Electronic Supplementary Information

Dithiafulvenyl-substituted phenylacetylene derivatives: synthesis and structure–property–reactivity relationships

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1. Experimental

1.1. *General*

Chemicals were purchased from commercial suppliers and used directly without purification. All reactions were conducted in standard, dry glassware and under an inert atmosphere of nitrogen unless otherwise noted. Evaporation and concentration were carried out with a water-aspirator. Flash column chromatography was performed with silica gel 60 (240-400 mesh). Thin-layer chromatography (TLC) was carried out with silica gel F254 covered on plastic sheets and visualized by UV light. Melting points were measured on a SRS OptiMelt melting point apparatus. ^{1}H and ^{13}C NMR spectra were measured on a Bruker Avance III 300 MHz multinuclear spectrometer. Chemical shifts (δ) are reported in ppm downfield relative to the signal of the internal reference $SiMe_4$. Coupling constants (J) are given in Hz. Infrared spectra (IR) were recorded on a Bruker Alfa spectrometer. HRMS analyses were performed on an Agilent 6230 TOF LC/MS instrument using an APPI ionizer and a QSTAR XL hybrid quadrupole/TOF mass spectrometer equipped with an o-MALDI ion source. UV-Vis absorption spectra were measured on a Cary 6000i spectrophotometer. Cyclic voltammetric analyses were carried out in a standard three-electrode setup controlled by a BASi epsilon workstation. Thione **3** was prepared according to literature procedures.[1]

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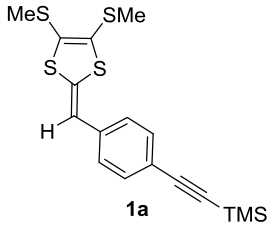
[1] (a) Steimecke, G.; Sieler, H. J.; Kirmse, R.; Hoyer, E. *Phosphor. Sulf.* **1979**, *7*, 49-55; (b) Bryce, M. R.; Moore, A. J. *Synthesis* **1991**, 26-28.

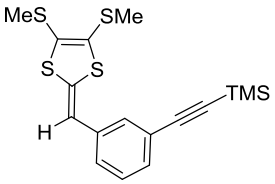
[2] (a) Chen, G.; Mahmud, I.; Dawe, L. N.; Daniels, L. M.; Zhao, Y. *J. Org. Chem.* **2011**, *76*, 2701-2715; (b) Chen, G.; Mahmud, I.; Dawe, L. N.; Zhao, Y. *Org. Lett.* **2010**, *12*, 704-707.

1.2. *Synthetic procedures*



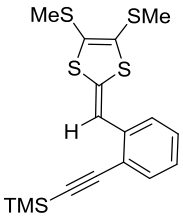
1a

***para*-Alkyne-DTF 1a**: A mixture of 4-(trimethylsilylethynyl)benzaldehyde **2a** (0.20 g, 0.99 mmol) and thione **3** (0.27 g, 1.2 mmol) in $P(OMe)_3$ (15 mL) was stirred and heated at 105 ˚C for 3 h. The excess $P(OMe)_3$ was removed by vacuum distillation. The residue was purified by silica column chromatography (CH_2Cl_2/hexanes, 1:9) to afford compound DTF **1a** (0.30 g, 0.79 mmol, 79%) as a yellow solid. m.p. 90-91 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.43 (d, *J* = 8.4 Hz, 2H), 7.12 (d, *J* = 8.2 Hz, 2H), 6.44 (s, 1H), 2.43 (d, *J* = 3.2 Hz, 6H), 0.25 (s, 9H) ppm. The data is consistent with literature report.[2]



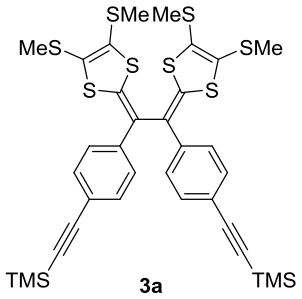
1b

***meta*-Alkyne-DTF 1b**: A mixture of 3-(trimethylsilylethynyl)benzaldehyde **2b** (0.20 g, 0.99 mmol) and thione **3** (0.27 g, 1.2 mmol) in $P(OMe)_3$ (15 mL) was stirred and heated at 105 ˚C for 3 h. The excess $P(OMe)_3$ was removed by vacuum distillation. The residue was purified by silica column chromatography (CH_2Cl_2/hexanes, 1:9) to afford compound DTF **1b** (0.29 g, 0.77 mmol, 78%) as a yellow liquid. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.29 (s, 1H), 7.28–7.26 (m, 2H), 7.19–7.14 (m, 1H), 6.41 (s, 1H), 2.44 (s, 3H), 2.42 (s, 3H), 0.26 (s, 9H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 136.3, 133.3, 130.3, 129.4, 128.4, 127.6, 126.6, 124.1, 123.5, 113.8, 104.9, 94.4, 19.1, 18.9 ppm; FTIR (neat) 2956, 2919, 2152, 1560, 1477, 1419, 1247, 840, 759, 685, 485 cm^{-1}; HRMS (APPI, positive) *m/z* $[M + H]^+$ calcd for $C_{17}H_{20}S_4Si$ 381.0290, found 381.0288.



1c

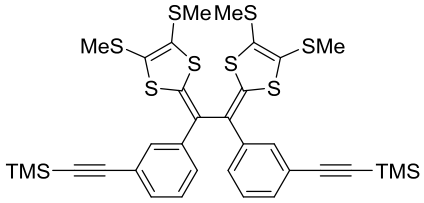
***ortho*-Alkyne-DTF 1c**: A mixture of 2-(trimethylsilylethynyl)benzaldehyde **2c** (0.20 g, 0.99 mmol) and thione **3** (0.27 g, 1.2 mmol) in $P(OMe)_3$ (15 mL) was stirred and heated at 105 ˚C for 3 h. The excess $P(OMe)_3$ was removed by vacuum distillation. The residue was purified by silica column chromatography (CH_2Cl_2/hexanes, 1:9) to afford compound DTF **1c** (0.28 g, 0.74 mmol, 75%) as a yellow liquid. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.45 (d, *J* = 7.5 Hz, 1H), 7.35–7.31 (m, 2H), 7.13–7.06 (m, 1H), 6.98 (s, 1H), 2.45 (s, 3H), 2.41 (s, 3H), 0.27 (s, 9H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 137.9, 134.3, 132.8, 128.5, 127.6, 125.5, 125.0, 124.2, 121.0, 113. 1, 103.5, 100.0, 19.0, 18.9 ppm; FTIR (neat) 2955, 2919, 2149, 1563, 1497, 1443, 1247, 1095, 838, 751, 644, 502 cm^{-1}; HRMS (APPI, positive) *m/z* $[M + H]^+$ calcd for $C_{17}H_{20}S_4Si$ 381.0290, found 381.0286.



3a

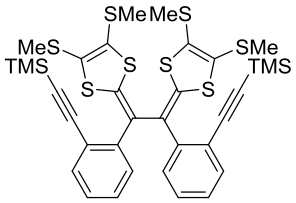
***para*-Alkyne-TTFV 3a**： A mixture of DTF **1a** (0.10 g, 0.26 mmol) and I_2 (0.20 g, 0.79 mmol) in CH_2Cl_2 (35 mL) was stirred at rt overnight. Then a satd $Na_2S_2O_3$ solution (aq, 30 mL) was added. The mixture was stirred for another 3 h at rt. The organic layer was separated, washed with H_2O, dried over $MgSO_4$, and concentrated under vacuum. The residue was purified by silica column chromatography (CH_2Cl_2/hexanes, 1:3) to afford compound TTFV **3a** (75.4 mg, 0.0995 mmol, 75%) as a yellow solid. m.p. 180-181 ˚C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.38 (d, *J* = 8.6 Hz, 4H), 7.30 (d, *J* = 8.7 Hz, 4H), 2.42 (s, 6H), 2.38 (s, 6H), 0.23 (s, 18H) ppm. The data is

consistent with literature report.[2]



3b

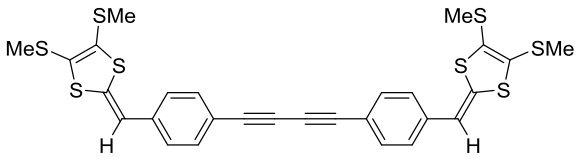
***meta*-Alkyne-TTFV 3b**: A mixture of DTF **1b** (0.10 g, 0.26 mmol) and I_2 (0.20 g, 0.79 mmol) in CH_2Cl_2 (35 mL) was stirred at rt overnight. Then a satd $Na_2S_2O_3$ solution (aq, 30 mL) was added. The mixture was stirred for another 3 h at rt. The organic layer was separated, washed with H_2O, dried over $MgSO_4$, and concentrated under vacuum. The residue was purified by silica column chromatography (CH_2Cl_2/hexanes, 1:3) to afford compound TTFV **3b** (73.1 mg, 0.0964 mmol, 73%) as a yellow solid. m.p. 51-52 ˚C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.47 (s, 2H), 7.32–7.27 (m, 4H), 7.25–7.21 (m, 2H), 2.41 (d, *J* = 5.3 Hz, 12H), 0.25 (s, 18H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 137.4, 137.2, 130.8, 129.9, 128.6, 128.1, 127.1, 125.2, 123.6, 123.5, 105.0, 94.5, 19.0, 18.9 ppm; FTIR (neat) 2953, 2917, 2152, 1523, 1489, 1419, 1246, 838, 757, 693, 468 cm^{-1}; HRMS (APPI, positive) *m/z* $[M + H]^+$ calcd for $C_{34}H_{38}S_8Si_2$ 759.0350, found 759.0360.



3c

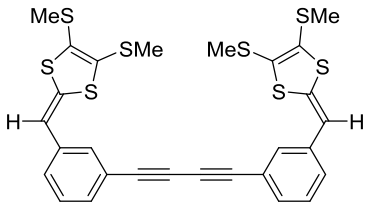
***ortho*-Alkyne-TTFV 3c**: A mixture of DTF **1c** (0.10 g, 0.26 mmol) and I_2 (0.20 g, 0.79 mmol) in CH_2Cl_2 (35 mL) was stirred at rt overnight. Then a satd $Na_2S_2O_3$ solution (aq, 30 mL) was added. The mixture was stirred for another 3 h at rt. The organic layer was separated, washed with H_2O, dried over $MgSO_4$, and concentrated under vacuum. The residue was purified by silica column chromatography (CH_2Cl_2/hexanes, 1:3) to afford compound TTFV **3c** (71.2 mg, 0.0939 mmol, 71%) as an orange solid. m.p. 99-100 ˚C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.35–7.27 (m, 4H),

7.18–7.06 (m, 4H), 2.46 (s, 6H), 2.35 (s, 6H), 0.25 (s, 18H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 141.3, 134.5, 133.2, 129.8, 128.5, 127.5, 126.9, 126.0, 123.2, 122.3, 104.5, 97.5, 19.0, 18.7 ppm; FTIR (neat) 2953, 2919, 2155, 1538, 1471, 1431, 1246, 835, 752, 669, 459 cm^{-1}; HRMS (APPI, positive) *m/z* $[M + H]^+$ calcd for $C_{34}H_{38}S_8Si_2$ 759.0350, found 759.0355.



4a

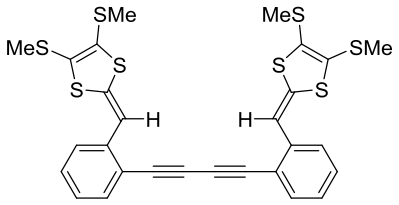
***para*-Diyne-DTF 4a**: A mixture of DTF **1a** (0.10 g, 0.26 mmol) and K_2CO_3·1.5 H_2O (0.13 g, 0.79 mmol) in THF/MeOH (30 mL, 1:1) was stirred at rt for 30 min, then concentrated under vacuum. The residue was dissolved in CH_2Cl_2 (30 mL), washed with H_2O, dried over $MgSO_4$ and filtered. Then a CH_2Cl_2 solution (5 mL) of CuI (0.15 g, 0.79 mmol) and TMEDA (0.16 mL, 1.1 mmol) was added. The mixture was stirred under air for 5 h at rt, then washed with H_2O, dried over $MgSO_4$, and concentrated under vacuum. The residue was purified by silica column chromatography (CH_2Cl_2/hexanes, 1:3) to afford compound DTF **4a** (50.4 mg, 0.0821 mmol, 63%) as a yellow solid. m.p. 170-171 ˚C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.49 (d, *J* = 8.4 Hz, 4H), 7.16 (d, *J* = 8.3 Hz, 4H), 6.46 (s, 2H), 2.44 (d, *J* = 2.4 Hz, 12H) ppm. The data is consistent with literature report.[2]



4b

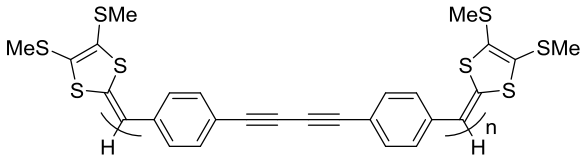
***meta*-Diyne-DTF 4b**: A mixture of DTF **1b** (0.10 g, 0.26 mmol) and K_2CO_3·1.5 H_2O (0.13 g, 0.79 mmol) in THF/MeOH (30 mL, 1:1) was stirred at rt for 30 min, then concentrated under vacuum. The residue was dissolved in CH_2Cl_2 (30 mL), washed with H_2O, dried over $MgSO_4$ and filtered. Then a CH_2Cl_2 solution (5 mL) of CuI

(0.15 g, 0.79 mmol) and TMEDA (0.16 mL, 1.1 mmol) was added. The mixture was stirred under air for 5 h at rt, then washed with H_2O, dried over $MgSO_4$, and concentrated under vacuum. The residue was purified by silica column chromatography (CH_2Cl_2/hexanes, 1:3) to afford compound DTF **4b** (52.2 mg, 0.0850 mmol, 65%) as a yellow solid. m.p. 109-110 ˚C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.36 (s, 2H), 7.35–7.30 (m, 4H), 7.23–7.18 (m, 2H), 6.42 (s, 2H), 2.44 (d, *J* = 2.3 Hz, 12H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 136.6, 134.1, 130.4, 129.8, 128.7, 127.6, 127.6, 124.3, 122.1, 113.3, 81.7, 74.1, 19.1, 18.9 ppm; FTIR (neat) 3041, 2916, 2851, 2145, 1732, 1569, 1494, 1416, 1312, 960, 887, 807, 680, 463 cm^{-1}; HRMS (APPI, positive) *m/z* $[M + H]^+$ calcd for $C_{28}H_{22}S_8$ 614.9560, found 614.9556.



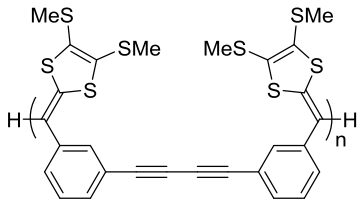
4c

***ortho*-Diyne-DTF 4c**: A mixture of DTF **1c** (0.10 g, 0.26 mmol) and K_2CO_3·1.5 H_2O (0.13 g, 0.79 mmol) in THF/MeOH (30 mL, 1:1) was stirred at rt for 30 min, then concentrated under vacuum. The residue was dissolved in CH_2Cl_2 (30 mL), washed with H_2O, dried over $MgSO_4$ and filtered. Then a CH_2Cl_2 solution (5 mL) of CuI (0.15 g, 0.79 mmol) and TMEDA (0.16 mL, 1.1 mmol) was added. The mixture was stirred under air for 5 h at rt, then washed with H_2O, dried over $MgSO_4$, and concentrated under vacuum. The residue was purified by silica column chromatography (CH_2Cl_2/hexanes, 1:3) to afford compound DTF **4c** (48.3 mg, 0.0787 mmol, 60%) as an orange solid. m.p. 124-125 ˚C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.55 (d, *J* = 7.5 Hz, 2H), 7.42–7.35 (m, 4H), 7.16–7.11 (m, 2H), 6.99 (s, 2H), 2.46 (s, 6H), 2.42 (s, 6H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 139.1, 135.7, 133.8, 129.3, 128.2, 125.6, 125.3, 123.9, 119.7, 112.4, 81.5, 79.0, 19.1, 19.0 ppm; FTIR (neat) 3053, 2917, 2852, 2133, 1735, 1545, 1496, 1415, 1311, 969, 890, 802, 742, 539, 497 cm^{-1}; HRMS (APPI, positive) *m/z* $[M + H]^+$ calcd for $C_{28}H_{22}S_8$ 614.9560, found 614.9560.



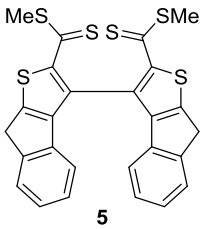
Poly-[**4a**]

***para*-Oligomers** Poly-[**4a**]: A mixture of DTF **4a** (20.0 mg, 0.0326 mmol) and I_2 (25.0 mg, 0.0984 mmol) in CH_2Cl_2 (25 mL) was stirred at rt overnight. Then a satd $Na_2S_2O_3$ solution (aq, 20 mL) was added. The mixture was stirred for another 3 h at rt. The organic layer was separated, washed with H_2O, dried over $MgSO_4$, and concentrated under vacuum to afford product poly-[**4a**] (19.6 mg, crude yield 98%) as a yellow solid. HRMS (MALDI, positive) *m/z* $[M + H]^+$ calcd for $C_{56}H_{42}S_{16}$ (n = 2) 1226.8891, found 1226.9838, calcd for $C_{84}H_{62}S_{24}$ (n = 3) 1838.8221, found 1838.9366, calcd for $C_{112}H_{82}S_{32}$ (n = 4) 2450.7552, found 2450.8962, calcd for $C_{140}H_{102}S_{40}$ (n = 5) 3062.6883, found 3062.8584.



Poly-[**4b**]

***meta*-Oligomers** Poly-[**4b**]: A mixture of DTF **4b** (20.0 mg, 0.0326 mmol) and I_2 (25.0 mg, 0.0984 mmol) in CH_2Cl_2 (25 mL) was stirred at rt overnight. Then a satd $Na_2S_2O_3$ solution (aq, 20 mL) was added. The mixture was stirred for another 3 h at rt. The organic layer was separated, washed with H_2O, dried over $MgSO_4$, and concentrated under vacuum to afford product poly-[**4b**] (19.2 mg, crude yield 96%) as a yellow solid. HRMS (MALDI, positive) *m/z* $[M + H]^+$ calcd for $C_{56}H_{42}S_{16}$ (n = 2) 1226.8891, found 1226.9348, calcd for $C_{84}H_{62}S_{24}$ (n = 3) 1838.8221, found 1838.8750, calcd for $C_{112}H_{82}S_{32}$ (n = 4) 2450.7552, found 2450.8115, calcd for $C_{140}H_{102}S_{40}$ (n = 5) 3062.6883, found 3062.7416.



5

Compound 5: A mixture of DTF **4c** (0.10 g, 0.16 mmol) and I_2 (0.12 g, 0.47 mmol) in CH_2Cl_2 (100 mL) was stirred at rt overnight. Then a satd $Na_2S_2O_3$ solution (aq, 90 mL) was added. The mixture was stirred for another 3 h at rt. The organic layer was separated, washed with H_2O, dried over $MgSO_4$, and concentrated under vacuum. The residue was purified by silica column chromatography (CH_2Cl_2/hexanes, 1:3) to afford compound **5** (25.1 mg, 0.0481 mmol, 30%) as a red solid. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.43 (d, *J* = 7.1 Hz, 2H), 7.15 – 7.02 (m, 4H), 6.70 (d, *J* = 7.3 Hz, 2H), 3.97 (s, 4H), 2.54 (s, 6H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 214.8, 152.9, 151.9, 148.3, 145.4, 138.3, 127.4, 127.3, 125.6, 124.7, 119.3, 35.6, 21.2 ppm; FTIR (neat) 3050, 2923, 2853, 1607, 1526, 1458, 1408, 1367, 1271, 1187, 1042, 732 cm^{-1}; HRMS (APPI, positive) *m/z* $[M + H]^+$ calcd for $C_{26}H_{18}S_6$ 522.9806, found 522.9808.

2. NMR Spectra of New Compounds

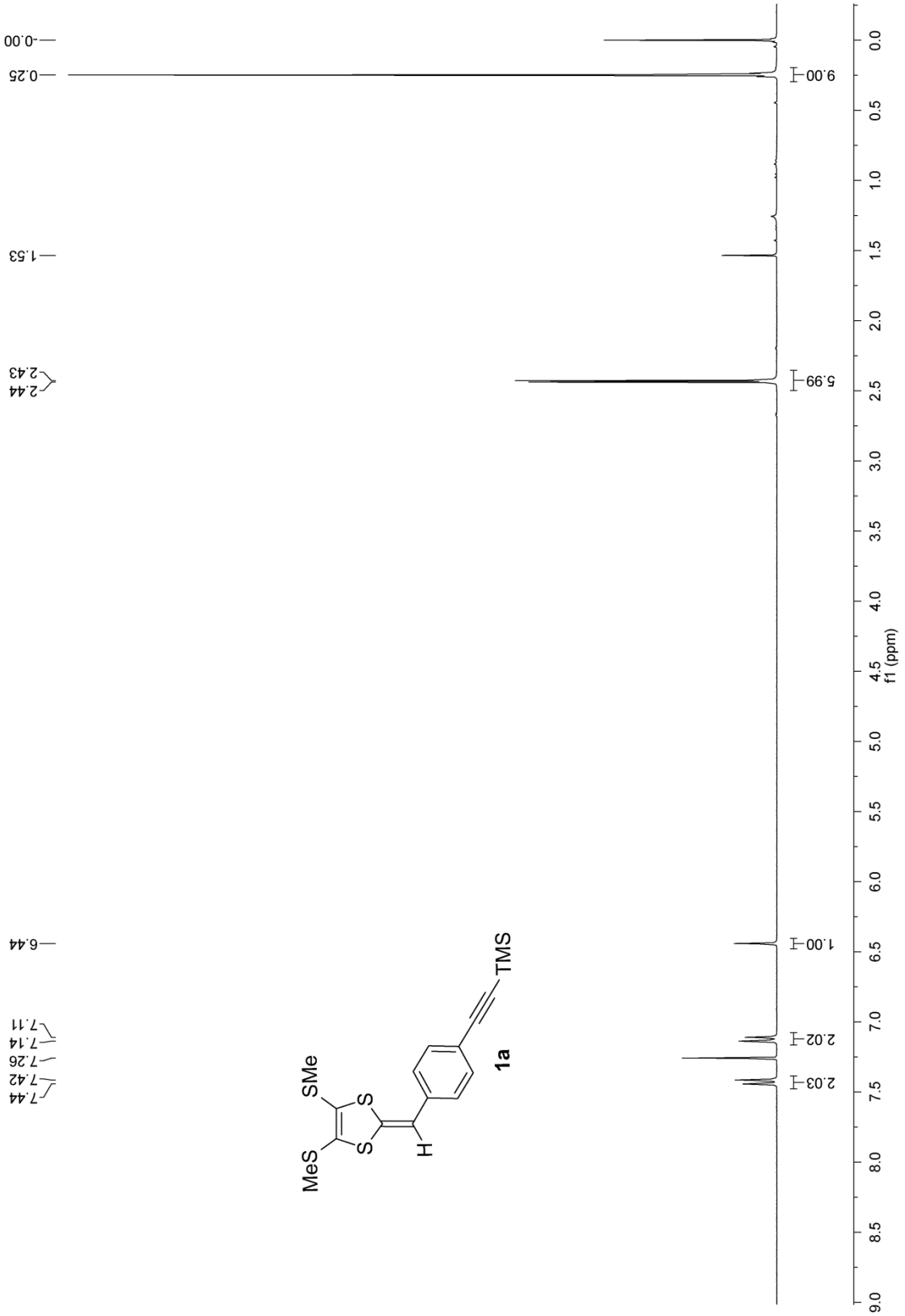


Fig. S-1 ^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound **1a**.

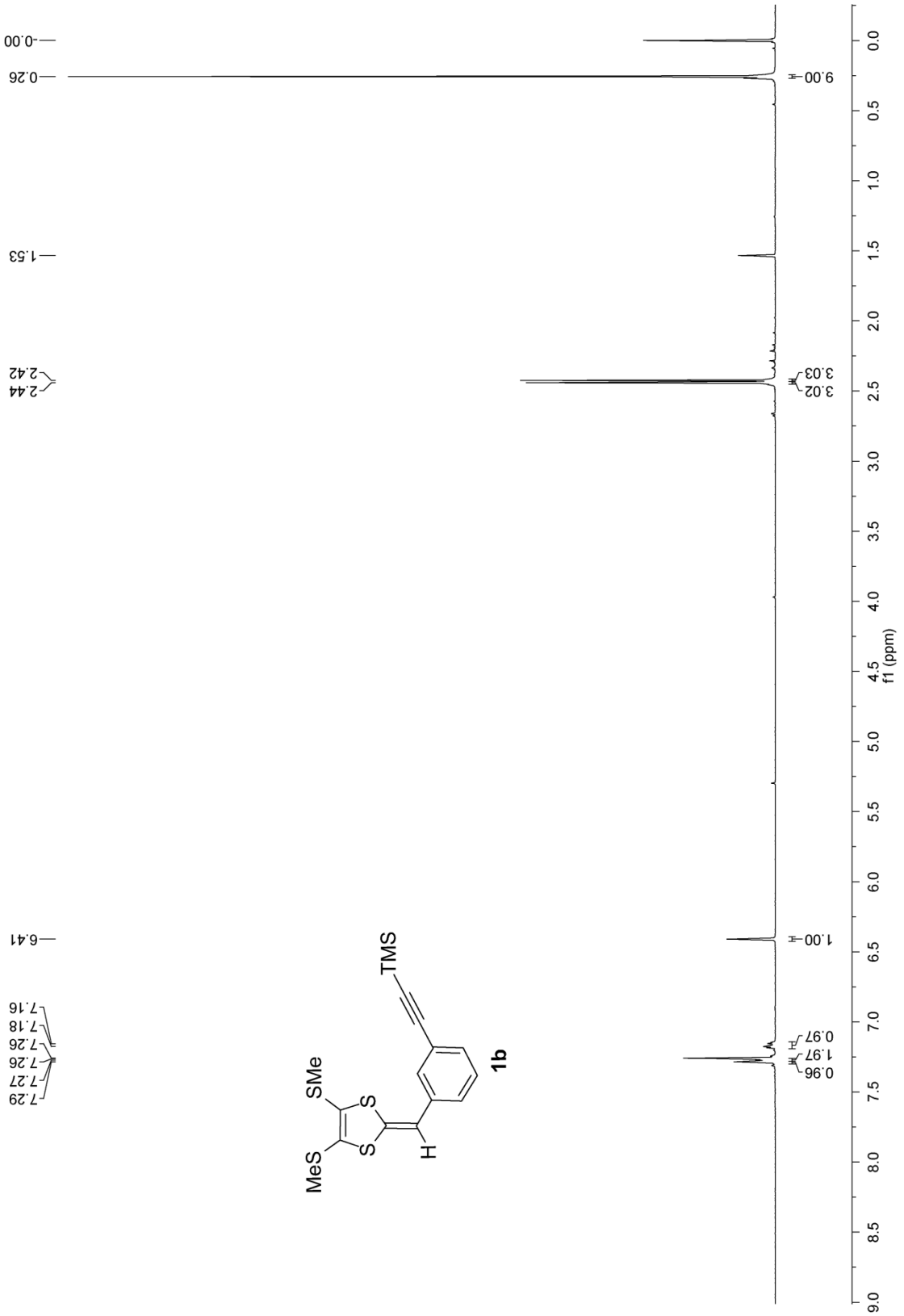


Fig. S-2 ^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound **1b**.

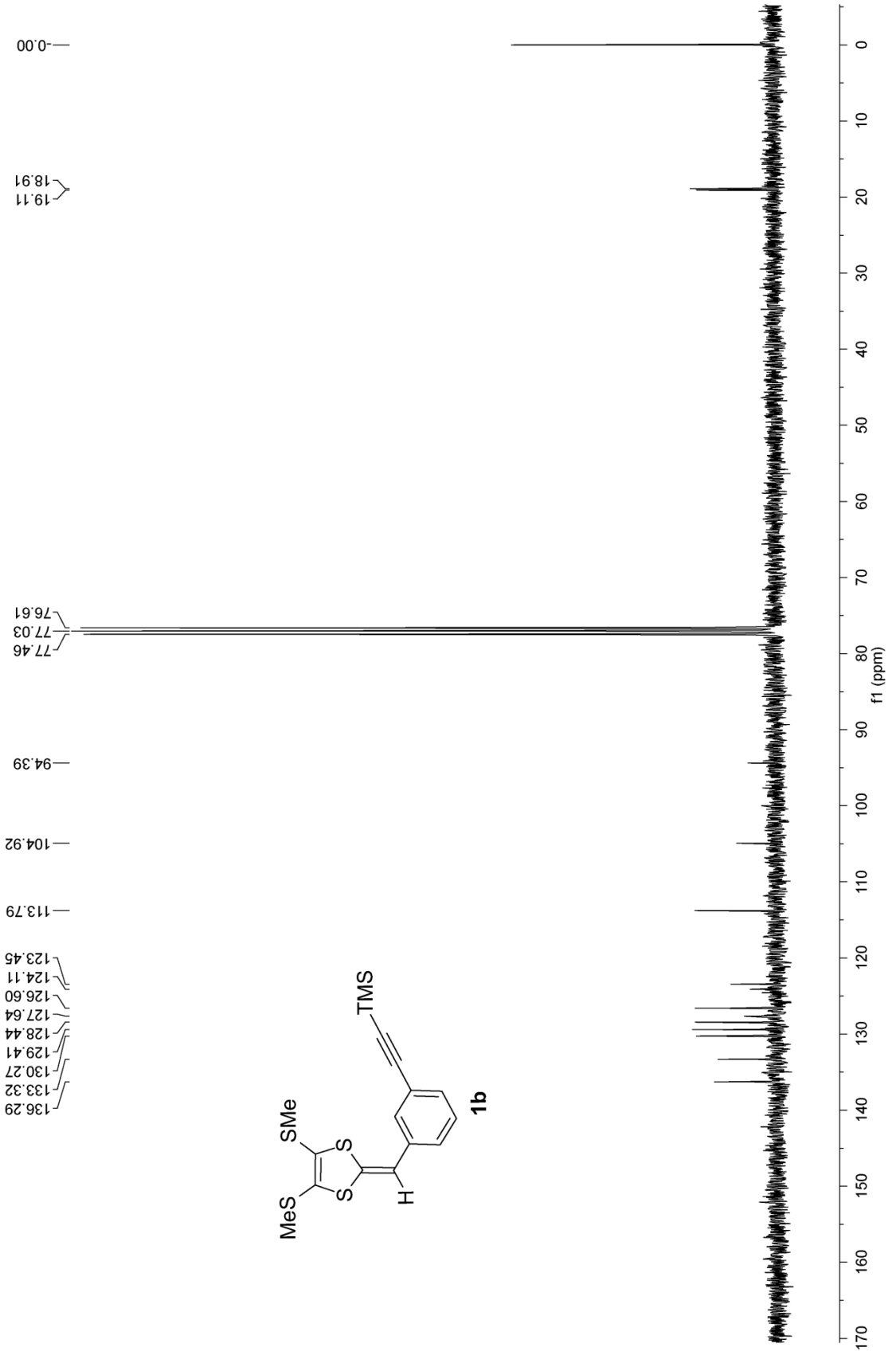


Fig. S-3 ^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound **1b**.

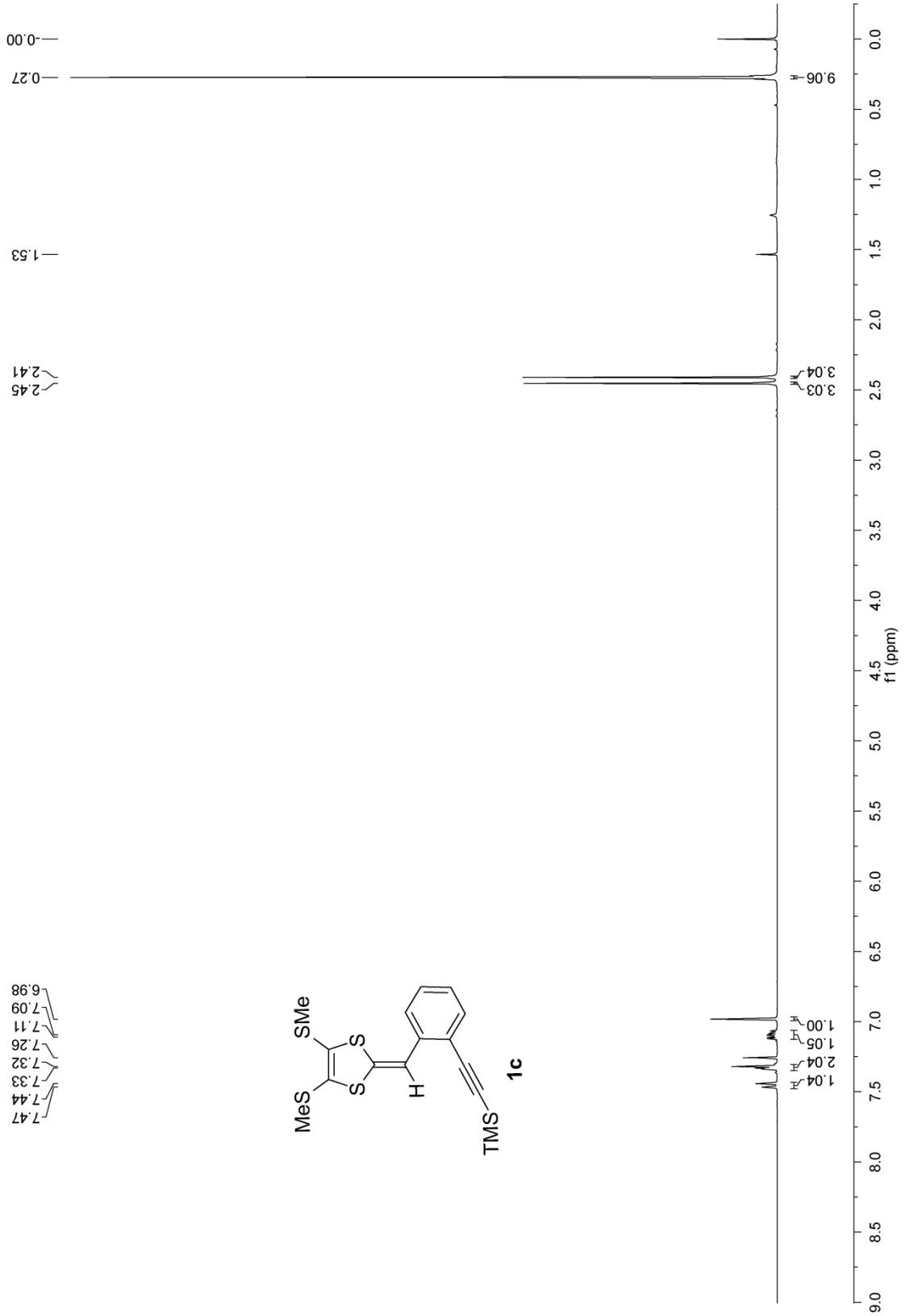


Fig. S-4 ^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound **1c**.

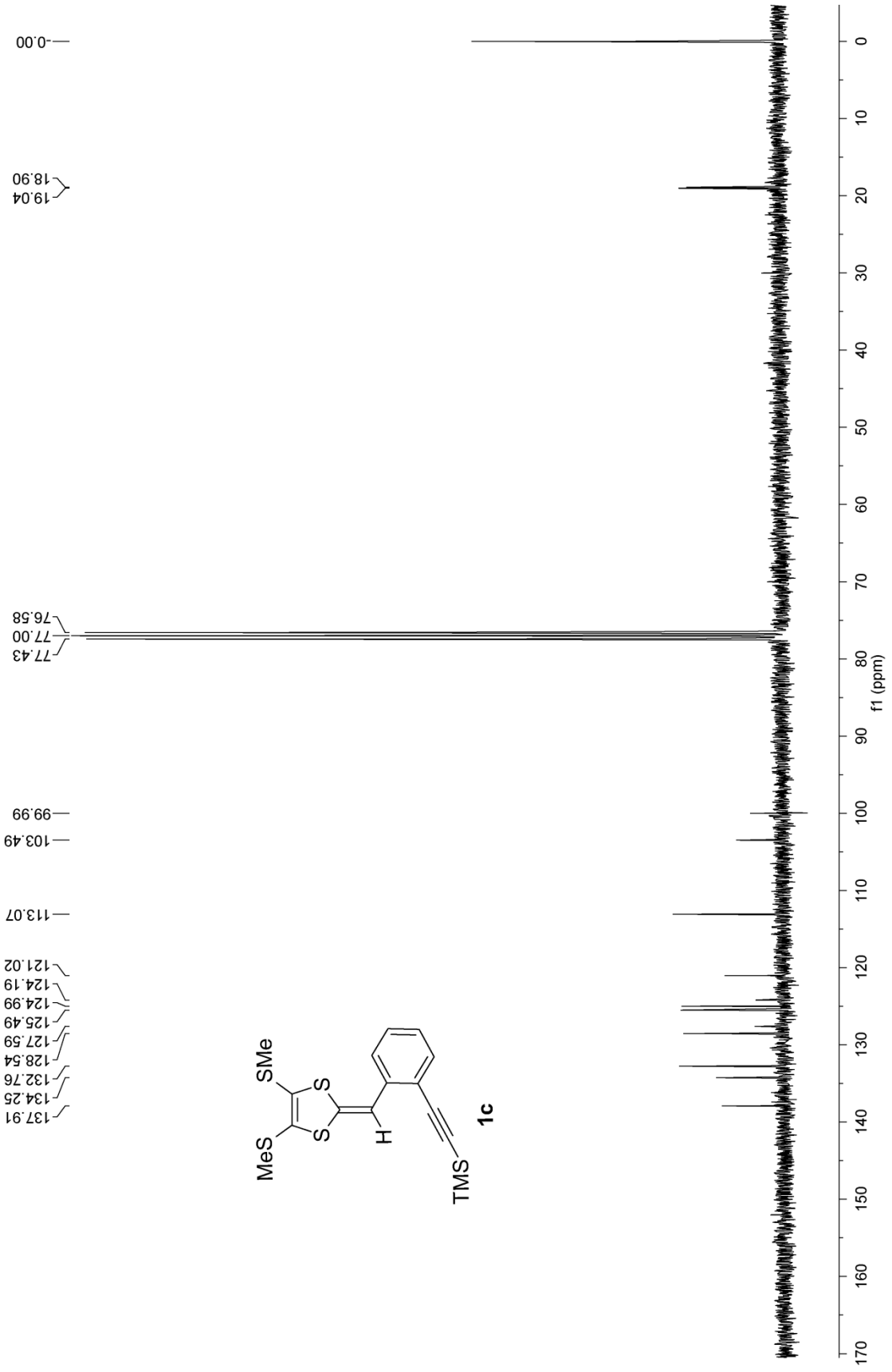


Fig. S-5 ^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound **1c**.

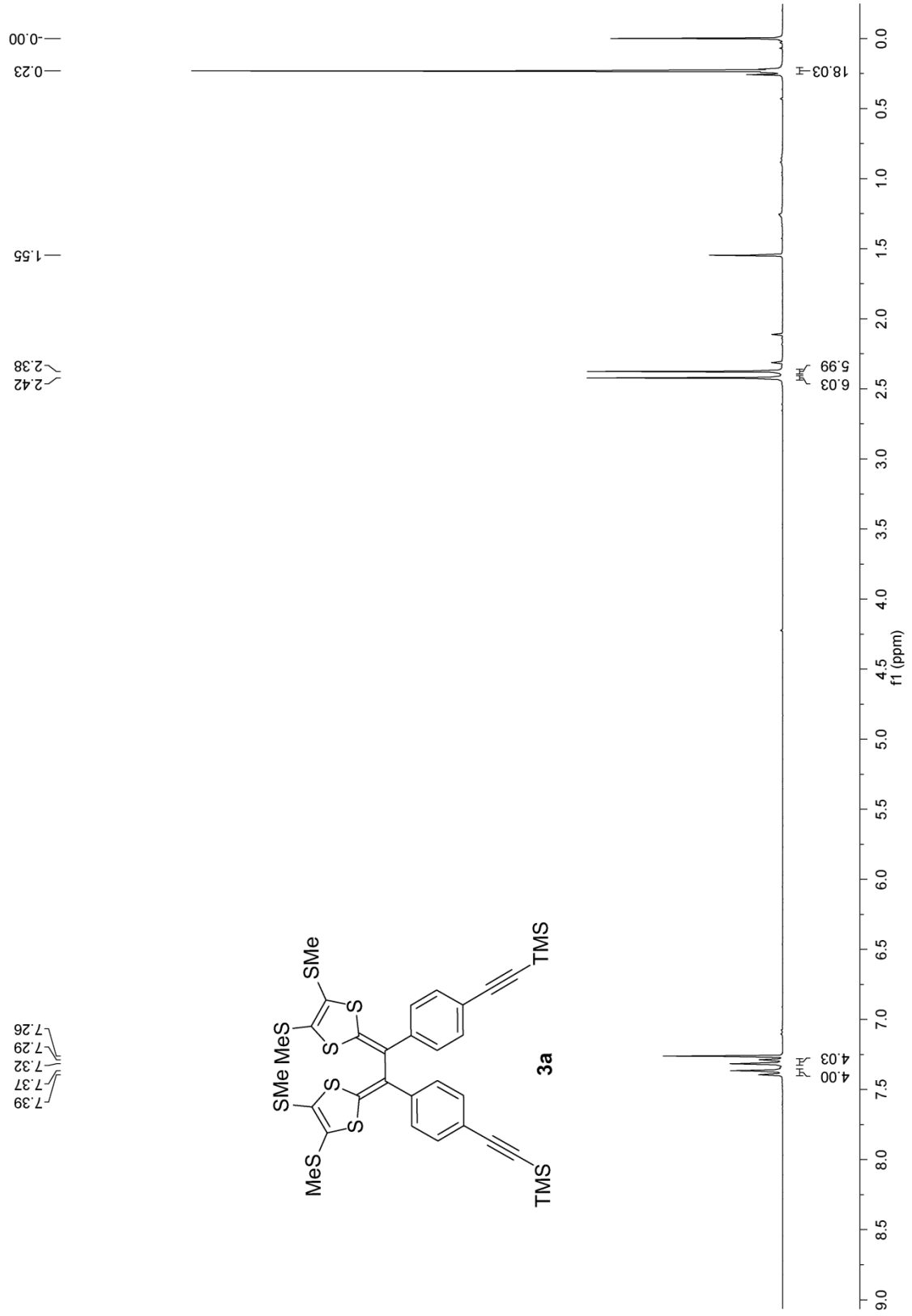


Fig. S-6 ^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound **3a**.

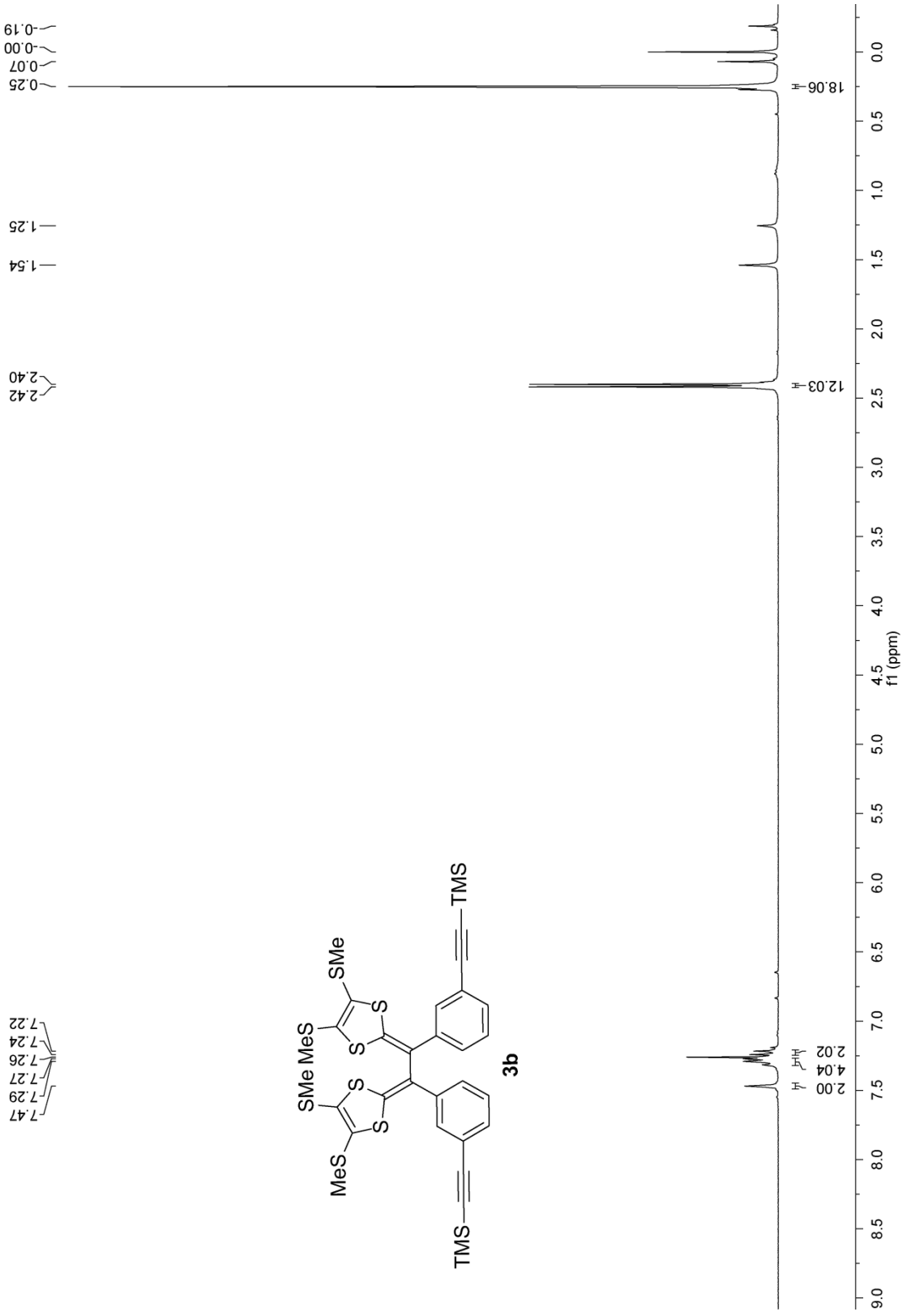


Fig. S-7 ^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound **3b**.

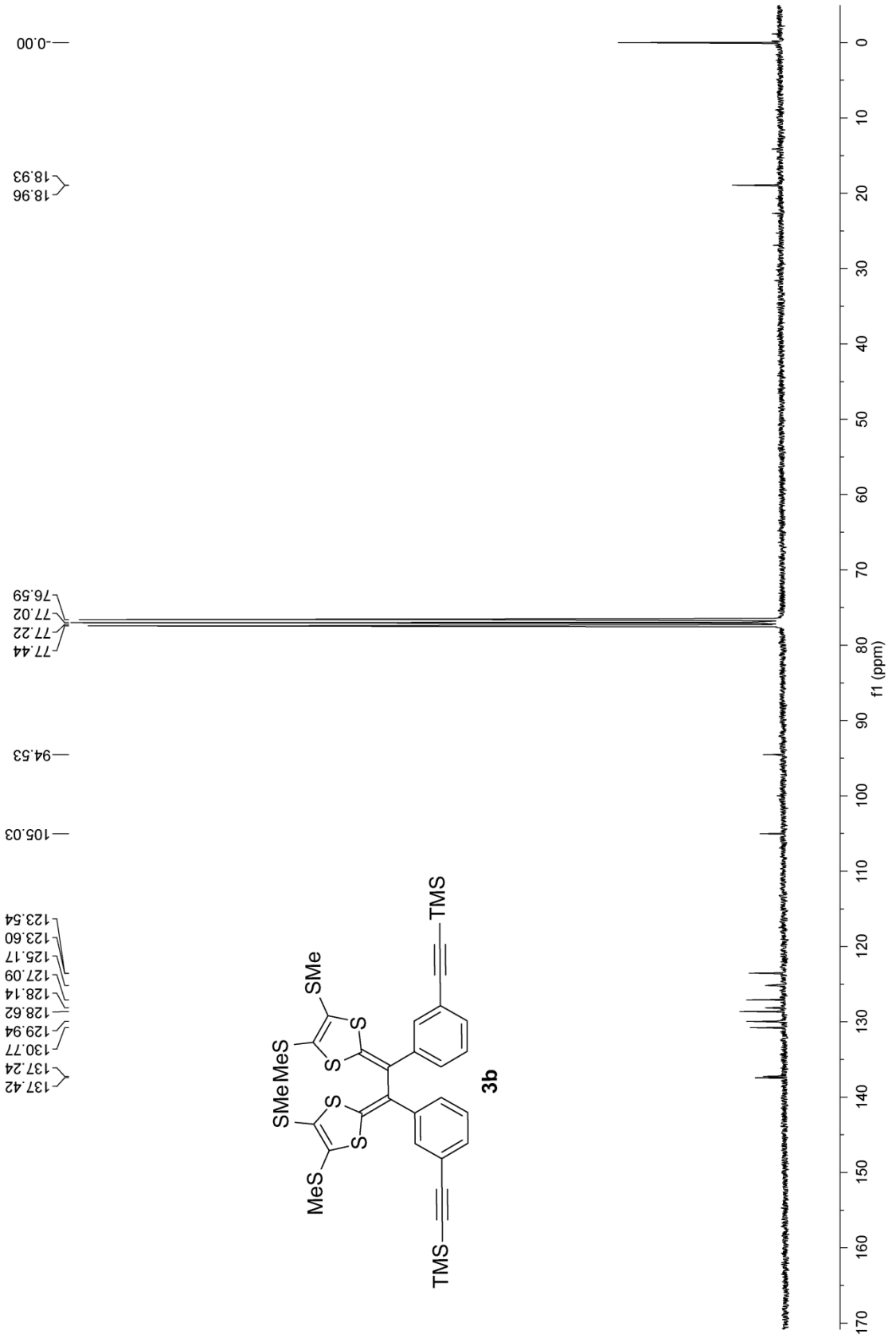


Fig. S-8 ^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound **3b**.

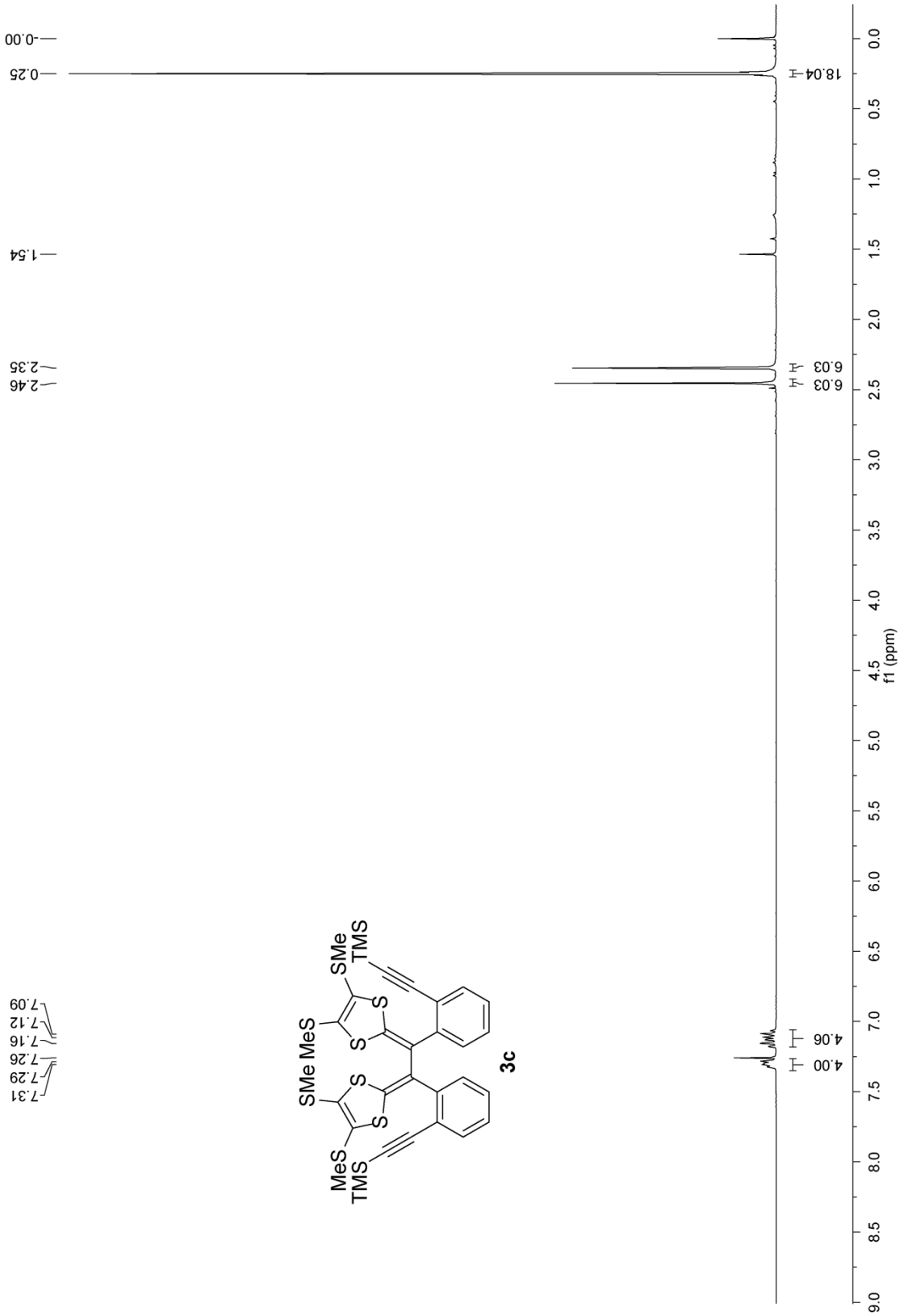


Fig. S-9 ^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound **3c**.

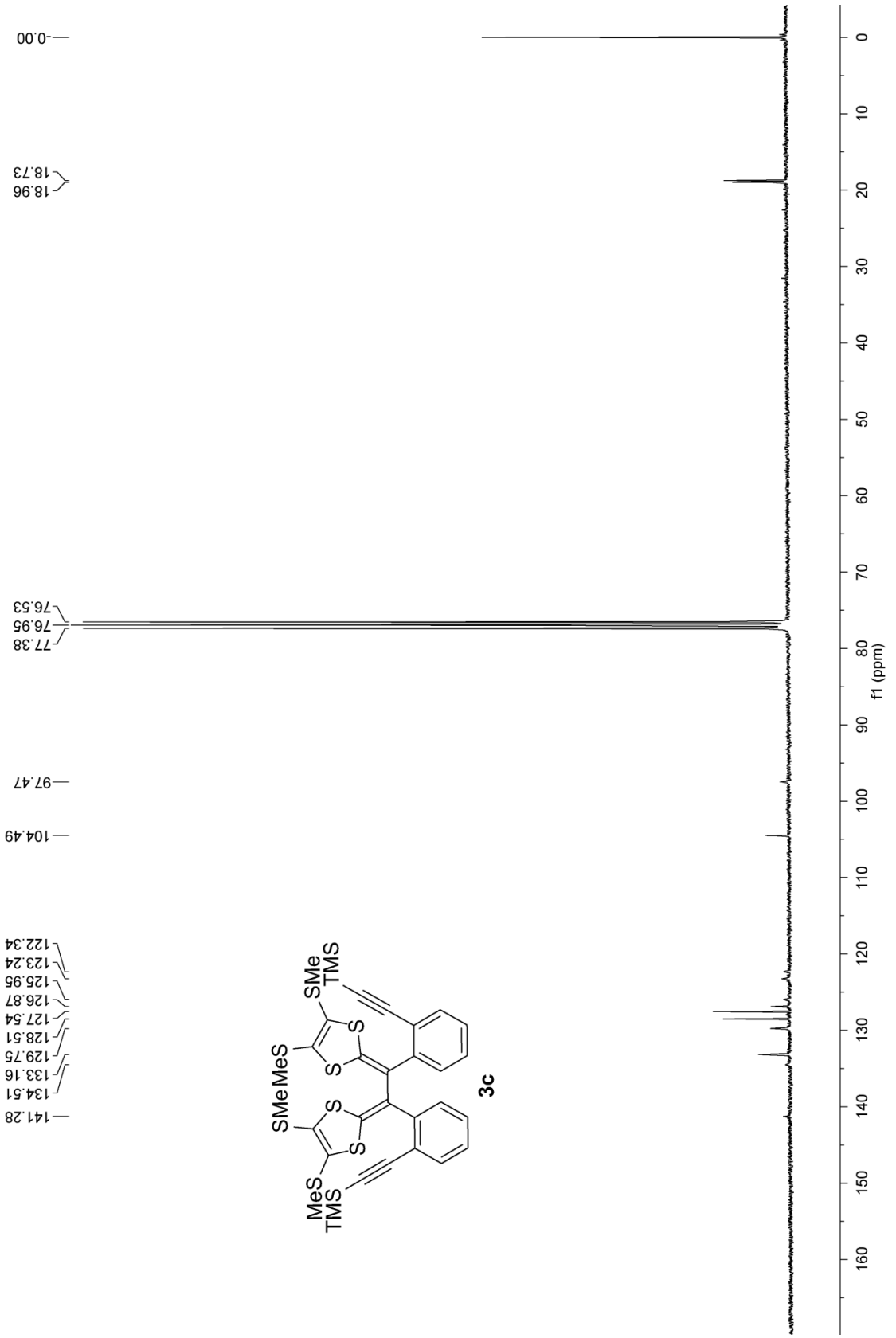


Fig. S-10 ^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound **3c**.

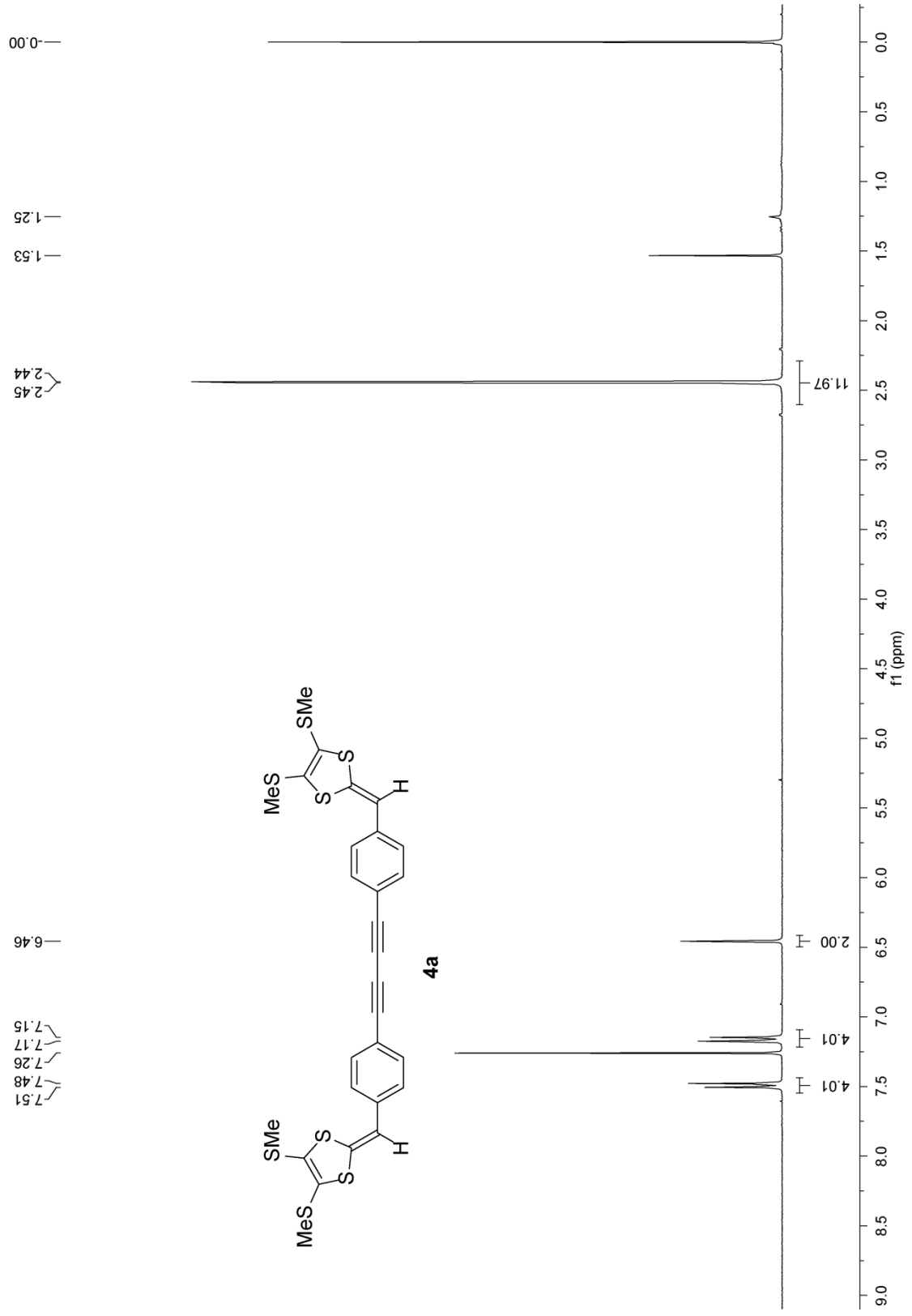


Fig. S-11 ^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound **4a**.

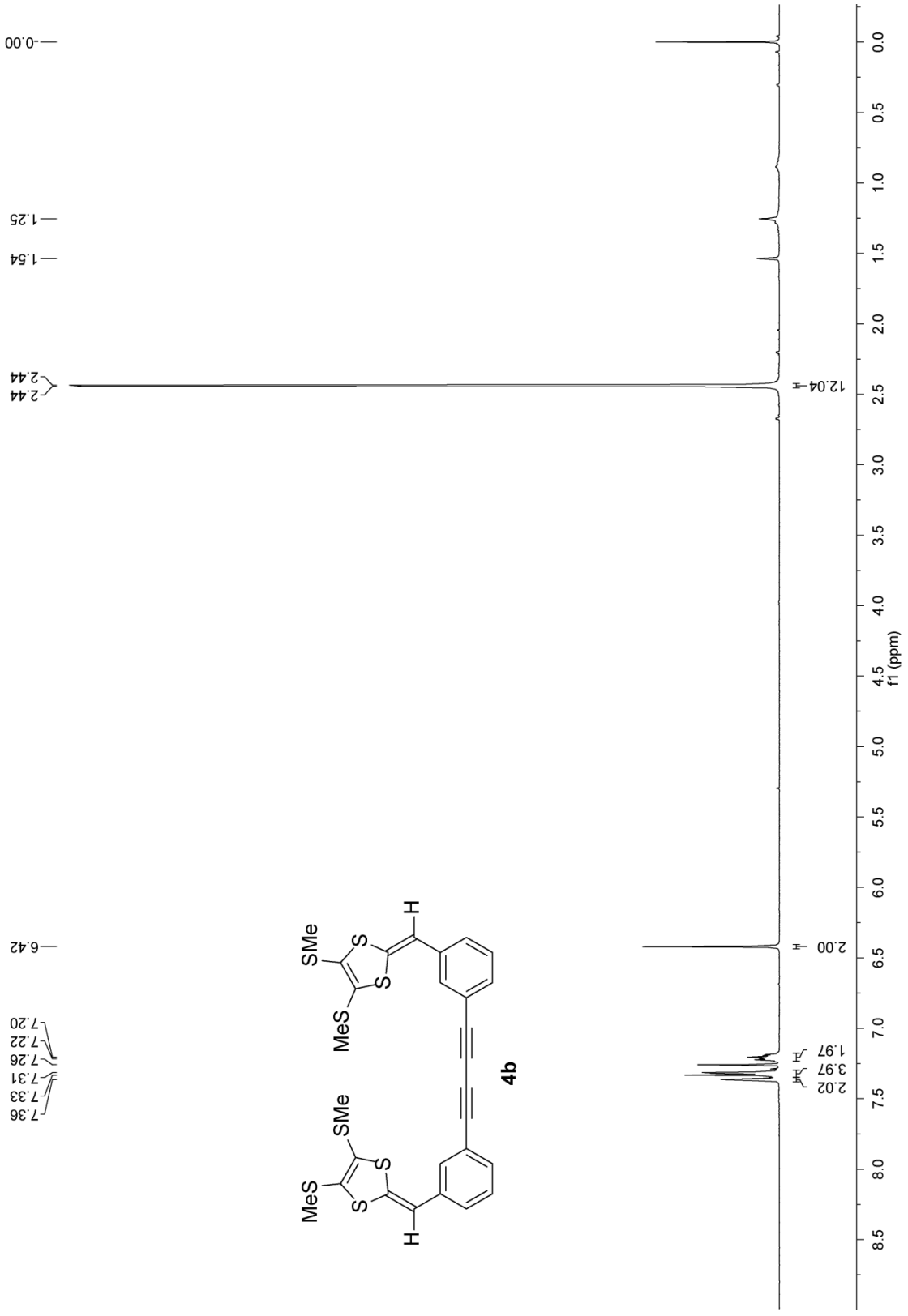


Fig. S-12 ^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound **4b**.

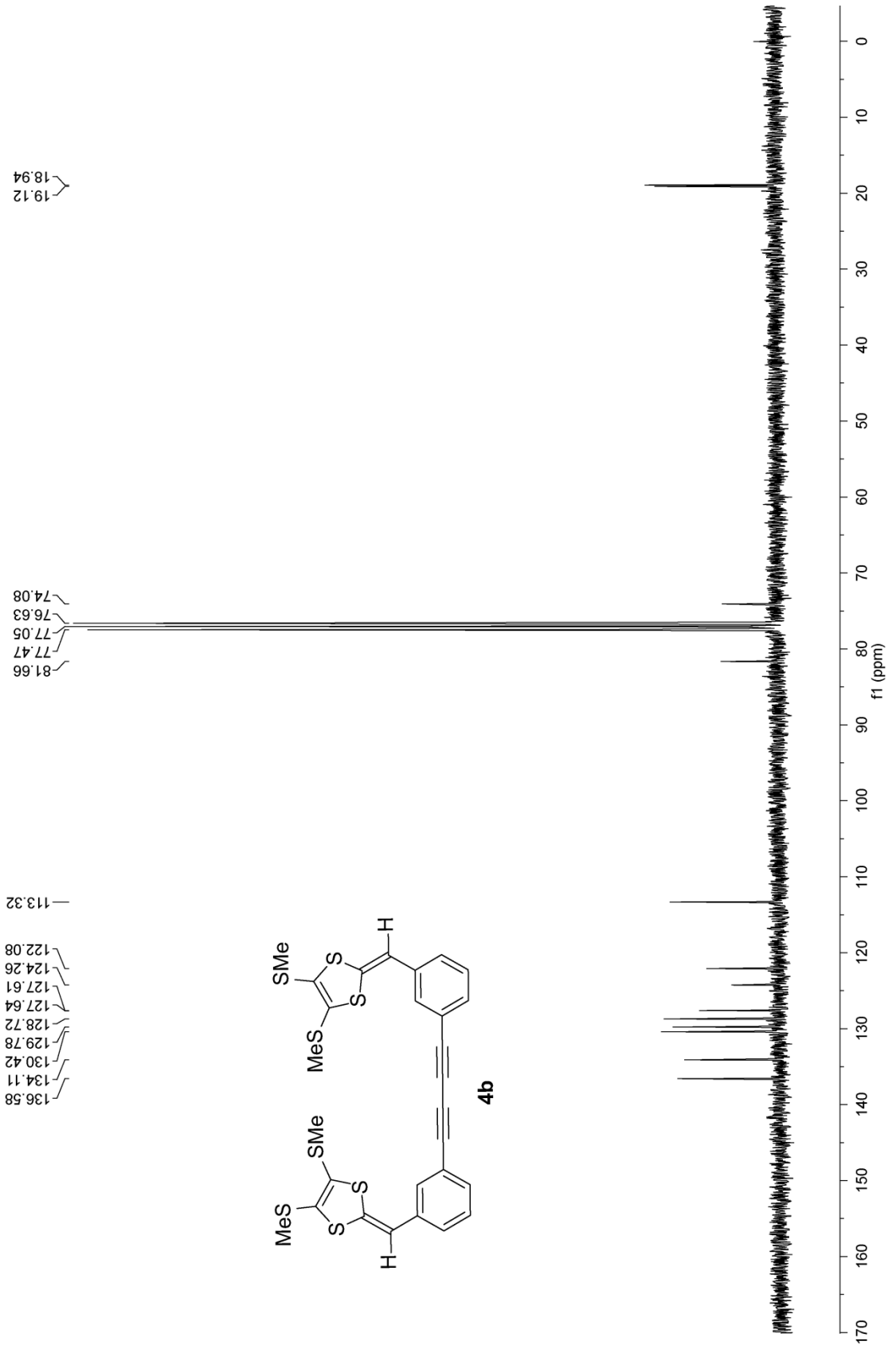


Fig. S-13 ^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound **4b**.

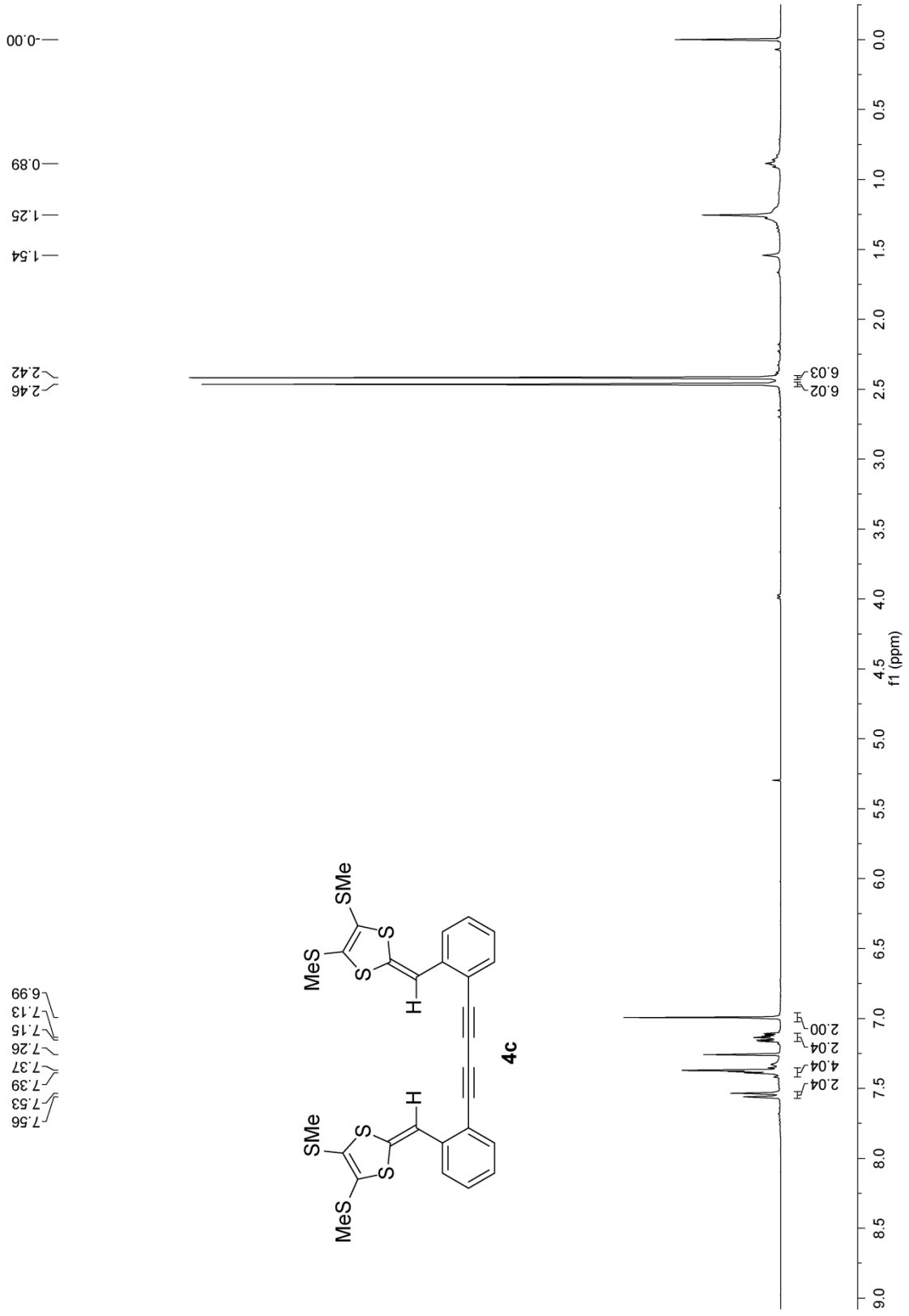


Fig. S-14 ^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound **4c**.

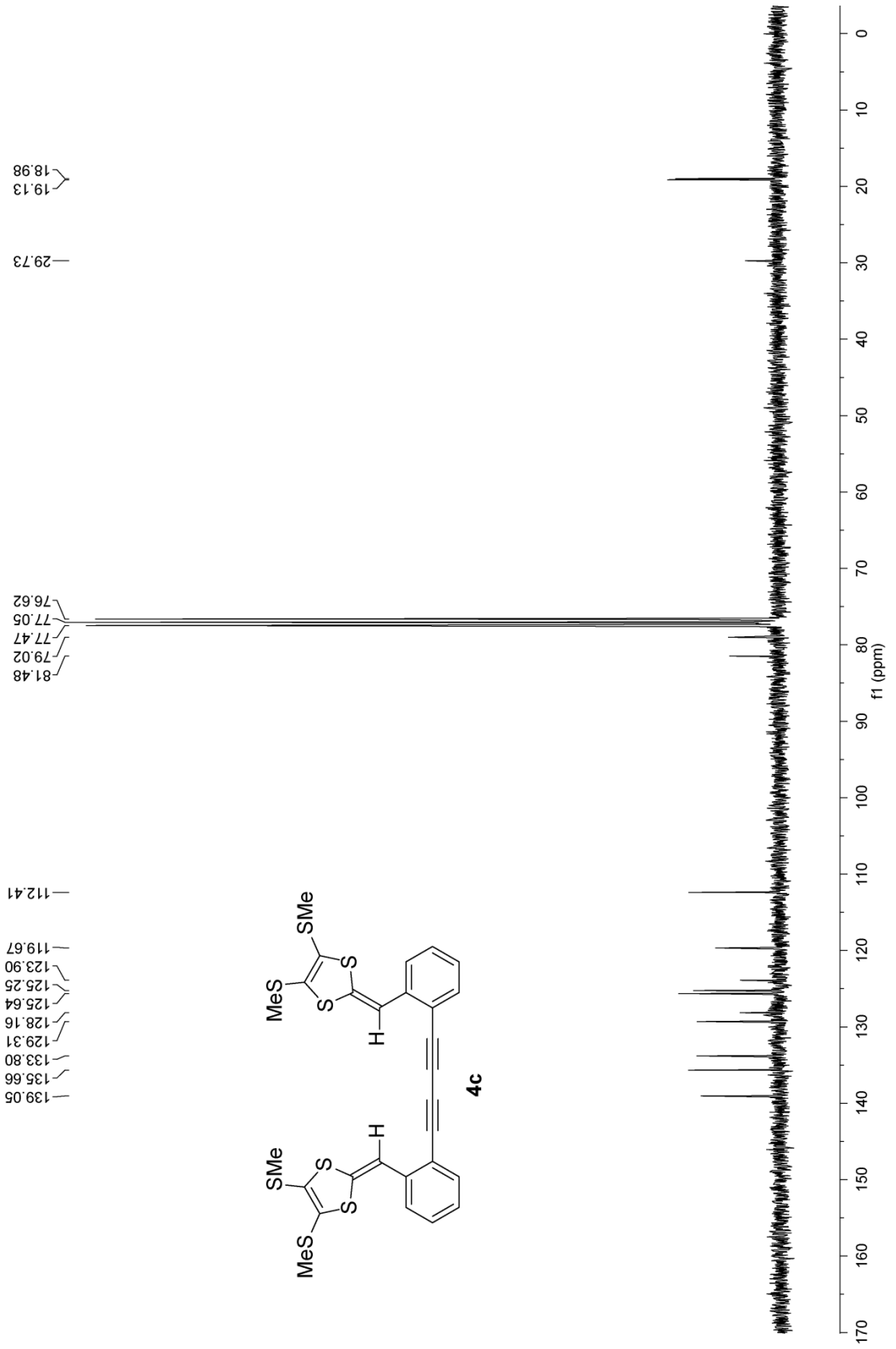


Fig. S-15 ^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound **4c**.

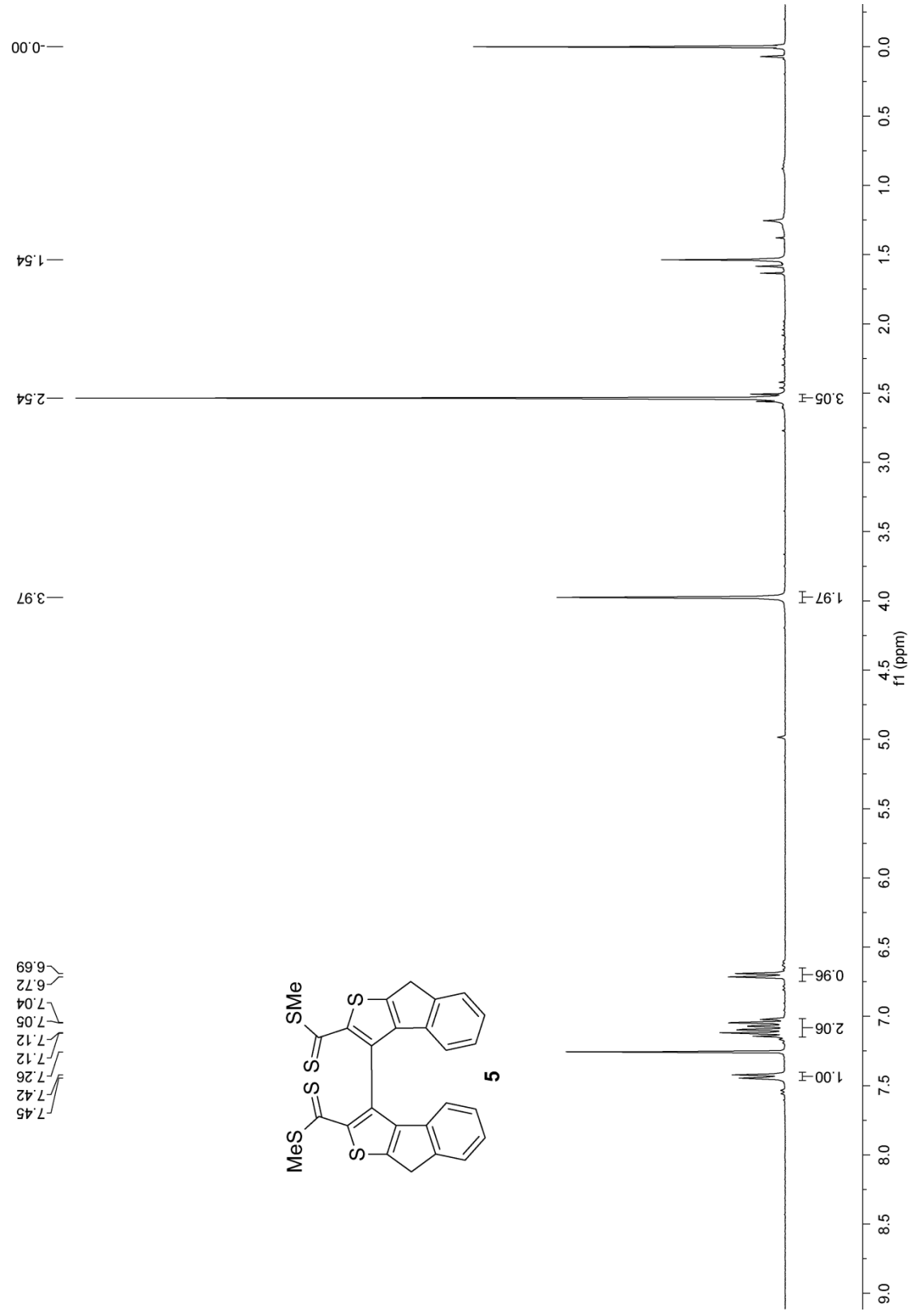


Fig. S-16 ^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound **5**.

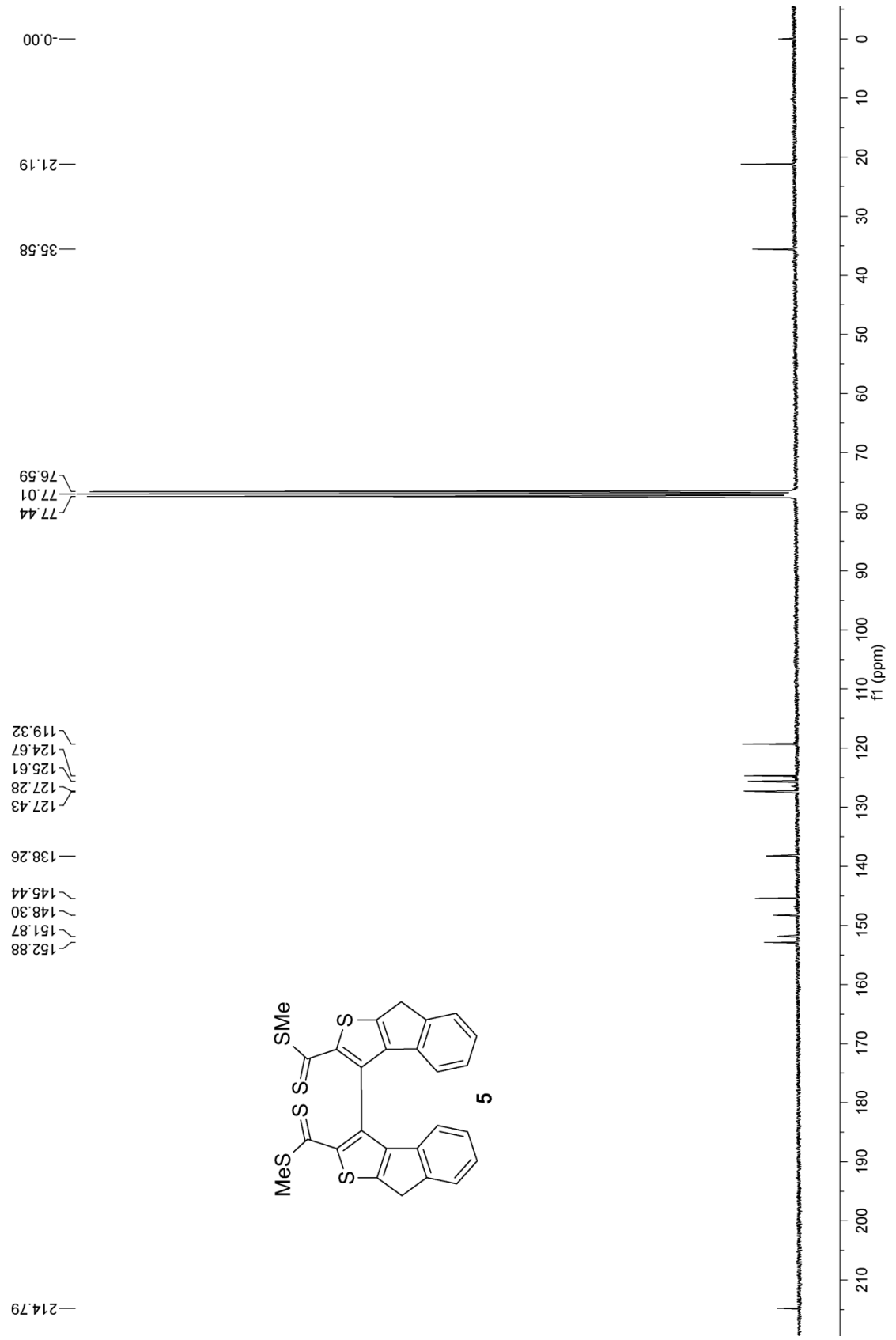


Fig. S-17 ^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound **5**.

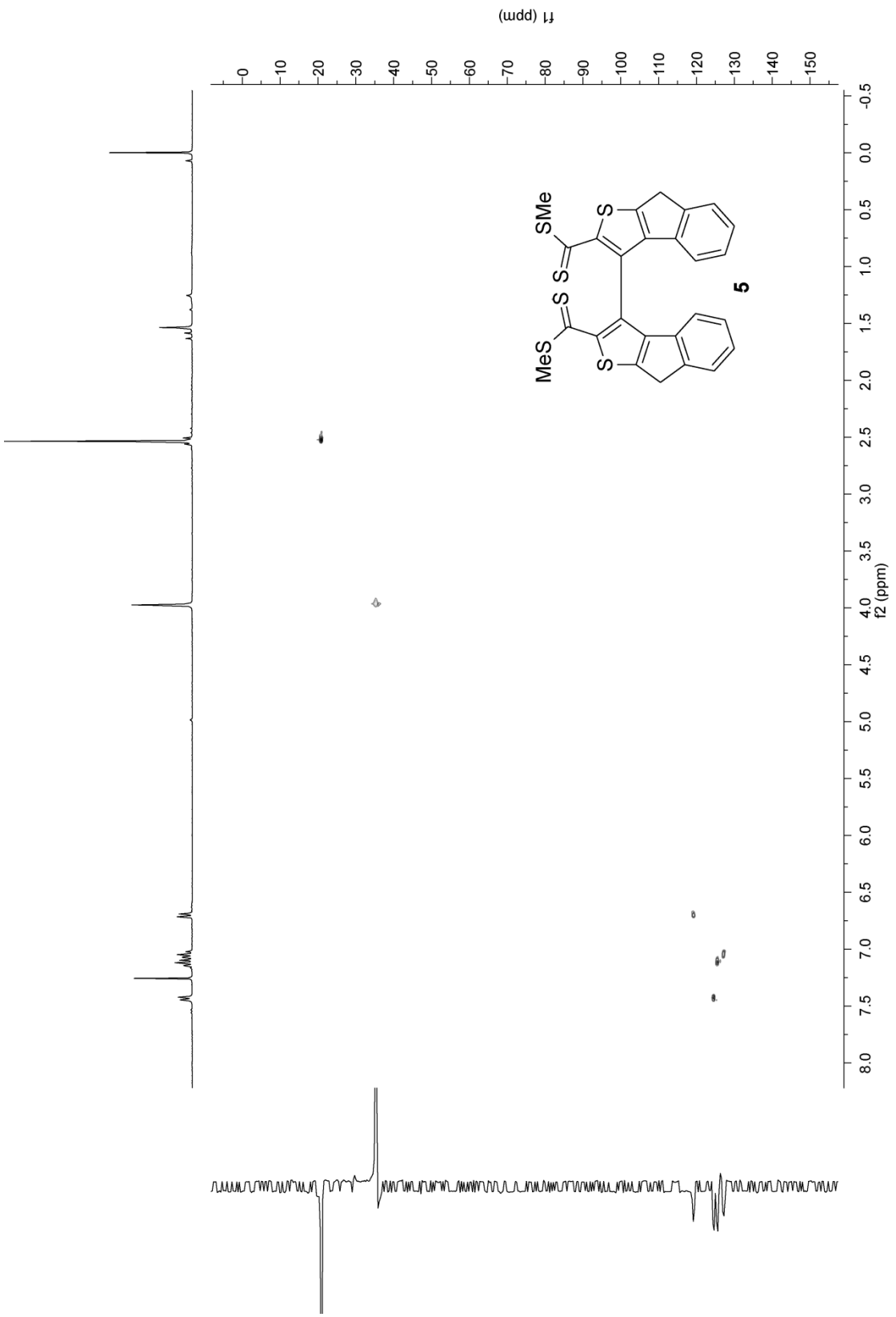


Fig. S-18 ^{1}H-^{13}C HSQC spectrum of compound **5**.

3. MALDI-TOF Mass Spectra of Poly-[4a], Poly-[4b] and Byproducts of Compound 5.

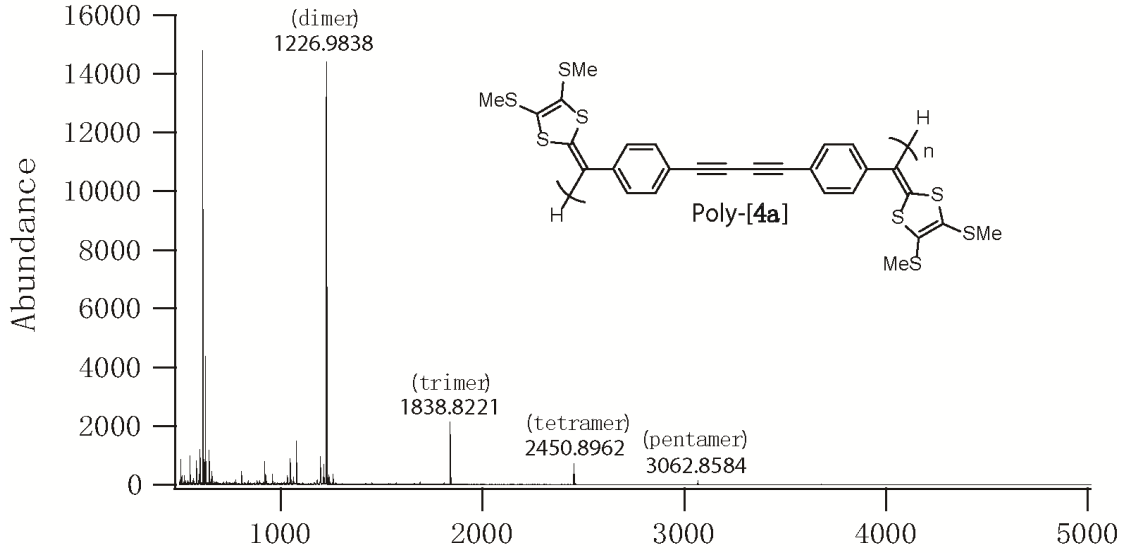


Fig. S-19 MALDI-TOF mass spectrum of poly-[**4a**].

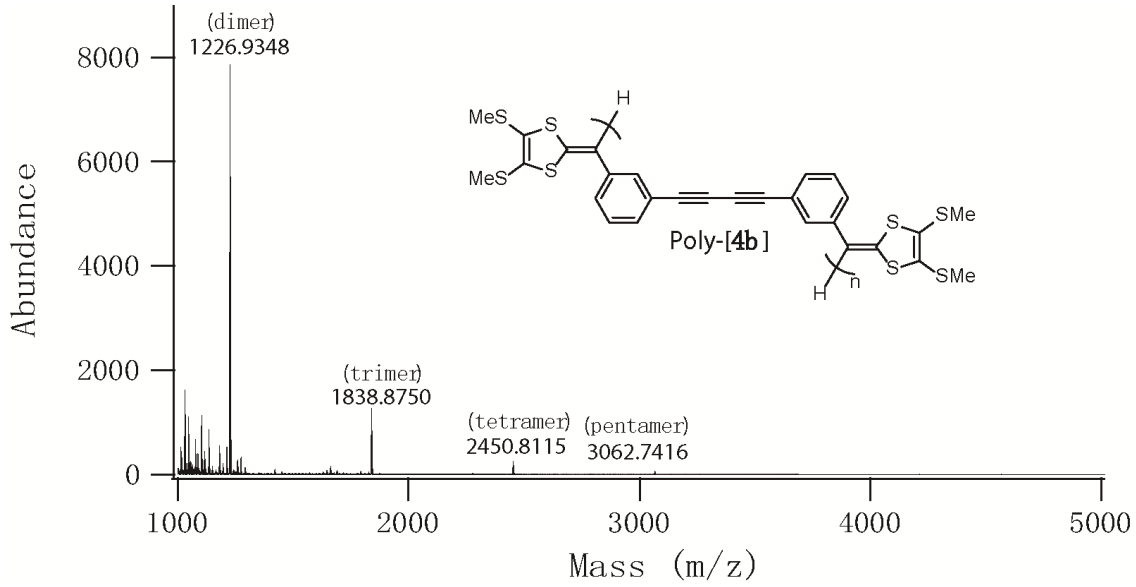


Fig. S-20 MALDI-TOF mass spectrum of poly-[**4b**].

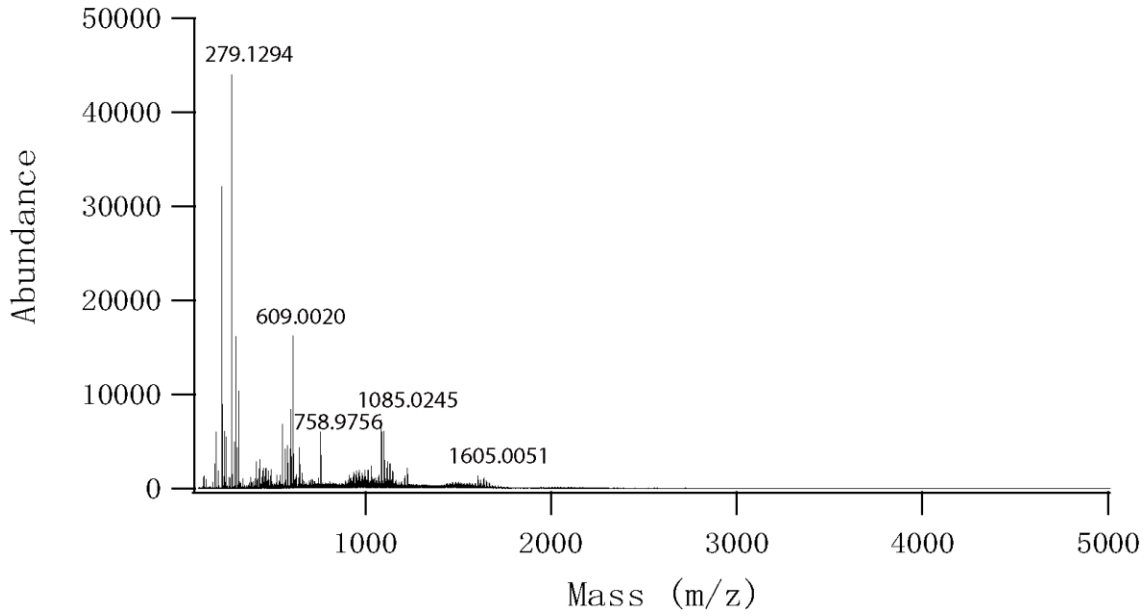


Fig. S-21 MALDI-TOF mass spectrum of byproducts of compound **5**.

4. UV-vis Spectrum of Compound 5.

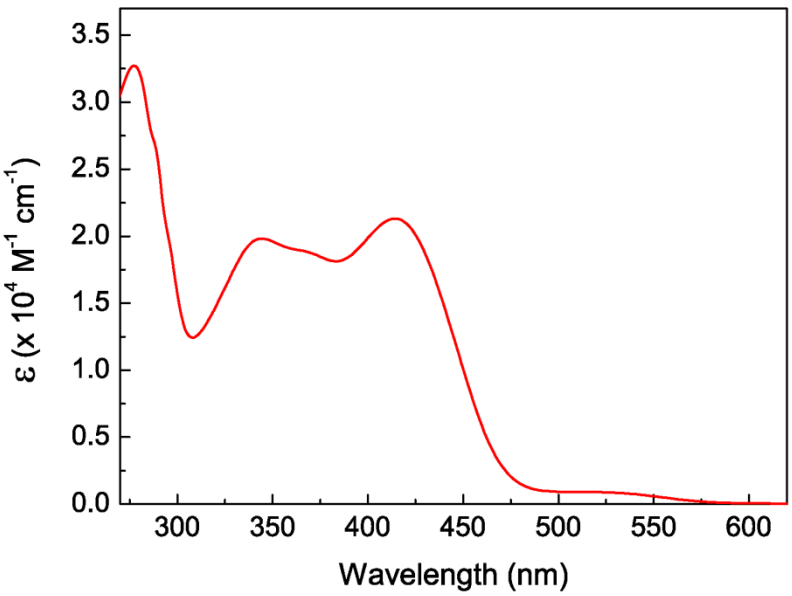


Fig. S-22 UV-vis spectrum of compound **5**, measured in CH_2Cl_2 at room temperature.

5. Cyclic Voltammogram of Compound 5.

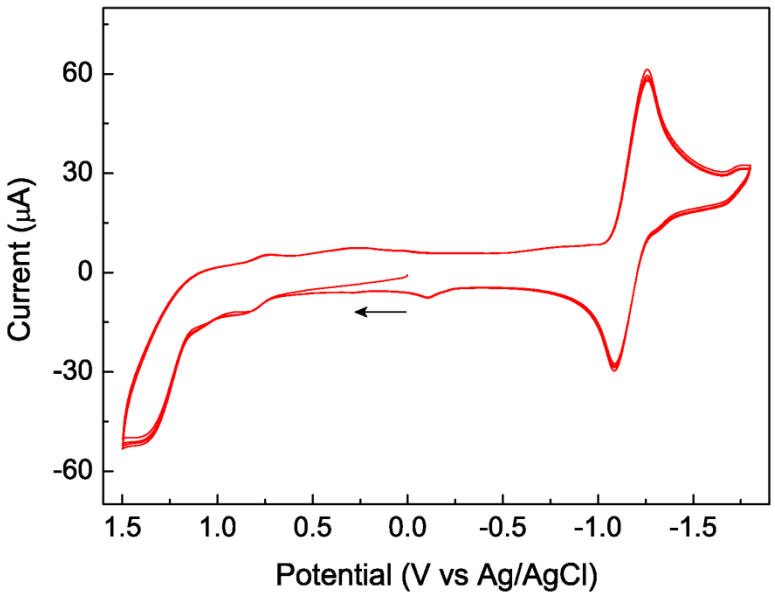


Fig. S-23 Cyclic voltammogram of compound **5**, measured in CH_2Cl_2 at room temperature. Experimental conditions: supporting electrolyte: Bu_4NBF_4 (0.1 M), working electrode: glassy carbon, counter electrode: Pt wire, reference electrode: Ag/AgCl (3 M NaCl), scan rate: 200 mV s^{-1}.

6. DFT Optimized Geometry of Compound 5

The geometry of compound **5** was optimized at the B3LYP/6-31G(d) level of theory using the Gaussian 09 software. The optimized Cartesian coordinates, energy, and dipolment are shown below. The frequency calculation shows no imaginary frequency, validating that the obtained structure is the true energy minimum.

E(RB3LYP) = -3390.73503484 a.u., dipole moment = 2.8873 Debye

H	-4.68963600	-3.60384900	1.91692400
C	-4.03152600	-3.21048200	1.14566900
C	-2.33096900	-2.19764700	-0.87151300
C	-3.07391100	-2.25308000	1.45007300
C	-4.14050500	-3.66516800	-0.17472300
C	-3.29832200	-3.16175400	-1.16960500
C	-2.21923900	-1.74376500	0.44353100
H	-4.88642800	-4.41409100	-0.42619500
H	-3.39589600	-3.52220400	-2.19003900
H	-1.68290700	-1.81191800	-1.65162500
C	-2.76479600	-1.60564200	2.79475200
H	-2.46777500	-2.34254200	3.55319900
H	-3.62935800	-1.06466700	3.20268100
C	-1.63914500	-0.68245800	2.41979500
C	-1.32907400	-0.76129300	1.07734700
S	-0.65742300	0.43569800	3.26918000
C	0.22605200	0.83423700	1.78556400
C	-0.26702900	0.10824000	0.69274400
C	1.28496700	1.82958100	1.90750700
S	1.70323600	2.48460700	3.38219400
S	2.07679900	2.29643100	0.39560000
C	3.30930800	3.51573600	0.94391800
H	2.82349500	4.37341500	1.41299300
H	3.82783300	3.82520800	0.03192400
H	4.01350400	3.06707800	1.64714200
C	0.26697700	0.10811300	-0.69274300
C	-0.22618500	0.83382400	-1.78572000
S	0.65722900	0.43494000	-3.26927900
C	1.32911600	-0.76138800	-1.07716100
C	1.63915300	-0.68283800	-2.41963300
C	2.76492000	-1.60596600	-2.79438700
H	3.62941100	-1.06497200	-3.20244200
H	2.46799100	-2.34307600	-3.55266600
C	3.07413300	-2.25304700	-1.44955900
C	3.29871800	-3.16102400	1.17034900

C	4.03186900	-3.21025800	-1.14493300
C	2.21942000	-1.74358900	-0.44312600
C	2.33123700	-2.19711700	0.87203200
C	4.14093700	-3.66459100	0.17557300
H	4.69001000	-3.60374100	-1.91610200
H	1.68314200	-1.81126200	1.65205300
H	4.88695900	-4.41335700	0.42721900
H	3.39636300	-3.52120200	2.19087200
C	-1.28520700	1.82903000	-1.90791700
S	-2.07643300	2.29694600	-0.39602600
S	-1.70411200	2.48298600	-3.38289700
C	-3.30930500	3.51570300	-0.94475300
H	-2.82377700	4.37309700	-1.41464200
H	-3.82751200	3.82577600	-0.03278200
H	-4.01372700	3.06645400	-1.64737300