ELECTRONIC SUPPORTING INFORMATION

Chiral Double stapled o-OPEs with intense circularly polarized luminiscence

Pablo Reiné,[a] Araceli G. Campaña,[a] Luis Alvarez de Cienfuegos,[a] Victor Blanco,[a] Sergio Abbate,[b] Antonio J. Mota, [c] Giovanna Longhi,*[b] Delia Miguel*[d] and Juan M. Cuerva*[a]

[a.] *Department of Organic Chemistry, University of Granada (UGR). C. U. Fuentenueva, 18071 Granada, Spain. email: jmcuerva@ugr.es*

[b.] *Department of Molecular and Translational Medicine, Università di Brescia, Brescia, Italy. Viale Europa 11 25123 Brescia, Italy. email: giovanna.longhi@unibs.it*

[c.] *Department of Inorganic Chemistry, University of Granada (UGR). C. U. Fuentenueva, 18071 Granada, Spain.*

[d.] *Department of Physical Chemistry, Faculty of Pharmacy, UGR. Cartuja Campus, 18071 Granada, Spain. Email: dmalvarez@ugr.es*

email: giovanna.longhi@unibs.it, dmalvarez@ugr.es, jmcuerva@ugr.es

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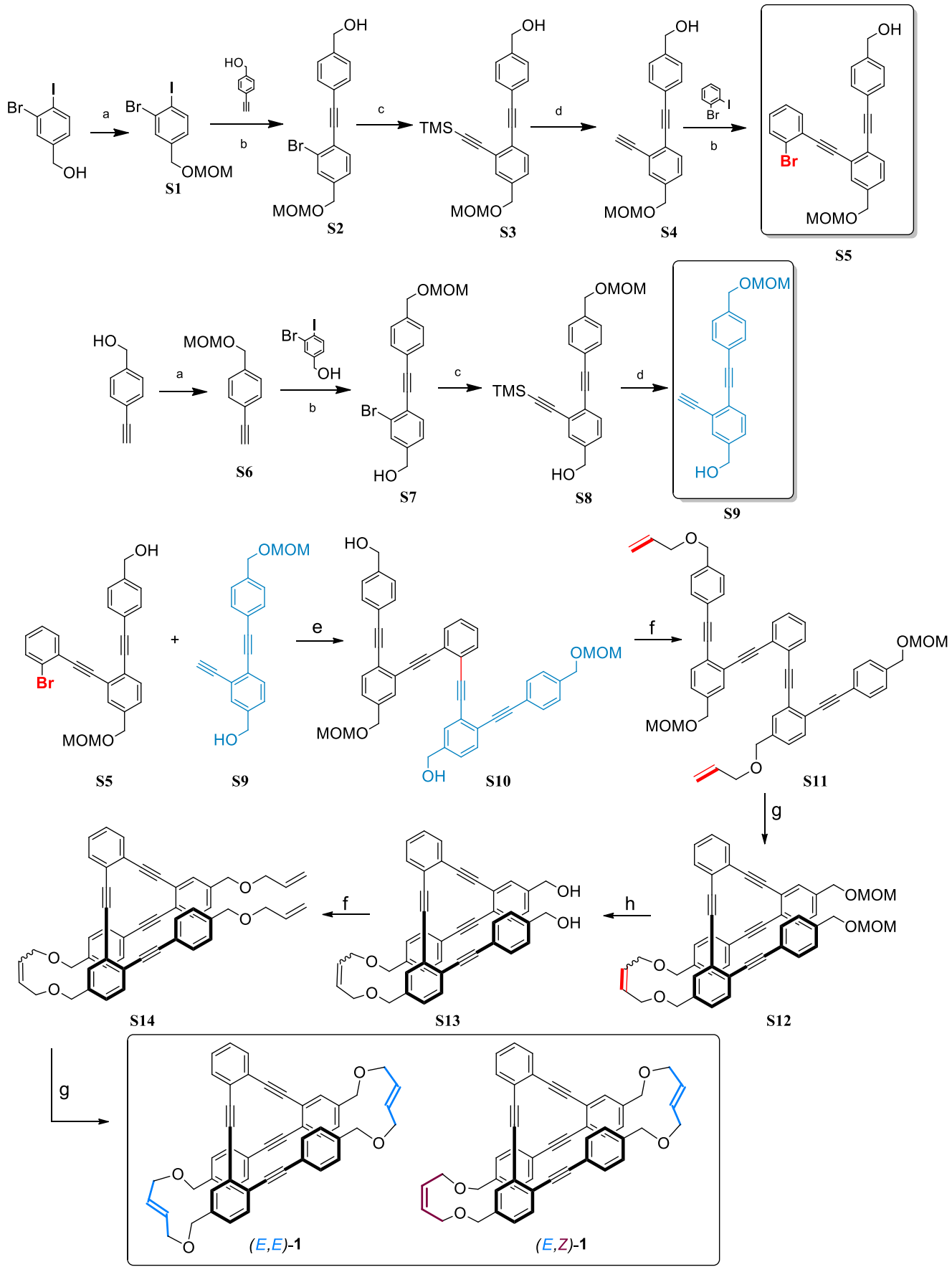
SYNTHETIC PART

General Details

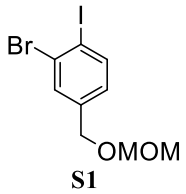
The following palladium catalysts, trans-dichlorobis(triphenylphosphine) palladium(II) ($Pd(PPh_3)_2Cl_2$) and trans-dichlorobis(acetonitrile)palladium(II) ($Pd(CH_3CN)_2Cl_2$), were prepared from palladium(II) chloride($PdCl_2$) according to previously described procedures.[S1] All reagents and solvents (CH_2Cl_2, EtOAc, hexane, THF, iPr_2NH, Et_3N, methanol, DMF, CH_3CN) were purchased from standard chemical suppliers and used without further purification. Dry THF was freshly distilled over Na/benzophenone. Thin-layer chromatography analysis was performed on aluminium-backed plates coated with silica gel 60 (230-240 mesh) with F254 indicator. The spots were visualized with UV light (254 nm and 360 nm) and/or stained with phosphomolybdic acid (10% ethanol solution) and subsequent heating. Chromatography purifications were performed with silica gel 60 (40-63 μm). ^1H and ^{13}C NMR spectra were recorded on Varian 400 or 500 MHz spectrometers, at a constant temperature of 298 K. Chemical shifts are reported in ppm using residual solvent peak as reference ($CDCl_3$: δ = 7.26 ppm, CD_2Cl_2: δ = 5.32 ppm, $(CD_3)_2CO$: δ = 2.05 ppm). Data are reported as follows: chemical shift, multiplicity (s: singlet, d: doublet, t: triplet, q: quartet, quint: quintuplet, hept: heptuplet, m: multiplet, dd: doublet of doublets, dt: doublet of triplets, td: triplet of doublets, bs: broad singlet), coupling constant (J in Hz) and integration; ^{13}C NMR spectra were recorded at 101 or 126 MHz using broadband proton decoupling and chemical shifts are reported in ppm using residual solvent peaks as reference ($CDCl_3$: δ = 77.16 ppm, CD_2Cl_2: δ = 54.00 ppm, $(CD_3)_2CO$: δ = 29.84 ppm). Carbon multiplicities were accomplished by DEPT techniques. High-resolution mass spectra (HRMS) were recorded using EI on a Micromass GCT Agilent Technologies 6890N (Waters), by APCI mass spectra carried out on a Bruker MAXIS II mass spectrometer or by ESI mass spectrometry carried out on a Waters Xevo G2-XS QTof mass spectrometer.

SYNTHESIS AND CHARACTERIZATION OF (E,E)-1 AND (E,Z)-1



Scheme S1. Synthesis of compounds (*E*,*E*)-**1** and (*E*,*Z*)-**1.** a) Methoxymethyl chloride, NaH, CH_3CN rt b) $Pd(PPh_3)_2Cl_2$, CuI, Et_3N/THF, rt c) $Pd(CH_3CN)_2Cl_2$, *t*$Bu_3P{\cdot}HBF_4$, CuI, trimethylsilyl acetylene, *i*Pr_2NH/THF, rt d) Bu_4NF, THF, rt e) $Pd(CH_3CN)_2Cl_2$, *t*$Bu_3P{\cdot}HBF_4$, CuI, *i*Pr_2NH/THF, 60ºC f) Allyl bromide, NaH, DMF, rt g) Grubbs Catalyst 1st generation, CH_2Cl_2, 45ºC h) p-Toluenesulfonic acid monohydrate, methanol, 65ºC.

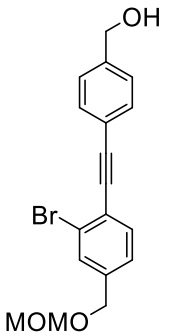
Compound S1.



S1

NaH (1.78 g, 44.6 mmol) was added to a solution of 3-bromo-4-iodobenzyl alcohol (2.79 g, 8.92 mmol) dissolved in 40 mL CH_3CN. The mixture was stirred during 15 min and then methoxymethyl chloride (1.3 mL, 17.8 mmol) was added. The reaction was stirred during 1 h at room temperature. The mixture was quenched with water, diluted with EtOAc, washed with water, dried over anhydrous Na_2SO_4 and the solvent was removed under reduced pressure. The residue was used without further purification to give **S1** (3.12 g, 98%) as a colourless oil. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.82 (d, *J* = 8.1 Hz, 1H), 7.63 (s, 1H), 6.98 (d, *J* = 8.2 Hz, 1H), 4.69 (s, 2H), 4.51 (s, 2H), 3.40 (s, 3H). **^{13}C NMR (101 MHz, $CDCl_3$)** δ 140.35 (CH), 140.29 (C), 131.9 (CH), 129.9 (C), 127.8 (CH), 99.9 (C), 96.0 (CH_2), 67.9 (CH_2), 55.7 (CH_3). **HRMS (EI):** *m*/*z* $[M]^+$ calcd for $C_9H_{10}O_2BrI$: 355.8909; found: 355.8922.

Compound S2.

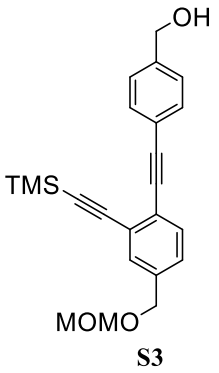


S2

A solution of 4-ethynylbenzyl alcohol (979 mg, 7.41 mmol) dissolved in 5 mL of THF was added dropwise during 1 h to a carefully degassed solution of $Pd(PPh_3)_2Cl_2$ (238 mg, 0.34 mmol), CuI (65 mg, 0.34 mmol) and **S1** (2.69 g, 6.74 mmol) in 10 mL of Et_3N. Afterwards, the reaction was stirred at room temperature under argon atmosphere during 24 h. The mixture was then diluted with EtOAc, washed

with saturated aq NH_4Cl solution, dried over anhydrous Na_2SO_4 and the solvent was removed under reduced pressure. The residue was purified by flash chromatography (SiO_2, EtOAc/Hexane 6:4) to give **S2** (1.97 g, 74%) as a yellow solid. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.63 (s, 1H), 7.57 (d, *J* = 8.2 Hz, 2H), 7.53 (d, *J* = 7.9 Hz, 1H), 7.36 (d, *J* = 8.2 Hz, 2H), 7.27 (d, *J* = 7.9 Hz, 1H), 4.71 (s, 4H), 4.58 (s, 2H), 3.41 (s, 3H). **^{13}C NMR (101 MHz, $CDCl_3$)** δ 141.6 (C), 140.0 (C), 133.2 (CH), 132.0 (CH), 131.6 (CH), 127.0 (CH), 126.3 (CH), 125.8 (C), 124.7 (C), 122.3 (C), 96.1 (CH_2), 93.9 (C), 88.2 (C), 68.2 (CH_2), 65.1 (CH_2), 55.7 (CH_3). **HRMS (EI):** *m*/*z* $[M]^+$ calcd for $C_{18}H_{17}O_3Br$: 360.0357; found: 360.0361.

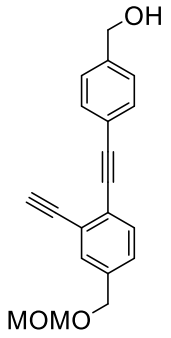
Compound S3.



S3

Trimethylsilyl acetylene (2.7 mL, 19.5 mmol) was added dropwise to a carefully degassed solution of $Pd(CH_3CN)_2Cl_2$ (127 mg, 0.49 mmol), CuI (93 mg, 0.49 mmol), P*t*Bu_3·HBF_4 (284 mg, 0.98 mmol) and **S2** (1.97 g, 4.88 mmol) in 10 mL of iPr_2NH and 10 mL of THF. Afterwards, the reaction was stirred at room temperature under argon atmosphere during 4 h. The mixture was then diluted with EtOAc, washed with saturated aq NH_4Cl solution, dried over anhydrous Na_2SO_4 and the solvent was removed under reduced pressure. The residue was purified by flash chromatography (SiO_2, EtOAc/Hexane 4:6) to give **S3** (1.89 g, 90%) as an orange solid. **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.55 (d, *J* = 8.2 Hz, 2H), 7.52 – 7.48 (m, 2H), 7.36 (d, *J* = 7.9 Hz, 2H), 7.28 (d, *J* = 7.9 Hz, 1H), 4.72 (s, 2H), 4.70 (s, 2H), 4.56 (s, 2H), 3.41 (s, 3H), 0.27 (s, 9H). **^{13}C NMR (126 MHz, $CDCl_3$)** δ 141.3 (C), 138.2 (C), 132.0 (CH), 131.9 (CH), 131.5 (CH), 127.6 (CH), 126.9 (CH), 125.8 (C), 125.4 (C), 122.7 (C), 103.5 (C), 98.8 (C), 96.0 (CH_2), 93.4 (C), 88.3 (C), 68.5 (CH_2), 65.1 (CH_2), 55.6 (CH_3), 0.2 (CH_3). **HRMS (ES):** *m*/*z* $[M+H]^+$ calcd for $C_{23}H_{27}O_3Si$: 379.1721; found: 379.1729.

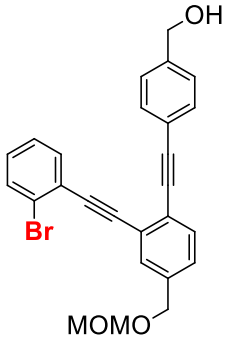
Compound S4.



S4

To a solution of **S3** (1.89 g, 5.00 mmol) in THF (10 ml) with 4-5 drops of water, Bu_4NF (2.14 g, 6.78 mmol) was added, and the mixture was stirred at room temperature until complete consumption of the starting material (TLC, 1 h). The solution was then diluted with EtOAc, washed with brine, dried over anhydrous Na_2SO_4 and the solvent was removed under reduced pressure. The residue was purified by flash chromatography (SiO_2, EtOAc/Hexane 4:6) to give **S4** (1.38 g, 90%) as a yellow solid. **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.56 (d, *J* = 8.2 Hz, 2H), 7.54 – 7.52 (m, 1H), 7.51 (s, 1H), 7.35 (d, *J* = 7.9 Hz, 2H), 7.32 (d, *J* = 8.2 Hz, 1H), 4.71 (s, 4H), 4.58 (s, 2H), 3.41 (s, 3H), 3.36 (s, 1H). **^{13}C NMR (126 MHz, $CDCl_3$)** δ 141.4 (C), 138.3 (C), 132.1 (CH), 132.0 (CH), 131.8 (CH), 128.0 (CH), 126.9 (CH), 125.6 (C), 124.8 (C), 122.5 (C), 96.0 (CH_2), 93.5 (C), 88.0 (C), 82.2 (C), 81.3 (CH), 68.4 (CH_2), 65.1 (CH_2), 55.6 (CH_3). **HRMS (ES):** *m/z* $[M+Na]^+$ calcd for $C_{20}H_{18}O_3Na$: 329.1144; found: 329.1154.

Compound S5.

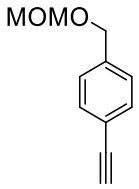


S5

A solution of **S4** (1.10 g, 3.59 mmol) dissolved in 5 mL of THF was added dropwise during 1 h to a carefully degassed solution of $Pd(PPh_3)_2Cl_2$ (111 mg, 0.16 mmol), CuI (60 mg, 0.32 mmol) and 2-bromoiodobenzene (1.07 g, 3.80 mmol) in 10 mL of Et_3N and 5 mL of THF. Afterwards, the reaction was stirred at room temperature under argon atmosphere during 24 h. The mixture was then diluted with EtOAc, washed with saturated aq NH_4Cl solution, dried over anhydrous Na_2SO_4 and the solvent was removed under reduced pressure. The residue was purified by flash chromatography (SiO_2, EtOAc/Hexane 4:6) to give **S5** (1.80 g, 99%) as an orange solid. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.67 – 7.52

(m, 6H), 7.38 – 7.33 (m, 3H), 7.33 – 7.27 (m, 1H), 7.20 (td, *J* = 7.6, 1.7 Hz, 1H), 4.75 (s, 2H), 4.72 (s, 2H), 4.63 (s, 2H), 3.45 (s, 3H). **^{13}C NMR (101 MHz, $CDCl_3$)** δ 141.4 (C), 138.3 (C), 133.7 (CH), 132.6 (CH), 132.2 (CH), 132.1 (CH), 131.4 (CH), 129.7 (CH), 127.8 (CH), 127.1 (CH), 126.9 (CH), 125.61 (C), 125.58 (C), 125.55 (C), 125.1 (C), 122.6 (C), 96.0 (CH_2), 93.6 (C), 92.7 (C), 92.0 (C), 88.3 (C), 68.5 (CH_2), 65.0 (CH_2), 55.6 (CH_3). **HRMS (ES):** *m*/*z* $[M+Na]^+$ calcd for $C_{26}H_{21}O_3NaBr$: 483.0558; found: 483.0572.

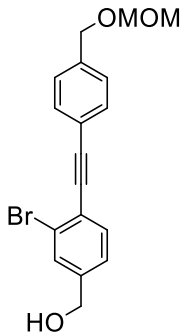
Compound S6.



S6

NaH (2.10 g, 52.5 mmol) was added to a solution of 4-ethynylbenzyl alcohol (1.39 g, 10.5 mmol) dissolved in 20 mL CH_3CN. The mixture was stirred during 15 min and then methoxymethyl chloride (1.6 mL, 21.0 mmol) was added. The reaction was stirred during 1 h at room temperature. The mixture was quenched with water, diluted with EtOAc, washed with water, dried over anhydrous Na_2SO_4 and the solvent was removed under reduced pressure. The residue was used without further purification to give **S6** (1.80 g, 97%) as a yellow oil. **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.48 (d, *J* = 8.2 Hz, 2H), 7.32 (d, *J* = 8.3 Hz, 2H), 4.70 (s, 2H), 4.59 (s, 2H), 3.41 (s, 3H), 3.07 (s, 1H). **^{13}C NMR (126 MHz, $CDCl_3$)** δ 138.9 (C), 132.3 (CH), 127.7 (CH), 121.5 (C), 95.9 (CH_2), 83.6 (C), 77.3 (CH), 68.8 (CH_2), 55.6 (CH_3). **HRMS (EI):** *m*/*z* $[M+H]^+$ calcd for $C_{11}H_{13}O_2$: 177.0916; found: 177.0901.

Compound S7.

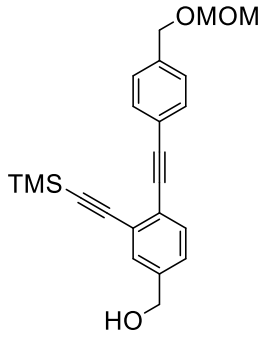


S7

A solution of **S6** (1.01 g, 5.75 mmol) dissolved in 5 mL of THF was added dropwise during 1 h to a carefully degassed solution of $Pd(PPh_3)_2Cl_2$ (167 mg, 0.24 mmol), CuI (91 mg, 0.48 mmol) and 3-bromo-4-iodobenzyl alcohol (1.50 g, 4.79 mmol) in 10 mL of Et_3N and 5 mL of THF. Afterwards, the reaction

was stirred at room temperature under argon atmosphere during 24 h. The mixture was then diluted with EtOAc, washed with saturated aq NH_4Cl solution, dried over anhydrous Na_2SO_4 and the solvent was removed under reduced pressure. The residue was purified by flash chromatography (SiO_2, EtOAc/Hexane 2:8) to give **S7** (1.54 g, 80%) as an orange solid. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.65 (s, 1H), 7.59 (d, *J* = 8.0 Hz, 2H), 7.55 (d, *J* = 7.9 Hz, 1H), 7.37 (d, *J* = 8.0 Hz, 2H), 7.31 – 7.26 (m, 1H), 4.74 (s, 2H), 4.70 (s, 2H), 4.63 (s, 2H), 3.44 (s, 3H). **^{13}C NMR (101 MHz, $CDCl_3$)** δ 142.8 (C), 138.7 (C), 133.3 (CH), 131.9 (CH), 130.7 (CH), 127.8 (CH), 125.9 (C), 125.5 (CH), 124.5 (C), 122.3 (C), 95.9 (CH_2), 93.8 (C), 88.1 (C), 68.9 (CH_2), 64.2 (CH_2), 55.6 (CH_3). **HRMS (EI):** *m*/*z* $[M]^+$ calcd for $C_{18}H_{17}O_3Br$: 360.0378; found: 360.0361.

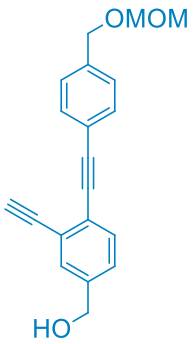
Compound S8.



S8

Trimethylsilyl acetylene (0.6 mL, 4.50 mmol) was added dropwise to a carefully degassed solution of $Pd(CH_3CN)_2Cl_2$ (97 mg, 0.37 mmol), CuI (71 mg, 0.37 mmol), P*t*Bu_3·HBF_4 (217 mg, 0.75 mmol) and **S7** (1.51 g, 4.18 mmol) in 8 mL of iPr_2NH and 5 mL of THF. Afterwards, the reaction was stirred at room temperature under argon atmosphere during 24 h. The mixture was then diluted with EtOAc, washed with saturated aq NH_4Cl solution, dried over anhydrous Na_2SO_4 and the solvent was removed under reduced pressure. The residue was purified by flash chromatography (SiO_2, EtOAc/Hexane 4:6) to give **S8** (1.01 g, 64%) as a yellow solid. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.58 – 7.47 (m, 4H), 7.35 (d, *J* = 8.0 Hz, 2H), 7.29 (d, *J* = 8.0 Hz, 1H), 4.72 (s, 2H), 4.68 (s, 2H), 4.61 (s, 2H), 3.42 (s, 3H), 0.27 (s, 9H). **^{13}C NMR (101 MHz, $CDCl_3$)** δ 140.9 (C), 138.5 (C), 132.0 (CH), 131.9 (CH), 130.7 (CH), 127.8 (CH), 126.8 (CH), 126.0 (C), 125.3 (C), 122.7 (C), 103.5 (C), 98.9 (C), 96.0 (CH_2), 93.5 (C), 88.3 (C), 69.0 (CH_2), 64.7 (CH_2), 55.6 (CH_3), 0.2 (CH_3). **HRMS (ES):** *m*/*z* $[M+H]^+$ calcd for $C_{23}H_{27}O_3Si$: 379.1728; found: 379.1729.

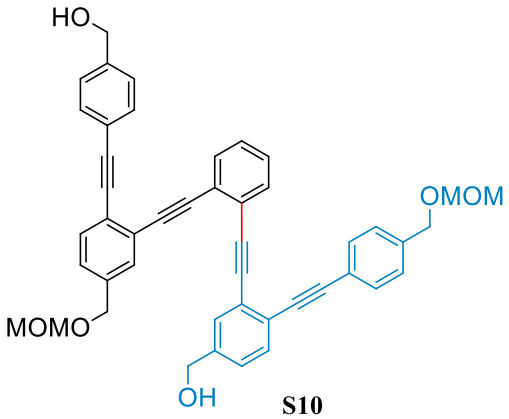
Compound S9.



S9

To a solution of **S8** (1.01 g, 2.67 mmol) in THF (10 ml) with 4-5 drops of water, Bu_4NF (1.13 g, 3.60 mmol) was added, and the mixture was stirred at room temperature until complete consumption of the starting material (TLC, 1 h). The solution was then diluted with EtOAc, washed with brine, dried over anhydrous Na_2SO_4 and the solvent was removed under reduced pressure. The residue was purified by flash chromatography (SiO_2, EtOAc/Hexane 4:6) to give **S9** (816 mg, 99%) as an orange oil. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.54 (d, *J* = 8.0 Hz, 2H), 7.52 – 7.48 (m, 2H), 7.33 (d, *J* = 8.0 Hz, 2H), 7.30 – 7.26 (m, 1H), 4.70 (s, 2H), 4.63 (s, 2H), 4.59 (s, 2H), 3.40 (s, 3H), 3.37 (s, 1H). **^{13}C NMR (101 MHz, $CDCl_3$)** δ 141.1 (C), 138.5 (C), 132.0 (CH), 131.9 (CH), 130.8 (CH), 127.8 (CH), 127.0 (CH), 125.4 (C), 124.8 (C), 122.5 (C), 95.9 (CH_2), 88.0 (C), 81.3 (CH), 68.9 (CH_2), 64.4 (CH_2), 55.5 (CH_3). **HRMS (ES):** *m/z* $[M+Na]^+$ calcd for $C_{20}H_{18}O_3Na$: 329.1145; found: 329.1154.

Compound S10.

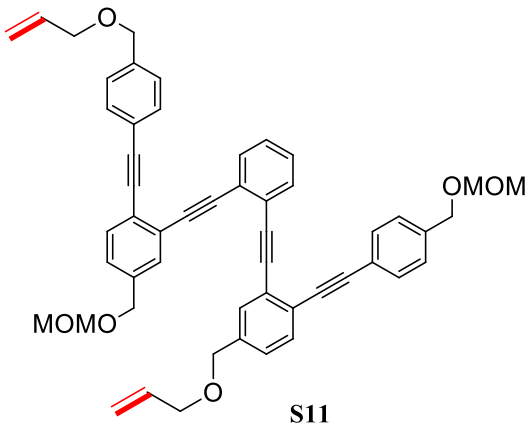


S10

S9 (694 mg, 2.26 mmol) was dissolved in 2 mL of THF and added dropwise during 1 h to a carefully degassed solution of $Pd(CH_3CN)_2Cl_2$ (56 mg, 0.22 mmol), CuI (41 mg, 0.22 mmol), P*t*Bu_3·HBF_4 (126 mg, 0.43 mmol) and **S5** (1.00 g, 2.17 mmol) in 10 mL of iPr_2NH. Afterwards, the reaction was stirred at 60ºC under argon atmosphere overnight. The mixture was then diluted with EtOAc, washed with saturated aq NH_4Cl solution, dried over anhydrous Na_2SO_4 and the solvent was removed under reduced pressure. The residue was purified by flash chromatography (SiO_2, EtOAc/Hexane 1:1) to give

S10 (900 mg, 60%) as an orange oil. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.61 (dd, *J* = 5.9, 3.3 Hz, 2H), 7.53 – 7.45 (m, 7H), 7.33 (dd, *J* = 5.9, 3.3 Hz, 2H), 7.29 – 7.20 (m, 7H), 4.70 (s, 2H), 4.65 (s, 4H), 4.56 (s, 4H), 4.52 (s, 2H), 3.41 (s, 3H), 3.37 (s, 3H). **^{13}C NMR (101 MHz, $CDCl_3$)** δ 141.3 (C), 141.1 (C), 138.3 (C), 137.9 (C), 132.14 (CH), 132.10 (CH), 132.0 (CH), 131.93 (CH), 131.86 (CH), 131.6 (CH), 130.6 (CH), 128.4 (CH), 128.3 (CH), 127.7 (CH), 127.6 (CH), 126.9 (CH), 126.6 (CH), 126.09 (C), 126.08 (C), 126.07 (C), 125.1 (C), 124.8 (C), 122.7 (C), 122.6 (C), 96.0 (CH_2), 95.9 (CH_2), 93.7 (C), 93.55 (C), 93.53 (C), 92.8 (C), 92.6 (C), 92.5 (C), 92.4 (C), 88.5 (C), 69.0 (CH_2), 68.5 (CH_2), 65.1 (CH_2), 64.4 (CH_2), 55.7 (CH_3), 55.6 (CH_3). **HRMS (ES):** *m*/*z* $[M+Na]^+$ calcd for $C_{46}H_{38}O_6Na$: 709.2568; found: 709.2566.

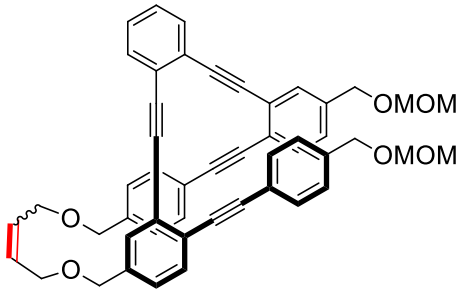
Compound S11.



S11

NaH (208 mg, 5.20 mmol) was added to a solution of **S10** (869 mg, 1.26 mmol) dissolved in 10 mL of DMF. The mixture was stirred during 15 min and then allyl bromide (0.45 mL, 5.20 mmol) was added. The reaction was stirred during 3 h at room temperature. The mixture was quenched with water, diluted with EtOAc, washed with brine (8x20 mL), dried over anhydrous Na_2SO_4 and the solvent was removed under reduced pressure. The residue was purified by flash chromatography (SiO_2, EtOAc/Hexane 4:6) to give **S11** (724 mg, 75%) as an orange oil. **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.63 (dd, *J* = 5.7, 3.4 Hz, 2H), 7.58 – 7.48 (m, 7H), 7.34 (dd, *J* = 5.7, 3.4 Hz, 2H), 7.31 – 7.24 (m, 7H), 6.03 – 5.86 (m, 2H), 5.35 – 5.27 (m, 2H), 5.25 – 5.18 (m, 2H), 4.71 (s, 2H), 4.68 (s, 2H), 4.58 (s, 2H), 4.51 (s, 2H), 4.50 (s, 2H), 4.44 (s, 2H), 4.02 (d, *J* = 5.6 Hz, 2H), 3.98 (d, *J* = 5.6 Hz, 2H), 3.42 (s, 3H), 3.39 (s, 3H). **^{13}C NMR (126 MHz, $CDCl_3$)** δ 138.8 (C), 138.6 (C), 138.3 (C), 138.1 (C), 134.75 (CH), 134.67 (CH), 132.22 (CH), 132.20 (CH), 132.1 (CH), 131.9 (CH), 131.85 (CH), 131.81 (CH), 131.6 (CH), 131.5 (CH), 128.3 (CH), 127.8 (CH), 127.7 (CH), 127.5 (CH), 127.42 (CH), 127.36 (CH), 126.00 (C), 125.99 (C), 125.97 (C), 125.89 (C), 125.0 (C), 124.9 (C), 122.7 (C), 122.5 (C), 117.4 (CH_2), 96.0 (CH_2), 95.9 (CH_2), 93.7 (C), 93.6 (C), 92.7 (C), 92.6 (C), 92.39 (C), 92.36 (C), 88.5 (C), 88.4 (C), 71.8 (CH_2), 71.4 (CH_2), 71.3 (CH_2), 68.9 (CH_2), 68.5 (CH_2), 55.5 (CH_3). **HRMS (ES):** *m*/*z* $[M+Na]^+$ calcd for $C_{52}H_{46}O_6Na$: 789.3179; found: 789.3192.

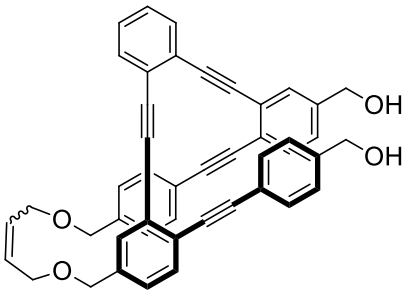
Compound S12.



S12

Grubbs catalyst 1st generation (250 mg, 0.30 mmol) was added into a Schlenk tube and carefully degassed. **S11** (724 mg, 0.94 mmol) was dissolved in 10 mL of CH_2Cl_2. Then, the mixture was diluted till 200 mL. The reaction was stirred at 45ºC during 5 h. Gas generated was carefully drained. The mixture was adsorbed on celite and purified by flash chromatography (SiO_2, EtOAc/Hexane 4:6) to give **S12**. Major isomer was a brown solid and was obtained in a 40% yield with the following spectroscopic data: **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.70 – 7.66 (m, 1H), 7.65 – 7.61 (m, 1H), 7.52 – 7.46 (m, 3H), 7.45 – 7.43 (m, 1H), 7.38 – 7.33 (m, 4H), 7.28 (d, *J* = 1.8 Hz, 1H), 7.24 – 7.18 (m, 2H), 7.18 – 7.12 (m, 5H), 5.76 (t, *J* = 4.7, 3.4 Hz, 2H), 4.71 (s, 2H), 4.69 (s, 2H), 4.55 (s, 2H), 4.48 (s, 2H), 4.46 (s, 2H), 4.28 (s, 2H), 3.87 (d, *J* = 3.9 Hz, 2H), 3.70 (d, *J* = 3.9 Hz, 2H), 3.42 (s, 3H), 3.42 (s, 3H). **^{13}C NMR (101 MHz, $CDCl_3$)** δ 138.1 (C), 138.0 (C), 137.8 (C), 137.7 (C), 133.0 (CH), 132.9 (CH), 132.14 (CH), 132.13 (CH), 131.9 (CH), 131.5 (CH), 131.2 (CH), 130.8 (CH), 128.9 (CH), 128.3 (CH), 128.0 (CH), 127.39 (CH), 127.37 (CH), 127.30 (CH), 127.1 (CH), 125.7 (C), 125.64 (C), 125.62 (C), 125.60 (C), 125.5 (C), 125.0 (C), 122.8 (C), 122.7 (C), 96.0 (CH_2), 95.9 (CH_2), 93.7 (C), 93.4 (C), 92.5 (C), 92.4 (C), 92.3 (C), 91.9 (C), 88.8 (C), 88.5 (C), 71.6 (CH_2), 71.1 (CH_2), 69.0 (CH_2), 68.4 (CH_2), 65.7 (CH_2), 63.7 (CH_2), 55.6 (CH_3), 55.5 (CH_3). **HRMS (ES):** *m*/*z* $[M+Na]^+$ calcd for $C_{50}H_{42}O_6Na$: 761.2875; found: 761.2879. Minor isomer was obtained as a brown solid in a 10% yield with the following spectroscopic data: **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.70 – 7.66 (m, 1H), 7.65 – 7.59 (m, 1H), 7.51 (d, *J* = 8.3 Hz, 2H), 7.47 – 7.39 (m, 3H), 7.39 – 7.33 (m, 3H), 7.30 – 7.27 (m, 1H), 7.24 – 7.13 (m, 7H), 5.58 – 5.55 (m, 2H), 4.71 (s, 2H), 4.67 (s, 2H), 4.57 (s, 4H), 4.47 (s, 2H), 4.14 (s, 4H), 3.87 (s, 2H), 3.42 (s, 3H), 3.40 (s, 3H). **^{13}C NMR (101 MHz, $CDCl_3$)** δ 140.3 (C), 138.5 (C), 138.0 (C), 137.7 (C), 132.65 (CH), 132.60 (CH), 132.1 (CH), 132.0 (CH), 131.9 (CH), 131.7 (CH), 131.4 (CH), 130.9 (CH), 130.6 (CH), 129.3 (CH), 128.3 (CH), 128.2 (CH), 127.5 (CH), 127.3 (CH), 127.2 (CH), 126.9 (CH), 125.85 (C), 125.80 (C), 125.73 (C), 125.67 (C), 125.2 (C), 125.1 (C), 122.8 (C), 122.4 (C), 95.95 (CH_2), 95.88 (CH_2), 93.45 (C), 93.41 (C), 92.4 (C), 92.2 (C), 92.1 (C), 91.9 (C), 88.53 (C), 88.48 (C), 72.6 (CH_2), 72.2 (CH_2), 70.1 (CH_2), 69.2 (CH_2), 69.0 (CH_2), 68.4 (CH_2), 55.5 (CH_3). **HRMS (ES):** *m*/*z* $[M+Na]^+$ calcd for $C_{50}H_{42}O_6Na$: 761.2875; found: 761.2879.

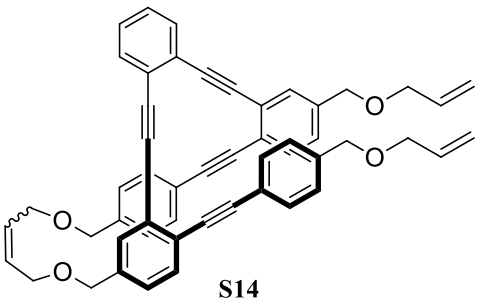
Compound S13.



S13

p-Toluenesulfonic acid monohidrate (9 mg, 0.05 mmol) and water (33 mg, 1.8 mmol) was added to a solution of **S12** (316 mg, 0.43 mmol) dissolved in 20 mL of methanol. The mixture was stirred during 8 h at reflux. The solvent was removed under reduced pressure and the residue was diluted with EtOAc, washed with brine, dried over anhydrous Na_2SO_4 and lastly the solvent was removed under reduced pressure. The residue was purified by flash chromatography (SiO_2, EtOAc/Hexane 1:1) to give **S13** a 8:2 mixture of isomers (109 mg, 39%) as a dark solid. **^{1}H NMR (500 MHz, Methanol-*d*$_4$)** δ 7.73 (dd, *J* = 5.7, 3.4 Hz, 1H), 7.68 (dd, *J* = 5.7, 3.4 Hz, 1H), 7.49 – 7.44 (m, 2H), 7.44 – 7.37 (m, 4H), 7.32 (d, *J* = 8.1 Hz, 1H), 7.27 – 7.17 (m, 7H), 7.17 – 7.12 (m, 2H), 5.83 – 5.78 (m, 2H, minor diastereomer), 5.69 (dt, *J* = 10.3, 5.0 Hz, 2H), 4.63 (s, 2H), 4.61 (s, 2H, minor diastereomer), 4.58 (s, 2H), 4.51 (s, 2H, minor diastereomer), 4.50 (s, 2H, minor diastereomer), 4.47 (s, 2H), 4.39 (s, 2H), 4.27 (s, 2H), 4.18 (d, *J* = 5.1 Hz, 2H), 4.01 – 3.94 (m, 2H). **^{13}C NMR (126 MHz, Methanol-*d*$_4$)** δ 141.5 (C), 141.3 (C), 140.1 (C), 138.6 (C), 132.1 (CH), 132.0 (CH), 131.44 (CH), 131.40 (CH), 131.38 (CH), 131.32 (CH), 131.28 (CH), 131.1 (CH), 130.3 (CH), 130.1 (CH), 129.8 (CH), 129.4 (CH), 128.18 (CH), 128.13 (CH), 127.3 (CH), 126.8 (CH), 126.6 (CH), 126.2 (CH), 126.1 (CH), 126.0 (CH), 125.6 (C), 125.5 (C), 125.4 (C), 125.2 (C), 125.0 (C), 124.4 (C), 122.3 (C), 122.0 (C), 93.0 (C), 92.5 (C), 92.15 (C), 92.10 (C), 91.5 (C), 91.0 (C), 88.0 (C), 87.5 (C), 71.4 (CH_2), 71.3 (CH_2), 69.5 (CH_2), 68.8 (CH_2), 63.5 (CH_2), 62.9 (CH_2). **HRMS (ES):** *m*/*z* $[M+Na]^+$ calcd for $C_{46}H_{34}O_4Na$: 673.2352; found: 673.2355.

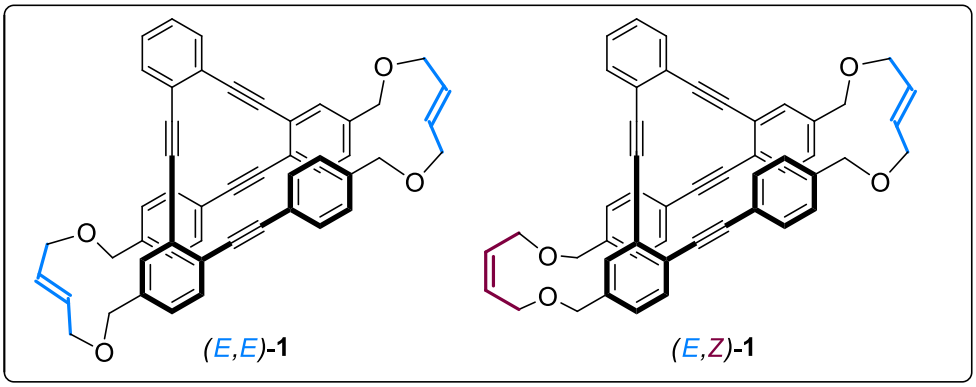
Compound S14.



S14

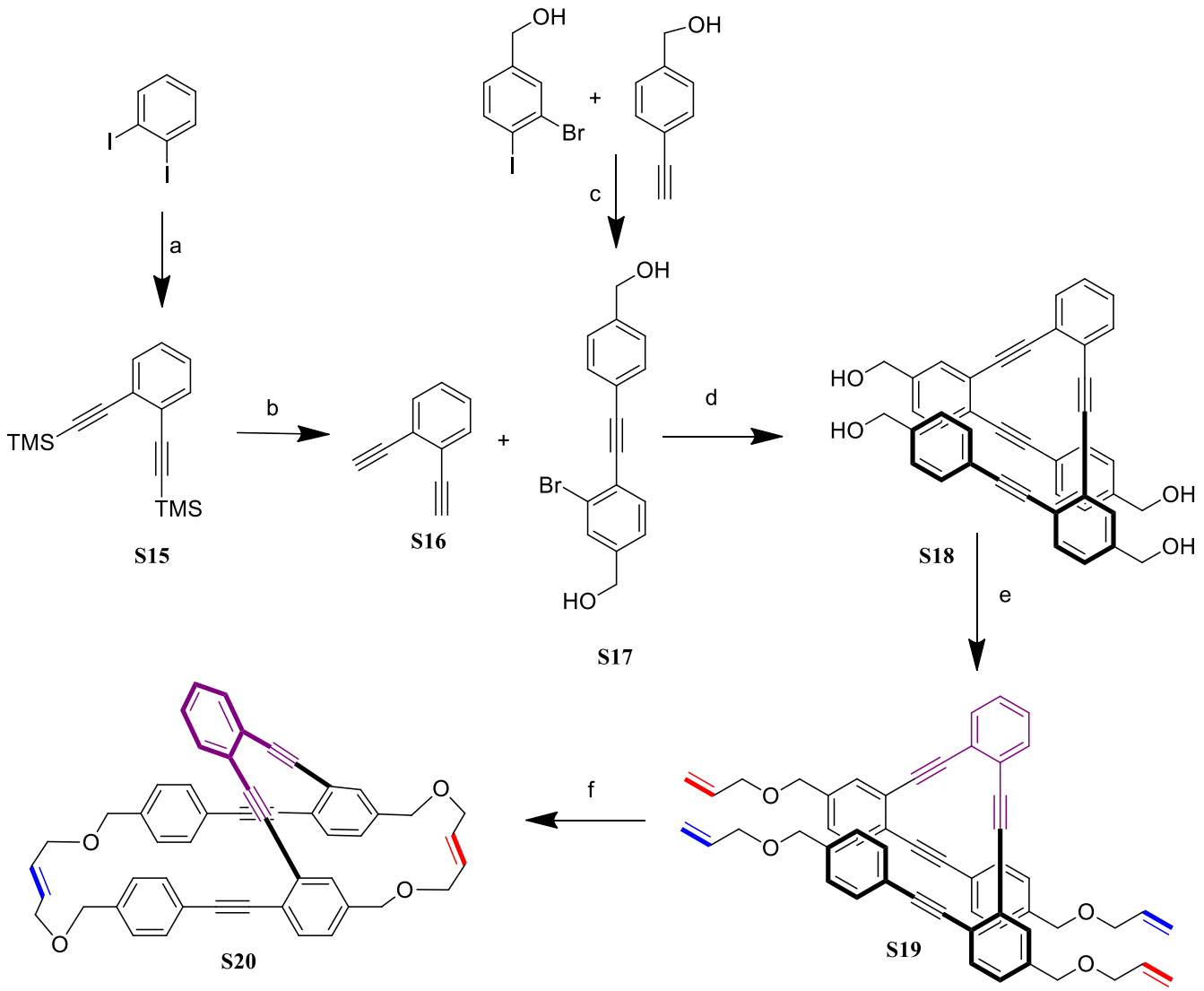
NaH (89 mg, 0.73 mmol) was added to a solution of **S13** (109 mg, 0.17 mmol) dissolved in 5 mL of DMF. The mixture was stirred during 15 min and then allyl bromide (89 mg, 0.73 mmol) was added. The reaction was stirred during 1 h at room temperature. The mixture was quenched with water, diluted with EtOAc, washed with brine (8x20 mL), dried over anhydrous Na_2SO_4 and the solvent was removed under reduced pressure. The residue was purified by flash chromatography (SiO_2, EtOAc/Hexane 4:6) to give **S14**. Major isomer was isolated as a dark solid in a 33% yield with the following spectroscopic data: **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.70 – 7.66 (m, 1H), 7.65 – 7.55 (m, 3H), 7.50 (d, *J* = 8.1 Hz, 2H), 7.47 – 7.42 (m, 2H), 7.37 – 7.33 (m, 4H), 7.24 – 7.12 (m, 6H), 6.02 – 5.89 (m, 2H), 5.76 (t, *J* = 4.1 Hz, 2H), 5.32 (d, *J* = 17.2 Hz, 2H), 5.23 (d, *J* = 11.6 Hz, 2H), 4.54 (d, *J* = 8.7 Hz, 2H), 4.48 (s, 2H), 4.46 (s, 2H), 4.40 (s, 2H), 4.28 (s, 2H), 4.05 – 4.00 (m, 2H), 3.87 (d, *J* = 4.6 Hz, 2H), 3.69 (d, *J* = 3.9 Hz, 2H). **^{13}C NMR (126 MHz, $CDCl_3$)** δ 138.3 (C), 138.2 (C), 138.04 (C), 137.98 (C), 134.8 (CH), 134.73 (CH), 134.68 (CH), 133.0 (CH), 132.9 (CH), 132.1 (CH), 131.9 (CH), 131.8 (CH), 131.4 (CH), 131.2 (CH), 130.8 (CH), 130.4 (CH), 128.9 (CH), 128.3 (CH), 128.1 (CH), 127.8 (CH), 127.4 (CH), 127.2 (CH), 127.1 (CH), 125.7 (C), 125.63 (C), 125.57 (C), 125.47 (C), 124.9 (C), 122.9 (C), 122.65 (C), 122.59 (C), 117.49 (CH_2), 117.42 (CH_2), 93.8 (C), 93.7 (C), 93.3 (C), 92.5 (C), 92.3 (C), 91.8 (C), 88.9 (C), 88.4 (C), 71.91 (CH_2), 71.87 (CH_2), 71.6 (CH_2), 71.5 (CH_2), 71.4 (CH_2), 71.1 (CH_2), 65.71 (CH_2), 63.68 (CH_2). **HRMS (ES):** *m*/*z* $[M+Na]^+$ calcd for $C_{52}H_{42}O_4Na$: 753.3016; found: 753.2981. Minor isomer was obteained as a dark solid in a 8% yield with the following spectroscopic data: **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.69 – 7.66 (m, 1H), 7.65 – 7.60 (m, 2H), 7.58 (t, *J* = 8.2 Hz, 1H), 7.51 (d, *J* = 8.2 Hz, 1H), 7.45 (d, *J* = 8.0 Hz, 1H), 7.42 (d, *J* = 8.0 Hz, 1H), 7.39 (d, *J* = 8.2 Hz, 1H), 7.37 – 7.33 (m, 3H), 7.28 – 7.27 (m, 1H), 7.24 – 7.19 (m, 5H), 7.18 – 7.13 (m, 1H), 6.03 – 5.89 (m, 2H), 5.60 – 5.55 (m, 2H), 5.38 – 5.27 (m, 2H), 5.26 – 5.19 (m, 2H), 4.57 (s, 2H), 4.54 (d, *J* = 9.7 Hz, 2H), 4.49 (s, 2H), 4.40 (s, 2H), 4.14 (s, 2H), 4.06 (dt, *J* = 5.6, 1.5 Hz, 2H), 4.04 (dt, *J* = 5.6, 1.5 Hz, 2H), 3.99 (dt, *J* = 5.6, 1.5 Hz, 2H), 3.89 – 3.86 (m, 2H). **^{13}C NMR (126 MHz, $CDCl_3$)** δ 140.3 (C), 138.45 (C), 138.42 (C), 138.2 (C), 134.8 (CH), 134.7 (CH), 132.7 (CH), 132.6 (CH), 132.0 (CH), 131.9 (CH), 131.8 (CH), 131.7 (CH), 131.3 (CH), 130.9 (CH), 130.6 (CH), 129.3 (CH), 128.3 (CH), 128.2 (CH), 127.8 (CH), 127.4 (CH), 127.2 (CH), 127.0 (CH), 125.85 (C), 125.80 (C), 125.76 (C), 125.6 (C), 125.2 (C), 125.0 (C), 122.7 (C), 122.4 (C), 117.45 (CH_2), 117.41 (CH_2), 93.5 (C), 93.4 (C), 92.4 (C), 92.3 (C), 92.1 (C), 91.8 (C), 88.6 (C), 88.4 (C), 72.6 (CH_2), 72.2 (CH_2), 71.9 (CH_2), 71.45 (CH_2), 71.40 (CH_2), 71.38 (CH_2), 70.1 (CH_2), 69.2 (CH_2). **HRMS (ES):** *m*/*z* $[M+Na]^+$ calcd for $C_{52}H_{42}O_4Na$: 753.3016; found: 753.2981.

Compounds (*E,E*)-1 and (*E,Z*)-1.



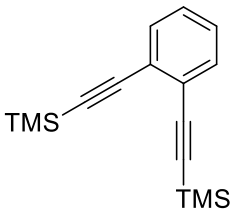
Grubbs catalyst 1st generation (18 mg, 0.02 mmol) was added into a Schlenk tube and carefully degassed. **S14** (50 mg, 0.07 mmol) was dissolved in 5 mL of CH_2Cl_2. Then, the mixture was diluted to 45 mL. The reaction was stirred at 45ºC during 4 h. Gas generated was carefully drained. The mixture was adsorbed on celite and purified by flash chromatography (SiO_2, EtOAc/Hexane 4:6). Then, we perform HPLC in order to isolate **(*E,E*)-1** and **(*E,Z*)-1**. (***E,E*)-1** was isolated as a white solid in a 28% yield with the following spectroscopic data: **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.65 (dd, *J* = 5.8, 3.3 Hz, 2H), 7.48 (d, *J* = 8.1 Hz, 4H), 7.38 (d, *J* = 7.9 Hz, 2H), 7.35 (dd, *J* = 5.8, 3.3 Hz, 2H), 7.26 (s, 2H), 7.19 (d, *J* = 8.1 Hz, 4H), 7.11 (dd, *J* = 8.1, 1.8 Hz, 2H), 5.76 – 5.64 (m, 4H), 4.63 (d, *J* = 13.6 Hz, 2H), 4.49 (d, *J* = 13.6 Hz, 2H), 4.40 (d, *J* = 12.5 Hz, 2H), 4.33 (d, *J* = 12.5 Hz, 2H), 4.20 (dd, *J* = 13.6, 5.0 Hz, 2H), 4.15 – 4.04 (m, 4H), 3.90 (dd, *J* = 13.6, 5.0 Hz, 2H). **^{13}C NMR (126 MHz, $CDCl_3$)** δ 139.56 (C), 138.35 (C), 132.64 (CH), 132.10 (CH), 131.58 (CH), 130.67 (CH), 129.47 (CH), 128.26 (CH), 127.27 (CH), 126.84 (CH), 126.06 (C), 125.89 (C), 125.22 (C), 122.73 (C), 93.42 (C), 92.65 (C), 92.10 (C), 88.36 (C), 72.29 (CH_2), 71.30 (CH_2), 70.19 (CH_2), 69.66 (CH_2). **HRMS (ES):** *m/z* [M+Na]$^+$ calcd for $C_{50}H_{38}O_4Na$: 725.2665; found: 725.2668. **(*E,Z*)-1** was isolated as a white solid in a 20% yield with the following spectroscopic data: **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.65 (ddd, *J* = 6.1, 5.2, 3.3 Hz, 2H), 7.45 – 7.38 (m, 6H), 7.37 – 7.34 (m, 2H), 7.33 (d, *J* = 1.7 Hz, 1H), 7.27 (d, *J* = 1.8 Hz, 1H), 7.13 (td, *J* = 8.4, 1.8 Hz, 2H), 7.08 (d, *J* = 8.4 Hz, 4H), 5.82 (qd, *J* = 3.3, 1.7 Hz, 2H), 5.77 – 5.72 (m, 2H), 4.56 (d, *J* = 13.5 Hz, 2H), 4.48 (d, *J* = 3.2 Hz, 2H), 4.46 (s, 1H), 4.45 (s, 1H), 4.44 (s, 1H), 4.42 (d, *J* = 2.7 Hz, 2H), 4.20 – 4.13 (m, 3H), 4.03 (d, *J* = 5.0 Hz, 2H), 3.98 (d, *J* = 5.0 Hz, 2H). **^{13}C NMR (126 MHz, $CDCl_3$)** δ 139.2 (C), 138.7 (C), 138.2 (C), 137.8 (C), 133.12 (CH), 133.06 (CH), 132.14 (CH), 132.07 (CH), 131.99 (CH), 131.88 (CH), 130.7 (CH), 130.6 (CH), 130.5 (CH), 130.0 (CH), 129.9 (CH), 129.7 (CH), 128.2 (CH), 127.5 (CH), 126.9 (CH), 126.8 (CH), 126.5 (CH), 125.95 (C), 125.90 (C), 125.64 (C), 125.57 (C), 125.3 (C), 125.0 (C), 122.8 (C), 122.6 (C), 93.6 (C), 93.4 (C), 92.63 (C), 92.59 (C), 92.3 (C), 92.2 (C), 88.4 (C), 88.3 (C), 71.5 (CH_2), 71.4 (CH_2), 71.2 (CH_2), 70.6 (CH_2), 70.03 (CH_2), 69.98 (CH_2), 66.3 (CH_2), 64.7 (CH_2). **HRMS (ES):** *m/z* [M+Na]$^+$ calcd for $C_{50}H_{38}O_4Na$: 725.2665; found: 725.2668.

Synthesis and characterization of new compound ***S20***



Scheme S2. Synthesis of compound S20. a) $Pd(PPh_3)_2Cl_2$, CuI, trimethylsilyl acetylene, Et_3N/THF, rt b) Bu_4NF, THF, rt c) $Pd(PPh_3)_2Cl_2$, CuI, Et_3N/THF, rt d) $Pd(CH_3CN)_2Cl_2$, *t*$Bu_3P{\cdot}HBF_4$, CuI, *i*Pr_2NH/THF, 60ºC e) Allyl bromide, NaH, DMF, rt f) Grubbs Catalyst 1st generation, CH_2Cl_2, 45ºC.

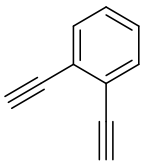
Compound S15.



S15

A solution of trimethylsiliyl acetylene (2.6 g, 4.4 mmol) was added dropwise during 1 h to a carefully degassed solution of $Pd(PPh_3)_2Cl_2$ (420 mg, 0.6 mmol), CuI (114 mg, 0.6 mmol) and 1,2-diiodobenzene (4 g, 12.1 mmol) in 24 mL of Et_3N and 4 mL of THF. Afterwards, the reaction was stirred at room temperature under argon atmosphere during 24 h. The mixture was then diluted with EtOAc, washed with saturated aq NH_4Cl solution, dried over anhydrous Na_2SO_4 and the solvent was removed under reduced pressure. The residue was purified by flash chromatography (SiO_2, Hexane) to give **S15** (2.77 g, 84%) as a yellow oil. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.46 (dd, *J* = 5.8, 3.4 Hz, 2H), 7.23 (dd, *J* = 5.8, 3.4 Hz, 2H), 0.28 (s, 18H). **^{13}C NMR (101 MHz, $CDCl_3$)** δ 132.4 (CH), 128.2 (CH), 125.9 (C), 103.4 (C), 98.6 (C), 0.2 (CH_3). **HRMS (EI):** *m*/*z* $[M]^+$ calcd for $C_{16}H_{22}Si$: 270.1260; found: 270.1247.

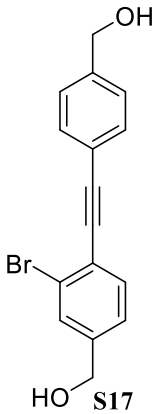
Compound S16.



S16

To a solution of **S15** (2.75 g, 10.2 mmol) in THF (5 ml) with 4-5 drops of water, Bu_4NF (9.65 g, 30.6 mmol) was added, and the mixture was stirred at room temperature until complete consumption of the starting material (TLC, 1 h). The solution was then diluted with diethylether, washed with brine, dried over anhydrous Na_2SO_4 and the solvent was removed under reduced pressure. The residue was purified by flash chromatography (SiO_2, Hexane) to give **S16** (900 mg, 70%) as a yellow oil. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.52 (dd, *J* = 5.8, 3.4 Hz, 2H), 7.31 (dd, *J* = 5.8, 3.4 Hz, 2H), 3.34 (s, 2H). **^{13}C NMR (101 MHz, $CDCl_3$)** δ 132.8 (CH), 128.6 (CH), 125.2 (C), 82.0 (C), 81.3 (CH). **HRMS (EI):** *m*/*z* $[M]^+$ calcd for $C_{10}H_6$: 126.0470; found: 126.0471.

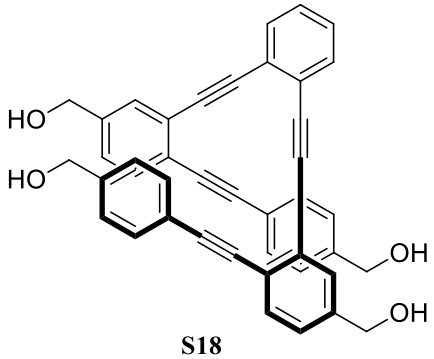
Compound S17.



S17

A solution of 4-ethynylnemzyl alcohol (422 mg, 3.30 mmol) was added dropwise during 1 h to a carefully degassed solution of $Pd(PPh_3)_2Cl_2$ (105 mg, 0.15 mmol), CuI (55 mg, 0.29 mmol) and 3-bromo-4-iodobenzyl alcohol (4 g, 12.1 mmol) in 10 mL of Et_3N and 2 mL of THF. Afterwards, the reaction was stirred at room temperature under argon atmosphere during 24 h. The mixture was then diluted with EtOAc, washed with saturated aq NH_4Cl solution, dried over anhydrous Na_2SO_4 and the solvent was removed under reduced pressure. The residue was purified by flash chromatography (SiO_2, EtOAc) to give **S17** (958 g, 92%) as a brown solid. **^{1}H NMR (500 MHz, MeOD)** δ 7.67 (s, 1H), 7.54 (d, *J* = 8.0 Hz, 2H), 7.51 (d, *J* = 8.2 Hz, 1H), 7.39 (d, *J* = 8.2 Hz, 2H), 7.33 (d, *J* = 7.9 Hz, 1H), 4.64 (s, 2H), 4.61 (s, 2H). **^{13}C NMR (126 MHz, MeOD)** δ 145.4 (C), 143.7 (C), 134.1 (CH), 132.6 (CH), 131.6 (CH), 128.0 (CH), 126.7 (CH), 126.3 (C), 125.1 (C), 123.0 (C), 94.4 (C), 88.6 (C), 64.7 (CH_2), 64.0 (CH_2). **HRMS (EI):** *m*/*z* $[M]^+$ calcd for $C_{16}H_{13}O_2Br$: 316.0099; found: 316.0096.

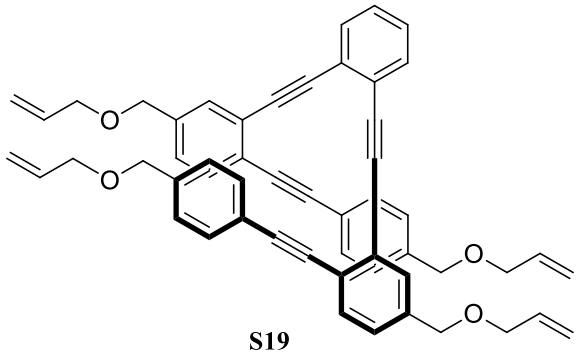
Compound S18.



S18

S16 (50 mg, 0.39 mmol) was dissolved in 1 mL of THF and added dropwise during 1 h to a carefully degassed solution of $Pd(CH_3CN)_2Cl_2$ (13 mg, 0.05 mmol), CuI (10 mg, 0.05 mmol), P*t*Bu$_3$·HBF_4 (29 mg, 0.1 mmol) and **S17** (444 mg, 1.56 mmol) in 4 mL of iPr_2NH. Afterwards, the reaction was stirred at 60ºC under argon atmosphere overnight. The mixture was then diluted with EtOAc, washed with saturated aq NH_4Cl solution, dried over anhydrous Na_2SO_4 and the solvent was removed under reduced pressure. The residue was purified by flash chromatography (SiO_2, MeOH/CH_2Cl_2 1:9) to give **S18** (200 mg, 20%) as a dark solid. **^{1}H NMR (400 MHz, MeOD)** δ 7.65 (dd, *J* = 5.8, 3.3 Hz, 1H), 7.53 – 7.50 (m, 2H), 7.47 (d, *J* = 8.2 Hz, 2H), 7.43 (dd, *J* = 5.8, 3.3 Hz, 1H), 7.37 – 7.29 (m, 3H), 4.62 (s, 2H), 4.57 (s, 2H). **^{13}C NMR (101 MHz, MeOD)** δ 143.25 (C), 143.18 (C), 133.1 (CH), 132.7 (CH), 132.6 (CH), 131.4 (CH), 129.6 (CH), 127.83 (CH), 127.81 (CH), 127.0 (C), 126.8 (C), 125.7 (C), 123.3 (C), 94.3 (C), 93.6 (C), 92.8 (C), 89.0 (C), 64.8 (CH_2), 64.3 (CH_2). **HRMS (ES):** *m*/*z* $[M+Na]^+$ calcd for $C_{42}H_{30}O_4Na$: 621.2042; found: 621.2032.

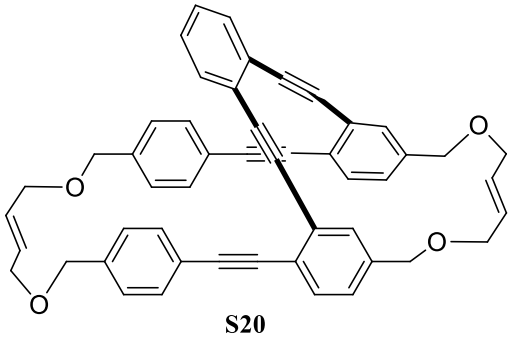
Compound S19.



S19

NaH (120 mg, 3.00 mmol) was added to a solution of **S18** (200 mg, 0.33 mmol) dissolved in 5 mL of DMF. The mixture was stirred during 15 min and then allyl bromide (0.26 mL, 3.00 mmol) was added. The reaction was stirred during 3 h at room temperature. The mixture was quenched with water, diluted with EtOAc, washed with brine (8x20 mL), dried over anhydrous Na_2SO_4 and the solvent was removed under reduced pressure. The residue was purified by flash chromatography (SiO_2, EtOAc/Hexane 2:8) to give **S19** (187 mg, 74%) as an orange oil. **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.65 (dd, *J* = 5.8, 3.3 Hz, 1H), 7.56 – 7.49 (m, 4H), 7.35 (dd, *J* = 5.8, 3.3 Hz, 1H), 7.32 – 7.26 (m, 3H), 5.95 (ddt *J* = 17.8, 16.0, 5.4 Hz, 2H), 5.37 – 5.27 (m, 2H), 5.26 – 5.18 (m, 2H), 4.52 (s, 2H), 4.45 (s, 2H), 4.04 (dt, *J* = 5.6, 1.5 Hz, 2H), 3.99 (dt, *J* = 5.6, 1.5 Hz, 2H). **^{13}C NMR (126 MHz, $CDCl_3$)** δ 138.7 (C), 138.5 (C), 134.7 (CH), 134.6 (CH), 132.2 (CH), 131.8 (CH), 131.6 (CH), 128.3 (CH), 127.5 (CH), 127.4 (CH), 126.0 (C), 125.9 (C), 124.9 (C), 122.5 (C), 117.43 (CH_2), 117.41 (CH_2), 93.7 (C), 92.6 (C), 92.3 (C), 88.4 (C), 71.8 (CH_2), 71.35 (CH_2), 71.34 (CH_2). **HRMS (ES):** *m*/*z* $[M+Na]^+$ calcd for $C_{54}H_{46}O_4Na$: 781.3294; found: 781.3290.

Compound S20.



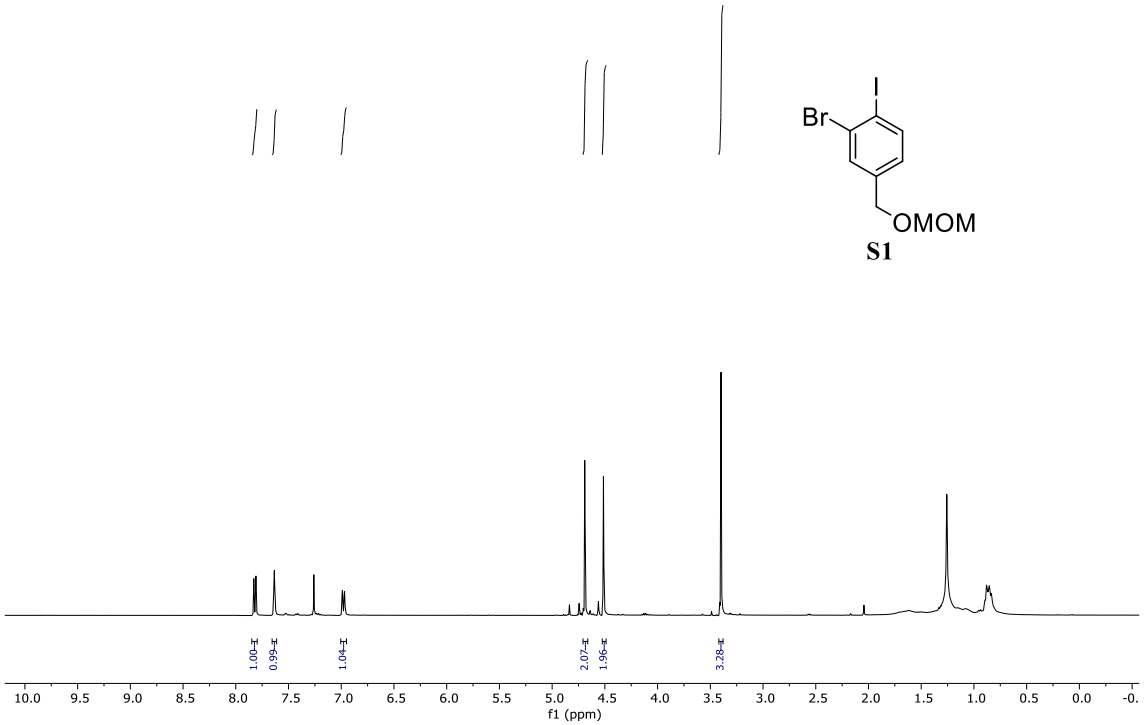
S20

Grubbs catalyst 1st generation (74 mg, 0.09 mmol) was added into a Schlenk tube and carefully degassed. **S19** (187 mg, 0.25 mmol) was dissolved in 5 mL of CH_2Cl_2. Then, the mixture was diluted till 90 mL. The reaction was stirred at 45ºC during 4 h. Gas generated was carefully drained. The mixture was adsorbed on celite and purified by flash chromatography (SiO_2, EtOAc/Hexane 4:6) to give **S20**

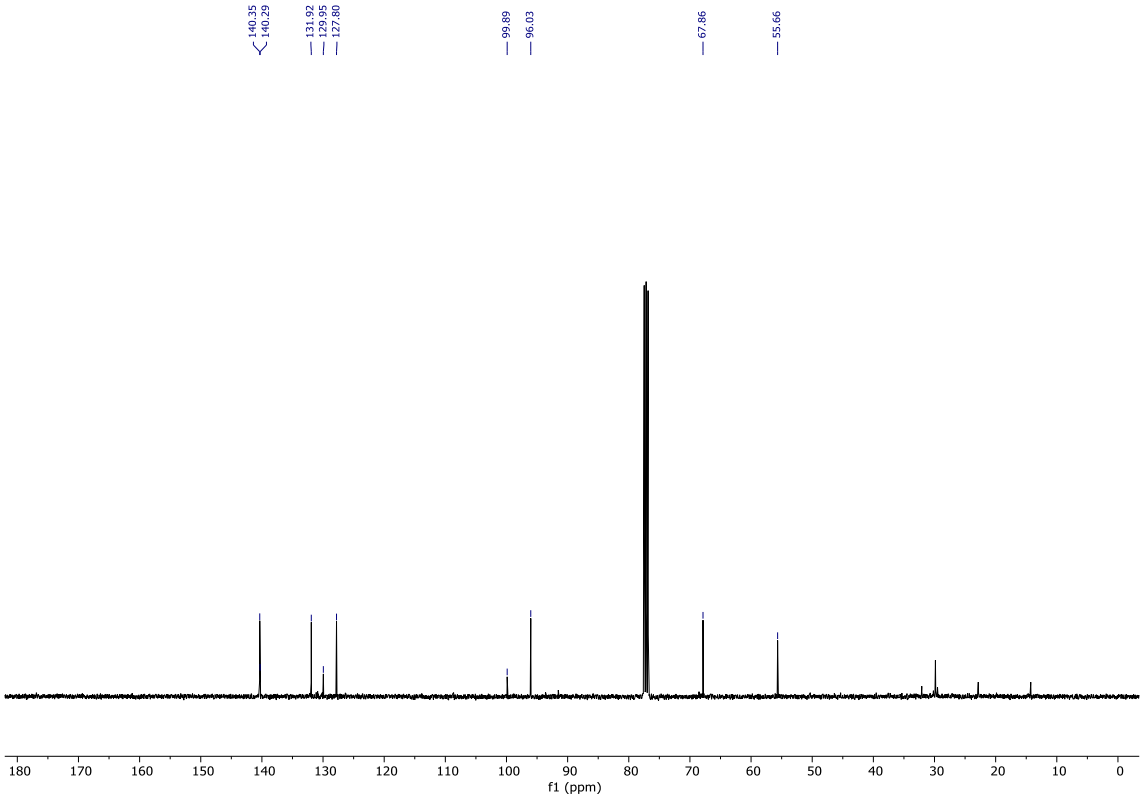
(116 mg, 66%) as a white solid. **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.62 – 7.58 (m, 2H), 7.45 (d, *J* = 8.0 Hz, 2H), 7.39 (d, *J* = 8.0 Hz, 1H), 7.33 (dd, *J* = 5.8, 3.3 Hz, 1H), 7.18 – 7.15 (m, 3H), 5.60 (ddt, *J* = 14.9, 2.9, 1.5 Hz, 2H), 4.43 (s, 2H), 4.39 (s, 2H), 4.03 – 4.02 (m, 2H), 3.98 – 3.96 (m, 2H). **^{13}C NMR (126 MHz, $CDCl_3$)** δ 139.3 (C), 139.2 (C), 131.8 (CH), 131.4 (CH), 131.1 (CH), 130.9 (CH), 129.7 (CH), 129.5 (CH), 128.4 (CH), 127.6 (CH), 127.5 (CH), 126.6 (C), 126.5 (C), 125.1 (C), 122.6 (C), 94.1 (C), 93.2 (C), 92.5 (C), 88.6 (C), 72.3 (CH_2), 72.0 (CH_2), 70.9 (CH_2), 70.7 (CH_2). **HRMS (ES):** *m*/*z* $[M+H]^+$ calcd for $C_{50}H_{39}O_4$: 703.2843; found: 703.2858.

^{1}H and ^{13}C NMR of new compounds

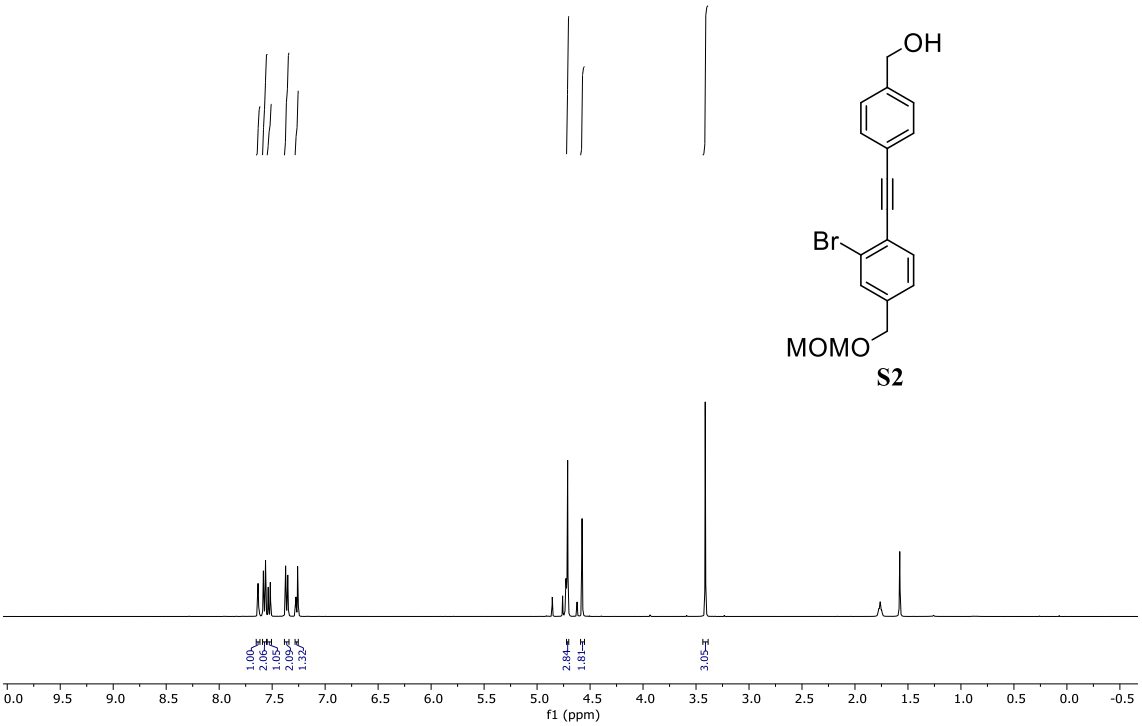
. ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of compound **S1**



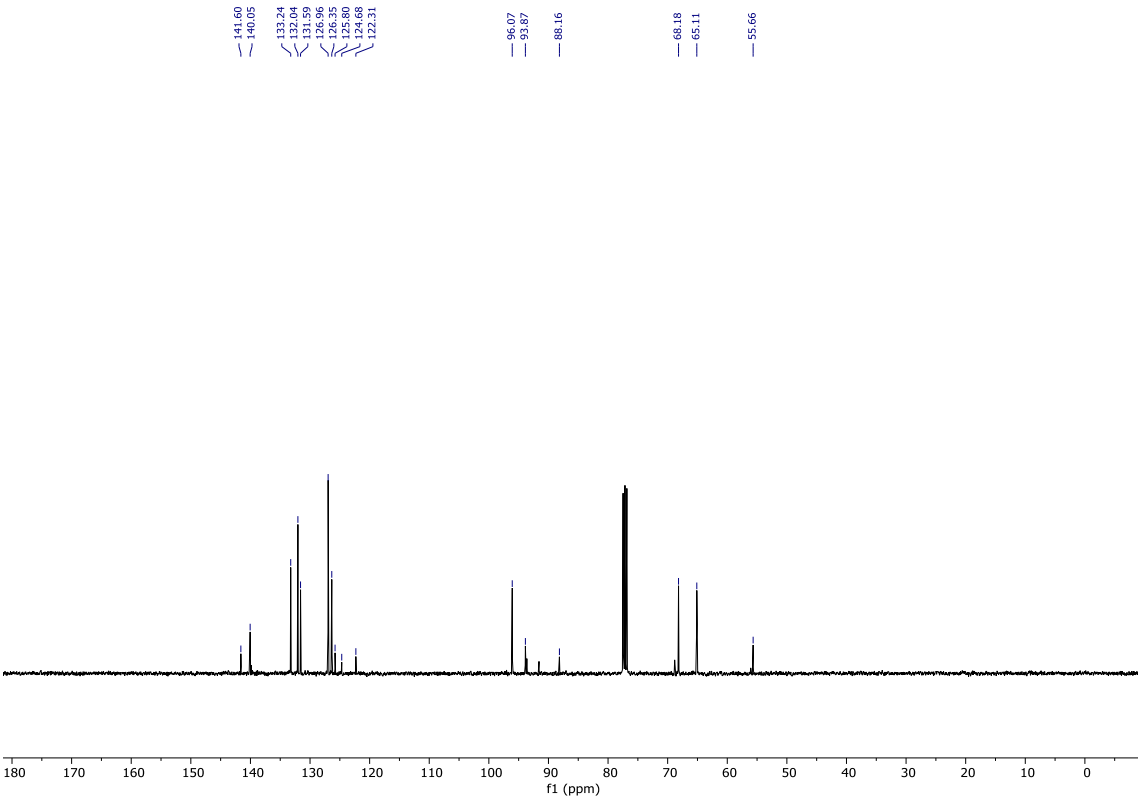
. ^{13}C NMR (126 MHz, $CDCl_3$) spectrum of compound **S1**



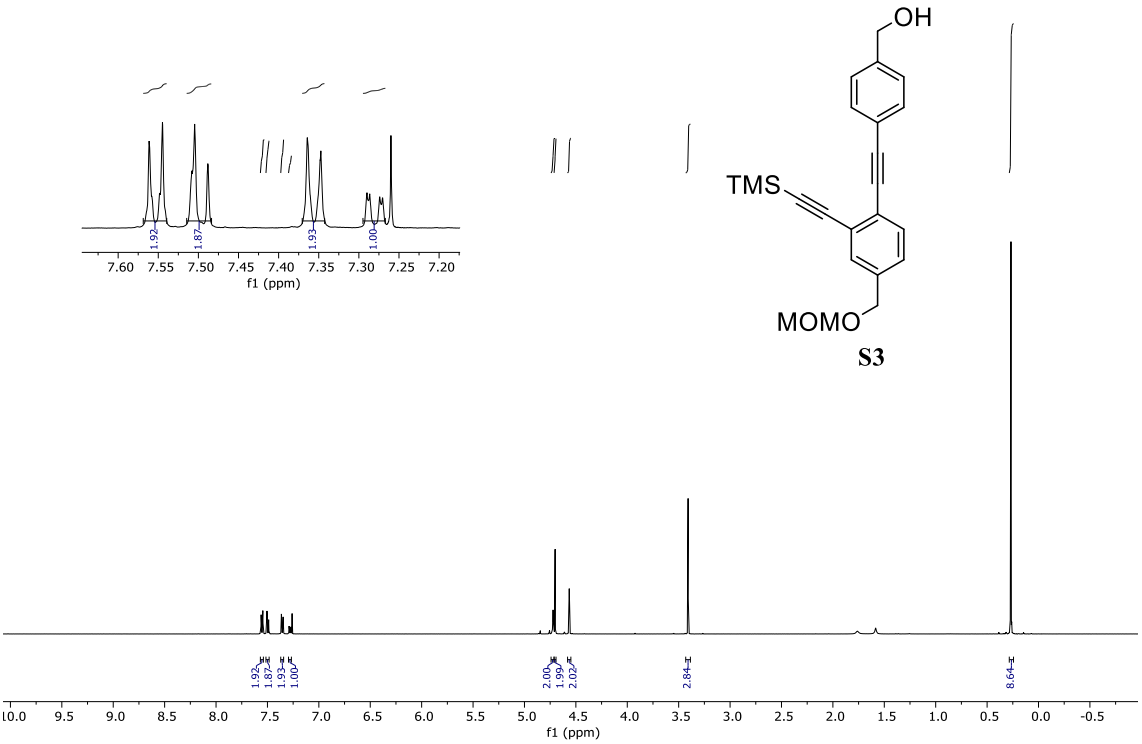
. **^{1}H NMR (500 MHz, $CDCl_3$)** spectrum of compound **S2**



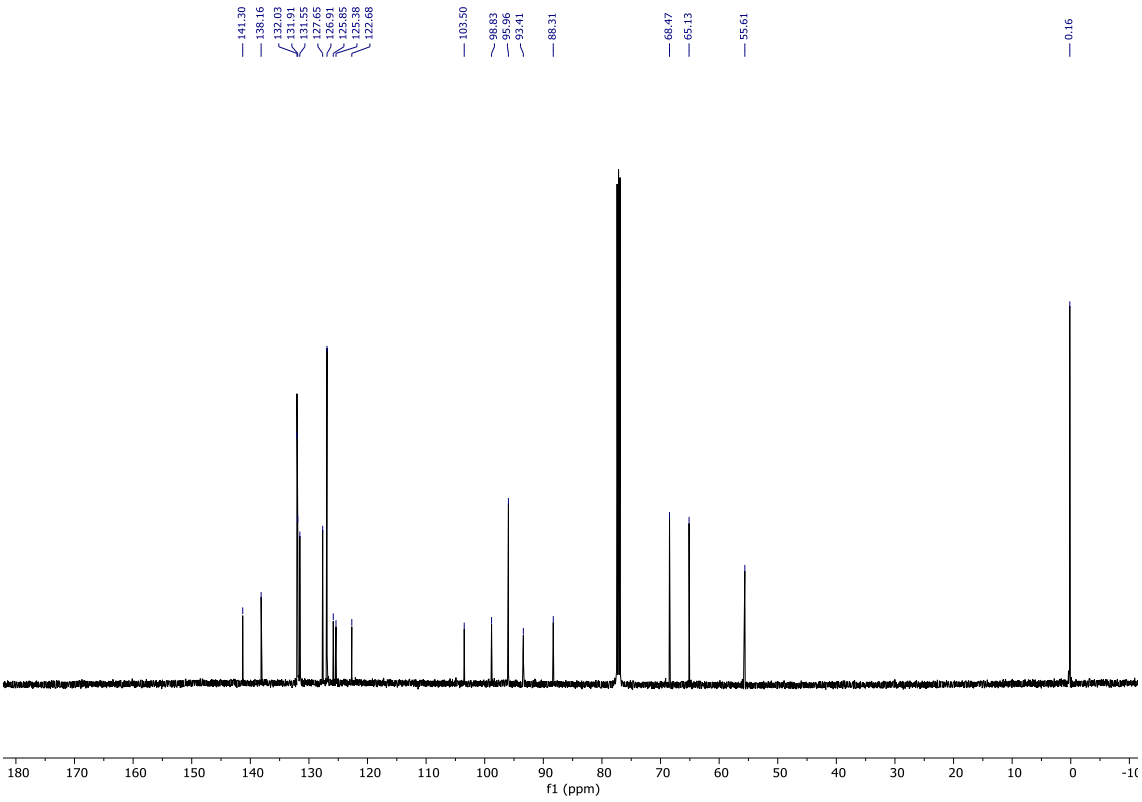
. **^{13}C NMR (126 MHz, $CDCl_3$)** spectrum of compound **S2**



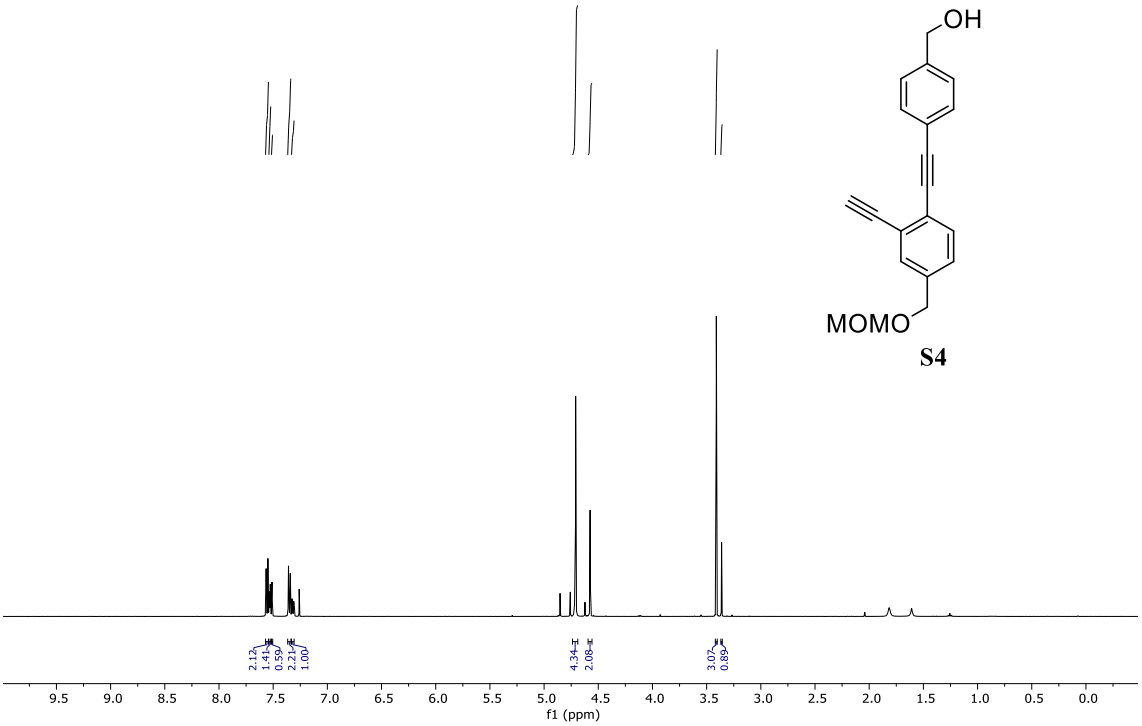
. **^{1}H NMR (500 MHz, $CDCl_3$)** spectrum of compound **S3**



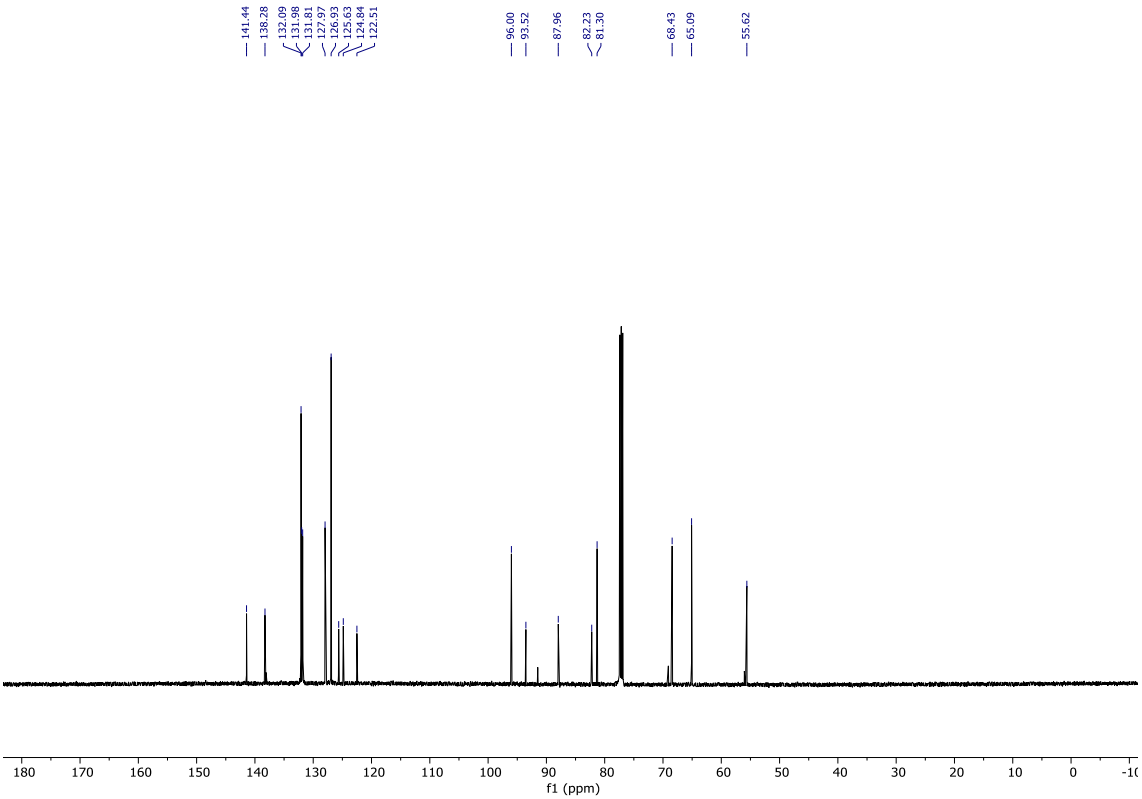
. **^{13}C NMR (126 MHz, $CDCl_3$)** spectrum of compound **S3**



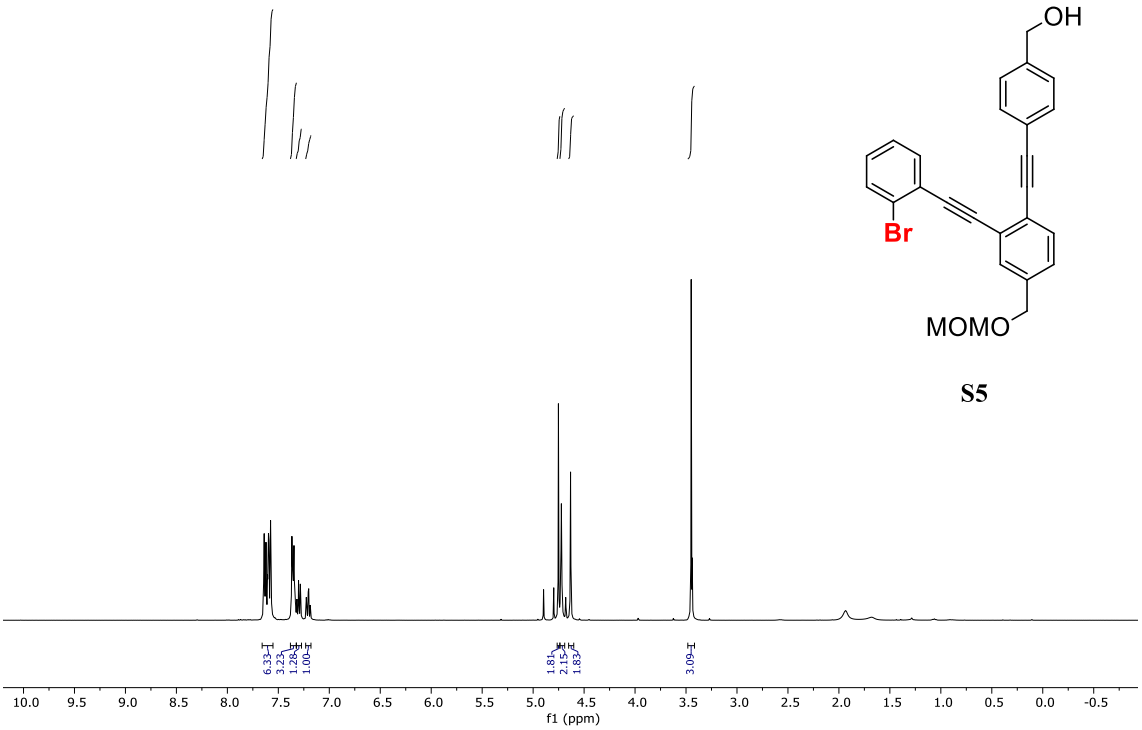
. **^{1}H NMR (500 MHz, $CDCl_3$)** spectrum of compound **S4**



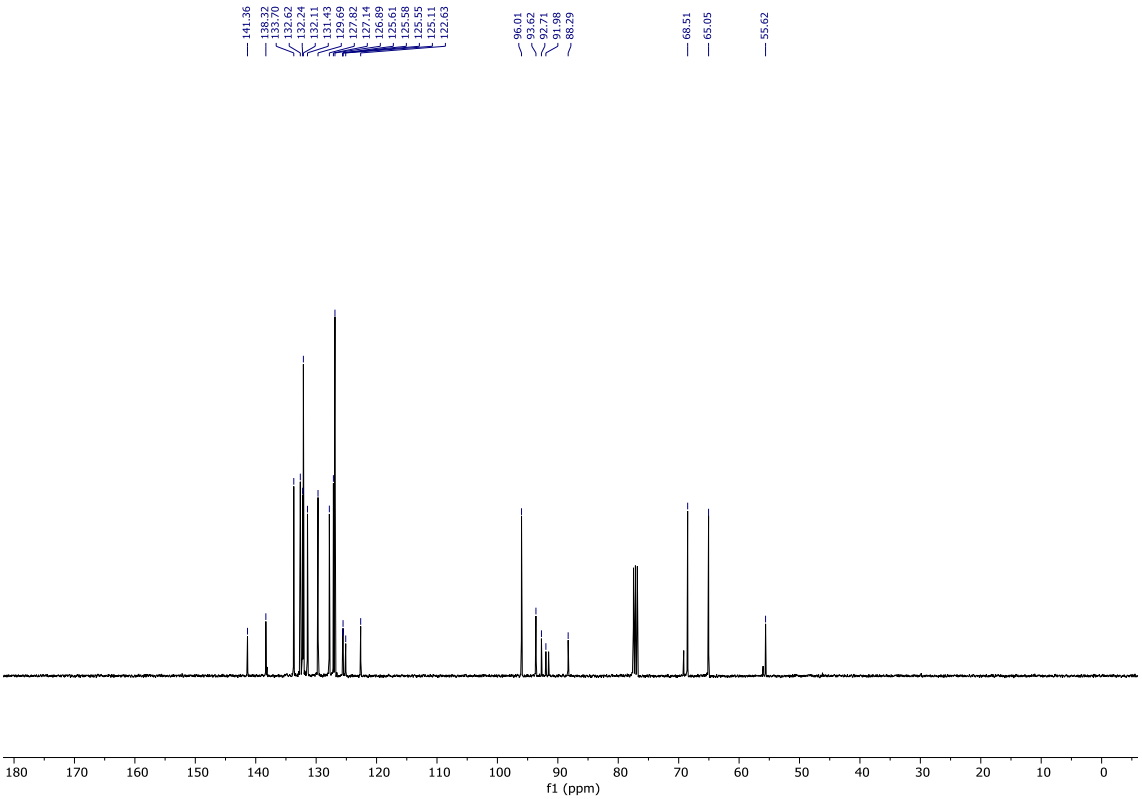
. **^{13}C NMR (126 MHz, $CDCl_3$)** spectrum of compound **S4**



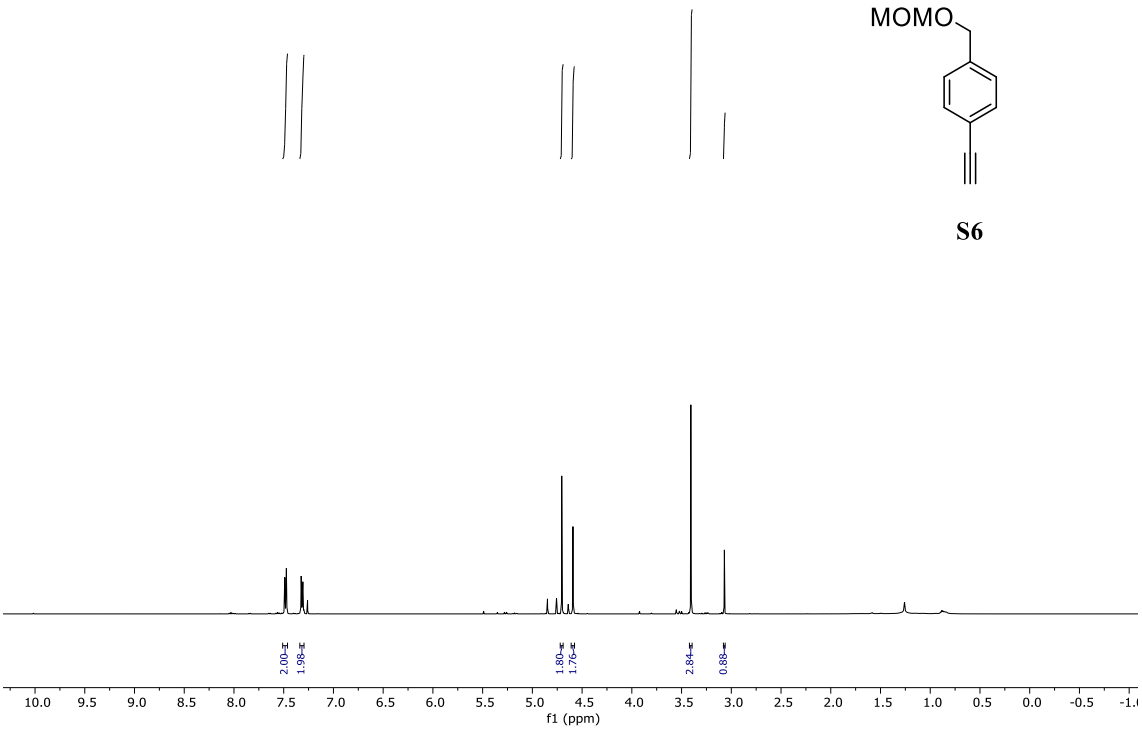
. **^{1}H NMR (500 MHz, $CDCl_3$)** spectrum of compound **S5**



. **^{13}C NMR (126 MHz, $CDCl_3$)** spectrum of compound **S5**

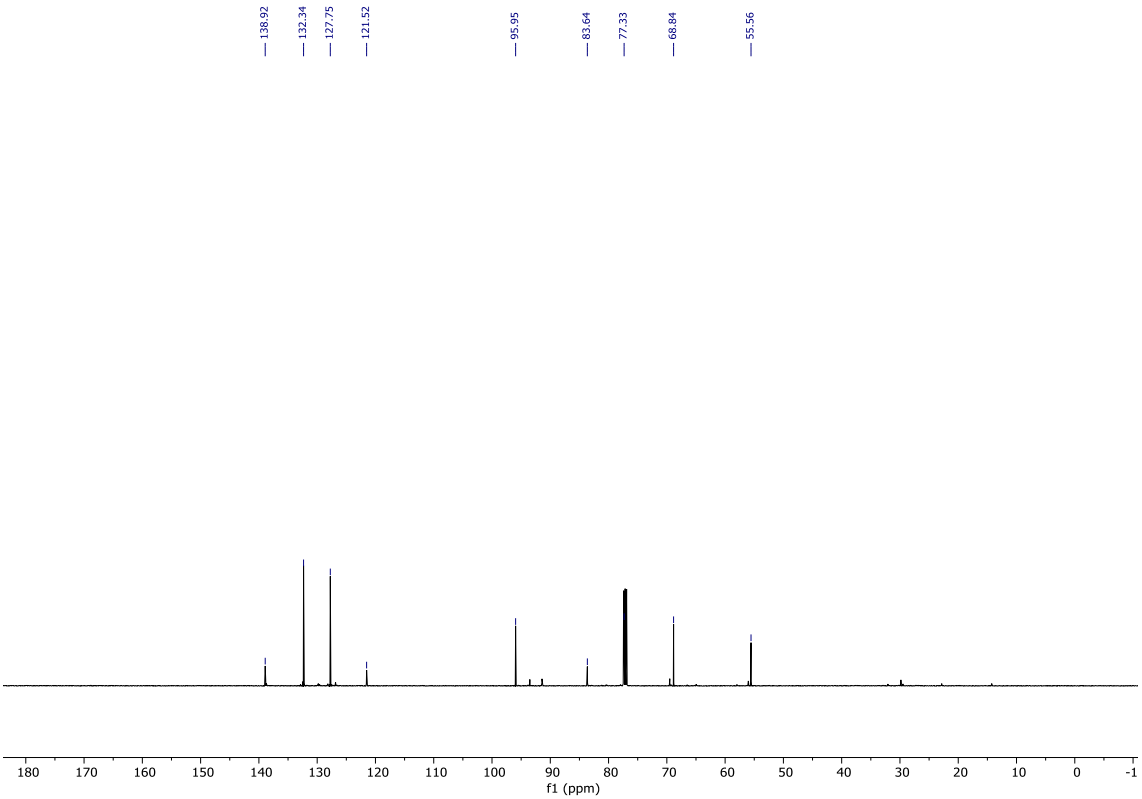


. **^{1}H NMR (500 MHz, $CDCl_3$)** spectrum of compound **S6**

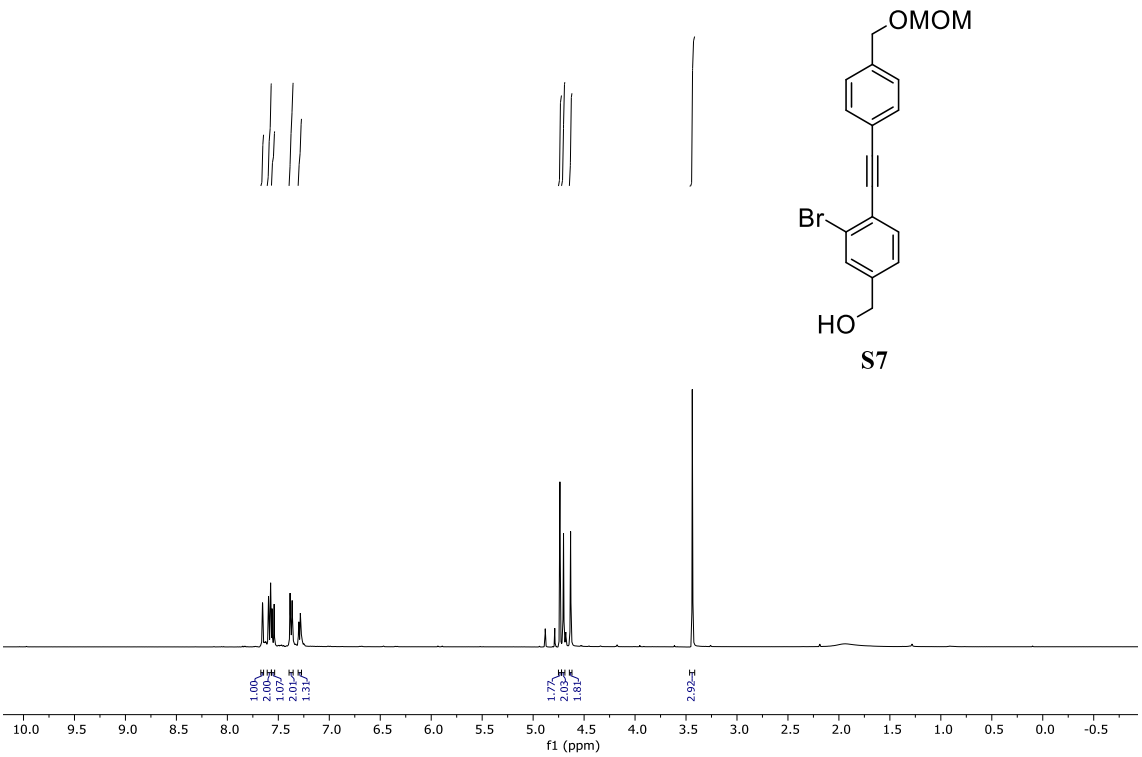


S6

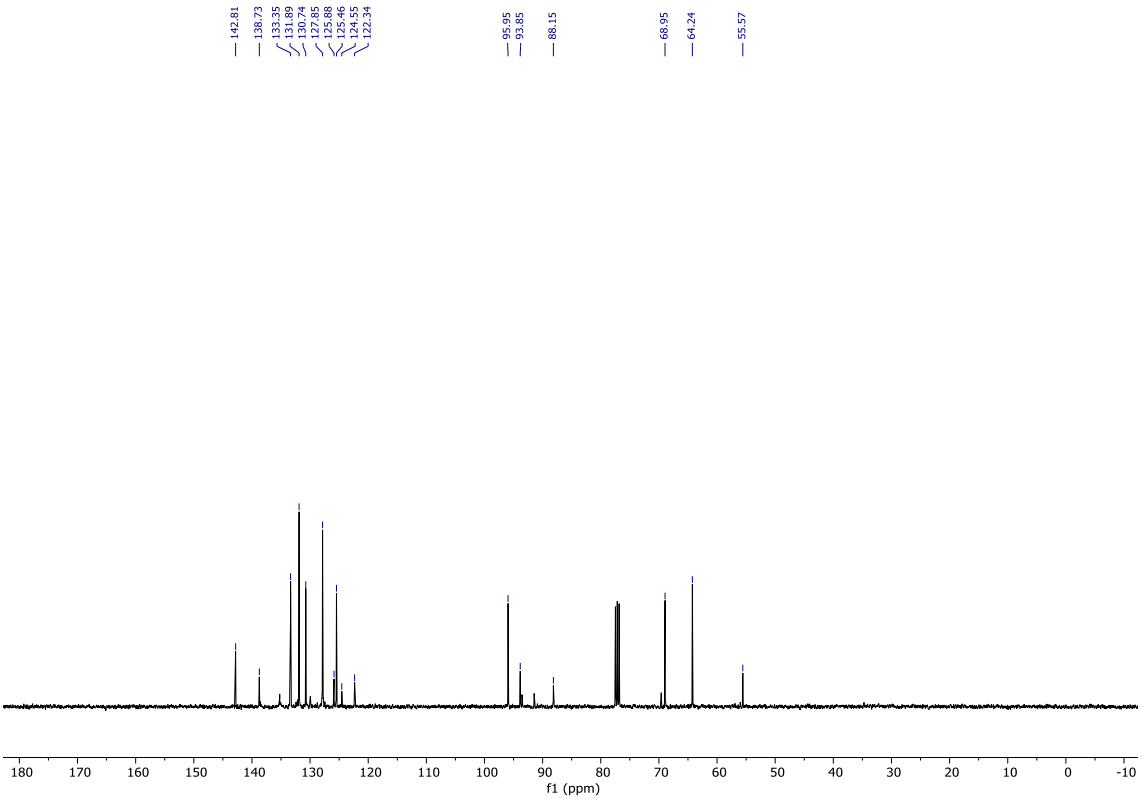
. **^{13}C NMR (126 MHz, $CDCl_3$)** spectrum of compound **S6**



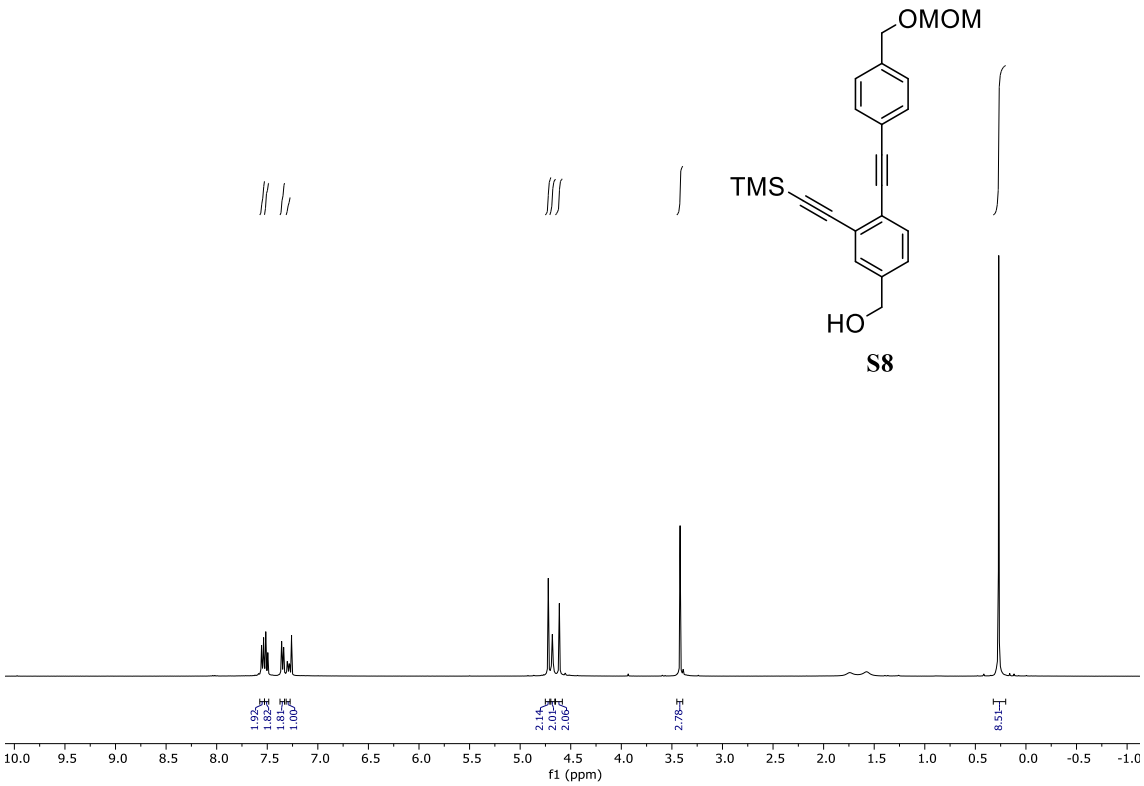
. ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of compound **S7**



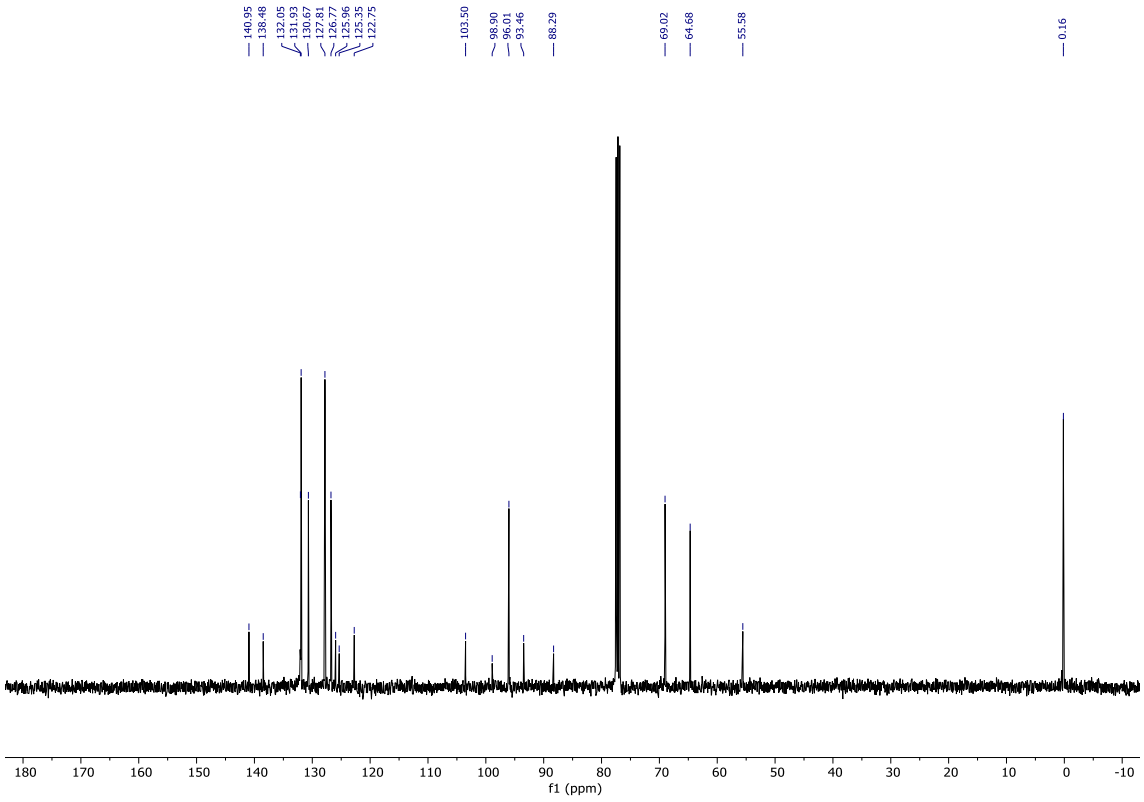
. ^{13}C NMR (126 MHz, $CDCl_3$) spectrum of compound **S7**



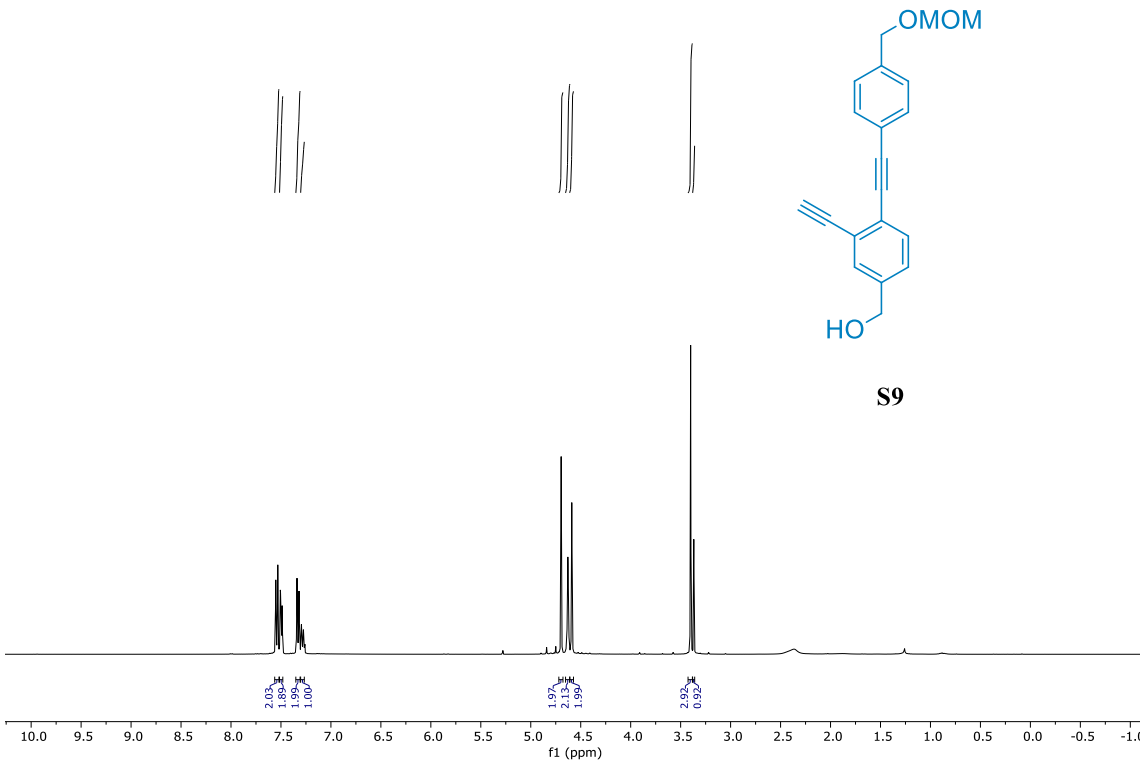
. **^{1}H NMR (500 MHz, $CDCl_3$)** spectrum of compound **S8**



. **^{13}C NMR (126 MHz, $CDCl_3$)** spectrum of compound **S8**

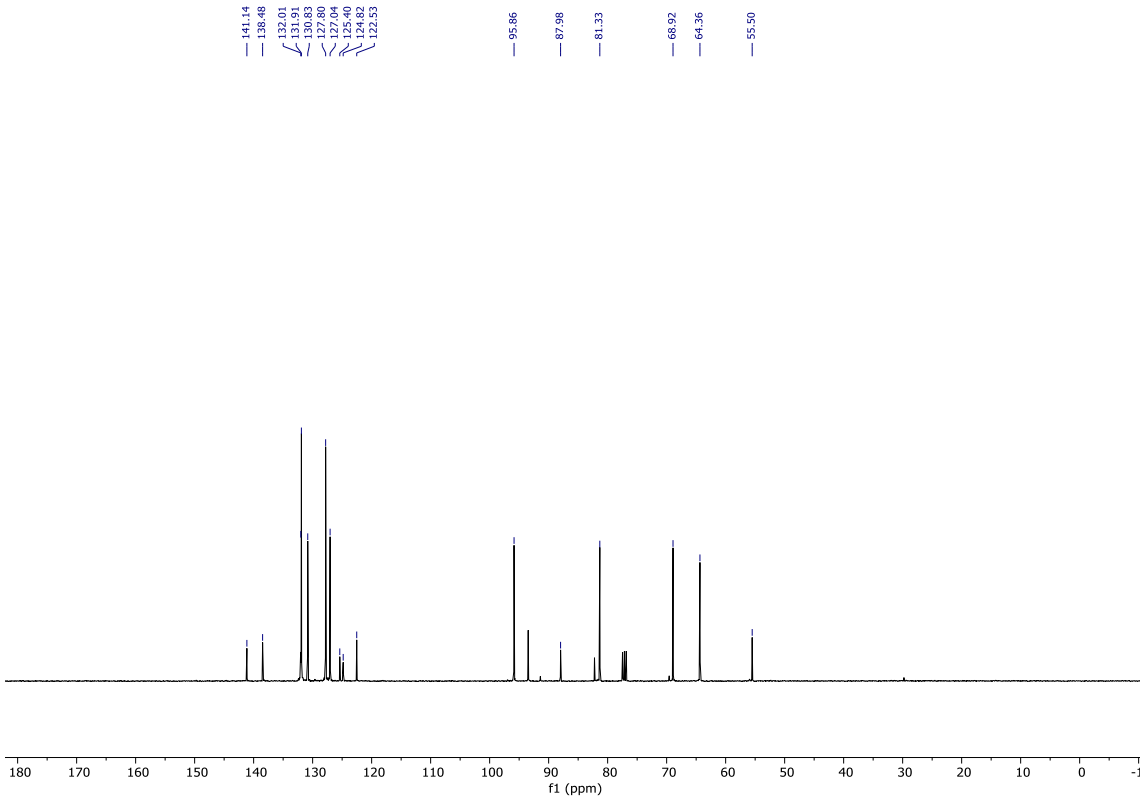


. **^{1}H NMR (500 MHz, $CDCl_3$)** spectrum of compound **S9**

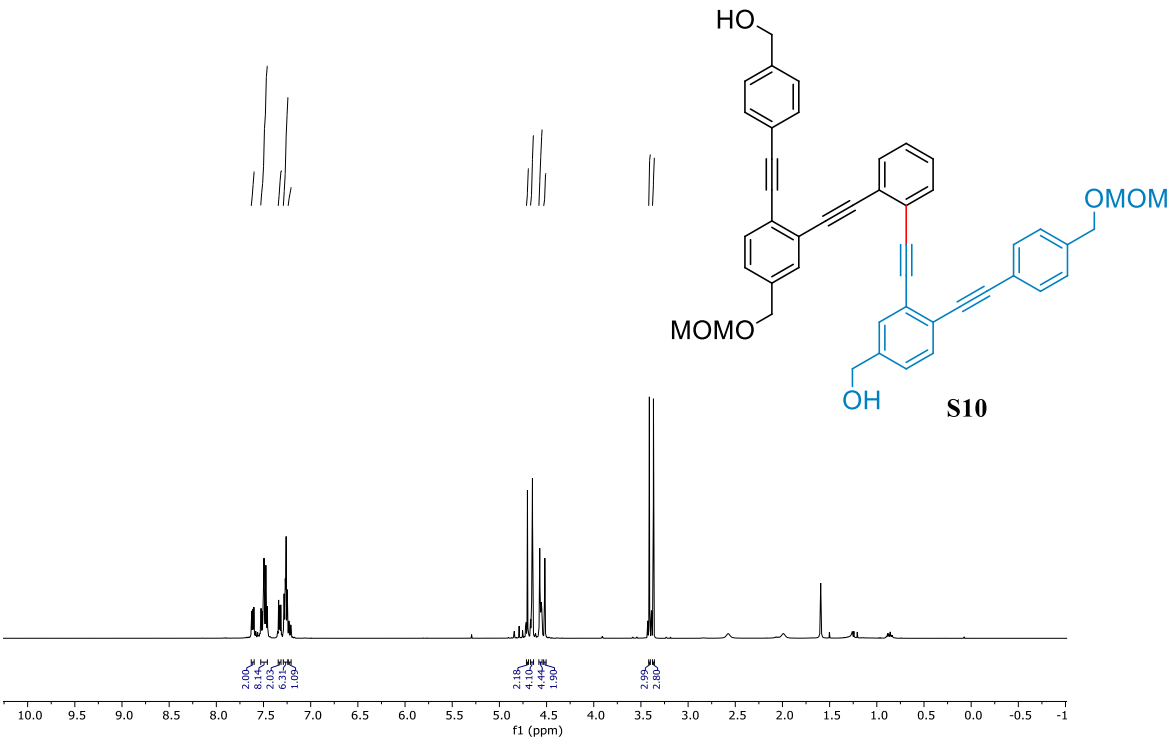


S9

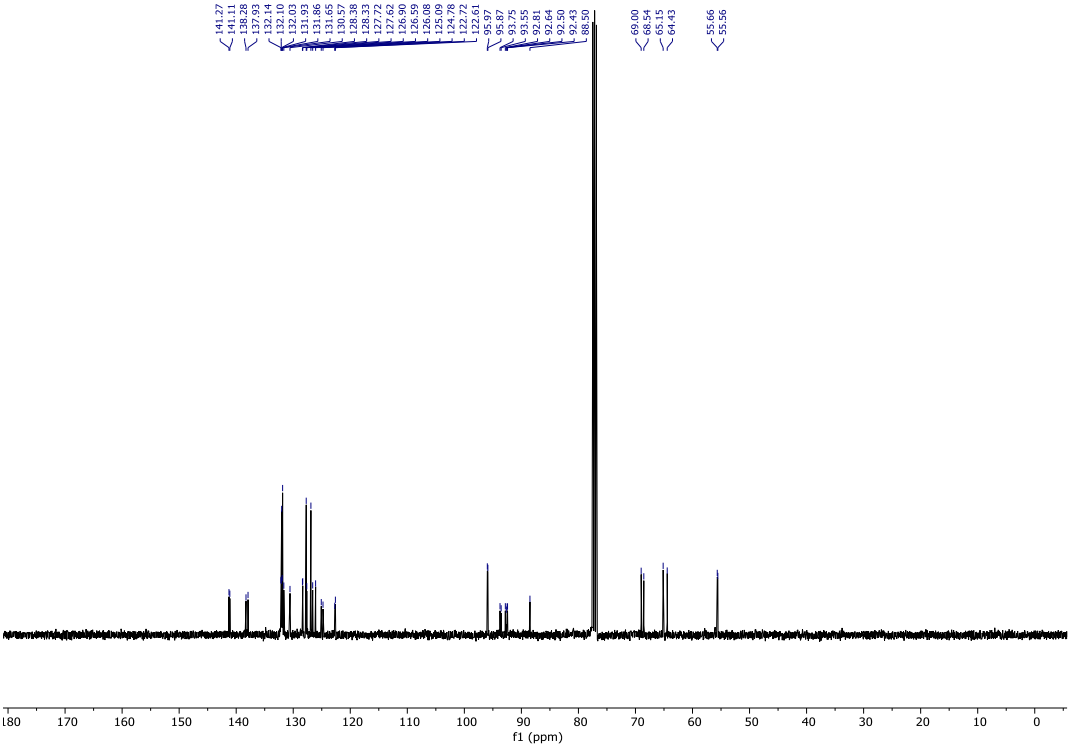
. **^{13}C NMR (126 MHz, $CDCl_3$)** spectrum of compound **S9**



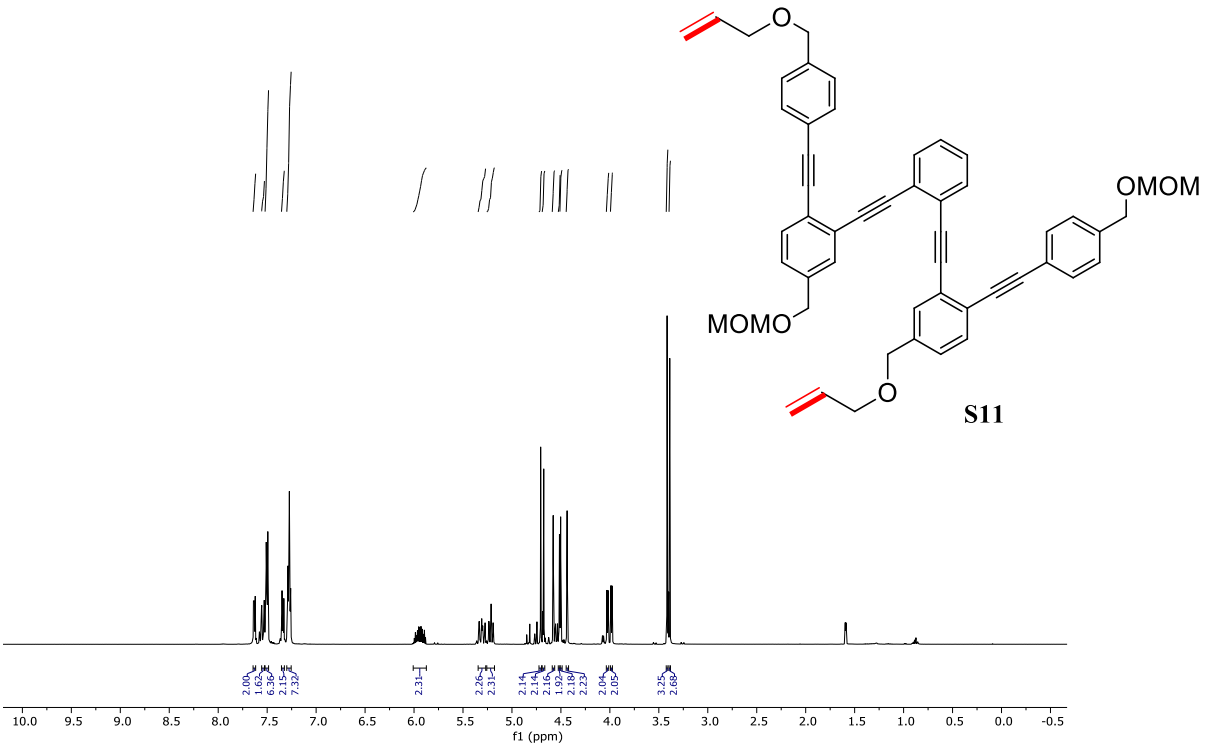
. **^{1}H NMR (500 MHz, $CDCl_3$)** spectrum of compound **S10**



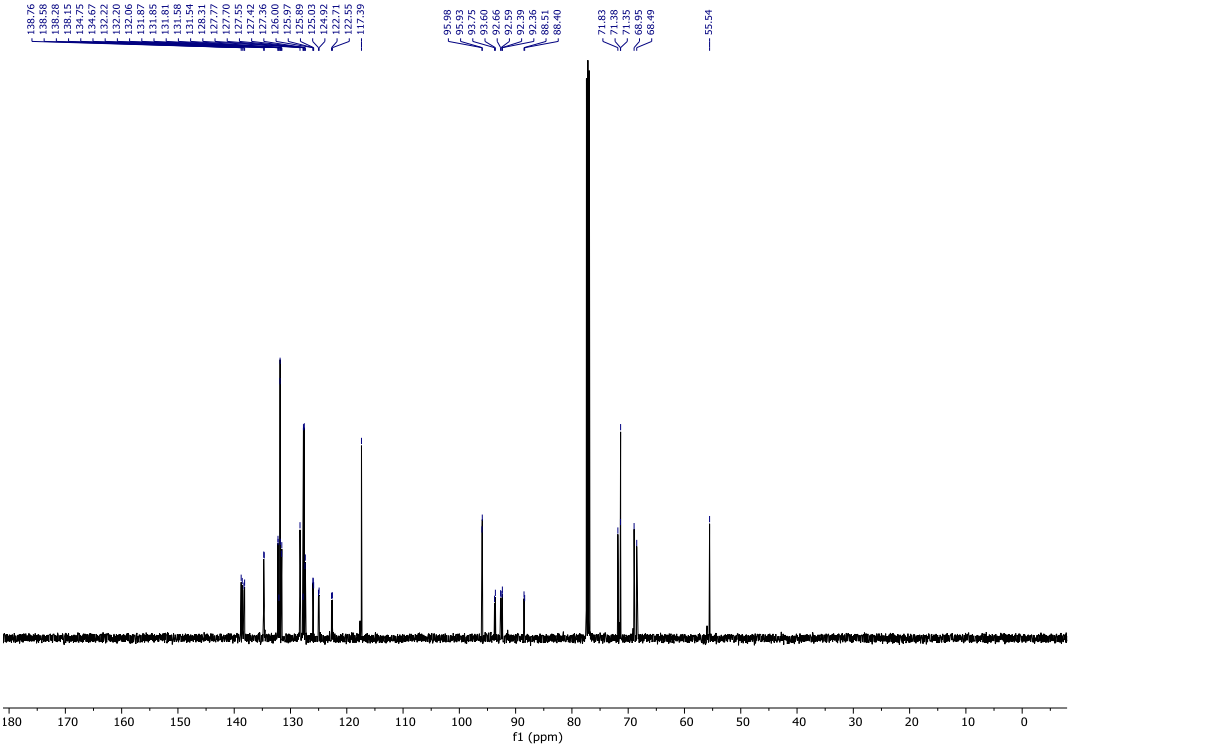
. **^{13}C NMR (126 MHz, $CDCl_3$)** spectrum of compound **S10**



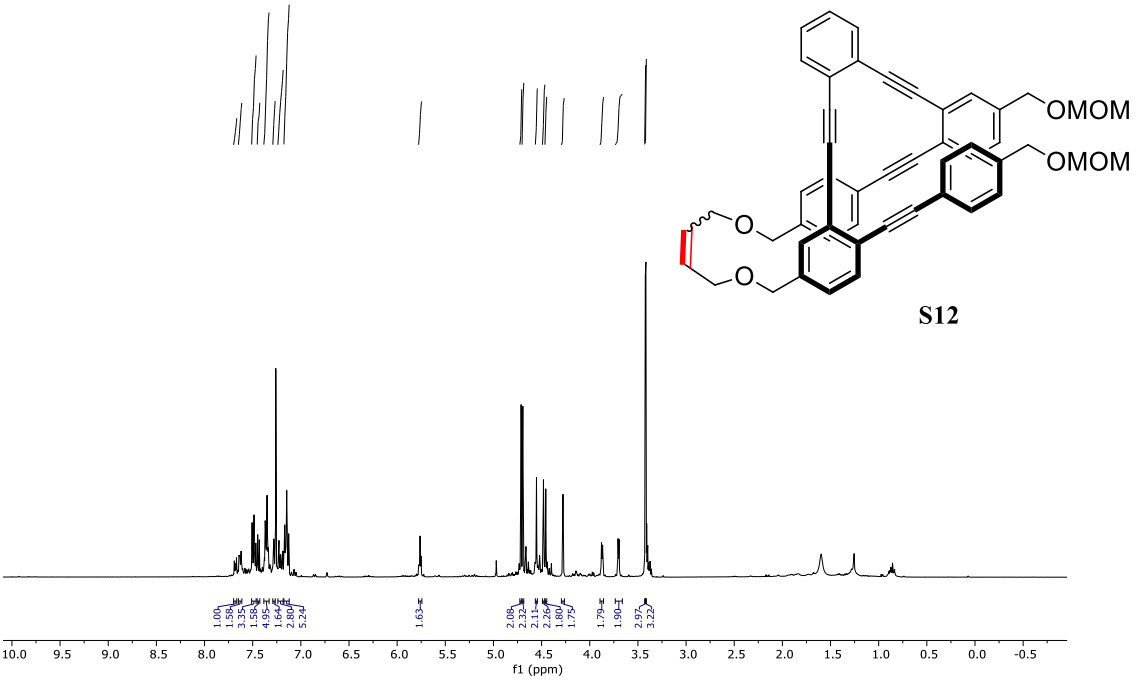
. **^{1}H NMR (500 MHz, $CDCl_3$)** spectrum of compound **S11**



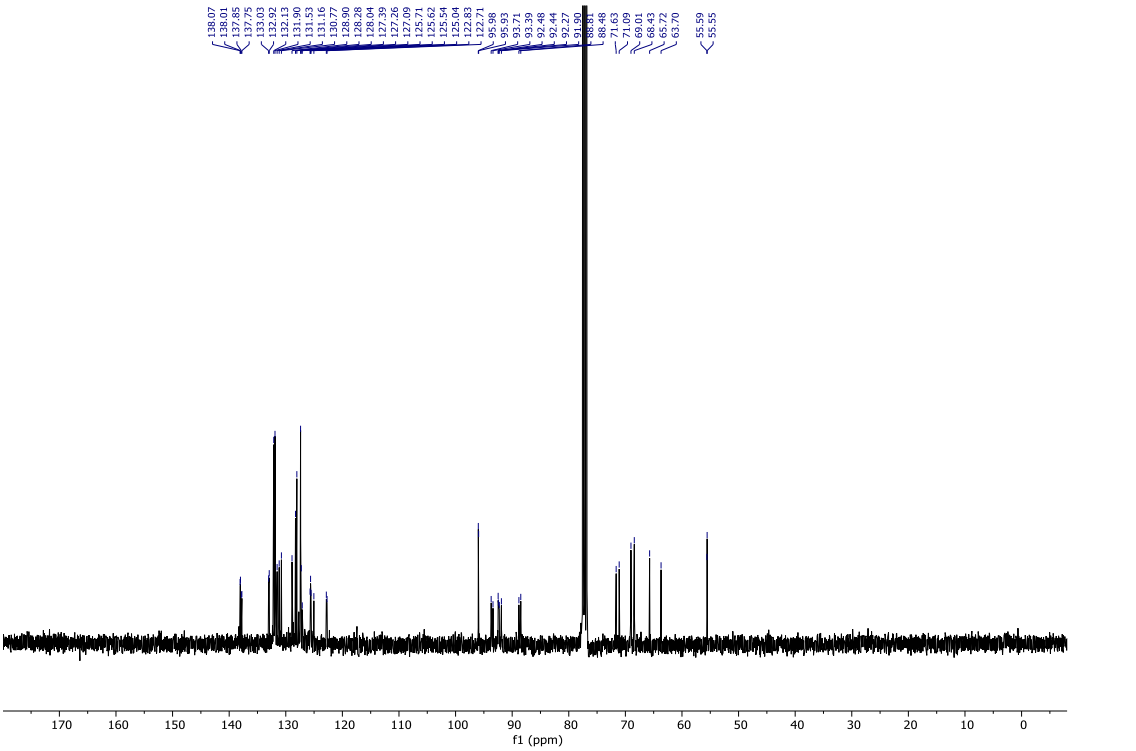
. **^{13}C NMR (126 MHz, $CDCl_3$)** spectrum of compound **S11**



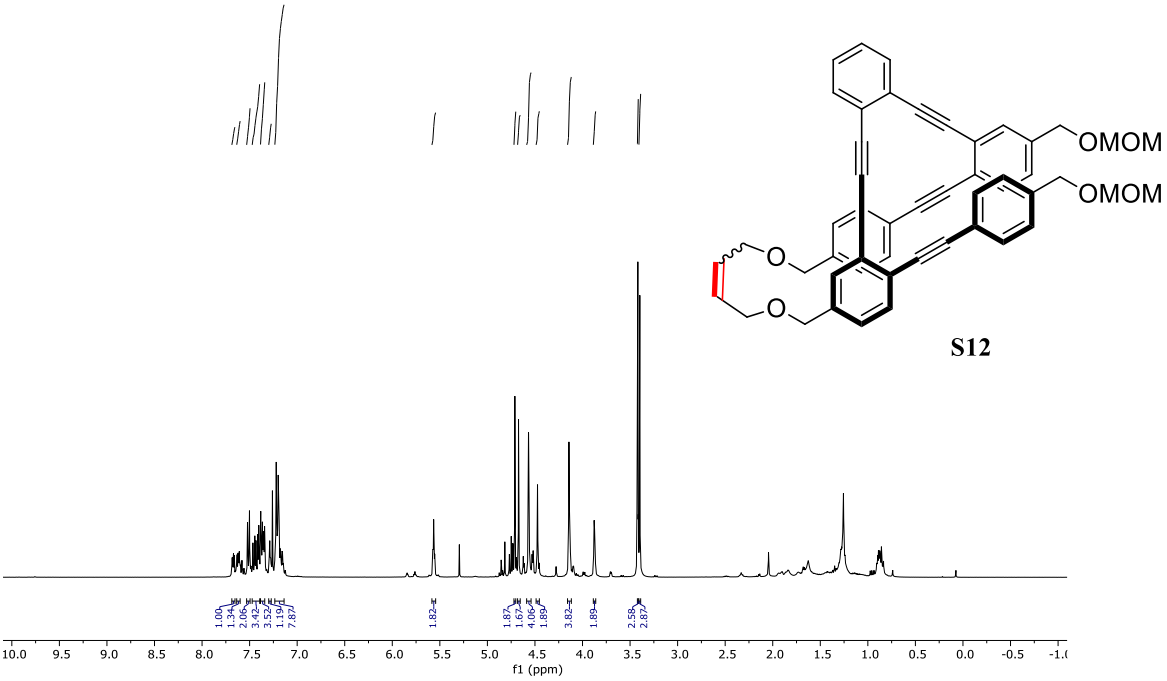
. **^{1}H NMR (500 MHz, $CDCl_3$)** spectrum of major isomer of compound **S12**



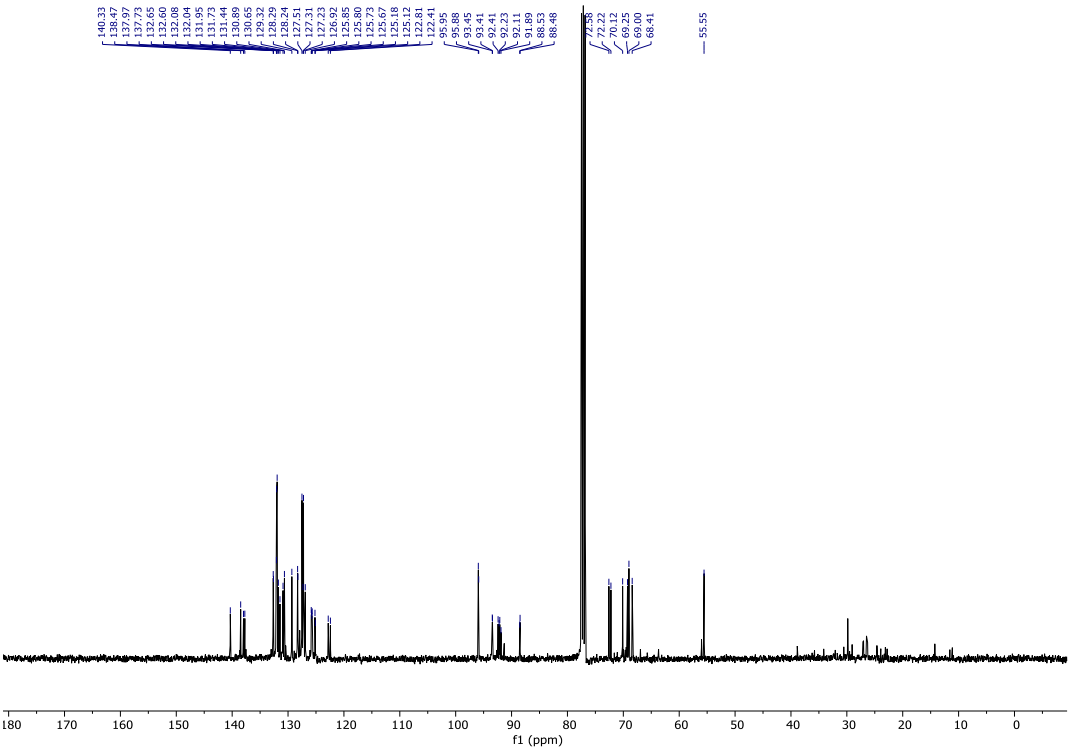
. **^{13}C NMR (126 MHz, $CDCl_3$)** spectrum of major isomer of compound **S12**



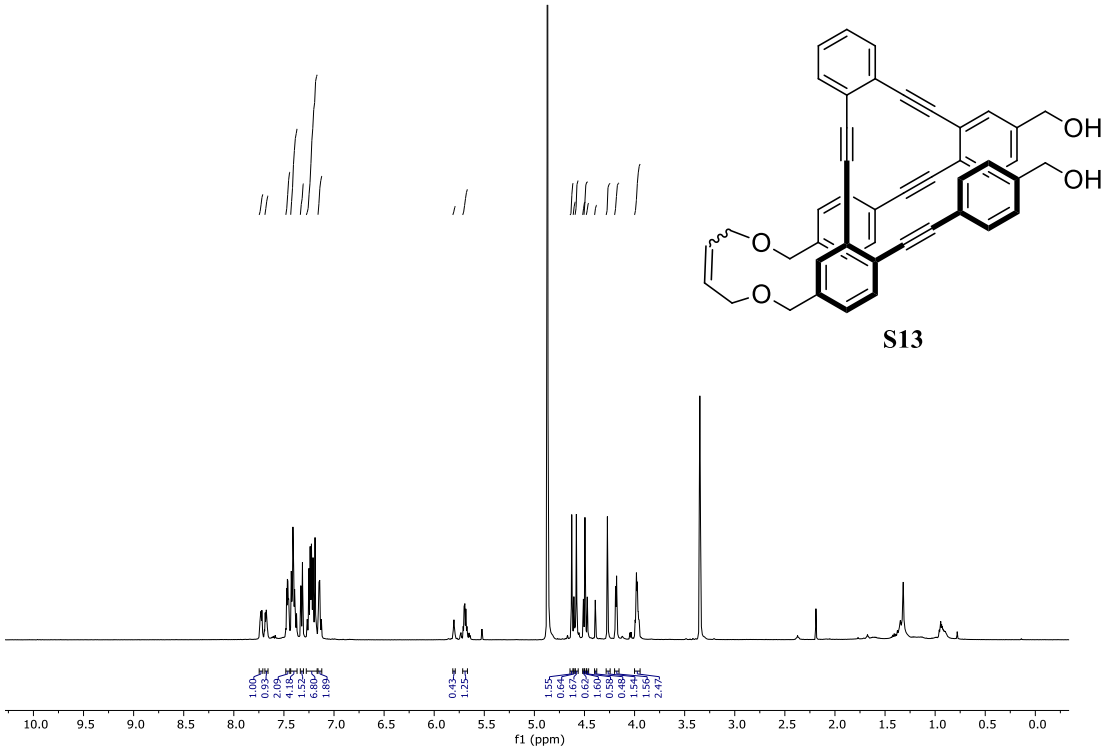
. **^{1}H NMR (500 MHz, $CDCl_3$)** spectrum of the minor isomer of compound **S12**



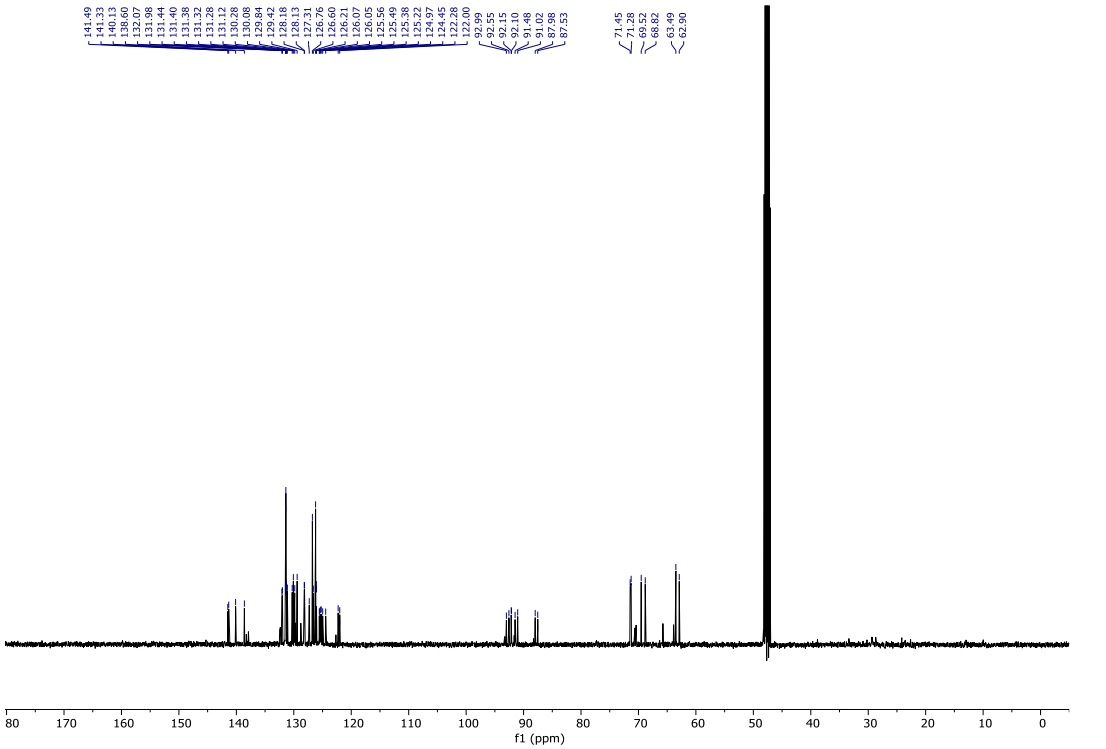
. **^{13}C NMR (126 MHz, $CDCl_3$)** spectrum of the minor isomer of compound **S12**



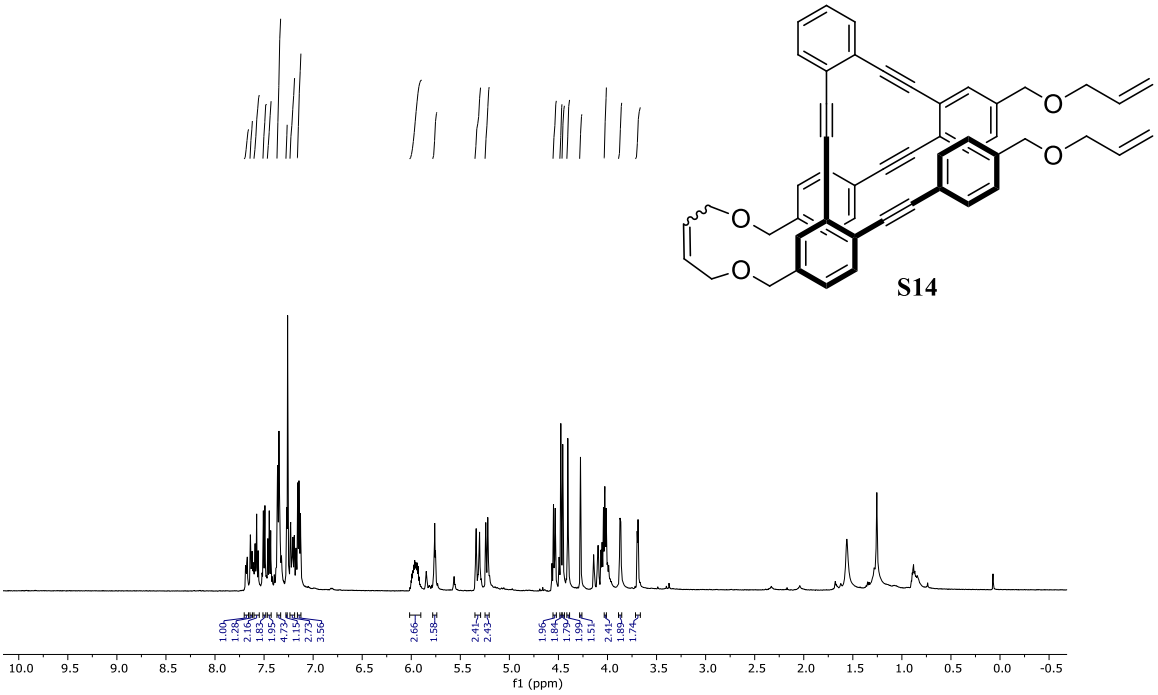
. ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of compound **S13**



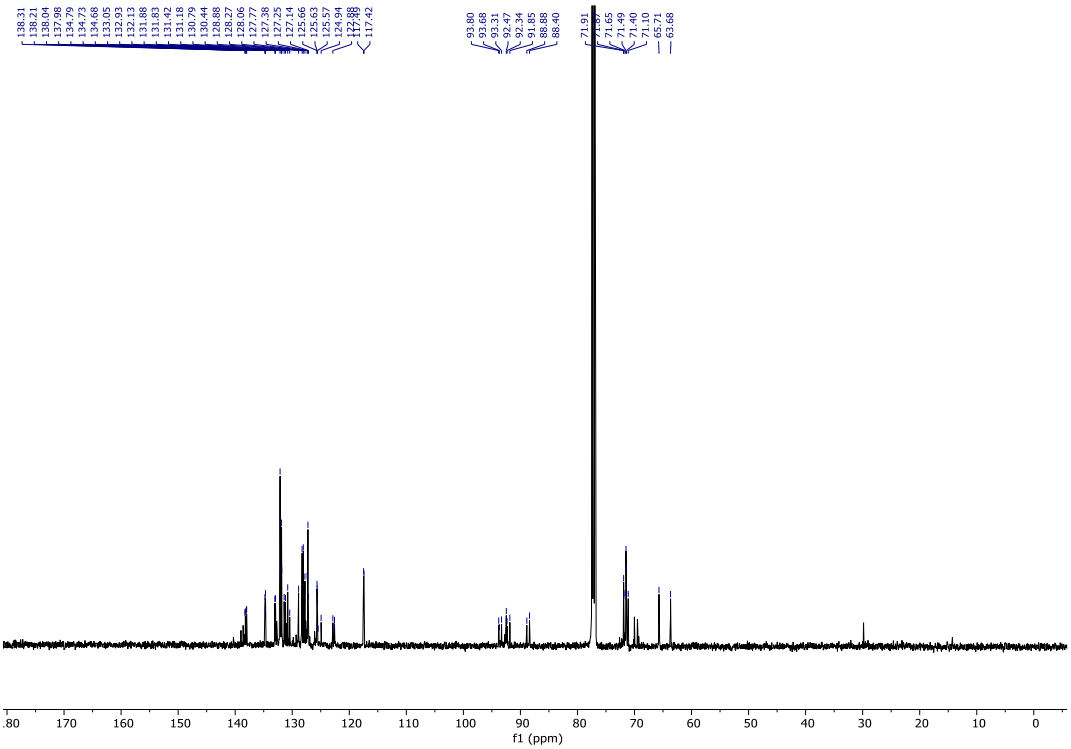
. ^{13}C NMR (126 MHz, $CDCl_3$) spectrum of compound **S13**



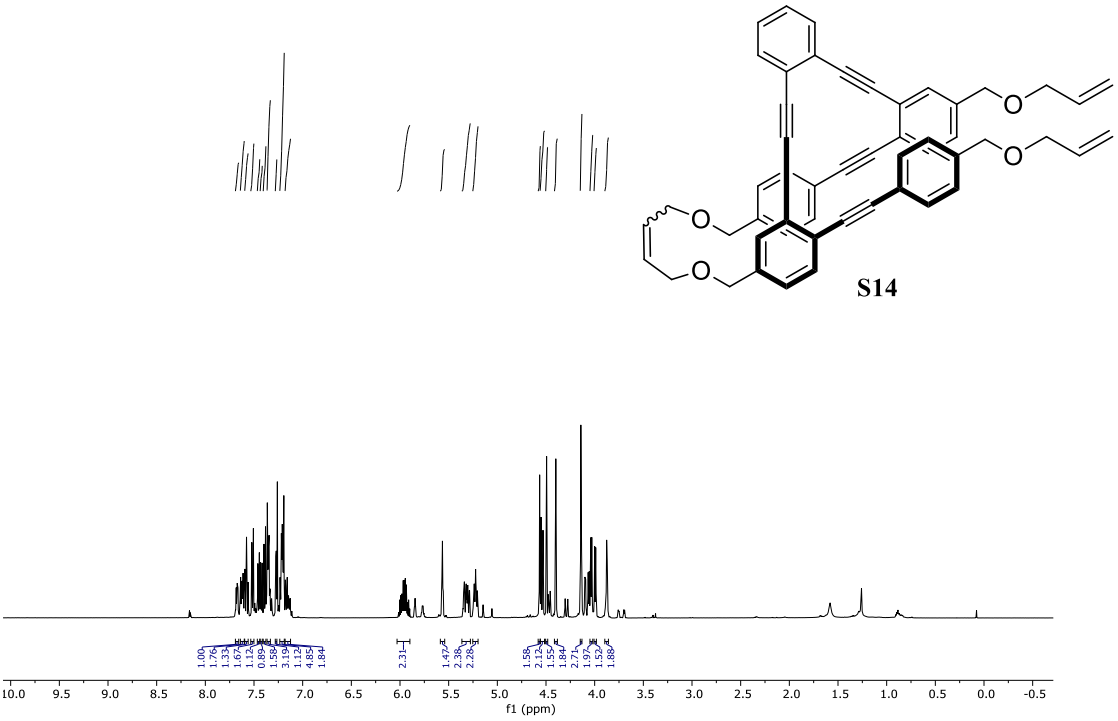
. **^{1}H NMR (500 MHz, $CDCl_3$)** spectrum of major isomer of compound **S14**



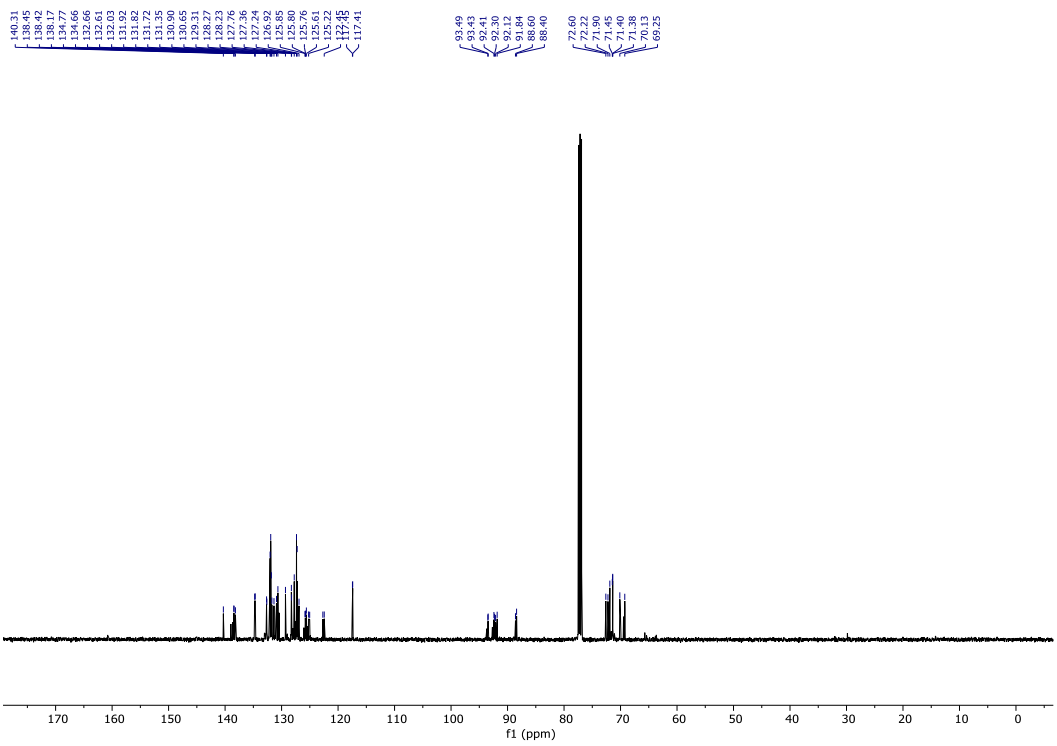
. **^{13}C NMR (126 MHz, $CDCl_3$)** spectrum of major isomer of compound **S14**



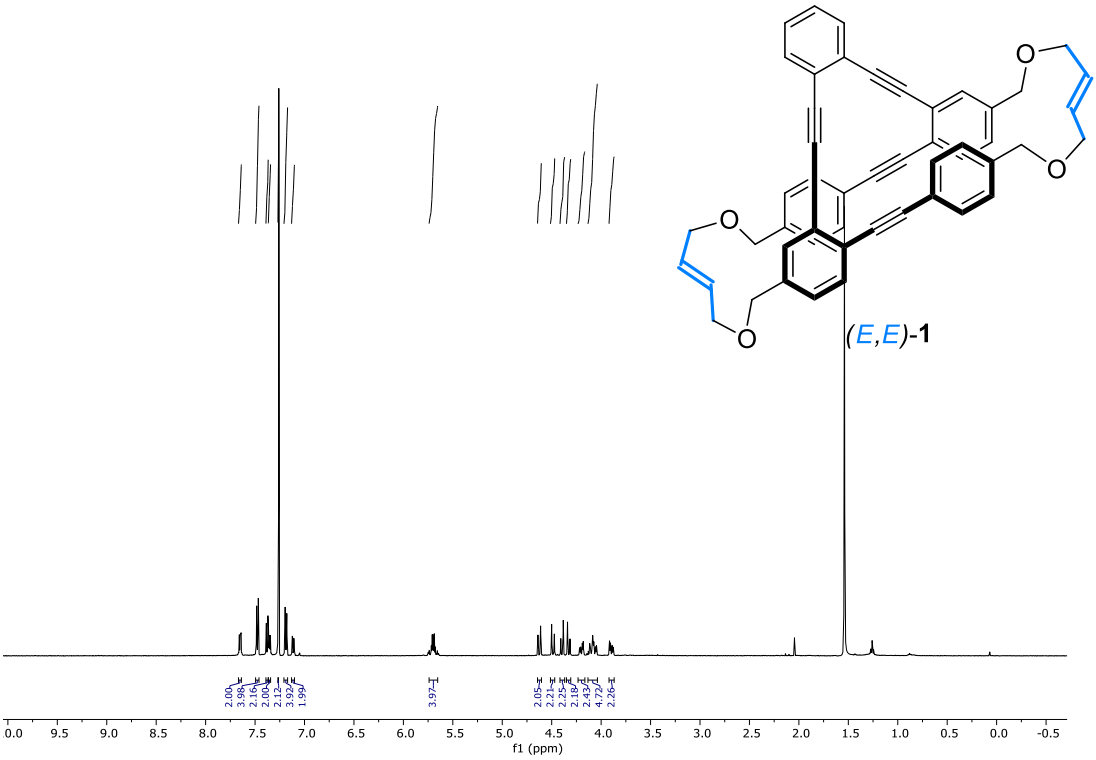
. **^{1}H NMR (500 MHz, $CDCl_3$)** spectrum of minor isomer of compound **S14**



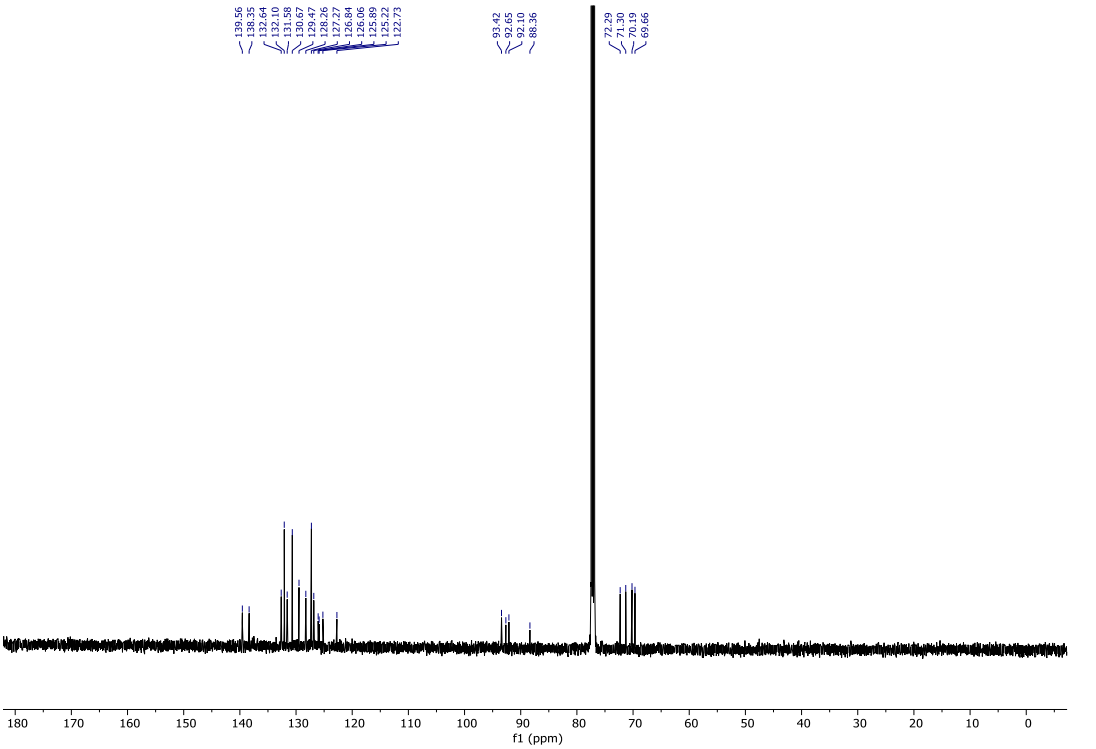
. **^{13}C NMR (126 MHz, $CDCl_3$)** spectrum of minor isomer of compound **S14**



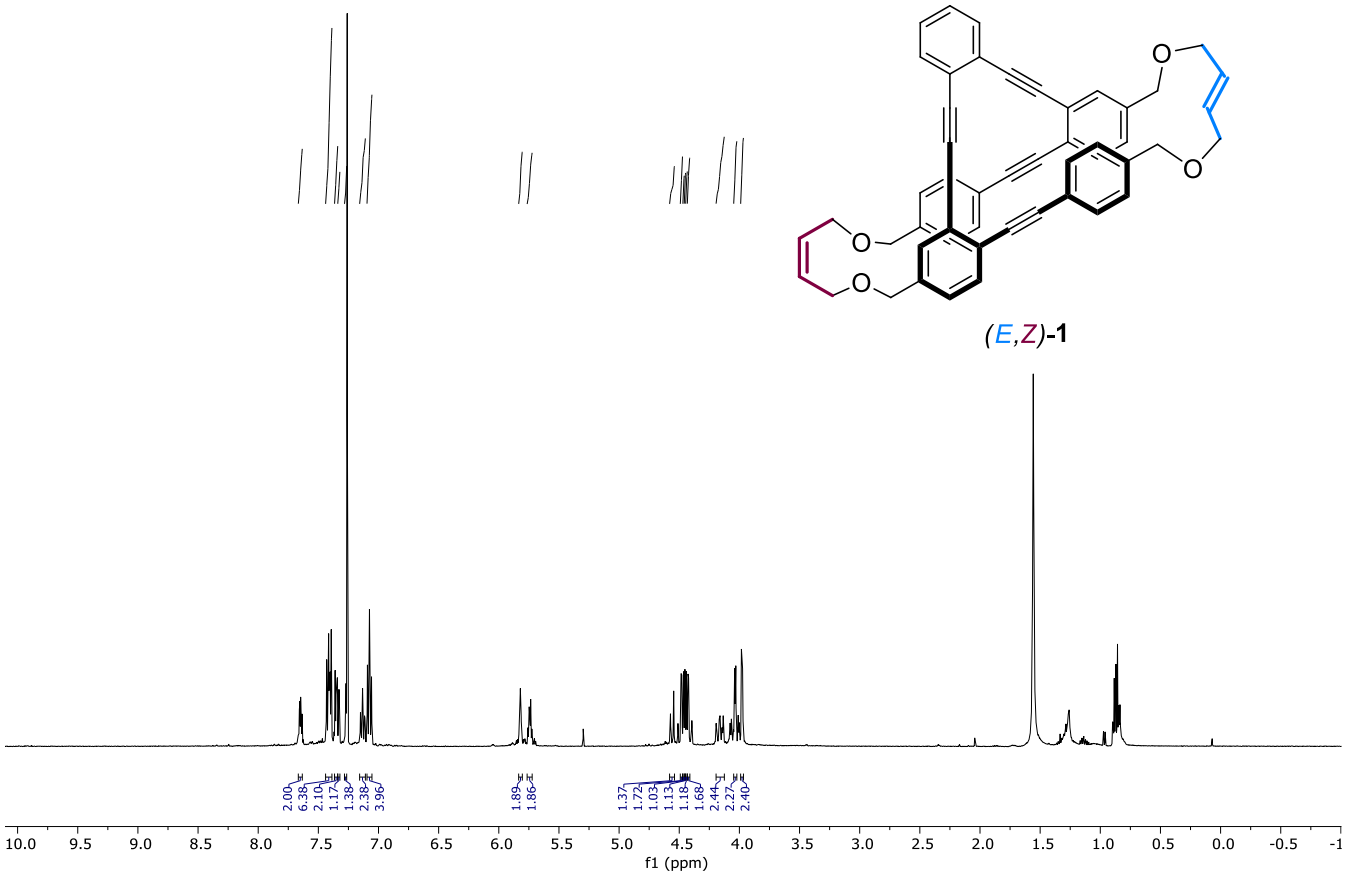
. **^{1}H NMR (500 MHz, $CDCl_3$)** spectrum of compound **(*E*,*E*)-1**



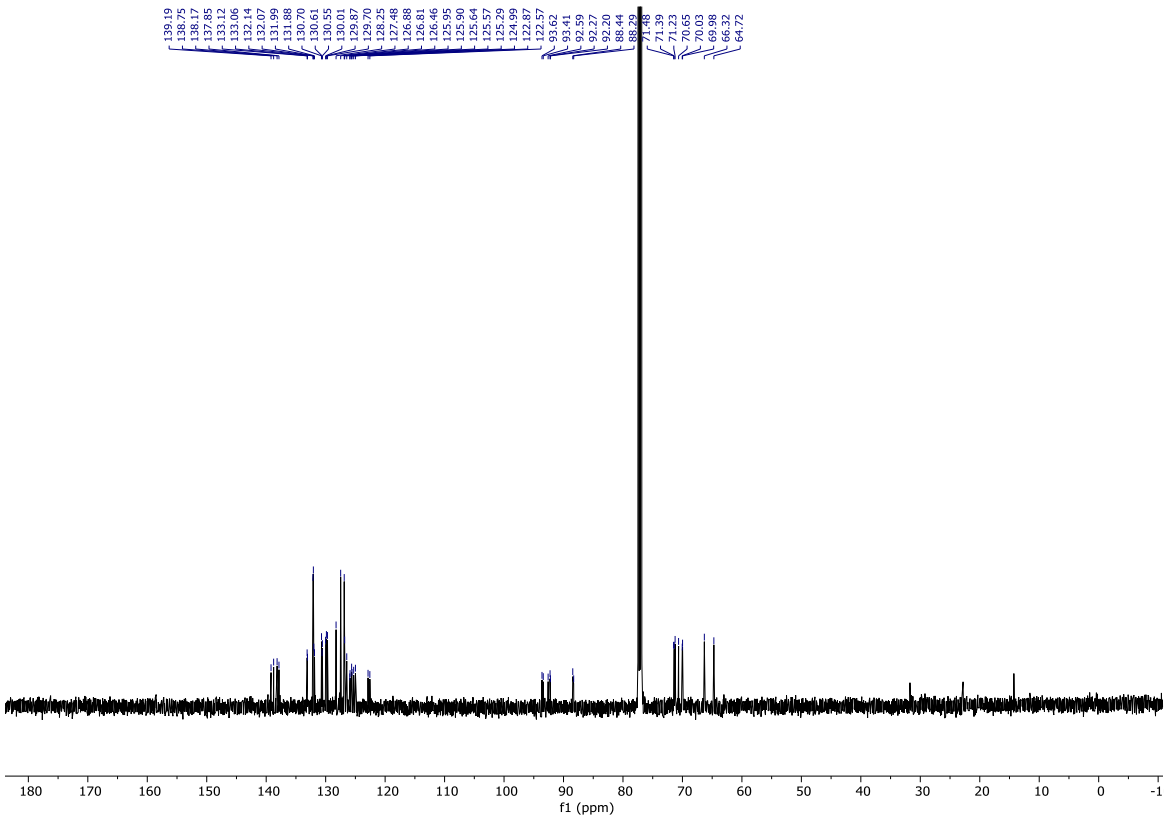
. **^{13}C NMR (126 MHz, $CDCl_3$)** spectrum of compound **(*E*,*E*)-1**



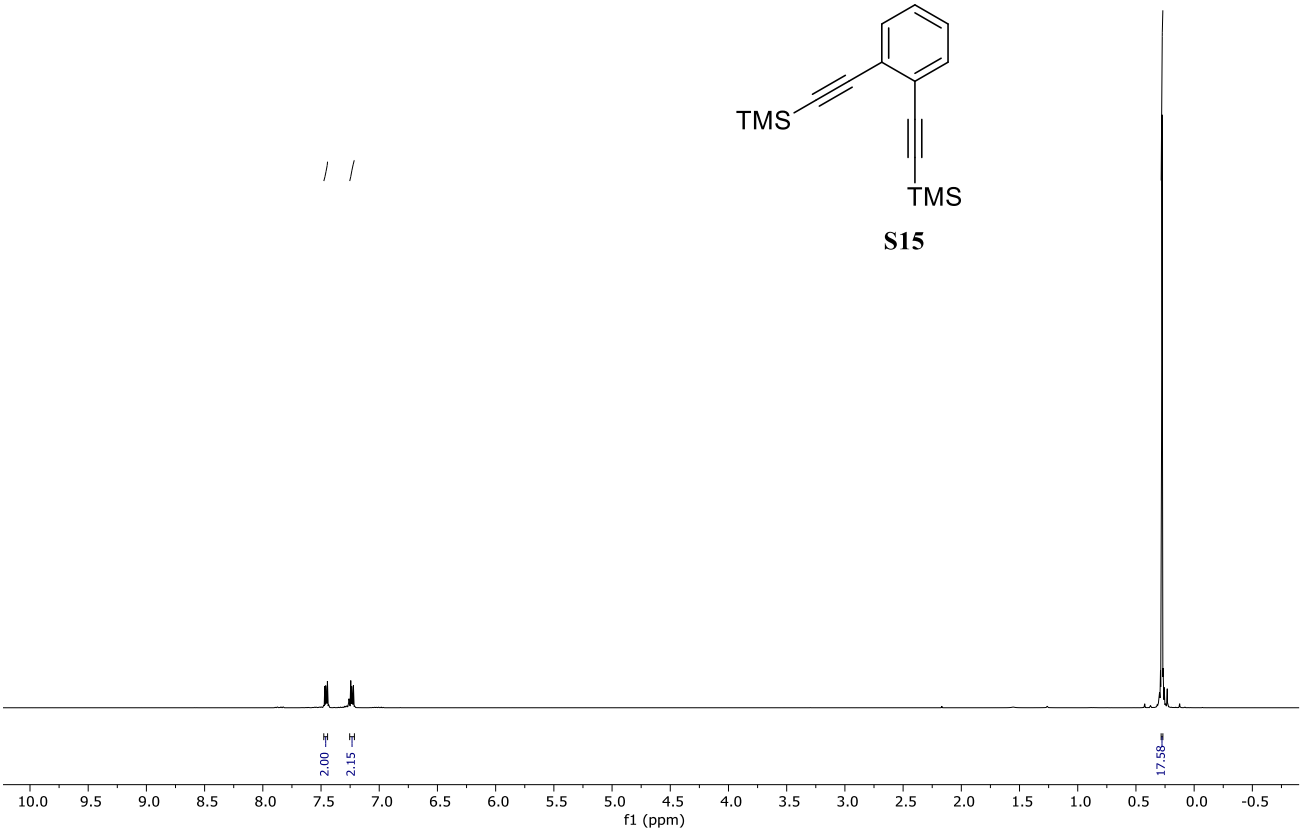
. **^{1}H NMR (500 MHz, $CDCl_3$)** spectrum of compound **(*E*,*Z*)-1**



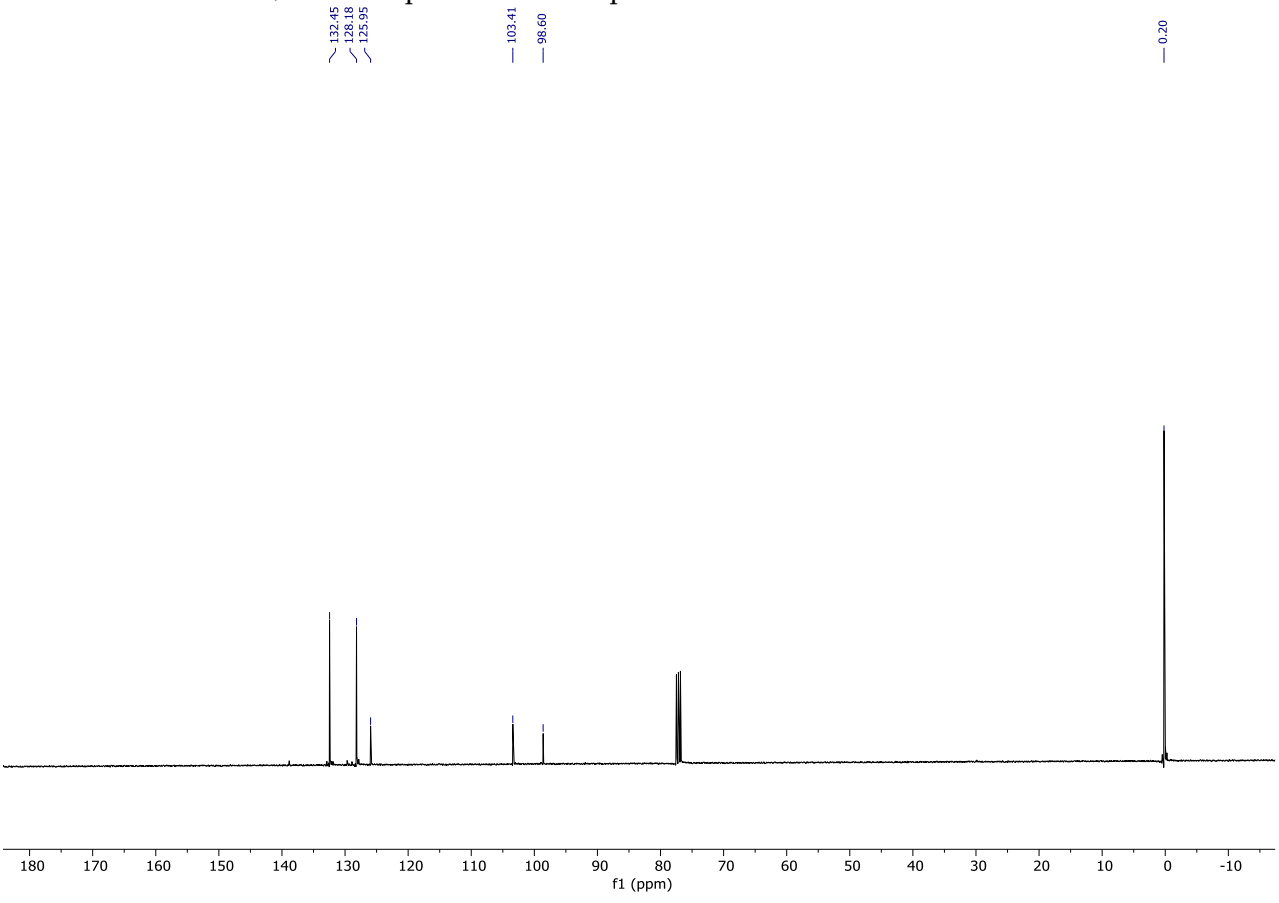
. **^{13}C NMR (126 MHz, $CDCl_3$)** spectrum of compound **(*E*,*Z*)-1**



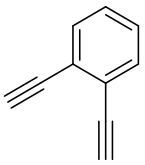
^{1}H NMR (500 MHz, $CDCl_3$) spectrum of compound **S15**



. **^{13}C NMR (126 MHz, $CDCl_3$)** spectrum of compound **S15**

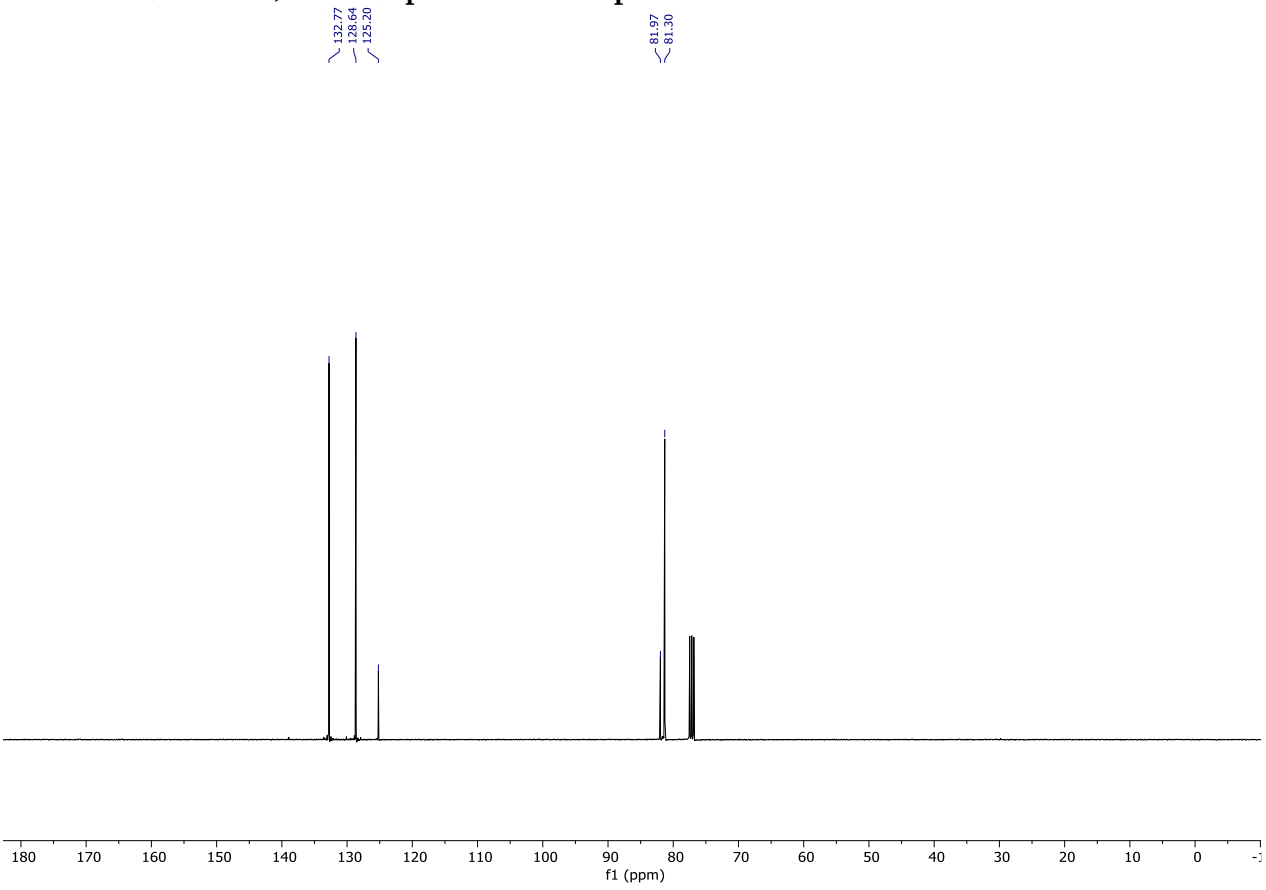


^{1}H NMR (500 MHz, $CDCl_3$) spectrum of compound S16

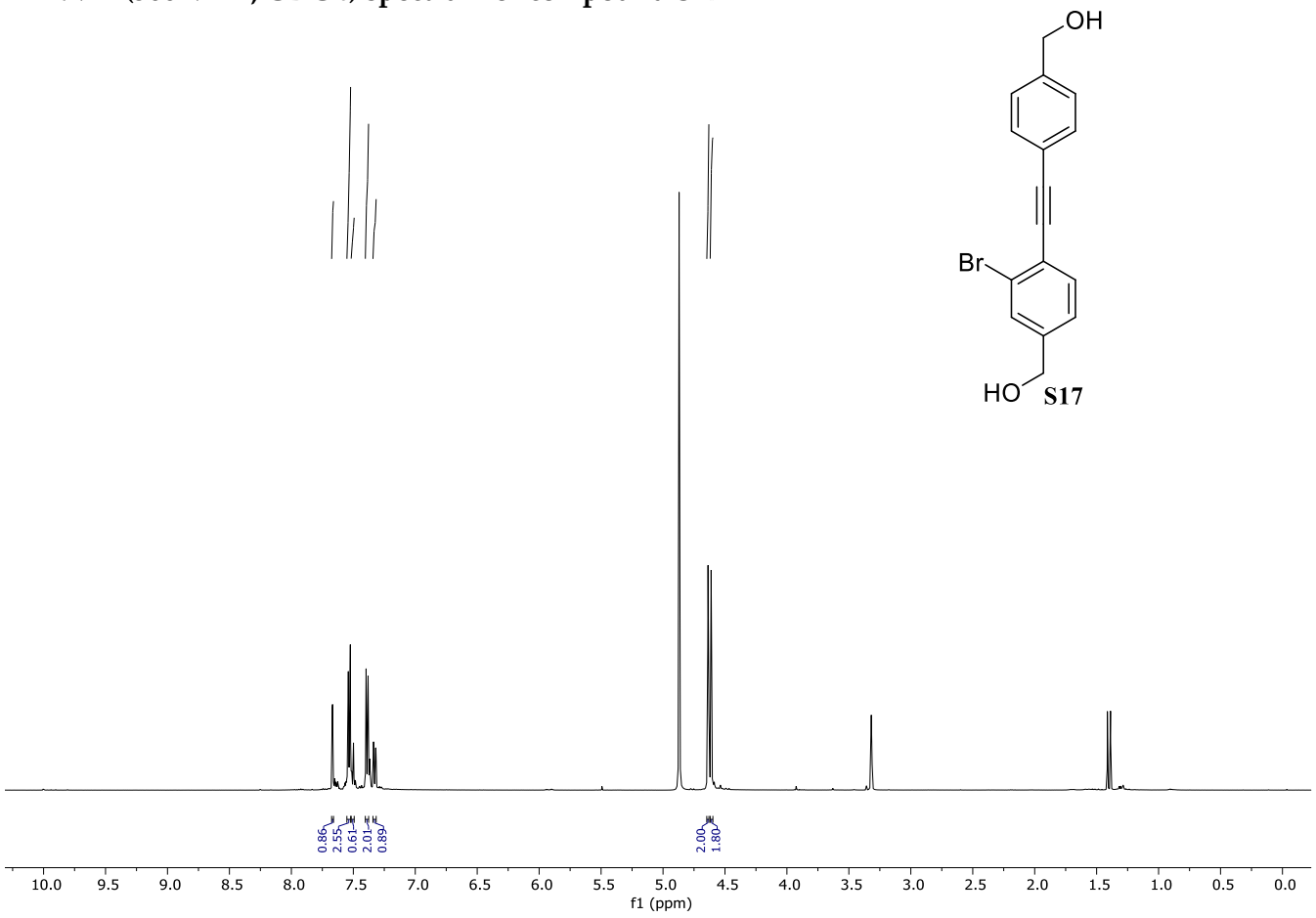


S16

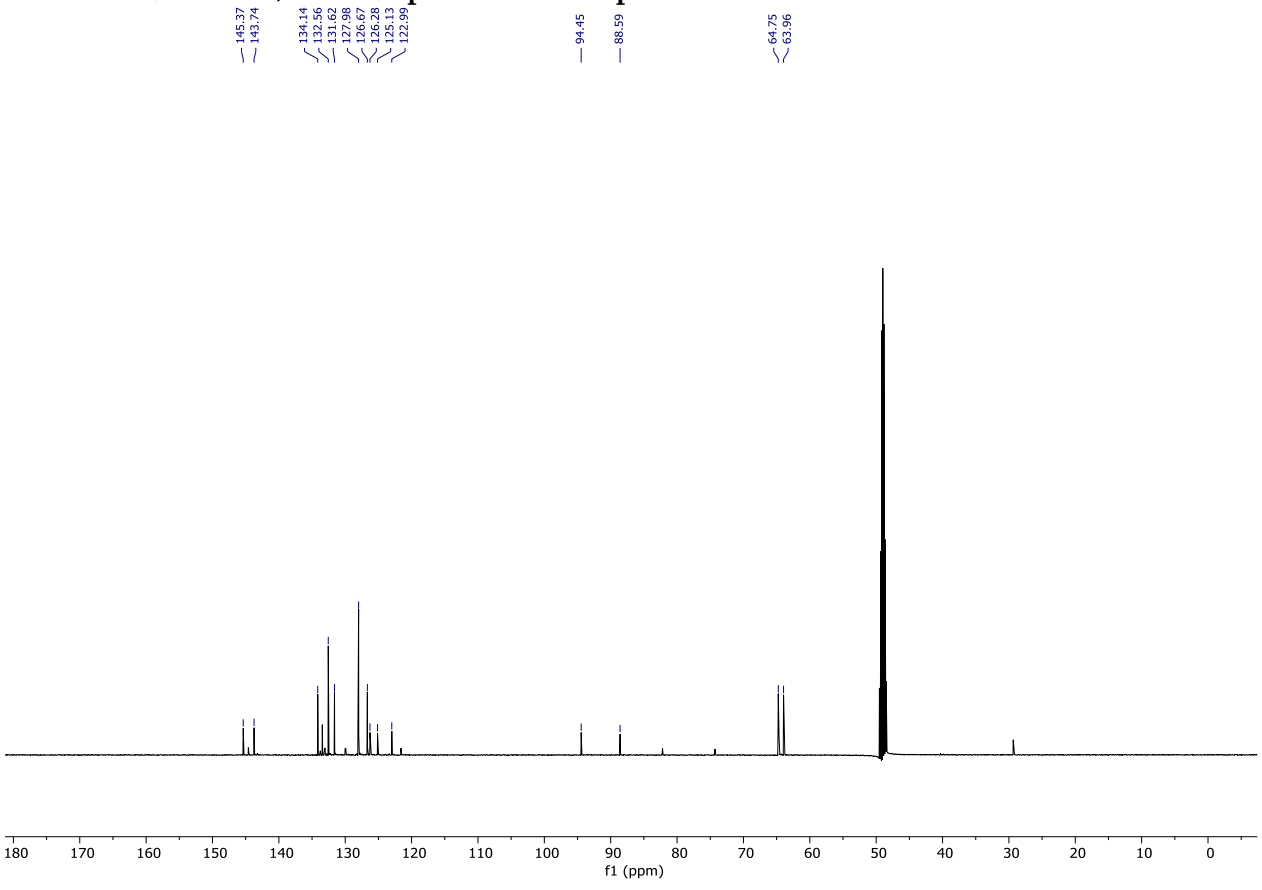
. ^{13}C NMR (126 MHz, $CDCl_3$) spectrum of compound S16



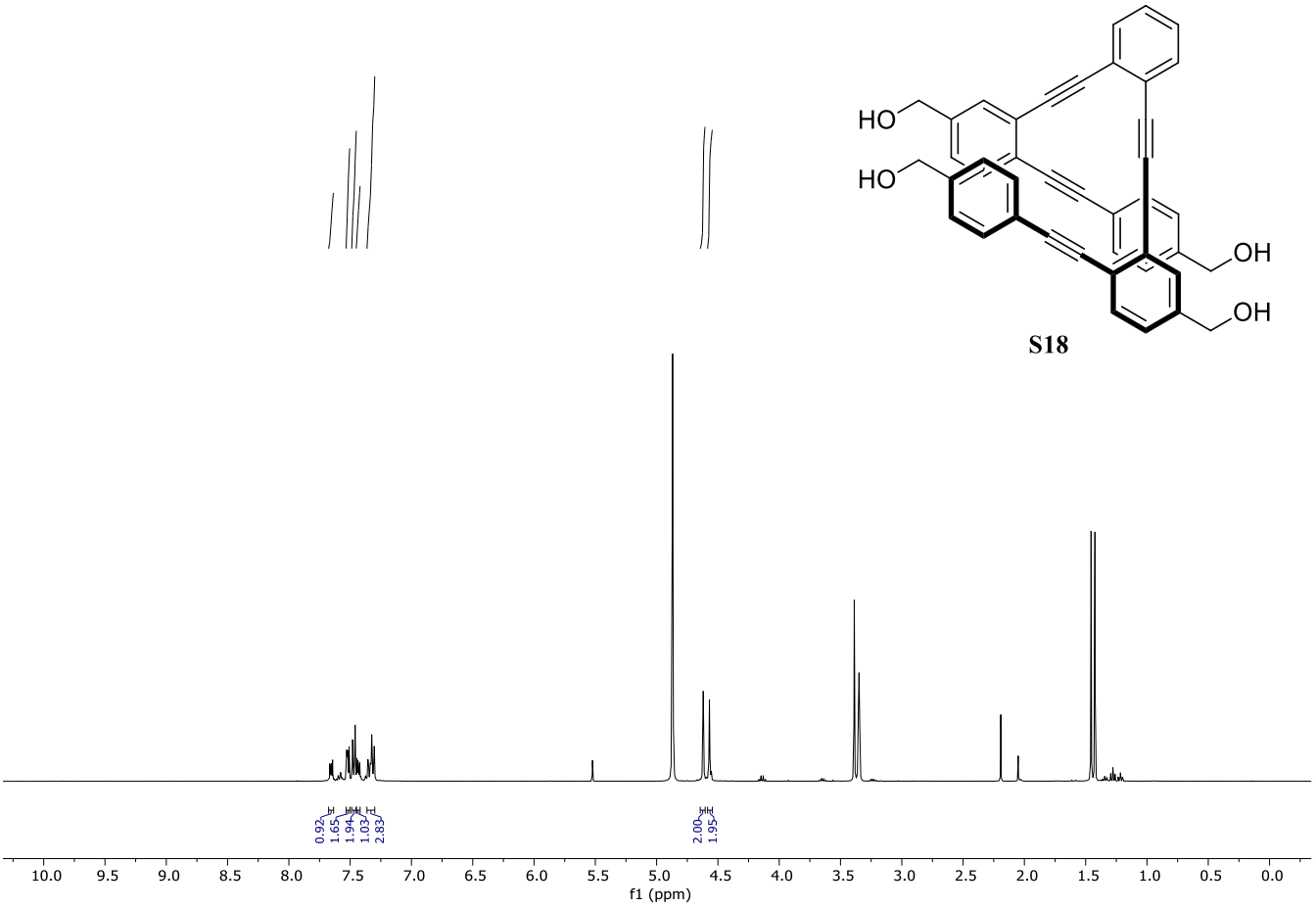
^{1}H NMR (500 MHz, $CDCl_3$) spectrum of compound S17



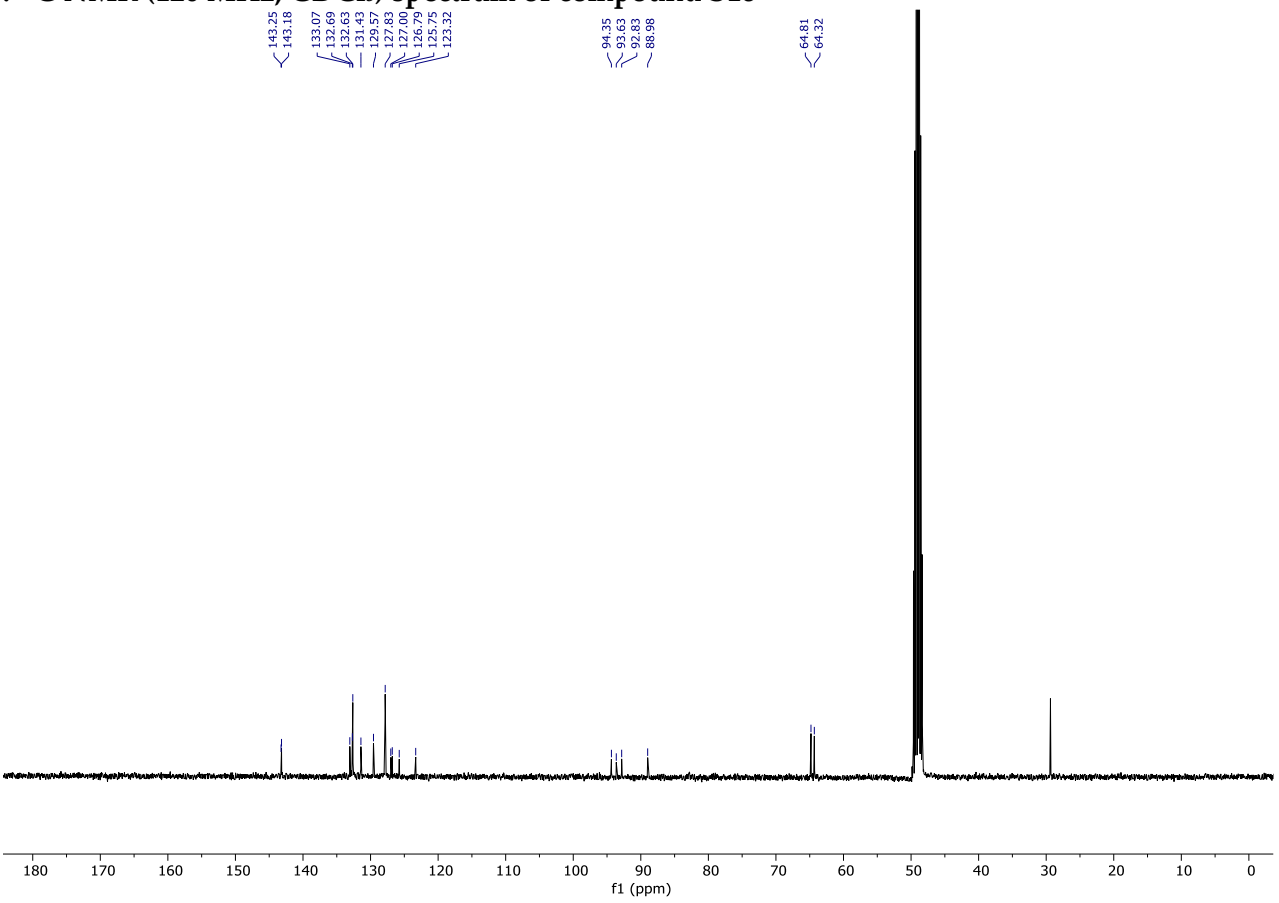
. ^{13}C NMR (126 MHz, $CDCl_3$) spectrum of compound S17



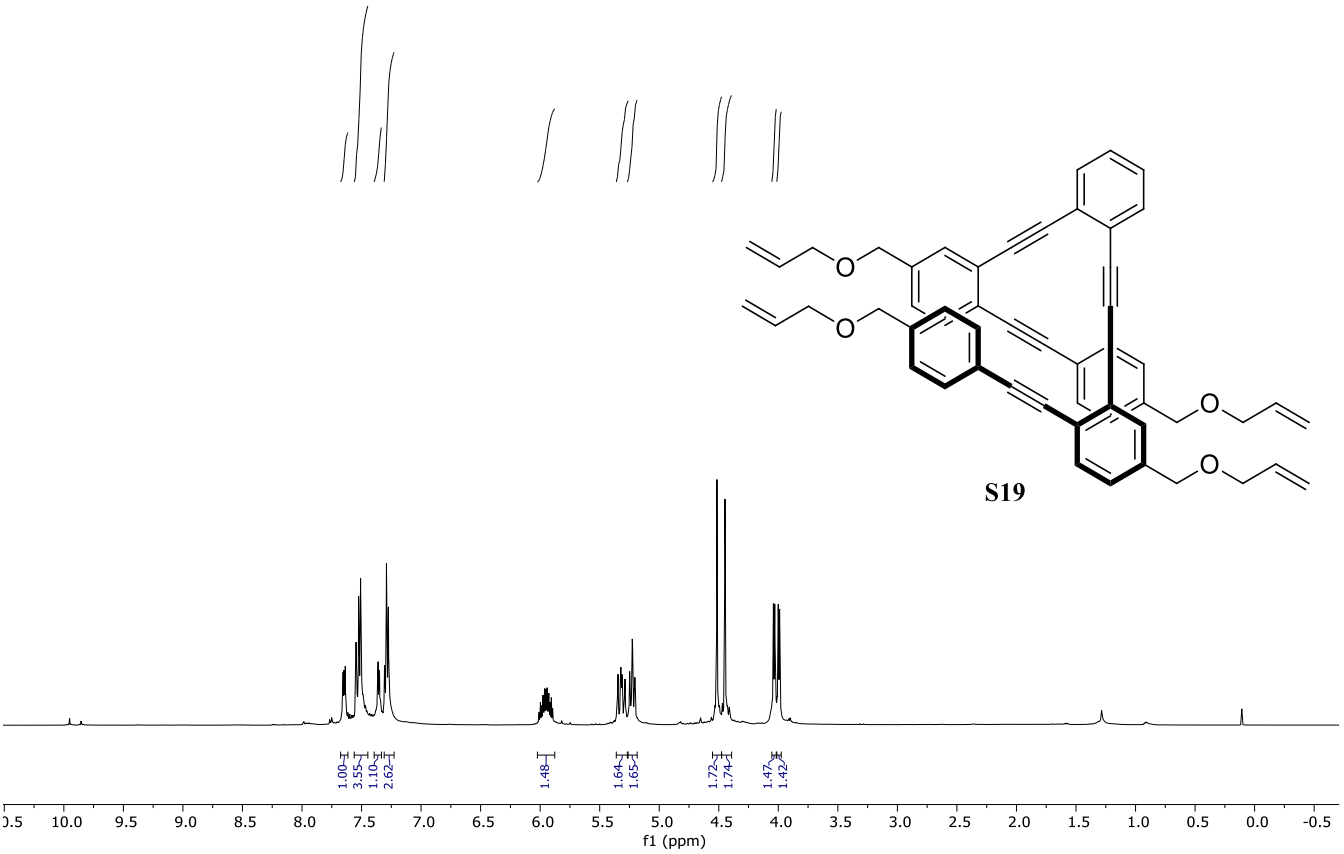
^{1}H NMR (500 MHz, $CDCl_3$) spectrum of compound S18



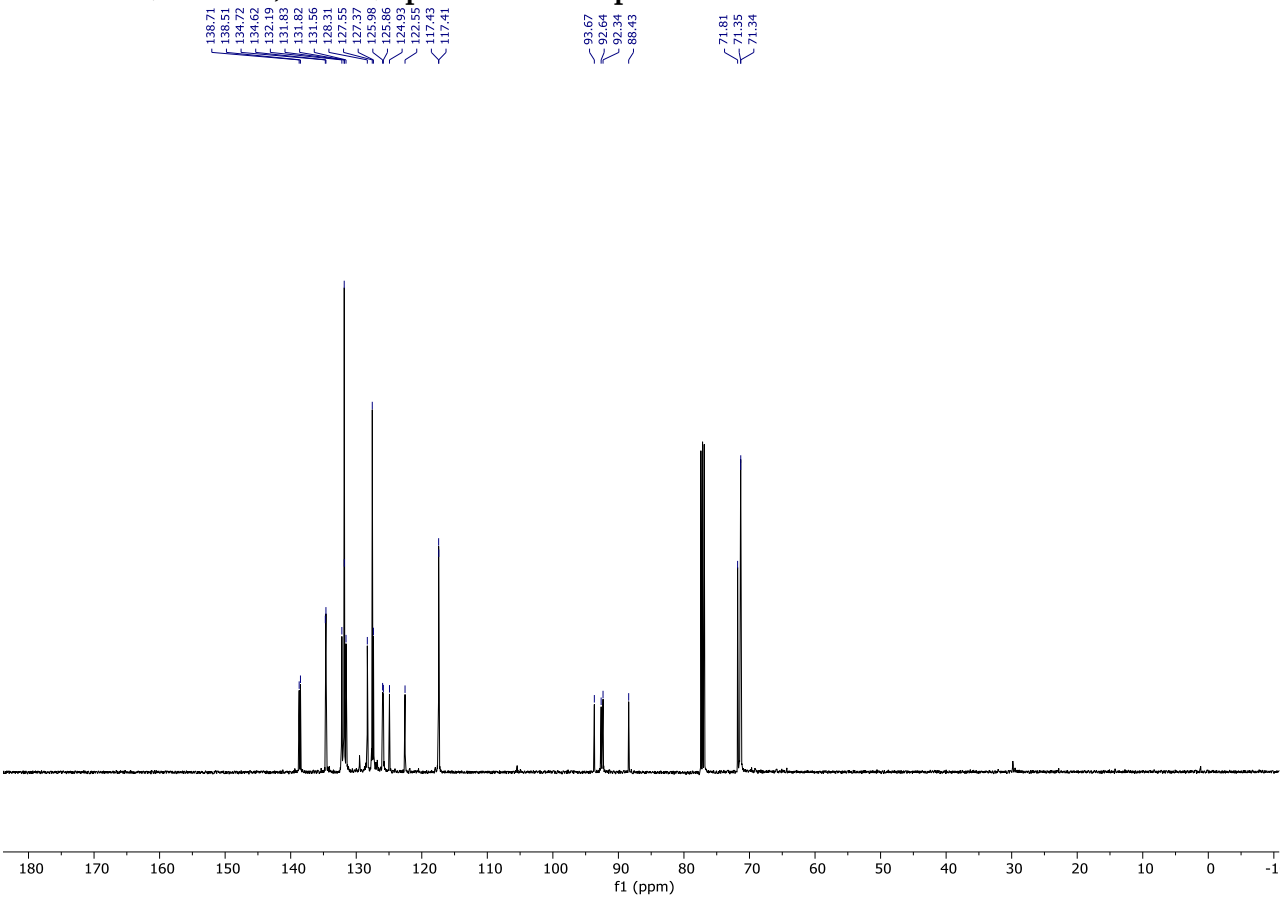
. ^{13}C NMR (126 MHz, $CDCl_3$) spectrum of compound S18



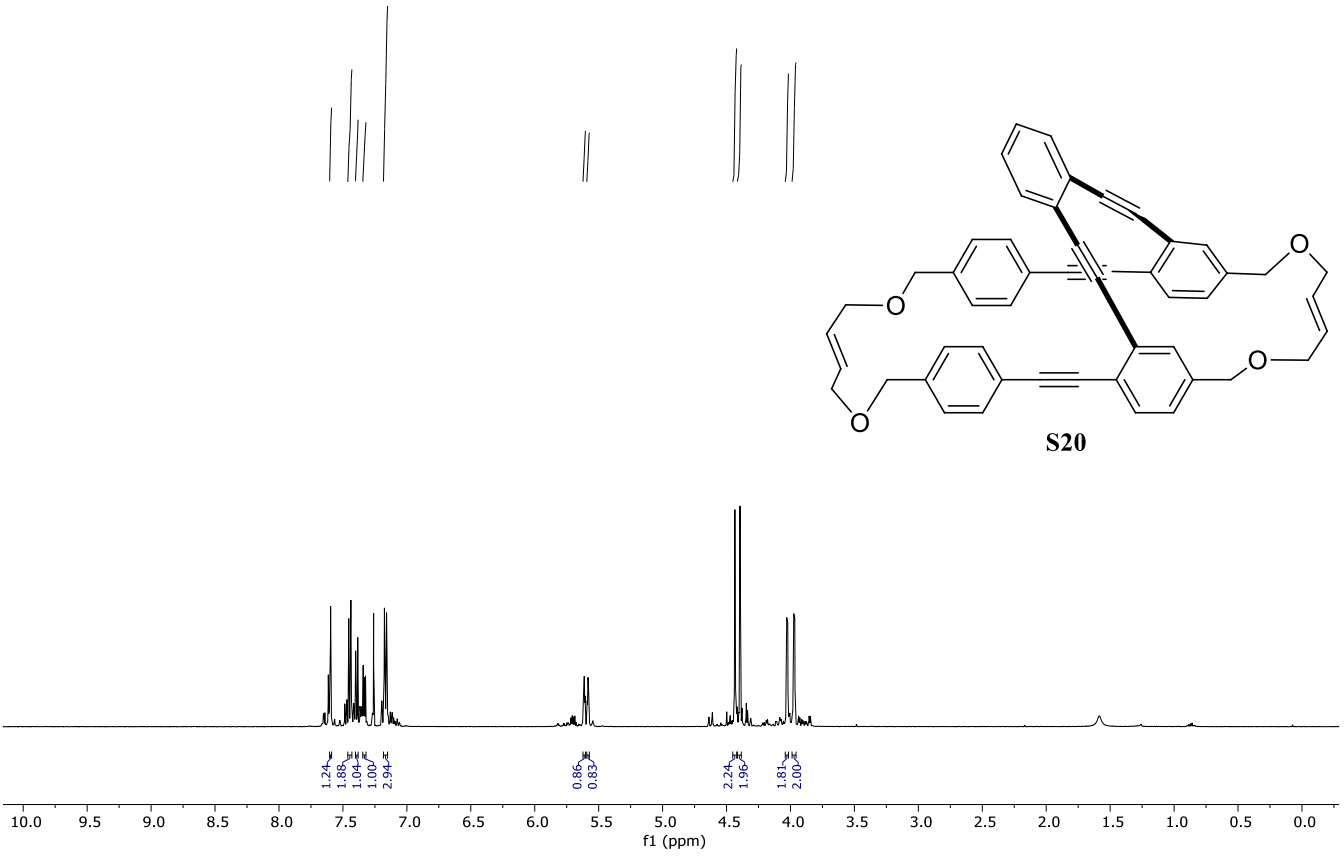
^{1}H NMR (500 MHz, $CDCl_3$) spectrum of compound S19



. ^{13}C NMR (126 MHz, $CDCl_3$) spectrum of compound S19

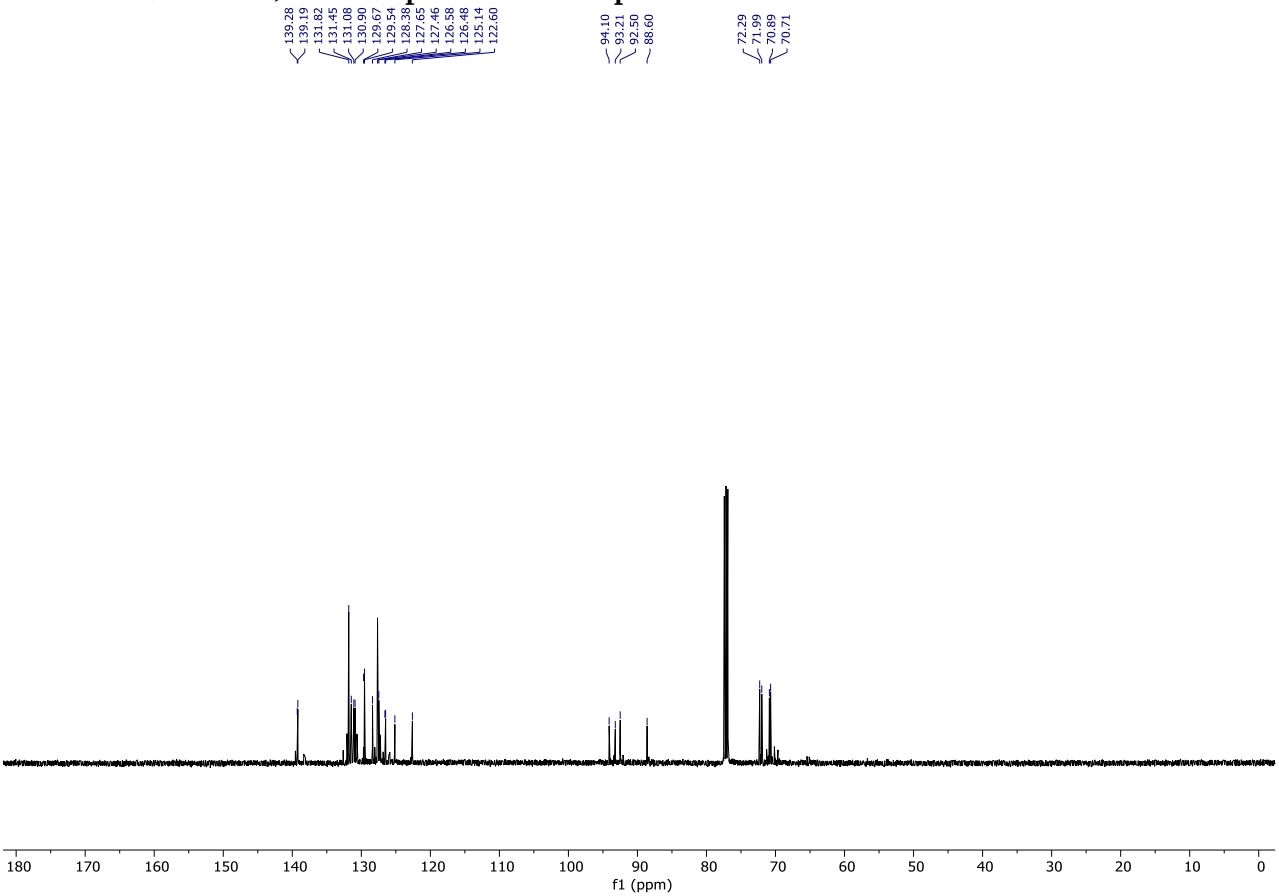


^{1}H NMR (500 MHz, $CDCl_3$) spectrum of compound S20



S20

. ^{13}C NMR (126 MHz, $CDCl_3$) spectrum of compound S20



HPLC ISOLATION OF (E,E)-1 AND (E,Z)-1

General details

HPLC analysis was carried out on an Agilent 1260 series using the following conditions: CHIRALPAK® IC analytical column (4,6x250mm) packed with cellulose tris-(3,5-dichlorophenylcarbamate) immobilized on silica gel (5μm). The column temperature was set at 20 °C. The flow was constant during operation (0.8 mL/min) and 350 nm was selected as reference wavelength for the peak detection. The mobile phase used was a 7:3 mixture of hexane:EtOAc.

HPLC chromatograms

Figure S1. HPLC chromatogram of (*P*,*E*,*E*)-**1** and (*M*,*E*,*E*)-**1**

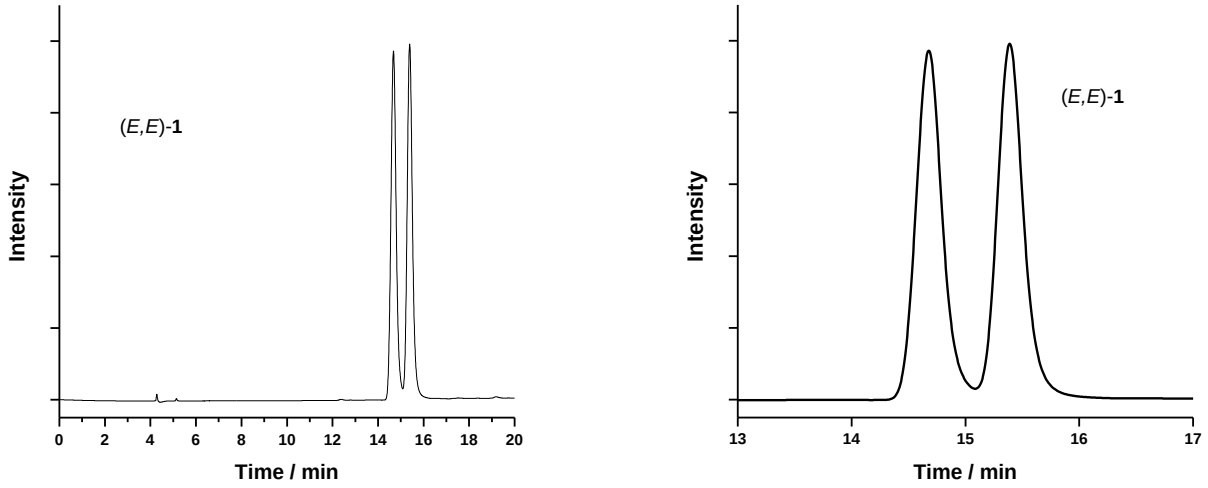
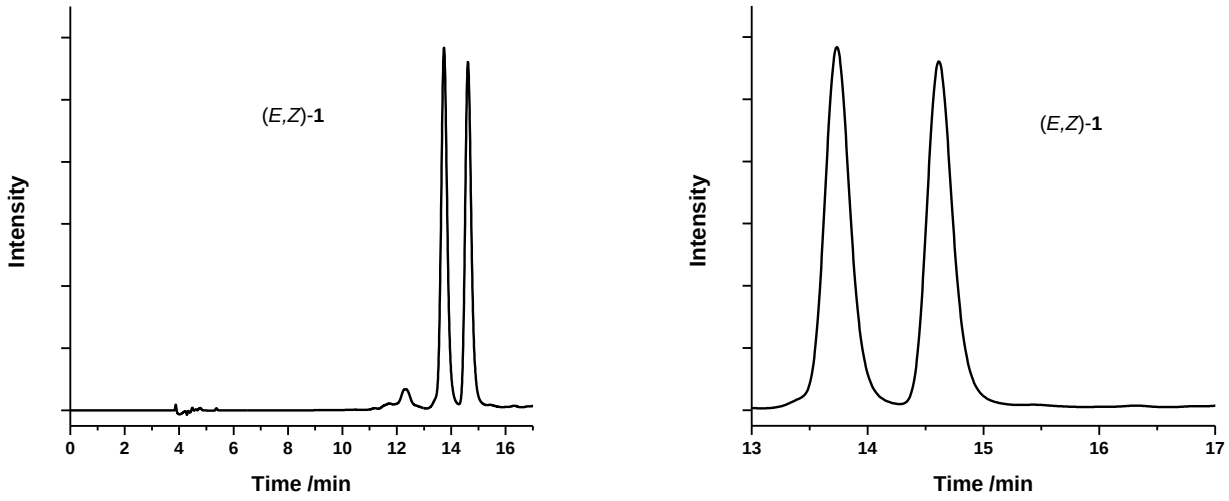


Figure S2. HPLC chromatogram of (*P*,*E*,*Z*)-**1** and (*M*,*E*,*Z*)-**1**

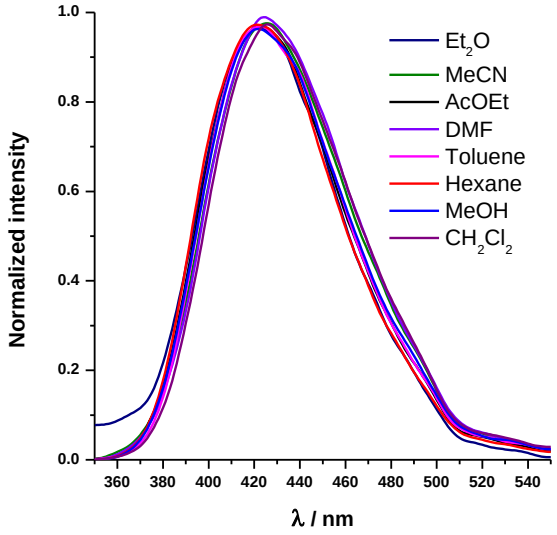


ABSORPTION AND STEADY-STATE FLUORESCENCE SPECTRA

Experimental Conditions

Absorption measurements were conducted in a UV-Visible double beam absorption spectrophotometer Lambda 650 (PerkinElemer, U. S. A) in 10 × 10 mm quartz cell cuvettes.
Steady-state fluorescence spectra were recorded using a JASCO FP-8300 spectrofluorometer in 10 × 10 mm cuvettes.

Figure S3. Normalized fluorescence spectra of compound (*E,Z*)-**1** in different solvents.



LIFETIMES, QUANTUM YIELDS and TRES DECONVOLUTION OF COMPOUNDS (E,E)-1 and (E,Z)-1

Quantum yields were determined by measuring both absorbance and fluorescence of compounds (*E,E*)-**1** and (*E,Z*)-**1** and quinine in 0.1 M H_2SO_4 as standard (Φr = 0.54).[S2] For the relative determination of the fluorescence quantum yield Φ the following formula was used:[S3,S4]

$$\Phi_x = \Phi_r \, \mathrm{x} \, \frac{F_x}{F_r} \, \mathrm{x} \, \frac{1-10^{-A_r(\lambda_{ex})}}{1-10^{-A_x(\lambda_{ex})}} \, \mathrm{x} \, \frac{n_x^2}{n_r^2} \qquad \text{(eq. S1)}$$

The subscripts ***x*** and ***r*** refer respectively to sample and reference (standard) fluorophore with known quantum yield Φ_r in a specific solvent; *F* stands for the spectrally corrected, integrated fluorescence spectra; $A(\lambda_{ex})$ denotes the absorbance at the used excitation wavelength λ_{ex}; and *n* represents the refractive index of the solvent (in principle at the average emission wavelength). To minimize inner filter effects, the absorbance at the excitation wavelength λ_{ex} was kept under 0.1. The measurements were performed using 10×10 mm cuvettes on non-degassed samples.

Time-resolved fluorescence decay traces were collected via the time-correlated single photon counting (TCSPC) method using a FluoTime 200 fluoromoter (PicoQuant, GmbH). The excitation source was a 325-nm LED using a 10 MHz excitation frequency. The full width at half maximum (fwhm) of the laser pulses was around 40 ps. The fluorescence emission was collected at a 90° geometry, focused at the detector after crossing through a polarizer (set at the magic angle), 2-mm slits, and a 2-nm bandwidth monochromator. TCSPC was achieved by a TimeHarp200 board, set at 36 ps/channel. Fluorescence decay traces were collected for the necessary time to reach 20,000 counts at the peak channel. For both compounds (*E*,*E*)-**1** and (*E*,*Z*)-**1** decay traces were collected at 415, 420 and 425 nm, where the maximum of emission was observed.

Time-resolved emission spectroscopy (TRES) of compounds (*E*,*E*)-**1** and (*E*,*Z*)-**1** in CH_2Cl_2 was performed by collecting 61 fluorescence decay traces in the 340-580 nm emission range ($\Delta\lambda_{em}$ = 4 nm) at 10 MHz excitation frequency during a fixed amount of time (500 s), to maintain the overall intensity information.

The fluorescence decay traces were fitted to a three -exponential function, by using a Levenberg-Marquard algorithm-based nonlinear least-squares error minimization deconvolution method iterative reconvolution methods (FluoFit 4.4 package, Picoquant GmbH). For each sample, the decay traces were fitted globally with the decay times linked as shared parameters, whereas the pre-exponential factors were local adjustable parameters. The quality of fittings was assessed by the value of the reduced chi-squared, χ^2, parameter and random distributions of the weighted residuals and the autocorrelation functions.

For the TRES (Time Resolved Emission Spectroscopy) analysis and the estimation of the species-associated emission spectra (SAEMS), the fitting procedure described above was performed, by fitting globally the 61 decay traces. The SAEMS of each species i at any given emission wavelength ($SAEMS_i(\lambda_{em})$) is given by the fluorescence intensity emitted by the species i ($A_{i,\lambda em} \times \tau_i$), normalized by the total intensity and corrected for the different detection sensitivity using the total intensity of the steady-state spectrum ($I_{ss,\lambda em}$):

$$SAEMS_i(\lambda_{em}) = \frac{A_{i,\lambda em} \times \tau_i}{\sum_i A_{i,\lambda em} \times \tau_i} \cdot I_{ss,\lambda em} \qquad \text{(eq. S2)}$$

The approximate contribution of each species can be assessed as the area under the SAEMS. This estimation assumes equal excitation rate for all the species, as the initial amount of each form in the excited state (after the pulse excitation) is unknown. Figures S1-S2 show the SAEMS of compounds (*E*,*E*)-**1** and (*E*,*Z*)-**1** dissolved in dichloromethane.

Table S0. Quantum yields and lifetimes (average of signals at 415,420 and 425 nm) of compounds (*E*,*E*)-**1** and (*E*,*Z*)-**1** in CH_2Cl_2 solutions.

COMPOUND	Φ	τ_1	τ_2	τ_3
(*E*,*Z*)-**1**	0.133±0.018	4.005±0.017	1.51±0.056	0.159±0.019
(*E*,*E*)-**1**	0.115±0.006	2.37±0.11	2.164±0.011	0.487±0.024

Figure S4. SAEMS spectra of compound (*E*,*E*)-**1** in CH_2Cl_2 solutions.

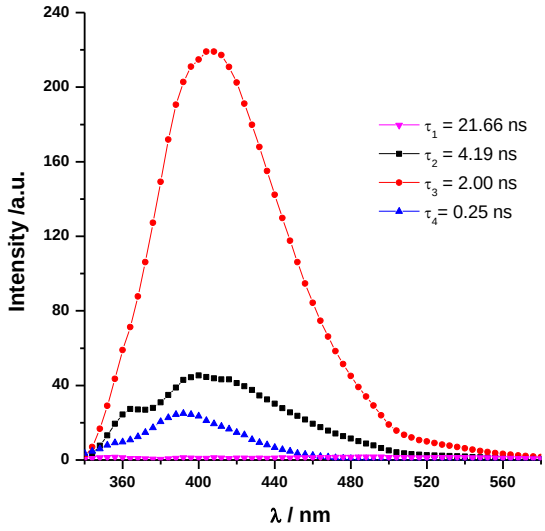
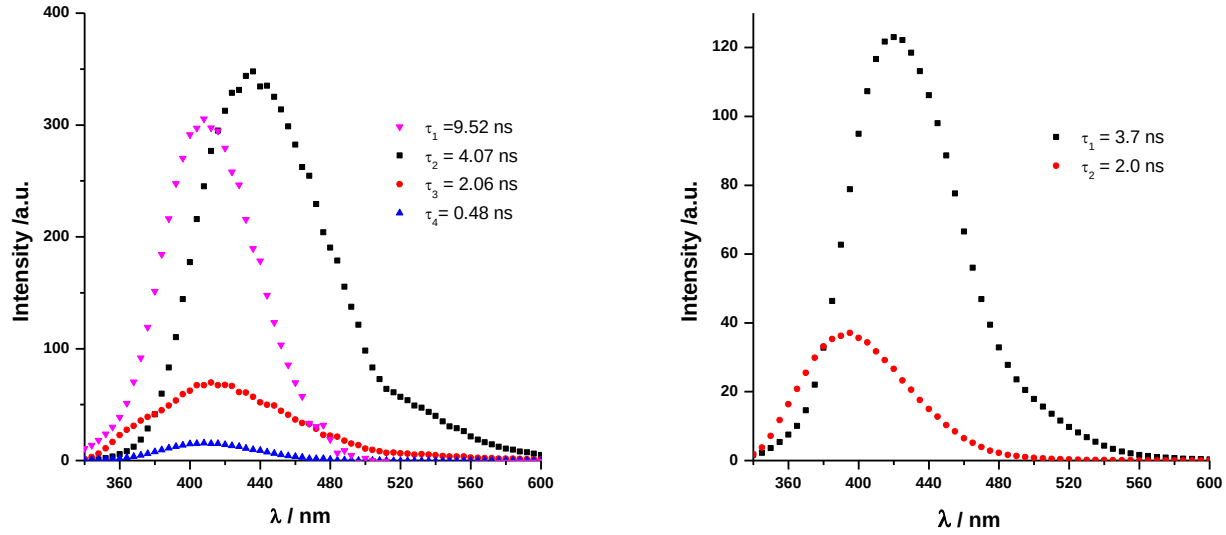


Figure S5. SAEMS spectra of compound (*E*,*Z*)-**1** in CH_2Cl_2 (left) and hexane (right) solutions.



In addition, lifetimes of compound (*E*,*Z*)-**1** in CH_3CN were also measured at the maxima of emission giving a biexponential decay with two species of 3.87 and 1.7ns. The fractional intensities of the positive decay components were 92% of the specie corresponding to the largest lifetime and 8% of

the shortest one. Finally, lifetimes were collected at higher wavelengths (between 480 and 525nm) and lifetimes of 4 and 2.1 ns were obtained in similar proportion to the previous ones.

CD and CPL MEASUREMENTS

Experimental

Circular Dichroism (CD) and Circularly Polarized Luminiscence (CPL) measurements were recorded in an Olis DSM172 spectrophotometer. The spectra were recorded at 8×10^{-5} M concentrations in HPLC grade solvents.

In CPL measurements, a fixed wavelength xenon-lamp (290 nm) as the excitation source was used. CPL spectra in Figure S6 were collected by accumulating 100 scans and with 0.5 s of integration time.

Fig. S6. g_{abs} values obtained for compounds (*E*,*E*)-**1** and (*E*,*Z*)-**1** in CH_2Cl_2 solutions.

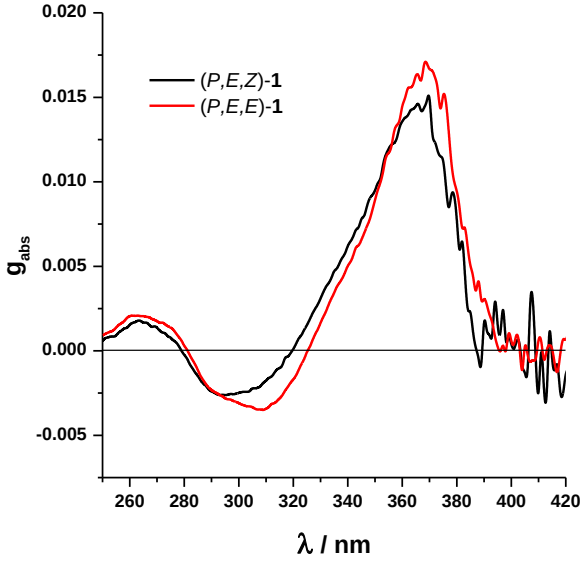


Fig. S7. g_{lum} values obtained for compounds (*E*,*E*)-**1** and (*E*,*Z*)-**1** in CH_2Cl_2 solutions.

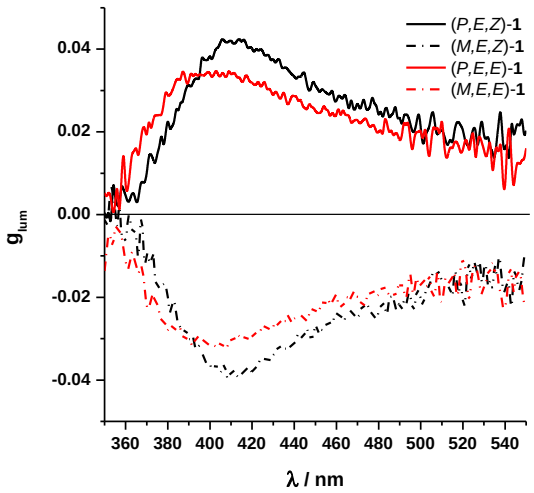


Fig. S8. (a) ΔI and (b) g_{lum} values obtained for compound (*E*,*Z*)-**1** at different temperatures

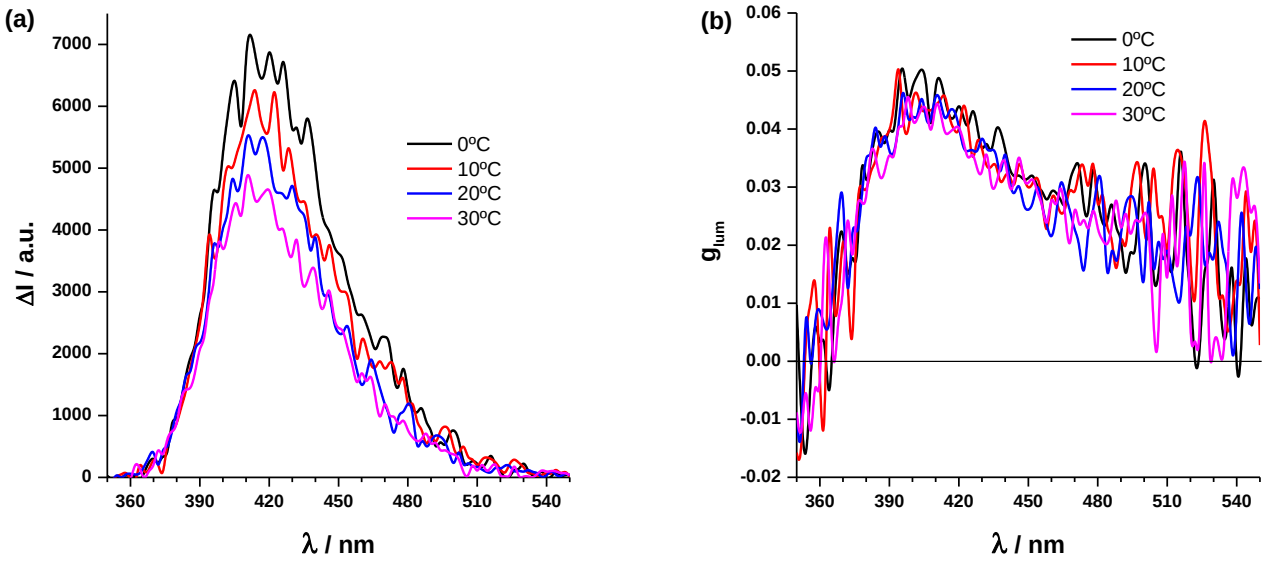
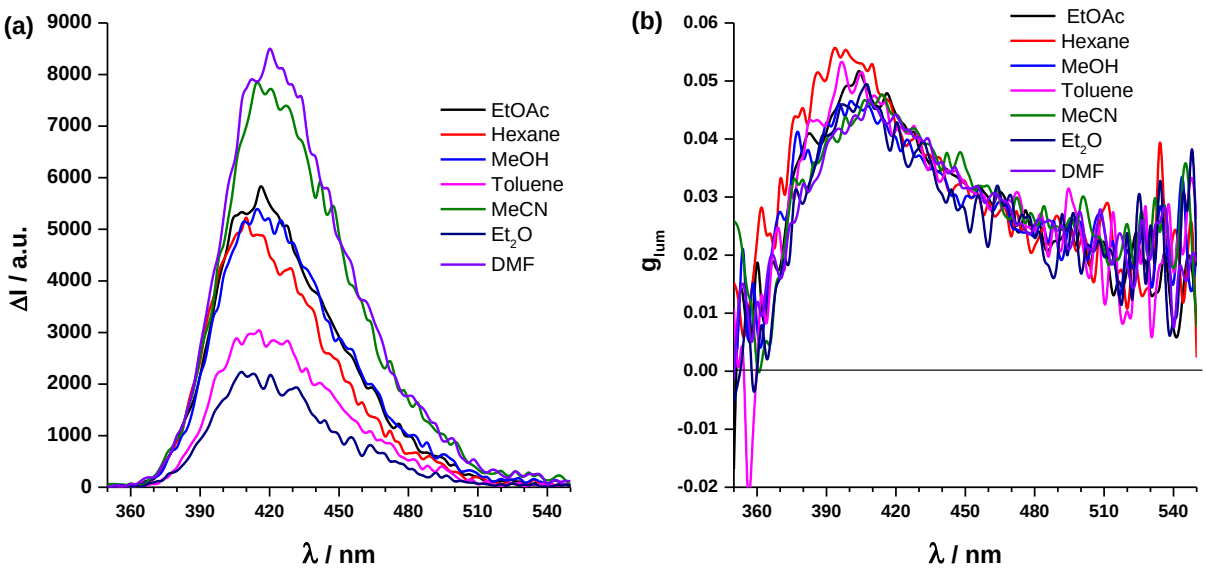


Fig. S9. (a) ΔI and (b) g_{lum} values obtained for compound (*E*,*Z*)-**1** in different solvents



	EtOAc	Hexane	MeOH	Toluene	MeCN	Et2O	DMF
g_{lum} (400 nm)	0.049	0.055	0.048	0.048	0.041	0.046	0.042

SINGLE CRISTAL X-RAY ANALYSIS

The X-ray diffraction data of both (*E*,*E*)-**1** and (*E*,*E*)-**S20** were collected on a Bruker D8 Venture diffractometer equipped with a Photon 100 detector using Cu radiation source. The structure was solved with SHELXT[S5] and refined using the full-matrix least-squares against F^2 procedure with SHELX 2018[S6] using the WinGX32[S7] software. C–H hydrogen atoms were placed in idealized positions (U_{eg}(H) = 1.2U_{eg}(C) or U_{eg}(H) = 1.5U_{eg}(C)) and were allowed to ride on their parent atoms.

Single crystals suitable for X-ray diffraction analysis of (*E*,*E*)-**1** were grown by diffusion of methanol into a CH_2Cl_2 solution of the compound. Summary of the X-ray diffraction measurement and refinement data: Chemical formula, $C_{50}H_{38}O_4$; *Mr*, 702.80; crystal size [mm^3], 0.382 × 0.081 x 0.042; temperature [K], 100(2); wavelength [Å], 1.54178 (Cu Kα), crystal system, monoclinic; space group, *Pc*; *a* [Å], 10.6708(3); *b* [Å], 20.4338(6); *c* [Å], 17.7611(6); α [°], 90; β [°], 104.773(2); γ [°], 90; *V* [$Å^3$], 3744.7(2); *Z*, 4; ρ_{calcd} [Mg m^{-3}], 1.247; μ [mm^{-1}], 0.613; F(000), 1480; θ range [°], 2.162 to 59.099; *hkl* ranges, -10/11, -22/22, -19/19; reflections collected, 51264; independent reflections, 9354; R_{int}, 0.0590; completeness to θ = 59.099°, 99.9%; absorption correction, numerical; refinement method; full-matrix least-squares on F^2; Final *R* indices [$I>2\sigma(I)$], R_1 = 0.0462, wR_2 = 0.1157; *R* indices (all data), R_1 = 0.0502, wR_2 = 0.1190; goodness-of-fit on F^2, 1.038; absolute structure parameter, 0.4(3).

CCDC-1902657 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via https://www.ccdc.cam.ac.uk/structures/?

Figure S10. Different views of the ORTEP-type[S8] drawing of the crystal structure of (*E*,*E*)-**1** showing the ellipsoids at ellipsoids at 50% probability: a) Front view; b) Side view; c) Top view. Color codes: C: gray, O: red, Hydrogen atoms have been omitted for clarity.

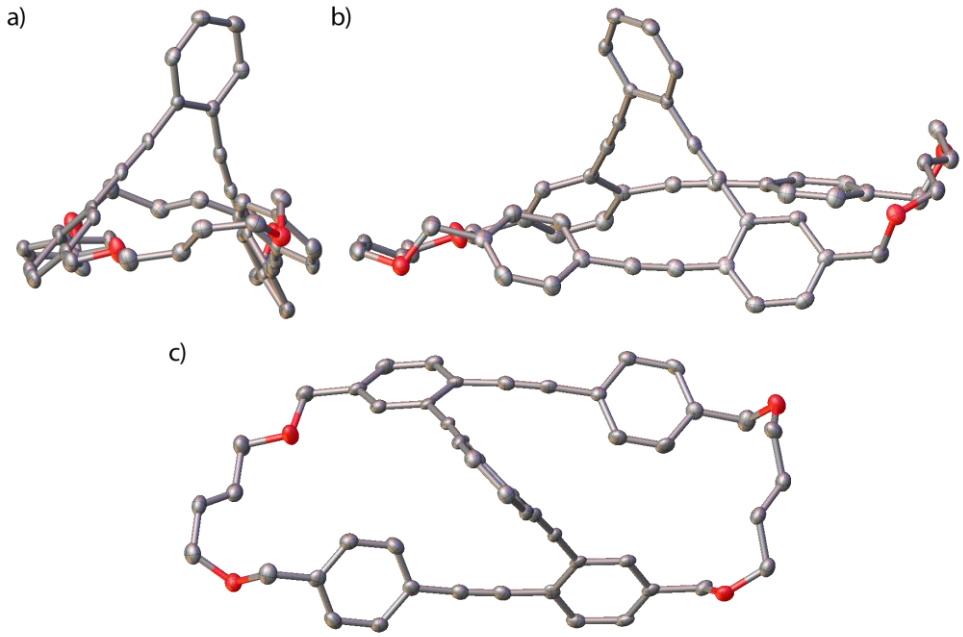


Table S1. Atomic coordinates for the X-ray diffraction structure of (*E*,*E*)-**1**

Atom	X	Y	Z
C	1.7292	21.4984	5.7155
H	1.245	21.9267	6.4649
H	1.3521	21.8489	4.8701
C	3.1526	21.858	5.7928
H	3.6867	21.7199	5.02
C	3.7407	22.3628	6.8644
H	3.1877	22.5528	7.613
C	5.1878	22.655	7.0018
H	5.3113	23.5991	7.2753
H	5.5791	22.0774	7.7043
C	7.2292	22.1318	5.8804
H	7.5918	22.6179	6.6624
H	7.6952	22.469	5.0744
C	7.5338	20.6647	6.0367
C	6.5364	19.7125	6.1929
H	5.628	19.9873	6.2408
C	6.8484	18.3618	6.2805
H	6.1532	17.7255	6.3967
C	8.1673	17.9347	6.1998
C	9.1702	18.891	6.0504
H	10.0787	18.6211	5.9961
C	8.8454	20.2315	5.9834
H	9.5412	20.8731	5.8959
C	8.5106	16.5371	6.2616
C	8.8036	15.3683	6.3441
C	9.1375	13.9951	6.5347
C	9.975	13.3024	5.6571
H	10.317	13.7504	4.8924
C	10.3172	11.9865	5.8769
H	10.8806	11.5353	5.2579
C	9.8424	11.3081	7.0018
C	8.9721	11.9803	7.8537
H	8.622	11.5216	8.6076
C	8.5986	13.3065	7.6356
C	10.2646	9.9124	7.347
H	11.0241	9.9499	7.9802
H	9.515	9.4488	7.7973
C	10.1049	7.8507	6.1964
H	10.2786	7.4245	7.0732
H	10.5577	7.3117	5.5006
C	8.642	7.8588	5.937
H	8.3207	8.4437	5.2614
C	7.7588	7.1171	6.5673

H	8.0657	6.5812	7.2901
C	6.2937	7.0578	6.2273
H	6.0377	7.8973	5.7694
H	6.1426	6.3115	5.5939
C	5.4929	7.9794	8.2401
H	6.4329	8.1716	8.4839
H	5.0096	7.734	9.0676
C	4.8702	9.232	7.6596
C	3.6689	9.1932	6.9589
H	3.2198	8.3626	6.851
C	3.1169	10.3354	6.4179
H	2.3124	10.2792	5.9156
C	3.7349	11.5778	6.6034
C	4.9282	11.6248	7.3264
H	5.3605	12.4587	7.4694
C	5.4829	10.4662	7.8331
H	6.3019	10.5145	8.312
C	3.2163	12.8079	6.0813
C	2.8952	13.9052	5.6966
C	2.6012	15.264	5.3669
C	1.857	15.6339	4.2557
H	1.5422	14.9632	3.6606
C	1.5652	16.9621	3.9947
H	1.0241	17.1857	3.2463
C	2.049	17.9715	4.8104
C	2.8328	17.616	5.913
H	3.1917	18.2989	6.4688
C	3.0955	16.2898	6.2118
C	1.7748	19.4223	4.5391
H	2.556	19.8334	4.091
H	0.9914	19.5094	3.9403
C	3.8128	15.9649	7.4209
C	4.3346	15.7626	8.4891
C	4.7721	15.6523	9.8407
C	3.9388	16.1877	10.8316
H	3.1052	16.5714	10.5875
C	4.3162	16.1611	12.1643
H	3.7496	16.533	12.8306
C	5.5306	15.5889	12.5198
H	5.799	15.5796	13.4308
C	6.3453	15.0331	11.5632
H	7.1664	14.633	11.8251
C	5.9884	15.0462	10.2134
C	6.8568	14.4447	9.2551
C	7.6627	13.9359	8.5217
O	1.5195	20.0823	5.7705
O	5.8517	22.423	5.7629
O	10.6496	9.1703	6.1988
O	5.4653	6.8788	7.3453
C	-0.1232	-3.8559	9.5676
H	-0.1049	-4.7025	10.0803
H	0.0988	-4.0665	8.626
C	-1.4932	-3.2796	9.6277
H	-2.1809	-3.715	9.138
C	-1.8176	-2.1966	10.3198
H	-1.1158	-1.759	10.7865
C	-3.1675	-1.6102	10.4332
H	-3.7603	-1.9693	9.7263
H	-3.5626	-1.8211	11.3152
C	-4.1667	0.5415	10.5483
H	-4.4896	0.3524	11.4646
H	-4.8825	0.2994	9.9085
C	-3.8268	1.9984	10.4126
C	-4.5079	2.9609	11.1459
H	-5.2203	2.6991	11.7168
C	-4.1622	4.2972	11.0532
H	-4.6409	4.941	11.5619
C	-3.1255	4.712	10.2254
C	-2.4514	3.7496	9.4457
C	-2.8191	2.401	9.5573
H	-2.3654	1.7495	9.0341
C	-2.6835	6.0729	10.2649
C	-2.2933	7.1968	10.4487
C	-1.7624	8.5025	10.7337
C	-2.6247	9.5937	10.9484
H	-3.5651	9.4863	10.8639
C	-2.0881	10.8258	11.285
H	-2.6698	11.5677	11.4085
C	-0.7264	11.0016	11.4465
C	0.1112	9.9083	11.2404
H	1.0491	10.012	11.3495
C	-0.3965	8.6762	10.8832
H	0.1933	7.9449	10.7384
C	-0.1546	12.34	11.8638
H	-0.7558	12.7469	12.5368
H	0.7227	12.1898	12.2976
C	1.0813	12.9285	9.8922
H	1.1451	13.6266	9.1937
H	0.8642	12.0726	9.444
C	2.4052	12.7977	10.5654
H	2.6428	13.457	11.2059
C	3.2655	11.8332	10.3336
H	3.0073	11.17	9.7054
C	4.6118	11.68	10.9622
H	5.3056	12.0018	10.3331
H	4.6579	12.2396	11.7782

C	4.1339	9.8266	12.4185
H	3.292	10.3385	12.5059
H	4.6571	9.9447	13.2502
C	3.823	8.3656	12.2176
C	3.2151	7.9283	11.0429
H	3.0089	8.5587	10.363
C	2.9039	6.5838	10.8471
C	3.1712	5.6479	11.8689
C	3.7795	6.1036	13.0419
H	3.9652	5.4895	13.7417
C	4.1146	7.4318	13.1999
H	4.5539	7.711	13.994
C	2.859	4.2788	11.6525
C	2.5863	3.1386	11.3554
C	2.236	1.839	10.8711
C	1.2336	1.7124	9.9094
H	0.7739	2.4862	9.6058
C	0.9055	0.4802	9.3976
H	0.2018	0.4166	8.7619
C	1.5719	-0.6661	9.784
C	2.8751	0.6784	11.3125
H	3.5397	0.7344	11.9889
C	2.5482	-0.5497	10.7715
H	2.9957	-1.3282	11.0791
C	1.2586	-1.9882	9.1348
H	0.5292	-1.8652	8.4773
H	2.0575	-2.3109	8.6475
C	2.3859	6.1342	9.5865
C	2.0243	5.7215	8.5217
C	1.7594	5.2533	7.1873
C	2.7276	5.4456	6.2067
H	3.5436	5.8745	6.4356
C	2.5244	5.0206	4.9015
H	3.1957	5.1549	4.2417
C	1.3345	4.3974	4.57
H	1.1815	4.1212	3.6748
C	0.3735	4.1787	5.5232
H	-0.4291	3.732	5.2804
C	0.5544	4.5976	6.8524
C	-0.4673	4.3483	7.8176
C	-1.3764	4.1113	8.5578
O	0.866	-2.9696	10.0937
O	-3.0134	-0.2043	10.2821
O	0.0199	13.264	10.7853
O	4.8803	10.3144	11.3077

Single crystals of (*E*,*E*)-**S20** were also grown by diffusion of methanol into a solution of the compound in dichloromethane. However due to the limited quality of the crystals obtained, no significant diffraction data could be collected at high angles giving a low data/parameter ratio. As a result, we believe that the data gathered does not meet the quality required for the publication of the structure as crystallographic data. Moreover, the structure shows some disorder in the alkyl chains that join the phenylene rings, which was modeled using PART instructions. However, the position and connectivity of the different atoms in the structure could be established with enough reliability to show that the compound obtained did not correspond to the target structure **1**, as the helicity of the structure is not maintained due to the connection between wrong ends. The structure and the XYZ atomic coordinates are shown in Figure S10 and Table S2, respectively.

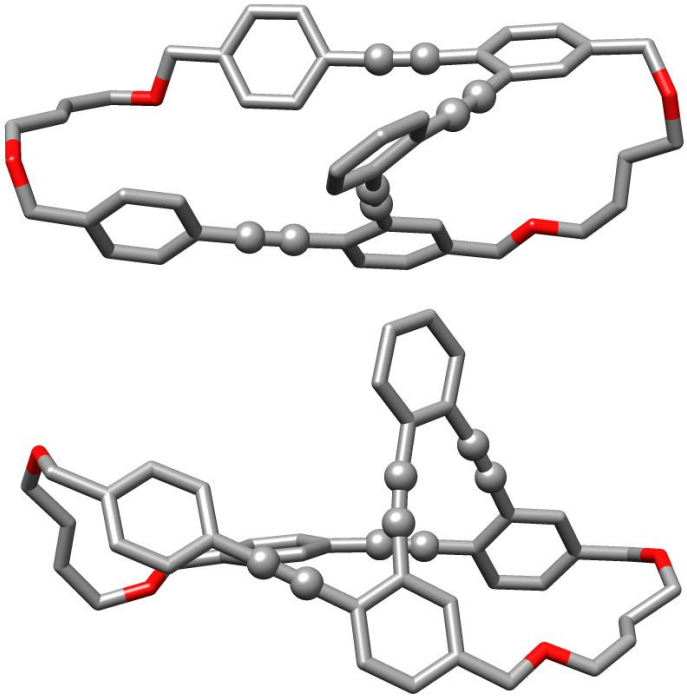


Figure S11. Top (top) and side (bottom) views of the X-ray diffraction structure of (*E*,*E*)-**S20**. Color codes: C: gray, O: red. Hydrogen atoms and disorder have been omitted for clarity.

Table S2. Atomic coordinates for the X-ray diffraction structure of (*E*,*E*)-**S20**

Atom	X	Y	Z
C	8.986311	3.608240	5.690491
C	9.167408	4.196077	6.930379
H	9.815581	3.836185	7.524216
C	8.430675	5.286904	7.321390
H	8.580505	5.675406	8.175461
C	7.469513	5.826925	6.477142
C	7.314691	5.265641	5.213941
H	6.684851	5.638883	4.608088
C	8.063830	4.174544	4.831672
H	7.944201	3.806331	3.964127
C	6.616518	6.885367	6.939636
C	5.881432	7.719486	7.404530
C	5.034863	8.702926	8.003132
C	4.344702	8.413958	9.186622
H	4.435424	7.557257	9.587199
C	3.536352	9.356608	9.773396
H	3.067209	9.137853	10.569990
C	3.391368	10.619992	9.227078
C	4.084600	10.922607	8.066043
H	4.002646	11.790802	7.689963
C	4.895165	9.987815	7.440357
C	5.628651	10.324809	6.256866
C	6.277667	10.576327	5.276338
C	7.112741	10.770950	4.125589
C	7.939171	11.874232	4.019822
H	7.908309	12.552538	4.685038
C	8.808761	11.997162	2.960440
H	9.366980	12.762720	2.889626
C	8.867700	11.012149	2.000483
H	9.485109	11.092081	1.282829
C	8.046290	9.916684	2.072137
H	8.091864	9.246885	1.400304
C	7.146041	9.783409	3.124148
C	6.222234	8.684711	3.191002
C	5.364038	7.842474	3.262656
C	4.256094	6.970297	3.357109
C	3.102979	7.430022	3.986566
H	3.101327	8.295828	4.378538
C	1.954447	6.650191	4.054106
C	2.006808	5.370992	3.505559
H	1.240032	4.813106	3.561374
C	3.130466	4.896538	2.893586
H	3.126097	4.018501	2.529968
C	4.284911	5.674441	2.787305
C	5.449574	5.176420	2.132477
C	6.445665	4.751815	1.598672
C	7.629500	4.217756	1.018584
C	7.587484	3.040918	0.289359
H	6.753306	2.611378	0.137702
C	8.729655	2.490843	-0.214276
H	8.672447	1.679534	-0.703323
C	9.956664	3.071235	-0.035998
C	10.007830	4.262319	0.668542
H	10.845737	4.689720	0.803193
C	8.858522	4.842006	1.182805
H	8.912209	5.668391	1.647921
C	9.779410	2.379218	5.336335
H	10.701703	2.640729	5.088066
H	9.830887	1.779803	6.122146
C	9.771927	0.439204	3.997537
H	9.063292	-0.165545	3.662152
H	10.119396	0.054149	4.840672
C	10.855180	0.474980	3.018724
H	11.291360	-0.353526	2.858925
C	11.296040	1.465693	2.353610
H	10.893934	2.306248	2.535454
C	12.362730	1.458938	1.325084
H	13.227078	1.588413	1.791298
H	12.383809	0.555875	0.921422
C	11.227793	2.452628	-0.548547
H	11.014591	1.532293	-0.845483
H	11.506106	2.959945	-1.351260
C	0.694467	7.162063	4.657508
H	0.027467	7.313420	3.941089
H	0.327737	6.480120	5.274864
C	0.577616	11.058161	8.840180
H	0.764627	10.439507	9.590096
H	-0.327188	11.434725	8.979443
C	-0.229019	8.950539	5.857455
H	-0.811181	9.180597	5.090775
H	-0.711961	8.272937	6.394140
C	-0.104218	10.068556	6.627135
H	-0.641026	10.793281	6.328554
C	0.584969	10.343512	7.664232
H	1.412400	9.882029	7.600841
C	2.475484	11.664594	9.825851
H	1.947935	11.254732	10.556859
H	3.021705	12.392000	10.215782
O	9.191031	1.708552	4.281582
O	0.897881	8.349051	5.353306
O	1.601626	12.203152	8.875150

C	0.475119	11.845413	8.163067
H	0.372311	12.446332	7.382382
H	-0.325096	11.946181	8.735974
O	12.305739	2.378830	0.291416
O	11.634346	1.445554	-0.047998

CHECKCIF of COMPOUND (E,E)-1

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) shelx

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: shelx

```
Bond precision:  C-C = 0.0067 A          Wavelength=1.54178

Cell:            a=10.6708(3)     b=20.4338(6)        c=17.7611(6)
                 alpha=90         beta=104.773(2)     gamma=90
Temperature:     100 K

                 Calculated                Reported
Volume           3744.7(2)                 3744.7(2)
Space group      P c                       P c
Hall group       P -2yc                    P -2yc
Moiety formula   C50 H38 O4                ?
Sum formula      C50 H38 O4                C50 H38 O4
Mr               702.80                    702.80
Dx,g cm-3        1.247                     1.247
Z                4                         4
Mu (mm-1)        0.613                     0.613
F000             1480.0                    1480.0
F000'            1484.23
h,k,lmax         11,22,19                  11,22,19
Nref             10814[ 5418]              9354
Tmin,Tmax        0.942,0.975               0.704,1.000
Tmin'            0.791

Correction method= # Reported T Limits: Tmin=0.704 Tmax=1.000
AbsCorr = NUMERICAL

Data completeness= 1.73/0.86      Theta(max)= 59.099

R(reflections)= 0.0462( 8906)     wR2(reflections)= 0.1190( 9354)

S = 1.038                 Npar= 973
```

```
The following ALERTS were generated. Each ALERT has the format
       test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.
```

Alert level B

```
THETM01_ALERT_3_B  The value of sine(theta_max)/wavelength is less than 0.575
           Calculated sin(theta_max)/wavelength =    0.5565
```

Author Response: Only relatively thin needles could be obtained upon crystallization, which gave only a diffraction pattern of moderate intensity. As a result, only noisy was observed at very high angles and this data was omitted.

Alert level C

```
STRVA01_ALERT_4_C           Flack test results are ambiguous.
          From the CIF: _refine_ls_abs_structure_Flack    0.400
          From the CIF: _refine_ls_abs_structure_Flack_su    0.300
PLAT089_ALERT_3_C Poor Data / Parameter Ratio (Zmax < 18) ........       5.57 Note
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ...............    0.00669 Ang.
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.557         4 Report
PLAT915_ALERT_3_C No Flack x Check Done: Low Friedel Pair Coverage        73 %
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/SigmaW > 10 Outliers ....         1 Check
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density.         0 Info
```

Alert level G

```
PLAT032_ALERT_4_G Std. Uncertainty on Flack Parameter Value High .     0.300 Report
PLAT371_ALERT_2_G Long   C(sp2)-C(sp1) Bond  C9       - C12      .      1.44 Ang.
PLAT371_ALERT_2_G Long   C(sp2)-C(sp1) Bond  C13      - C14      .      1.43 Ang.
PLAT371_ALERT_2_G Long   C(sp2)-C(sp1) Bond  C19      - C50      .      1.43 Ang.
PLAT371_ALERT_2_G Long   C(sp2)-C(sp1) Bond  C29      - C32      .      1.43 Ang.
PLAT371_ALERT_2_G Long   C(sp2)-C(sp1) Bond  C33      - C34      .      1.43 Ang.
PLAT371_ALERT_2_G Long   C(sp2)-C(sp1) Bond  C39      - C41      .      1.44 Ang.
PLAT371_ALERT_2_G Long   C(sp2)-C(sp1) Bond  C42      - C43      .      1.42 Ang.
PLAT371_ALERT_2_G Long   C(sp2)-C(sp1) Bond  C48      - C49      .      1.43 Ang.
PLAT371_ALERT_2_G Long   C(sp2)-C(sp1) Bond  C59      - C62      .      1.43 Ang.
PLAT371_ALERT_2_G Long   C(sp2)-C(sp1) Bond  C60      - C100     .      1.44 Ang.
PLAT371_ALERT_2_G Long   C(sp2)-C(sp1) Bond  C63      - C64      .      1.44 Ang.
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PLAT371_ALERT_2_G Long   C(sp2)-C(sp1) Bond  C83      - C84      .      1.43 Ang.
PLAT371_ALERT_2_G Long   C(sp2)-C(sp1) Bond  C92      - C93      .      1.44 Ang.
PLAT371_ALERT_2_G Long   C(sp2)-C(sp1) Bond  C98      - C99      .      1.43 Ang.
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still       92% Note
PLAT916_ALERT_2_G Hooft y and Flack x Parameter Values Differ by .      0.10 Check
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   1 ALERT level B = A potentially serious problem, consider carefully
   7 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  19 ALERT level G = General information/check it is not something unexpected

   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data


18 ALERT type 2 Indicator that the structure model may be wrong or deficient
 7 ALERT type 3 Indicator that the structure quality may be low
 2 ALERT type 4 Improvement, methodology, query or suggestion
 0 ALERT type 5 Informative message, check
```

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

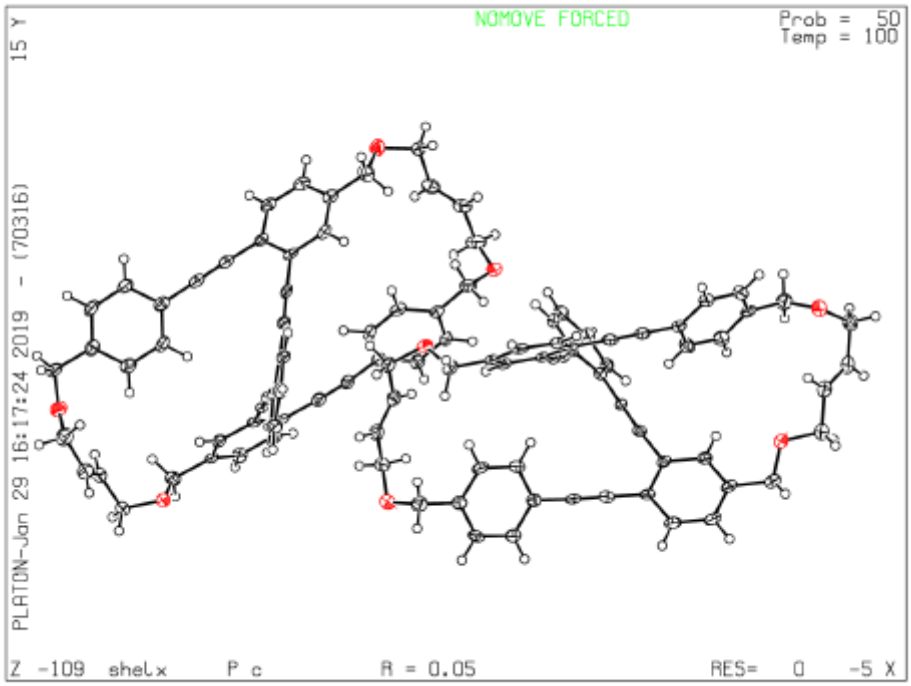
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 06/01/2019; check.def file version of 19/12/2018

Datablock shelx - ellipsoid plot



THEORETICAL CALCULATIONS

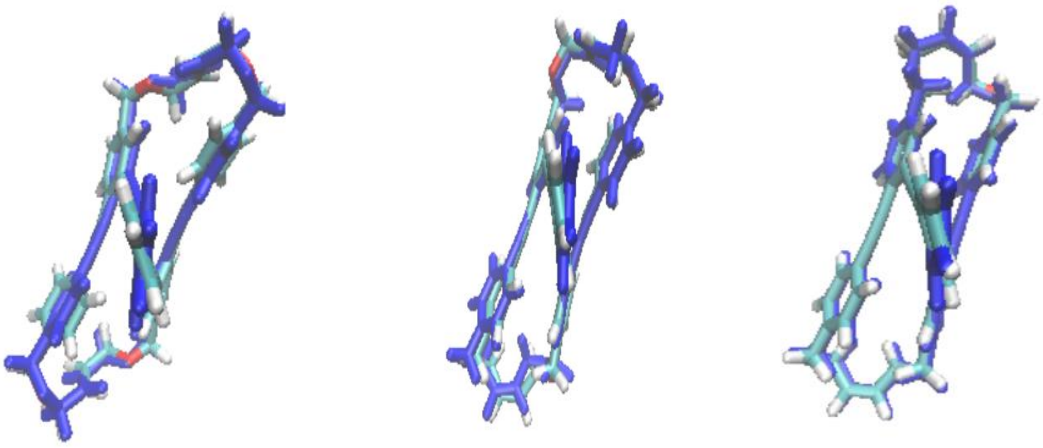
Methods of calculations

DFT and TD-DFT calculations have been performed using Gaussian program[S9] to obtain optimized structures of the ground and first excited singlet state, dipole and rotational strengths. The M06-2X functional and def2-SVP basis set have been used. Calculated CD and absorption spectra have been obtained assuming Gaussian bands, 0.2 eV bandwidth. 20nm wavelength red-shift has been applied to calculated spectra.

Comparison of calculated structures

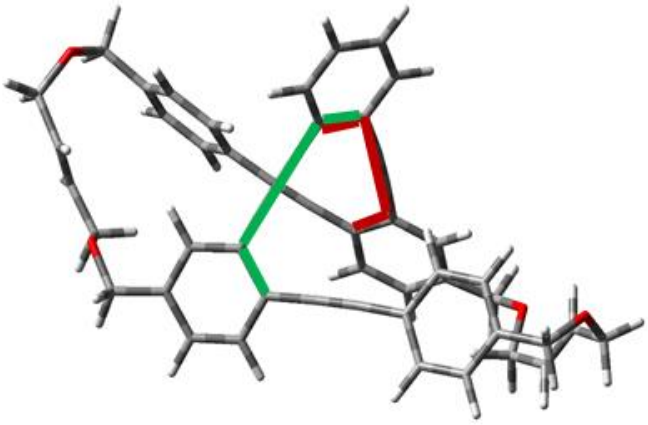
Figure S12. Superposition of the optimized structures in the ground (dark blue) and first excited state (coloured by the atom type) for the three compounds (*E*-*E*)-**1** (left) (*E*-*Z*)-**1** (center) and (*Z*-*Z*)-**1** (right).

(*E*,*E*)-**1** (*E*,*Z*)-**1** (*Z*,*Z*)-**1**



It is known that diphenylacetylene moieties are quite flexible[S10]. In particular calculations show differences between ground and excited state structures as illustrated by the figure above and as indicated by the dihedral angles τ1 and τ2 reported below. In fact, in all cases the dihedral angles within the diphenylacetylene bridge moiety (defined in the figure below), imparting some strain to the structure, show changes considering ground and excited state, while the diphenylacetylenes connected by the O-CH_2-CH=CH-CH_2-O staples show high conformational flexibility. A detailed analysis of the phenyl-O-CH_2-CH=CH-CH_2-O-phenyl conformations is beyond the scope of this work, but in all tested cases a decrease in τ1 and τ2 value in the excited state is obtained.

Figure S13. Definition of the relevant dihedral angles angles τ1 (green) and τ2 (red) for the comparison of ground and excited state geometry.



	τ1	τ2
(*E*-*E*)-**1**-**G**	38	38
(*E*-*E*)-**1**-**E**	19	19
(*E*-*Z*)-**1**-**G**	29	31
(*E*-*Z*)-**1**-**E**	21	15
(*Z*-*Z*)-**1**-**G**	34	30
(*Z*-*Z*)-**1**-**E**	14	19

Calculated spectroscopic properties

On the optimized structures, dipole and rotational strengths have been calculated as illustrated in Table S3, together with absorption and CD spectra plotted in figure S14. These calculations permit, inter alia, to assign the absolute configuration to the separated enantiomers and to account for the observed high g_{lum} value. The values of g_{abs} reported in the table are overestimated due to the fact that in all cases the second transition bears a rotational strength of opposite sign (see Figure S11), and also because of some flexibility of the structures.

Table S3: Parameters characterizing the spectroscopic properties for the examined compounds, and for the model molecules used for comparison to test the variation of dissymmetry factor with different staples:
Transition energy (eV) and transition wavelength (nm), magnitude of the electric and magnetic transition dipole moments, $|\langle 0|\mu|e\rangle|$, $|\langle 0|m|e\rangle|$ (atomic units), and angle formed by $\langle 0|\mu|e\rangle$ and $\langle 0|m|e\rangle$; Dipole Strength (D 10^{-40} esu^2 cm^2), Rotational Strengths (R 10^{-40} esu^2 cm^2), dissymmetry ratio.

	eV	nm	|μ| (a.u.)	|m|(a.u.)	angle	R	D	G	g_{lum}/g_{abs}
(*E*-*E*)-1-G	3.74	331	1.68	3.24	21	1245	181839	2.7E-02	**1.18**
(*E*-*E*)-1-E	2.82	439	1.38	3.02	15	1001	123531	3.2E-02	
(*E*-*Z*)-1-G	3.68	337	1.33	3.42	22	1045	114811	3.6E-02	**0.98**
(*E*-*Z*)-1-E	2.78	447	1.14	3.06	29	752	84173	3.6E-02	
(*Z*-*Z*)-1-G	3.71	334	1.29	3.46	11	1079	108186	4.0E-02	**0.80**
(*Z*-*Z*)-1-E	2.98	416	1.32	3.50	37	902	113116	3.2E-02	
model1-G	3.78	328	1.19	3.44	5	1009	91735	4.4E-02	**0.57**
model1-E	3.03	409	1.47	3.21	40	885	140332	2.5E-02	
model2-G	3.77	329	1.53	3.58	14	1296	150607	3.4E-02	**1.62**
model2-E	2.77	447	0.94	3.93	30	801	57409	5.6E-02	
model3-G	3.73	333	1.26	3.40	18	1006	102141	3.9E-02	**0.86**
model3-E	2.97	418	1.29	3.15	25	905	107315	3.4E-02	

Beside compound **1**, other model molecules have been considered through calculations (see Figure S11): an open model compound composed of four diphenylacetylene units shaped analogously as the synthesized compounds **1** but without staples (**model1**: no staple) and two molecules with shorter staples (**model2:** staple O-CH_2-CH_2-O and **model3:** staple O-$C(CH_3)_2$-O). For **model1**, the analogous dihedral angles τ1 and τ2 change from 32° in the ground state to 16° in the excited state.

Figure S14. Calculated structure of **model1**, **model2** and **model3**

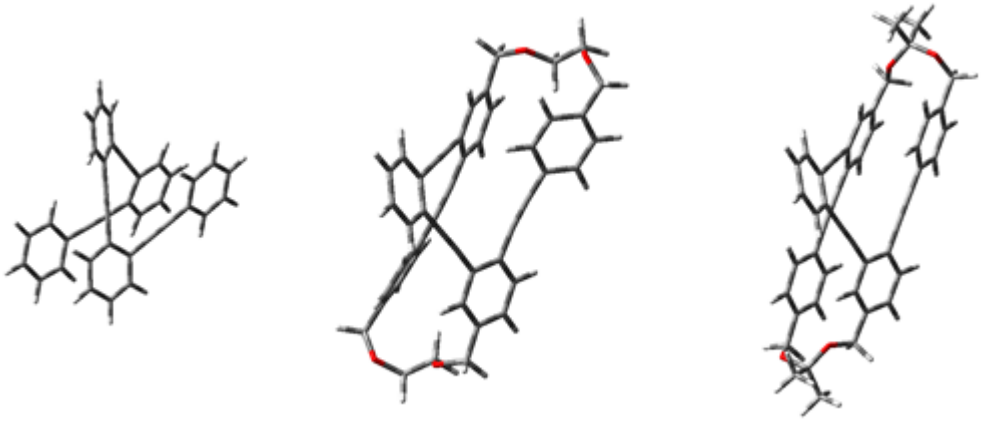
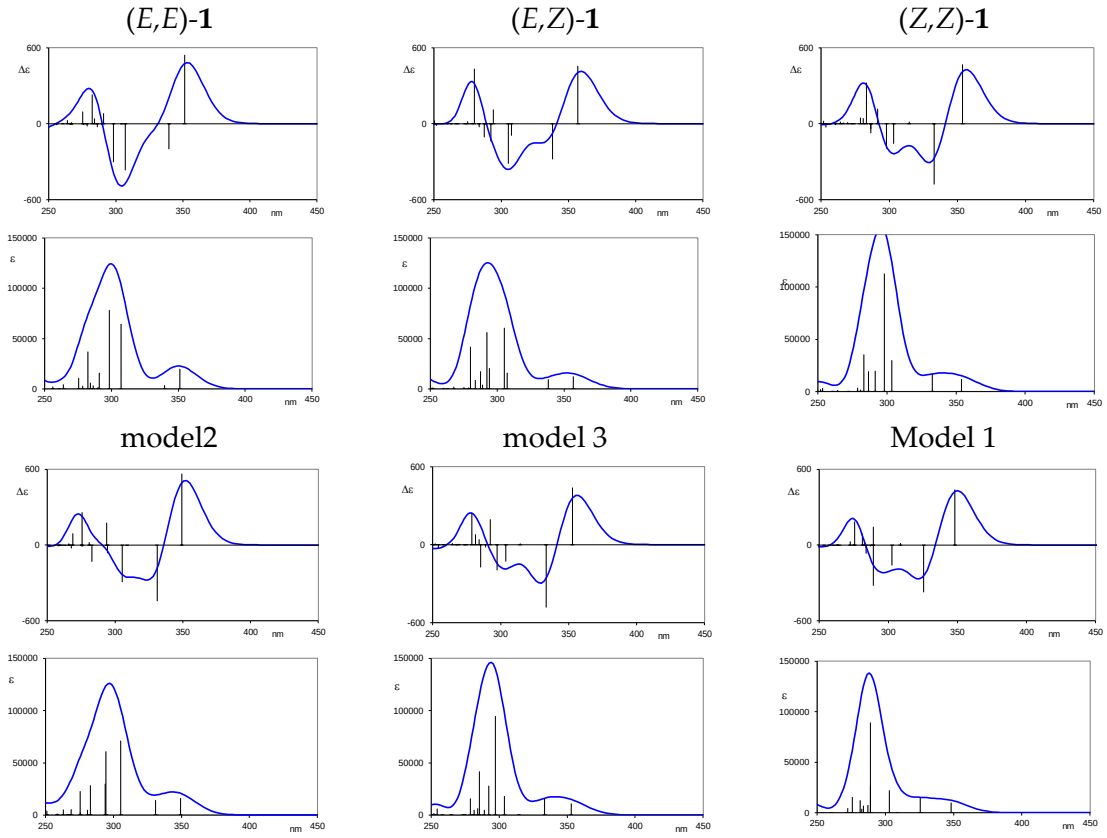
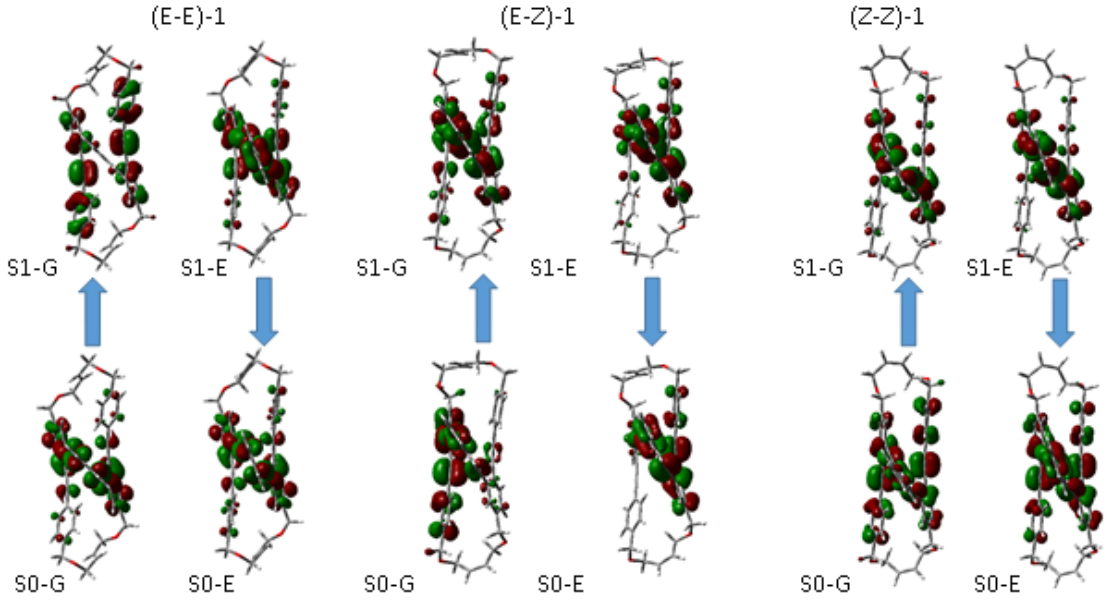


Figure S15. Calculated CD and absorption spectra of compounds reported in Table S3. All calculated spectra have been red shifted by 20 nm.



All transitions responsible of the first absorption band and of the emission band involve only the HOMO and LUMO states that are illustrated in figure **S15**.

Figure S16. Representation of the HOMO LUMO orbitals involved in the first absorption S0→S1 (S0-G, S1-G calculated in the ground state geometry) and in the emissive transition S1→S0 (S0-E, S1-E calculated in the first excited state geometry).



For (Z,Z)-**1** S0→S1 presents some charge transfer character from the bridge to the lateral diphenylacetylene groups, the emission process appears instead more localized on the bridge, in all cases the bridge of two fused *orto* diphenylacetylene is highly involved in the transitions

Considering calculated spectra in comparison with the experimental ones reported in Figure 4, we obtain a good correspondence and configuration assignment. The open compound has been optimized also by fixing the two torsional angles τ1 and τ2 at 20° and 50°.

Atomic coordinates of the DFT optimized structures

Optimized structures of the model molecule and the three compounds shown in Table 1 in the ground (G) and excited state (E). m062x/def2SVP, pcm dichloromethane

Model-G

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.567348	5.733350	-0.408094
2	6	0	1.131888	4.529940	-0.816796
3	6	0	0.573567	3.305215	-0.417508
4	6	0	-0.573423	3.305310	0.417338
5	6	0	-1.131667	4.530129	0.816445
6	6	0	-0.567054	5.733444	0.407565
7	6	0	1.152289	2.069116	-0.852144
8	6	0	-1.152210	2.069310	0.852175
9	6	0	1.636935	1.015529	-1.217396
10	6	0	-1.636887	1.015791	1.217581
11	6	0	-2.212247	-0.237351	1.603860
12	6	0	2.212230	-0.237615	-1.603768
13	6	0	3.602490	-0.356291	-1.753034
14	6	0	4.177309	-1.579904	-2.076319
15	6	0	3.370375	-2.706541	-2.253167
16	6	0	1.989832	-2.604300	-2.119103
17	6	0	1.389848	-1.375258	-1.801578
18	6	0	-1.389911	-1.375027	1.801660
19	6	0	-1.989949	-2.604061	2.119119
20	6	0	-3.370500	-2.706254	2.253143
21	6	0	-4.177388	-1.579579	2.076315
22	6	0	-3.602515	-0.355977	1.753088
23	6	0	-0.034681	-1.269505	-1.699891
24	6	0	-1.244393	-1.166610	-1.636289
25	6	0	0.034625	-1.269303	1.700020
26	6	0	1.244339	-1.166428	1.636423
27	6	0	2.669208	-1.017993	1.561270
28	6	0	3.248551	0.257879	1.681367
29	6	0	4.629085	0.407162	1.594620
30	6	0	5.445886	-0.707748	1.391448
31	6	0	4.876295	-1.976260	1.275295
32	6	0	3.495469	-2.135206	1.357274
33	6	0	-2.669255	-1.018099	-1.561156

34	6	0	-3.495591	-2.135294	-1.357364
35	6	0	-4.876411	-1.976278	-1.275418
36	6	0	-5.445922	-0.707714	-1.391403
37	6	0	-4.629046	0.407177	-1.594375
38	6	0	-3.248517	0.257825	-1.681086
39	1	0	1.012275	6.676120	-0.728280
40	1	0	2.014175	4.521904	-1.457357
41	1	0	-2.013952	4.522242	1.457012
42	1	0	-1.011923	6.676288	0.727613
43	1	0	4.226203	0.523844	-1.593291
44	1	0	3.819702	-3.669281	-2.500150
45	1	0	1.353467	-3.477533	-2.265837
46	1	0	-1.353620	-3.477322	2.265841
47	1	0	-3.819870	-3.668983	2.500090
48	1	0	-4.226190	0.524188	1.593362
49	1	0	2.601986	1.123260	1.833846
50	1	0	5.072084	1.400022	1.686419
51	1	0	5.511684	-2.848383	1.113144
52	1	0	3.043852	-3.123189	1.257714
53	1	0	-3.044038	-3.123320	-1.257939
54	1	0	-5.511858	-2.848388	-1.113426
55	1	0	-5.071983	1.400077	-1.686044
56	1	0	-2.601895	1.123190	-1.833414
57	1	0	5.260372	-1.658708	-2.178817
58	1	0	6.528191	-0.586634	1.324727
59	1	0	-5.260457	-1.658343	2.178781
60	1	0	-6.528222	-0.586542	-1.324707

Model-E

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.675061	5.689084	-0.232566
2	6	0	1.325847	4.507899	-0.485885
3	6	0	0.668504	3.256489	-0.296009
4	6	0	-0.668843	3.256504	0.295961
5	6	0	-1.326145	4.507977	0.485843
6	6	0	-0.675296	5.689113	0.232553
7	6	0	1.232466	2.066549	-0.732900
8	6	0	-1.232827	2.066606	0.732795
9	6	0	1.664540	0.991483	-1.171360
10	6	0	-1.664877	0.991505	1.171283
11	6	0	-2.171108	-0.229106	1.617547
12	6	0	2.171032	-0.229140	-1.617514

13	6	0	3.567888	-0.397693	-1.828565
14	6	0	4.081412	-1.623884	-2.196688
15	6	0	3.227615	-2.730779	-2.372877
16	6	0	1.859106	-2.592710	-2.187485
17	6	0	1.299721	-1.354033	-1.828987
18	6	0	-1.299588	-1.353933	1.828840
19	6	0	-1.858796	-2.592743	2.187262
20	6	0	-3.227231	-2.730990	2.372842
21	6	0	-4.081225	-1.624140	2.196928
22	6	0	-3.567945	-0.397872	1.828870
23	6	0	-0.105138	-1.203289	-1.699119
24	6	0	-1.315772	-1.060942	-1.619977
25	6	0	0.105193	-1.202967	1.698965
26	6	0	1.315838	-1.060475	1.619904
27	6	0	2.736413	-0.948303	1.524037
28	6	0	3.371731	0.303698	1.647199
29	6	0	4.755176	0.394734	1.557131
30	6	0	5.526608	-0.752943	1.344823
31	6	0	4.904305	-1.994562	1.214677
32	6	0	3.518485	-2.096653	1.301054
33	6	0	-2.736365	-0.948653	-1.524050
34	6	0	-3.518518	-2.096883	-1.300811
35	6	0	-4.904325	-1.994649	-1.214378
36	6	0	-5.526522	-0.752998	-1.344725
37	6	0	-4.755004	0.394562	-1.557296
38	6	0	-3.371564	0.303374	-1.647425
39	1	0	1.183411	6.637814	-0.407802
40	1	0	2.342580	4.504735	-0.880630
41	1	0	-2.342888	4.504855	0.880563
42	1	0	-1.183604	6.637866	0.407788
43	1	0	4.225164	0.457778	-1.668616
44	1	0	3.640627	-3.698346	-2.660233
45	1	0	1.192891	-3.443294	-2.336424
46	1	0	-1.192447	-3.443252	2.336027
47	1	0	-3.640098	-3.698635	2.660147
48	1	0	-4.225348	0.457538	1.669113
49	1	0	2.763187	1.195726	1.804718
50	1	0	5.239587	1.367442	1.654777
51	1	0	5.501825	-2.890771	1.040825
52	1	0	3.025704	-3.063888	1.193069
53	1	0	-3.025824	-3.064145	-1.192676
54	1	0	-5.501918	-2.890768	-1.040318
55	1	0	-5.239326	1.367297	-1.655113
56	1	0	-2.762949	1.195315	-1.805165
57	1	0	5.156778	-1.738631	-2.339719
58	1	0	6.612763	-0.675516	1.277485
59	1	0	-5.156550	-1.739067	2.340123

60	1	0	-6.612667	-0.675464	-1.277327

(E-E)-1-G

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.504241	0.482974	5.783446
2	6	0	-1.010863	0.964127	4.579830
3	6	0	-0.515905	0.487870	3.357186
4	6	0	0.515905	-0.487870	3.357186
5	6	0	1.010863	-0.964127	4.579830
6	6	0	0.504241	-0.482974	5.783446
7	6	0	-1.040741	0.963072	2.110924
8	6	0	1.040741	-0.963072	2.110924
9	6	0	-1.437554	1.324545	1.020388
10	6	0	1.437554	-1.324545	1.020388
11	6	0	1.869663	-1.700322	-0.293127
12	6	0	-1.869663	1.700322	-0.293127
13	6	0	-2.205660	3.028538	-0.586980
14	6	0	-2.666116	3.389745	-1.854431
15	6	0	-2.736782	2.416640	-2.855584
16	6	0	-2.401248	1.094471	-2.585186
17	6	0	-1.984293	0.709458	-1.303183
18	6	0	1.984293	-0.709458	-1.303183
19	6	0	2.401248	-1.094471	-2.585186
20	6	0	2.736782	-2.416640	-2.855584
21	6	0	2.666116	-3.389745	-1.854431
22	6	0	2.205660	-3.028538	-0.586980
23	6	0	-1.762966	-0.674517	-1.007793
24	6	0	-1.690148	-1.858971	-0.740358
25	6	0	1.762966	0.674517	-1.007793
26	6	0	1.690148	1.858971	-0.740358
27	6	0	1.719995	3.254975	-0.407603
28	6	0	1.114905	3.736899	0.767915
29	6	0	1.235112	5.076730	1.119835
30	6	0	1.963073	5.964118	0.320927
31	6	0	2.544348	5.490807	-0.858614
32	6	0	2.425659	4.153775	-1.225335
33	6	0	2.165974	7.401055	0.756186
34	6	0	-0.734387	7.546658	-0.137782
35	6	0	-0.504241	7.198312	-1.402980
36	6	0	-3.171147	4.794986	-2.105385
37	8	0	-2.424116	5.788369	-1.459981
38	6	0	-1.234563	6.114727	-2.129251

39	8	0	1.079024	7.971179	1.436320
40	6	0	-1.719995	-3.254975	-0.407603
41	6	0	-2.425659	-4.153775	-1.225335
42	6	0	-2.544348	-5.490807	-0.858614
43	6	0	-1.963073	-5.964118	0.320927
44	6	0	-1.235112	-5.076730	1.119835
45	6	0	-1.114905	-3.736899	0.767915
46	6	0	3.171147	-4.794986	-2.105385
47	8	0	2.424116	-5.788369	-1.459981
48	6	0	-2.165974	-7.401055	0.756186
49	8	0	-1.079024	-7.971179	1.436320
50	6	0	1.234563	-6.114727	-2.129251
51	6	0	0.504241	-7.198312	-1.402980
52	6	0	-0.102373	-8.558557	0.593764
53	6	0	0.734387	-7.546658	-0.137782
54	6	0	0.102373	8.558557	0.593764
55	1	0	-0.899858	0.861664	6.726505
56	1	0	-1.802524	1.713775	4.572445
57	1	0	1.802524	-1.713775	4.572445
58	1	0	0.899858	-0.861664	6.726505
59	1	0	-2.123745	3.788476	0.192452
60	1	0	-3.076075	2.693416	-3.856073
61	1	0	-2.477426	0.336250	-3.364965
62	1	0	2.477426	-0.336250	-3.364965
63	1	0	3.076075	-2.693416	-3.856073
64	1	0	2.123745	-3.788476	0.192452
65	1	0	0.563137	3.044148	1.404366
66	1	0	0.760299	5.450652	2.028773
67	1	0	3.100053	6.177865	-1.501360
68	1	0	2.891632	3.790595	-2.142280
69	1	0	3.017577	7.433109	1.455139
70	1	0	2.444905	8.015233	-0.120068
71	1	0	-1.519815	7.031244	0.422674
72	1	0	0.301653	7.683944	-1.966135
73	1	0	-4.196608	4.874134	-1.712586
74	1	0	-3.221336	4.983173	-3.193220
75	1	0	-1.457213	6.436526	-3.164904
76	1	0	-0.569739	5.228463	-2.210543
77	1	0	-2.891632	-3.790595	-2.142280
78	1	0	-3.100053	-6.177865	-1.501360
79	1	0	-0.760299	-5.450652	2.028773
80	1	0	-0.563137	-3.044148	1.404366
81	1	0	4.196608	-4.874134	-1.712586
82	1	0	3.221336	-4.983173	-3.193220
83	1	0	-3.017577	-7.433109	1.455139
84	1	0	-2.444905	-8.015233	-0.120068
85	1	0	0.569739	-5.228463	-2.210543

86	1	0	1.457213	-6.436526	-3.164904
87	1	0	-0.301653	-7.683944	-1.966135
88	1	0	0.522870	-9.177030	1.252087
89	1	0	-0.599250	-9.226388	-0.133865
90	1	0	1.519815	-7.031244	0.422674
91	1	0	-0.522870	9.177030	1.252087
92	1	0	0.599250	9.226388	-0.133865

(E-E)-1-E

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.235692	0.673389	5.580145
2	6	0	-0.494051	1.325005	4.399624
3	6	0	-0.300354	0.666002	3.151276
4	6	0	0.300354	-0.666002	3.151276
5	6	0	0.494051	-1.325005	4.399624
6	6	0	0.235692	-0.673389	5.580145
7	6	0	-0.736711	1.206206	1.949879
8	6	0	0.736711	-1.206206	1.949879
9	6	0	-1.147572	1.574363	0.841640
10	6	0	1.147572	-1.574363	0.841640
11	6	0	1.631206	-1.899104	-0.425885
12	6	0	-1.631206	1.899104	-0.425885
13	6	0	-1.953325	3.236699	-0.782762
14	6	0	-2.439650	3.537123	-2.040306
15	6	0	-2.561467	2.508025	-3.003751
16	6	0	-2.262305	1.195272	-2.683548
17	6	0	-1.833370	0.847820	-1.388294
18	6	0	1.833370	-0.847820	-1.388294
19	6	0	2.262305	-1.195272	-2.683548
20	6	0	2.561467	-2.508025	-3.003751
21	6	0	2.439650	-3.537123	-2.040306
22	6	0	1.953325	-3.236699	-0.782762
23	6	0	-1.697805	-0.509850	-1.009041
24	6	0	-1.685381	-1.678477	-0.648403
25	6	0	1.697805	0.509850	-1.009041
26	6	0	1.685381	1.678477	-0.648403
27	6	0	1.753164	3.053450	-0.273769
28	6	0	1.652157	3.449660	1.076120
29	6	0	1.764260	4.788464	1.422691
30	6	0	2.003488	5.767563	0.448381
31	6	0	2.099466	5.376119	-0.889437

32	6	0	1.967719	4.040213	-1.255138
33	6	0	2.183318	7.209445	0.870218
34	6	0	-0.678661	7.428613	0.093587
35	6	0	-0.525651	7.427112	-1.230795
36	6	0	-2.945393	4.927320	-2.361928
37	8	0	-2.355462	5.933497	-1.586440
38	6	0	-1.200995	6.479589	-2.169698
39	8	0	1.147572	7.689701	1.694311
40	6	0	-1.753164	-3.053450	-0.273769
41	6	0	-1.967719	-4.040213	-1.255138
42	6	0	-2.099466	-5.376119	-0.889437
43	6	0	-2.003488	-5.767563	0.448381
44	6	0	-1.764260	-4.788464	1.422691
45	6	0	-1.652157	-3.449660	1.076120
46	6	0	2.945393	-4.927320	-2.361928
47	8	0	2.355462	-5.933497	-1.586440
48	6	0	-2.183318	-7.209445	0.870218
49	8	0	-1.147572	-7.689701	1.694311
50	6	0	1.200995	-6.479589	-2.169698
51	6	0	0.525651	-7.427112	-1.230795
52	6	0	-0.102414	-8.342130	0.997211
53	6	0	0.678661	-7.428613	0.093587
54	6	0	0.102414	8.342130	0.997211
55	1	0	-0.412644	1.179859	6.529539
56	1	0	-0.894809	2.339355	4.396354
57	1	0	0.894809	-2.339355	4.396354
58	1	0	0.412644	-1.179859	6.529539
59	1	0	-1.825686	4.030950	-0.045235
60	1	0	-2.922457	2.750180	-4.005662
61	1	0	-2.390705	0.404596	-3.423626
62	1	0	2.390705	-0.404596	-3.423626
63	1	0	2.922457	-2.750180	-4.005662
64	1	0	1.825686	-4.030950	-0.045235
65	1	0	1.490323	2.691294	1.842931
66	1	0	1.676353	5.089704	2.468566
67	1	0	2.270447	6.131678	-1.660175
68	1	0	2.039899	3.744825	-2.302823
69	1	0	3.110722	7.291124	1.459389
70	1	0	2.304509	7.847524	-0.023390
71	1	0	-1.360552	6.708922	0.557071
72	1	0	0.175654	8.130412	-1.695811
73	1	0	-4.027285	4.954187	-2.153322
74	1	0	-2.823217	5.133352	-3.440431
75	1	0	-1.461338	7.000709	-3.110482
76	1	0	-0.481828	5.677581	-2.440359
77	1	0	-2.039899	-3.744825	-2.302823
78	1	0	-2.270447	-6.131678	-1.660175

79	1	0	-1.676353	-5.089704	2.468566
80	1	0	-1.490323	-2.691294	1.842931
81	1	0	4.027285	-4.954187	-2.153322
82	1	0	2.823217	-5.133352	-3.440431
83	1	0	-3.110722	-7.291124	1.459389
84	1	0	-2.304509	-7.847524	-0.023390
85	1	0	0.481828	-5.677581	-2.440359
86	1	0	1.461338	-7.000709	-3.110482
87	1	0	-0.175654	-8.130412	-1.695811
88	1	0	0.547042	-8.769101	1.773781
89	1	0	-0.518449	-9.176801	0.402598
90	1	0	1.360552	-6.708922	0.557071
91	1	0	-0.547042	8.769101	1.773781
92	1	0	0.518449	9.176801	0.402598

(E-Z)-1-G

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	7.237465	-2.632064	-1.620027
2	1	0	7.724978	-2.257754	-2.530349
3	1	0	7.659411	-3.626941	-1.391328
4	6	0	7.463495	-1.675389	-0.478139
5	6	0	7.577348	-0.360321	-0.666524
6	6	0	7.648066	0.645961	0.438703
7	1	0	8.548261	1.278630	0.324102
8	1	0	6.778141	1.321938	0.336176
9	6	0	6.838578	0.648405	2.658124
10	1	0	7.070572	1.725935	2.732391
11	1	0	7.097307	0.185928	3.621581
12	6	0	5.360143	0.462787	2.387518
13	6	0	4.820883	-0.827403	2.284659
14	1	0	5.483757	-1.691374	2.374580
15	6	0	3.455069	-1.018577	2.102162
16	1	0	3.039417	-2.026044	2.039744
17	6	0	2.595637	0.090287	2.006770
18	6	0	3.141237	1.383456	2.057415
19	1	0	2.478159	2.244334	1.960347
20	6	0	4.508347	1.561570	2.249146
21	1	0	4.918167	2.572623	2.306017
22	6	0	1.169769	-0.042019	1.903939
23	6	0	-0.045569	-0.009268	1.875513
24	6	0	-1.465534	0.181157	1.885678
25	6	0	-2.322111	-0.683555	2.578617

26	1	0	-1.901589	-1.561635	3.069645
27	6	0	-3.686298	-0.415501	2.671215
28	1	0	-4.338269	-1.080714	3.238490
29	6	0	-4.230127	0.722332	2.069418
30	6	0	-3.390484	1.575327	1.353372
31	1	0	-3.802078	2.459015	0.859841
32	6	0	-2.019689	1.320018	1.243785
33	6	0	-5.695949	1.078615	2.213252
34	1	0	-5.773697	2.040508	2.743407
35	1	0	-6.137714	1.229821	1.209393
36	6	0	-7.001393	-0.891109	2.170822
37	1	0	-7.271878	-1.691412	2.877019
38	1	0	-6.259575	-1.310233	1.466436
39	6	0	-8.692742	-0.814661	0.271940
40	6	0	-8.073780	-1.886629	-0.577182
41	1	0	-7.103573	-2.203932	-0.160183
42	1	0	-8.727786	-2.771501	-0.582955
43	6	0	-7.148547	-0.378898	-2.167853
44	1	0	-7.501769	0.487276	-1.578943
45	1	0	-7.290833	-0.125714	-3.229703
46	6	0	-5.671650	-0.586886	-1.903880
47	6	0	-5.123993	-1.871897	-1.833486
48	1	0	-5.777636	-2.737786	-1.949948
49	6	0	-3.761733	-2.050373	-1.619642
50	1	0	-3.343122	-3.055324	-1.552417
51	6	0	-2.905816	-0.940582	-1.507953
52	6	0	-3.450918	0.350019	-1.610768
53	1	0	-2.790200	1.215355	-1.541363
54	6	0	-4.820533	0.517914	-1.785870
55	1	0	-5.235837	1.527366	-1.844825
56	6	0	-1.500159	-1.154429	-1.316701
57	6	0	-0.321223	-1.422638	-1.184155
58	6	0	1.036141	-1.867680	-1.084289
59	6	0	1.284212	-3.231455	-0.863744
60	1	0	0.436848	-3.905216	-0.734256
61	6	0	2.583347	-3.724924	-0.834087
62	1	0	2.752960	-4.791726	-0.674552
63	6	0	3.671390	-2.868828	-1.025488
64	6	0	3.438923	-1.509157	-1.231881
65	1	0	4.289305	-0.839973	-1.373219
66	6	0	2.137231	-0.990396	-1.252977
67	6	0	5.087248	-3.378945	-0.960643
68	1	0	5.482949	-3.160700	0.049112
69	1	0	5.105729	-4.477005	-1.085825
70	6	0	1.929546	0.416341	-1.428738
71	6	0	1.755151	1.613260	-1.550066
72	6	0	1.530620	3.021585	-1.691215

73	6	0	2.398864	3.803951	-2.468398
74	1	0	3.248217	3.322477	-2.953718
75	6	0	2.178084	5.168730	-2.622987
76	1	0	2.861713	5.761648	-3.231606
77	6	0	1.083245	5.776020	-2.003661
78	1	0	0.907776	6.845390	-2.125759
79	6	0	0.213737	5.017975	-1.226283
80	1	0	-0.640190	5.485588	-0.735405
81	6	0	0.423116	3.640910	-1.055432
82	6	0	-0.462769	2.864848	-0.239193
83	6	0	-1.183822	2.179617	0.460013
84	8	0	5.863399	-2.746418	-1.943712
85	8	0	7.653765	0.021930	1.697866
86	8	0	-6.423719	0.134754	2.949359
87	8	0	-7.941881	-1.512124	-1.933582
88	1	0	-9.616147	-0.377496	-0.123052
89	1	0	7.462874	-2.053556	0.547468
90	1	0	7.590912	0.049767	-1.683335
91	6	0	-8.232229	-0.399011	1.455074
92	1	0	-8.797009	0.356399	2.012291

(E-Z)-1-E

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	6.881397	-3.224566	-1.296586
2	1	0	7.335473	-3.152508	-2.294307
3	1	0	7.244888	-4.154392	-0.823989
4	6	0	7.256940	-2.019207	-0.470709
5	6	0	7.405993	-0.812476	-1.018806
6	6	0	7.647391	0.450693	-0.253760
7	1	0	8.549257	0.961433	-0.640024
8	1	0	6.797714	1.132178	-0.449389
9	6	0	7.091193	1.113221	1.944317
10	1	0	7.347265	2.157409	1.690330
11	1	0	7.444387	0.925175	2.968992
12	6	0	5.592195	0.920256	1.876829
13	6	0	5.047393	-0.351480	2.109277
14	1	0	5.718280	-1.185849	2.326175
15	6	0	3.674898	-0.555962	2.079749
16	1	0	3.253893	-1.544968	2.268065
17	6	0	2.803431	0.525359	1.808890
18	6	0	3.354361	1.802225	1.552713
19	1	0	2.685178	2.635529	1.332471

20	6	0	4.729751	1.986227	1.587078
21	1	0	5.146314	2.977249	1.392159
22	6	0	1.400013	0.352991	1.784243
23	6	0	0.171584	0.266459	1.819476
24	6	0	-1.223387	0.332294	1.888723
25	6	0	-2.000823	-0.631618	2.573462
26	1	0	-1.505043	-1.518454	2.970013
27	6	0	-3.346805	-0.428184	2.786754
28	1	0	-3.935261	-1.158530	3.343274
29	6	0	-3.993958	0.753915	2.322228
30	6	0	-3.285454	1.670706	1.581508
31	1	0	-3.780033	2.555114	1.173662
32	6	0	-1.904067	1.474281	1.297954
33	6	0	-5.433467	1.025153	2.705830
34	1	0	-5.441958	1.648075	3.614320
35	1	0	-5.929456	1.608898	1.908241
36	6	0	-6.673698	-0.809929	1.890134
37	1	0	-6.903418	-1.833089	2.223904
38	1	0	-5.909447	-0.892470	1.090380
39	6	0	-8.611610	-0.470377	0.285620
40	6	0	-8.258139	-1.624908	-0.607232
41	1	0	-7.314108	-2.089534	-0.274229
42	1	0	-9.041181	-2.395235	-0.541388
43	6	0	-7.328563	-0.215818	-2.286148
44	1	0	-7.644208	0.715184	-1.782910
45	1	0	-7.436571	-0.053170	-3.369600
46	6	0	-5.874948	-0.483667	-1.962172
47	6	0	-5.371084	-1.790081	-1.974691
48	1	0	-6.046644	-2.618045	-2.198435
49	6	0	-4.032045	-2.036363	-1.700591
50	1	0	-3.648338	-3.057355	-1.703096
51	6	0	-3.149813	-0.970957	-1.435916
52	6	0	-3.651393	0.341677	-1.444177
53	1	0	-2.972486	1.173583	-1.255488
54	6	0	-5.002557	0.573449	-1.685960
55	1	0	-5.383545	1.597668	-1.669491
56	6	0	-1.767003	-1.251602	-1.185773
57	6	0	-0.609062	-1.573765	-0.989365
58	6	0	0.722606	-2.055711	-0.801537
59	6	0	0.927992	-3.407352	-0.494968
60	1	0	0.059044	-4.055511	-0.376606
61	6	0	2.212633	-3.928205	-0.357479
62	1	0	2.345305	-4.986118	-0.123366
63	6	0	3.333524	-3.108751	-0.535085
64	6	0	3.150589	-1.762637	-0.837886
65	1	0	4.023081	-1.118995	-0.970781
66	6	0	1.860010	-1.205874	-0.956168

67	6	0	4.737109	-3.632494	-0.377299
68	1	0	5.181169	-3.167581	0.523449
69	1	0	4.727222	-4.725571	-0.213572
70	6	0	1.728599	0.181929	-1.179494
71	6	0	1.707575	1.401052	-1.352144
72	6	0	1.652062	2.783962	-1.550478
73	6	0	2.722761	3.481840	-2.168864
74	1	0	3.632453	2.930167	-2.409667
75	6	0	2.597501	4.811385	-2.501734
76	1	0	3.421173	5.326327	-2.997326
77	6	0	1.389760	5.515260	-2.230257
78	1	0	1.300794	6.562840	-2.519997
79	6	0	0.348373	4.892964	-1.588925
80	1	0	-0.565471	5.436575	-1.347095
81	6	0	0.459821	3.530596	-1.177740
82	6	0	-0.479746	2.917164	-0.365430
83	6	0	-1.199448	2.291022	0.428907
84	8	0	5.485569	-3.300980	-1.519194
85	8	0	7.786789	0.205736	1.123584
86	8	0	-6.153002	-0.137523	3.014103
87	8	0	-8.190285	-1.281388	-1.977030
88	1	0	-9.514776	0.089017	0.020898
89	1	0	7.351848	-2.116029	0.614114
90	1	0	7.325356	-0.694296	-2.106074
91	6	0	-7.921416	-0.126672	1.375489
92	1	0	-8.284505	0.693949	2.003819

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	7.604273	-1.954621	-2.386607
2	1	0	7.760108	-1.241764	-3.217304
3	1	0	7.782467	-2.961222	-2.796982
4	6	0	8.618904	-1.667135	-1.307371
5	6	0	7.368038	-2.491050	0.768884
6	1	0	6.413003	-2.378565	0.232715
7	1	0	7.553522	-3.571593	0.876781
8	6	0	6.818771	-0.670454	2.175375
9	1	0	7.324105	-0.017371	1.437343
10	1	0	7.105688	-0.300792	3.172015
11	6	0	5.315757	-0.545719	2.021174
12	6	0	4.724069	0.719292	1.911152
13	1	0	5.356127	1.610817	1.888031

14	6	0	3.342717	0.857081	1.843492
15	1	0	2.886734	1.845344	1.762639
16	6	0	2.517560	-0.281690	1.864075
17	6	0	3.112736	-1.549840	1.953091
18	1	0	2.477977	-2.436962	1.964821
19	6	0	4.495515	-1.676018	2.042604
20	1	0	4.949876	-2.662830	2.140304
21	6	0	1.087975	-0.172370	1.820379
22	6	0	-0.127631	-0.133047	1.822063
23	6	0	-1.557578	-0.147284	1.900111
24	6	0	-2.220385	-1.311864	2.316325
25	1	0	-1.629033	-2.198871	2.545446
26	6	0	-3.604167	-1.339007	2.458741
27	1	0	-4.100407	-2.244766	2.808882
28	6	0	-4.369866	-0.203760	2.176972
29	6	0	-3.723908	0.955051	1.749506
30	1	0	-4.305673	1.849524	1.514252
31	6	0	-2.331591	1.002424	1.604594
32	6	0	-5.874029	-0.192829	2.363284
33	1	0	-6.130750	0.549788	3.134226
34	1	0	-6.357313	0.138933	1.424083
35	6	0	-6.703465	-2.316067	1.737763
36	1	0	-6.796744	-3.309801	2.202845
37	1	0	-5.874170	-2.371007	1.009126
38	6	0	-8.326793	-2.128684	-0.208801
39	6	0	-7.459694	-2.780248	-1.247364
40	1	0	-6.439595	-2.946582	-0.862020
41	1	0	-7.873766	-3.767109	-1.503330
42	6	0	-6.895491	-0.765712	-2.369252
43	1	0	-7.408816	-0.176879	-1.587144
44	1	0	-7.112102	-0.279405	-3.332860
45	6	0	-5.401665	-0.724882	-2.121325
46	6	0	-4.592773	-1.832164	-2.397649
47	1	0	-5.054126	-2.749600	-2.767004
48	6	0	-3.216300	-1.769659	-2.209023
49	1	0	-2.592825	-2.639803	-2.418445
50	6	0	-2.611288	-0.580140	-1.766784
51	6	0	-3.421742	0.538191	-1.508376
52	1	0	-2.957150	1.467374	-1.175342
53	6	0	-4.800794	0.454424	-1.667521
54	1	0	-5.421793	1.326838	-1.447904
55	6	0	-1.185935	-0.515139	-1.614686
56	6	0	0.027732	-0.498515	-1.536377
57	6	0	1.459603	-0.530612	-1.514831
58	6	0	2.133800	-1.748390	-1.692532
59	1	0	1.546780	-2.659725	-1.811389
60	6	0	3.523830	-1.804061	-1.733826

61	1	0	4.034620	-2.754425	-1.886485
62	6	0	4.280664	-0.636569	-1.598905
63	6	0	3.622934	0.576961	-1.407408
64	1	0	4.199848	1.496719	-1.287917
65	6	0	2.226141	0.650613	-1.357077
66	6	0	5.785521	-0.642196	-1.675548
67	1	0	6.111300	0.081244	-2.447396
68	1	0	6.201150	-0.286499	-0.711274
69	6	0	1.607897	1.920582	-1.121687
70	6	0	1.135619	3.017814	-0.896478
71	6	0	0.564412	4.302965	-0.624993
72	6	0	1.158313	5.470887	-1.127605
73	1	0	2.065344	5.385506	-1.726550
74	6	0	0.596480	6.717167	-0.870218
75	1	0	1.068611	7.615858	-1.268650
76	6	0	-0.569220	6.816832	-0.106601
77	1	0	-1.010719	7.793583	0.094169
78	6	0	-1.169787	5.670139	0.402498
79	1	0	-2.077043	5.739938	1.003129
80	6	0	-0.614503	4.405263	0.155759
81	6	0	-1.221342	3.222213	0.686896
82	6	0	-1.712884	2.202070	1.128463
83	8	0	6.257257	-1.923453	-1.986945
84	8	0	7.286246	-1.987884	2.087294
85	8	0	-6.386784	-1.425826	2.786600
86	8	0	-7.427148	-2.060727	-2.462901
87	1	0	-9.319493	-1.822445	-0.556156
88	1	0	9.570247	-1.275206	-1.680682
89	6	0	-8.000020	-1.937280	1.072310
90	1	0	-8.736858	-1.494138	1.751067
91	6	0	8.513231	-1.876077	0.008674
92	1	0	9.376461	-1.632319	0.638562

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	7.808170	-1.957993	-2.169172
2	1	0	8.066459	-1.185433	-2.917175
3	1	0	8.030747	-2.931790	-2.633760
4	6	0	8.688175	-1.774028	-0.959362
5	6	0	7.141128	-2.561915	0.933623
6	1	0	6.256071	-2.364205	0.309299
7	1	0	7.234040	-3.655745	1.023912

8	6	0	6.566939	-0.744546	2.332241
9	1	0	7.150587	-0.114323	1.632960
10	1	0	6.817491	-0.399403	3.347831
11	6	0	5.085299	-0.528436	2.102458
12	6	0	4.572452	0.775840	2.019247
13	1	0	5.255959	1.627543	2.059556
14	6	0	3.208741	0.999161	1.902579
15	1	0	2.814612	2.014953	1.841305
16	6	0	2.312874	-0.091017	1.857454
17	6	0	2.833724	-1.398558	1.906209
18	1	0	2.147909	-2.245482	1.858637
19	6	0	4.201719	-1.609309	2.036022
20	1	0	4.595525	-2.624050	2.105787
21	6	0	0.902487	0.089902	1.792162
22	6	0	-0.320974	0.132114	1.776921
23	6	0	-1.733852	0.135417	1.834766
24	6	0	-2.417147	-0.998923	2.311184
25	1	0	-1.835687	-1.876896	2.594884
26	6	0	-3.794059	-0.997854	2.459240
27	1	0	-4.299872	-1.870574	2.872118
28	6	0	-4.554167	0.139315	2.103618
29	6	0	-3.910371	1.259922	1.614577
30	1	0	-4.485824	2.142510	1.325465
31	6	0	-2.498996	1.295371	1.455675
32	6	0	-6.061946	0.153370	2.273099
33	1	0	-6.335229	0.961512	2.968138
34	1	0	-6.536162	0.390254	1.301187
35	6	0	-6.827082	-2.044646	1.848038
36	1	0	-6.939567	-2.979792	2.418582
37	1	0	-5.959016	-2.172933	1.176290
38	6	0	-8.330552	-2.123549	-0.194630
39	6	0	-7.396651	-2.885741	-1.091268
40	1	0	-6.399818	-2.992671	-0.630214
41	1	0	-7.789432	-3.900733	-1.252806
42	6	0	-6.739379	-1.023985	-2.399360
43	1	0	-7.262574	-0.349186	-1.697373
44	1	0	-6.915774	-0.632675	-3.413473
45	6	0	-5.252892	-0.984889	-2.113836
46	6	0	-4.452160	-2.121509	-2.290821
47	1	0	-4.922109	-3.059203	-2.592510
48	6	0	-3.079057	-2.059389	-2.095009
49	1	0	-2.461457	-2.947241	-2.235486
50	6	0	-2.464515	-0.840745	-1.738916
51	6	0	-3.271338	0.300845	-1.562525
52	1	0	-2.801977	1.246843	-1.291600
53	6	0	-4.647411	0.218578	-1.735837
54	1	0	-5.261858	1.110202	-1.587399

55	6	0	-1.048312	-0.762653	-1.596723
56	6	0	0.170033	-0.719294	-1.511207
57	6	0	1.586714	-0.703433	-1.489373
58	6	0	2.308114	-1.891474	-1.701817
59	1	0	1.751773	-2.818259	-1.847091
60	6	0	3.694696	-1.898240	-1.744197
61	1	0	4.240757	-2.823746	-1.921941
62	6	0	4.414825	-0.698595	-1.568759
63	6	0	3.729714	0.482188	-1.351064
64	1	0	4.277838	1.415817	-1.207465
65	6	0	2.311847	0.523338	-1.299298
66	6	0	5.920858	-0.668056	-1.624462
67	1	0	6.244467	0.061486	-2.391339
68	1	0	6.312895	-0.303361	-0.653598
69	6	0	1.685849	1.749550	-1.059187
70	6	0	1.264724	2.893193	-0.840633
71	6	0	0.775361	4.183348	-0.667542
72	6	0	1.575368	5.316474	-0.999022
73	1	0	2.610154	5.148995	-1.300756
74	6	0	1.045147	6.582739	-0.989836
75	1	0	1.666473	7.433902	-1.270428
76	6	0	-0.322069	6.792166	-0.639823
77	1	0	-0.734080	7.801780	-0.655619
78	6	0	-1.112798	5.736498	-0.260532
79	1	0	-2.147869	5.896708	0.043806
80	6	0	-0.588190	4.411637	-0.206468
81	6	0	-1.310107	3.362185	0.344021
82	6	0	-1.869921	2.404104	0.892384
83	8	0	6.425226	-1.939157	-1.926008
84	8	0	6.958851	-2.086077	2.252680
85	8	0	-6.572814	-1.038378	2.804443
86	8	0	-7.293639	-2.311840	-2.378438
87	1	0	-9.301783	-1.878669	-0.637878
88	1	0	9.702603	-1.437495	-1.196170
89	6	0	-8.084269	-1.765607	1.068688
90	1	0	-8.863712	-1.250663	1.640791
91	6	0	8.405791	-2.013705	0.325010
92	1	0	9.201243	-1.849363	1.060892

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