Electronic Supplementary Information for

Synthesis and characterization of bis(dithiafulvenyl)-substituted fluorenones and fluorenylidene-1,3-dithioles

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1. NMR Spectra for New Compounds

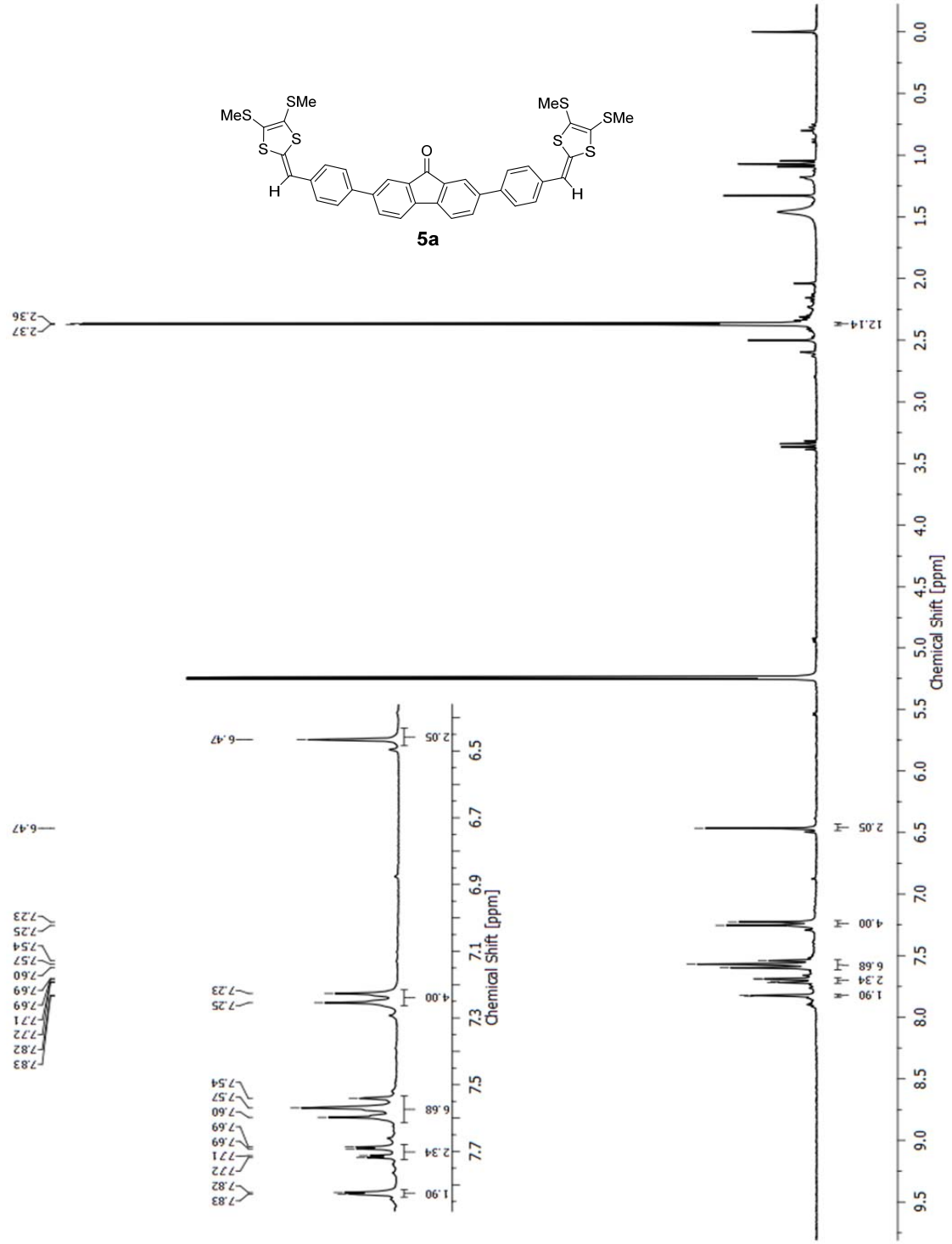

Fig. S-1. ^{1}H NMR (300 MHz, CD_2Cl_2) spectrum of compound **5a**.

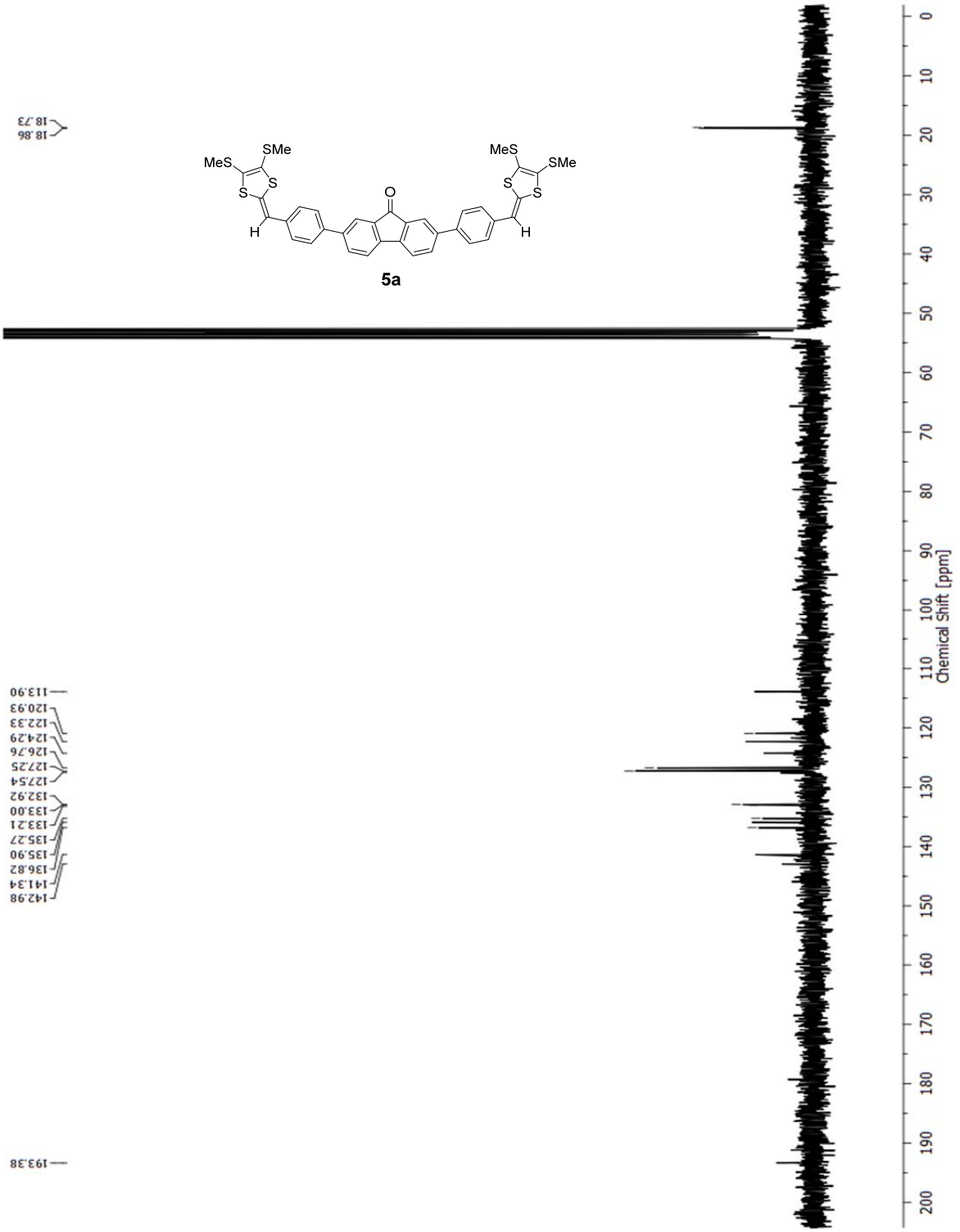

Fig. **S-2** ^{13}C NMR (75 MHz, CD_2Cl_2) spectrum of compound **5a**.

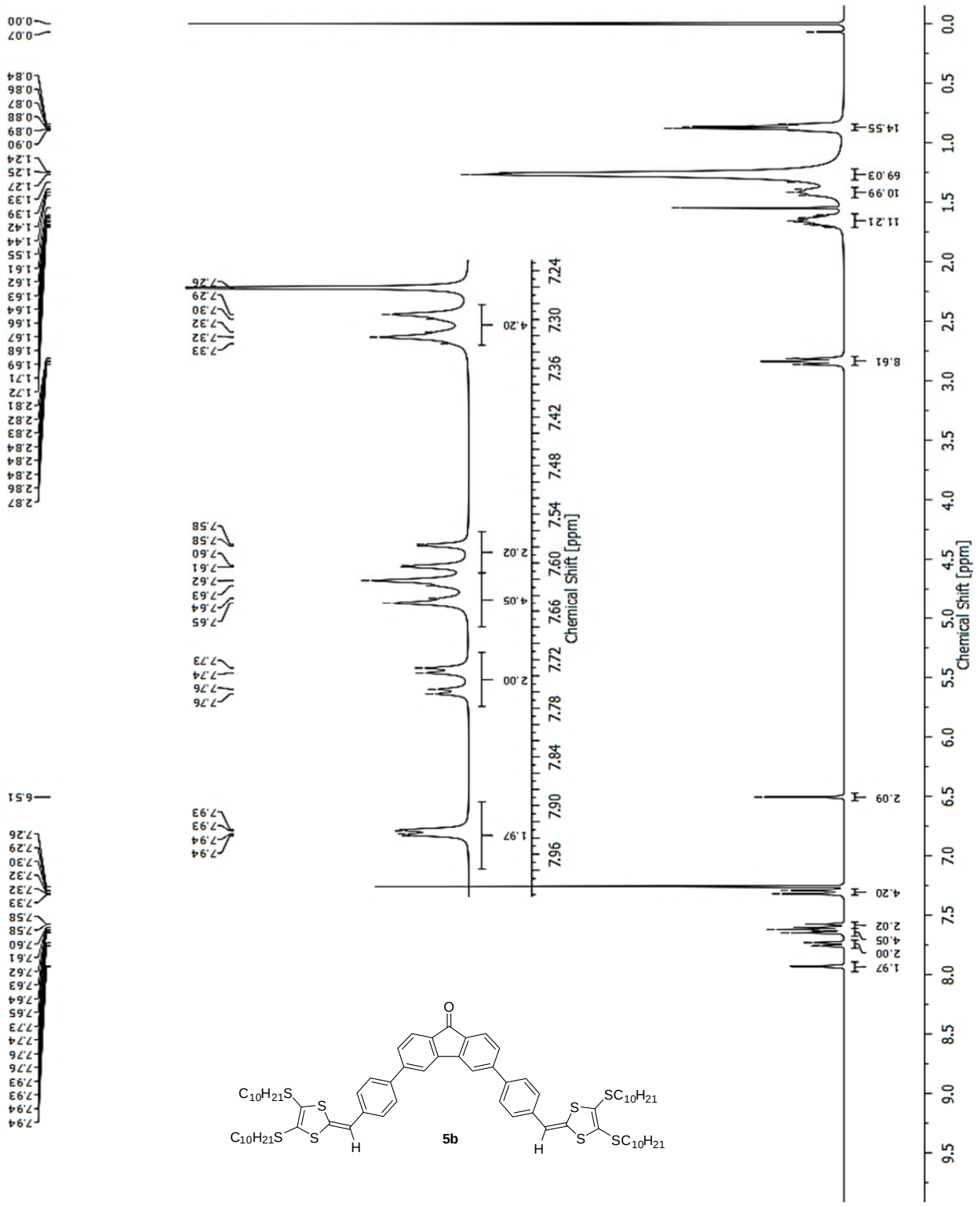

Fig. S-3 ^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound **5b**.

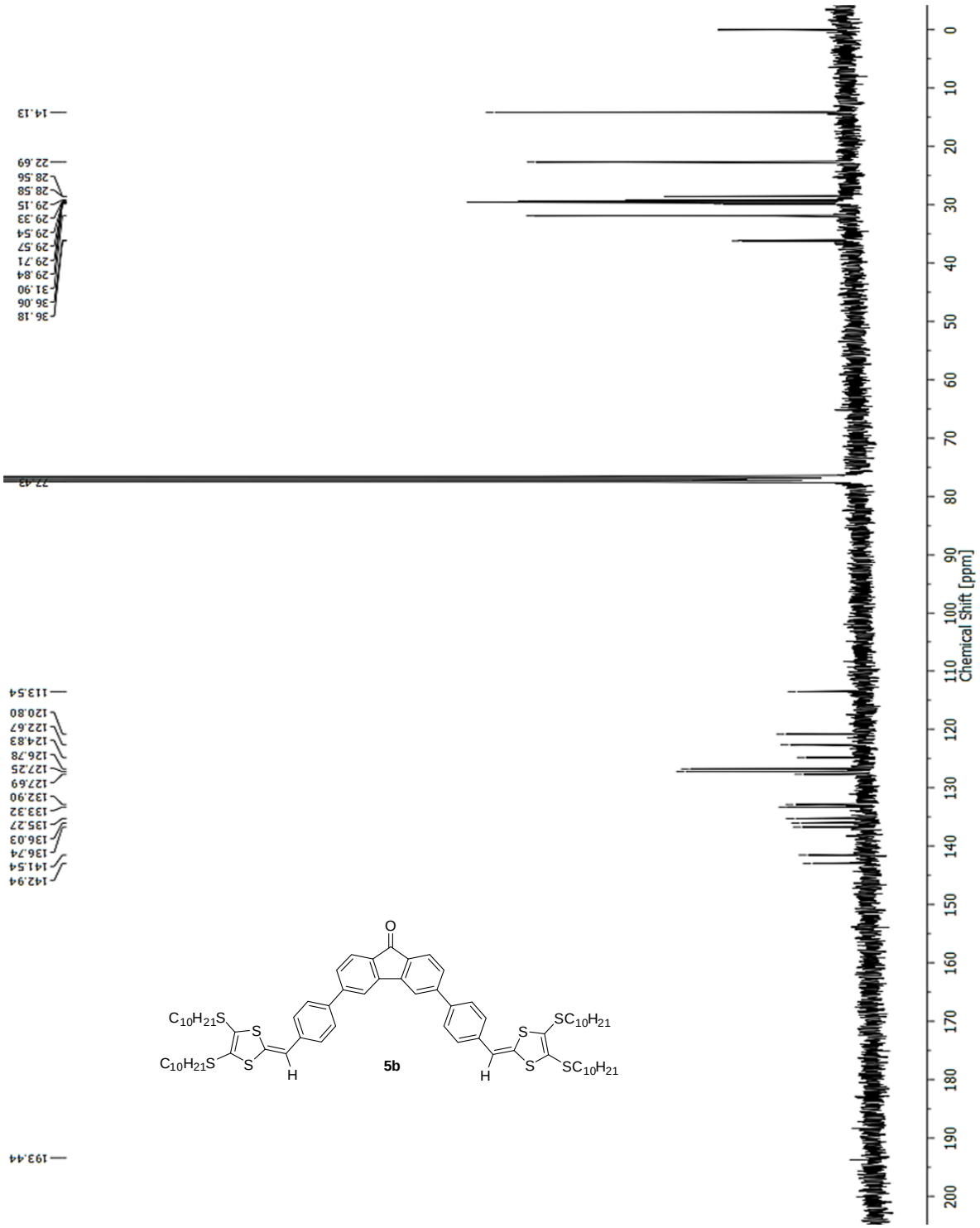

Fig. S-4 ^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound **5b**.

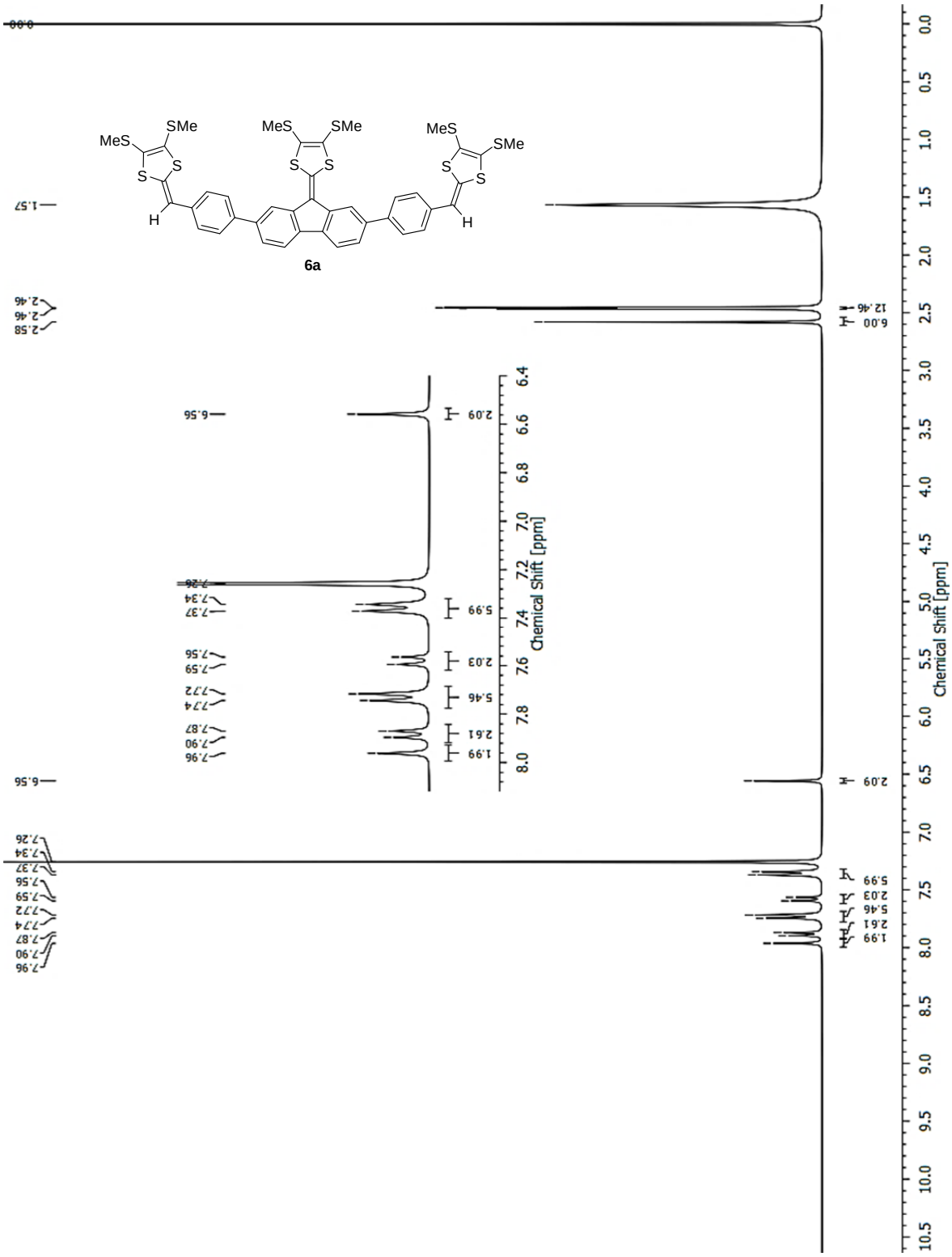

Fig. S-5 ^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound **6a**.

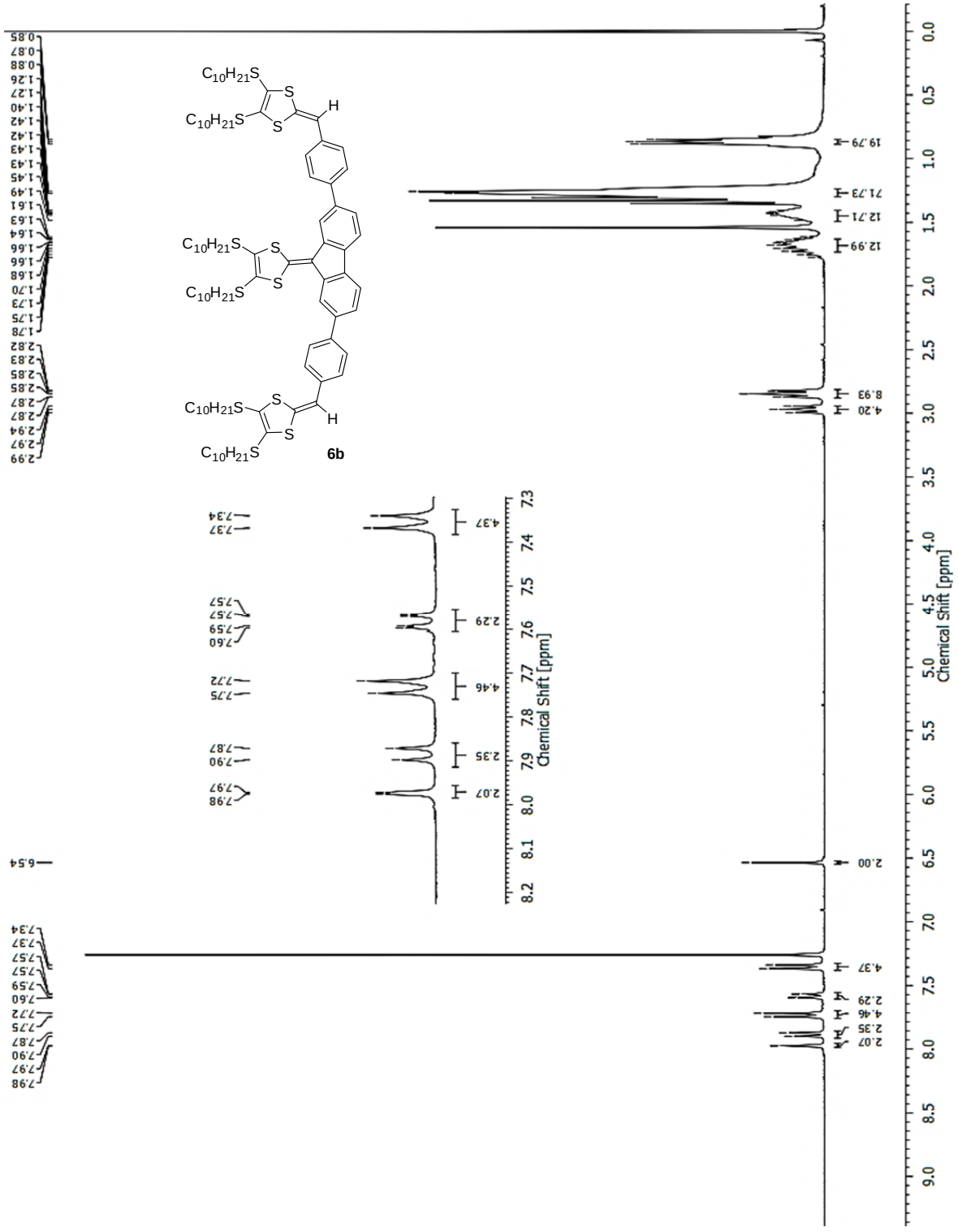

Fig. S-6 ^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound **6b**.

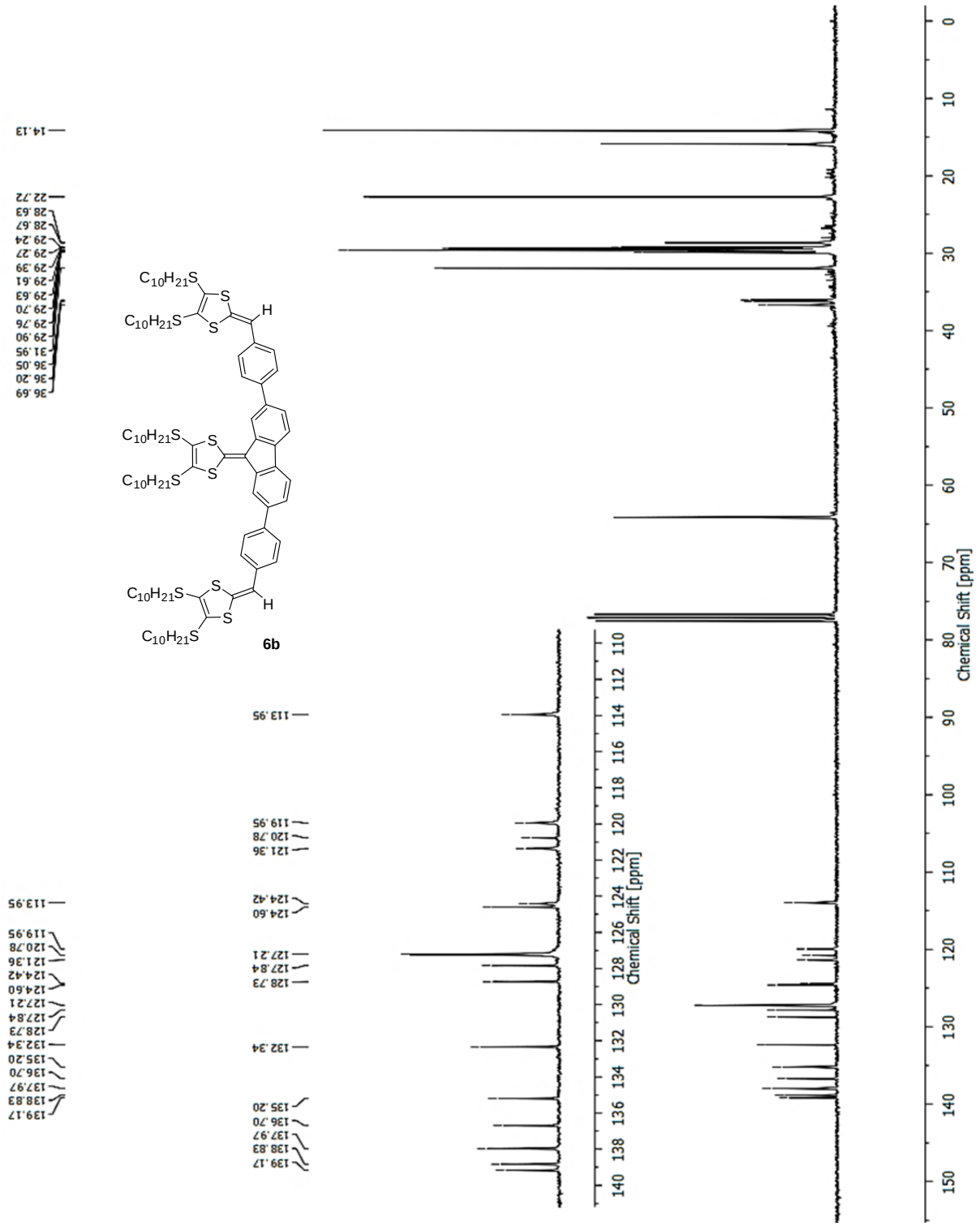

Fig. S-7 ^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound **6b**.

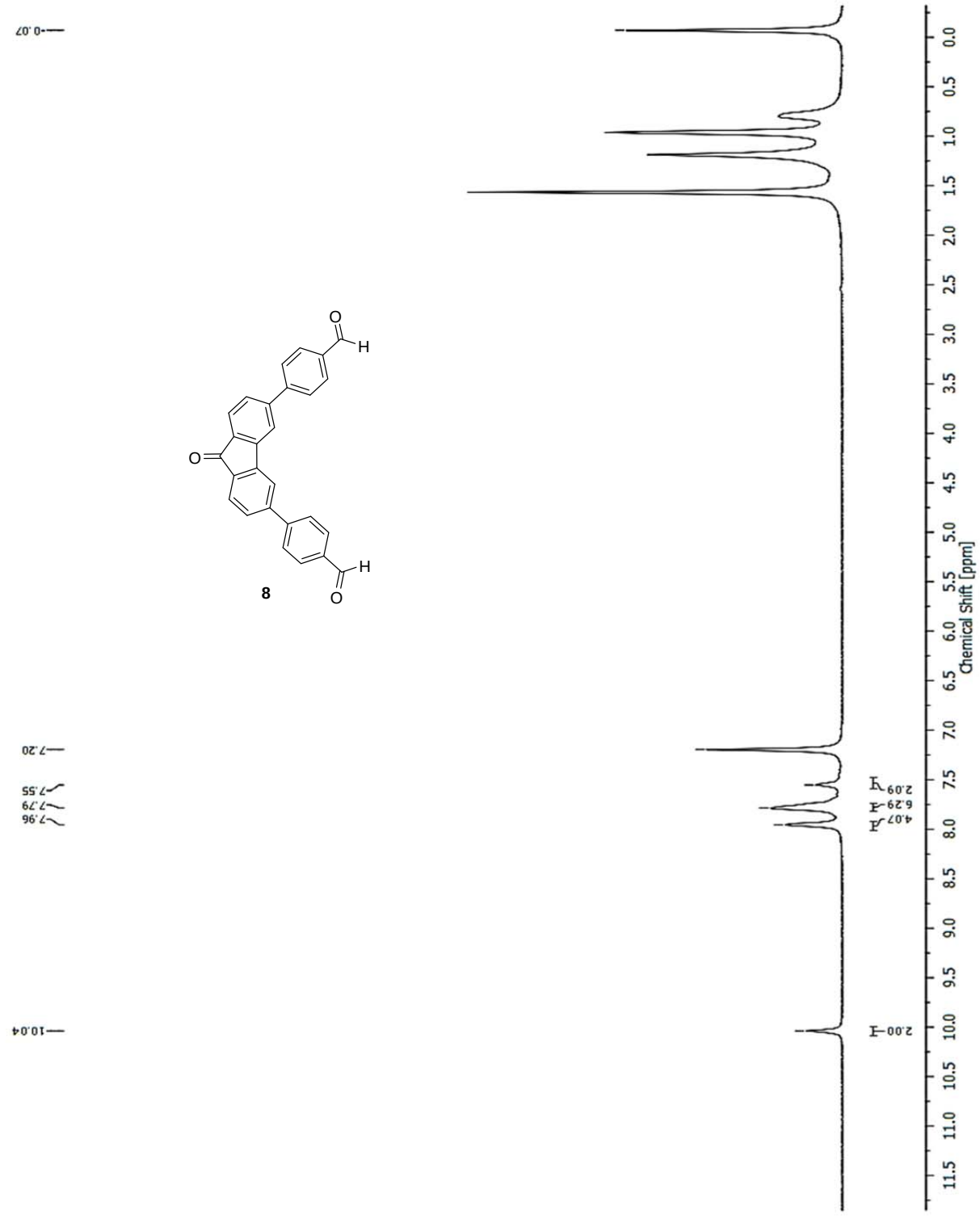

Fig. S-8 ^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound **8**.

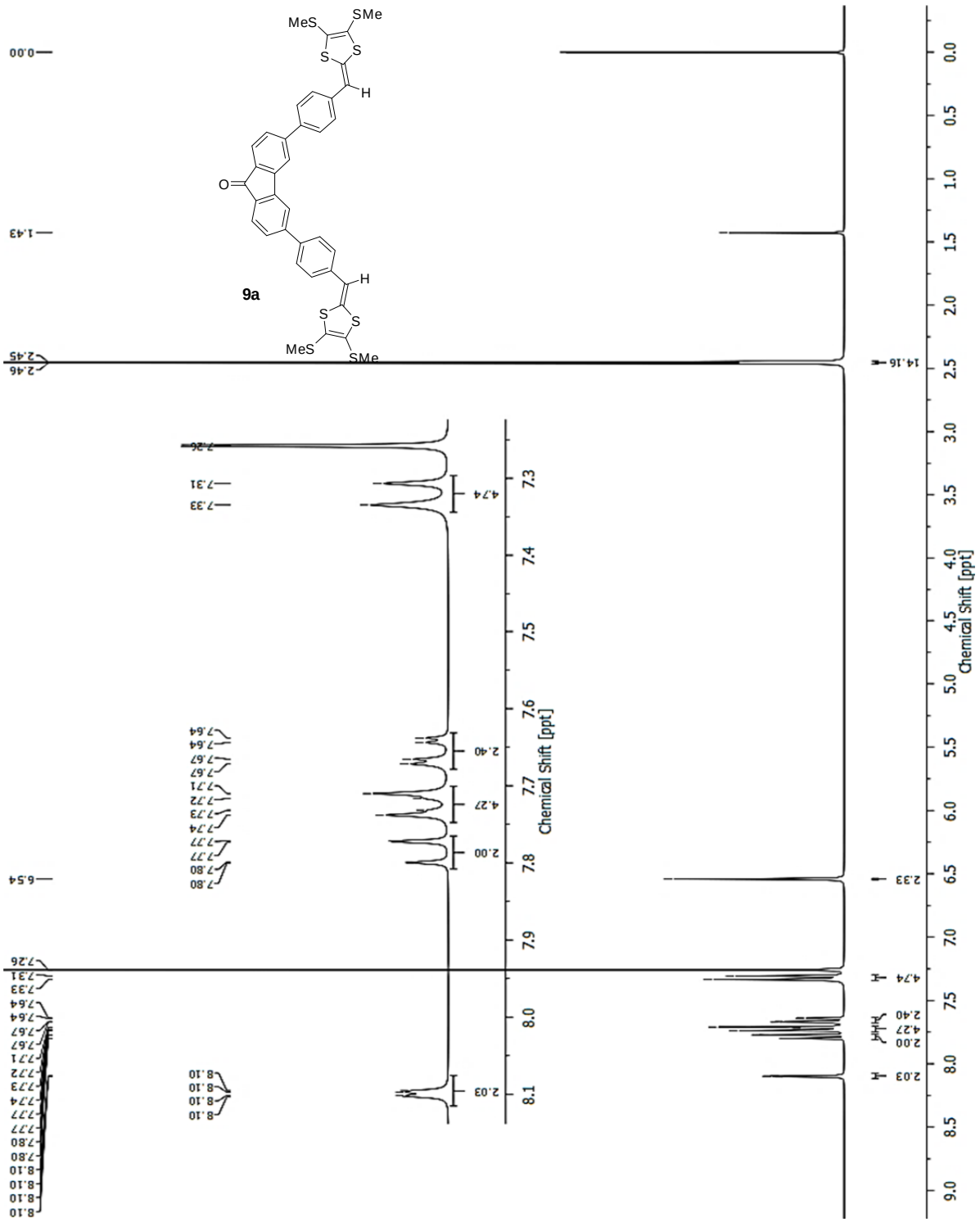

Fig. S-9 ^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound **9a**.

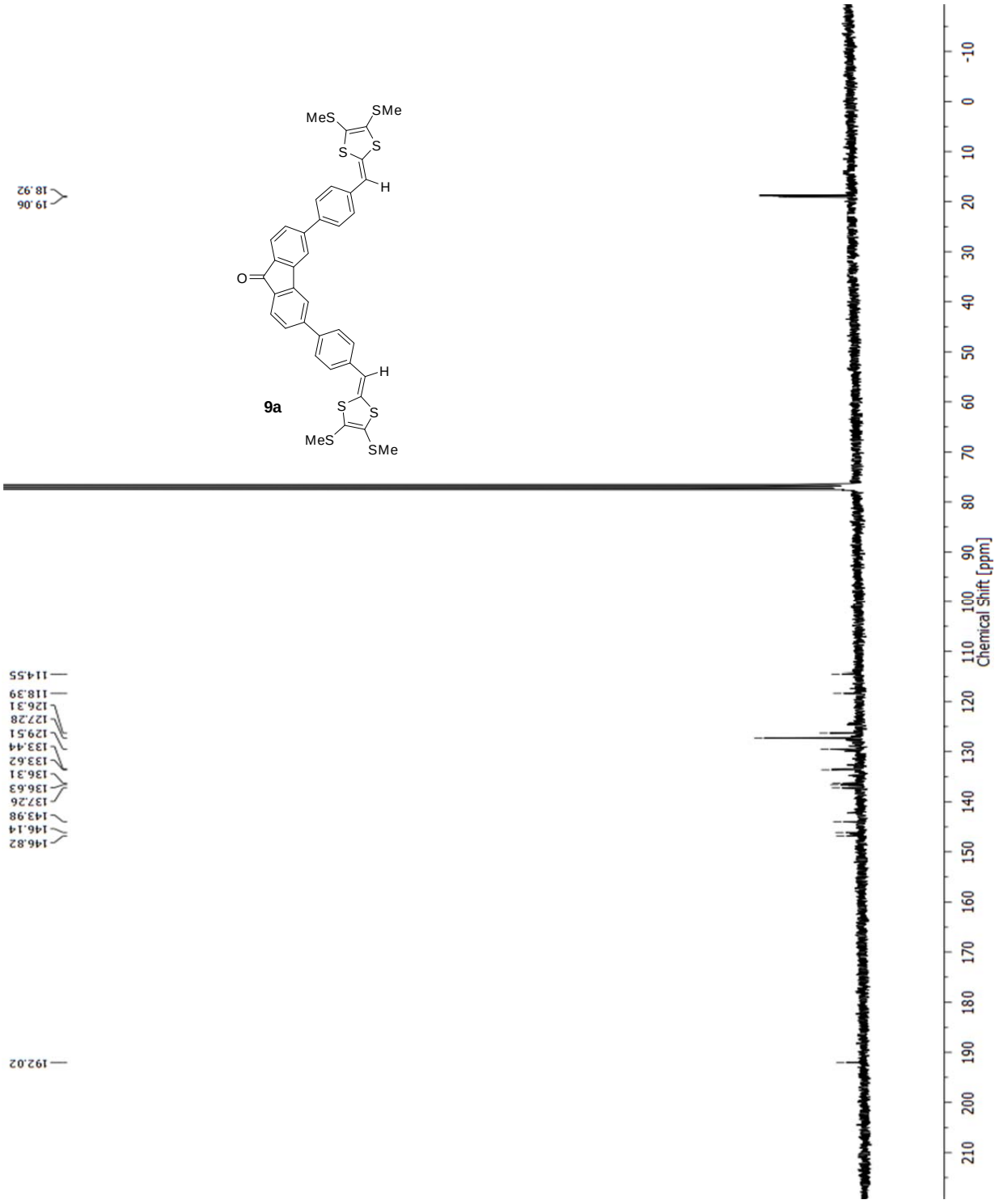

Fig. S-10 ^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound **9a**.

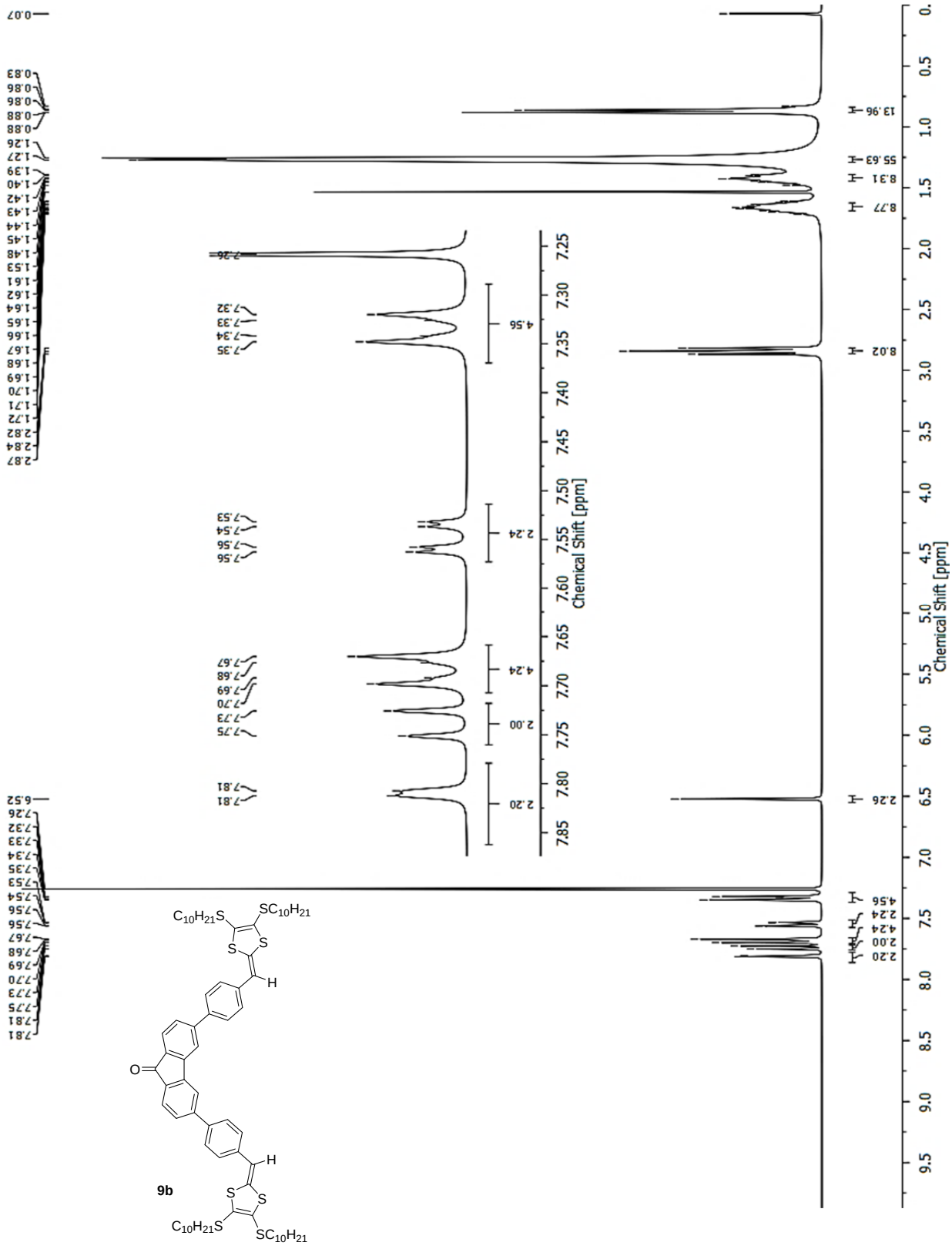

Fig. S-11 ^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound **9b**.

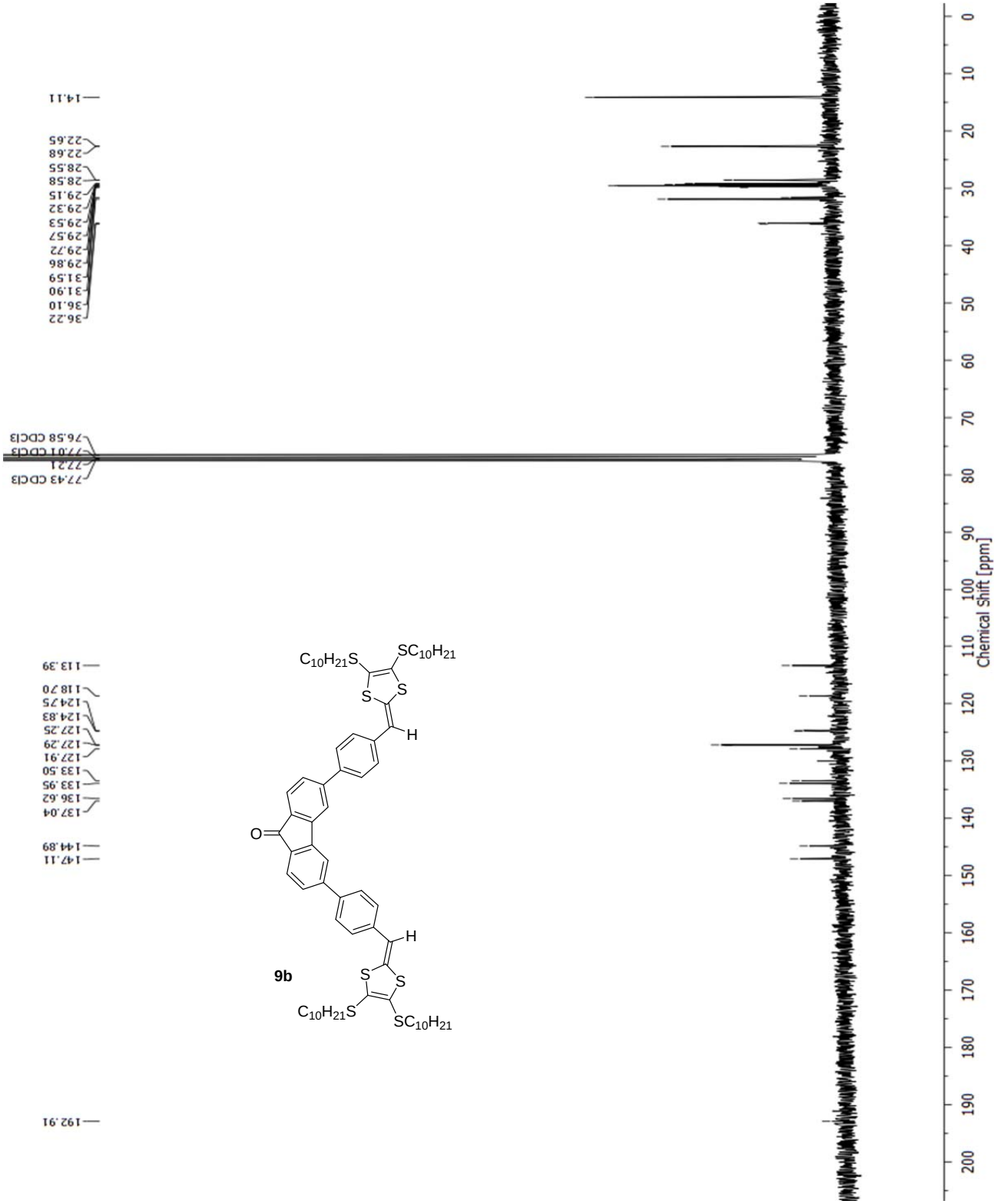

Fig. S-12 ^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound **9b**.

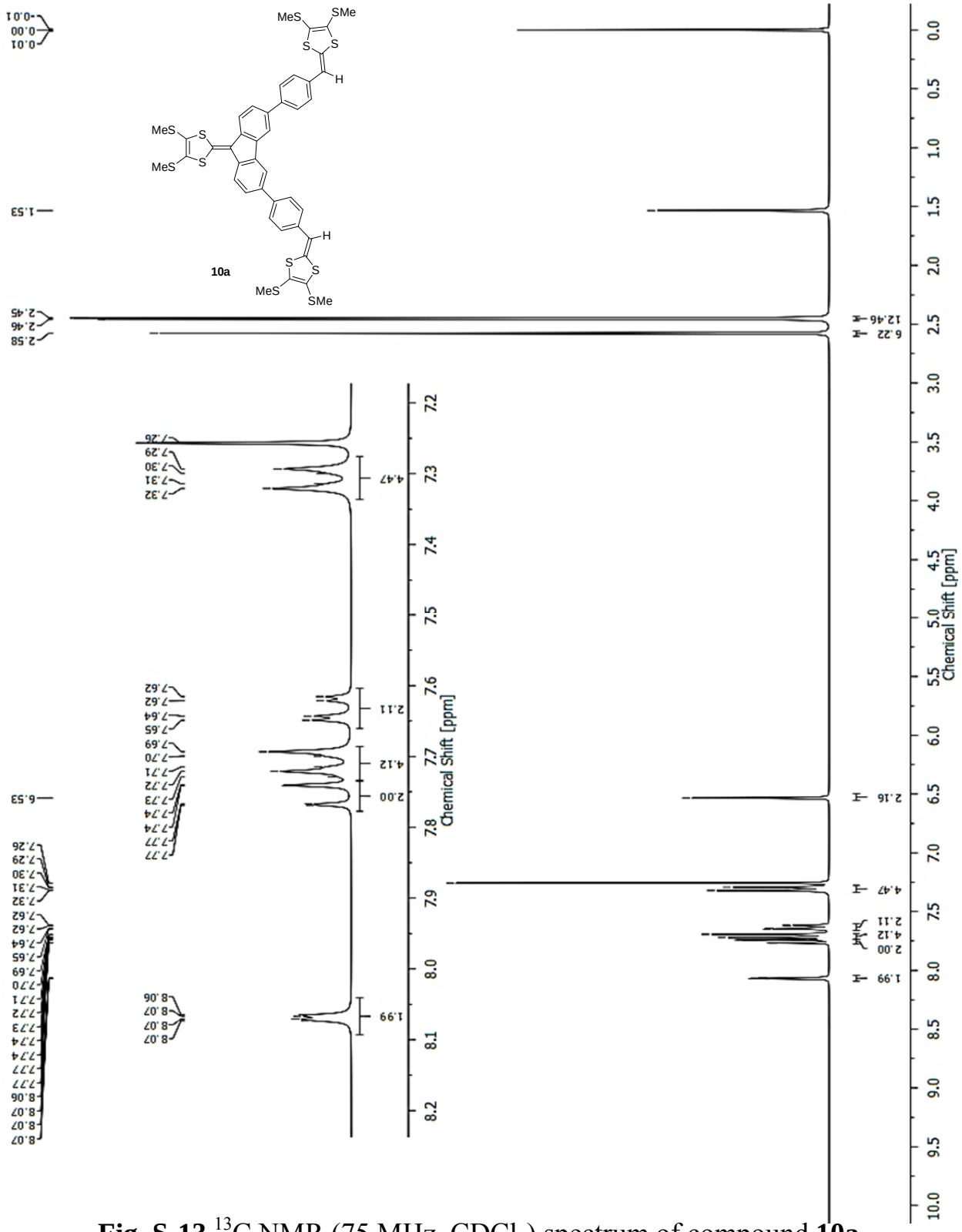

Fig. S-13 ^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound **10a**.

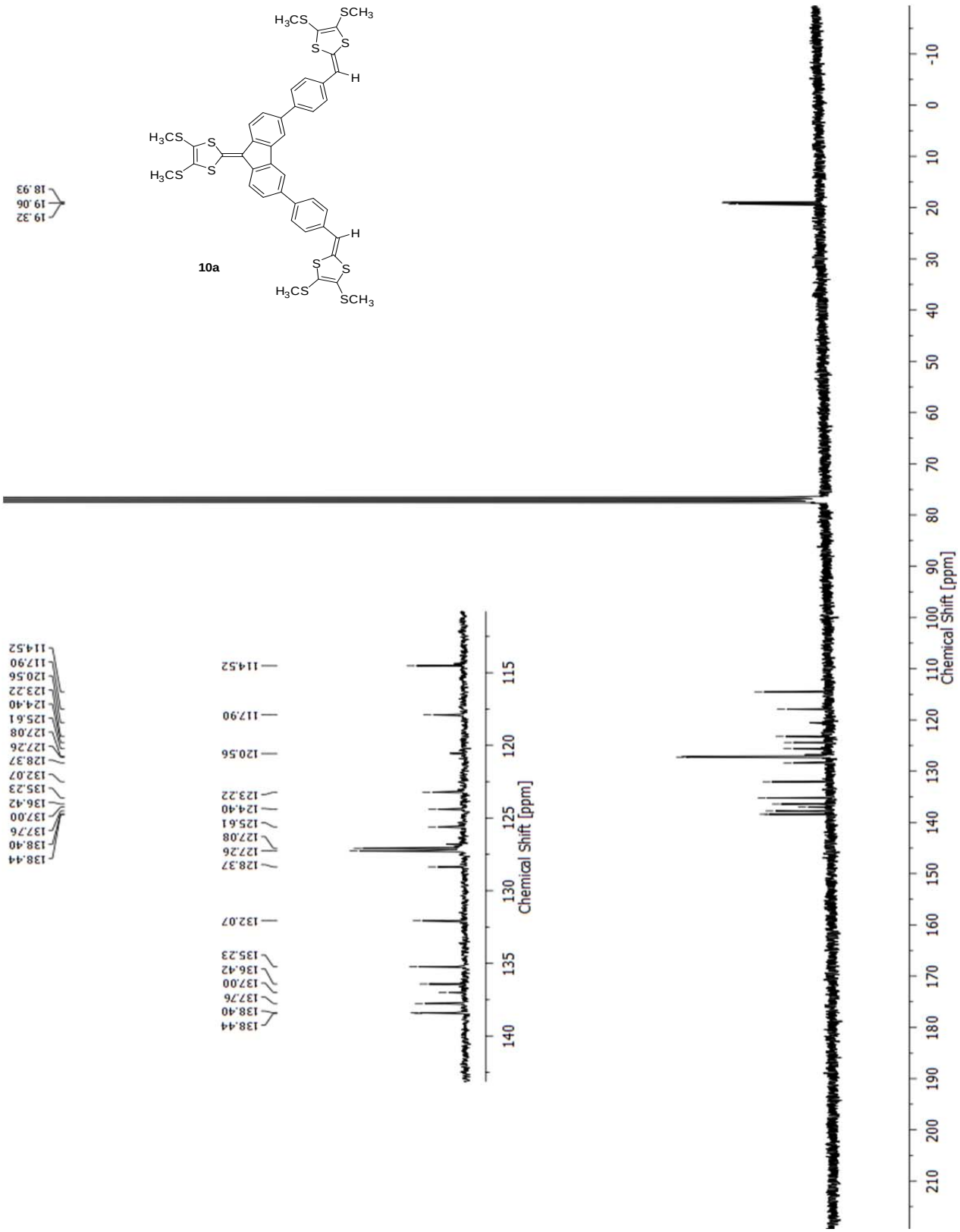

Fig. S-14 ^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound **10a**.

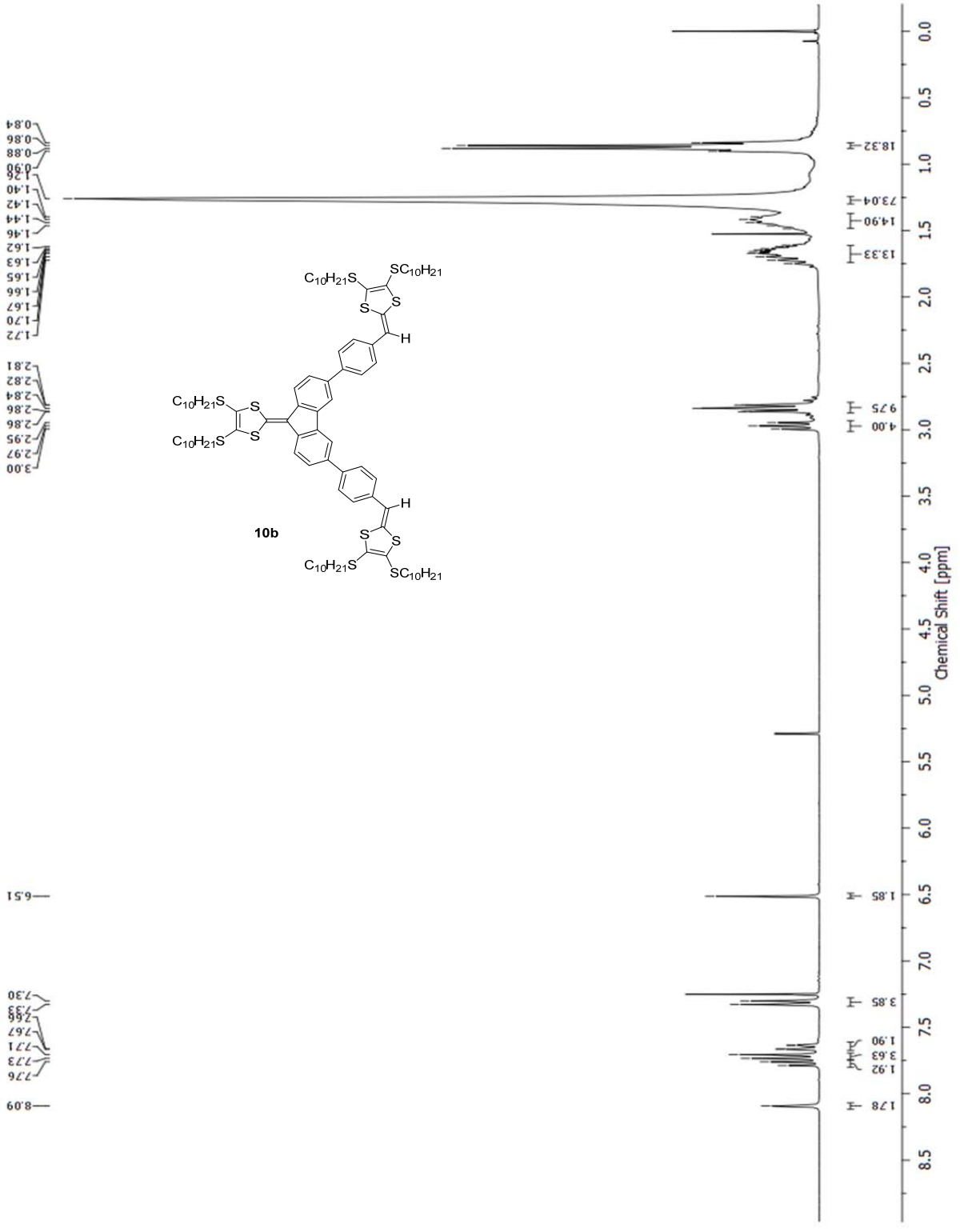

Fig. S-15 ^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound **10b**.

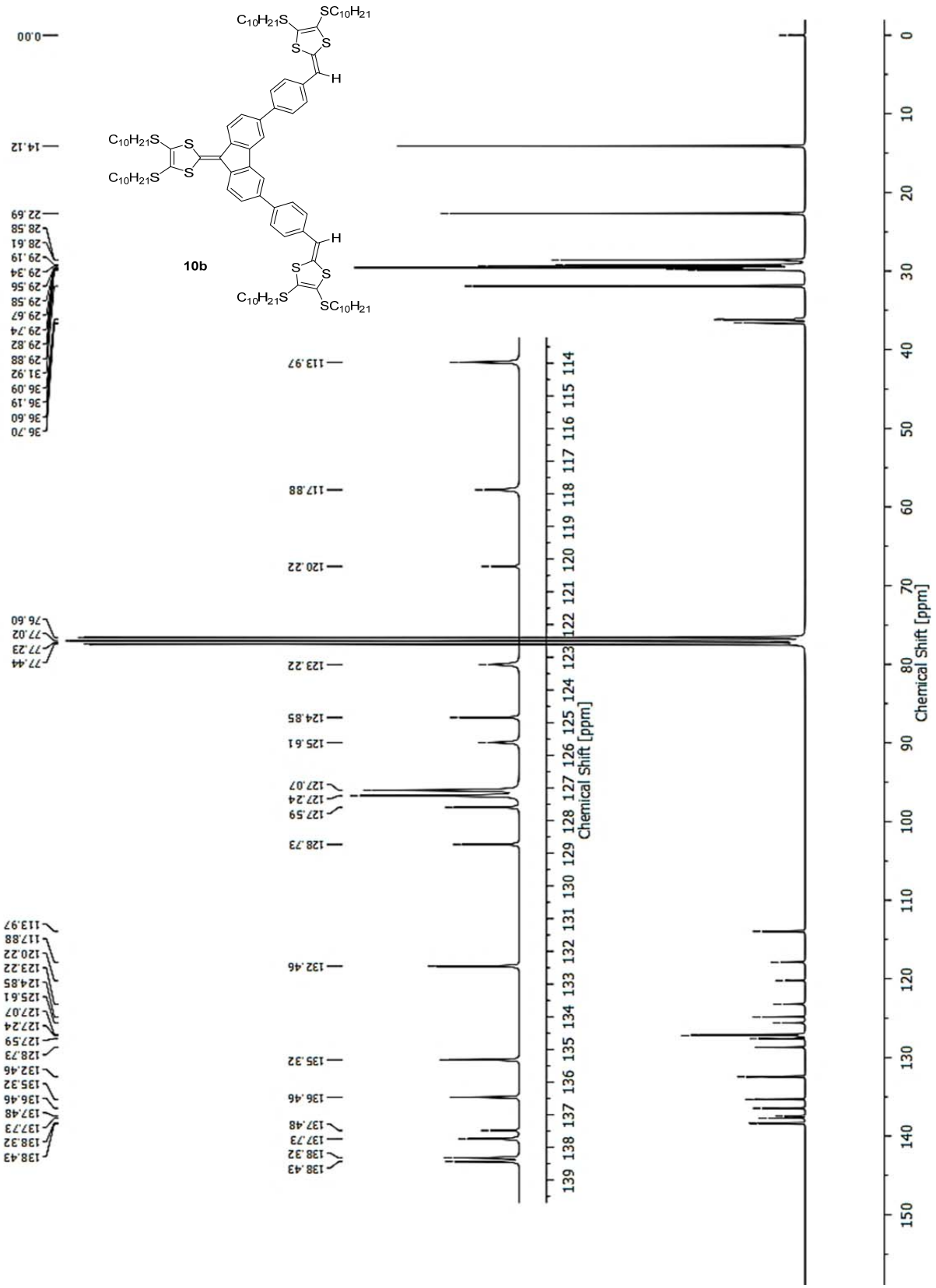

Fig. S-16 ^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound **10b**.

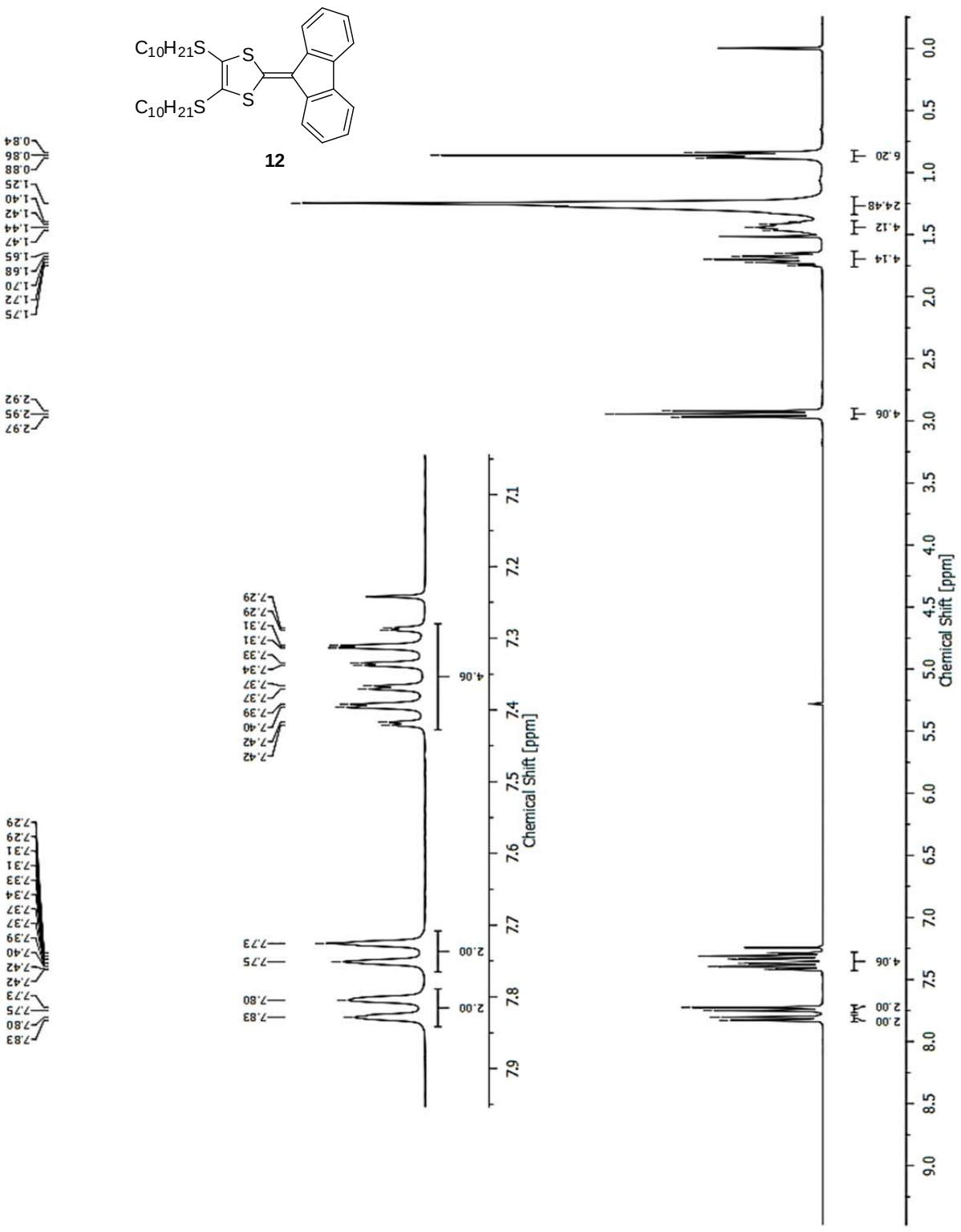

Fig. S-17 ^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound **12**.

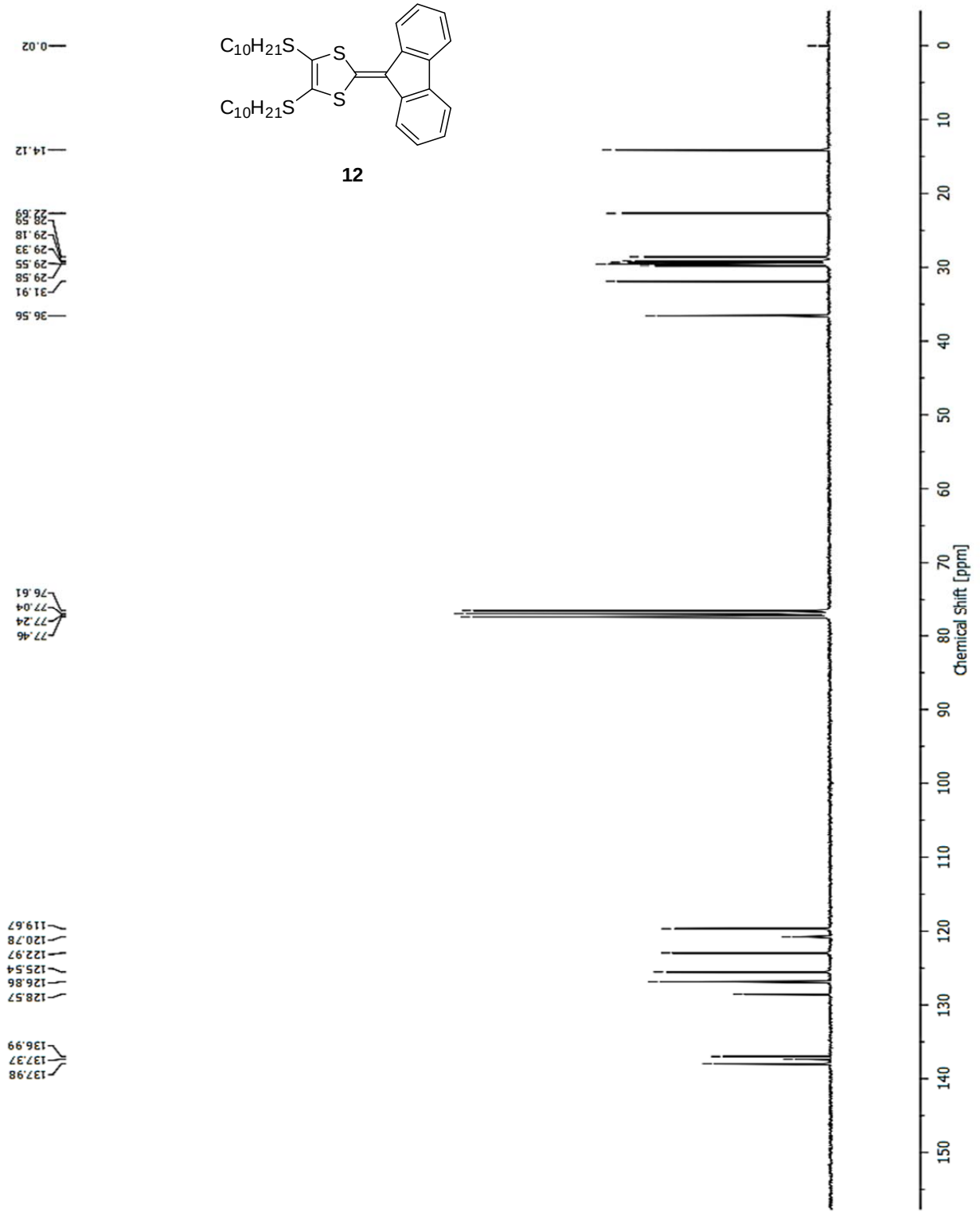

Fig. S-18 ^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound **12**.

2. UV-Vis Absorption Data

Table S-1 Summary of UV-Vis absorption data

entry	λmax /nm (ε / mol^{-1} L cm^{-1})
5a	442 (4.38×10^2), 390 (4.23×10^3), 285 (3.23×10^3), 225 (3.49×10^3)
5b	442 (4.38×10^2), 395 (3.67×10^3), 291 (2.75×10^3), 225 (3.49×10^3)
6a	388 (2.25×10^3), 347 (2.83×10^3), 265 (3.69×10^3), 228 (3.96×10^3)
6b	414 (3.58×10^3), 388 (3.98×10^3), 270 (3.23×10^3)
9a	439 (2.37×10^3), 350 (3.32×10^3), 271 (3.74×10^3), 227 (3.28×10^3)
9b	445 (5.05×10^2), 285 (4.10×10^3), 228 (2.62×10^3)
10a	430 (2.21×10^3), 371 (1.91×10^3), 278 (2.38×10^3)
10b	443 (4.06×10^3), 285 (5.45×10^3)
12	413 (2.06×10^3), 398 (1.93×10^3), 251 (4.39×10^3)

3. Crystallographic Data for Compounds 5a, 10a, and 12

Table S-2 Crystal data and structure refinement for **5a**

Empirical formula	$C_{37}H_{28}OS_8$
Formula weight	745.07
Temperature/K	100(2)
Crystal system	triclinic
Space group	*P*-1
a/Å	12.8667(2)
b/Å	19.3354(3)
c/Å	20.7609(3)
α/°	99.0250(10)
β/°	99.0750(10)
γ/°	97.7900(10)
Volume/Å^3	4968.66(13)
Z	6
ρ_{calc}g/cm^3	1.494
μ/mm^{-1}	5.242
F(000)	2316.0
Crystal size/mm^3	0.2 × 0.07 × 0.07
Radiation	Cu *K*α (λ = 1.54184)
2θ range for data collection/°	4.384 to 154.85
Index ranges	$-16 \le h \le 15$, $-24 \le k \le 24$, $-25 \le l \le 26$
Reflections collected	97458
Independent reflections	20586 [R_{int} = 0.0494, R_{sigma} = 0.0365]
Data/restraints/parameters	20586/26/1360
Goodness-of-fit on F^2	1.047
Final *R* indexes [I>=2σ (I)]	R_1 = 0.0743, wR_2 = 0.1938
Final *R* indexes [all data]	R_1 = 0.0956, wR_2 = 0.2122
Largest diff. peak/hole / e Å^{-3}	1.10/-1.24

Table S-3 Crystal data and structure refinement for **10a**

Empirical formula	$C_{85}H_{70}Cl_2S_{24}$
Formula weight	1931.75
Temperature/K	173.01(10)
Crystal system	triclinic
Space group	*P*-1
a/Å	9.43840(10)
b/Å	20.8406(3)
c/Å	22.59980(10)
α/°	89.3300(10)
β/°	83.4290(10)
γ/°	83.1130(10)
Volume/Å^3	4384.35(8)
Z	2
ρ_{calc}g/cm^3	1.463
μ/mm^{-1}	6.361
F(000)	1996.0
Crystal size/mm^3	0.18 × 0.05 × 0.05
Radiation	Cu *K*α (λ = 1.54184)
2θ range for data collection/°	3.936 to 155.314
Index ranges	$-11 \le h \le 11$, $-26 \le k \le 22$, $-28 \le l \le 28$
Reflections collected	32975
Independent reflections	32975 [R_{sigma} = 0.0143]
Data/restraints/parameters	32975/0/1013
Goodness-of-fit on F^2	1.036
Final *R* indexes [*I*>=2σ (I)]	R_1 = 0.0539, wR_2 = 0.1514
Final *R* indexes [all data]	R_1 = 0.0605, wR_2 = 0.1570
Largest diff. peak/hole / e Å^{-3}	1.11/-0.98

Table S-4 Crystal data and structure refinement for **12**

Empirical formula	$C_{36}H_{50}S_4$
Formula weight	611.00
Temperature/K	100(2)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	9.32000(10)
b/Å	10.2529(2)
c/Å	35.0079(5)
β/°	92.2020(10)
Volume/Å^3	3342.78(9)
Z	4
ρ_{calc}g/cm^3	1.214
μ/mm^{-1}	2.770
F(000)	1320.0
Crystal size/mm^3	0.25 × 0.05 × 0.04
Radiation	Cu $K\alpha$ (λ = 1.54184)
2θ range for data collection/°	5.052 to 155.036
Index ranges	$-11 \le h \le 8$, $-12 \le k \le 12$, $-43 \le l \le 44$
Reflections collected	56658
Independent reflections	6956 [R_{int} = 0.1055, R_{sigma} = 0.0473]
Data/restraints/parameters	6956/0/363
Goodness-of-fit on F^2	1.058
Final R indexes [I>=2σ (I)]	R_1 = 0.0638, wR_2 = 0.1731
Final R indexes [all data]	R_1 = 0.0758, wR_2 = 0.1868
Largest diff. peak/hole / e Å^{-3}	0.63/-0.70