, potassium trifluoromethanesulfonate] and Tokyo Chemical Industry Co [3,5-dibromopyridine, 3-ethynylpyridine, copper(I) iodide, tetrabutylammonium fluoride solution (1 M in tetrahydrofuran), 3-bromoiodobenzene, 1,3-diiodobenzene, 1,3-diethynylbenzene, sodium 1-butanesulfonate, 4,4'-biphenyldisulfonic acid].

NMR analyses. Spectra were measured on a JEOL 400 MHz NMR ECX-400 spectrometer equipped with a 5-mm broadband 40TH5AT/FG2 autotunable universal probe, a 400 MHz Bruker Avance III NMR spectrometer equipped with a 5-mm BBFO probehead, a Bruker Avance III 500 MHz NMR spectrometer equipped with a 5-mm nitrogen-cooled ^{1}H, ^{13}C, ^{15}N Prodigy probehead and a Bruker Avance III HD 800 MHz NMR spectrometer, equipped with a cryogenically cooled, 5 mm ^{1}H, ^{13}C, ^{15}N triple-resonance TCI probehead. All signals were internally referenced to the solvent residue ($CDCl_3$: 7.26 ppm, D_2O: 4.79 ppm, CD_3CN: 1.96 ppm) or tetramethylsilane. NMR solvents ($CDCl_3$ with or without 0.03% of tetramethylsilane, D_2O and CD_3CN) were purchased from Sigma-Aldrich and Eurisotop.

HR-MS analyses. HR-MS analyses were performed on an Agilent 6560 ESI-IM-QTOF mass spectrometer equipped with AJS ESI ion source.

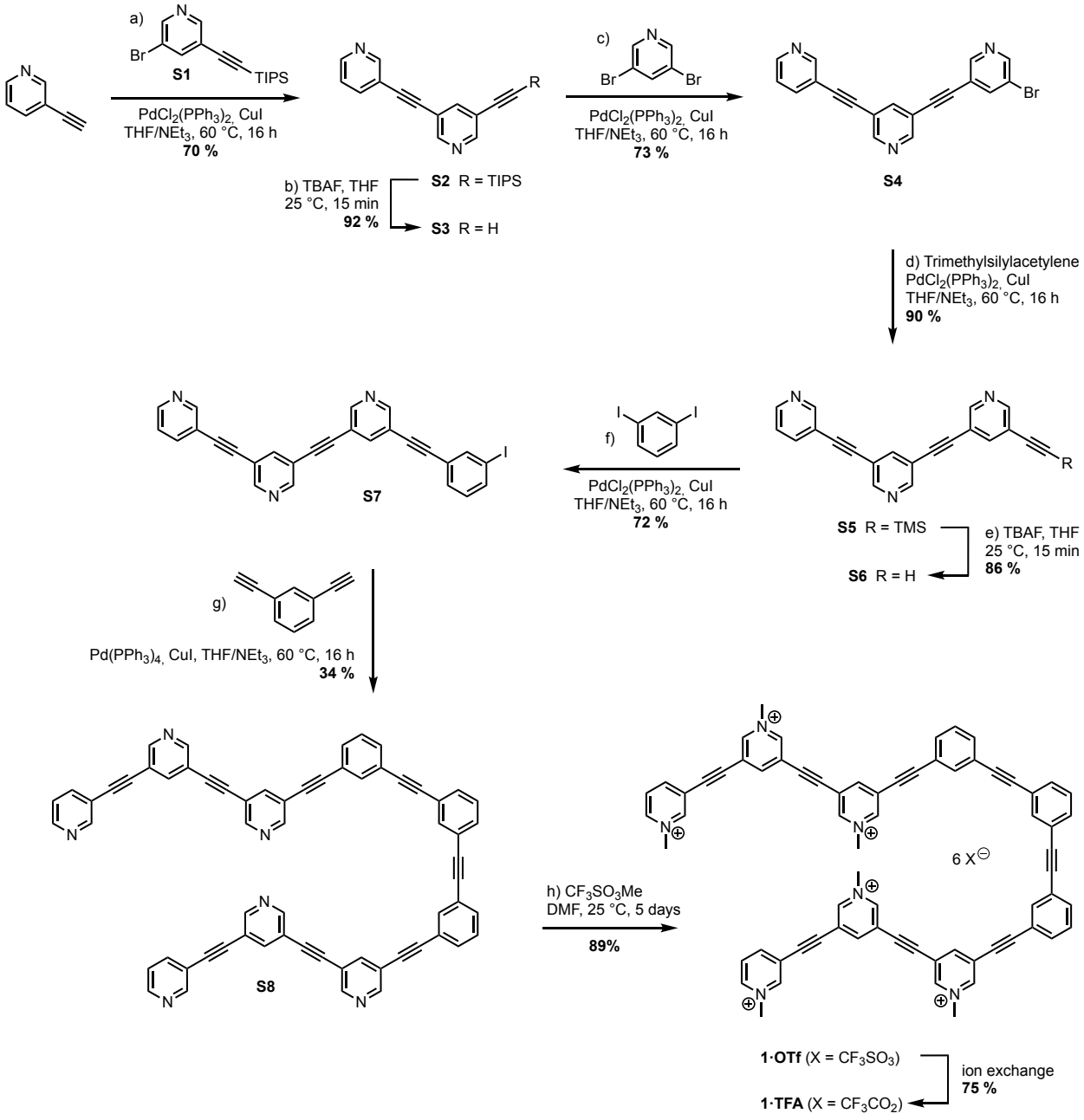
UHPLC-MS analyses. UHPLC-MS analyses were performed on an Agilent 6530-QTOF mass spectrometer (ionisation mode: ESI+) equipped with an Agilent 1290 UHPLC inlet, UV detector and Autosampler.

Melting Point. Melting points were measured on a Büchi Melting point B-540/B-545.

Preparative HPLC. Water soluble compounds were purified by HPLC Shimadzu LC-8A system equipped with a Shimadzu array detector SPD-M20A using a Gemini 10 µm C18 column 110 Å, 100 x 21.20 mm 10 micron from Phenomenex. Eluents: solution A (99.9% water, 0.1 % trifluoroacetic acid), solution B (100% acetonitrile). Gradient: 0 min, 5% B; 1 min, 5% B; 15 min, 100% B. Flow rate: 12 mL/min.

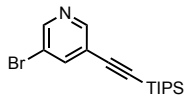
List of abbreviations. DOSY: Diffusion-ordered spectroscopy; DMF: N,N-Dimethylformamide, equiv.: equivalents; ESI-IM-QTOF: Electrospray Ionisation – Ion Mobility – Quadrupole Time-of-Flight; EXSY: Exchange spectroscopy; HR-MS: High-Resolution Mass Spectrometry; NMR: Nuclear Magnetic Resonance; OTf: Triflate; ROESY: rotating frame Overhauser effect spectroscopy; TBAF: Tetra-*n*-butylammonium fluoride; TFA: Trifluoroacetic acid; TIPS: Triisopropylsilyl; TMS: Trimethylsilyl; UHPLC: Ultra-High Performance Liquid Chromatography; UV: Ultraviolet.

2. Synthesis of strand 1



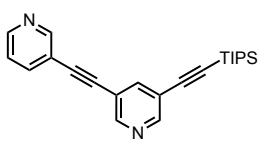
Scheme S1 | General procedure for the synthesis of strand 1.

Compound S1



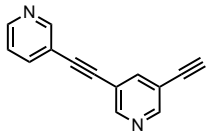
The synthesis of **S1** was adapted from a published procedure.[S1] 3,5-Dibromopyridine (1.0 g, 4.2 mmol), (triisopropylsilyl)acetylene (1.0 mL, 4.7 mmol), $PdCl_2(PPh_3)_2$ (190 mg, 0.06 mmol) and CuI (23 mg, 0.03 mmol) were dissolved in triethylamine (10 mL) under nitrogen atmosphere. The mixture was stirred 16 h at 50 °C and concentrated by rotary evaporation. The crude product was redissolved in dichloromethane, washed with a saturated solution of Na_2CO_3, dried over Na_2SO_4, filtered, and concentrated by rotary evaporation. The residue was purified by silica gel column chromatography (gradient pentane/ethyl acetate = 100/0 to 30/70) to yield **S1** (1.4 g, 97 %) as a yellow oil. Spectral data closely match those previously reported in the literature.[S1]

Compound S2



3-Ethynylpyridine (242 mg, 2.4 mmol), **S1** (783 mg, 2.3 mmol), $PdCl_2(PPh_3)_2$ (84 mg, 0.1 mmol) and CuI (12 mg, 0.06 mmol) were dissolved in triethylamine (3 mL) and tetrahydrofuran (3 mL) at 0 °C under nitrogen atmosphere. The reaction mixture was stirred 16 h at 60 °C, concentrated by rotary evaporation, and the resulting residue was purified by silica gel column chromatography (gradient pentane/ethyl acetate = 100/0 to 50/50) to yield **S2** (581.0 mg, 70 %) as a colorless oil. Melting point: 67-68 °C. ^{1}H NMR (400 MHz, $CDCl_3$ + 0.03 % tetramethylsilane, 293 K): δ 8.78 (br d, J = 1.7 Hz, 1H), 8.67 (d, J = 2.1 Hz, 1H), 8.64 (d, J = 2.1 Hz, 1H), 8.59 (dd, J = 4.9, 1.7 Hz, 1H), 7.90 (t, J = 2.1 Hz, 1H), 7.82 (dt, J = 8.1, 1.7 Hz, 1H), 7.32 (ddd, J = 8.1, 4.9, 0.8 Hz, 1H), 1.13 (m, 21H). ^{13}C NMR (100 MHz, $CDCl_3$ + 0.03 % TMS, 293 K): δ 152.4, 151.9, 150.9, 149.3, 141.3, 138.7, 123.3, 120.5, 119.6, 119.4, 102.4, 96.2, 89.8, 88.5, 18.7, 11.3. HR- HR-MS (ESI+) *m/z* calculated for $C_{23}H_{28}N_2Si^+$ $[M]^+$ = 361.2024, found 360.2022, Δ = -0.58 ppm.

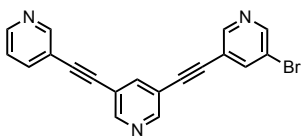
Compound S3



Tetrabutylammonium fluoride (1 M in tetrahydrofuran, 720 µL) was added to a solution of **S2** (795 mg, 2.2 mmol) in tetrahydrofuran (150 mL). The reaction mixture was stirred for 15 min at 25 °C and concentrated by rotary evaporation. The residue was purified by silica gel column chromatography (gradient pentane/ethyl acetate = 100/0 to 60/40) to yield **S3** (403 mg, 92 %) as a white solid. Melting point: 107-108 °C. ^{1}H NMR (400 MHz, $CDCl_3$ + 0.03 % tetramethylsilane, 293 K): δ 8.78 (br s, 1H), 8.70 (d, J = 2.0 Hz, 1H), 8.66 (d, J = 2.0 Hz, 1H), 8.60 (br d, J = 5.0 Hz, 1H), 7.91 (t, J = 2.0 Hz, 1H), 7.82 (dt, J = 7.8, 2.0 Hz, 1H), 7.32 (dd, J = 7.8, 5.0 Hz, 1H), 3.26 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$ + 0.03 % tetramethylsilane, 293 K): δ 152.4, 151.9, 151.5, 149.4, 141.4, 138.7, 123.3, 119.5, 119.2, 90.0, 88.2, 81.6, 79.5. HR-MS (ESI+) *m/z* calculated

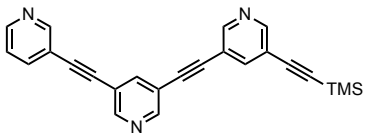
for $C_{14}H_9N_2$ $[M]^+$ = 204.0687, found 204.0695, Δ = -3.76 ppm.

Compound S4



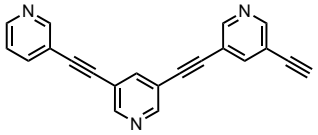
Compound **S3** (127 mg, 0.6 mmol), 3,5-dibromopyridine (966 mg, 4,1 mmol), $PdCl_2(PPh_3)_2$ (72 mg, 0.1 mmol) and CuI (11 mg, 0.03 mmol) were dissolved in dry triethylamine (10 mL) and tetrahydrofuran (10 mL) at 0 °C under nitrogen atmosphere. The reaction mixture was stirred for 8 h at 25 °C and 16 h at 60 °C before being concentrated by rotary evaporation. The crude product was redissolved in dichloromethane, washed with a saturated solution of Na_2CO_3, dried over Na_2SO_4, filtered, and concentrated by rotary evaporation. The residue was purified by silica gel column chromatography (gradient pentane/ethyl acetate = 100/0 to 0/100) to yield **S4** (481 mg, 73 %) as a white solid. Melting point: 189-190 °C. ^{1}H NMR (400 MHz, $CDCl_3$ + 0.03 % tetramethylsilane, 293 K): δ 8.79 (br s, 1H), 8.74 (d, *J* = 2.0 Hz, 1H), 8.72 (d, *J* = 2.0 Hz, 1H), 8.68 (d, *J* = 2.0 Hz, 1H), 8.66 (d, *J* = 2.0 Hz, 1H), 8.61 (br d, *J* = 4.9 Hz, 1H), 7.98 (t, *J* = 2.0 Hz, 1H), 7.97 (t, *J* = 2.0 Hz, 1H), 7.83 (dt, *J* = 7.9, 2.0 Hz, 1H), 7.33 (dd, *J* = 7.9, 4.9Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$ + 0.03 % tetramethylsilane, 293 K): δ 152.5, 151.7, 151.4, 150.6, 150.4, 149.5, 140.9, 138.7, 123.3, 120.9, 120.3, 119.7, 119.5, 119.2, 90.3, 89.5, 88.2. HR-MS (ESI+) *m/z* calculated for $C_{14}H_{11}BrN_3$ $[M]^+$ = 359.0058, found 359.0062, Δ = -1.19 ppm.

Compound S5



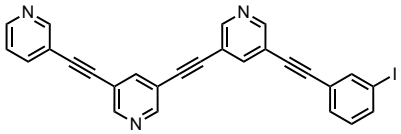
Compound **S4** (1.90 g, 5.27 mmol, 1.00 equiv.), $PdCl_2(PPh_3)_2$ (0.185 g, 0.263 mmol, 0.05 equiv.), CuI (50 mg, 0.263 mmol, 0.05 equiv.) in dry degassed tetrahydrofuran (25 mL) at 0 °C was added trimethylsilylacetylene (1.12 mL, 7.91 mmol, 1.5 equiv.) and Et_3N (2.5 mL, 15.82 mmol, 3.00 equiv.). The resulting mixture was then allowed to stir overnight at 60 °C and monitored by thin-layer chromatography. After completion, the reaction mixture was filtered through celite. The resulting organic phase was diluted in dichloromethane (50 mL) and washed with a saturation solution of NH_4Cl. The combined organic layers were washed with brine (100 mL), dried (Na_2SO_4), filtered and concentrated. The residue was purified by flash chromatography (hexane/ethyl acetate = 30/70) to give product **S5** (1.79 g, 90%) as a white solid. Melting point: 188-190 °C. ^{1}H NMR (500 MHz, $CDCl_3$, 298 K): δ 8.80 (s, 1H), 8.74 (dd, *J* = 2.0 , 2.0 Hz, 2H), 8.68 (dd, *J* = 2.0 Hz, 2H), 8.62 (d, *J* = 4.8 Hz, 1H), 7.98 (br d, *J* = 2.0 Hz, 1H), 7.91 (br d, *J* = 2.0 Hz, 1H), 7.86-7.84 (m, 1H), 7.34 (dd, *J* = 4.7, 4.9 Hz, 1H), 0.28 (s, 9H). ^{13}C NMR (126 MHz, $CDCl_3$, 298 K): δ 152.37, 151.86, 151.42, 151.28, 150.94, 149.36, 141.18, 140.77, 138.62, 123.16, 120.14, 119.59, 119.44, 119.33, 118.97, 100.29, 99.64, 90.08, 89.17, 88.73, 88.16, -0.25. HR-MS (ESI+) *m/z* calculated for $C_{24}H_{19}N_3Si^+$ $[M+H]^+$ = 378.1426, found 378.1424, Δ = -1.56 ppm.

Compound S6



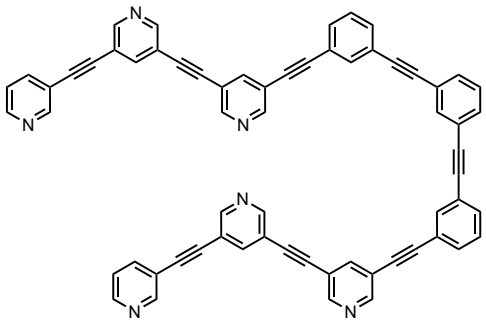
To a stirred solution of substrate **S5** (1.75 g, 4.63 mmol, 1.00 equiv.) in tetrahydrofuran/methanol (1:2, 30 mL) was added K_2CO_3 (1.27 g, 9.27 mmol, 2.00 equiv.). The resulting mixture was stirred at room temperature for 15 min at 25 °C and monitored by thin-layer chromatography. After completion, the reaction mixture was filtered, concentrated and subjected to column chromatography (hexane/ethyl acetate = 20/80) to give product **S6** as a white solid (1.216 g, 86%). Melting point: 189-190 °C. ^{1}H NMR (500 MHz, $CDCl_3$, 298 K): δ 8.81 (br d, *J* = 2.0 1H), 8.76-8.74 (m, 3H), 8.70 (d, *J* = 2.0 Hz, 1H), 8.62 (dd, *J* = 2.0, 2.0 Hz, 1H), 8.0 (br t, *J* = 2.0 Hz, 1H), 7.94 (br t, *J* = 2.0 Hz, 1H), 7.87-7.85 (m, 1H), 7.35 (dd, *J* = 4.0, 5.0 Hz, 1H), 3.29 (s, 1H). ^{13}C NMR (126 MHz, $CDCl_3$, 298 K): δ 152.38, 152.06, 151.49, 151.45, 151.30, 149.38, 141.37, 140.81, 138.62, 123.17, 119.61, 119.43, 119.24, 119.15, 90.12, 88.95, 88.14, 81.66, 79.34. HR-MS (ESI+) *m/z* calculated for $C_{21}H_{11}N_3^+$ $[M+H]^+$ = 306.1031, found 306.1028, Δ = 0.38 ppm.

Compound S7



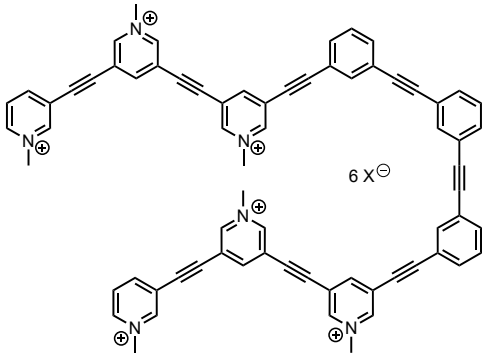
Compound **S6** (1.0 g, 3.27 mmol, 1.00 equiv.), $Pd(PPh_3)_4$ (0.189 g, 0.163 mmol, 0.05 equiv.), CuI (31 mg, 0.163 mmol, 0.05 equiv.) in dry degassed THF (25 mL) at 0 °C was added 1,3-diiodobenzene (1.18 mL, 3.60 mmol, 1.1 equiv.) and Et_3N (1.4 mL, 9.82 mmol, 3.00 equiv.). The resulting mixture was then allowed to stir overnight at 60 °C and monitored by thin-layer chromatography. After completion, the reaction mixture was filtered through celite. The resulting organic phase was diluted in dichloromethane (50 mL) and washed with a saturated solution of NH_4Cl. The combined organic layers were washed with brine (100 mL), dried (Na_2SO_4), filtered and concentrated. The residue was purified by flash chromatography (hexane/ethyl acetate = 20/80) to give product **S7** (1.2 g, 72 %) as a white solid. Melting point: 186-188 °C. ^{1}H NMR (500 MHz, $CDCl_3$, 298 K): δ 8.82 (br d, *J* = 2.0, 1H), 8.76-8.73 (m, 4H), 8.63 (dd, *J* = 2.0, 2.0 Hz, 1H), 8.0 (br t, *J* = 2.0 Hz, 1H), 7.97 (br t, *J* = 2.0 Hz, 1H), 7.93 (br t, *J* = 2.0 Hz, 1H), 7.87-7.85 (m, 1H), 7.75-7.73 (m, 1H), 7.54-7.52 (m, 1H), 7.35(dd, *J* = 5.0, 5.0 Hz, 1H), 7.14 (t, *J* = 8.0 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$, 298 K): δ 152.37, 151.49, 151.31, 151.10, 149.37, 140.82, 140.75, 140.30, 138.64, 138.11, 130.86, 130.02, 124.21, 123.19, 119.88, 119.63, 119.44, 119.30, 119.20, 93.78, 91.80, 90.12, 89.12, 88.93, 88.16, 86.16. HR-MS (ESI+) *m/z* calculated for $C_{27}H_{14}N_3I^+$ $[M+H]^+$ = 508.0310, found 508.0305, Δ = -0.46 ppm.

Compound S8



Compound **S7** (1.80 g, 3.56 mmol, 2.00 equiv.), $Pd(PPh_3)_4$ (0.205 g, 0.178 mmol, 0.1 equiv.), CuI (33 mg, 0.178 mmol, 0.1 equiv.) in dry degassed tetrahydrofuran (25 mL) at 0 °C was added 1,3-diethynylbenzene (0.237 mL, 1.78 mmol, 1.0 equiv.) and Et_3N (1.5 mL, 10.68 mmol, 6.00 equiv.). The resulting mixture was then allowed to stir overnight at 60 °C and monitored by thin-layer chromatography. After completion, the reaction mixture concentrated by rotary evaporation. The crude product was diluted in dichloromethane (50 mL) and washed with a saturated solution of NH_4Cl. The combined organic layers were washed with brine (100 mL), dried (Na_2SO_4), filtered and concentrated. The residue was purified by flash chromatography (dichloromethane/methanol = 95/5) to give product **S8** (568 g, 34 %) as a pale-yellow solid. Melting point: >400 °C (decomposition). ^{1}H NMR (500 MHz, $CDCl_3$, 298 K): δ 8.82 (br t, *J* = 3.0, 2H), 8.77-8.73 (m, 8H), 8.63 (br d, *J* = 5.0 Hz, 2H), 8.0 (br t, *J* = 6.0 Hz, 4H), 7.86 (br t, *J* = 6.0 Hz, 2H), 7.76 (br t, *J* = 3.0 Hz, 2H), 7.58-7.53 (m, 5H), 7.43-7.39 (m, 3H), 7.37-7.33 (m, 4H). ^{13}C NMR (126 MHz, $CDCl_3$, 298 K): δ 152.37, 151.54, 151.45, 151.31, 150.99, 149.35, 140.78, 138.64, 138.63, 135.41, 134.75, 133.17, 132.43, 132.16, 131.62, 128.70, 123.48, 123.18, 122.58, 120.07, 119.60, 119.44, 119.31, 119.16, 90.11, 89.19, 88.89, 88.18. HR-MS (ESI+) *m/z* calculated for $C_{64}H_{33}N_6^+$ $[M+H]^+$ = 885.2762, found 885.2732, Δ = 3.39 ppm.

Strand 1



Methyl triflate (120 µL, 1.1 mmol) was added to a solution of **S7** (40 mg, 0.05 mmol) in dry N,N-dimethylformamide (2 mL) under argon atmosphere. The mixture was stirred 24 h at 60 °C, and reaction progress was monitored by LC–MS. Upon completion, water (10 mL) was added, and the mixture was lyophilized to obtain a crude solid. The residue was redissolved in water (5 mL), cooled to 0 °C, and centrifuged. The resulting precipitate was collected and washed with dichloromethane (**1·OTf**, 75 mg, 89% yield).

Ion exchange was performed on preparative HPLC to afford salt of **1·CF_3CO_2** as a beige solid (50 mg, 75% yield). Melting point: >400 °C (decomposition). ^{1}H NMR (500 MHz, CD_3CN, 298 K): δ 9.08 (br t, *J* = 2.0, 2H), 9.04 (br t, *J* = 2.0, 2H), 9.01-8.99 (m, 4H), 8.93 (br t, *J* = 1.0 Hz, 2H), 8.83 (br t, *J* = 2.0 Hz, 2H), 8.74 (br t, *J* = 2.0 Hz, 2H), 8.72-8.70 (m, 2H), 8.65 (br t, *J* = 2.0 Hz, 1H), 8.63 (br t, *J* = 2.0 Hz, 1H) 8.12-8.09 (m, 2H), 7.83 (t, *J* = 2.0 Hz, 2H), 7.77 (t, *J* = 1.0 Hz, 1H), 7.73-7.68 (m, 4H), 7.63 (dd, *J* = 1.0, 2.0 Hz, 2H), 7.57-7.48 (m, 3H), 4.40 (s, 6H), 4.37 (s, 6H), 4.36 (s, 6H), ^{13}C NMR (126 MHz, CD_3CN, 298 K): δ 160.6, 160.3, 150.2, 149.6, 149.1, 149.0, 148.8, 148.5, 147.8, 147.0, 135.5, 135.1, 134.5, 133.2, 132.9, 130.5, 130.3, 129.4, 124.5,

124.0, 123.6, 123.4, 123.1, 122.9, 122.0, 120.7, 116.0, 90.2, 89.5, 89.3, 88.8, 82.4, 50.2, 50.0, 49.7. HR-MS (ESI+) *m/z* calculated for $C_{80}H_{50}F_{15}N_6O_{10}^+$ $[M+5CF_3CO_2]^+$ = 1539.3344, found 1539.3328, Δ = -1.04 ppm.

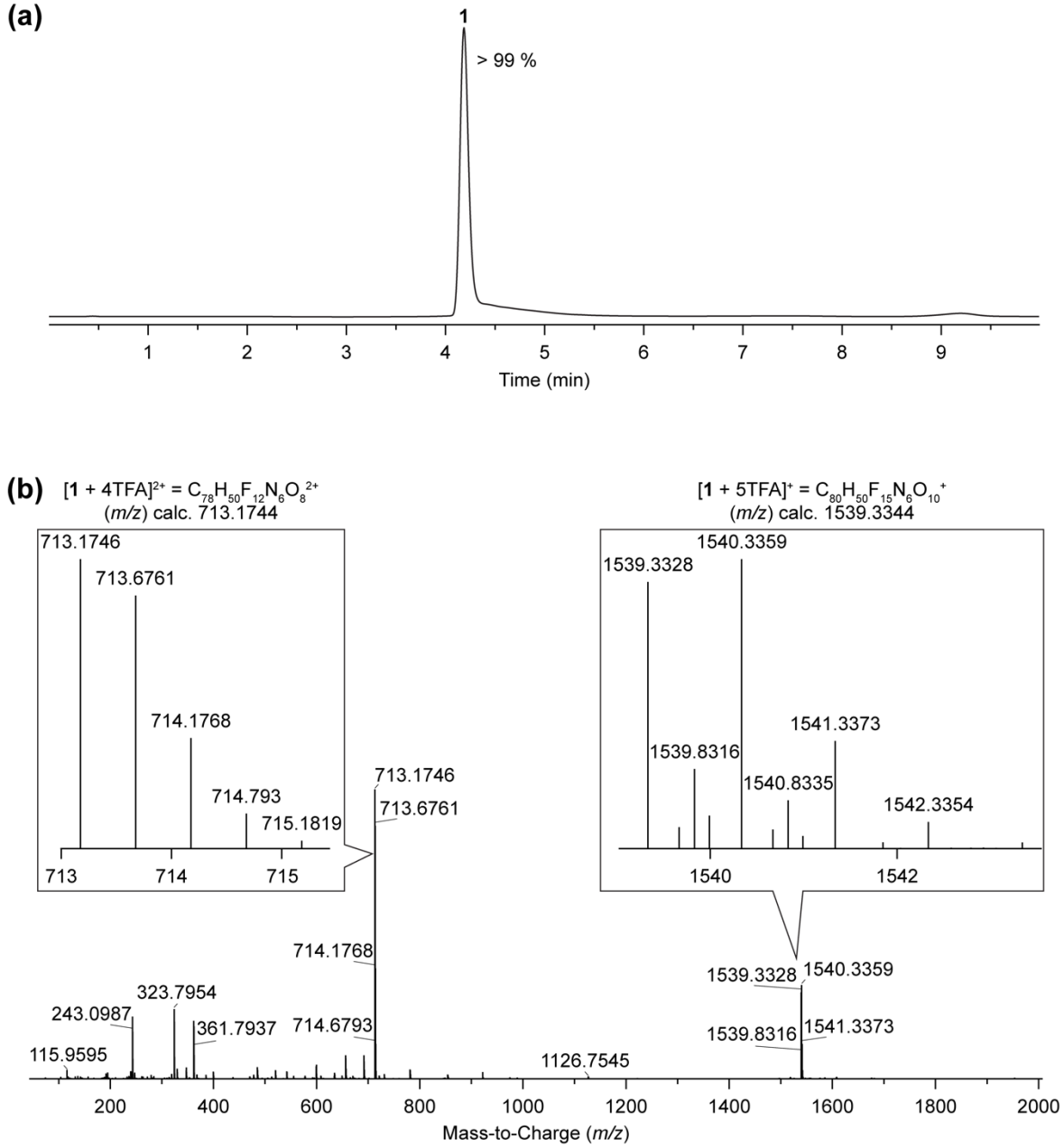


Figure S1 | UHPLC-MS characterization of strand 1. Tandem **(a)** Reverse-phase UHPLC chromatogram and **(b)** MS spectrum of strand **1**. Absorbance was recorded at 254 nm.

3. NMR characterization of unfolded strand 1 in CD_3CN

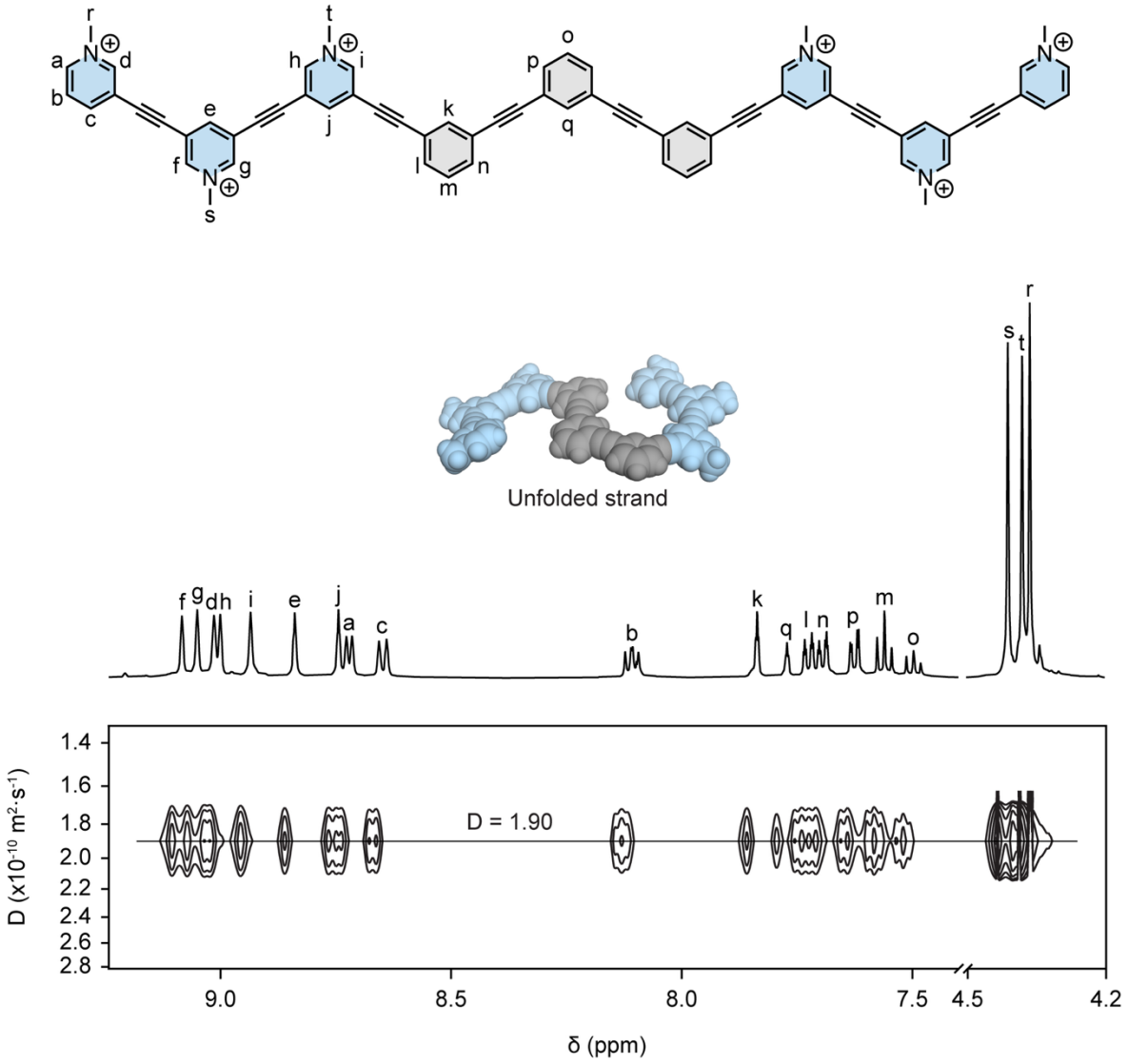


Figure S2 | Expansion of ^{1}H and DOSY NMR spectra of unfolded strand 1·TFA in CD_3CN (5 mM, 500 MHz, 298 K). Hydrodynamic radius r_H = 12.0 Å was calculated using the Stokes-Einstein equation.

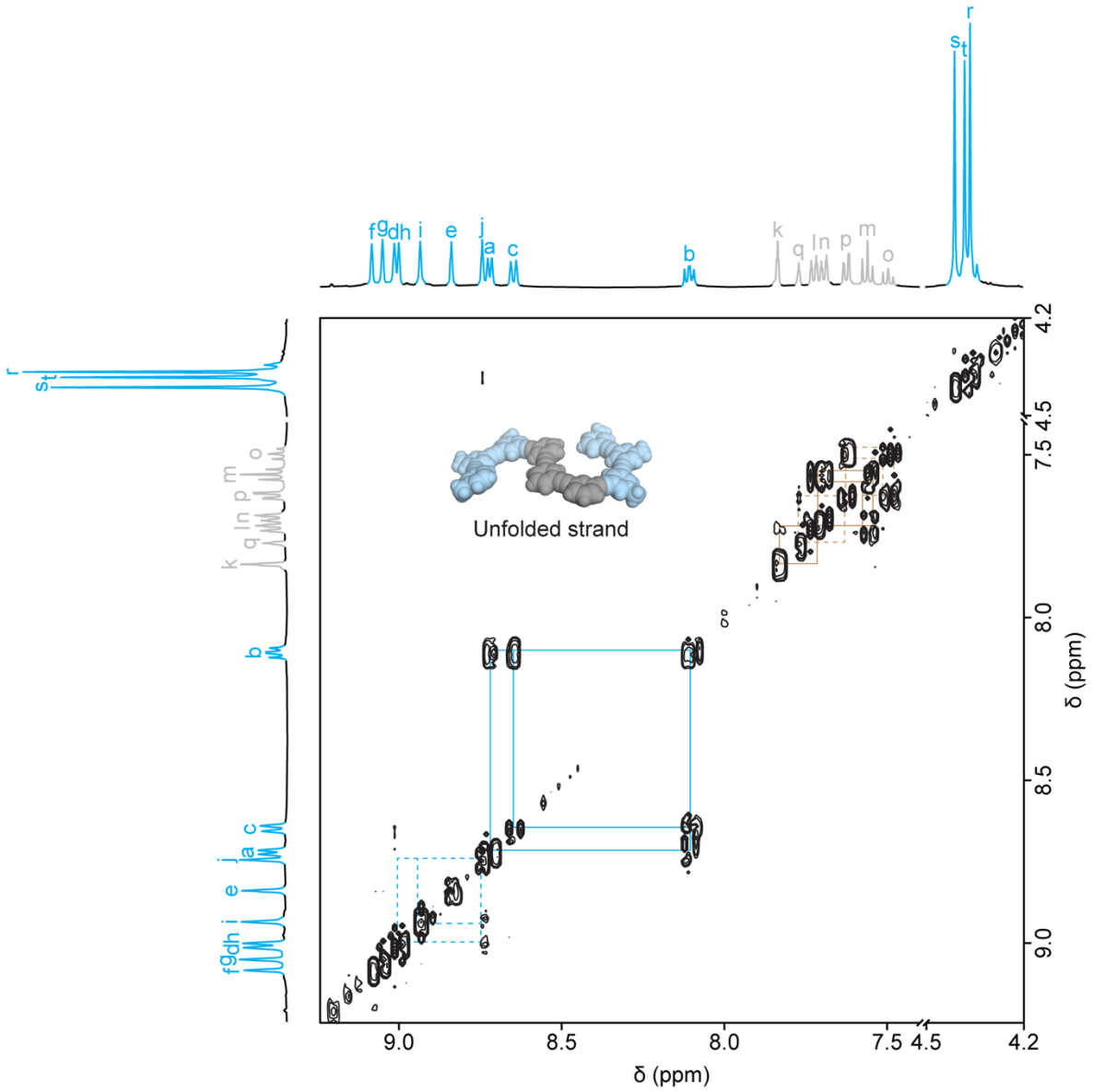


Figure S3 | Expansion of 2D ^{1}H-^{1}H COSY NMR spectrum of unfolded strand 1·TFA in CD_3CN (5 mM, 500 MHz, 298 K).

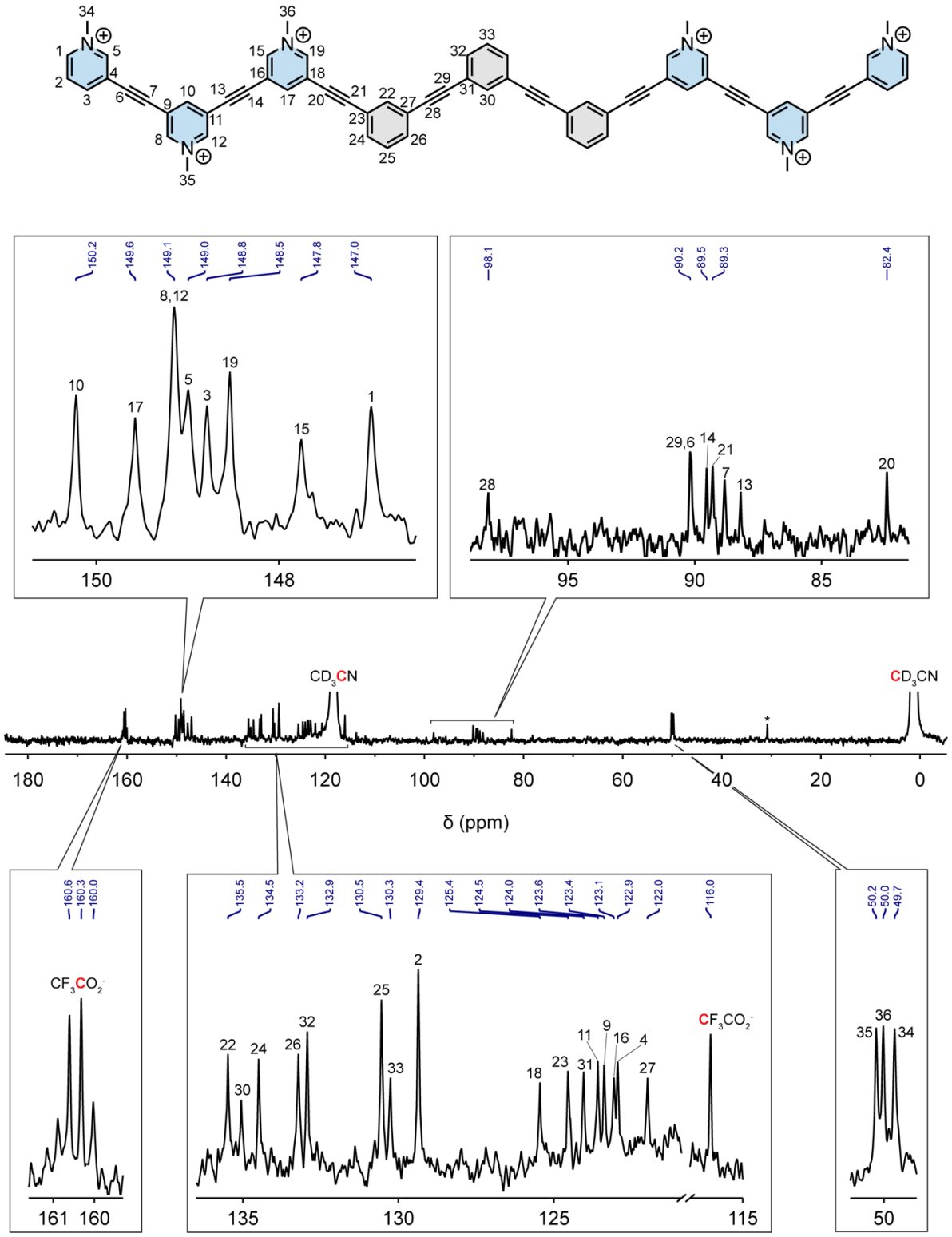


Figure S4 | ^{13}C NMR spectrum of unfolded strand 1·TFA in CD_3CN (5 mM, 126 MHz, 298 K). Assigned ^{13}C NMR chemical shifts are denoted onto the 1·TFA structure.

4. NMR characterization of double helix $(1)_2$ in D_2O

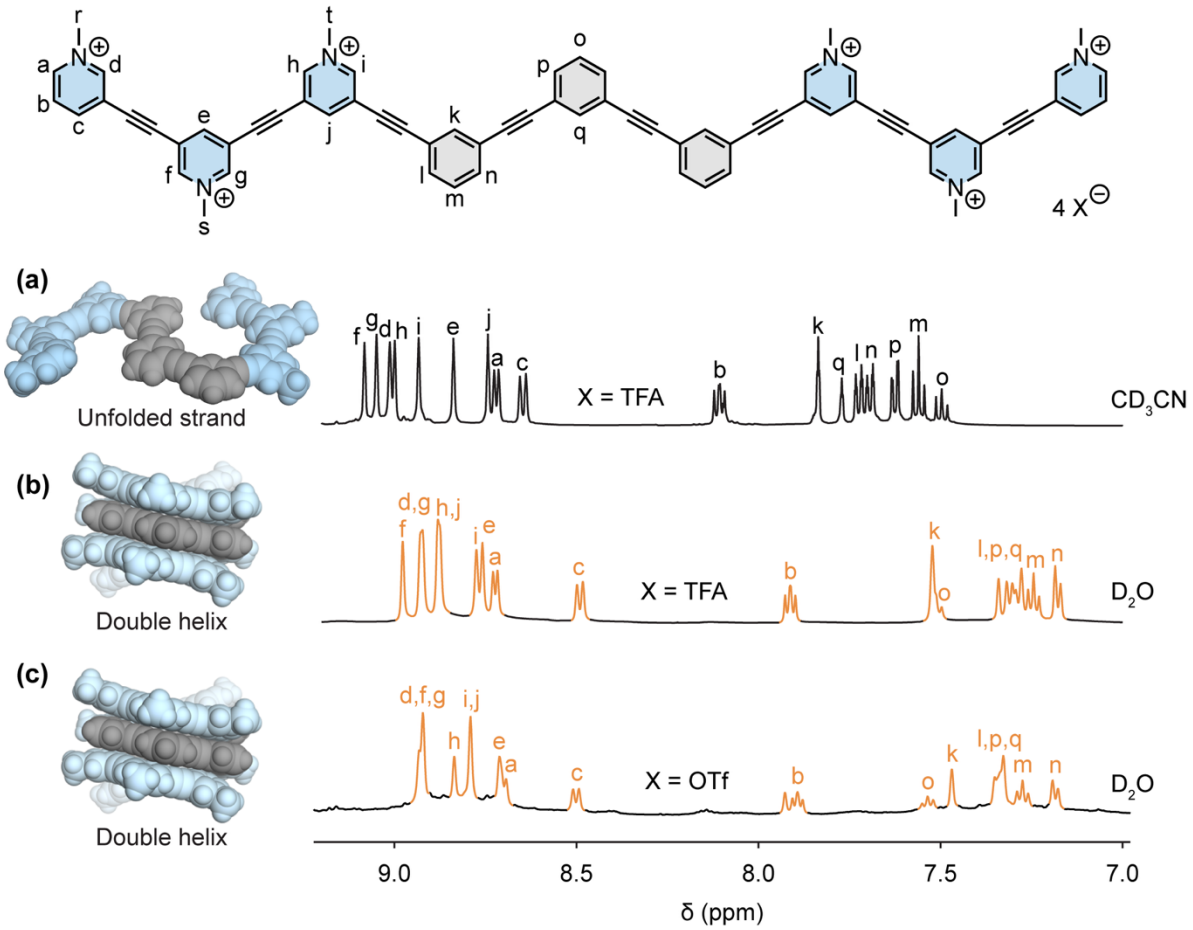


Figure S5 | Solvent-dependent ^{1}H NMR spectra of strand 1. Comparison between the ^{1}H NMR spectra of **a,** unfolded strand **1·TFA** in CD_3CN (5 mM); **b,** double helix $(\mathbf{1})_2$**·TFA** in D_2O (10 mM); and **c,** double helix $(\mathbf{1})_2$**·OTf** in D_2O (3 mM). All the spectra were recorded at 500 MHz and 298 K.

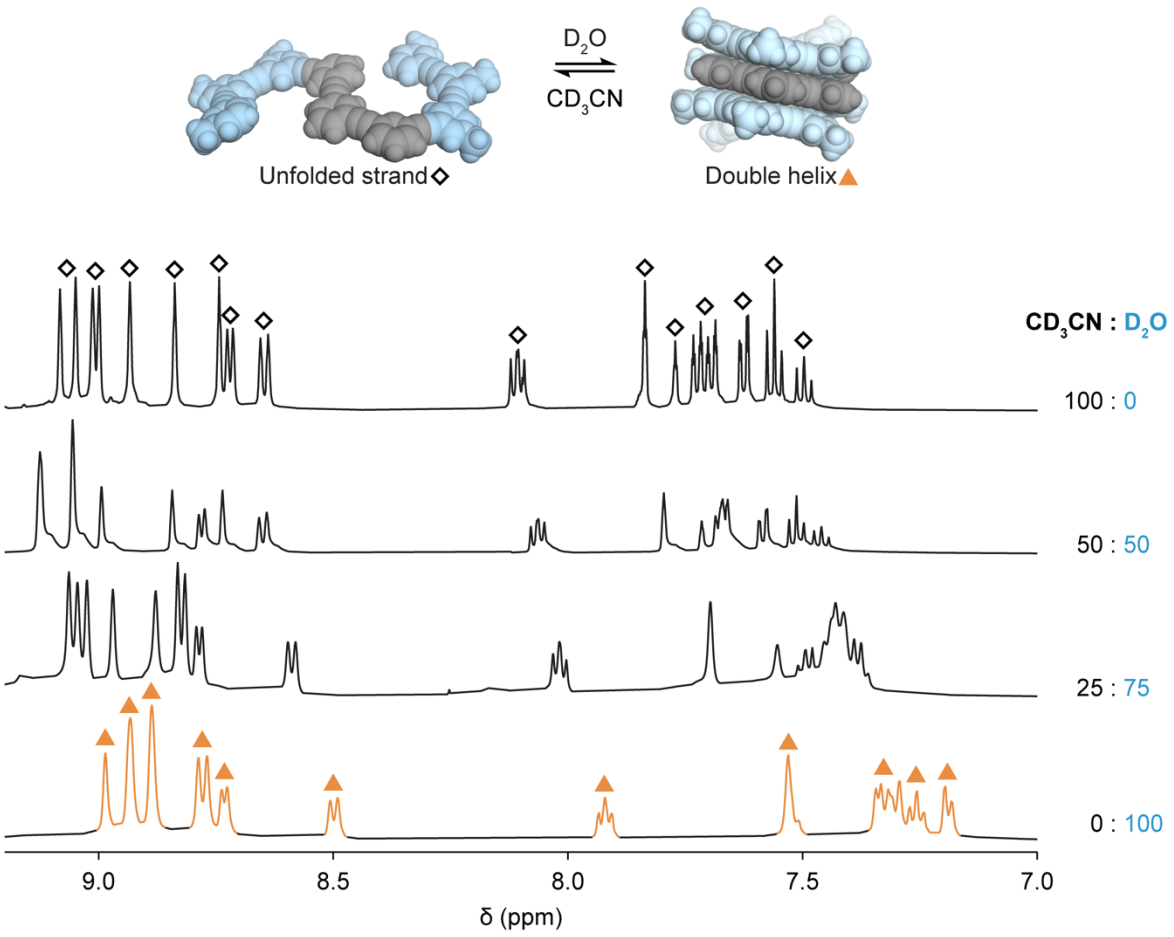


Figure S6 | Expansion of aromatic ^{1}H NMR spectral region of 1·TFA in CD_3CN / D_2O mixtures (5 mM, 500 MHz, 298 K). The signals corresponding to the unfolded strand and double helix are labelled with empty diamonds and orange triangles, respectively.

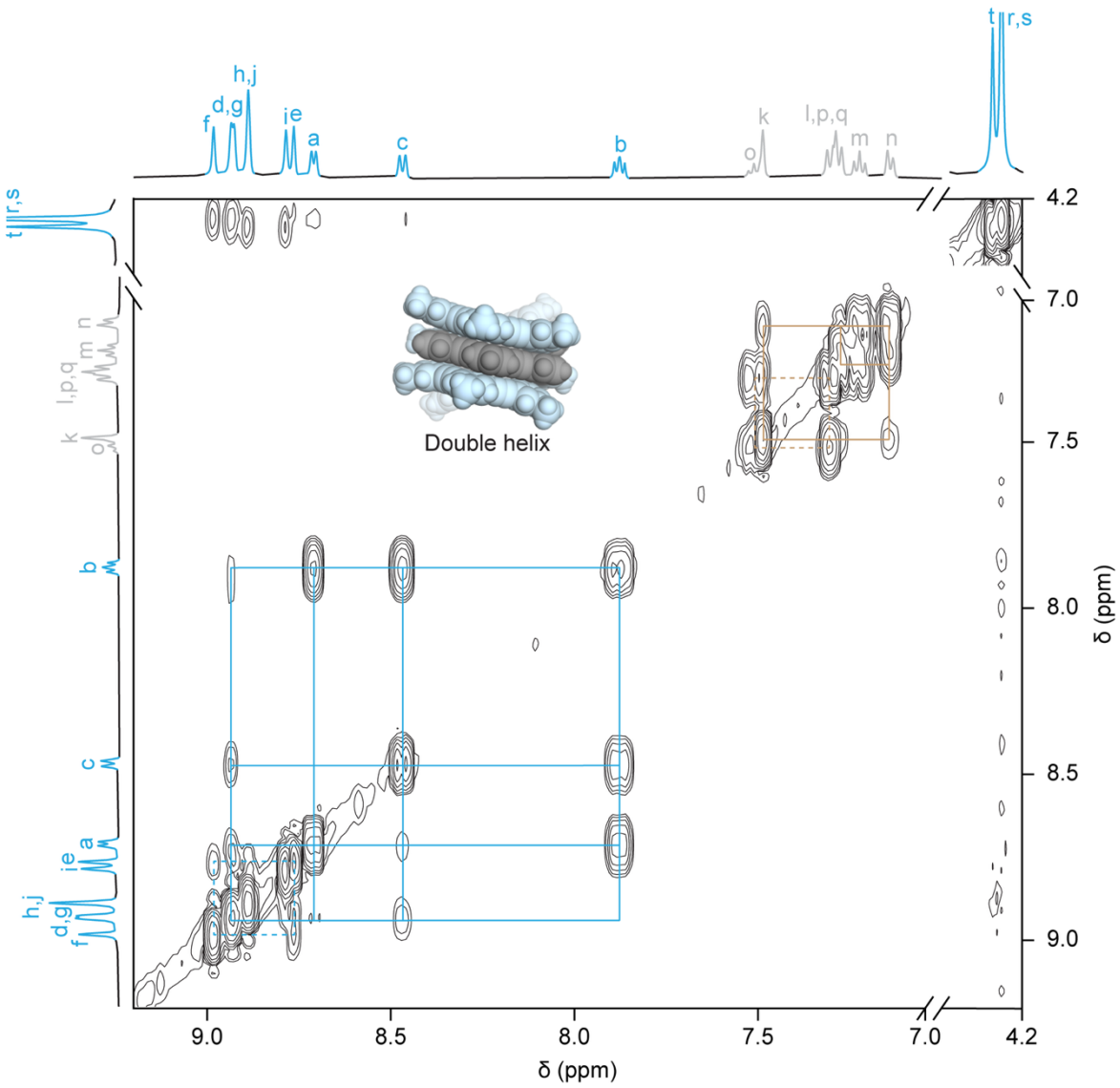


Figure S7 | Expansion of selected regions in 2D ^{1}H-^{1}H COSY NMR spectrum of double helix $(1)_2$·TFA in D_2O (10 mM, 500 MHz, 278 K).

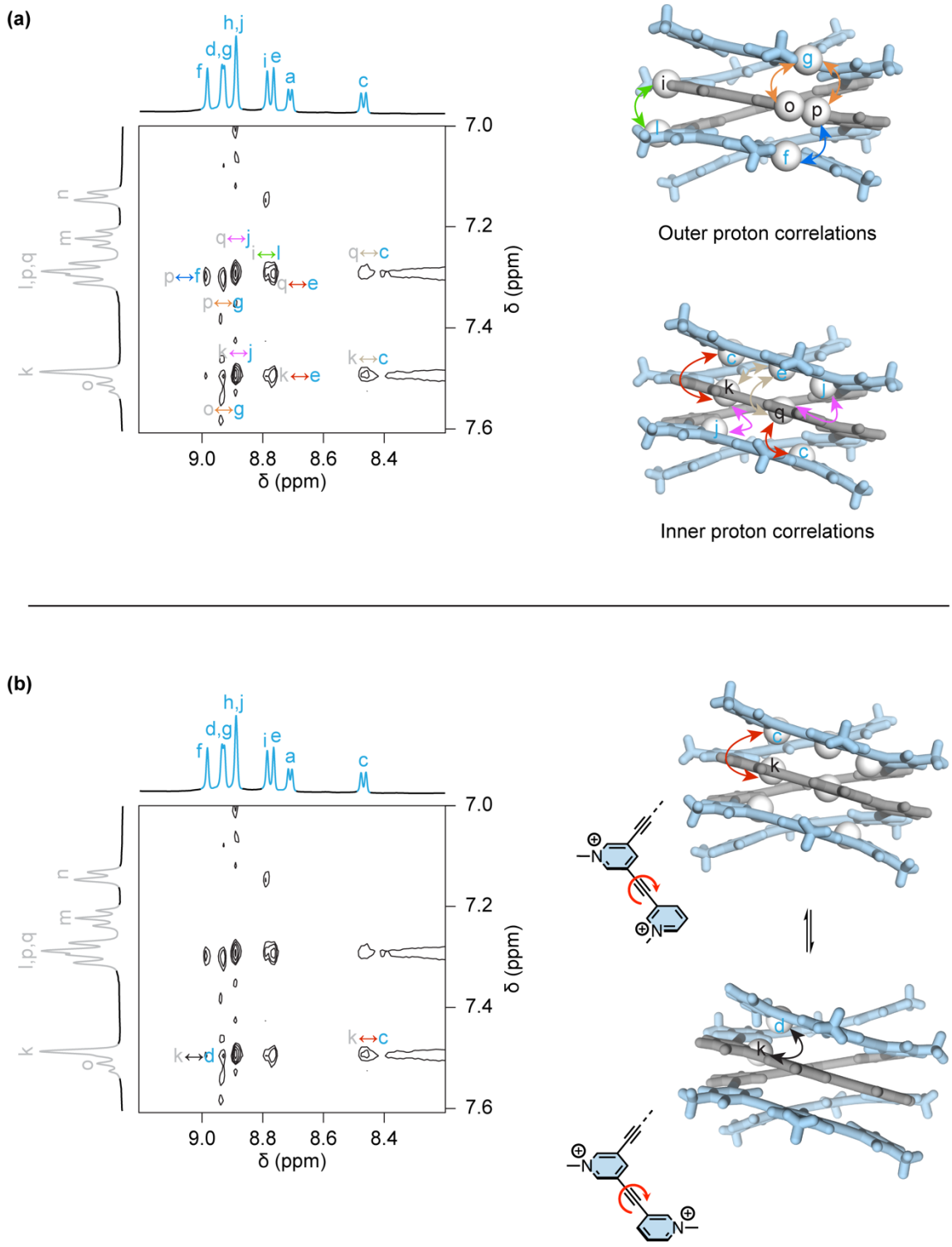


Figure S8 | Expansion of 2D ^{1}H-^{1}H ROESY NMR spectrum of double helix $(1)_2$·TFA in D_2O (10 mM, 500 MHz, 278 K, 100 ms mixing time). a, Key ROE correlations between protons of stacked pyridinium (colored in blue) and phenylene (colored in gray) residues. **b,** Rotation of the terminal pyridinium residue around the acetylene bond results in the appearance of additional ROE correlations between stacked pyridinium and phenylene residues.

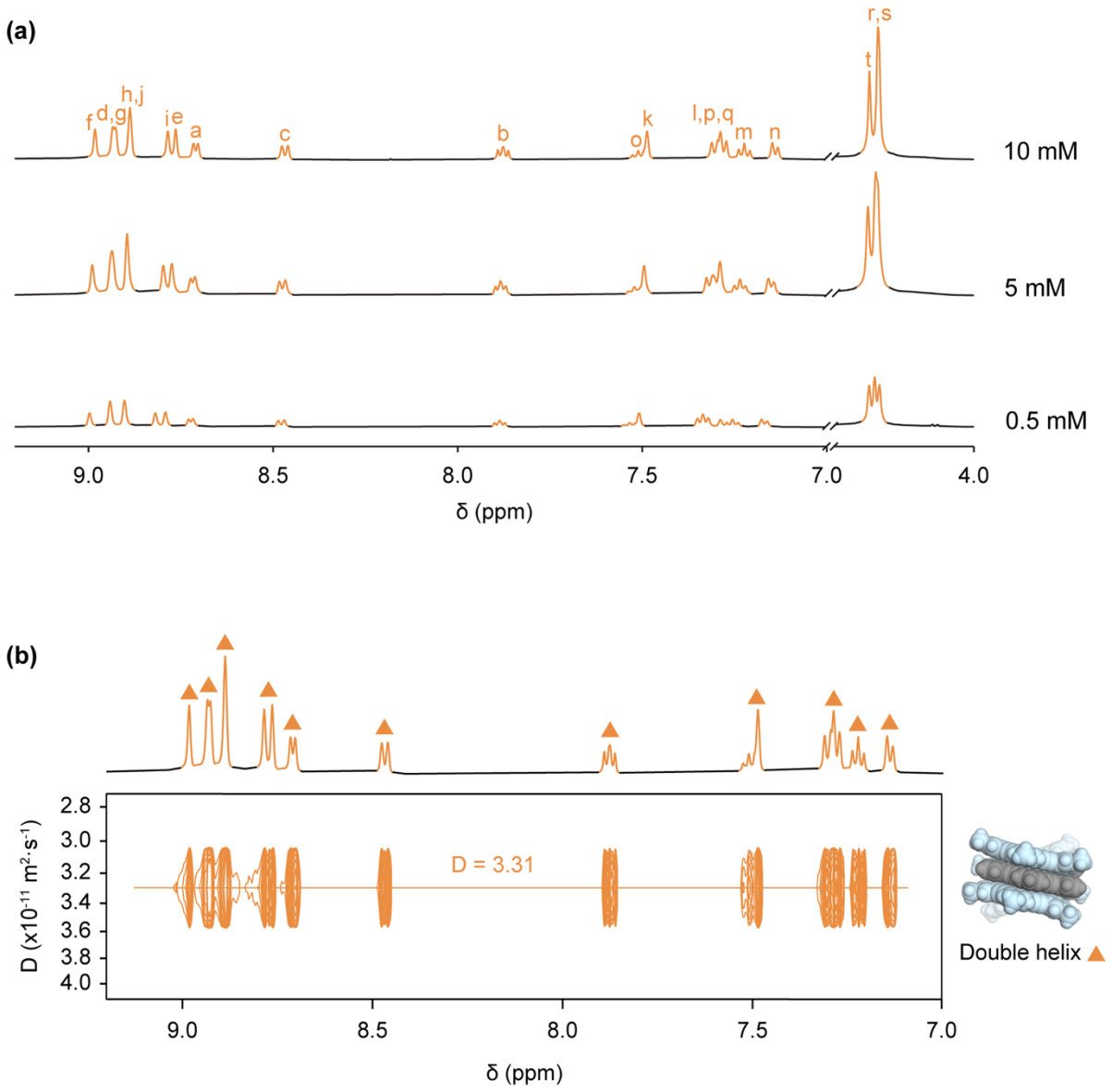


Figure S9 | Concentration-dependent ^{1}H and DOSY NMR spectra of double helix (1)$_2$·TFA. **a,** Concentration-dependent ^{1}H NMR spectra of **1·TFA** between 0.5 mM and 10 mM in D_2O (500 MHz, 278 K). **b,** ^{1}H DOSY NMR spectrum (500 MHz, D_2O, 278 K) of the double helix assembled from **1·TFA** (10 mM) in D_2O. The signals corresponding to the double helix are labelled with orange triangles. Its hydrodynamic radius r_H = 8.4 Å was calculated using the Stokes-Einstein equation.

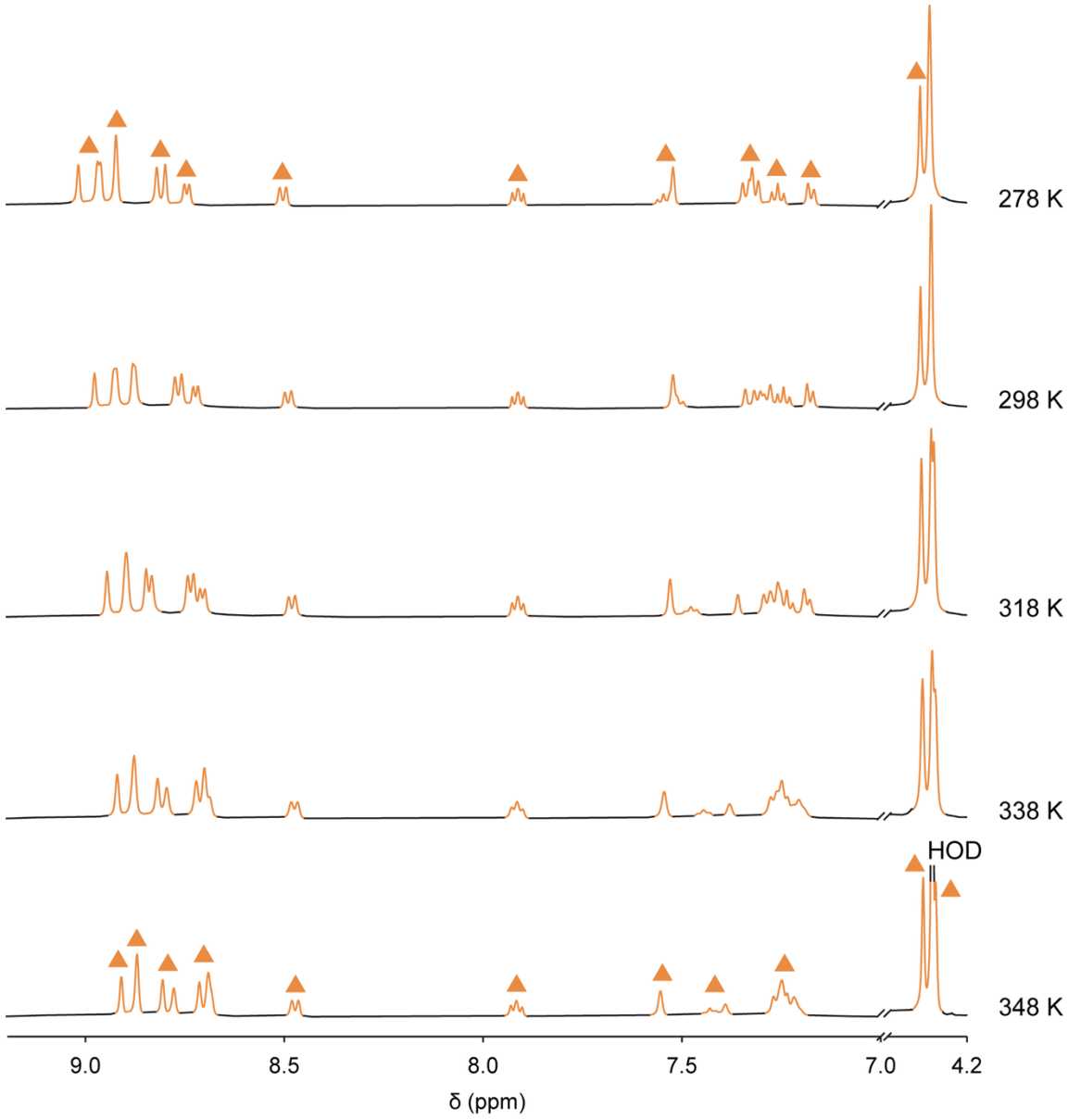


Figure S10 | Variable temperature ^{1}H NMR spectra (500 MHz) of a 10 mM solution of 1·TFA in D_2O between 278 K and 348 K. The signals corresponding to the double helix are labelled with orange triangles.

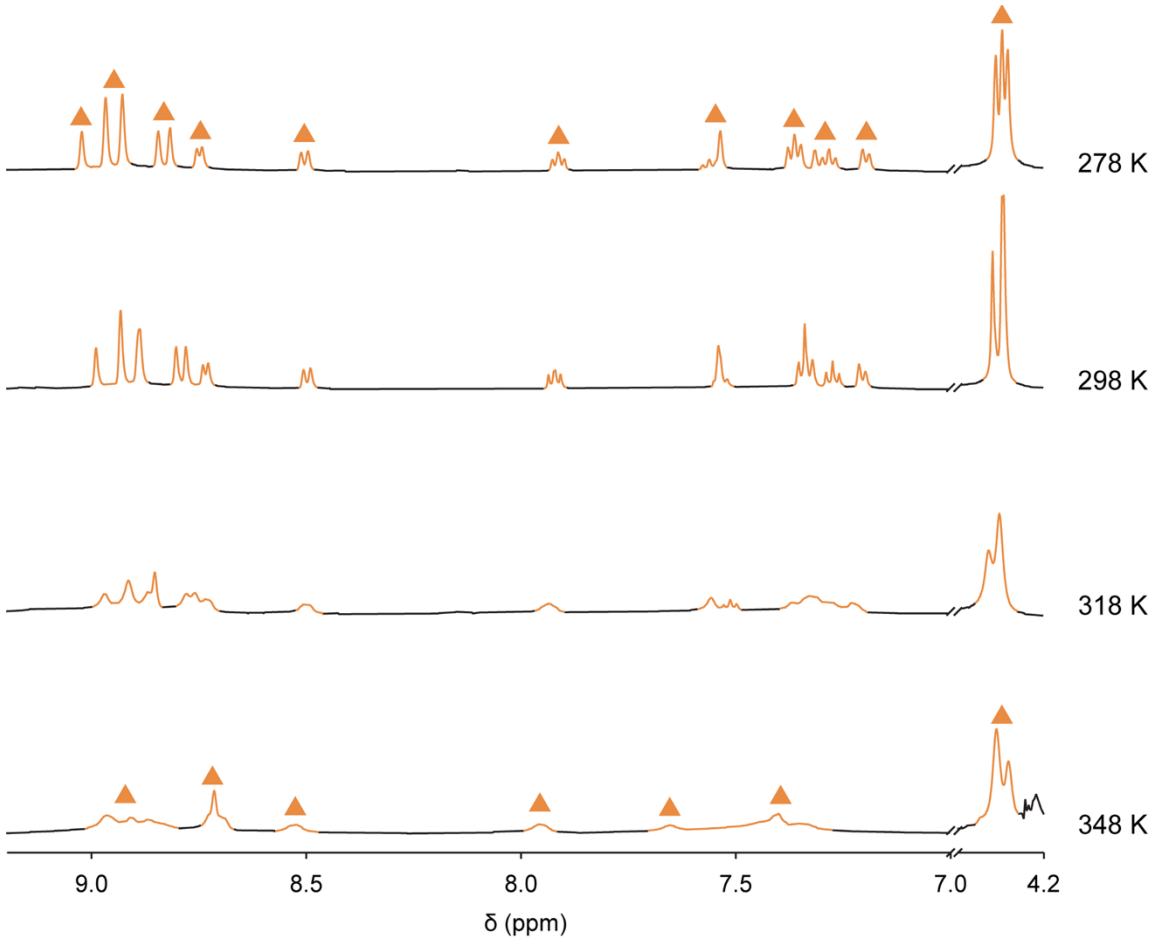


Figure S11 | Variable temperature ^{1}H NMR spectra (500 MHz) of a 0.5 mM solution of 1·TFA in D_2O between 278 K and 348 K. The signals corresponding to the double helix are labelled with orange triangles.

5. Host-guest studies with double helix $(1)_2$·TFA

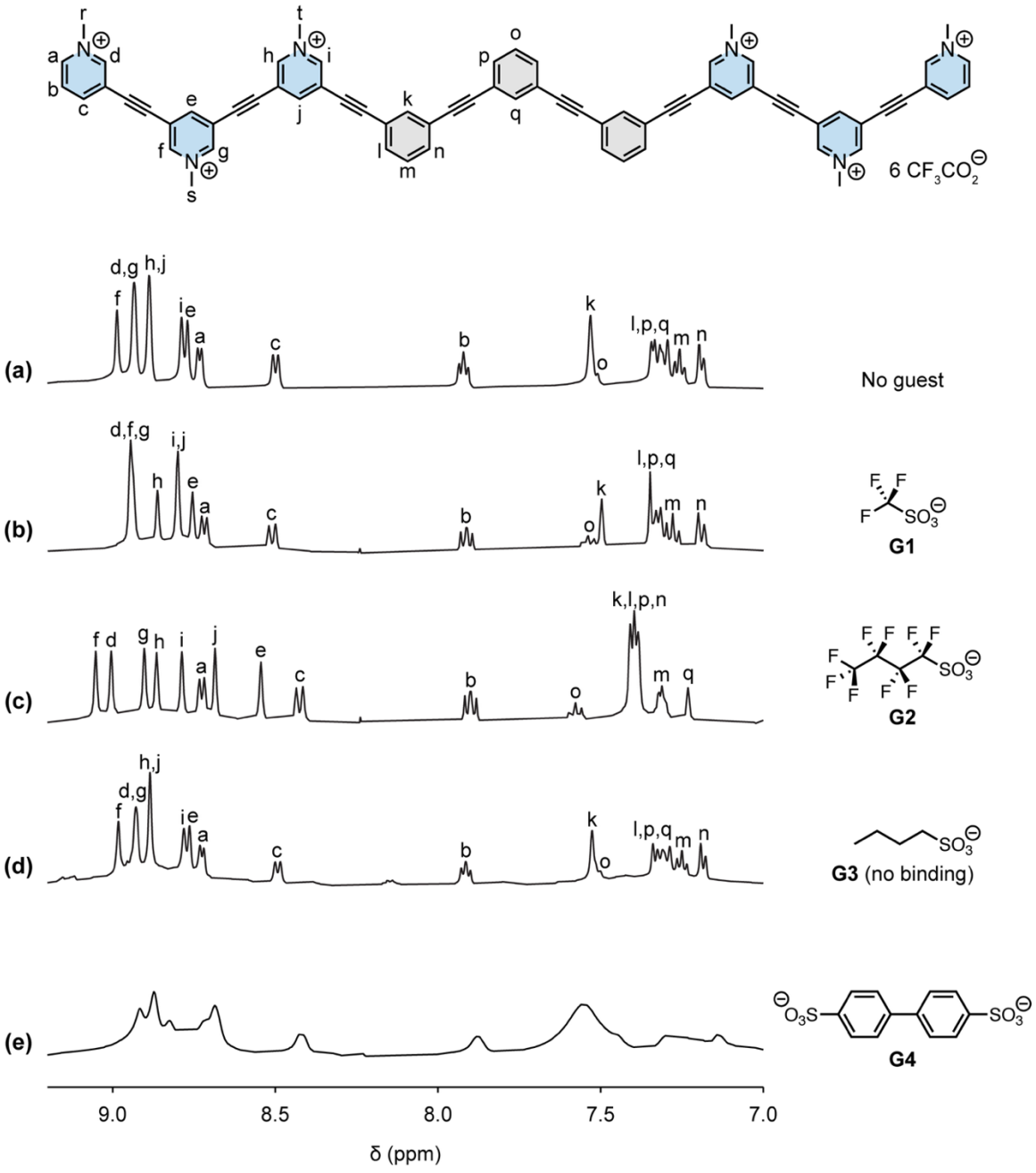


Figure S12 | ^{1}H NMR spectra of 1·TFA aromatic region (5 mM in D_2O, 500 MHz, 298 K) after addition of different guests. a, No guest added. **b,** After addition of 6.0 equiv. of potassium trifluoromethanesulfonate **G1**. **c,** After addition of 3.0 equiv. of potassium perfluorobutanesulfonate **G2**. **d,** After addition of 3.0 equiv. of sodium butanesulfonate **G3**. **e,** After addition of 2.0 equiv. of sodium 4,4'-biphenyldisulfonate **G4** (the sample precipitates above 2 equiv. of **G4**).

5.1. Titration with potassium trifluoromethanesulfonate (G1)

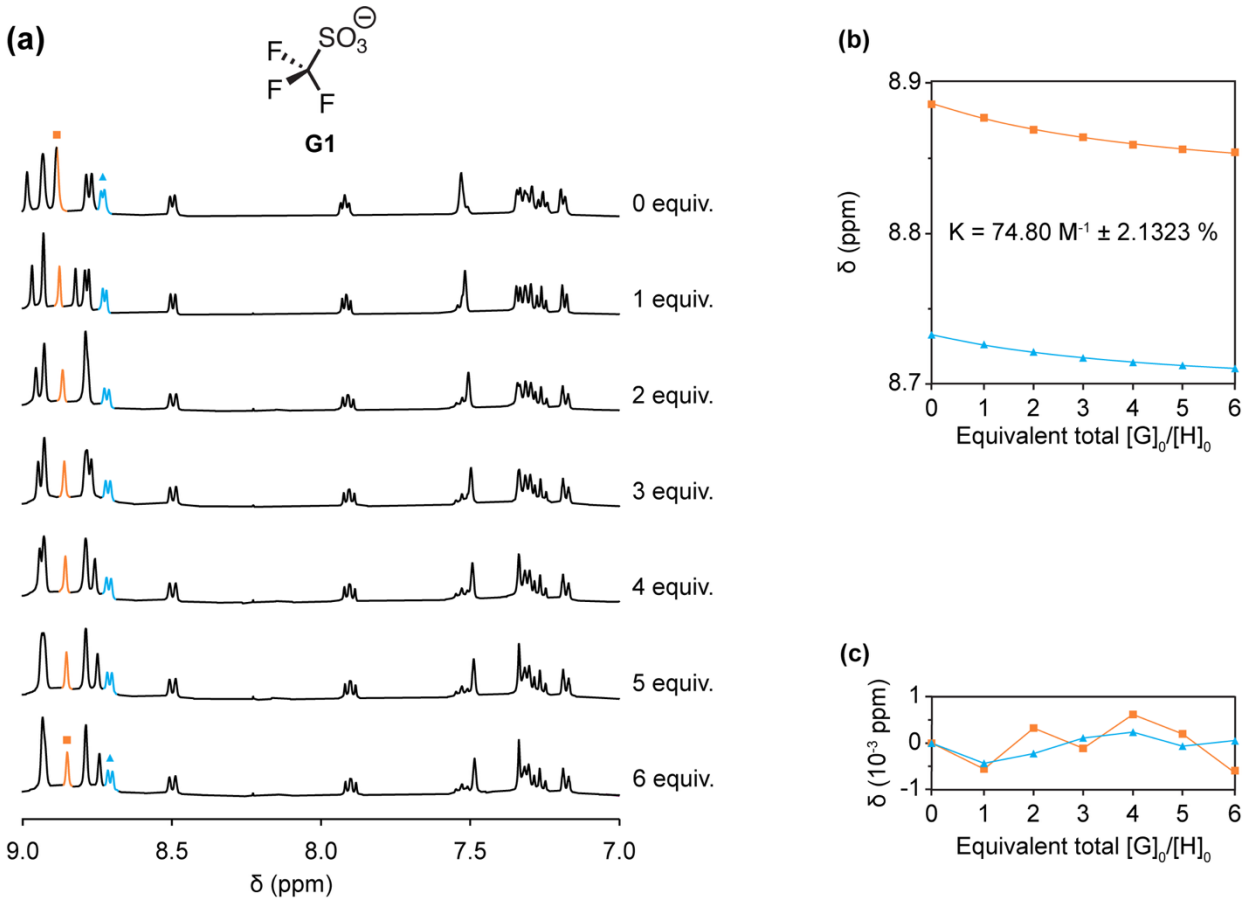


Figure S13 | ^{1}H NMR titration (400 MHz, 298 K) of potassium trifluoromethanesulfonate G1 into a 5 mM-solution of 1·TFA in D_2O. a, Selected region of the ^{1}H NMR spectra recorded during the titration. **b,** Chemical shift changes recorded as a function of guest equivalents. **c,** Residuals from the curve fitting. Association constant was obtained by fitting the data with *BindFit*.[S2]

5.2. Titration with potassium perfluorobutanesulfonate (G2)

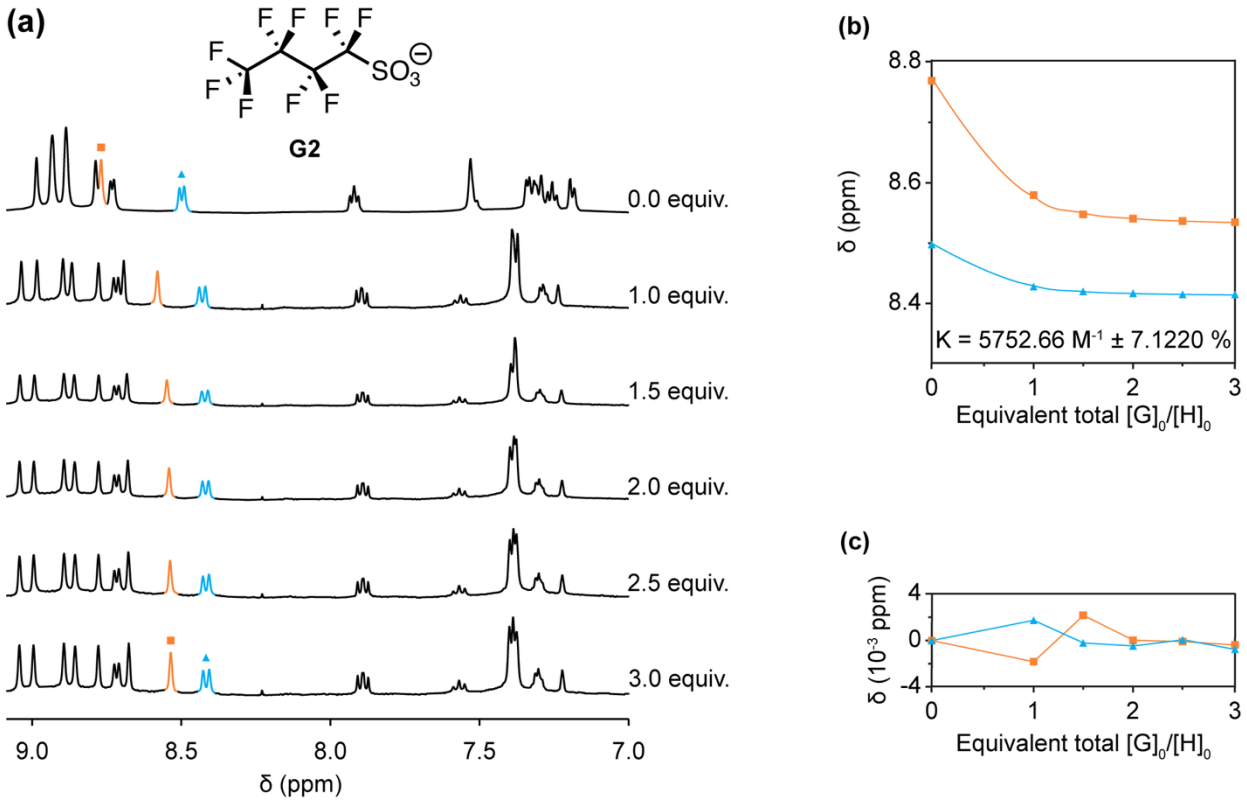
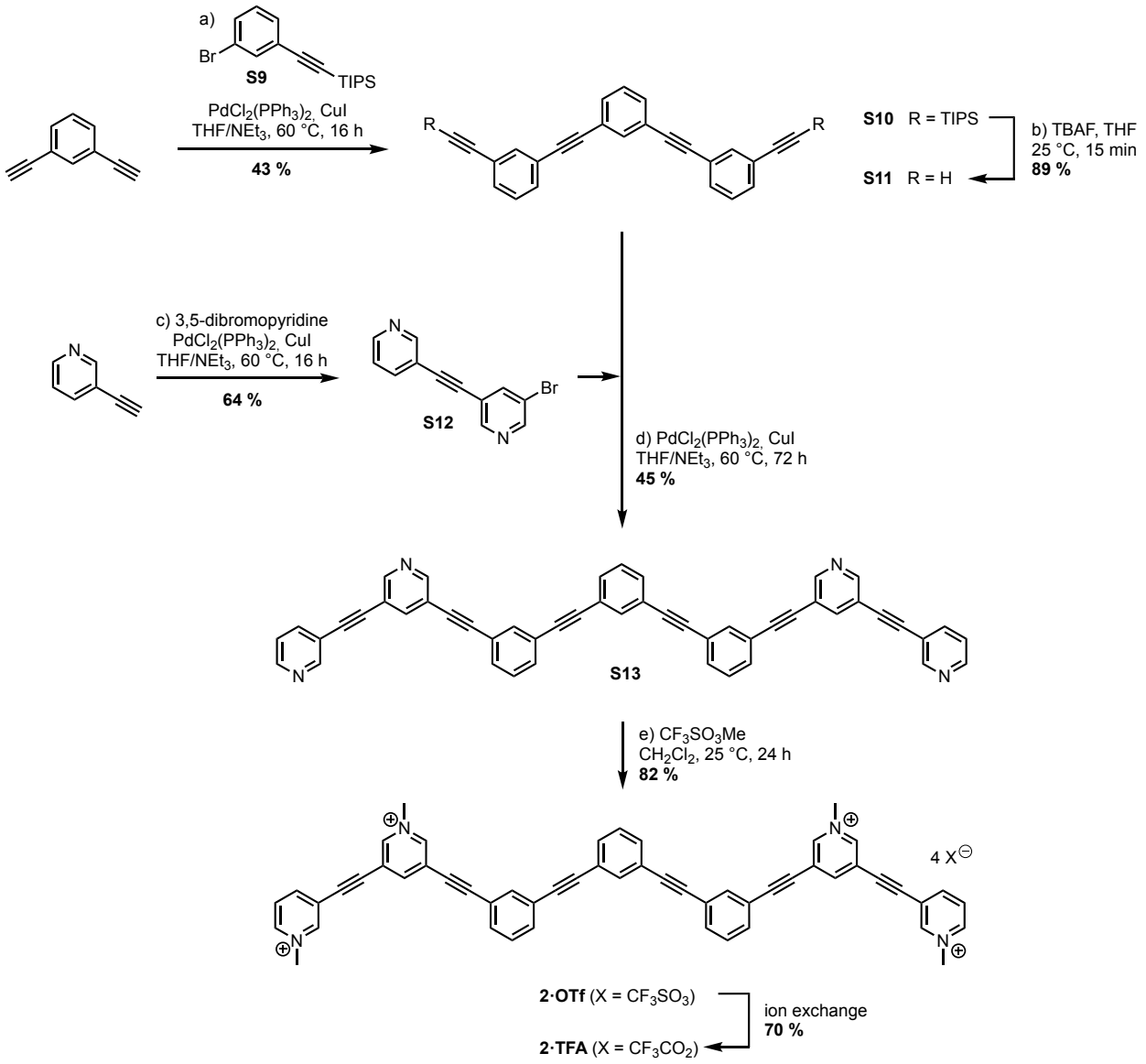


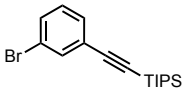
Figure S14 | ^{1}H NMR titration (400 MHz, 298 K) of potassium perfluorobutanesulfonate G2 into a 5 mM-solution of 1·TFA in D_2O. a, Selected region of the ^{1}H NMR spectra recorded during the titration. **b,** Chemical shift changes recorded as a function of guest equivalents. **c,** Residuals from the curve fitting. Association constant was obtained by fitting the data with *BindFit*.[S2]

6. Synthesis of strand 2



Scheme S2 | General procedure for the synthesis of strand 2.

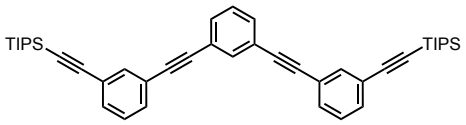
Compound S9



The synthesis of **S9** was adapted from a published procedure.[S3] 3-bromoiodobenzene (735 µL, 5.7 mmol), (triisopropylsilyl)acetylene (1.4 mL, 6.4 mmol), $PdCl_2(PPh_3)_2$ (206 mg, 0.3 mmol), and CuI (30 mg, 0.2 mmol) were

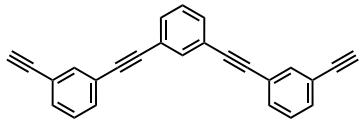
dissolved in dry triethylamine (18 mL) at 0 °C under nitrogen atmosphere. The reaction mixture was stirred 16 h at 25 °C, concentrated by rotary evaporation, and the resulting residue was purified by silica gel column chromatography (100% cyclohexane) to yield **S9** (1.9 g, 97 %) as a colorless oil. Spectral data closely match those previously reported in the literature.[S3]

Compound S10



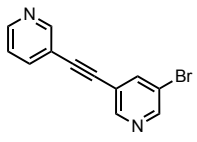
The synthesis of **S10** was adapted from a published procedure.[S4] 1,3-diethynylbenzene (263 µL, 2.0 mmol), **S9** (1.5 g, 4.4 mmol), $PdCl_2(PPh_3)_2$ (139 mg, 0.2 mmol), and CuI (20 mg, 0.1 mmol) were dissolved in dry triethylamine (10 mL) and tetrahydrofuran (10 mL) at 0 °C under nitrogen atmosphere. The reaction mixture was stirred 16 h at 60 °C, concentrated by rotary evaporation, and the resulting residue was purified by silica gel column chromatography (gradient hexane/dichloromethane = 100/0 to 90/10) to yield **S10** (551 mg, 43 %) as a colorless oil. Spectral data closely match those previously reported in the literature.[S4]

Compound S11



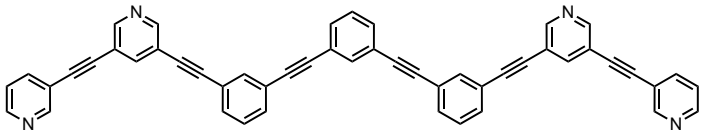
The synthesis of **S11** was adapted from a published procedure.[S4] Tetrabutylammonium fluoride (1 M in tetrahydrofuran, 4.6 mL) was added to a solution of **S10** (829 mg, 1.3 mmol) in tetrahydrofuran (150 mL). The reaction mixture was stirred for 15 min at 25 °C and concentrated by rotary evaporation. The crude product was first washed with plenty of CH_3OH. The residue was then redissolved in dichloromethane, washed with water, dried over Na_2SO_4, filtered and concentrated by rotary evaporation to yield **S11** (376 mg, 89 %) as a white solid. Spectral data closely match those previously reported in the literature.[S4]

Compound S12



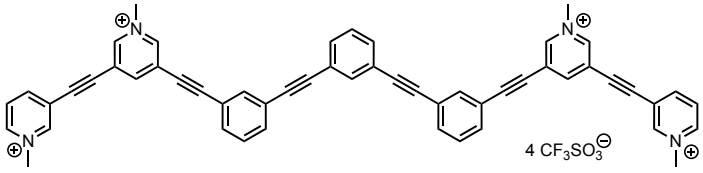
3-Ethynylpyridine (1.0 g, 9.8 mmol), 3,5-dibromopyridine (3.0 g, 12.8 mmol), $PdCl_2(PPh_3)_2$ (341 mg, 0.5 mmol) and CuI (53 mg, 0.3 mmol) were dissolved in dry triethylamine (35 mL) and tetrahydrofuran (43 mL) at 0 °C under nitrogen atmosphere. The reaction mixture was stirred 16 h at 60 °C, concentrated by rotary evaporation, and the resulting residue was purified by silica gel column chromatography (gradient hexane/ethyl acetate = 100/0 to 50/50) to yield **S12** (1.6 g, 64 %) as a white solid. Melting point: 91-92 °C. ^{1}H NMR (400 MHz, $CDCl_3$ + 0.03 % tetramethylsilane, 293 K): δ 8.78 (br d, J = 1.5 Hz, 1H), 8.68 (d, J = 2.0 Hz, 1H), 8.65 (d, J = 2.0 Hz, 1H), 8.61 (br dd, J = 4.9, 1.5 Hz, 1H), 7.99 (t, J = 2.0 Hz, 1H), 7.83 (dt, J = 7.9, 2.0 Hz, 1H), 7.33 (ddd, J = 7.9, 4.9, 0.7 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$ + 0.03 % tetramethylsilane, 293 K): δ 152.5, 150.4, 150.3, 149.5, 140.9, 138.8, 123.3, 121.2, 120.3, 119.4, 90.5, 87.7. HR-MS (ESI+) *m/z* calculated for $C_{12}H_7BrN_2^+$ $[M]^+$ = 257.9793, found 257.9798, Δ = -2.02 ppm.

Compound S13



Compounds **S11** (395 mg, 1.2 mmol), **S12** (624 mg, 2.4 mmol), $PdCl_2(PPh_3)_2$ (86 mg, 0.1 mmol) and CuI (14 mg, 0.07 mmol) were dissolved in dry triethylamine (10 mL) and tetrahydrofuran (10 mL) at 0 °C under nitrogen atmosphere. The reaction mixture was stirred for 72 h at 60 °C and concentrated by rotary evaporation. The solid residue was dissolved in dichloromethane, washed with a saturated solution of Na_2CO_3, dried over Na_2SO_4, filtered, and concentrated by rotary evaporation. The resulting solid was washed several times with petroleum ether and methanol to yield **S13** (372 mg, 45 %) as a beige solid. Melting point: >400 °C (decomposition). ^{1}H NMR (400 MHz, $CDCl_3$ + 0.03 % tetramethylsilane, 293 K): δ 8.79 (br d, *J* = 1.5 Hz, 2H), 8.71 (d, *J* = 2.0 Hz, 2H), 8.70 (d, *J* = 2.0 Hz, 2H), 8.60 (br dd, *J* = 5.0, 1.5 Hz, 2H), 7.96 (t, *J* = 2.0 Hz, 2H), 7.83 (dt, *J* = 8.0, 2.0 Hz, 2H), 7.73 (t, *J* = 1.5 Hz, 1H), 7.72 (t, *J* = 1.5 Hz, 2H), 7.55-7.49 (m, 6H), 7.38 (t, *J* = 8.0 Hz, 2H), 7.34 (t, *J* = 8.0 Hz, 1H), 7.32 (ddd, *J* = 8.0, 5.0, 1.0 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$ + 0.03 % tetramethylsilane, 293 K): δ 152.5, 151.4, 151.1, 149.4, 140.8, 138.7, 134.9, 134.8, 132.2, 131.7, 128.8, 128.7, 123.7, 123.4, 123.3, 122.7, 120.1, 119.6, 92.7, 89.9, 89.4, 89.0, 88.5, 85.8. HR-MS (ESI+) *m/z* calculated for $C_{50}H_{27}N_4^+$ $[M+H]^+$ = 683.2231, found 683.2238, Δ = -1,02 ppm.

Strand 2



Methyl triflate (154 µL, 1.4 mmol) was added to a solution of **S13** (169 mg, 0.3 mmol) in dry dichloromethane (120 mL) under nitrogen atmosphere. The mixture was stirred 24 h at 25 °C before being concentrated by rotary evaporation. The crude product was washed with dichloromethane to yield **2·OTf** (270 mg, 82 %) as a beige solid. Melting point: >400 °C (decomposition). ^{1}H NMR (500 MHz, CD_3CN, 298 K): δ 9.01 (br s, 2H), 8.94 (br s, 2H), 8.91 (br s, 2H), 8.74 (br s, 2H), 8.71 (br d, *J* = 6.3 Hz, 2H), 8.65 (br d, *J* = 8.2 Hz, 2H), 8.99 (br t, *J* = 7.2 Hz, 2H), 7.84 (br t, *J* = 1.7 Hz, 2H), 7.77 (br t, *J* = 1.6 Hz, 1H), 7.71 (br dt, *J* = 7.8, 1.3 Hz, 2H), 7.69 (br dt, *J* = 7.9, 1.4 Hz, 2H), 7.62 (br dd, *J* = 7.8, 1.7 Hz, 2H), 7.55 (t, *J* = 7.8 Hz, 2H), 7.49 (t, *J* = 7.8 Hz, 1H), 4.37 (s, 6H), 4.36 (s, 6H). ^{13}C NMR (126 MHz, CD_3CN, 298 K): δ 149.6, 149.1, 148.6, 148.5, 147.7, 146.9, 135.6, 135.2, 134.5, 133.2, 132.9, 130.6, 130.3, 129.4, 125.4, 124.6, 124.1, 123.4, 123.1, 122.1, 98.1, 90.2, 89.8, 89.4, 88.6, 82.6, 50.0, 49.8. HR-MS (ESI+) *m/z* calculated for $C_{57}H_{38}F_9N_4O_9S_3^+$ $[M+3CF_3SO_3]^+$ = 1189.1652, found 1189.1686, Δ = -2.86 ppm.

Ion exchange was performed on preparative HPLC. Strand **2·TFA** (169 mg, 70 %) was isolated as a beige solid. HR-MS (ESI+) *m/z* calculated for $C_{60}H_{38}F_9N_4O_6^+$ $[M+3CF_3CO_2]^+$ = 1081.2643, found 1081.2623, Δ = 1.85 ppm.

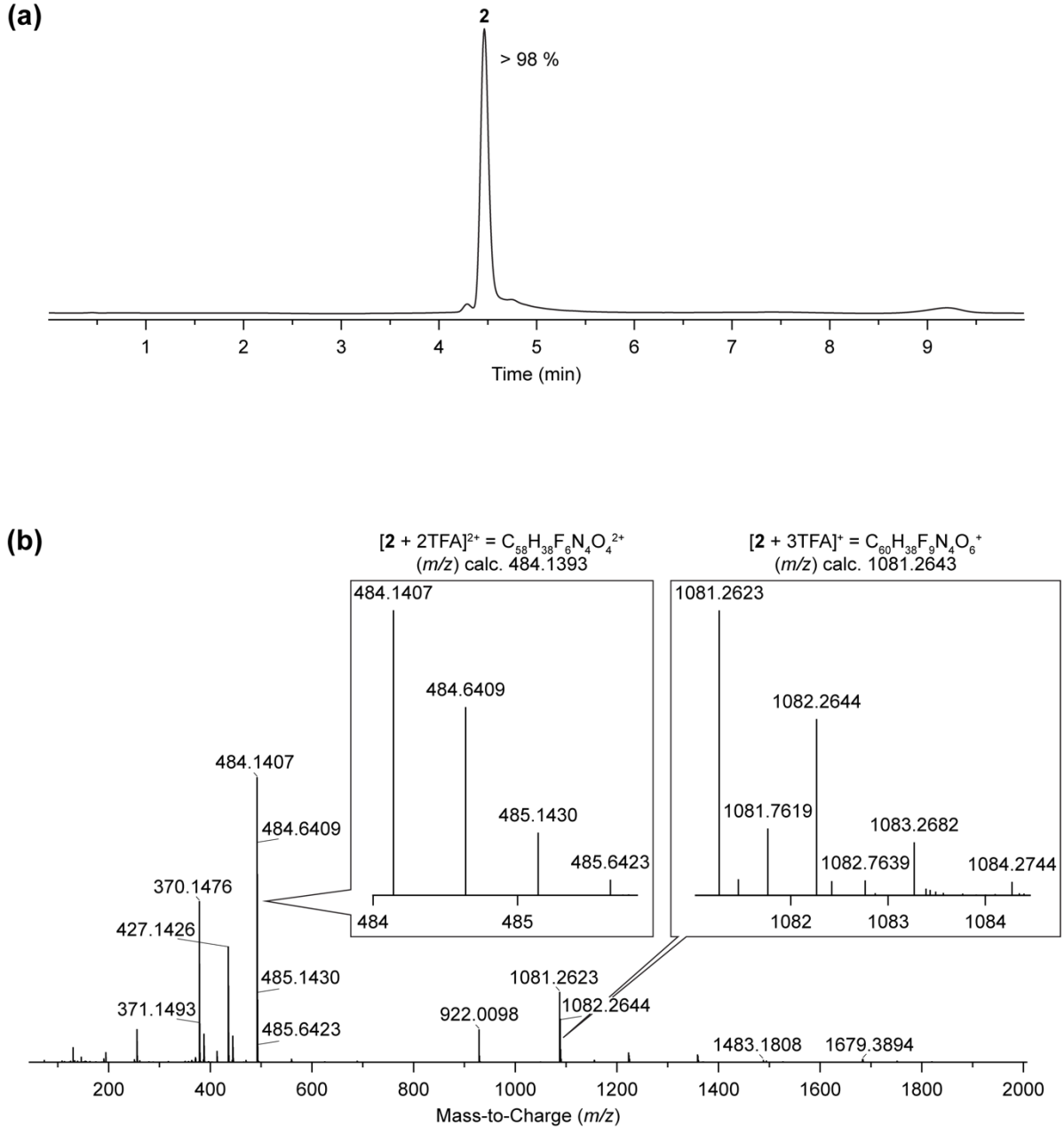


Figure S15 | UHPLC-MS characterization of strand 2. Tandem **a,** Reverse-phase UHPLC chromatogram and **b,** MS spectrum of strand **2**. Absorbance was recorded at 254 nm.

7. NMR Characterization of unfolded strand 2 in CD_3CN

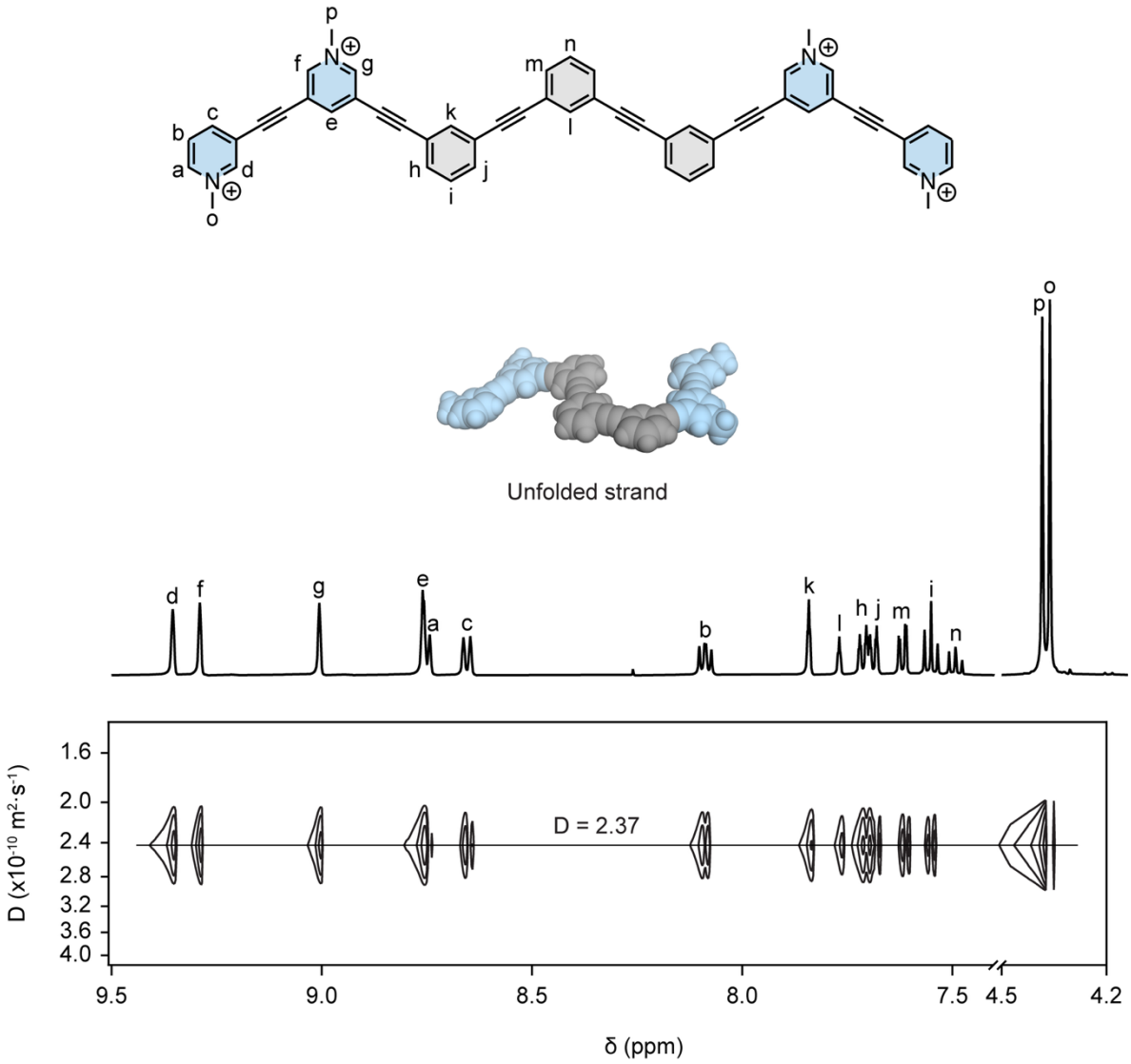


Figure S16 | Expansion of ^{1}H and DOSY NMR spectra of unfolded strand 2·TFA in CD_3CN (5 mM, 500 MHz, 298 K). Similar experiment was performed on strand 2·OTf. The hydrodynamic radii of unfolded strand 2·OTf and unfolded strand 2·TFA were found to be r_H = 10.3 Å and r_H = 10.8 Å, respectively, using the Stokes-Einstein equation.

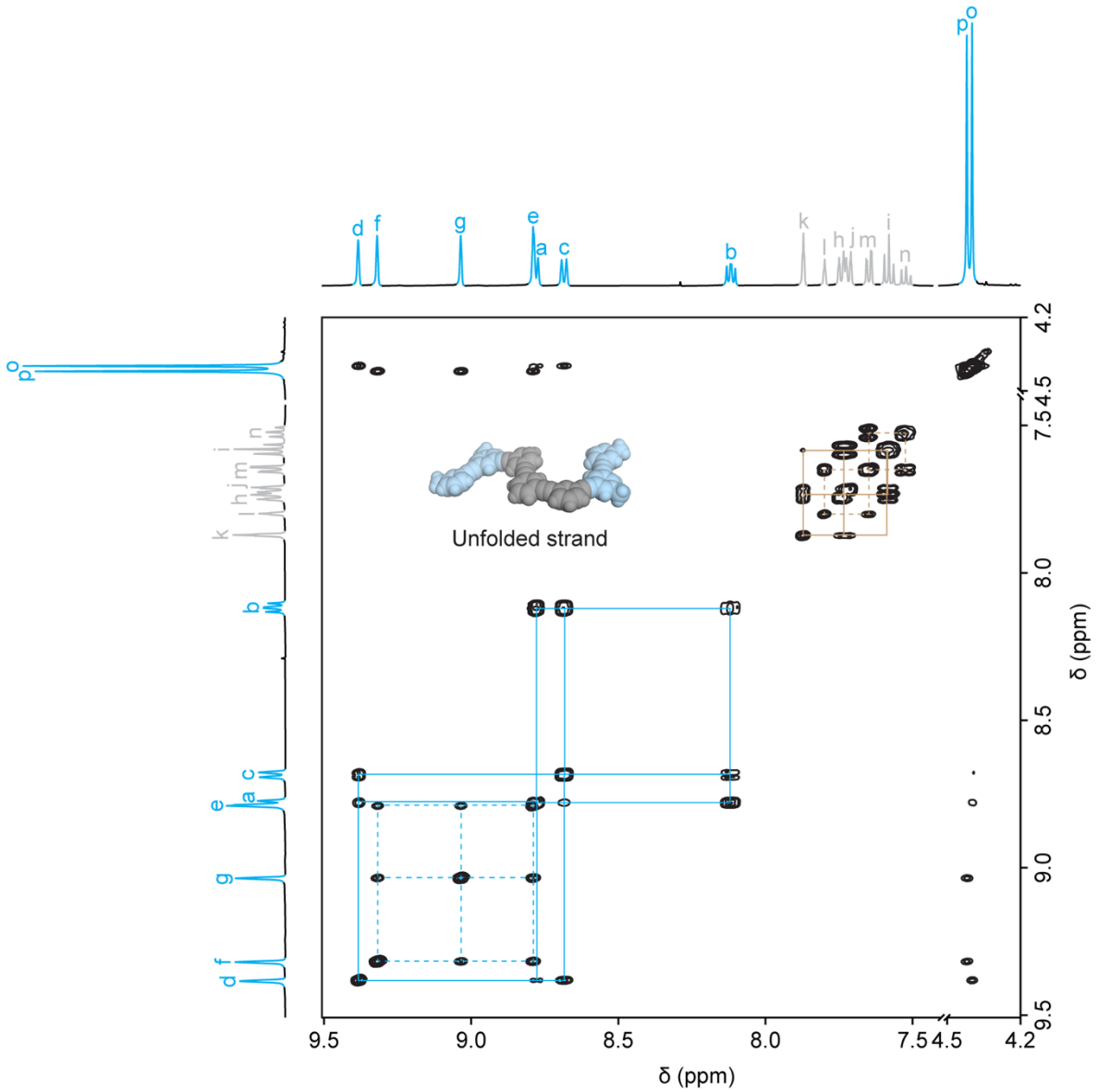


Figure S17 | Expansion of selected regions in 2D ^{1}H-^{1}H COSY NMR spectrum of unfolded strand 2·TFA in CD_3CN (5 mM, 500 MHz, 298 K).

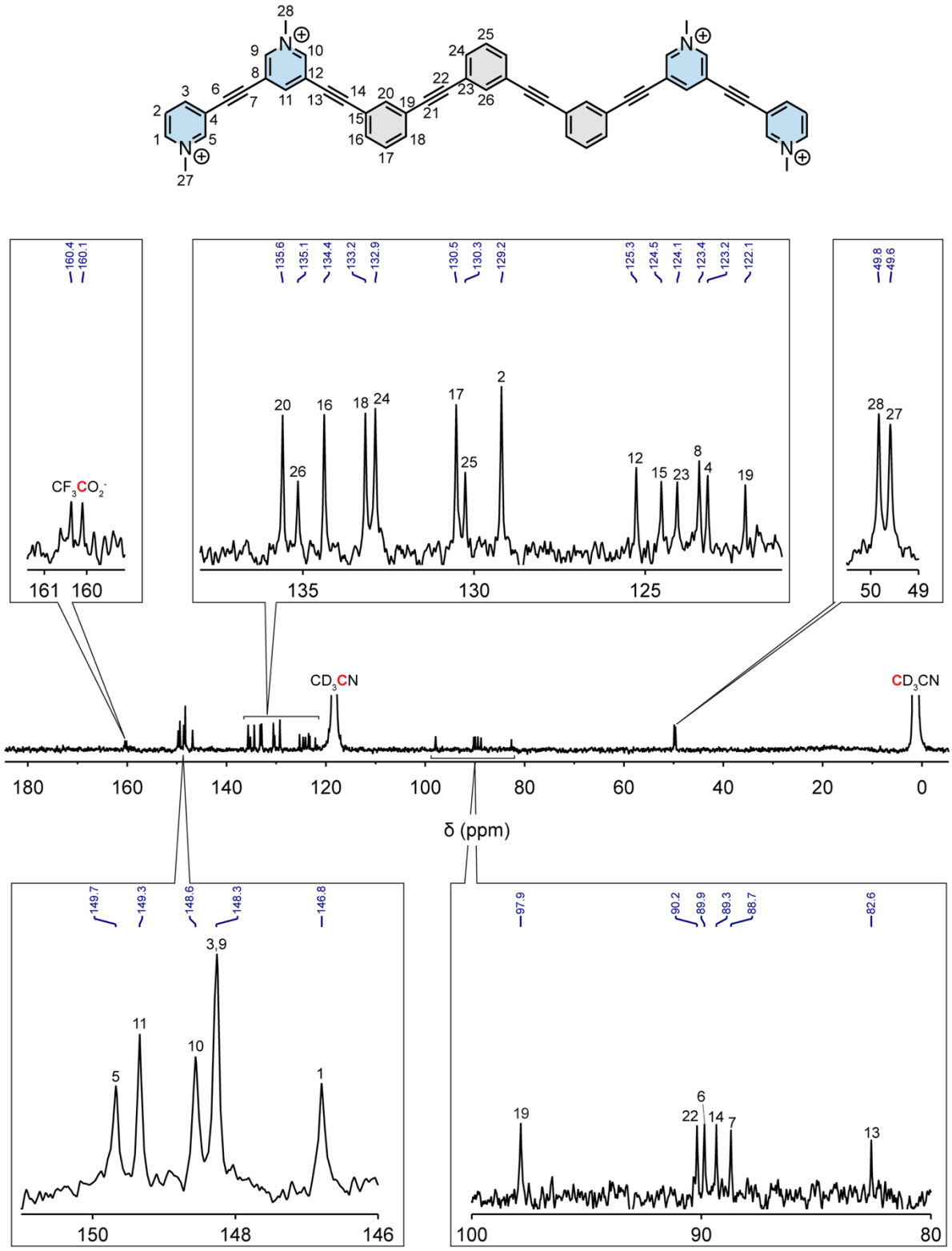


Figure S18 | ^{13}C NMR spectrum of unfolded strand 2·TFA in CD_3CN (5 mM, 126 MHz, 298 K).

8. NMR characterization of double helix $(2)_2$ and triple helix $(2)_3$ in D_2O

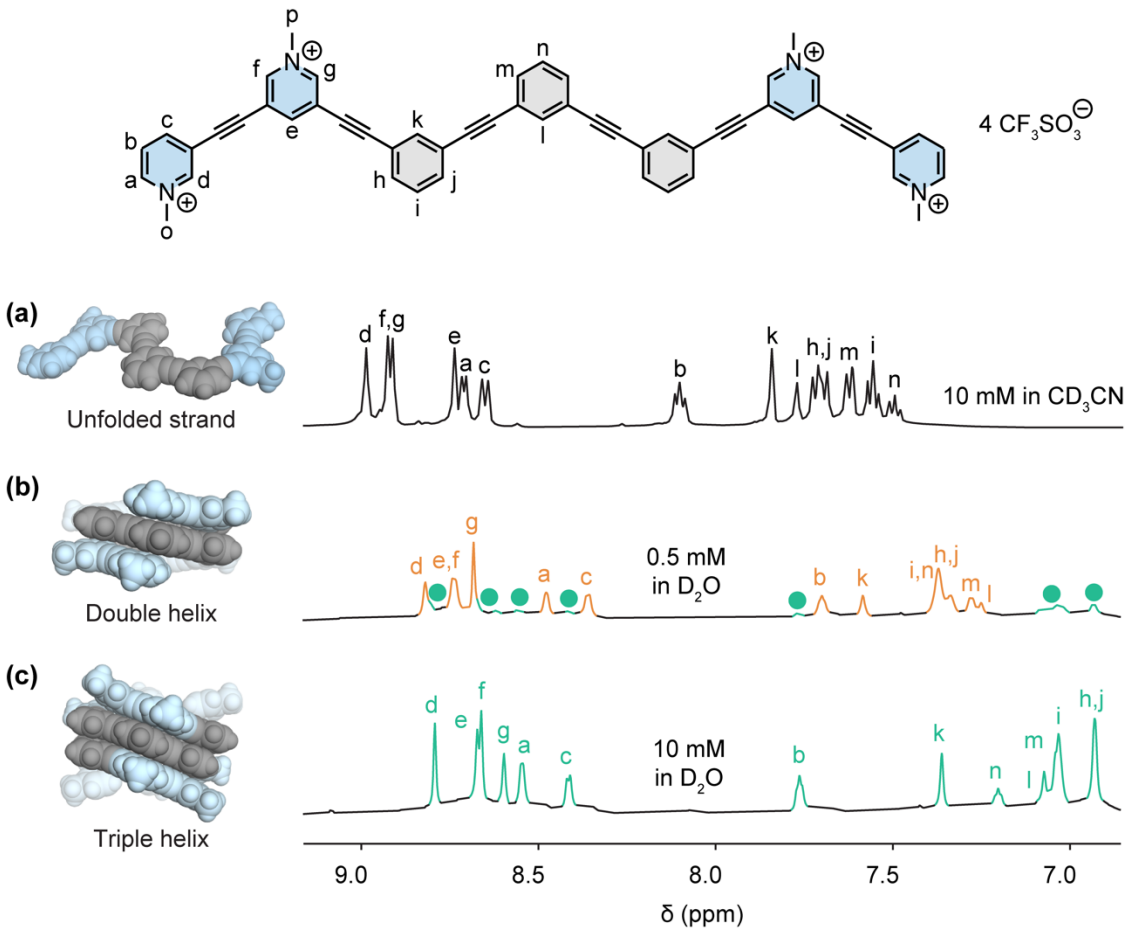


Figure S19 | Solvent-dependent ^{1}H NMR spectra of strand 2. Comparison between the ^{1}H NMR spectra of **a,** unfolded strand **2·OTf** in CD_3CN (10 mM, 500 MHz, 298 K); **b,** double helix $(\mathbf{2})_2$**·OTf** in D_2O (0.5 mM, 800 MHz, 288 K); and **c,** triple helix $(\mathbf{2})_3$**·OTf** in D_2O (10 mM, 800 MHz, 288 K). In spectrum **b**, the signals corresponding to the triple helix are labelled with green circles.

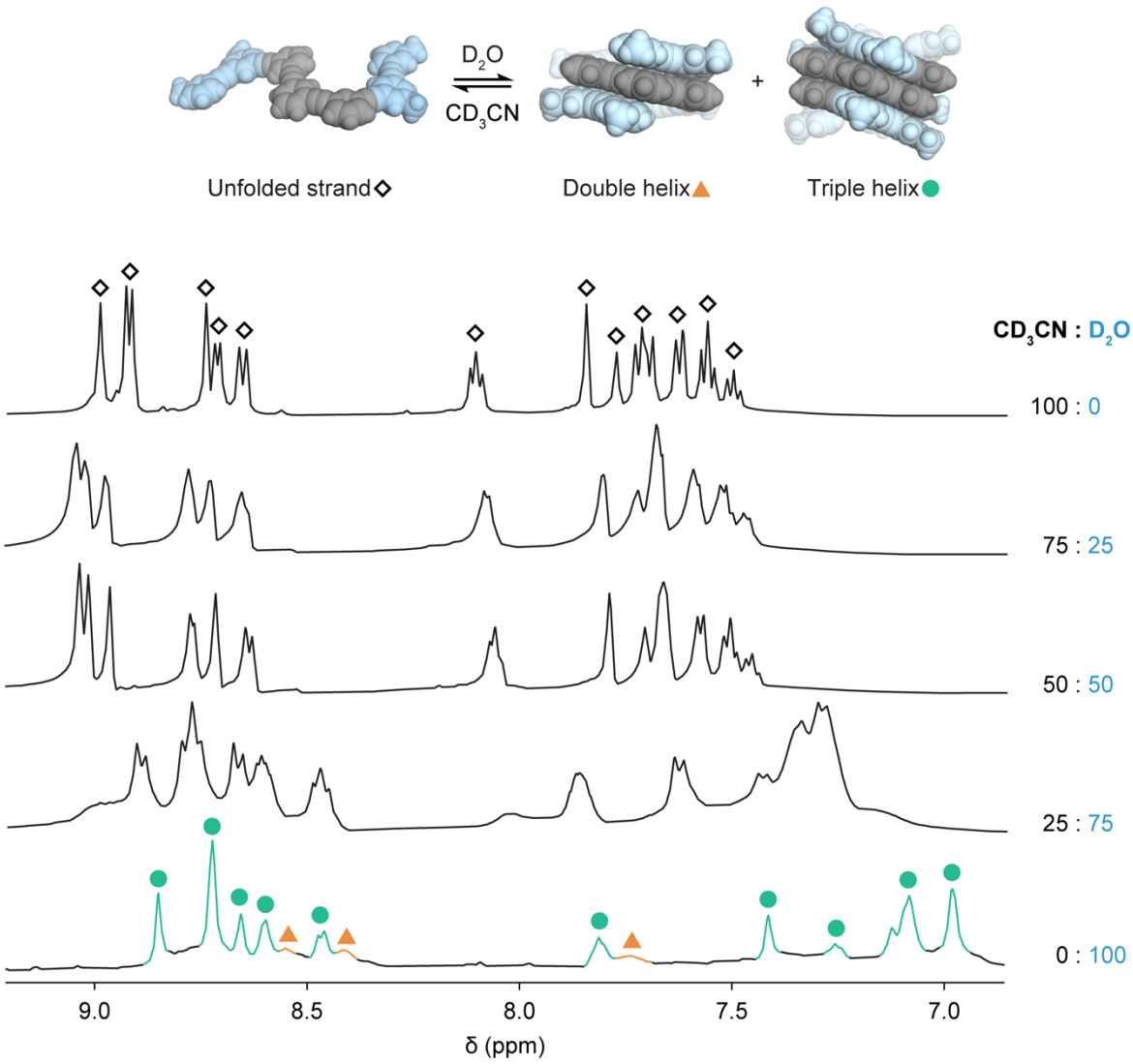


Figure S20 | ^{1}H NMR spectra of 2·OTf aromatic protons in CD_3CN / D_2O mixtures (5 mM, 500 MHz, 298 K). The signals corresponding to the unfolded strand, double helix and triple helix are labelled with empty diamonds, orange triangles and green circles, respectively.

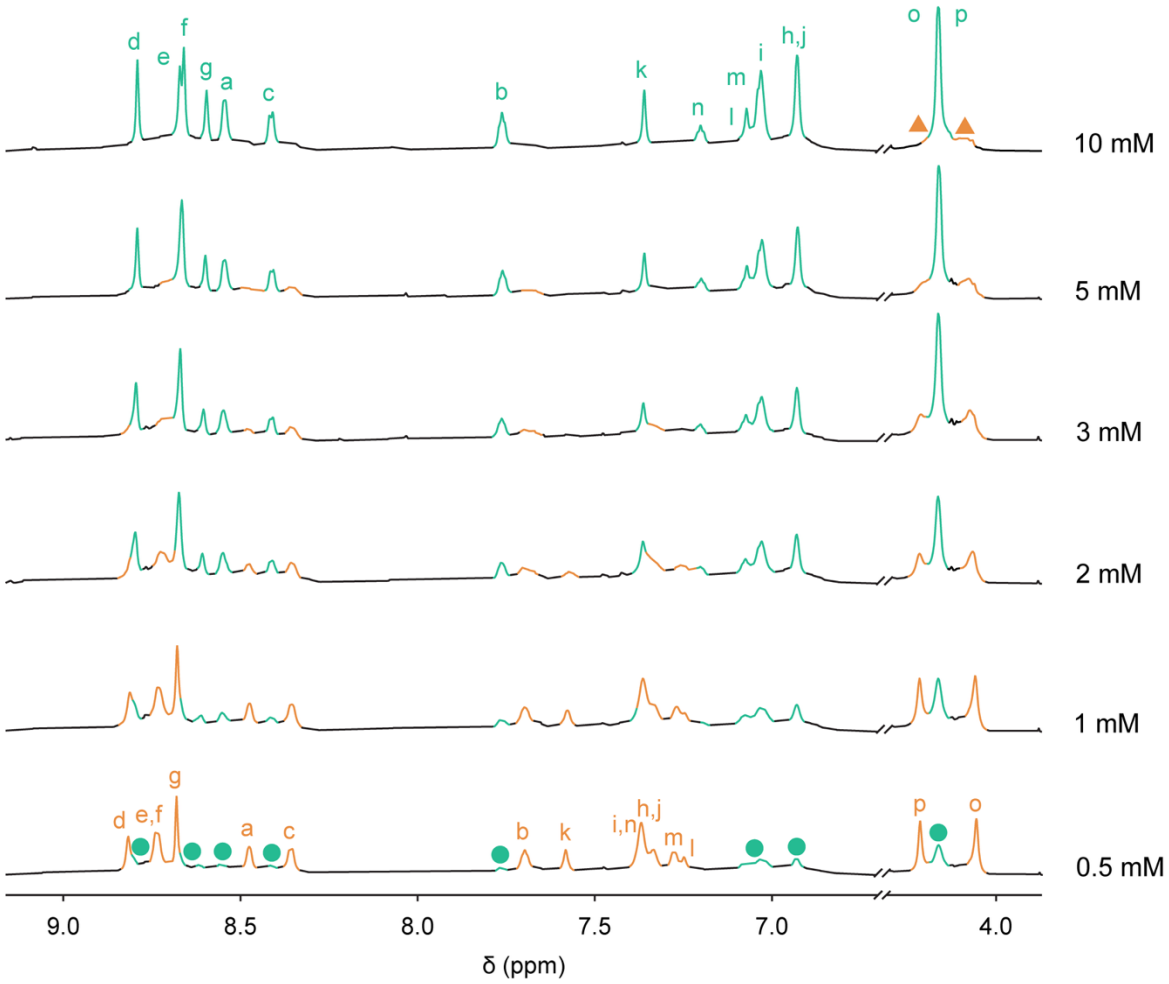


Figure S21 | Concentration-dependent ^{1}H NMR spectra of 2·OTf between 0.5 mM and 10 mM in D_2O (800 MHz, 288 K). The triple helix is the main species observed at high concentration and dissociates into the double helix upon dilution.

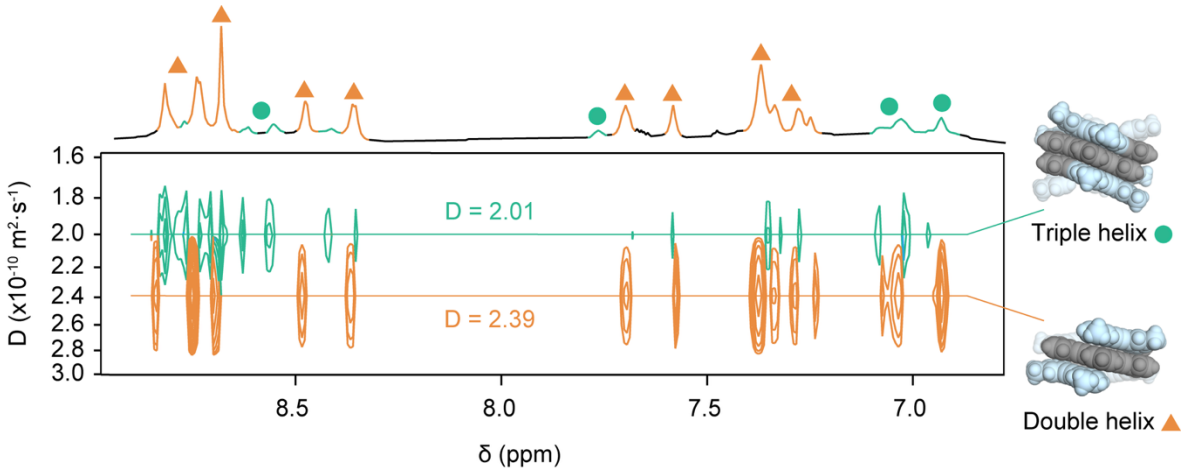


Figure S22 | ^{1}H DOSY NMR spectrum (800 MHz, D_2O, 288 K) of the double and triple helices assembled from 2·OTf (0.5 mM) in D_2O. The signals corresponding to the double and triple helices are labelled with orange triangles and green circles, respectively. The hydrodynamic radii of the double and triple helices were found to be r_H = 8.1 Å and r_H = 9.4 Å, respectively, using the Stokes-Einstein equation.

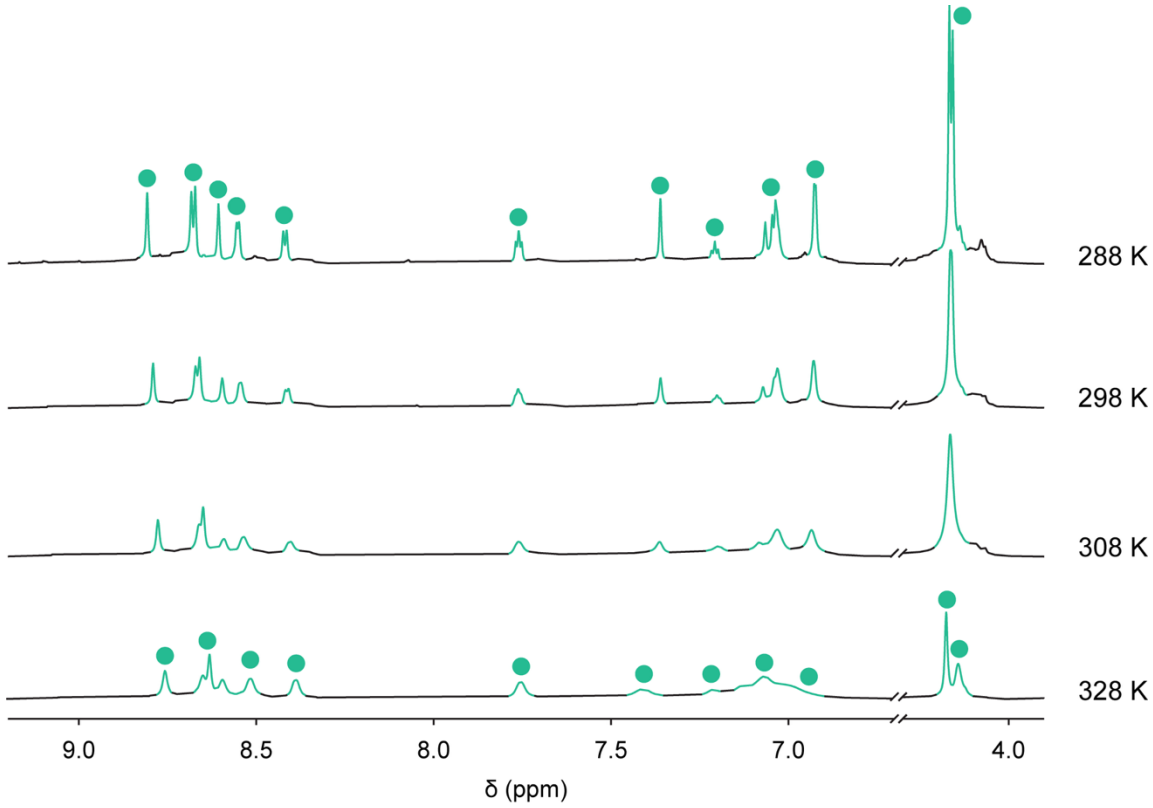


Figure S23 | Variable temperature ^{1}H NMR spectra of 2·OTf between 288 K and 328 K in D_2O (800 MHz, 10 mM). The triple helix (signals labelled with green circles) remains intact at high temperature when strand concentration is sufficiently high.

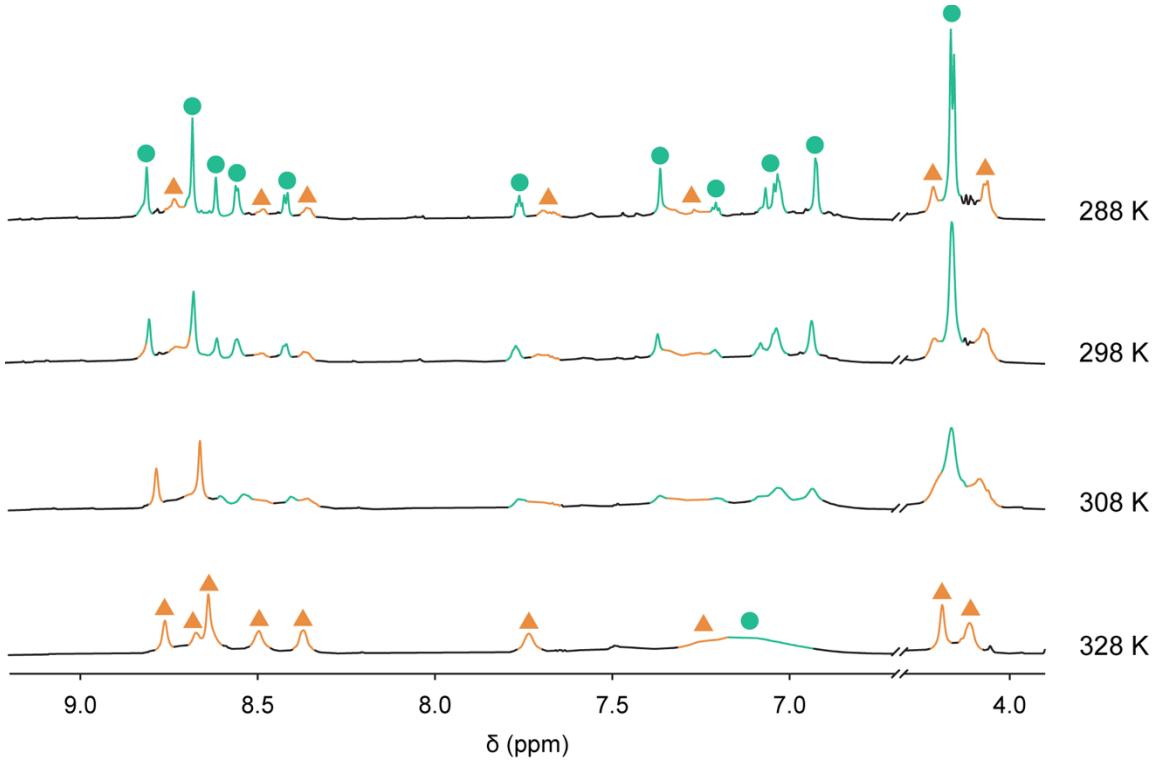


Figure S24 | Variable temperature ^{1}H NMR spectra of 2·OTf between 288 K and 328 K in D_2O (800 MHz, 3 mM). The spectra show the temperature-dependent interconversion between double and triple helix (signals labelled with orange triangles and green circles, respectively) at low strand concentration.

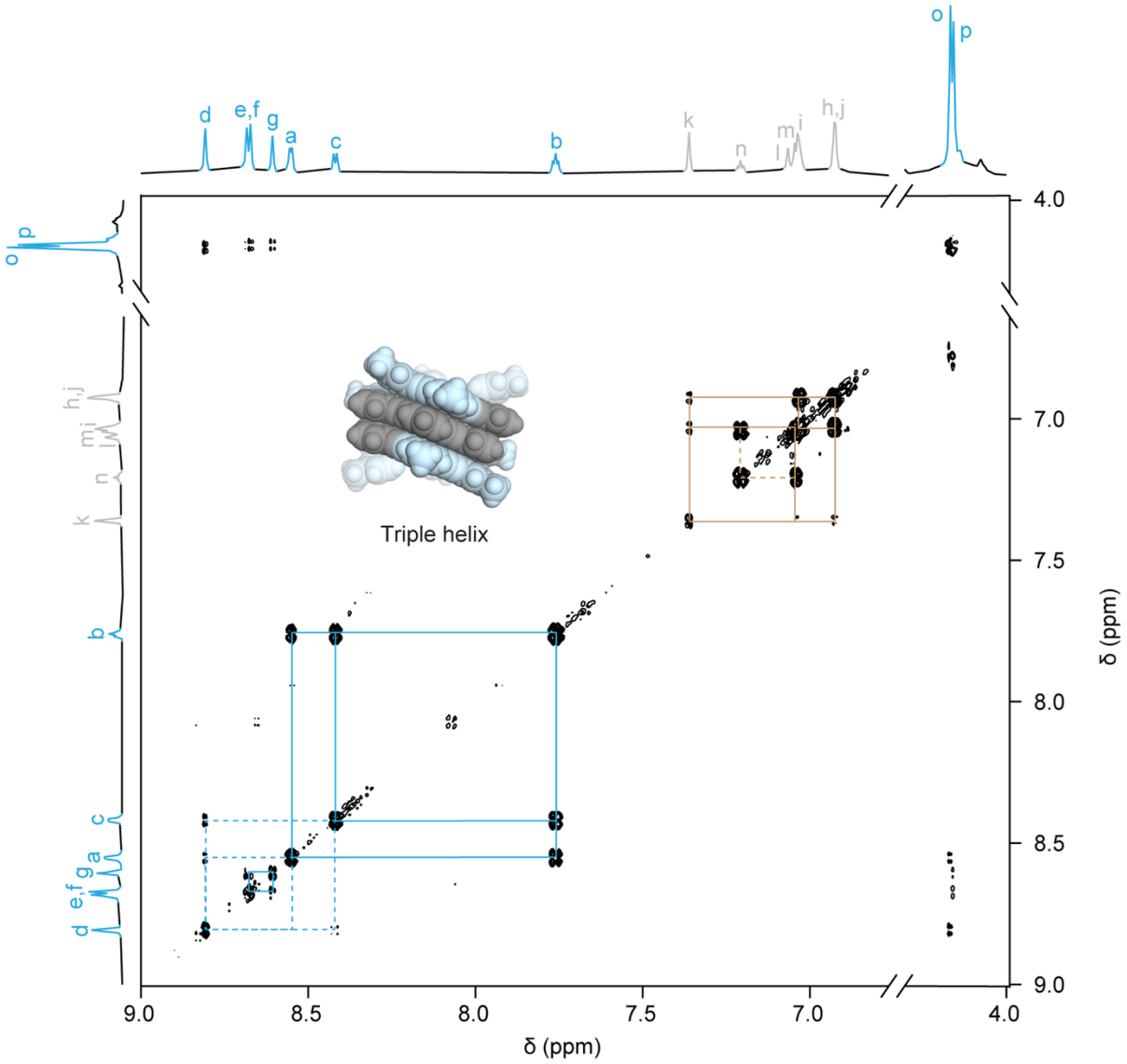


Figure S25 | 2D ^{1}H-^{1}H COSY from selected spectral regions of triple helix $(2)_3 \cdot$OTf in D_2O (10 mM, 800 MHz, 288 K).

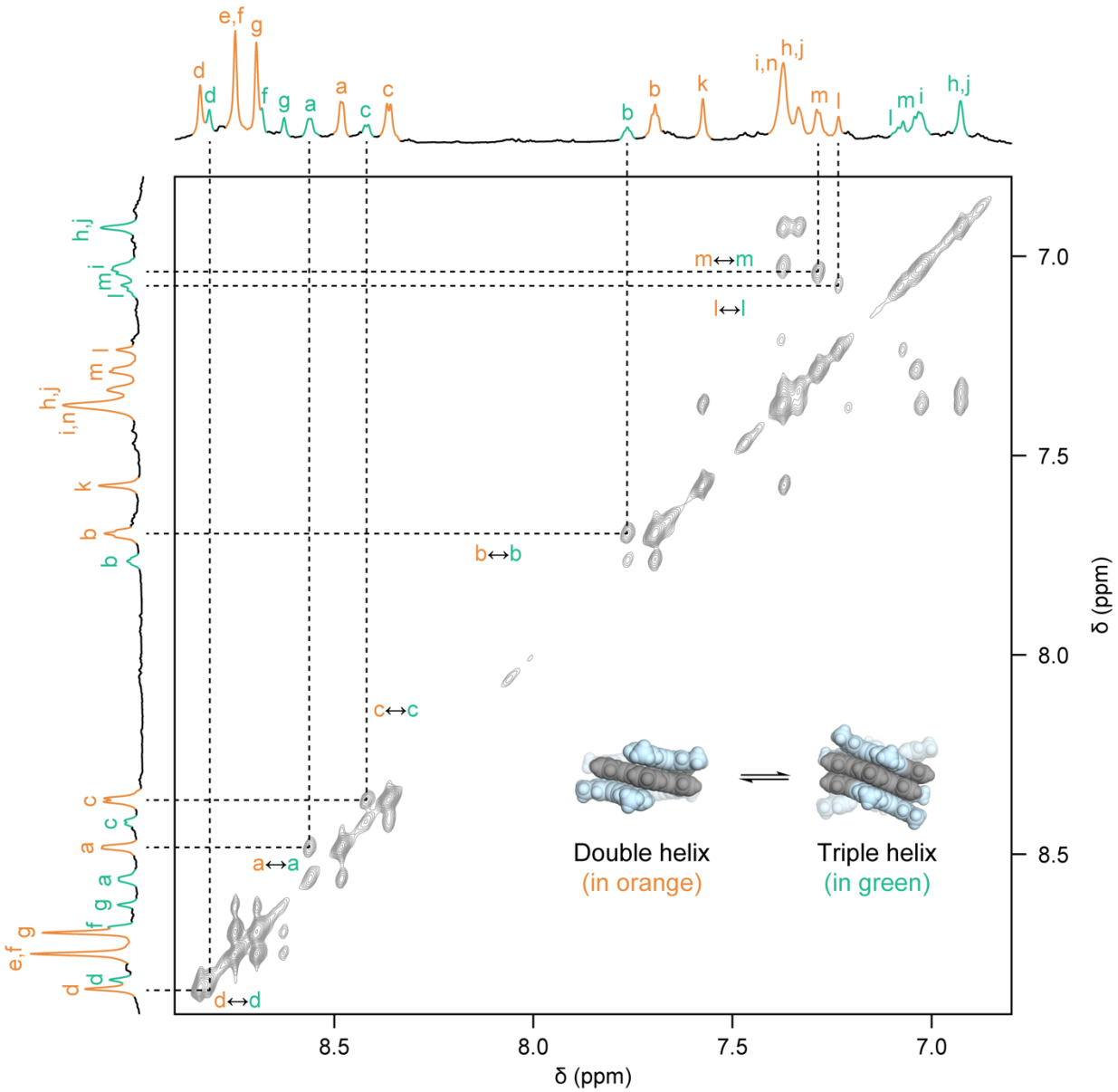


Figure S26 | 2D ^{1}H-^{1}H ROESY NMR spectrum from aromatic region of 2·OTf at 0.5 mM in D_2O (800 MHz, 288 K, 200 ms mixing time). The dotted lines highlight exchange cross-peaks between the protons of the double and triple helices, colored in orange and green, respectively. The ROE cross-peak correlations are shown on the following figures.

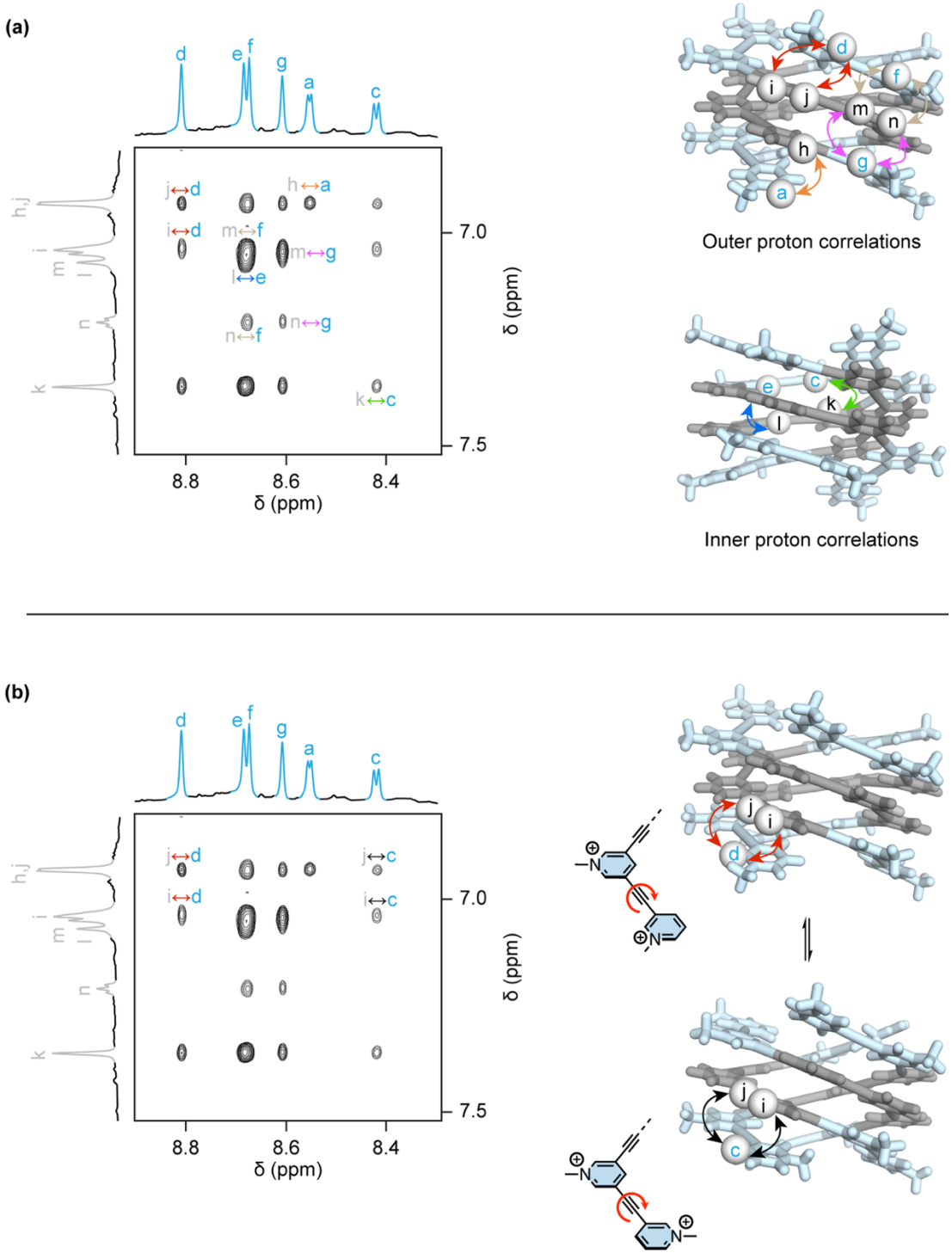


Figure S27 | Expansion of aromatic region in 2D ^{1}H-^{1}H ROESY NMR spectrum of triple helix $(2)_3$·OTf in D_2O (10 mM, 800 MHz, 288 K, 200 ms mixing time). a, Highlighted key correlations between protons of stacked pyridinium (colored in blue) and phenylene (colored in gray) residues. **b,** Rotation of the terminal pyridinium residue around the acetylene bond results in the appearance of additional 2D correlations between stacked pyridinium and phenylene residues.

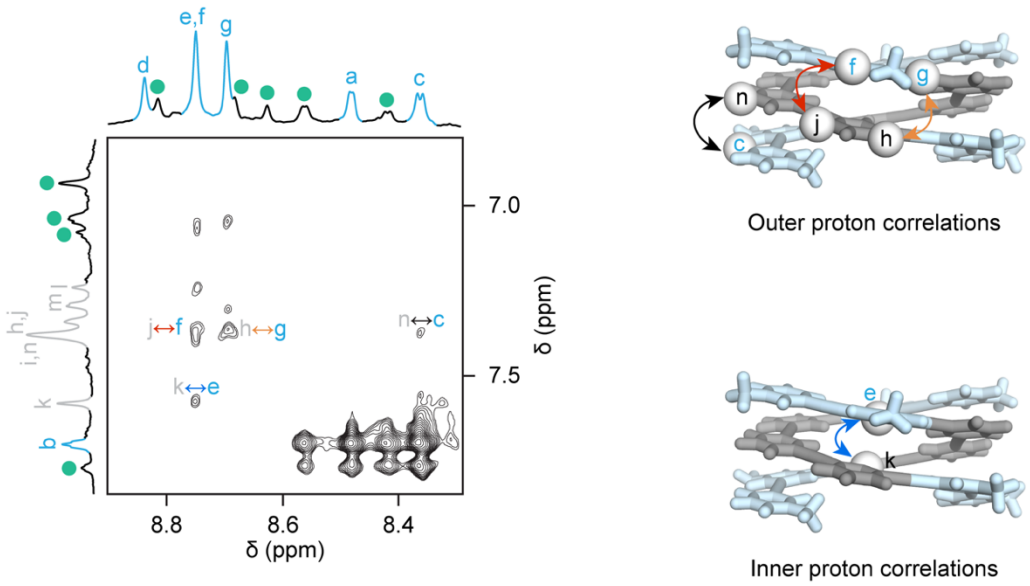


Figure S28 | Aromatic region of 2D ^{1}H-^{1}H ROESY NMR spectrum of double helix $(2)_2$·OTf in D_2O (0.5 mM, 800 MHz, 288 K, 200 ms mixing time). Key correlations between protons of stacked pyridinium (colored in blue) and phenylene (colored in gray) residues are highlighted. The signals corresponding to the triple helix are labelled with green circles.

9. Host-guest studies with triple helix $(2)_3 \cdot TFA$

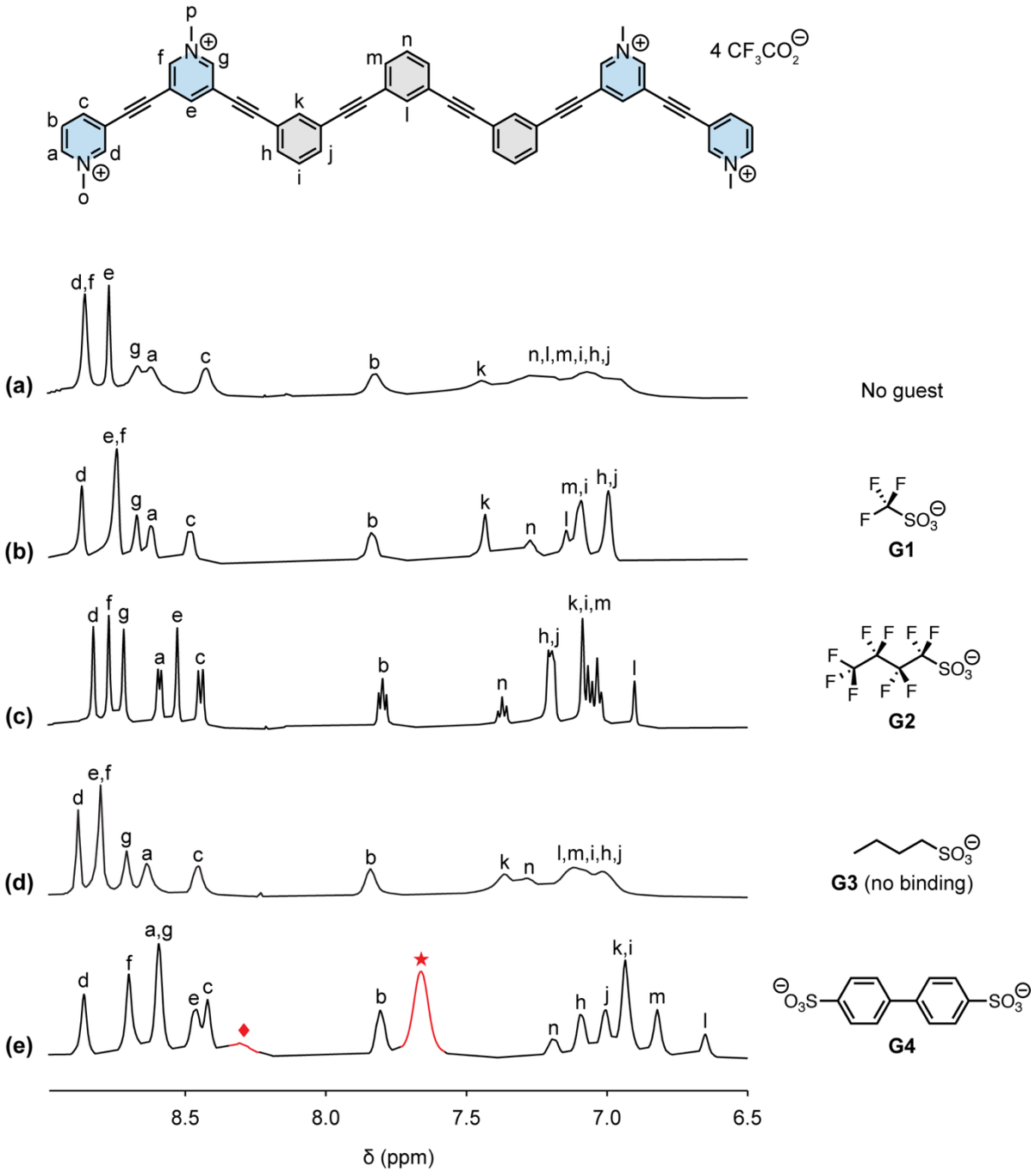


Figure S29 | Aromatic region of ^{1}H NMR spectra of 2·TFA (5 mM in D_2O, 500 MHz, 298 K) after addition of different guests. a, No guest added. **b,** After addition of 10.0 equiv. of potassium trifluoromethanesulfonate **G1**. **c,** After addition of 5.0 equiv. of potassium perfluorobutanesulfonate **G2**. **d,** After addition of 3.9 equiv. of sodium butanesulfonate **G3**. **e,** After addition of 5.5 equiv. of sodium 4,4'-biphenyldisulfonate **G4**. The signals corresponding to bound and free guest **G4** are labelled with a red diamond and a star, respectively.

9.1. Titration with potassium trifluoromethanesulfonate (G1)

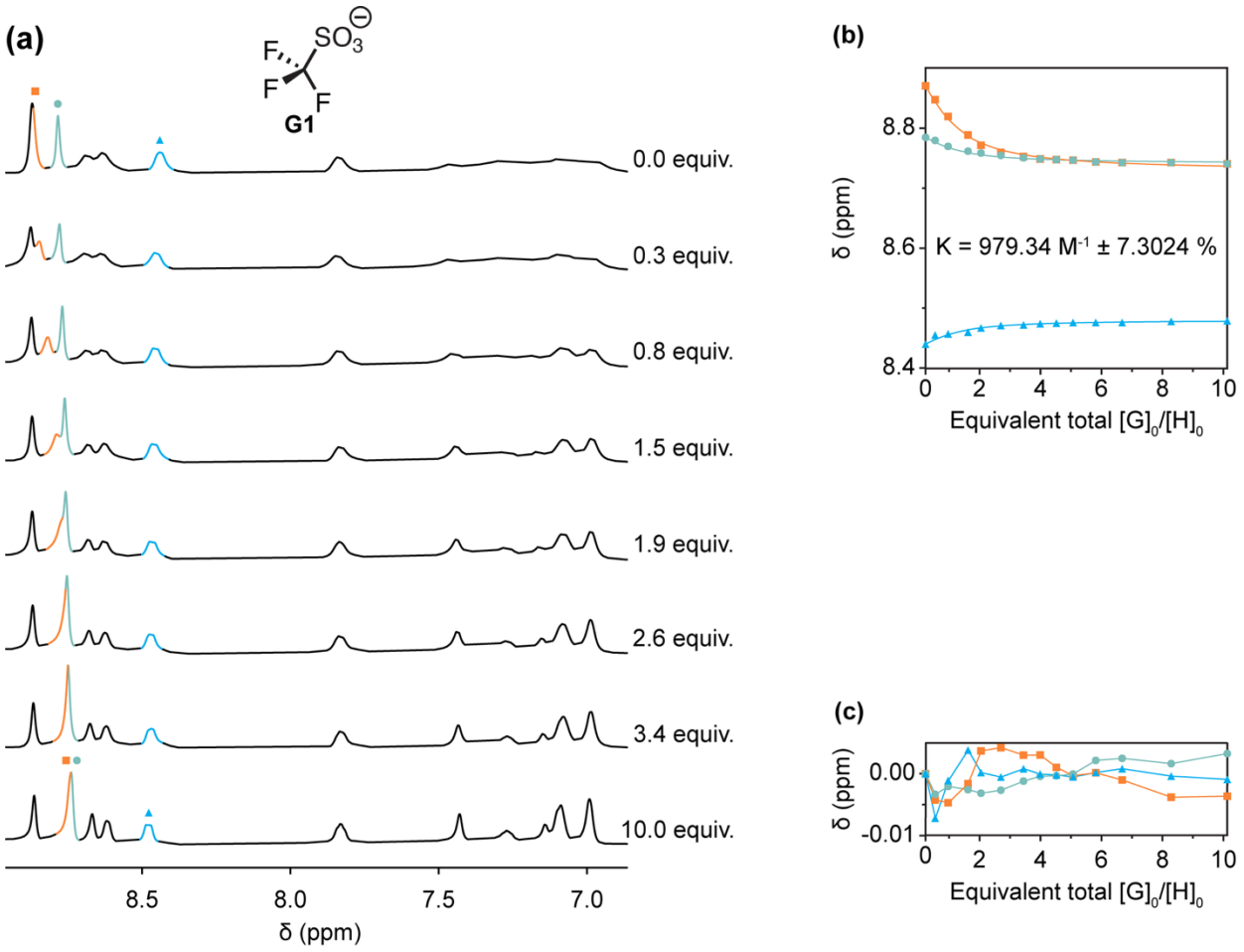


Figure S30 | ^{1}H NMR titration (500 MHz, 298 K) of potassium trifluoromethanesulfonate G1 into a 5 mM-solution of 2·TFA in D_2O. a, Selected region of the ^{1}H NMR spectra recorded during the titration. **b,** Chemical shift changes recorded as a function of guest equivalents. **c,** Residuals from the curve fitting. Association constant was obtained by fitting the data with *BindFit*.[S2]

9.2. Titration with potassium perfluorobutanesulfonate (G2)

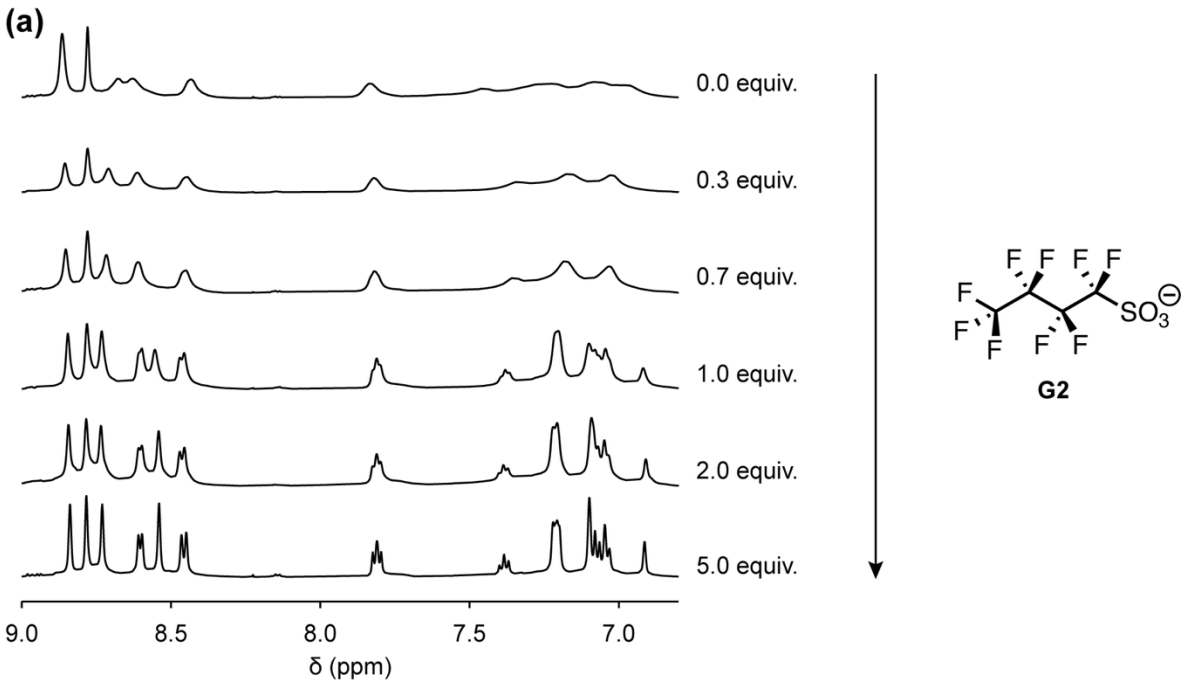


Figure S31 | ^{1}H NMR titration (500 MHz, 298 K) of potassium perfluorobutanesulfonate G2 into a 5 mM-solution of 2·TFA in D_2O.

1.1. Titration with sodium 4,4'-biphenyldisulfonate (G4)

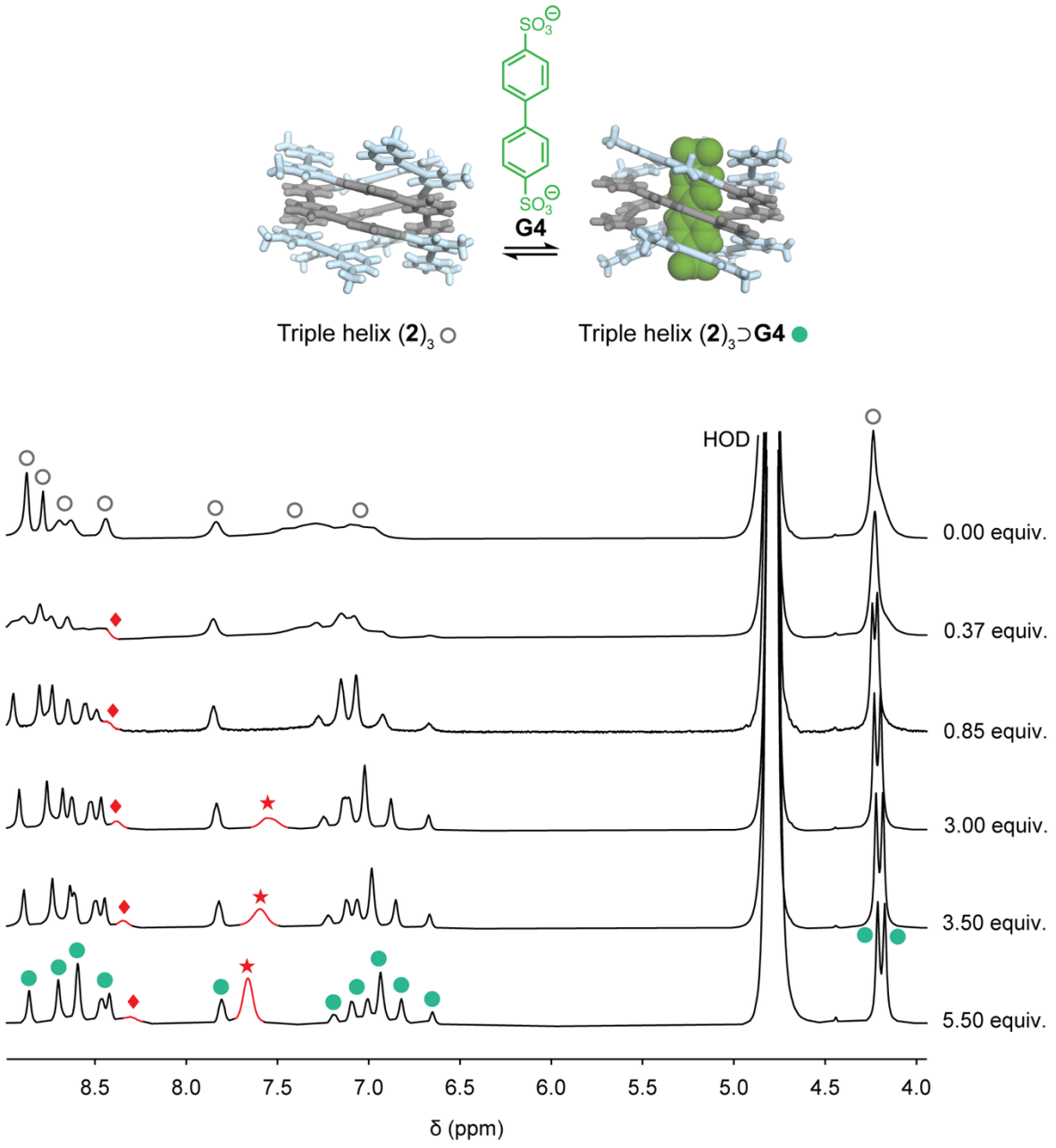


Figure S32 | ^{1}H NMR titration (500 MHz, 298 K) of sodium 4,4'-biphenyldisulfonate G4 into a 5 mM-solution 2·TFA in D_2O. The NMR signals of the resulting complex remain relatively broad, presumably due to dynamic deformations of the triple helix induced by electrostatic attraction between **G4** and the pyridinium units, as evidenced by DFT modeling. This bulky guest appears to occupy the cavity more completely than **G2**, slowing the exchange between free and bound guests on the NMR timescale. The signals corresponding to the bound and free guest are labelled with a red diamond and a red star, respectively.

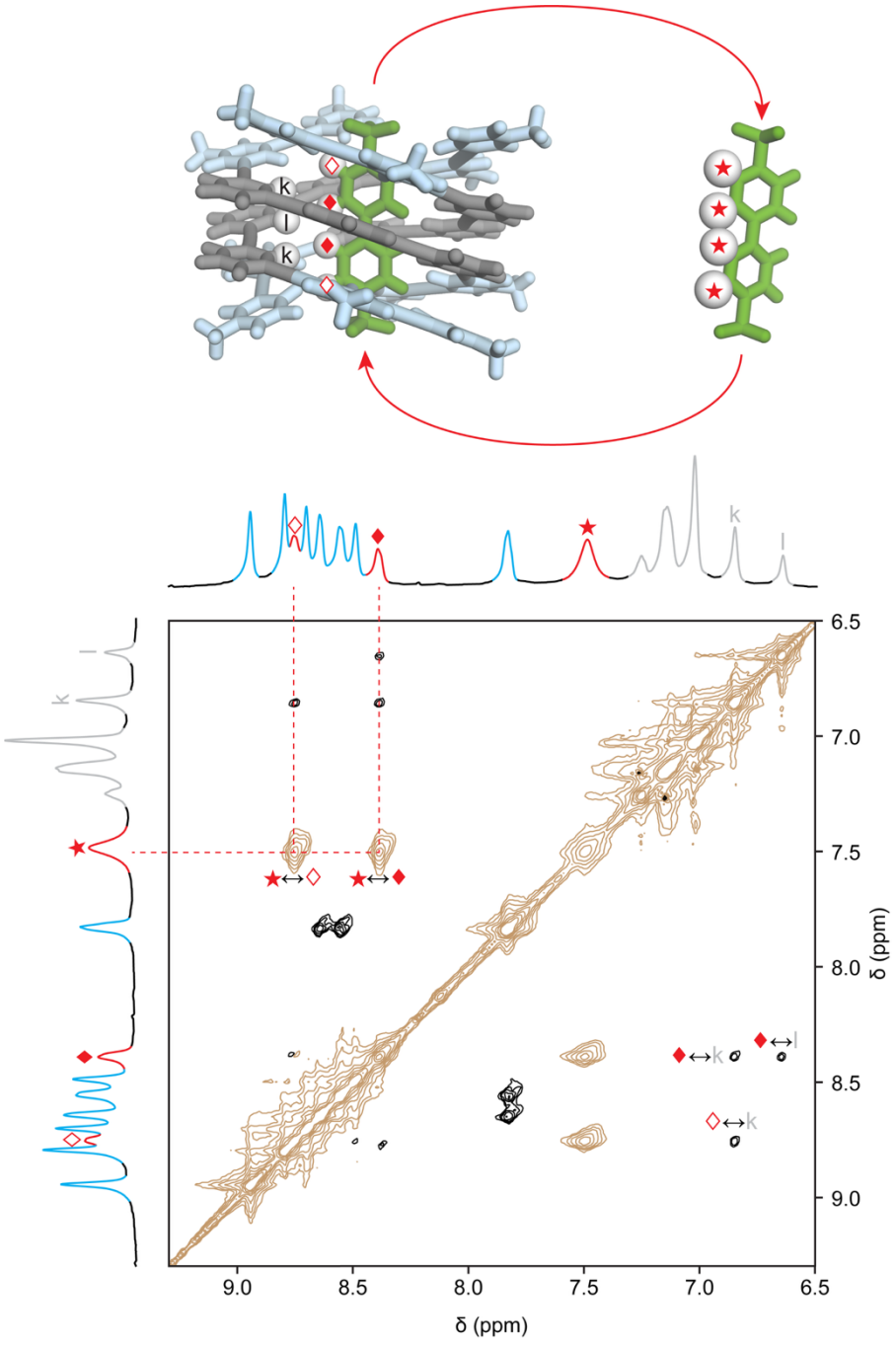


Figure S33 | Expansion of selected spectral regions from 2D ^{1}H-^{1}H ROESY of 2·TFA at 5 mM in D_2O (500 MHz, 100 ms mixing time) recorded at low temperature (278 K) in the presence of 5.5 equiv. of sodium 4,4'-biphenyldisulfonate G4. The dotted lines highlight exchange cross-peaks bound and free guest protons, labelled with red diamonds and star, respectively. ROE correlations between the bound guest and the inner phenylene protons of the triple helix (*k* and *l*) are also observable.

10. Concentration- and temperature dependent double-to-triple helix transformation in the presence of guests G1-G4

10.1. Concentration- and temperature dependent double-to-triple helix transformation in the presence of potassium trifluoromethanesulfonate (G1)

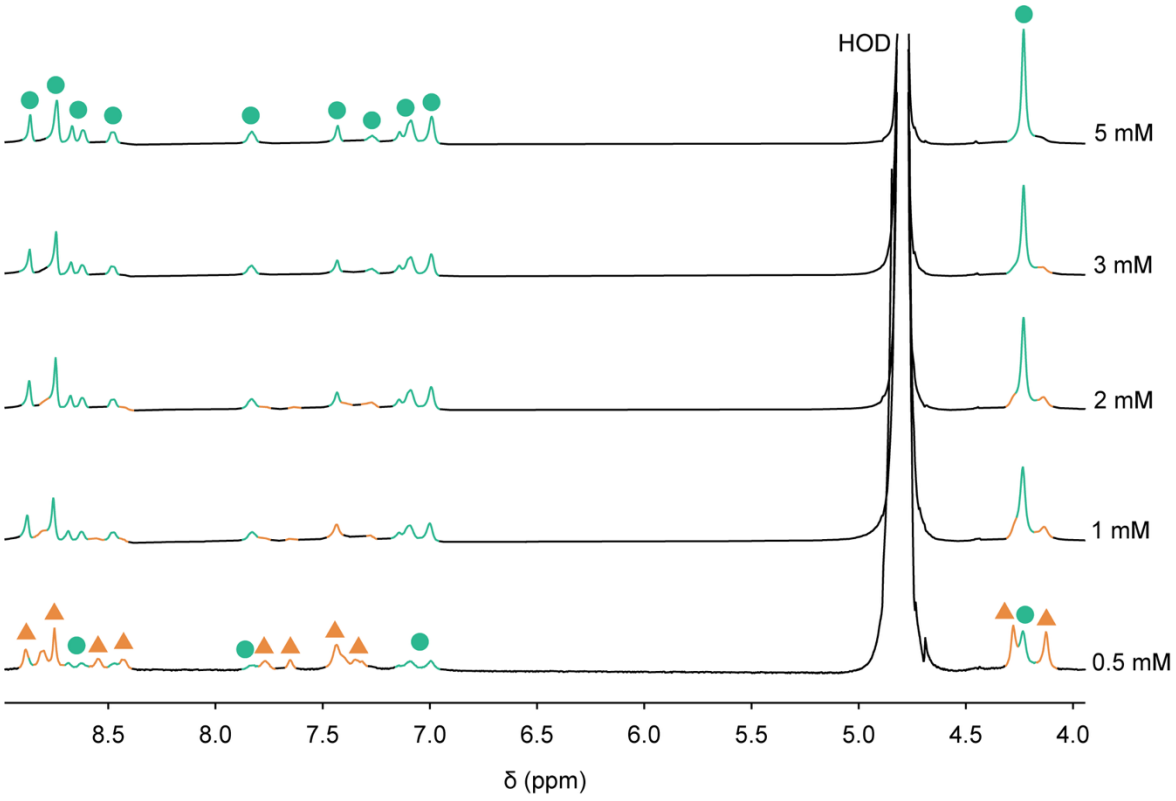


Figure S34 | Concentration-dependent ^{1}H NMR spectra of 2·TFA between 0.5 mM and 5 mM in D_2O (500 MHz, 298 K) in the presence of 10 equiv. of potassium trifluoromethanesulfonate G1. The signals corresponding to the double and triple helices are labelled with orange triangles and green circles, respectively.

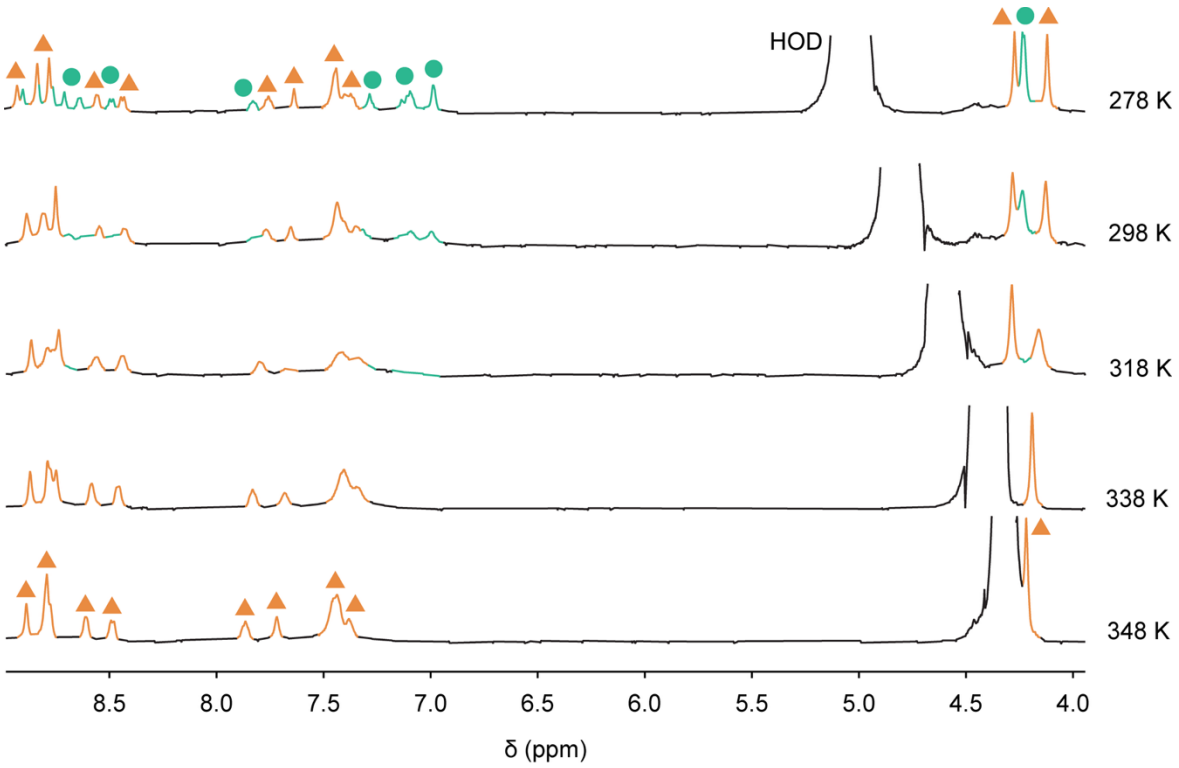


Figure S35 | Variable temperature ^{1}H NMR spectra of 2·TFA between 278 K and 348 K in D_2O (500 MHz, 0.5 mM) in the presence of 10 equiv. of potassium trifluoromethanesulfonate G1. The signals corresponding to the double and triple helices are labelled with orange triangles and green circles, respectively.

10.2. Concentration- and temperature-dependent double-to-triple helix transformation in the presence of potassium perfluorobutanesulfonate (G2)

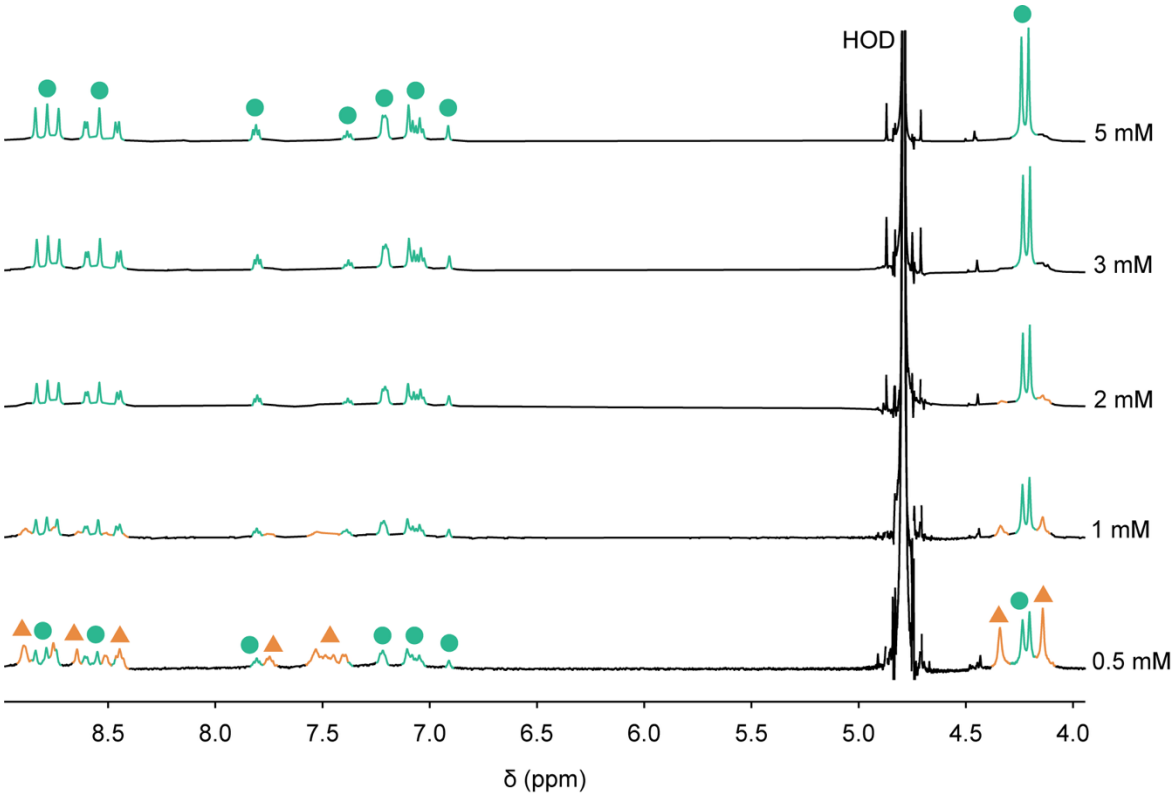


Figure S36 | Concentration-dependent ^{1}H NMR spectra of 2·TFA between 0.5 mM and 5 mM in D_2O (500 MHz, 298 K) in the presence of 5 equiv. of potassium perfluorobutanesulfonate G2. The signals corresponding to the double and triple helices are labelled with orange triangles and green circles, respectively.

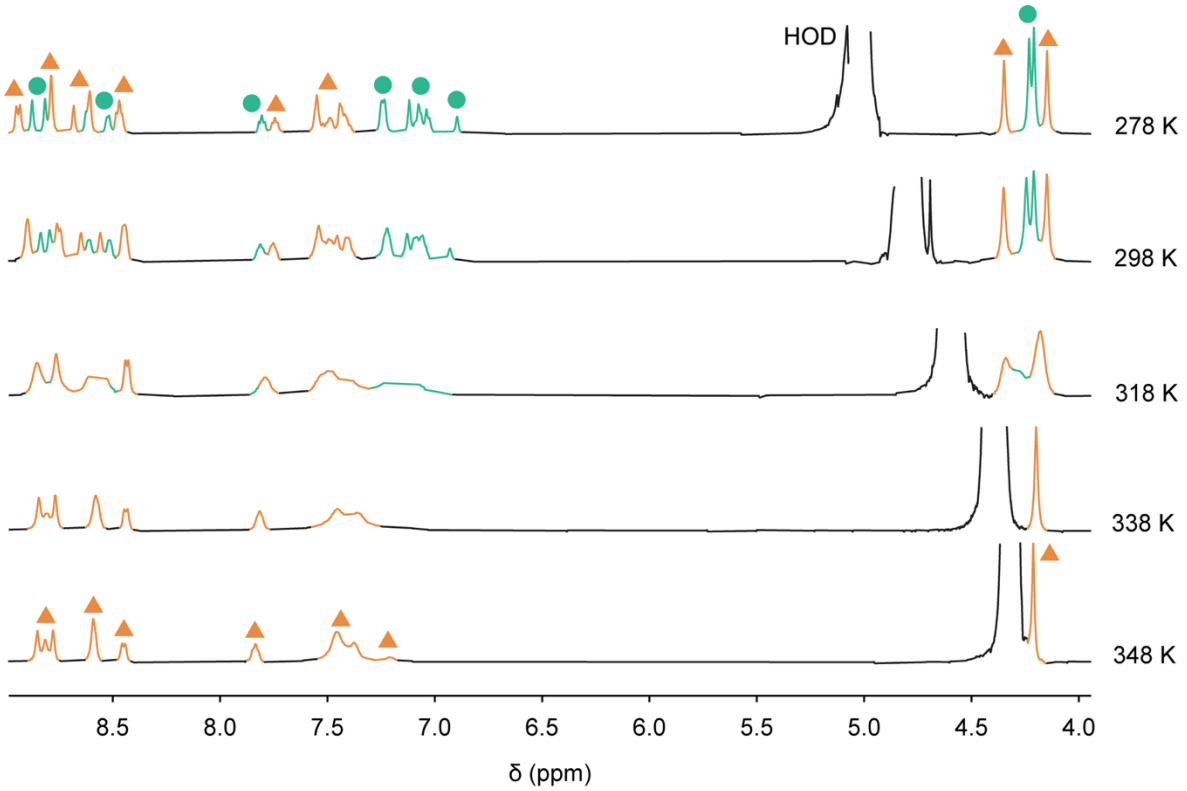


Figure S37 | Variable temperature ^{1}H NMR spectra of 2·TFA between 278 K and 348 K in D_2O (500 MHz, 0.5 mM) in the presence of 5 equiv. of potassium perfluorobutanesulfonate G2. The signals corresponding to the double and triple helices are labelled with orange triangles and green circles, respectively.

10.3. Concentration- and temperature-dependent double-to-triple helix transformation in the presence of sodium 4,4'-biphenyldisulfonate guest (G4)

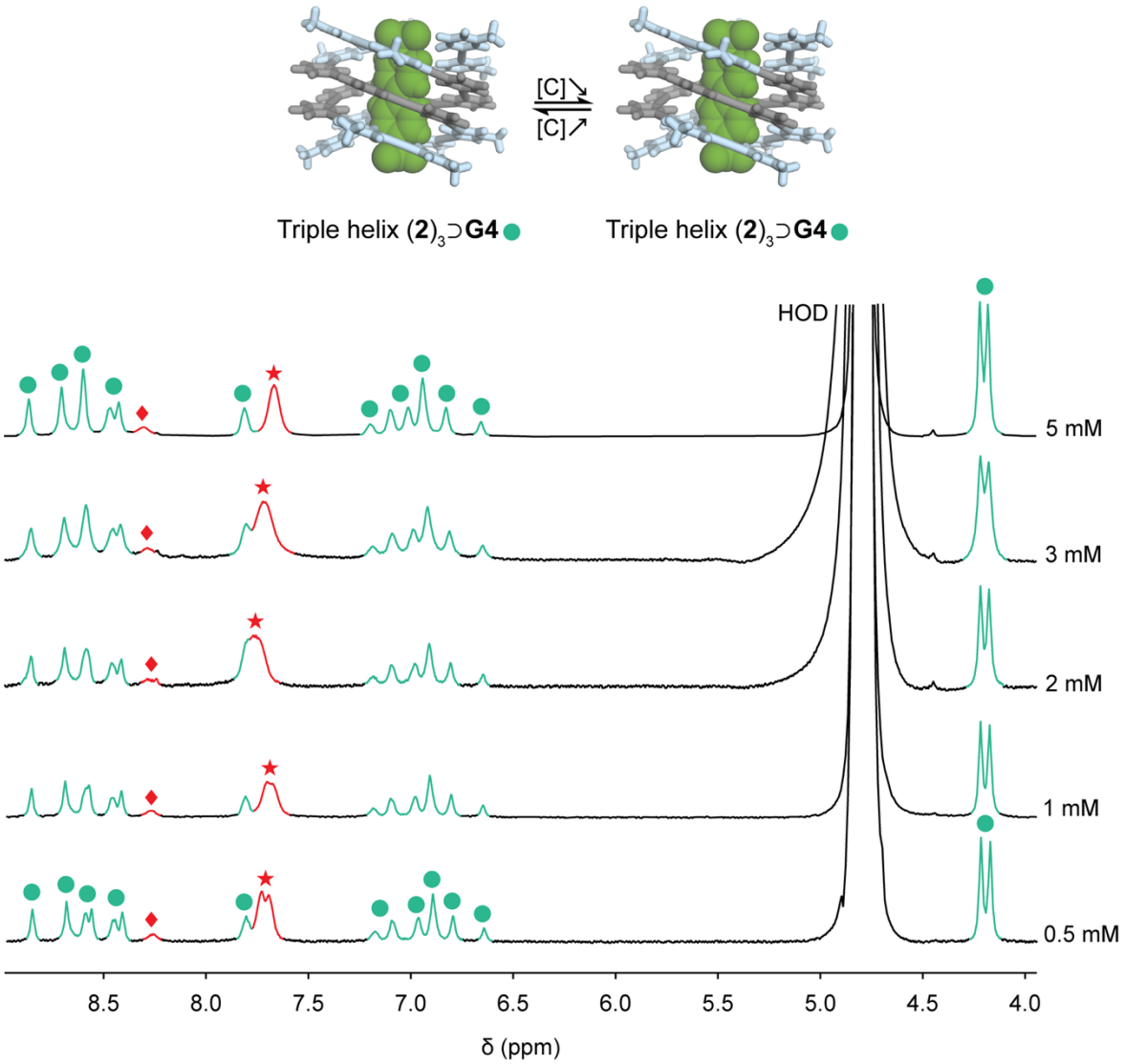


Figure S38 | Concentration-dependent ^{1}H NMR spectra of 2·TFA between 0.5 mM and 5 mM in D_2O (500 MHz, 298 K) in the presence of 5.5 equiv. of sodium 4,4'-biphenyldisulfonate G4. No switch was observed in the conditions.

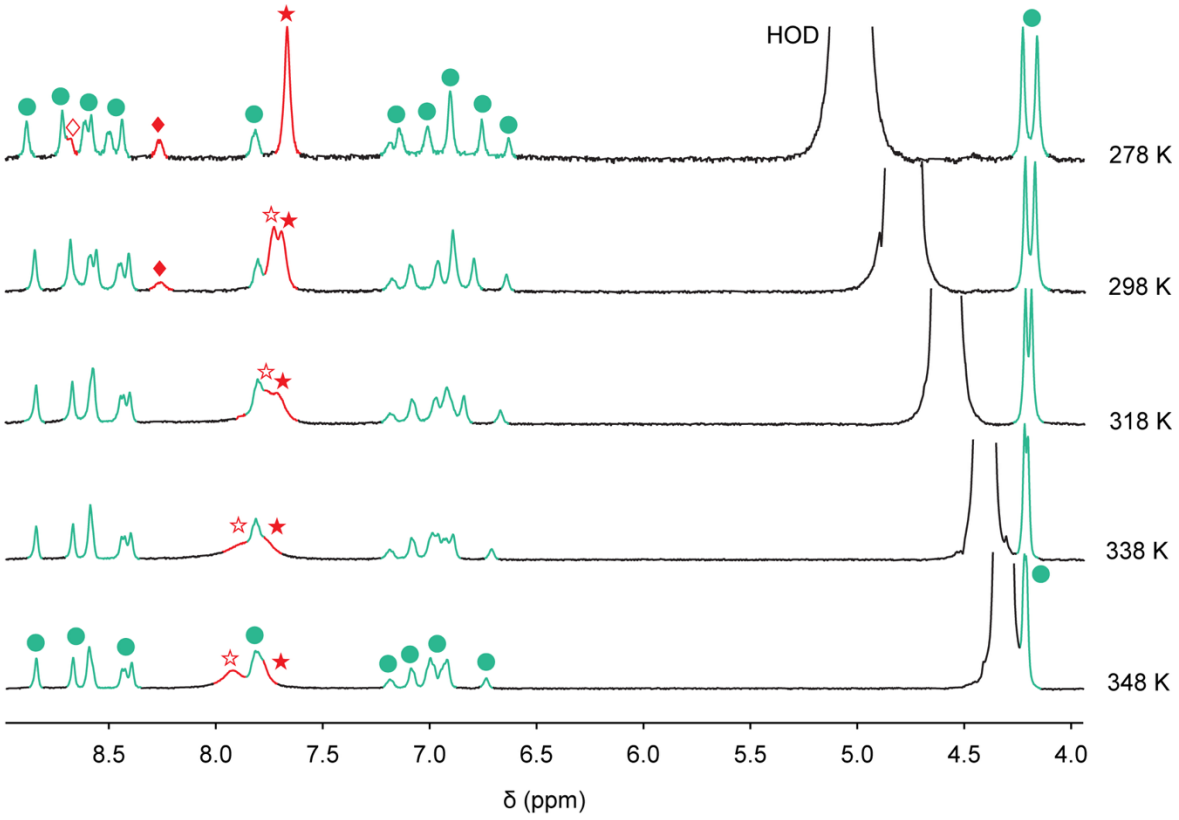


Figure S39 | Variable temperature ^{1}H NMR spectra of 2·TFA between 278 K and 348 K in D_2O (500 MHz, 0.5 mM) in the presence of 5.5 equiv. of sodium 4,4'-biphenyldisulfonate G4. No switch was observed in the conditions.

11. ^{1}H and ^{13}C NMR spectra of the synthesized compounds

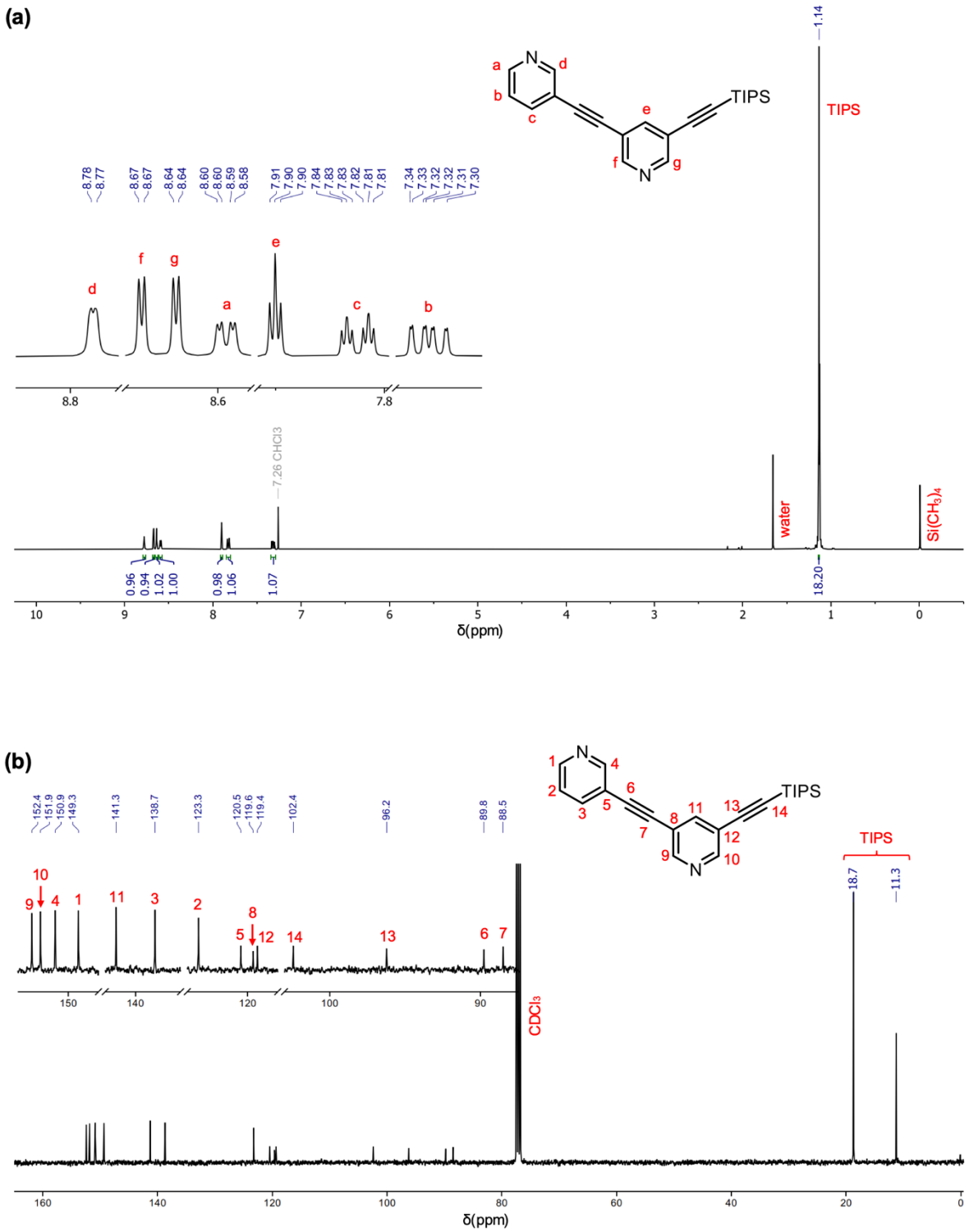


Figure S40 | NMR characterization of S2. a, ^{1}H NMR (400 MHz, $CDCl_3$ + 0.03 % tetramethylsilane, 293 K) and **b,** ^{13}C NMR (100 MHz, $CDCl_3$ + 0.03 % tetramethylsilane, 293 K).

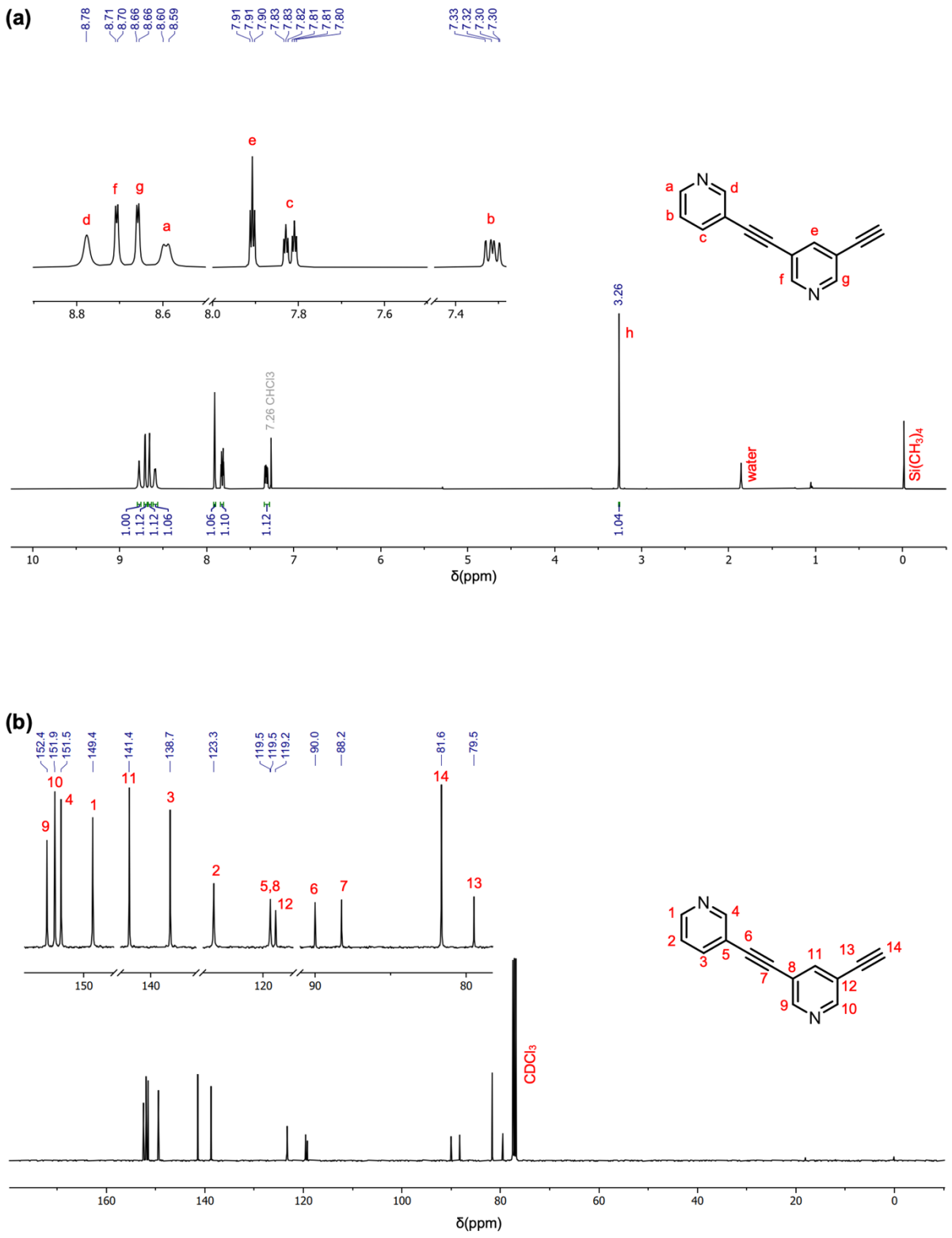


Figure S41. | NMR characterization of S3. a, ^{1}H NMR (400 MHz, $CDCl_3$ + 0.03 % tetramethylsilane, 293 K) and **b,** ^{13}C NMR (100 MHz, $CDCl_3$ + 0.03 % tetramethylsilane, 293 K).

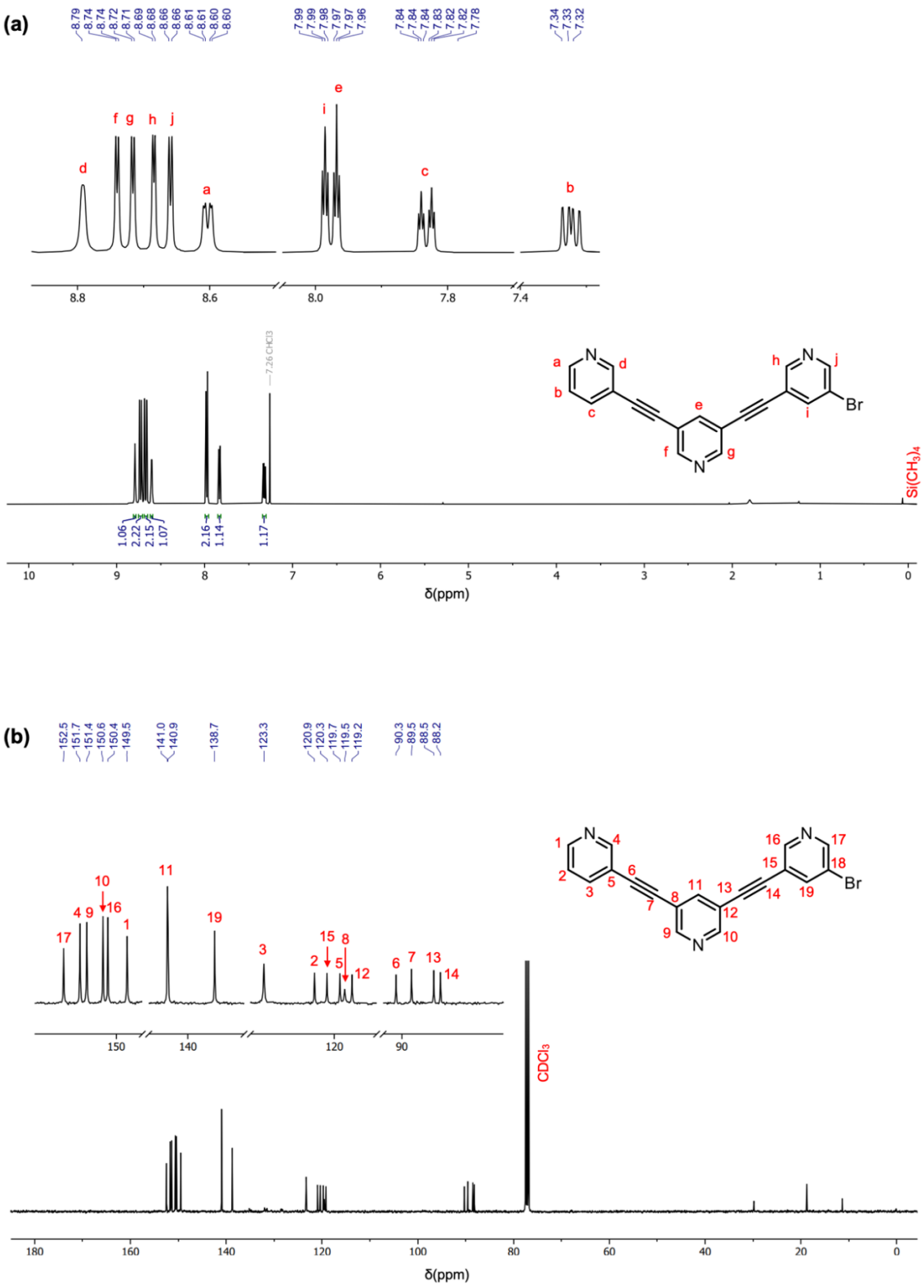


Figure S42 | NMR characterization of S4. a, ^{1}H NMR (400 MHz, $CDCl_3$ + 0.03 % tetramethylsilane, 293 K) and **b,** ^{13}C NMR (100 MHz, $CDCl_3$ + 0.03 % tetramethylsilane, 293 K).

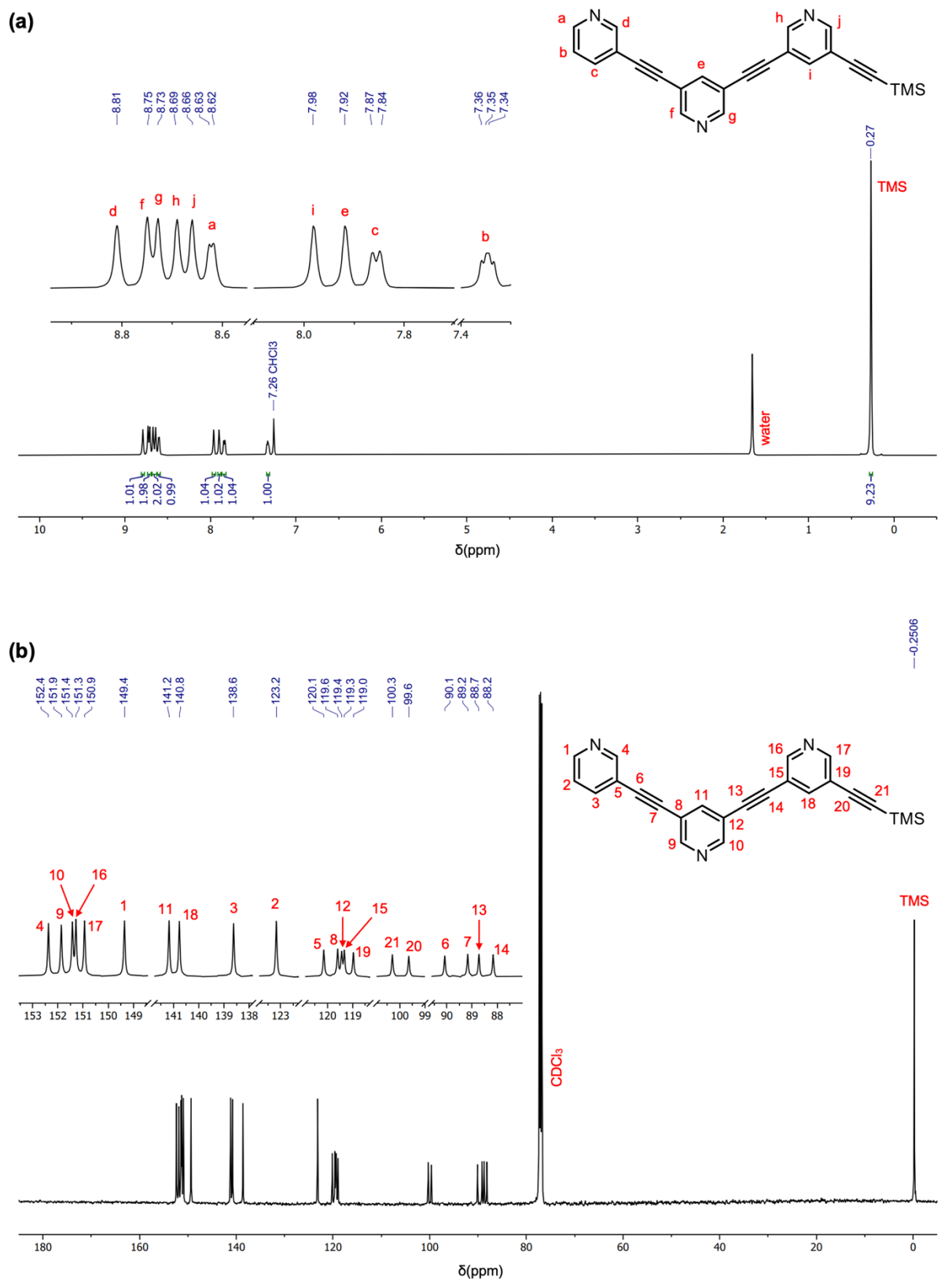


Figure S43 | NMR characterization of S5. a, ^{1}H NMR (500 MHz, $CDCl_3$, 298 K) and **b,** ^{13}C NMR (126 MHz, $CDCl_3$, 298 K).

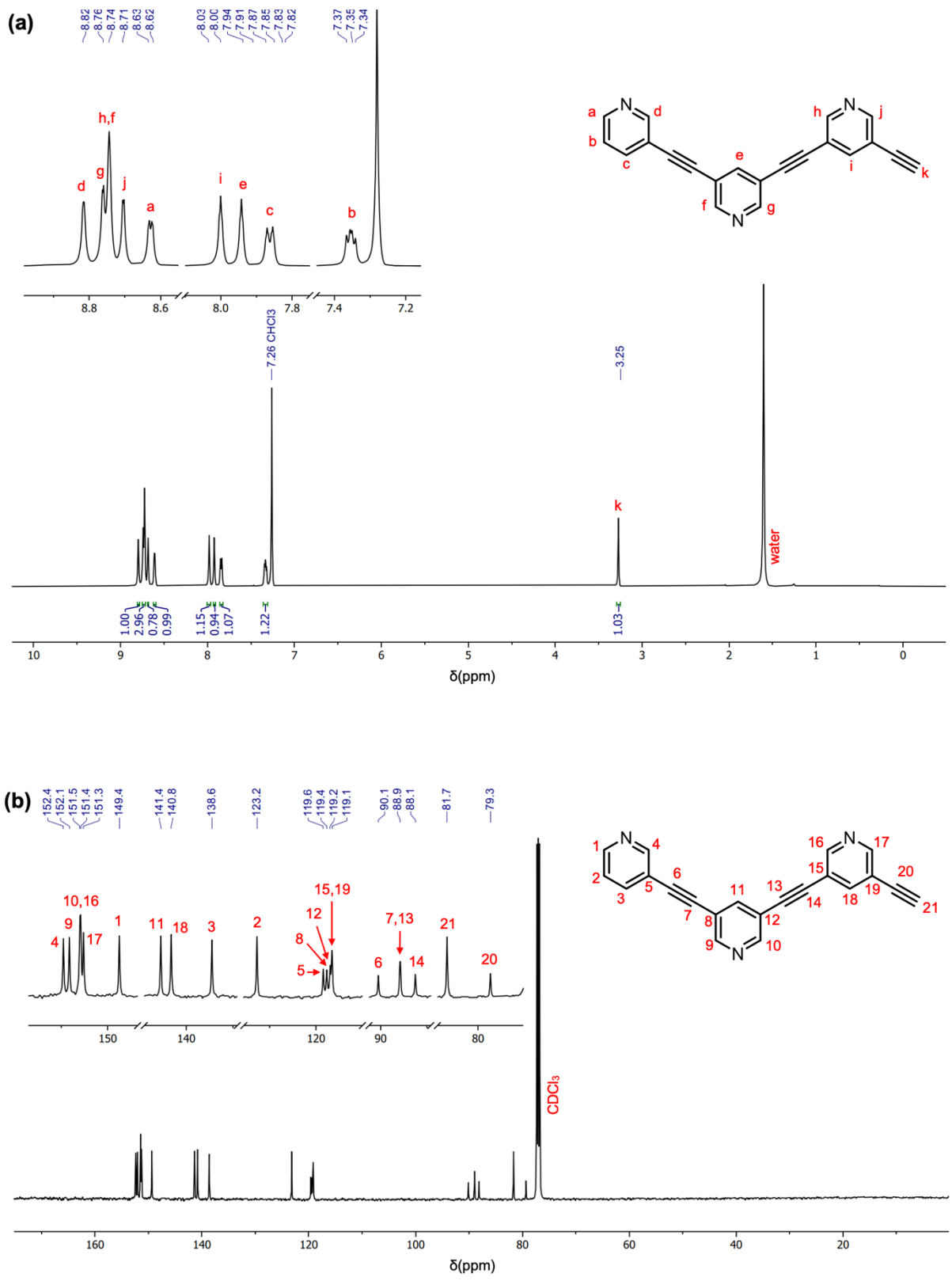


Figure S44 | NMR characterization of S6. a, ^{1}H NMR (500 MHz, $CDCl_3$, 298 K) and **b,** ^{13}C NMR (126 MHz, $CDCl_3$, 298 K).

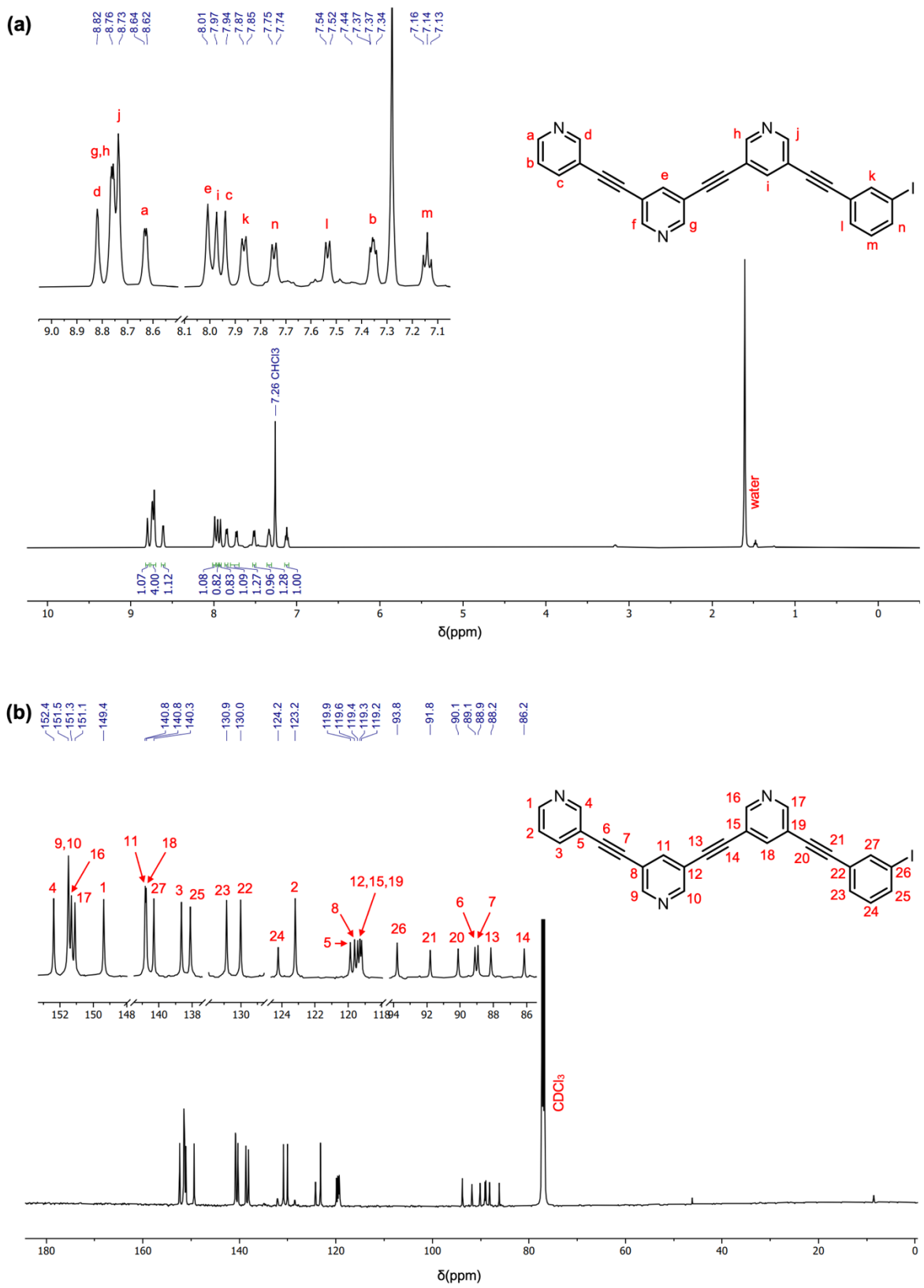


Figure S45 | NMR characterization of S7. a, ^{1}H NMR (500 MHz, $CDCl_3$, 298 K) and **b,** ^{13}C NMR (126 MHz, $CDCl_3$, 298 K).

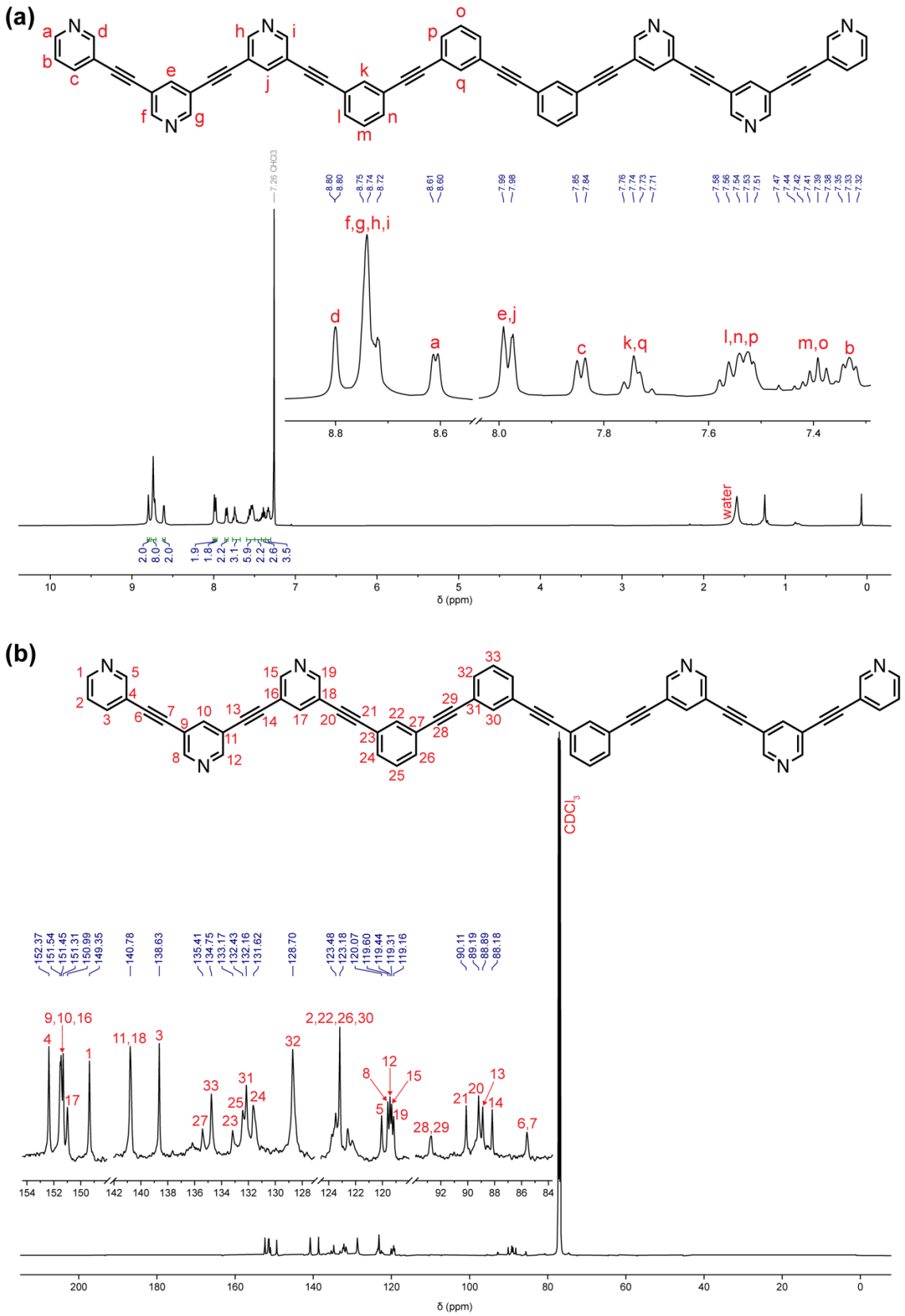


Figure S46 | NMR characterization of S8. a, ^{1}H NMR (500 MHz, $CDCl_3$, 298 K) and **b,** ^{13}C NMR (126 MHz, $CDCl_3$, 298 K).

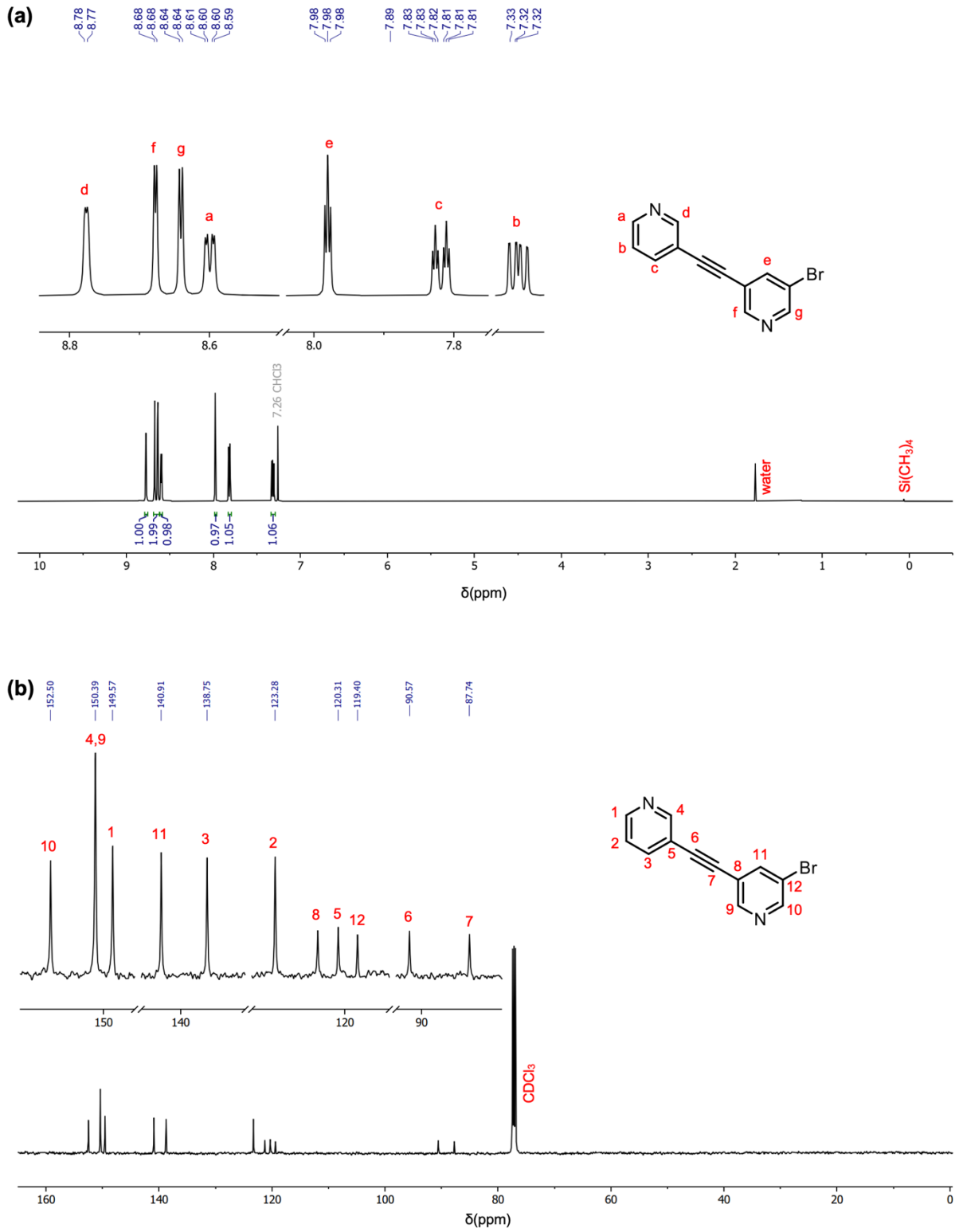


Figure S47 | NMR characterization of S12. a, ^{1}H NMR (400 MHz, $CDCl_3$ + 0.03 % tetramethylsilane, 293 K) and **b,** ^{13}C NMR (100 MHz, $CDCl_3$+ 0.03 % tetramethylsilane, 293 K).

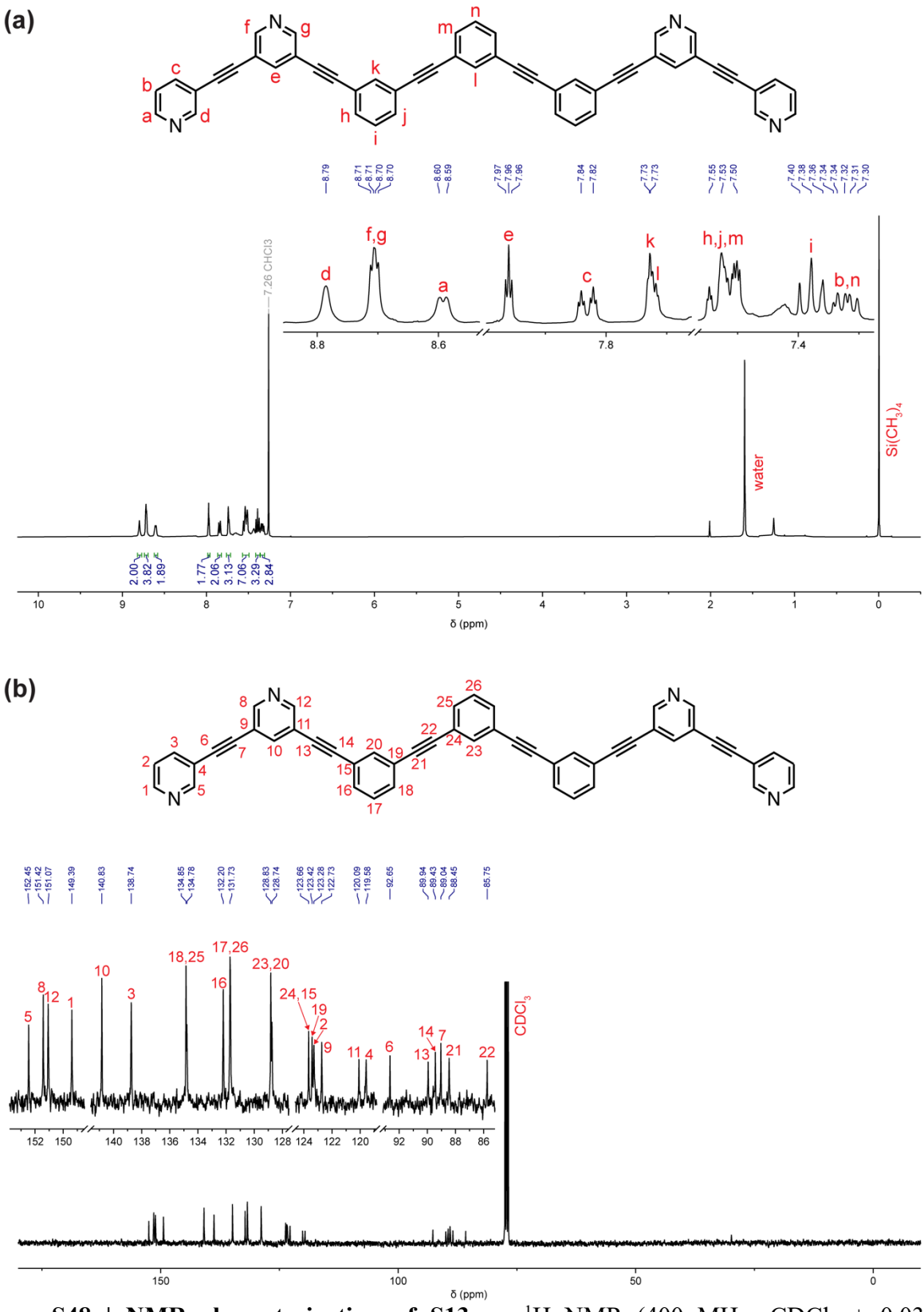


Figure S48 | NMR characterization of S13. a, ^{1}H NMR (400 MHz, $CDCl_3$ + 0.03 % tetramethylsilane, 293 K) and **b,** ^{13}C NMR (100 MHz, $CDCl_3$+ 0.03 % tetramethylsilane, 293 K).

12. DFT calculations

All geometries of $(\mathbf{1})_2$, $(\mathbf{2})_2$, $(\mathbf{2})_3$, $(\mathbf{2})_3\supset\mathbf{G2}$, and $(\mathbf{2})_3\supset\mathbf{G4}$ were optimized without symmetry constraints. Initial structures were manually constructed and pre-optimized using Grimme's GFN2-xTB program.[S5] The final re-optimizations were performed at the BP86-D4-COSMO/def2-TZVP[S6–8] level of theory using the TURBOMOLE 7.7 program suite in a water solvent.[S9] The solvent effects were modeled using the COSMO model[S10] with the default TURBOMOLE parameters. The D4 dispersion correction[S7] was included to account for crucial London dispersion forces, which are essential for the stabilization of these supramolecular complexes, given the dominance of stacking interactions.

Cartesian coordinates for $(\mathbf{1})_2$

N	-3.0102992	-1.9543833	-7.4652450
C	8.3565201	-0.2134676	1.0538048
N	-4.2485828	2.5810286	7.1616838
C	-5.0608227	-3.7909471	4.0552030
C	-5.9205448	-3.6726462	5.1532185
H	-6.9727803	-3.4232905	5.0479238
N	-5.4662314	-3.8760252	6.4040518
C	-4.1706617	-4.1989022	6.6438743
C	-3.2780584	-4.3281195	5.5941847
C	-3.7131591	-4.1245107	4.2890921
H	-3.0256277	-4.2244503	3.4509478
C	-5.5555725	-3.5629954	2.7508830
C	-5.9647499	-3.3591985	1.6235638
C	-6.4038845	-3.1057599	0.3053870
C	-7.7704479	-2.9823111	0.0332516
H	-8.5349623	-3.0924585	0.7973791
N	-8.1973397	-2.7331915	-1.2235154
C	-7.3399879	-2.5891339	-2.2522059
H	-7.7729958	-2.3911202	-3.2287176
C	-5.9587966	-2.7033083	-2.0452699
C	-5.4879190	-2.9628733	-0.7505607
H	-4.4199381	-3.0548442	-0.5643969
C	-5.0706832	-2.5419224	-3.1327659
C	-4.2959627	-2.3921419	-4.0582302
C	-3.3883618	-2.1970118	-5.1235336
C	-3.8645611	-2.1482843	-6.4380980
H	-4.9131376	-2.2782859	-6.6900458
C	-1.6876143	-1.7917821	-7.2707221
H	-1.0782487	-1.6378995	-8.1568551
C	-1.1454481	-1.8314054	-5.9776891
C	-2.0122995	-2.0370229	-4.8929672
C	0.2429702	-1.6508319	-5.7977127
C	1.4386214	-1.4773079	-5.6395866
C	2.8273769	-1.2678954	-5.4657696
C	3.6802955	-1.2175814	-6.5887230
H	3.2599851	-1.3411185	-7.5863313
C	5.0481547	-1.0162196	-6.4109833
C	5.5817918	-0.8621222	-5.1320882
H	6.6519131	-0.7080196	-4.9995617
C	4.7390216	-0.9018073	-4.0003692
C	3.3598265	-1.1077653	-4.1737133
H	2.7020766	-1.1449328	-3.3070475
C	5.2817632	-0.7290764	-2.7038854
C	5.7682564	-0.5625117	-1.5981238

C	6.3629848	-0.3693002	-0.3275302
C	7.7684654	-0.4008290	-0.1961565
H	8.3834720	-0.5741543	-1.0788995
C	7.5684667	0.0050561	2.1837988
H	8.0331201	0.1481722	3.1584062
C	6.1626175	0.0452619	2.0687143
C	5.5652670	-0.1427707	0.8094115
C	5.3619798	0.2781397	3.2135104
C	4.6871540	0.4888687	4.2069942
C	3.9106153	0.7380068	5.3642149
C	4.5047321	0.6990736	6.6447085
H	5.5680837	0.4772676	6.7321998
C	3.7349715	0.9409581	7.7813979
C	2.3758103	1.2326953	7.6703096
H	1.7786375	1.4276426	8.5598029
C	1.7721390	1.2886270	6.3967987
C	2.5403255	1.0329816	5.2478734
H	2.0746979	1.0681158	4.2643038
C	0.3998370	1.6138858	6.2732786
C	-0.7796338	1.9036470	6.1764095
C	-2.1516387	2.2159192	6.0746977
C	-2.9302082	2.3001460	7.2358831
H	-2.5164344	2.1582540	8.2304376
C	-4.8689592	2.7864611	5.9838550
H	-5.9328599	3.0035508	6.0180870
C	-4.1440583	2.7321895	4.7851469
C	-2.7736016	2.4409495	4.8331921
C	-4.8086690	2.9721589	3.5603988
C	-5.3795251	3.1889029	2.5084414
C	-6.0434379	3.4315443	1.2849301
C	-7.4407979	3.4942105	1.2590179
H	-8.0511895	3.3829681	2.1508095
N	-8.0934303	3.7160959	0.0982861
C	-7.4386703	3.8804278	-1.0669708
H	-8.0450021	4.0521720	-1.9520045
C	-6.0378634	3.8410614	-1.1061505
C	-5.3347598	3.6113928	0.0852295
H	-4.2473649	3.5764665	0.0819488
C	-5.3693183	4.0319603	-2.3365948
C	-4.7924896	4.2019789	-3.3942259
N	-4.2244893	4.5168596	-7.0023592
C	-2.8861955	4.7194911	-7.0780144
C	-2.1205047	4.7712077	-5.9248439
H	-1.0506919	4.9484061	-6.0085279
C	-2.7277061	4.6059770	-4.6854066
H	-2.1431774	4.6453402	-3.7681180
C	-4.1182286	4.3891749	-4.6223325
C	-4.8449781	4.3537407	-5.8178348
H	-5.9212187	4.2066307	-5.8429993
H	-2.4722523	4.8411624	-8.0760307
H	5.7102764	-0.9801018	-7.2758832
H	9.4419846	-0.2353241	1.1540069
H	4.4812050	-0.1141143	0.7135618
H	-1.6207539	-2.0722689	-3.8783773
H	-2.1922065	2.3928714	3.9148139
H	4.1965658	0.9100691	8.7686244
H	-3.8969177	-4.3550005	7.6841628
H	-2.2455270	-4.5957936	5.8070626
N	3.0100876	1.9541333	-7.4695010
C	-8.3541046	0.2152297	1.0546297
N	4.2499759	-2.5840898	7.1612097
C	5.0553733	3.7925572	4.0520523
C	5.9143486	3.6735663	5.1505215
H	6.9666085	3.4240710	5.0457299
N	5.4592324	3.8760299	6.4012506
C	4.1634823	4.1986051	6.6403510
C	3.2716121	4.3286126	5.5901005
C	3.7075801	4.1260918	4.2851464
H	3.0207088	4.2265813	3.4465066
C	5.5509022	3.5650488	2.7479853
C	5.9604815	3.3612226	1.6208532

C	6.3998888	3.1071431	0.3029668
C	7.7665031	2.9848275	0.0308742
H	8.5308954	3.0962597	0.7949287
N	8.1937319	2.7355225	-1.2257798
C	7.3366207	2.5900984	-2.2543067
H	7.7696628	2.3920002	-3.2308008
C	5.9553395	2.7033523	-2.0473673
C	5.4840291	2.9630926	-0.7529488
H	4.4160105	3.0550587	-0.5668829
C	5.0680113	2.5416371	-3.1353369
C	4.2948364	2.3921768	-4.0621132
C	3.3879760	2.1969998	-5.1279611
C	3.8643636	2.1483340	-6.4424413
H	4.9129790	2.2784128	-6.6942663
C	1.6874227	1.7913752	-7.2750374
H	1.0781014	1.6374087	-8.1611889
C	1.1451141	1.8307284	-5.9820250
C	2.0120553	2.0363999	-4.8973983
C	-0.2431040	1.6498746	-5.8017233
C	-1.4384997	1.4761660	-5.6420427
C	-2.8272928	1.2677645	-5.4680986
C	-3.6797021	1.2185839	-6.5915098
H	-3.2586225	1.3417899	-7.5888245
C	-5.0478504	1.0189837	-6.4145426
C	-5.5822033	0.8656976	-5.1358559
H	-6.6526011	0.7133489	-5.0038083
C	-4.7398938	0.9037387	-4.0037386
C	-3.3602918	1.1077352	-4.1762928
H	-2.7027441	1.1428958	-3.3094042
C	-5.2834750	0.7311325	-2.7075878
C	-5.7703546	0.5644517	-1.6020269
C	-6.3632540	0.3707251	-0.3306667
C	-7.7684504	0.4023634	-0.1965151
H	-8.3851541	0.5758570	-1.0780501
C	-7.5638369	-0.0028994	2.1830968
H	-8.0265290	-0.1451848	3.1587502
C	-6.1582478	-0.0438575	2.0651389
C	-5.5633235	0.1437259	0.8046957
C	-5.3561629	-0.2772084	3.2088039
C	-4.6820708	-0.4890655	4.2025376
C	-3.9072795	-0.7396410	5.3605412
C	-4.5030934	-0.7000657	6.6401640
H	-5.5662533	-0.4764474	6.7264576
C	-3.7353048	-0.9436122	7.7778417
C	-2.3764386	-1.2374506	7.6684842
H	-1.7809891	-1.4336819	8.5588538
C	-1.7710717	-1.2937078	6.3957951
C	-2.5373769	-1.0366753	5.2459599
H	-2.0706060	-1.0723360	4.2630075
C	-0.3989534	-1.6199634	6.2733271
C	0.7805349	-1.9093560	6.1757927
C	2.1529023	-2.2202486	6.0740195
C	2.9312063	-2.3047193	7.2353079
H	2.5169196	-2.1644192	8.2298918
C	4.8707690	-2.7879794	5.9833839
H	5.9347324	-3.0042670	6.0176150
C	4.1461707	-2.7333314	4.7844228
C	2.7754043	-2.4435414	4.8323955
C	4.8113975	-2.9720923	3.5597122
C	5.3829597	-3.1880554	2.5079493
C	6.0469138	-3.4300421	1.2842648
C	7.4443167	-3.4922095	1.2577505
H	8.0552134	-3.3807268	2.1491732
N	8.0965373	-3.7138886	0.0967385
C	7.4415038	-3.8776259	-1.0684134
H	8.0475965	-4.0488408	-1.9537379
C	6.0407156	-3.8384805	-1.1070387
C	5.3379598	-3.6097351	0.0846832
H	4.2505549	-3.5754657	0.0817235
C	5.3719676	-4.0292057	-2.3373832
C	4.7956494	-4.1996773	-3.3952259

N	4.2281763	-4.5175081	-7.0032708
C	2.8900719	-4.7214851	-7.0787884
C	2.1243737	-4.7727227	-5.9255984
H	1.0547190	-4.9509830	-6.0090874
C	2.7314149	-4.6059283	-4.6863261
H	2.1468118	-4.6450769	-3.7690455
C	4.1217214	-4.3878891	-4.6233406
C	4.8484670	-4.3526852	-5.8188682
H	5.9246396	-4.2047672	-5.8439450
H	2.4763906	-4.8447421	-8.0767351
H	-5.7095290	0.9837698	-7.2798072
H	-9.4393395	0.2374059	1.1569290
H	-4.4794624	0.1148520	0.7065180
H	1.6205290	2.0714356	-3.8827157
H	2.1939212	-2.3956354	3.9140299
H	-4.1982412	-0.9121634	8.7644484
H	3.8886982	4.3536951	7.6804958
H	2.2389236	4.5960217	5.8025687
C	-9.5718442	3.7712056	0.1246798
H	-9.8782086	4.6023665	0.7681038
H	-9.9365527	3.9241960	-0.8928238
H	-9.9508263	2.8259957	0.5275246
C	-9.6540690	-2.6380753	-1.4676629
H	-10.0749814	-3.6494862	-1.4588996
H	-10.1054178	-2.0377725	-0.6719406
H	-9.8185972	-2.1683025	-2.4397845
C	5.0249505	-4.5015067	-8.2489268
H	5.2103773	-5.5357284	-8.5601225
H	4.4594792	-3.9739294	-9.0220647
H	5.9735468	-3.9938660	-8.0565334
C	9.5749514	-3.7692963	0.1224064
H	9.9388327	-3.9256447	-0.8949194
H	9.9542848	-2.8228556	0.5219565
H	9.8815452	-4.5984908	0.7682600
C	-6.3956516	-3.7693073	7.5483504
H	-7.3155716	-3.2841879	7.2146697
H	-6.6127611	-4.7773874	7.9184071
H	-5.9175869	-3.1789531	8.3363304
C	-3.5602639	-1.9228984	-8.8389442
H	-2.7566705	-1.6722746	-9.5341661
H	-3.9710481	-2.9107455	-9.0721686
H	-4.3525635	-1.1682751	-8.8838809
C	3.5603856	1.9214002	-8.8430034
H	2.7575427	1.6683540	-9.5380613
H	3.9698574	2.9094649	-9.0776410
H	4.3538210	1.1679230	-8.8863301
C	-5.0210077	2.6569950	8.4213830
H	-4.9145224	1.7077400	8.9567608
H	-4.6198710	3.4757775	9.0276641
H	-6.0698622	2.8422946	8.1816355
C	6.3886580	3.7696329	7.5456134
H	7.3035983	3.2731107	7.2149078
H	6.6160865	4.7784759	7.9074137
H	5.9057868	3.1903657	8.3387597
C	9.6505819	2.6416192	-1.4694946
H	10.0728458	3.6521978	-1.4458965
H	10.1000351	2.0293351	-0.6817657
H	9.8154079	2.1855842	-2.4480672
C	5.0221608	-2.6598667	8.4210872
H	4.9180249	-1.7095082	8.9549734
H	4.6187517	-3.4763649	9.0289862
H	6.0706300	-2.8481196	8.1816834
C	-5.0214177	4.4997765	-8.2478782
H	-5.2100204	5.5336367	-8.5583465
H	-4.4548096	3.9742677	-9.0215626
H	-5.9685699	3.9892879	-8.0558777

Cartesian coordinates for $(2)_2$

N	-2.2229435	-2.6413441	-6.9139460
C	9.1283864	0.8672370	0.9814647
N	-3.5687004	2.1793254	7.3053312
H	-4.7999040	-4.0058942	2.0162087
C	-5.1666565	-3.9649189	0.9935691
C	-6.4933425	-4.2749400	0.7422517
H	-7.1966002	-4.5611290	1.5197747
N	-6.9756796	-4.2470939	-0.5237140
C	-6.1912178	-3.9148275	-1.5674624
H	-6.6529585	-3.9240955	-2.5509739
C	-4.8441491	-3.5913587	-1.3717308
C	-4.3296849	-3.6174779	-0.0599065
H	-3.2834796	-3.3721238	0.1152052
C	-4.0379574	-3.2592037	-2.4844276
C	-3.3295467	-2.9974880	-3.4382744
C	-2.5034666	-2.7095802	-4.5482657
C	-2.9985603	-2.9059855	-5.8442077
H	-3.9987124	-3.2809229	-6.0411014
C	-0.9617317	-2.1817581	-6.7856332
H	-0.4123171	-1.9996314	-7.7049385
C	-0.4040632	-1.9697697	-5.5170961
C	-1.1922812	-2.2377188	-4.3857571
C	0.9195321	-1.4925491	-5.4089601
C	2.0645774	-1.0827810	-5.3265619
C	3.3936812	-0.5999588	-5.2579996
C	4.1256636	-0.3785440	-6.4453737
H	3.6654957	-0.5981087	-7.4080958
C	5.4286547	0.1101131	-6.3769930
C	6.0248961	0.3694484	-5.1438981
H	7.0467381	0.7434925	-5.0940380
C	5.3107767	0.1404286	-3.9471681
C	3.9888259	-0.3334077	-4.0118640
H	3.4227195	-0.4913168	-3.0956217
C	5.9268242	0.3643646	-2.6917347
C	6.4757039	0.5204826	-1.6140681
C	7.1104966	0.6691791	-0.3565531
C	8.5169493	0.7533643	-0.2660820
H	9.1160121	0.7288284	-1.1754724
C	8.3646960	0.9211309	2.1454980
H	8.8450805	1.0229763	3.1178823
C	6.9551545	0.8587851	2.0702079
C	6.3369176	0.7185025	0.8168414
C	6.1659532	0.9808691	3.2396494
C	5.4965540	1.1577670	4.2437892
C	4.7301882	1.3616601	5.4177849
C	5.3549286	1.3833387	6.6851704
H	6.4350094	1.2559143	6.7502709
C	4.5942396	1.5625793	7.8387034
C	3.2117572	1.7163176	7.7601288
H	2.6154058	1.8474426	8.6621584
C	2.5748185	1.7048410	6.4997464
C	3.3381590	1.5342230	5.3312134
H	2.8470636	1.5316910	4.3592885
C	1.1694904	1.8448365	6.4067154
C	-0.0423613	1.9405000	6.3232040
C	-1.4460247	2.0297917	6.2203086
C	-2.2256785	2.1104162	7.3834333
H	-1.7902101	2.1214988	8.3788295
C	-4.2169980	2.1617902	6.1224403
H	-5.3008281	2.2256320	6.1553697
C	-3.4979390	2.0897808	4.9234015
C	-2.0972123	2.0228195	4.9760814
C	-4.1975244	2.0936630	3.6948553
C	-4.8115414	2.1186402	2.6445504
C	-5.5221538	2.2004140	1.4249108
C	-6.9210476	2.2203967	1.4422878
H	-7.4948624	2.1605591	2.3633256
N	-7.6212117	2.3377282	0.2965774
C	-7.0010267	2.4305192	-0.9040498
H	-7.6449665	2.5322099	-1.7736467
C	-5.6177736	2.4077411	-0.9807848

C	-4.8646921	2.2903027	0.1812173
H	-3.7767703	2.2760057	0.1421770
H	-5.1425885	2.4939935	-1.9549656
H	5.9918161	0.2790013	-7.2946027
H	10.2148258	0.9239298	1.0460348
H	5.2523873	0.6577936	0.7528860
H	-0.7880532	-2.0812663	-3.3879367
H	-1.5182396	1.9653742	4.0567754
H	5.0847856	1.5763500	8.8119755
N	2.8233843	2.6962016	-6.5167156
C	-9.2487760	-1.1860835	-0.0501134
N	3.5079209	-1.7852753	6.1534035
H	4.3837653	3.8118294	2.6845664
C	4.8577650	3.7841117	1.7062758
C	6.2098730	4.0683301	1.6065934
H	6.8315247	4.3189128	2.4622383
N	6.8248575	4.0570843	0.3993326
C	6.1494622	3.7698039	-0.7306587
H	6.7142158	3.7909730	-1.6585522
C	4.7821854	3.4742648	-0.6887545
C	4.1309747	3.4807304	0.5610216
H	3.0673953	3.2553086	0.6180168
C	4.0940066	3.1897619	-1.8907173
C	3.4911980	2.9690232	-2.9243603
C	2.8017487	2.7212192	-4.1334235
C	3.4596815	2.9329575	-5.3524371
H	4.4813868	3.2958806	-5.4139875
C	1.5508096	2.2514489	-6.5575891
H	1.1213969	2.0903202	-7.5423696
C	0.8330592	2.0258503	-5.3744475
C	1.4741758	2.2662749	-4.1470975
C	-0.4955865	1.5559406	-5.4477566
C	-1.6403262	1.1443835	-5.5302306
C	-2.9607349	0.6477769	-5.6540618
C	-3.5099438	0.4196344	-6.9353545
H	-2.9199121	0.6520666	-7.8212249
C	-4.7996938	-0.0931437	-7.0565274
C	-5.5598433	-0.3755946	-5.9225774
H	-6.5696012	-0.7725339	-6.0209832
C	-5.0304956	-0.1387451	-4.6348262
C	-3.7250683	0.3676722	-4.5072208
H	-3.3030833	0.5440039	-3.5191440
C	-5.8033404	-0.3994795	-3.4760499
C	-6.4657867	-0.6045823	-2.4728077
C	-7.1796177	-0.8204510	-1.2684226
C	-8.5814629	-0.9882400	-1.2585104
H	-9.1329996	-0.9574108	-2.1973818
C	-8.5504369	-1.2216994	1.1558437
H	-9.0769409	-1.3765606	2.0967181
C	-7.1477680	-1.0585895	1.1613164
C	-6.4723516	-0.8587099	-0.0545863
C	-6.3987905	-1.0961111	2.3624900
C	-5.7007066	-1.1259199	3.3619016
C	-4.8692331	-1.1551567	4.5085299
C	-5.4232053	-1.1047057	5.8060381
H	-6.5046555	-1.0490277	5.9255123
C	-4.5904215	-1.1303528	6.9241638
C	-3.2064863	-1.2012213	6.7780397
H	-2.5572513	-1.2308760	7.6523916
C	-2.6381703	-1.2474856	5.4861545
C	-3.4735141	-1.2251204	4.3553542
H	-3.0363199	-1.2583184	3.3587335
C	-1.2314187	-1.3127025	5.3319092
C	-0.0186189	-1.3694264	5.2193895
C	1.3815972	-1.5014894	5.0964924
C	2.1745009	-1.6052906	6.2486585
H	1.7562300	-1.5733004	7.2509599
C	4.1357297	-1.8572338	4.9622629
H	5.2097506	-2.0176971	4.9805940
C	3.4033742	-1.7631639	3.7717356
C	2.0145968	-1.5733834	3.8430553

C	4.0602499	-1.9186576	2.5281431
C	4.5872940	-2.1333623	1.4520495
C	5.1682729	-2.4248396	0.1958789
C	6.5623310	-2.4416081	0.0610589
H	7.2312507	-2.2466451	0.8946278
N	7.1325357	-2.7226657	-1.1249923
C	6.3850311	-3.0057147	-2.2208254
H	6.9328213	-3.2291730	-3.1329694
C	5.0038595	-3.0168785	-2.1411034
C	4.3808831	-2.7177946	-0.9338495
H	3.2955201	-2.7221317	-0.8486517
H	4.4268011	-3.2706578	-3.0271438
H	-5.2226135	-0.2651011	-8.0461230
H	-10.3314010	-1.3115988	-0.0484213
H	-5.3915500	-0.7318149	-0.0564314
H	0.9449893	2.0974868	-3.2115669
H	1.4265018	-1.5029148	2.9301053
H	-5.0272316	-1.1066132	7.9227087
C	-9.0964979	2.4184263	0.3567204
H	-9.3867544	3.4733947	0.4183626
H	-9.5110681	1.9677231	-0.5484902
H	-9.4449887	1.8814195	1.2424404
C	-8.3808024	-4.6385132	-0.7675073
H	-8.4334097	-5.7314728	-0.8298572
H	-8.9954497	-4.2807661	0.0629071
H	-8.7153108	-4.1926235	-1.7071439
C	8.6050158	-2.7232147	-1.2526248
H	8.8925992	-1.9967838	-2.0199682
H	9.0451611	-2.4537535	-0.2901615
H	8.9319090	-3.7257966	-1.5476066
C	-2.7566476	-2.8970025	-8.2700488
H	-2.3370930	-2.1595470	-8.9593935
H	-2.4632894	-3.9076807	-8.5747248
H	-3.8458635	-2.8152640	-8.2405455
C	3.5272377	2.9663549	-7.7898970
H	3.1931587	2.2425848	-8.5378244
H	3.2822622	3.9839928	-8.1138835
H	4.6031424	2.8745394	-7.6236199
C	-4.3656211	2.2942117	8.5465693
H	-3.7489228	1.9796200	9.3914874
H	-4.6718081	3.3390346	8.6694087
H	-5.2478417	1.6533947	8.4588975
C	8.2593391	4.4075543	0.3199932
H	8.3540260	5.4993305	0.3259447
H	8.7738259	3.9823122	1.1859881
H	8.6728559	4.0001486	-0.6054549
C	4.2930979	-1.9796388	7.3932766
H	3.8400207	-1.3900431	8.1940738
H	4.2738414	-3.0445127	7.6511761
H	5.3208180	-1.6542240	7.2156182

Cartesian coordinates for $(2)_3$

N	13.4166874	4.6717909	14.8731962
C	6.0604755	16.8237679	13.1825327
C	12.2054420	13.0112449	0.6561597
H	11.9083119	4.4980964	11.8832825
C	12.2002338	4.9129400	12.8452765
C	13.0505056	4.1861889	13.6606259
H	13.4555595	3.2148888	13.3871084
C	12.9776033	5.8647758	15.3152207
H	13.3101623	6.1772460	16.3007565
C	12.1237657	6.6458379	14.5264000
C	11.7274489	6.1498167	13.2696233
C	11.6856955	7.9010459	15.0079561
C	11.3120134	8.9836925	15.4188670
C	10.8314951	10.2219167	15.9044719
C	10.9713391	10.5334794	17.2632357
N	10.4706897	11.6860232	17.7529581

C	9.8407711	12.5815638	16.9661348
H	9.4619420	13.4777653	17.4491980
C	9.6825059	12.3407517	15.5938714
C	10.1909027	11.1432863	15.0619364
H	10.0809172	10.9277093	14.0009748
C	9.0131920	13.2892124	14.7920851
C	8.4149619	14.1011324	14.1079157
C	7.6912715	15.0351727	13.3293249
C	6.7970516	15.9287371	13.9549324
H	6.6929467	15.9108219	15.0387592
C	6.2107285	16.8552693	11.7977897
H	5.6376991	17.5617079	11.1987415
C	7.1204294	15.9832126	11.1610285
C	7.8520391	15.0659883	11.9327478
C	7.2936500	16.0433534	9.7571666
C	7.4311361	16.1270341	8.5481735
C	7.5446721	16.2629643	7.1433799
C	6.6742393	17.1369653	6.4553727
H	5.9275965	17.6974973	7.0173237
C	6.7734207	17.2730476	5.0718567
C	7.7315695	16.5568838	4.3546810
H	7.8055228	16.6666064	3.2736529
C	8.6145058	15.6844261	5.0267719
C	8.5132718	15.5402851	6.4220394
H	9.1881334	14.8667544	6.9477993
C	9.5900053	14.9658521	4.2932534
C	10.4168802	14.3615524	3.6315454
C	11.3715699	13.6754827	2.8420502
C	11.2640010	13.6809516	1.4339121
H	10.4352745	14.2093668	0.9645951
C	13.2671600	12.3362902	1.2534534
H	14.0066824	11.8166537	0.6456934
C	13.3929667	12.3300233	2.6594359
C	12.4386854	12.9920737	3.4495850
C	14.4892111	11.6732384	3.2675105
C	15.4541169	11.1218674	3.7683586
C	16.5616373	10.4472221	4.3234152
C	17.1861452	9.4294905	3.5875740
H	16.8609820	9.1451820	2.5912303
N	18.2378527	8.7592348	4.0987087
C	18.8837371	7.7089518	3.2811747
C	18.7339367	9.0328874	5.3222976
H	19.5850434	8.4431777	5.6510613
C	18.1655245	10.0468424	6.1033242
C	17.0646820	10.7551573	5.5985724
H	16.6027043	11.5400899	6.1935087
C	18.7079668	10.3315962	7.3772009
C	19.1782553	10.5812559	8.4710809
N	21.1559173	10.2458979	11.5395752
C	22.1497470	9.3122478	12.1104181
C	20.8010010	11.3461898	12.2459217
C	19.8923619	12.2504143	11.7215591
H	19.6300371	13.1326768	12.3005299
C	19.3376241	12.0218211	10.4682324
H	18.6203881	12.7199743	10.0404357
C	19.7136505	10.8722475	9.7460699
C	20.6408943	9.9958478	10.3201923
H	20.9856372	9.0973255	9.8162040
H	21.2704740	11.4668273	13.2190844
H	5.3687861	17.5144510	13.6642831
H	8.5502812	14.3837253	11.4511017
H	11.0559853	6.7349783	12.6440193
H	12.5249297	12.9739437	4.5344586
H	6.0993869	17.9454411	4.5401758
H	12.1103386	13.0146267	-0.4294377
H	22.0271157	8.3335403	11.6397628
H	21.9855448	9.2389515	13.1890064
H	23.1544819	9.7006905	11.9093487
H	18.1358921	7.2725844	2.6138500
H	19.2926531	6.9451478	3.9474748
H	19.6880712	8.1670557	2.6946270

C	14.3151954	3.8603196	15.7211423
H	13.8011413	2.9305127	15.9872357
H	14.5575625	4.4257134	16.6236630
H	15.2254977	3.6345899	15.1561534
H	11.4549341	9.8676996	17.9721644
C	10.5682689	11.9495702	19.2062509
H	11.4806482	11.4853412	19.5881469
H	9.6901551	11.5152773	19.6972189
H	10.5935168	13.0299549	19.3675562
N	4.2053786	13.8415600	14.1905354
C	9.1908910	10.8926502	1.1411775
C	18.7043648	7.5061803	11.5822099
H	6.3479292	11.2744243	14.4319136
C	5.7566670	12.0559461	13.9604012
C	4.9656990	12.8712100	14.7529388
H	4.9069769	12.7786568	15.8344606
C	4.1993308	14.0484255	12.8589905
H	3.5543681	14.8398347	12.4876032
C	4.9859185	13.2594130	12.0126018
C	5.7767040	12.2424428	12.5835458
C	4.9750689	13.5023803	10.6204850
C	4.9855763	13.7081479	9.4213304
C	5.0075306	13.9287123	8.0253531
C	4.1041765	14.8321241	7.4484667
H	3.3746574	15.3872093	8.0309862
N	4.1037328	15.0335359	6.1163616
C	4.9657665	14.3977947	5.2949891
C	5.9034783	13.4931404	5.8085736
C	5.9174020	13.2598649	7.1952126
H	6.6316232	12.5596963	7.6236513
C	6.8063759	12.8447816	4.9412646
C	7.6037554	12.2967834	4.1999971
C	8.5183726	11.6312697	3.3507201
C	8.2981119	11.5825218	1.9574683
H	7.4282462	12.0813382	1.5323289
C	10.2979392	10.2459017	1.6863679
H	10.9907947	9.7026715	1.0451327
C	10.5356163	10.2947510	3.0771192
C	9.6428741	10.9969015	3.9039304
C	11.6527479	9.6277293	3.6370021
C	12.6083662	9.0364861	4.1102709
C	13.7208729	8.3108383	4.6040593
C	14.2934938	7.2939573	3.8093830
H	13.8741281	7.0821190	2.8266404
C	15.3856244	6.5669812	4.2805411
C	15.9262360	6.8378414	5.5352703
H	16.7822211	6.2726845	5.9039777
C	15.3701370	7.8548250	6.3434641
C	14.2648795	8.5871154	5.8711416
H	13.8321361	9.3732719	6.4877814
C	15.9395192	8.1114351	7.6152388
C	16.4800730	8.2708701	8.6973960
C	17.1303515	8.3920040	9.9498958
C	18.0757262	7.4180823	10.3421543
H	18.3028426	6.5921661	9.6691090
C	18.4160658	8.5592863	12.4477272
H	18.8957577	8.6236688	13.4235743
C	17.4905987	9.5510523	12.0610471
C	16.8463955	9.4626592	10.8134753
C	17.2191913	10.6340738	12.9294289
C	17.0114076	11.5659098	13.6867371
C	16.7605142	12.6320753	14.5747507
C	17.2599849	12.5764895	15.8846896
H	17.8497321	11.7411516	16.2509033
N	17.0237443	13.5789187	16.7533429
C	17.5987985	13.5095937	18.1148988
C	16.2972817	14.6644180	16.4132203
H	16.1624291	15.4250122	17.1766136
C	15.7674324	14.7795275	15.1229339
C	16.0068593	13.7536546	14.1945678
H	15.6028930	13.8249502	13.1868943

C	14.9969248	15.9134073	14.7795183
C	14.3202356	16.8771018	14.4741887
C	13.5454226	18.0017136	14.1090721
C	13.3505025	18.3676575	12.7622396
H	13.8058094	17.7760153	11.9698239
C	12.5823230	19.4869919	12.4650285
H	12.4212361	19.8044894	11.4375366
C	12.0123393	20.2214717	13.4921914
N	12.2073062	19.8587666	14.7833964
C	11.6366947	20.6949851	15.8609743
C	12.9498857	18.7815203	15.1057917
H	13.0641543	18.5637050	16.1641275
H	19.4188896	6.7390763	11.8799913
H	15.8174898	5.7811306	3.6604213
H	16.1238218	10.2222451	10.5204856
H	11.4071800	21.1089855	13.3266521
H	9.8222644	11.0488605	4.9763274
H	9.0213383	10.8574726	0.0652628
H	6.3920030	11.6120293	11.9442741
H	10.6654244	21.0755648	15.5346508
H	12.3209530	21.5284787	16.0558669
H	11.5228943	20.0854831	16.7607129
H	17.8356785	12.4683471	18.3454996
H	16.8658264	13.8998984	18.8266932
H	18.5088215	14.1189563	18.1399351
C	3.3463128	14.6759621	15.0572083
H	3.1192131	15.6102086	14.5375851
H	3.8788304	14.8797843	15.9906128
H	2.4197420	14.1293340	15.2662432
H	4.8839964	14.6185821	4.2345037
C	3.1407498	15.9842782	5.5193964
H	2.4909408	15.4369826	4.8288490
H	3.6984932	16.7553502	4.9774504
H	2.5492810	16.4362746	6.3181512
N	7.8633917	8.0210738	3.1484022
C	16.3398515	6.7485524	14.6891805
C	8.5977214	18.8664068	15.1751038
H	6.2280947	9.5706218	5.6311993
C	7.0142359	9.0013654	5.1410700
C	6.9079040	8.7409516	3.7846201
H	6.0717234	9.0763073	3.1763930
C	8.9386881	7.5457309	3.8063824
H	9.6548812	6.9714798	3.2251422
C	9.0966079	7.7777722	5.1767609
C	8.1104629	8.5256253	5.8503349
C	10.2245308	7.2513283	5.8468072
C	11.1784929	6.7798258	6.4363981
C	12.2808222	6.2278585	7.1269243
C	13.0202288	5.1971323	6.5347410
H	12.7826965	4.7878062	5.5571173
N	14.0711357	4.6557471	7.1853573
C	14.4494610	5.0792244	8.4073612
H	15.3055975	4.5826045	8.8546366
C	13.7503758	6.1080898	9.0567427
C	12.6518424	6.6862932	8.4011610
H	12.0913654	7.4884397	8.8764495
C	14.1698340	6.5324302	10.3344563
C	14.5536653	6.8873612	11.4354081
C	15.0082303	7.2523377	12.7242597
C	15.9088249	6.4090138	13.4088363
H	16.2617867	5.4979979	12.9273227
C	15.8906897	7.9174372	15.2991399
H	16.2262644	8.1786440	16.3020183
C	15.0002739	8.7793086	14.6208793
C	14.5623969	8.4406528	13.3298151
C	14.5570077	9.9678977	15.2496316
C	14.1980578	10.9796291	15.8283019
C	13.8010301	12.1377812	16.5396631
C	14.1845456	12.2980813	17.8906504
H	14.7734302	11.5197195	18.3751055
C	13.8066117	13.4397479	18.5929447

C	13.0264540	14.4215584	17.9839317
H	12.7186538	15.3059198	18.5406211
C	12.6156556	14.2675847	16.6422809
C	13.0248002	13.1327183	15.9189925
H	12.7294859	13.0188876	14.8772290
C	11.7731408	15.2345896	16.0397802
C	11.0162309	16.0513725	15.5429774
C	10.1769727	17.0297820	14.9550843
C	9.3832035	17.8756197	15.7605932
H	9.3944023	17.7485764	16.8426474
C	8.5896137	19.0400008	13.7930944
H	7.9849383	19.8219602	13.3358439
C	9.3728967	18.1980212	12.9750134
C	10.1553319	17.1877392	13.5593362
C	9.3908104	18.3778951	11.5719798
C	9.4223480	18.5439126	10.3648710
C	9.4540424	18.7296980	8.9671172
C	8.5498030	19.6151686	8.3602472
H	7.8111513	20.1752787	8.9263278
N	8.5727260	19.8131186	7.0283148
C	9.4467723	19.1720382	6.2235861
H	9.3984923	19.4031086	5.1633814
C	10.3720658	18.2725835	6.7644544
C	10.3726255	18.0510781	8.1510602
H	11.0859355	17.3569361	8.5902913
C	11.2915108	17.6182122	5.9134595
C	12.0929323	17.0614747	5.1867841
C	15.0576859	15.1420096	4.0062281
H	15.9091604	14.5768816	4.3780604
C	14.9030780	15.3025134	2.6388067
N	13.8568334	16.0090364	2.1473948
C	13.7493008	16.2204231	0.6880660
C	12.9415066	16.5678767	2.9635175
H	12.1374012	17.1239809	2.4892445
C	13.0513093	16.4422074	4.3522350
C	14.1339512	15.7078339	4.8764561
H	14.2402323	15.5937370	5.9539177
H	14.1082198	13.5603137	19.6334593
H	17.0391461	6.0994291	15.2156563
H	13.8762274	9.0972571	12.7977818
H	15.5964110	14.8951329	1.9075646
H	10.7538365	16.5317640	12.9297237
H	7.9870676	19.5138381	15.8041847
H	8.2118007	8.7172492	6.9172137
H	14.1397171	15.3380612	0.1745084
H	14.3396244	17.1038255	0.4189120
H	12.6996059	16.3775442	0.4284280
C	7.6201949	20.7617225	6.4116178
H	6.9607914	21.1548906	7.1880945
H	7.0386760	20.2305367	5.6510198
H	8.1877265	21.5752171	5.9481437
C	7.6908891	7.7039585	1.7145372
H	8.6708743	7.5020683	1.2753513
H	7.2214486	8.5576734	1.2189655
H	7.0499179	6.8194120	1.6277280
C	14.8041804	3.5409944	6.5459315
H	14.8493758	3.7213458	5.4684326
H	14.2662622	2.6080053	6.7476625
H	15.8113991	3.4919946	6.9669313

Cartesian coordinates for $(2)_3 \supset$G2

N	12.6736955	4.6118072	13.5766391
C	6.3202599	17.0317355	12.7954772
C	12.2454712	12.5150488	0.5403767
H	11.0564337	5.2322952	10.7062608
C	11.4228480	5.4037790	11.7158605
C	12.2166319	4.4380279	12.3124934
H	12.5044396	3.5128930	11.8190659

C	12.3783222	5.7181341	14.2858316
H	12.7764917	5.7776257	15.2949638
C	11.5916849	6.7285725	13.7244417
C	11.1020321	6.5613692	12.4134242
C	11.3050225	7.9014438	14.4580083
C	11.0364449	8.9427743	15.0252912
C	10.6448208	10.1868958	15.5655295
C	10.7723892	10.4594380	16.9339467
N	10.3473949	11.6389994	17.4326283
C	9.8098707	12.5973426	16.6477386
H	9.5061342	13.5176773	17.1385327
C	9.6658492	12.3907316	15.2685683
C	10.0931843	11.1670939	14.7270088
H	9.9778180	10.9526469	13.6642429
C	9.0859113	13.3890172	14.4584094
C	8.5558024	14.2233842	13.7451407
C	7.8933188	15.1922656	12.9559241
C	6.9948483	16.0905270	13.5687146
H	6.8377956	16.0456766	14.6454959
C	6.5363066	17.1010984	11.4225140
H	6.0162880	17.8463453	10.8218461
C	7.4421829	16.2154024	10.7965447
C	8.1132078	15.2548933	11.5689174
C	7.6560035	16.3077653	9.3996107
C	7.8000420	16.4276645	8.1942950
C	7.9153435	16.5675181	6.7899125
C	7.1046727	17.4966134	6.0999717
H	6.4046412	18.1177025	6.6577972
C	7.2004924	17.6108474	4.7145345
C	8.0903469	16.8135409	3.9953044
H	8.1564333	16.9004501	2.9116299
C	8.9067576	15.8799164	4.6690498
C	8.8168143	15.7680271	6.0666289
H	9.4397447	15.0473773	6.5904597
C	9.8044919	15.0543923	3.9501658
C	10.5700785	14.3352174	3.3313311
C	11.4802914	13.5180601	2.6189425
C	11.3276817	13.3025983	1.2322930
H	10.4856089	13.7557253	0.7109573
C	13.3331252	11.9461261	1.1990834
H	14.0596472	11.3450610	0.6540405
C	13.5042347	12.1612182	2.5835776
C	12.5656544	12.9310802	3.2896206
C	14.6295782	11.6374731	3.2609405
C	15.6164118	11.2201779	3.8422498
C	16.7381956	10.7152664	4.5296965
C	17.6052883	9.8176504	3.8948291
H	17.4693835	9.4999395	2.8648745
N	18.6700270	9.3107493	4.5526695
C	19.5602015	8.3756493	3.8298036
C	18.9477958	9.6412104	5.8281204
H	19.8257805	9.1852958	6.2759331
C	18.1319819	10.5521286	6.5146634
C	17.0164461	11.0859403	5.8578448
H	16.3712972	11.7948324	6.3724585
C	18.4602016	10.9288070	7.8377961
C	18.7662185	11.2966202	8.9568570
N	20.3758639	11.4032230	12.2509456
C	21.2528150	10.5530601	13.0838281
C	19.9666626	12.5988422	12.7447913
C	19.1296193	13.4123693	12.0013056
H	18.8283368	14.3764378	12.4055275
C	18.7023414	12.9973180	10.7437501
H	18.0501500	13.6284388	10.1422370
C	19.1438186	11.7593920	10.2386925
C	19.9911520	10.9775111	11.0337736
H	20.3775969	10.0170190	10.7038421
H	20.3433546	12.8673447	13.7288420
H	5.6240587	17.7225898	13.2694785
H	8.8050561	14.5594480	11.0972794
H	10.4825464	7.3413920	11.9706225

H	12.6873833	13.0851713	4.3594061
H	6.5659090	18.3217516	4.1855539
H	12.1147103	12.3479072	-0.5285016
H	21.4993174	9.6455367	12.5283438
H	20.7244238	10.3019206	14.0100259
H	22.1659112	11.1106562	13.3163611
H	18.9461059	7.6101600	3.3456734
H	20.2464285	7.9176003	4.5451872
H	20.1190447	8.9403961	3.0760138
C	13.4863487	3.5451459	14.1986369
H	12.8152565	2.7527091	14.5490342
H	14.0387512	3.9666346	15.0418327
H	14.1773239	3.1463041	13.4505921
H	11.1839814	9.7463388	17.6423074
C	10.4341912	11.8720842	18.8928452
H	11.3145662	11.3539321	19.2805357
H	9.5287702	11.4734107	19.3645892
H	10.5108673	12.9466402	19.0745754
N	5.9502024	12.0241937	15.5590340
C	9.0805226	10.8166091	1.9725789
C	18.9031033	7.0757747	11.7098172
H	7.3869322	9.0932563	14.7852623
C	6.9417781	10.0733677	14.6276914
C	6.5255716	10.8083743	15.7264728
H	6.6181443	10.4538231	16.7502011
C	5.7579431	12.5476191	14.3318037
H	5.2720931	13.5189952	14.2833853
C	6.1703398	11.8540763	13.1910826
C	6.7739026	10.5899122	13.3487124
C	6.0005778	12.4280679	11.9125824
C	5.9076903	12.8964329	10.7948311
C	5.8637505	13.3710888	9.4657071
C	4.9683550	14.3801566	9.0986586
H	4.2810563	14.8443006	9.8007939
N	4.9156392	14.8085204	7.8194672
C	5.7112502	14.2949712	6.8625865
C	6.6448869	13.2931826	7.1695016
C	6.7235358	12.8341481	8.4931999
H	7.4357080	12.0609092	8.7821026
C	7.4624090	12.7653311	6.1488610
C	8.1395442	12.2718113	5.2633347
C	8.8786892	11.6103817	4.2548232
C	8.4033205	11.5723531	2.9262493
H	7.5047869	12.1267657	2.6584989
C	10.2346439	10.1122174	2.3116740
H	10.7577909	9.5181831	1.5638120
C	10.7439334	10.1777961	3.6255757
C	10.0561910	10.9267078	4.5945121
C	11.9397691	9.5091763	3.9767767
C	12.9889015	8.9658641	4.2769825
C	14.1947746	8.3063551	4.6129681
C	14.8378347	7.4723925	3.6723199
H	14.4117895	7.3607441	2.6761450
C	15.9960906	6.7831449	4.0270085
C	16.5310596	6.9039428	5.3080488
H	17.4208413	6.3433928	5.5930017
C	15.9174529	7.7563413	6.2521241
C	14.7546665	8.4607155	5.8926737
H	14.2745249	9.1166388	6.6171744
C	16.4593186	7.8834725	7.5533533
C	16.9299629	7.9620319	8.6754805
C	17.4733617	8.0187084	9.9808867
C	18.3852285	7.0318256	10.4175597
H	18.6735953	6.2331287	9.7353086
C	18.5384758	8.0975526	12.5836162
H	18.9365958	8.1277416	13.5969233
C	17.6472193	9.1036338	12.1532999
C	17.1086010	9.0532674	10.8562311
C	17.3248458	10.1794722	13.0120293
C	17.0919762	11.1263688	13.7435259
C	16.8211565	12.2271676	14.5807437

C	17.2410591	12.2081656	15.9187354
H	17.7765272	11.3689570	16.3532046
N	16.9917313	13.2545795	16.7310051
C	17.4838262	13.2160951	18.1263332
C	16.3298481	14.3499419	16.3062812
H	16.1812130	15.1470342	17.0285507
C	15.8813628	14.4330066	14.9812408
C	16.1357015	13.3605931	14.1129840
H	15.7951186	13.4044063	13.0806675
C	15.1827853	15.5843097	14.5537534
C	14.5800388	16.5783180	14.1945768
C	13.9017472	17.7464914	13.7762131
C	13.7903950	18.0999676	12.4168622
H	14.2416204	17.4680337	11.6535016
C	13.1198532	19.2667414	12.0693523
H	13.0282196	19.5775008	11.0312924
C	12.5675600	20.0620017	13.0604344
N	12.6838227	19.7119316	14.3646239
C	12.1371050	20.6116010	15.4033289
C	13.3280567	18.5883960	14.7352996
H	13.3850705	18.3841215	15.8008335
H	19.5969324	6.3037910	12.0411566
H	16.4750271	6.1267892	3.3004888
H	16.4088846	9.8196824	10.5279848
H	12.0398418	20.9898503	12.8551107
H	10.4315977	10.9663223	5.6141290
H	8.7035913	10.7748286	0.9511224
H	7.1056824	10.0377853	12.4721724
H	11.2058099	21.0495295	15.0349582
H	12.8710481	21.4006209	15.6020795
H	11.9524838	20.0336664	16.3121070
H	17.5609239	12.1735066	18.4441736
H	16.7793046	13.7590089	18.7619101
H	18.4678757	13.6966933	18.1603467
C	5.5547510	12.8194931	16.7414282
H	4.5860863	13.2882691	16.5456891
H	6.3124793	13.5916622	16.9215783
H	5.4808253	12.1552917	17.6056856
H	5.5861790	14.6866629	5.8572901
C	3.9697835	15.8943368	7.4795681
H	2.9595840	15.5820902	7.7622927
H	4.0180967	16.0820371	6.4047540
H	4.2530689	16.7931605	8.0383132
N	6.0818611	9.4788213	4.8844343
C	15.8769590	6.4940769	14.1317100
C	8.9512327	18.9986071	14.7798057
H	5.4283552	10.0496430	8.1239944
C	5.9930395	9.7425654	7.2461816
C	5.4160848	9.8820849	5.9959169
H	4.4225619	10.2953293	5.8387145
C	7.3111539	8.9354553	4.9606368
H	7.7698485	8.6209174	4.0269563
C	7.9426995	8.7781304	6.1994418
C	7.2673669	9.1972215	7.3619239
C	9.2268845	8.1944497	6.2812419
C	10.3107922	7.6668154	6.4431990
C	11.5227468	7.0335144	6.7994302
C	12.1293036	6.0944944	5.9569854
H	11.7307936	5.8318839	4.9813096
N	13.2354863	5.4364622	6.3618119
C	13.8121115	5.6703417	7.5586684
H	14.6941964	5.0840323	7.8008088
C	13.2640025	6.6127952	8.4397549
C	12.1025584	7.2982943	8.0489522
H	11.6199600	8.0054733	8.7245594
C	13.8404800	6.8434008	9.7058824
C	14.2448095	7.0481987	10.8366237
C	14.6793664	7.2574985	12.1657384
C	15.4959316	6.3020479	12.8056954
H	15.8194794	5.4193556	12.2556761
C	15.4712036	7.6299771	14.8283098

H	15.7752017	7.7787985	15.8636818
C	14.6735883	8.6067316	14.1924650
C	14.2734877	8.4095214	12.8616271
C	14.2958575	9.7793139	14.8888297
C	14.0023092	10.7902383	15.5044165
C	13.6737567	11.9528759	16.2412834
C	14.0319930	12.0573591	17.6043183
H	14.5513249	11.2295547	18.0858279
C	13.7159112	13.2087643	18.3218189
C	13.0238968	14.2574774	17.7168156
H	12.7651244	15.1492809	18.2860789
C	12.6390642	14.1608717	16.3625021
C	12.9865673	13.0143055	15.6268070
H	12.7067067	12.9418370	14.5768996
C	11.8816472	15.1905036	15.7525169
C	11.1911443	16.0513509	15.2341341
C	10.4303554	17.0757680	14.6195697
C	9.6589618	17.9683385	15.3953027
H	9.6262375	17.8456115	16.4772726
C	9.0036870	19.1697091	13.3984699
H	8.4629431	19.9846408	12.9195484
C	9.7686902	18.2840144	12.6094925
C	10.4658036	17.2309293	13.2242721
C	9.8564508	18.4647841	11.2091899
C	9.9500696	18.6380003	10.0062731
C	10.0286257	18.8266295	8.6104969
C	9.1921282	19.7634956	7.9853437
H	8.4868447	20.3778216	8.5373653
N	9.2419073	19.9445080	6.6512137
C	10.0745523	19.2343820	5.8623138
H	10.0471588	19.4498136	4.7980720
C	10.9371689	18.2847595	6.4227728
C	10.9166785	18.0893525	7.8118450
H	11.5882800	17.3659043	8.2673956
C	11.8044816	17.5535688	5.5789575
C	12.5501246	16.9458214	4.8337683
C	15.4296877	15.0020016	3.4841890
H	16.3376934	14.4931389	3.7991657
C	15.1195876	15.0489207	2.1347639
N	14.0082666	15.6979636	1.7101314
C	13.7409310	15.7940156	0.2586809
C	13.1720440	16.3004277	2.5776168
H	12.3081257	16.8061767	2.1554125
C	13.4346847	16.2824791	3.9520888
C	14.5916235	15.6187734	4.4056061
H	14.8302586	15.6105655	5.4675210
H	13.9968045	13.2849731	19.3721474
H	16.5049493	5.7543351	14.6274400
H	13.6462438	9.1490906	12.3667858
H	15.7398366	14.5986704	1.3642026
H	11.0474419	16.5391495	12.6177933
H	8.3558091	19.6810728	15.3856894
H	7.7451712	9.0832848	8.3343224
H	14.0475467	14.8596203	-0.2187938
H	14.3205194	16.6309993	-0.1470578
H	12.6732809	15.9674936	0.1047574
C	8.3765993	20.9680901	6.0251017
H	7.5477041	21.1906931	6.7008944
H	8.0011869	20.5771696	5.0753456
H	8.9745256	21.8693346	5.8499048
C	5.4270637	9.6368714	3.5682669
H	6.1085803	9.2896173	2.7887720
H	5.1829564	10.6939230	3.4183236
H	4.5103464	9.0383472	3.5584967
C	13.7959880	4.3799736	5.4896938
H	13.6222215	4.6543777	4.4462996
H	13.2890172	3.4361483	5.7202399
H	14.8665705	4.2894302	5.6877575
S	9.5171962	9.8474575	10.6347967
C	10.9745278	11.0452071	10.4536477
F	10.9754441	11.8979701	11.5188957

F	12.1368906	10.3234994	10.4895101
C	10.9592140	11.9023519	9.1471732
F	10.0214901	12.8837686	9.2769721
C	12.3368248	12.5835512	8.8043933
C	12.2322424	13.7749419	7.7860898
F	11.6530297	14.8456270	8.3601027
F	13.4648105	14.1195253	7.3781802
F	11.5063297	13.4179808	6.7052730
F	12.9030891	13.0716341	9.9376594
F	13.1658184	11.6539083	8.2603192
F	10.6154167	11.1138476	8.0932225
O	9.5756091	9.5261443	12.0678170
O	8.3543220	10.6436098	10.2253861
O	9.8611434	8.7333707	9.7445605

Cartesian coordinates for $(2)_3 \supset$G4

N	12.7841943	4.7198481	13.3921910
C	5.3979342	16.5514387	12.0961354
C	12.5568833	11.0456533	1.1971463
H	10.8905822	4.6901326	10.6262786
C	11.3452885	5.0814124	11.5336593
C	12.2118186	4.2712189	12.2469660
H	12.4717430	3.2604353	11.9424158
C	12.5377593	5.9564239	13.8628459
H	13.0283572	6.2373896	14.7907062
C	11.6799360	6.8195457	13.1717083
C	11.0683452	6.3664730	11.9870392
C	11.4363102	8.1168274	13.6764791
C	11.2038838	9.2278470	14.1130355
C	10.8600860	10.4953403	14.6313696
C	11.2965117	10.8712514	15.9094611
N	10.9181354	12.0525406	16.4380776
C	10.1465345	12.9257514	15.7561269
H	9.8981665	13.8552182	16.2607325
C	9.6888263	12.6156086	14.4698460
C	10.0441561	11.3771110	13.9069911
H	9.6550675	11.0903024	12.9271516
C	8.8644894	13.5171148	13.7635831
C	8.1361197	14.2360519	13.1015616
C	7.2710975	15.0244910	12.3069088
C	6.2740602	15.8244386	12.9002863
H	6.1982645	15.8757167	13.9856333
C	5.5102356	16.5113198	10.7088136
H	4.8285685	17.0880873	10.0848235
C	6.5165235	15.7295492	10.1007073
C	7.3884664	14.9826234	10.9077976
C	6.6582794	15.6765954	8.6928623
C	6.8179166	15.5989739	7.4860406
C	7.0287865	15.4605808	6.0924926
C	6.1443119	16.0446043	5.1599115
H	5.2957124	16.6286110	5.5154525
C	6.3597035	15.8706887	3.7936457
C	7.4395683	15.1172203	3.3346788
H	7.5979200	14.9761169	2.2662983
C	8.3328619	14.5267793	4.2539686
C	8.1255962	14.7102617	5.6313505
H	8.8131127	14.2604173	6.3455117
C	9.4287147	13.7517380	3.8032175
C	10.3744328	13.0815424	3.4250668
C	11.4744239	12.3188673	2.9639402
C	11.4685733	11.7830121	1.6577206
H	10.6023323	11.9469653	1.0182898
C	13.6649965	10.8357894	2.0142785
H	14.5193242	10.2652035	1.6528078
C	13.6885307	11.3701427	3.3214805
C	12.5877577	12.1028973	3.7953313
C	14.8321275	11.1648088	4.1293911
C	15.8470051	10.9562139	4.7728404

C	17.0327598	10.5885819	5.4423893
C	17.8679132	9.6415004	4.8300350
H	17.6472240	9.2151380	3.8557037
N	18.9960702	9.2247951	5.4360177
C	19.8654665	8.2452640	4.7487558
C	19.3705395	9.6940517	6.6424413
H	20.2949017	9.3025929	7.0566942
C	18.5970591	10.6607055	7.2984718
C	17.4140367	11.1086885	6.6926356
H	16.7970538	11.8596640	7.1820525
C	19.0645054	11.1483767	8.5430498
C	19.5742698	11.5307030	9.5799734
N	21.5209956	11.3514844	12.6777899
C	22.2673756	10.3409051	13.4562305
C	21.5140635	12.6369816	13.1152243
C	20.8650816	13.6174705	12.3884893
H	20.8627481	14.6464915	12.7395549
C	20.2143438	13.2865604	11.2030300
H	19.7284673	14.0676346	10.6125822
C	20.2138791	11.9473765	10.7725403
C	20.8897951	10.9941564	11.5450535
H	20.9446401	9.9464162	11.2616821
H	22.0553314	12.8298076	14.0384223
H	4.6241031	17.1635395	12.5582522
H	8.1579606	14.3684358	10.4437462
H	10.4032073	7.0398112	11.4443628
H	12.5980434	12.5091430	4.8051609
H	5.6721534	16.3186852	3.0764446
H	12.5408562	10.6269088	0.1911288
H	22.0805855	9.3539233	13.0278724
H	21.9312866	10.3755689	14.4969728
H	23.3355293	10.5770237	13.4000084
H	19.2590328	7.6692572	4.0460763
H	20.3135937	7.5854035	5.4968301
H	20.6487246	8.7905763	4.2106344
C	13.6835349	3.8165260	14.1401383
H	13.0835956	3.0182856	14.5907386
H	14.1914592	4.3883632	14.9194217
H	14.4122085	3.3885349	13.4446267
H	11.9160211	10.2308892	16.5308628
C	11.3219271	12.3805804	17.8244268
H	12.2845777	11.9070086	18.0326232
H	10.5574313	11.9961871	18.5092674
H	11.4014436	13.4659502	17.9213126
N	5.5605347	12.4170242	15.4536825
C	9.5126391	9.0888957	2.5943740
C	19.2316654	8.1554043	13.1750304
H	7.4939288	9.6806522	15.3104601
C	6.8952003	10.5142769	14.9487932
C	6.3356713	11.3841411	15.8696750
H	6.4678437	11.2831348	16.9443122
C	5.3151498	12.6271431	14.1465499
H	4.6688913	13.4635707	13.8939736
C	5.8772384	11.7933663	13.1738482
C	6.6773658	10.7110859	13.5893921
C	5.6580537	12.0675560	11.8065051
C	5.5284725	12.3156884	10.6235807
C	5.4379083	12.5376649	9.2322597
C	4.3703592	13.2696033	8.7001619
H	3.5920610	13.7132911	9.3150106
N	4.2659346	13.4418867	7.3650908
C	5.1595228	12.9139948	6.5030070
C	6.2555248	12.1776441	6.9762357
C	6.4072653	12.0127636	8.3641015
H	7.2706647	11.4567558	8.7428829
C	7.1744608	11.5928652	6.0830550
C	7.9863208	10.9962081	5.3968747
C	8.9214738	10.2659473	4.6296670
C	8.6018331	9.8522196	3.3194473
H	7.6394732	10.1255506	2.8885638
C	10.7452620	8.7492493	3.1463646

H	11.4615469	8.1623392	2.5724824
C	11.0863546	9.1768937	4.4485646
C	10.1629837	9.9278675	5.1946177
C	12.3488402	8.8283906	4.9873408
C	13.4470142	8.4979118	5.4022844
C	14.6966156	8.0185075	5.8650336
C	15.4336565	7.1077470	5.0752284
H	15.0630323	6.8298243	4.0893595
C	16.6180064	6.5578013	5.5620429
C	17.0979464	6.9109049	6.8219495
H	18.0139078	6.4672873	7.2105335
C	16.3983507	7.8529098	7.6068980
C	15.1975393	8.4004154	7.1209772
H	14.6428640	9.1137060	7.7275935
C	16.9058656	8.2285550	8.8745610
C	17.3800109	8.5182114	9.9603493
C	17.9121851	8.8071047	11.2403090
C	18.7552837	7.8826196	11.8943569
H	19.0148360	6.9492859	11.3964320
C	18.9051163	9.3484576	13.8176293
H	19.2764271	9.5587267	14.8199187
C	18.0942413	10.2993942	13.1629639
C	17.5920755	10.0127032	11.8827094
C	17.8328172	11.5614766	13.7514708
C	17.6575319	12.6826753	14.1964882
C	17.5258462	14.0317158	14.5926029
C	18.5770450	14.6612205	15.2649511
H	19.4752527	14.1312569	15.5694694
N	18.5141091	15.9718795	15.5707240
C	19.6752733	16.6177159	16.2202014
C	17.4506215	16.7280117	15.2358623
H	17.4920754	17.7802094	15.5026159
C	16.3580092	16.1564643	14.5786983
C	16.3926597	14.7926238	14.2662216
H	15.5514716	14.3287399	13.7590766
C	15.2591226	16.9716785	14.2181181
C	14.3374078	17.6937539	13.8906986
C	13.2897585	18.5610146	13.4988573
C	12.9969773	18.8156146	12.1460098
H	13.5790793	18.3353248	11.3623638
C	11.9727738	19.6965517	11.8201352
H	11.7322128	19.9184132	10.7827413
C	11.2517856	20.3145386	12.8282377
N	11.5396193	20.0571241	14.1266061
C	10.7837976	20.7595119	15.1846770
C	12.5250158	19.2063161	14.4752769
H	12.6942626	19.0633738	15.5390423
H	19.8632496	7.4254818	13.6809774
H	17.1661445	5.8366288	4.9558330
H	16.9624150	10.7356580	11.3716986
H	10.4504126	21.0243432	12.6415371
H	10.3943068	10.2439278	6.2109887
H	9.2620682	8.7594206	1.5863981
H	7.1302469	10.0648222	12.8388529
H	9.7545445	20.9037760	14.8450214
H	11.2566277	21.7314040	15.3671743
H	10.8030443	20.1557929	16.0952661
H	20.2182034	15.8662828	16.7991227
H	19.3142099	17.4116783	16.8793269
H	20.3210839	17.0392239	15.4409379
C	4.9961860	13.3403453	16.4620443
H	4.2164841	13.9436040	15.9914495
H	5.7986845	13.9831790	16.8417239
H	4.5722602	12.7509669	17.2802605
H	4.9857557	13.0933162	5.4456540
C	3.1696496	14.2874305	6.8437812
H	2.2539046	14.0628998	7.3975255
H	3.0329106	14.0762024	5.7808009
H	3.4424494	15.3394205	6.9898461
N	4.3378437	9.3575453	7.1990258
C	15.9331736	6.4553148	13.0594524

C	8.3702397	18.4289566	13.7285942
H	4.7217563	9.2099954	10.5260297
C	4.9800776	9.1102373	9.4745274
C	4.0472908	9.4774353	8.5177272
H	3.0603664	9.8617641	8.7628398
C	5.5213755	8.8630183	6.7802341
H	5.6631614	8.7764842	5.7064761
C	6.4959437	8.4744721	7.7021715
C	6.2175453	8.6178994	9.0778521
C	7.7285679	7.9384216	7.2713604
C	8.8061822	7.4438477	7.0025414
C	10.1063771	6.8988282	6.9050627
C	10.5267475	6.1574244	5.7968131
H	9.8981815	5.9785767	4.9291006
N	11.7589738	5.6057806	5.7817744
C	12.6219273	5.7419251	6.8105418
H	13.5813557	5.2413954	6.7144728
C	12.2696672	6.4989003	7.9342569
C	10.9964363	7.0886294	7.9725944
H	10.6807068	7.6871778	8.8330616
C	13.1588619	6.6787812	9.0163399
C	13.8196865	6.8852076	10.0194878
C	14.4996373	7.1472206	11.2323317
C	15.3631728	6.1967564	11.8142298
H	15.5688780	5.2636128	11.2911958
C	15.6799991	7.6528352	13.7265667
H	16.1280132	7.8476943	14.6998376
C	14.8565364	8.6315863	13.1315625
C	14.2584341	8.3635888	11.8905857
C	14.6215608	9.8787999	13.7573834
C	14.4175387	10.9673967	14.2669709
C	14.1514941	12.2138953	14.8817260
C	14.7425527	12.5492422	16.1197492
H	15.4252331	11.8467770	16.5958205
C	14.4473108	13.7697518	16.7237191
C	13.5592633	14.6636739	16.1278974
H	13.3182305	15.6085553	16.6129841
C	12.9593165	14.3434651	14.8903100
C	13.2714812	13.1229707	14.2680994
H	12.8116687	12.8660101	13.3163608
C	12.0169816	15.2254423	14.3036965
C	11.1675238	15.9689623	13.8412974
C	10.1742931	16.8457909	13.3385976
C	9.3341097	17.5553298	14.2250894
H	9.4445038	17.4089972	15.2991904
C	8.2192176	18.6172448	12.3553037
H	7.4686161	19.3051699	11.9693247
C	9.0417456	17.9078802	11.4581180
C	10.0147488	17.0238355	11.9566790
C	8.9161639	18.0727718	10.0590878
C	8.8385972	18.1798795	8.8479223
C	8.7897999	18.2375160	7.4395357
C	7.7544705	18.9216462	6.7852975
H	6.9658197	19.4418777	7.3211932
N	7.7039670	18.9608058	5.4398285
C	8.6255080	18.3445704	4.6674986
H	8.5053200	18.4362497	3.5918869
C	9.6827186	17.6458802	5.2583387
C	9.7633427	17.5966273	6.6591227
H	10.5791454	17.0590391	7.1377590
C	10.6504890	16.9952495	4.4604137
C	11.5036226	16.4041351	3.8261770
C	14.6882802	14.6778468	2.9728875
H	15.6472573	14.4018154	3.4054295
C	14.4164832	14.3299384	1.6601225
N	13.2303870	14.6639250	1.0963209
C	12.9855348	14.3263444	-0.3218920
C	12.2879326	15.3358641	1.7864341
H	11.3664446	15.5676571	1.2592464
C	12.5095802	15.7116115	3.1146252
C	13.7378935	15.3694425	3.7142239

H	13.9332153	15.6468177	4.7487262
H	14.9073354	14.0245344	17.6783114
H	16.5906768	5.7153197	13.5146180
H	13.5934787	9.1014502	11.4464866
H	15.1189289	13.7957625	1.0260116
H	10.6512656	16.4812992	11.2595017
H	7.7221444	18.9666888	14.4203580
H	6.9679697	8.3295827	9.8112798
H	13.4825344	13.3795333	-0.5493790
H	13.3969771	15.1260749	-0.9483423
H	11.9086570	14.2384866	-0.4853810
C	6.6101017	19.6959942	4.7681343
H	5.9255765	20.0805595	5.5267598
H	6.0859923	19.0088477	4.0955104
H	7.0445165	20.5215879	4.1949948
C	3.3206619	9.7283508	6.1916246
H	2.7477396	8.8346408	5.9199998
H	3.8240515	10.1272612	5.3064908
H	2.6499788	10.4761304	6.6233890
C	12.2015992	4.8843351	4.5697132
H	12.6459296	5.6083522	3.8755759
H	11.3357240	4.4056620	4.1055370
H	12.9412914	4.1326240	4.8553619
S	18.1159869	16.3511812	11.2591669
O	18.7991135	15.9005692	12.4910204
O	17.6673081	17.7536970	11.3039937
O	18.8792536	16.0047085	10.0349240
C	16.7004908	13.9741872	11.3033904
C	16.6224739	15.3601277	11.1375981
C	15.3924106	15.9548929	10.8508094
H	15.3499356	17.0347175	10.7145822
C	14.2500107	15.1674038	10.7120840
H	17.6486672	13.5104120	11.5687381
C	15.5577654	13.1963134	11.1787804
H	15.6076057	12.1254800	11.3703089
C	14.3155129	13.7720705	10.8596193
C	13.1337833	12.9117886	10.6686220
C	13.2754957	11.6163685	10.1366103
H	14.2623521	11.2685809	9.8288172
C	11.8451143	13.3467446	11.0224874
H	11.7142119	14.3301231	11.4753882
C	10.7409087	12.5150860	10.8615626
H	9.7492241	12.8471761	11.1655374
C	10.9057606	11.2275929	10.3456854
C	12.1758456	10.7797301	9.9768376
H	12.2937215	9.7751847	9.5695474
H	13.3049478	15.6389989	10.4399540
S	9.4817427	10.1661446	10.1257151
O	9.0250555	10.4078521	8.7409695
O	8.5071425	10.6091593	11.1478577
O	9.9776273	8.7893118	10.3434962

13. References

1. Dubbaka, S. R., Kienle, M., Mayr, H. & Knochel, P. Copper(I)-Mediated Oxidative Cross-Coupling between Functionalized Alkynyl Lithium and Aryl Magnesium Reagents. *Angew. Chem. Int. Ed.* **46**, 9093–9096 (2007).
2. BindFit v0.5 | Supramolecular. http://app.supramolecular.org/bindfit/.
3. Moreno, J., Grubert, L., Schwarz, J., Bléger, D. & Hecht, S. Efficient Sensitized Z→E Photoisomerization of an Iridium(III)-Azobenzene Complex over a Wide Concentration Range. *Chem. – Eur. J.* **23**, 14090–14095 (2017).
4. Leung, S. Y.-L., Tam, A. Y.-Y., Tao, C.-H., Chow, H. S. & Yam, V. W.-W. Single-Turn Helix–Coil Strands Stabilized by Metal···Metal and π–π Interactions of the Alkynylplatinum(II) Terpyridyl Moieties in meta-Phenylene Ethynylene Foldamers. *J. Am. Chem. Soc.* **134**, 1047–1056 (2012).
5. Bannwarth, C., Ehlert, S. & Grimme, S. GFN2-xTB—An Accurate and Broadly Parametrized Self-Consistent Tight-Binding Quantum Chemical Method with Multipole Electrostatics and Density-Dependent Dispersion Contributions. *J. Chem. Theory Comput.* **15**, 1652–1671 (2019).
6. Becke, A. D. Density-functional exchange-energy approximation with correct asymptotic behavior. *Phys. Rev. A* **38**, 3098–3100 (1988).
7. Caldeweyher, E. *et al.* A generally applicable atomic-charge dependent London dispersion correction. *J. Chem. Phys.* **150**, 154122 (2019).

8. Weigend, F. & Ahlrichs, R. Balanced basis sets of split valence, triple zeta valence and quadruple zeta valence quality for H to Rn: Design and assessment of accuracy. *Phys. Chem. Chem. Phys.* **7**, 3297–3305 (2005).
9. TURBOMOLE V7.7. A development of University of Karlsruhe and Forschungszentrum Karlsruhe GmbH, 1989–2007; TURBOMOLE GmbH: Karlsruhe, Germany (2022).
10. Klamt, A. & Schüürmann, G. COSMO: a new approach to dielectric screening in solvents with explicit expressions for the screening energy and its gradient. *J. Chem. Soc. Perkin Trans. 2* 799–805 (1993).