Electronic Supplementary Information for

Molecular tuning of the crystallization-induced emission enhancement of diphenyl-dibenzofulvene luminogens

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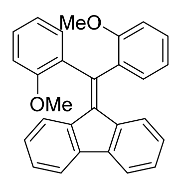
1. Synthetic Procedures

1.1 General procedures for Suzuki-Miyaura cross coupling of 9-(dibromomethylene)-9*H*-fluorene (10) with arylboronic acids (11a-c)

9-(Dibromomethylene)-9H-fluorene **(10)** was prepared according to the literature method.[1] To a solution of **10** (2.00 g, 5.95 mmol) and an arylboronic acid (2.25 g, 14.9 mmol) in THF (40 mL) and deionized water (14 mL) was added K_2CO_3 (4.00 g, 29.8 mmol). The reaction mixture was bubbled with N_2 flow for 10 min, and $Pd(PPh_3)_4$ (0.270 g, 0.238 mmol) was added. Under N_2 protection, the mixture was stirred and heated at 80 °C for 12 h. The formation of desired product was monitored by TLC analysis. After completion of the reaction, the mixture was cooled to rt and poured to a separatory funnel including water, and extracted with CH_2Cl_2 (3×20 mL) three times. The combined organic layers were dried over $MgSO_4$, filtered and concentrated under reduced pressure. The resulting residue was purified by silica gel column chromatography using CH_2Cl_2/hexanes as eluent.

9-(Bis(2-methoxyphenyl)methylene)-9*H*-fluorene (5a):



5a

Compound **5a** was prepared according to the general Suzuki-Miyaura cross coupling procedures and purified by silica gel column chromatography (CH_2Cl_2/hexanes, 40:60) as a colorless solid (1.35 g, 3.45 mmol, 58%). m.p.: 197.2−201.4 °C; IR (neat): 3051, 2923, 2852, 1621, 1578, 1500, 1444, 1179, 1117, 1024, 779, 750 cm^{-1}; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.66 (d, *J* = 7.5 Hz, 2H), 7.54 (dd, *J* = 7.5, 1.8 Hz, 2H), 7.36 (td, *J* = 7.5, 1.8 Hz, 2H), 7.21 (td, *J* = 7.5, 1.1 Hz, 2H), 7.03 (td, *J* = 7.5, 1.0 Hz, 2H), 6.99–6.89 (m, 4H), 6.41 (d, *J* = 7.9 Hz, 2H), 3.72 (s, 6H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ 156.35, 140.38, 139.03, 138.66, 135.25, 131.06, 130.56, 128.98, 127.38, 126.70. 124.57, 121.08, 119.04, 111.53, 55.65 ppm; HRMS (APPI-TOF, positive mode): *m/z* calcd for $C_{44}H_{36}O_4$ $[M]^+$ 390.16198, found 390.16365.

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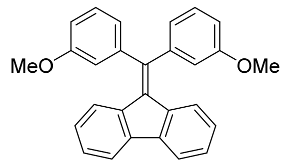
[1] X. Zhang, S. B. Hassine, N. Richy, O. Mongin, M. Blanchard-Desce, F. Paul and C. O. Paul-Roth, *New J. Chem.*, 2020, **44**, 4144-4157.

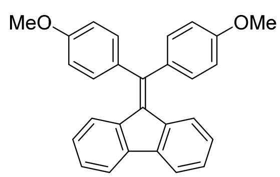
9-(Bis(3-methoxyphenyl)methylene)-9*H*-fluorene (5b)



5b

Compound **5b** was prepared according to the general Suzuki-Miyaura cross coupling procedures and purified by silica gel column chromatography (CH_2Cl_2/hexanes, 35:65) as a yellow solid (1.45 g, 3.71 mmol, 62%). m.p.: 159−162 °C; IR (neat): 3047, 2963, 2834, 1585, 1483, 1289, 1193, 1126, 1083, 856, 777, 704 cm^{-1}; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.68 (d, *J* = 6.9 Hz, 2H), 7.30 (dd, *J* = 8.4, 7.5 Hz, 2H), 7.24 (td, *J* = 7.5, 0.9 Hz, 2H), 7.00−6.92 (m, 8H), 6.68 (d, *J* = 8.1 Hz, 2H), 3.77 (s, 6H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ 159.94, 144.90, 144.08, 140.50, 138.54, 134.12, 129.93, 127.70, 126.51, 125.11, 121.84, 119.20, 114.66, 113.97, 55.34 ppm; HRMS (APPI-TOF, positive mode): *m/z* calcd for $C_{28}H_{22}O_2$ $[M]^+$ 390.1619, found 390.1622.

9-(Bis(4-methoxyphenyl)methylene)-9*H*-fluorene (5c)



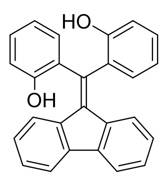
5c

Compound **5c** was prepared according to the general Suzuki-Miyaura cross coupling procedures and purified by silica gel column chromatography (CH_2Cl_2/hexanes, 35:65) as a yellow solid (1.97 g, 5.04 mmol, 85%). m.p.: 130−149 °C; IR (neat): 3048, 2997, 2834, 1600, 1503, 1455, 1274, 1170, 783, 750, 735, 694 cm^{-1}; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.71 (d, *J* = 7.5 Hz, 2H), 7.30−7.20 (m, 6H), 6.90−6.98 (m, 6H), 6.80 (d, *J* = 7.8 Hz, 2H), 3.87 (s, 6H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ 159.91, 145.55, 140.19, 139.19, 135.60, 133.26, 131.93, 127.12, 126.23, 124.56, 119.20, 114.03, 55.33 ppm; HRMS (APPI-TOF, positive mode): *m/z* calcd for $C_{28}H_{23}O_2$ $[M + H]^+$ 391.1698, found 391.1689.

1.2 General procedures for the demethylation reactions to prepare 12a-c

To an ice-cooled solution of **DP-DBF** derivative (**5a–c**) (1.00 g, 2.56 mmol) in dry CH_2Cl_2 (25 mL), a fresh solution of BBr_3 (2.67 mL, 25.2 mmol) in dry CH_2Cl_2 (5 mL) was added dropwise. The resulting reaction mixture was stirred at 0 ºC for ca. 3 h and then the ice bath was removed. The reaction was continued at rt for another 1 h. The progress of the reaction was monitored by TLC analysis. Upon completion, the reaction was quenched very carefully with water. The resulting mixture was then diluted with brine and extracted with CH_2Cl_2 (3×20 mL) three times. The combined organic layers were dried over $MgSO_4$, filtered, and concentrated under reduced pressure, resulting in demethylated products (**12a–c**) without further purification.

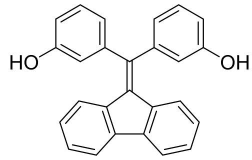
2,2'-((9*H*-fluoren-9-ylidene)methylene)diphenol (12a)



12a

Compound **12a** was prepared according to the general demethylation procedures as a brownish creamy solid (0.790 g, 2.18 mmol, 85%). m.p.: > 215.6 °C (decomp). IR (neat): 3475, 3374, 3054,1575, 1486, 1445, 1339, 1271, 1211, 1179, 1100, 1033, 876, 855, 759, 734 cm^{-1}; ^{1}H NMR (300 MHz, acetone-d_6): δ 8.64 (s, 2H), 7.78 (d, J = 7.3 Hz, 2H), 7.41 (dd, J = 7.8, 1.7 Hz, 2H), 7.34 (td, J = 7.5, 1.7 Hz, 2H), 7.28 (td, J = 7.5, 1.0 Hz, 2H), 7.08−7.01 (m, 4H), 6.96 (td, J = 7.9, 1.2 Hz, 2H), 6.50 (d, J = 7.8 Hz, 2H) ppm; ^{13}C NMR (75 MHz, acetone-d_6): δ 152.95, 140.60, 137.92, 137.62, 129.50, 129.26, 128.96, 128.27, 126.93, 126.67, 124.66, 121.18, 119.29, 116.31 ppm; HRMS (ESI-TOF, negative mode): *m/z* calcd for $C_{26}H_{18}O_2$ $[M]^-$ 362.1307, found 362.1299.

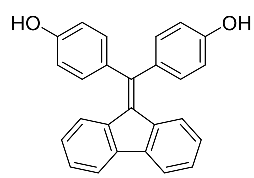
3,3'-((9*H*-fluoren-9-ylidene)methylene)diphenol (12b)



12b

Compound **12b** was prepared according to the general demethylation procedures as a creamy solid (0.550 g, 1.52 mmol, 59%). m.p.: > 207.4 °C (decomp). IR (neat): 3263, 3.054, 2922, 1580, 1489, 1443, 1353, 1263, 1244, 1196, 1180, 1124, 931, 776, 747, 729 cm^{-1}; ^{1}H NMR (300 MHz, acetone- *d*6): δ 8.44 (s, 1H), 7.79 (d, *J* = 7.5 Hz, 2H), 7.32 (t, *J* = 8.0 Hz, 2H), 7.27 (td, *J* = 7.3, 1.0 Hz, 2H), 6.99–6.87 (m, 8H), 6.73 (d, *J* = 8.1 Hz, 2H), 5.61 (s, 1H) ppm; ^{13}C NMR (75 MHz, acetone-d_6): δ 157.82, 145.58, 144.27, 140.40, 138.43, 130.06, 127.83, 126.45, 125.03, 119.87, 119.26, 115.66, 115.05 ppm (one aromatic signal missing due to coincidental overlap); HRMS (ESI-TOF, negative mode): *m/z* calcd for $C_{26}H_{18}O_2$ $[M]^-$ 362.1307, found 362.1297.

4,4'-((9*H*-fluoren-9-ylidene)methylene)diphenol (12c)



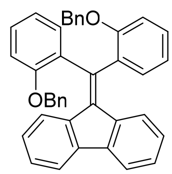
12c

Compound **12c** was prepared according to the general demethylation procedures as an orange solid (0.620 g, 1.71 mmol, 67%). m.p. > 261 °C (decomp). IR (neat): 3333, 3053, 2921, 1687, 1602, 1585, 1505, 1429, 1367, 1218,1132, 1106, 968, 835, 777 cm^{-1}; ^{1}H NMR (300 MHz, acetone-d_6): δ 7.78 (d, *J* = 7.5 Hz, 2H), 7.26–7.18 (m, 6H), 6.99–6.92 (m, 6H), 6.83 (d, *J* = 7.8 Hz, 2H) ppm; ^{13}C NMR (75 MHz, acetone-d_6): δ 152.92, 146.73, 140.04, 139.21, 134.49, 131.66, 127.34, 127.11, 126.17, 124.44, 119.16, 115.46 ppm; HRMS (APPI-TOF, negative mode): *m/z* calcd for $C_{26}H_{18}O_2$ $[M]^-$ 362.1307, found 362.13232.

1.3 General procedures for the benzylation reactions to prepare 8a-c

To the solution of a hydroxylated **DP-DBF** (**12a-c**) (0.500 g, 1.38 mmol) in DMF (15 mL) K_2CO_3 (0.570 g, 4.14 mmol) was added. The resulting mixture was stirred at rt for 15 min, and benzyl bromide (0.410 mL, 3.44 mmol) was then added dropwise. The reaction was further heated to 100 ºC for 12 h, and was monitored by TLC analysis. Upon completion, the reaction was quenched with water and extracted with ethyl acetate (3 × 20 mL). The combined organic layers were washed with water, brine, dried over $MgSO_4$, and concentrated under reduced pressure. The residue was subjected to silica gel column chromatography using CH_2Cl_2/hexanes as eluent, affording pure compounds **8a–c**, respectively.

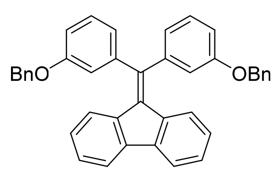
9-(Bis(2-(benzyloxy)phenyl)methylene)-9*H*-fluorene (8a)



8a

Compound **8a** was obtained according to the general benzylation procedures as a creamy white solid (0.50 g, 0.92 mmol, 67%). m.p.: 165.3–170.5 °C. IR (neat): 3056, 3030, 2928, 2915, 2873, 1591, 1484, 1443, 1288, 1234, 1160, 1115, 1080, 998, 780 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ 7.68 (d, J = 7.2 Hz, 2H), 7.46 (dd, J = 7.5, 1.5 Hz, 2H), 7.32–7.08 (m,14H), 6.96 (d, J = 8.1 Hz, 2H), 6.91 (d, J = 7.5 Hz, 4H), 6.44 (d, J = 7.8 Hz, 2H), 5.01 (s, 4H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ ppm 155.49, 140.39, 139.61, 138.77, 137.03, 131.90, 130.94, 128.94, 128.26, 127.93, 127.54, 127.35, 126.59, 124.85, 121.13, 119.02, 113.09, 112.74, 70.14 ppm; HRMS (APPI-TOF, positive mode): *m/z* calcd for $C_{40}H_{30}O_2$ $[M]^+$ 542.2246, found 542.2236.

9-(Bis(3-(benzyloxy)phenyl)methylene)-9*H*-fluorene (8b)

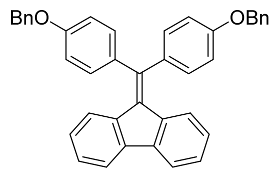


8b

Compound **8b** was obtained according to the general benzylation procedures as a yellow solid (0.54 g, 1.0 mmol, 73%). m.p.: 163.6–167.2 °C. IR (neat): 3057, 3029, 2925, 2859, 1582, 1481, 1431, 1377, 1315, 1285, 1213, 1155, 1027, 1003, 776 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ 7.69 (d, J = 7.5 Hz, 2H), 7.41–7.27 (m, 14H), 7.24 (td, J = 7.4, 1.0 Hz, 2H), 7.03–6.91 (m, 6H), 6.68

(d, J = 8.1 Hz, 2H), 5.02 (s, 4H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ 159.18, 144.72, 144.07, 140.50, 138.50, 136.78, 134.16, 129.97, 128.54, 127.97, 127.70, 127.58, 126.53, 125.12, 122.12, 119.20, 115.64, 114.94, 70.06 ppm; HRMS (APPI-TOF, positive mode): *m/z* calcd for $C_{40}H_{30}O_2$ $[M]^+$ 542.2246, found 542.2244.

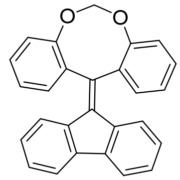
9-(Bis(4-(benzyloxy)phenyl)methylene)-9*H*-fluorene (8c)



8c

Compound **8c** was obtained according to the general benzylation procedures as a yellow solid (0.580 g, 1.06 mmol, 78%). m.p.: 192.2−194.0 °C. IR (neat): 3090, 3028, 2920, 2869, 1600, 1502, 1465, 1448, 1379, 1287, 1233, 1171, 1108, 1003, 969, 860, 824, 790 cm^{-1}; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.71 (d, J = 7.5 Hz, 2H), 7.49−7.33 (m, 10H), 7.32−7.19 (m, 6H), 7.02−6.93 (m, 6H), 6.79 (d, J = 8.7 Hz, 2H), 5.12 (s, 4H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ 159.14, 145.45, 140.20, 139.14, 136.78, 135.82, 133.41, 131.86, 128.59, 128.12, 127.64, 127.15, 126.24, 124.58, 119.12, 114.96, 70.12 ppm; HRMS (APPI-TOF, positive mode): *m/z* calcd for $C_{40}H_{30}O_2$ $[M]^+$ 542.2246, found 542.2242.

12-(9*H*-fluoren-9-ylidene)-12*H*-dibenzo[*d,g*][1,3]dioxocine (9)



9

A suspension of compound **12a** (0.30 g, 0.83 mmol) and Cs_2CO_3 (0.22 g, 2.48 mmol) in DMF (10 mL) was stirred at rt for 15 min. To this mixture was added CH_2I_2 (0.10 mL, 1.2 mmol) dropwise. The reaction mixture was then heated to 100 ºC for 8 h. The reaction was monitored by TLC analysis. Upon completion, the reaction was quenched with water and extracted with ethyl acetate (3 × 15 mL). The organic layers were combined, washed with water and brine, dried over $MgSO_4$, and concentrated under reduced pressure. The resulting residue was purified by silica gel column chromatography (CH_2Cl_2/hexanes, 50:50) to give pure compound **9** as a creamy white solid (0.15 g, 0.40 mmol, 50%). m.p.: 227.4–235.1 °C. IR (neat): 3053, 2999, 2955, 2852, 1619, 1597, 1571, 1483, 1435, 1273, 1235, 1182, 1143, 1046, 1000, 964, 877, 852, 781 cm^{-1}; ^{1}H NMR (300 MHz, CD_2Cl_2): δ 7.62 (d, *J* = 7.6 Hz, 2H), 7.30–7.24 (m, 4H), 7.20 (td, *J* = 7.5, 0.9 Hz, 2H), 7.09–7.04 (m, 4H), 6.88 (td, *J* = 7.5, 1.4 Hz, 2H), 6.52 (d, *J* = 8.1 Hz, 2H), 6.27 (d, *J* = 7.5 Hz, 1H), 5.36 (d, *J* = 7.5 Hz, 1H) ppm; ^{13}C NMR (75 MHz, CD_2Cl_2): δ 153.63, 140.70, 137.51, 136.09, 129.97, 129.50, 128.30, 126.89, 124.98, 123.88, 120.98, 119.38, 93.74 ppm (two aromatic signals missing due to coincidental overlap); HRMS (APPI-TOF, positive mode): *m/z* calcd for $C_{27}H_{18}O_2$ $[M]^+$ 374.1307, found 374.1313.

2. NMR Spectra for New Compounds

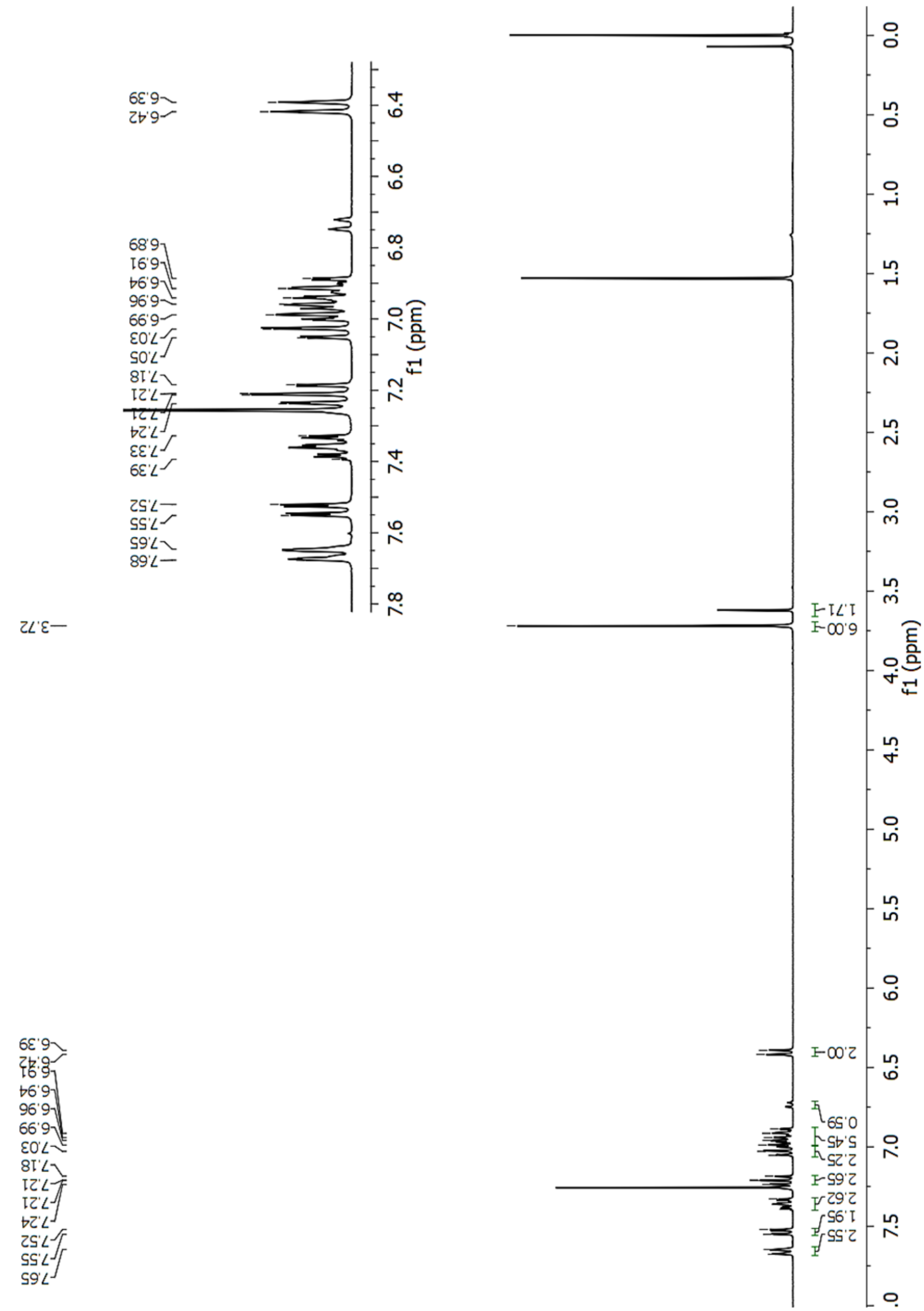


Fig. S-1 ^{1}HNMR (300 MHz, $CDCl_3$) of compound **5a.**

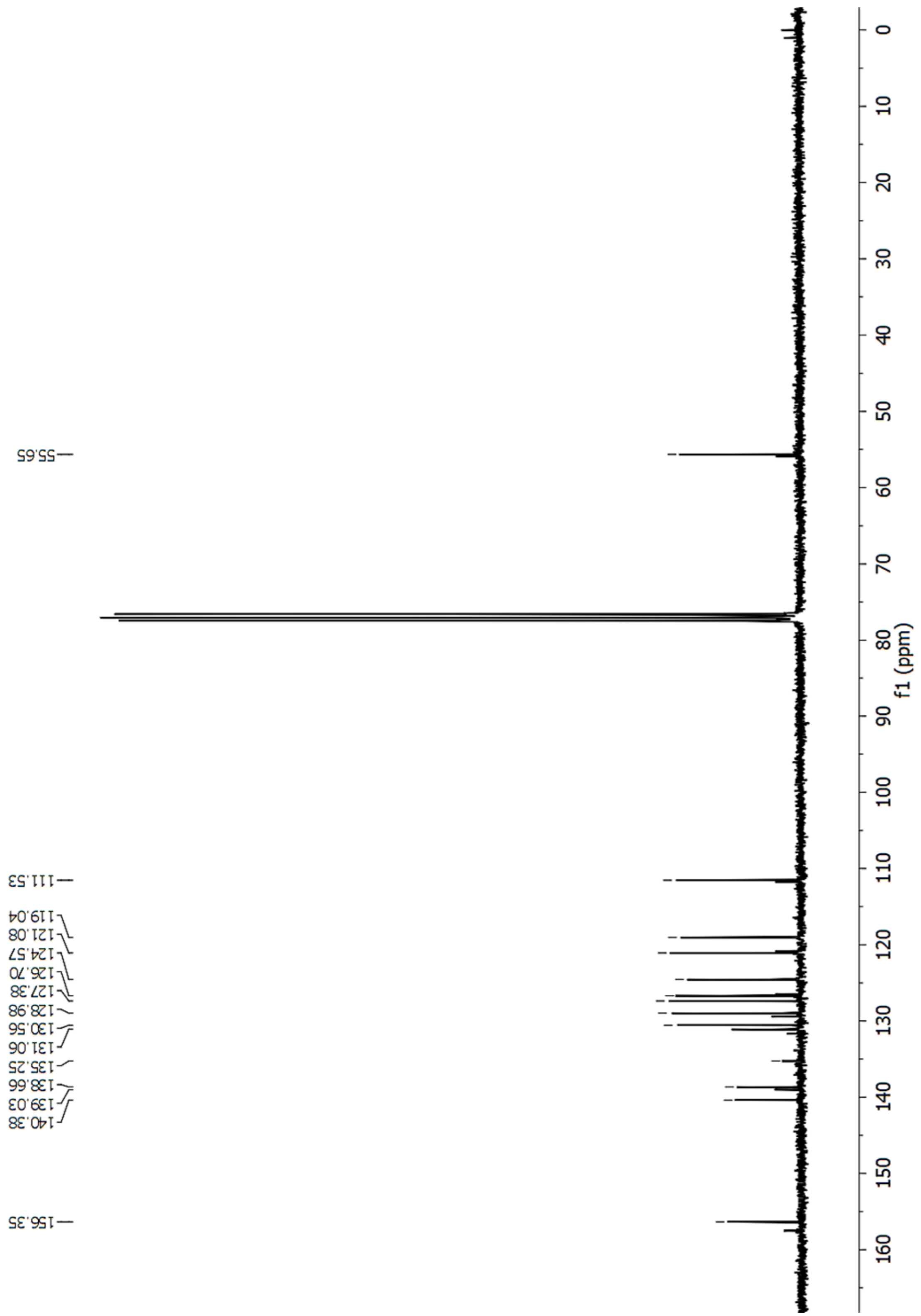


Fig. S-2 ^{13}CNMR (75 MHz, $CDCl_3$) of compound **5a.**

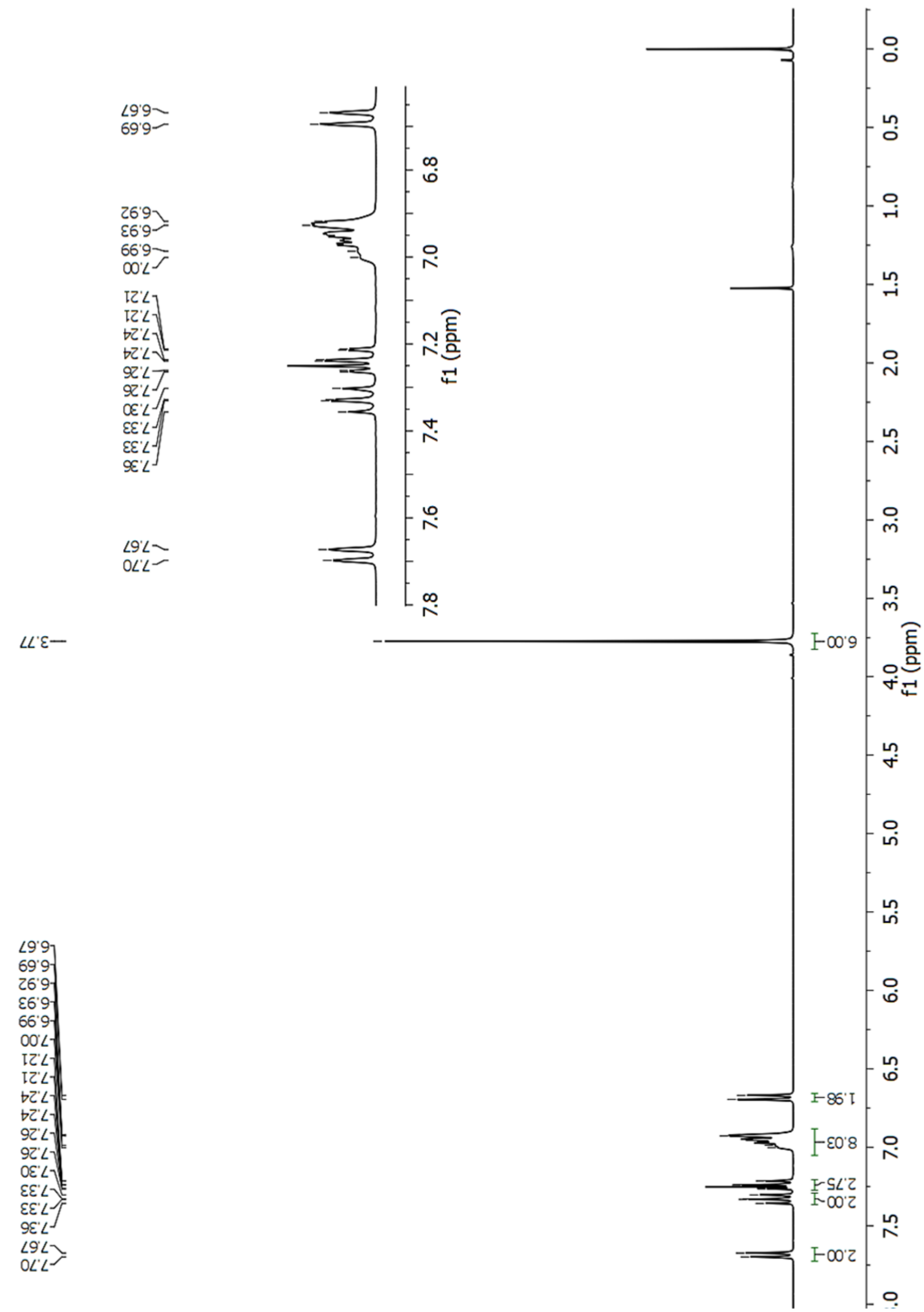


Fig. S-3 ^{1}HNMR (300 MHz, $CDCl_3$) of compound **5b.**

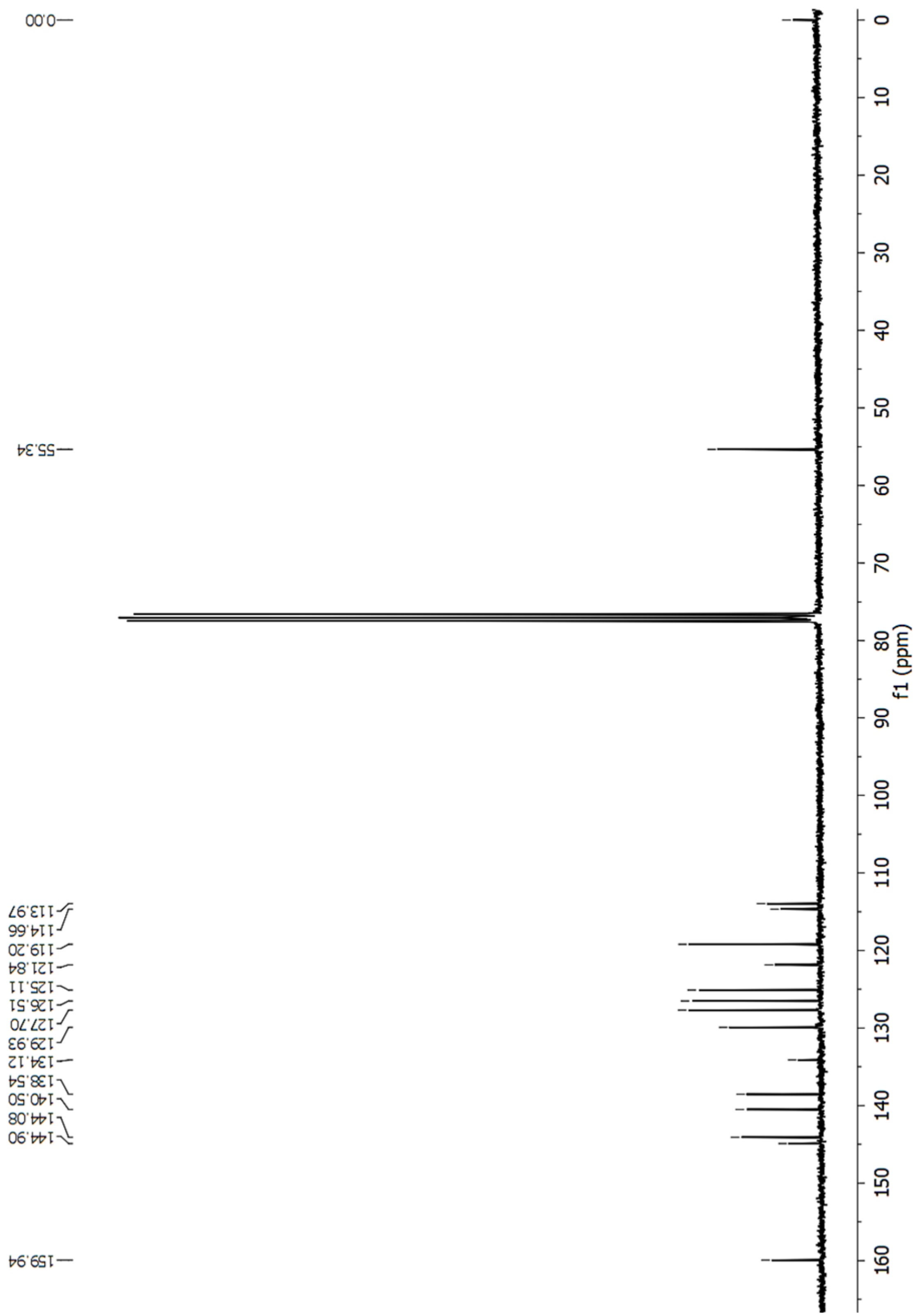


Fig. S-4 ^{13}CNMR (75 MHz, $CDCl_3$) of compound **5b.**

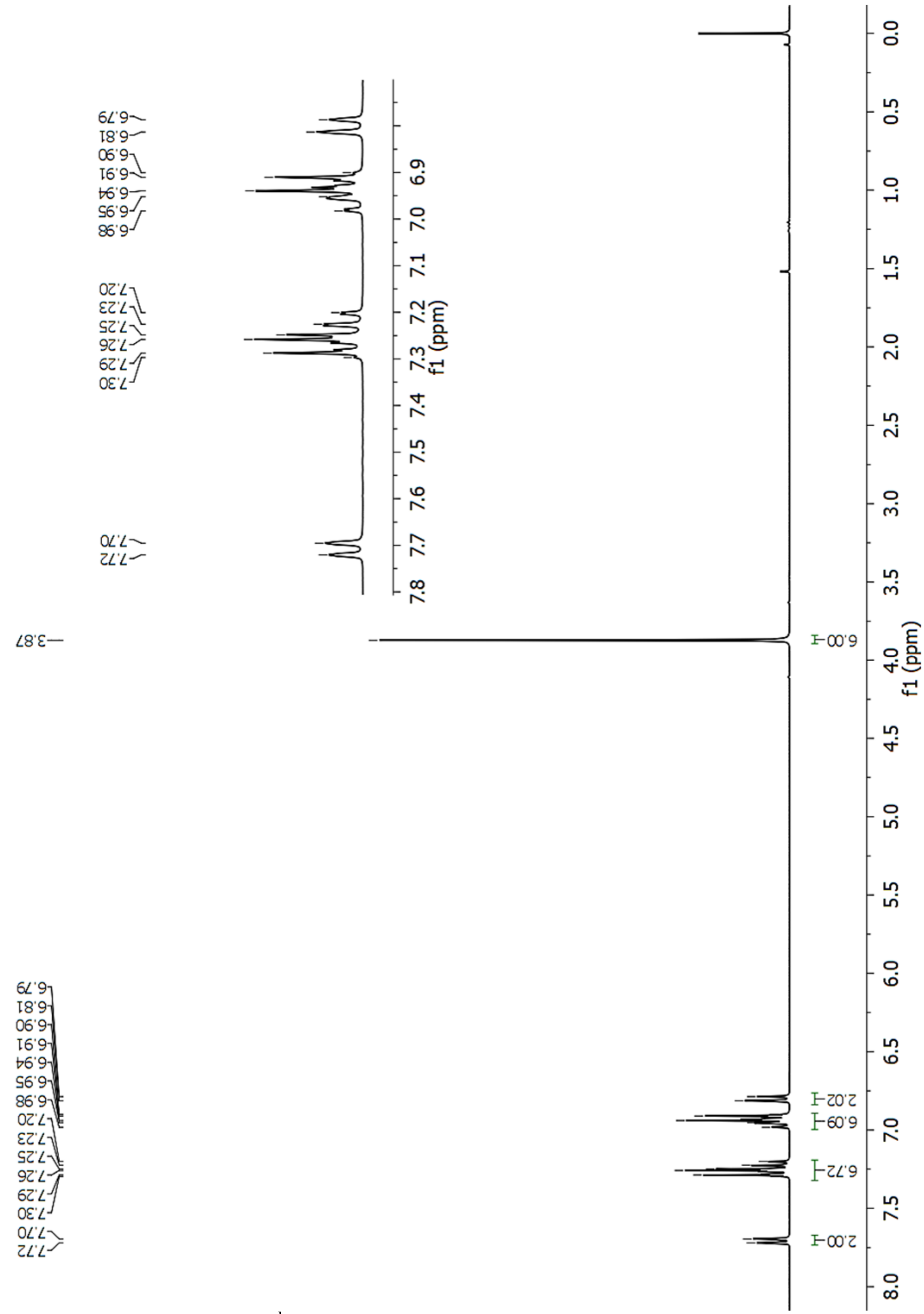


Fig. S-5 [1]HNMR (300 MHz, $CDCl_3$) of compound **5c.**

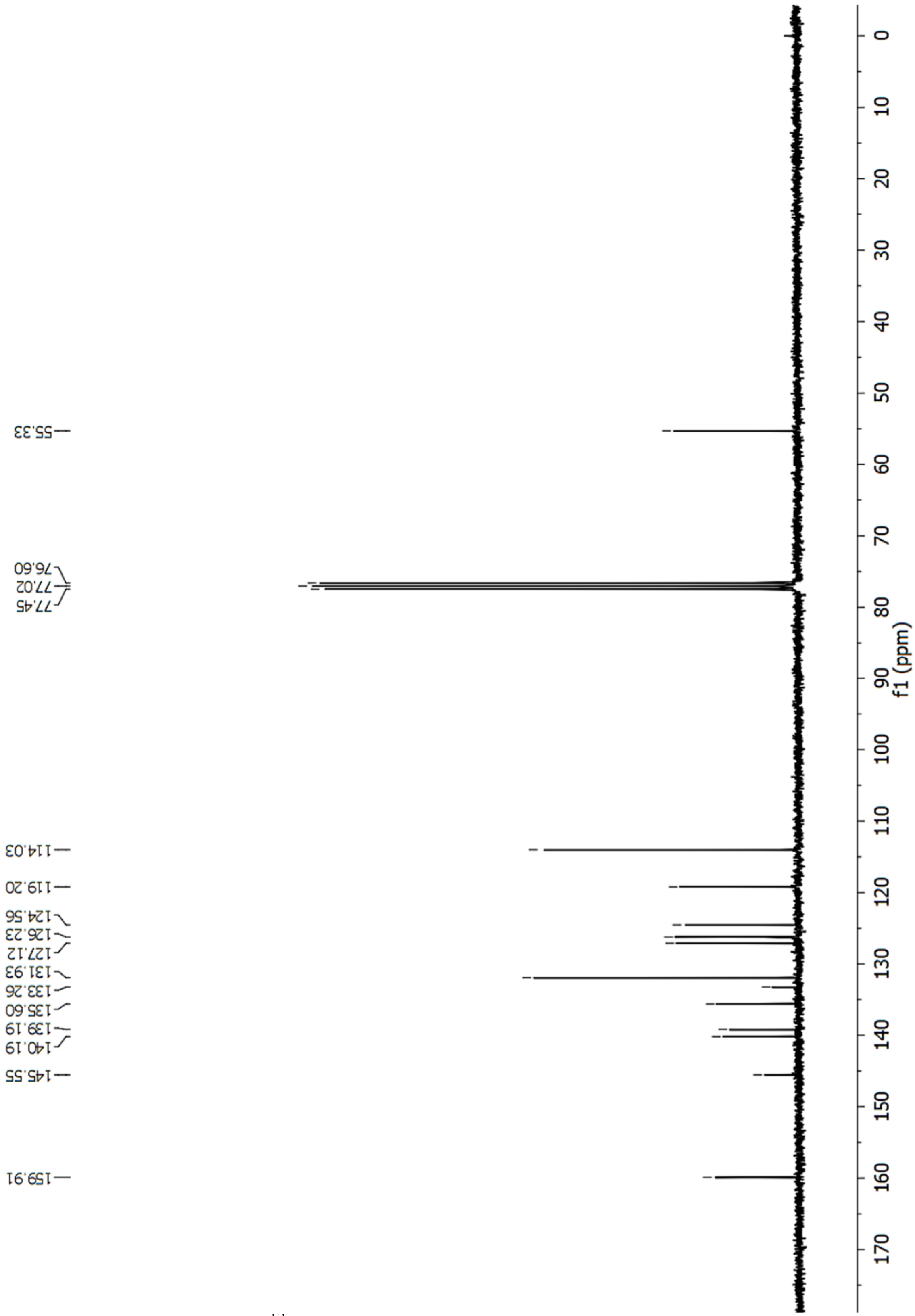


Fig. S-6 ^{13}CNMR (75 MHz, $CDCl_3$) of compound **5c.**

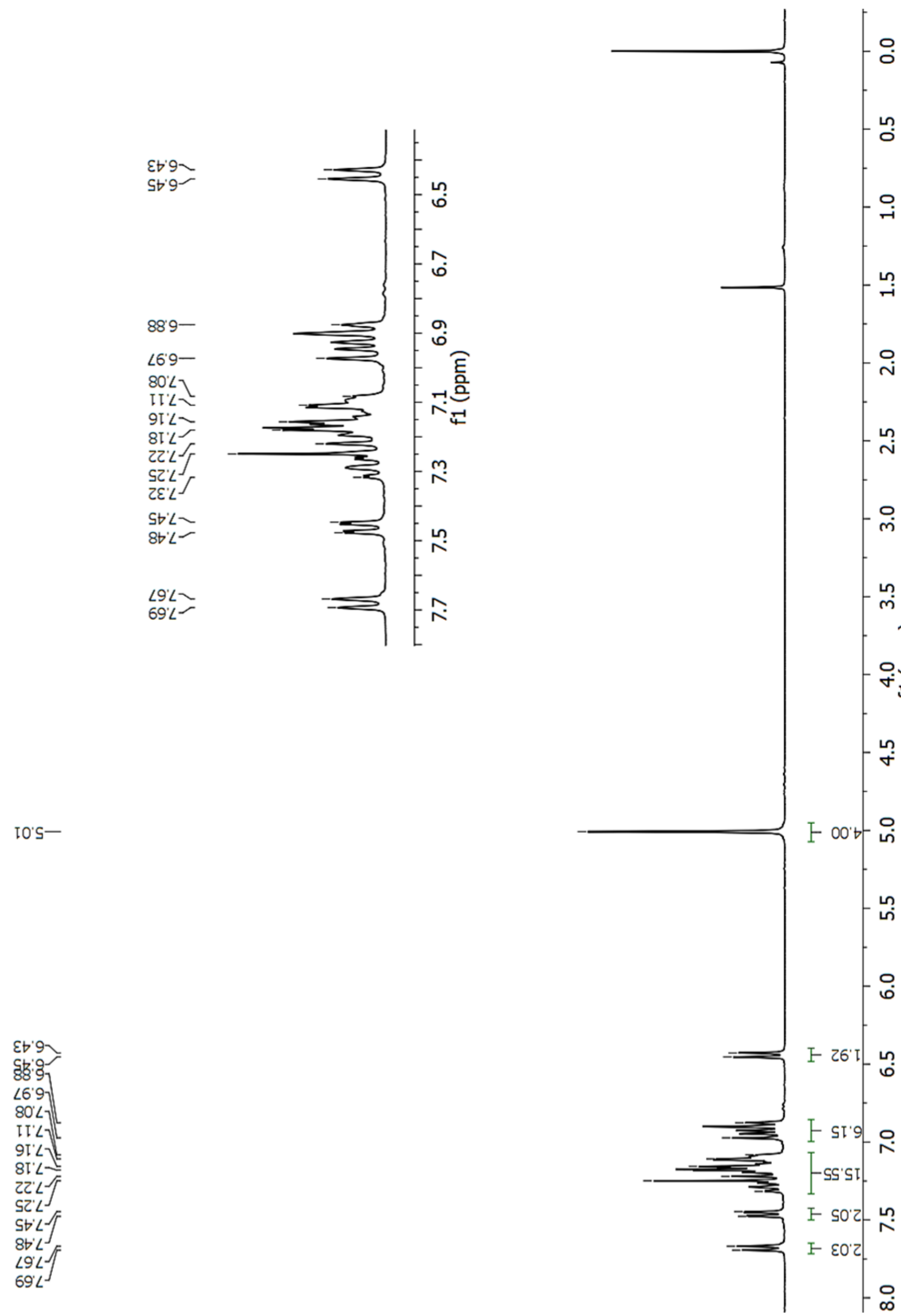


Fig. S-7 ^{1}HNMR (300 MHz, $CDCl_3$) of compound **8a.**

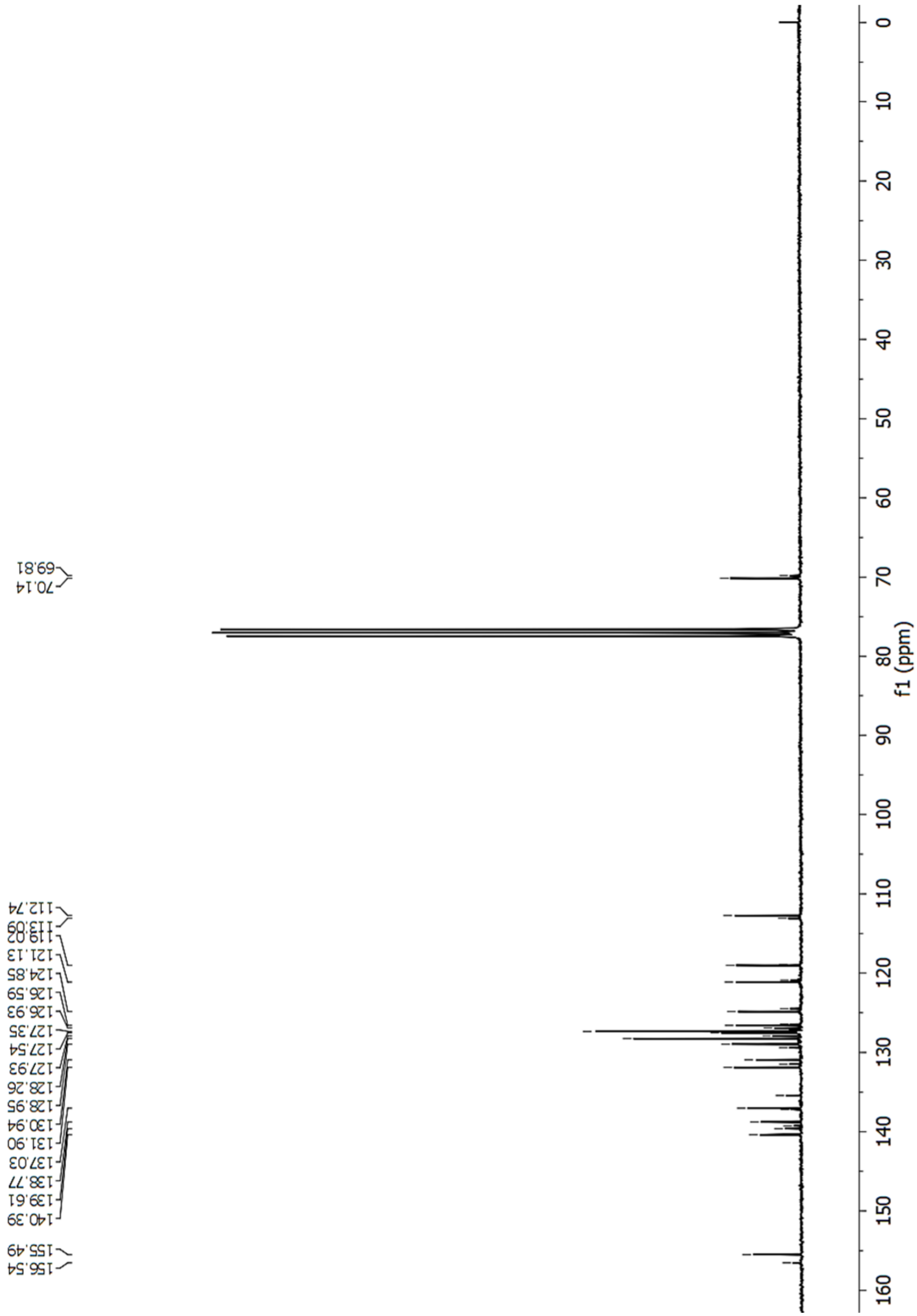


Fig. S-8 ^{13}CNMR (75 MHz, $CDCl_3$) of compound **8a.**

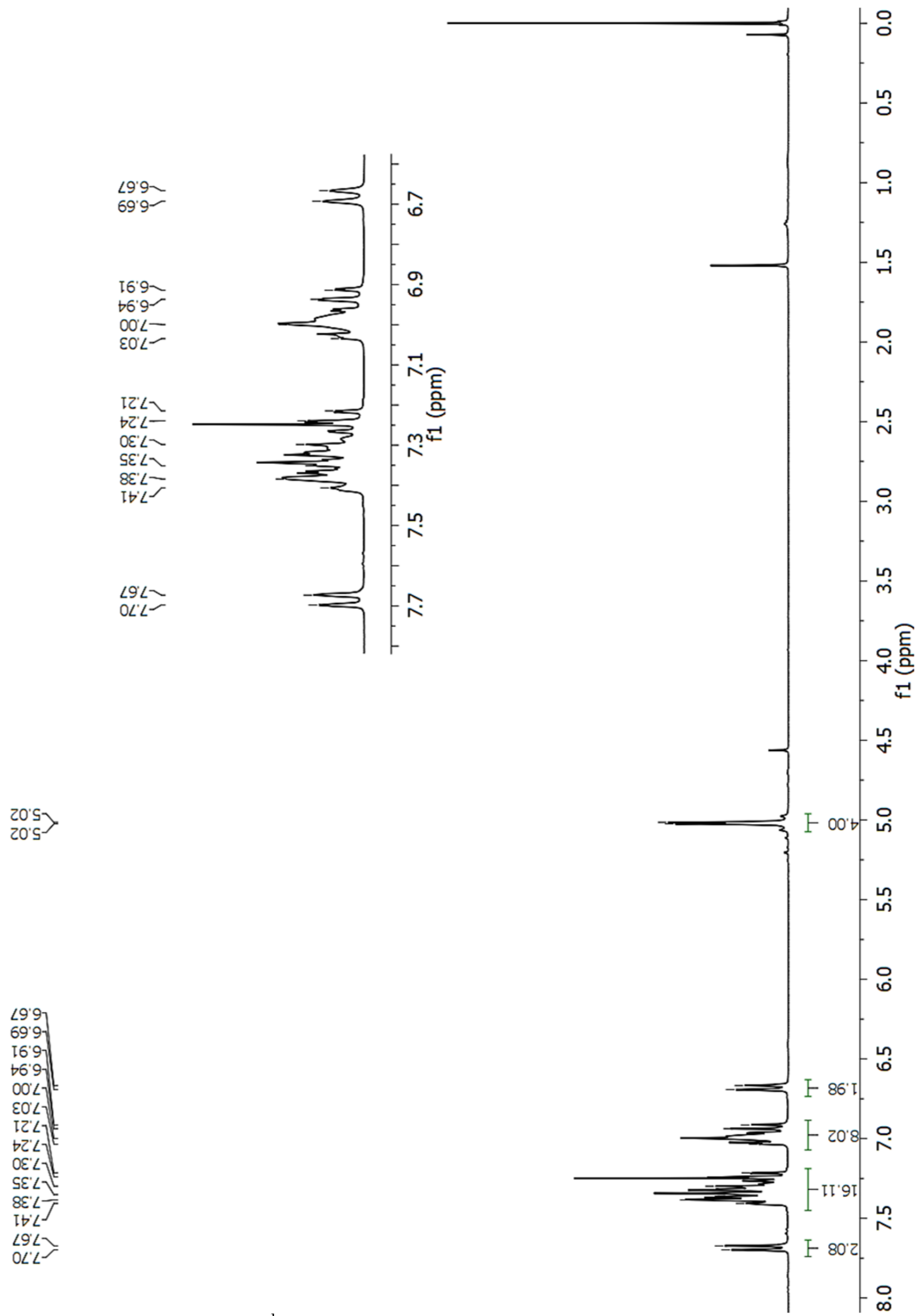


Fig. S-9 [1]HNMR (300 MHz, $CDCl_3$) of compound **8b.**

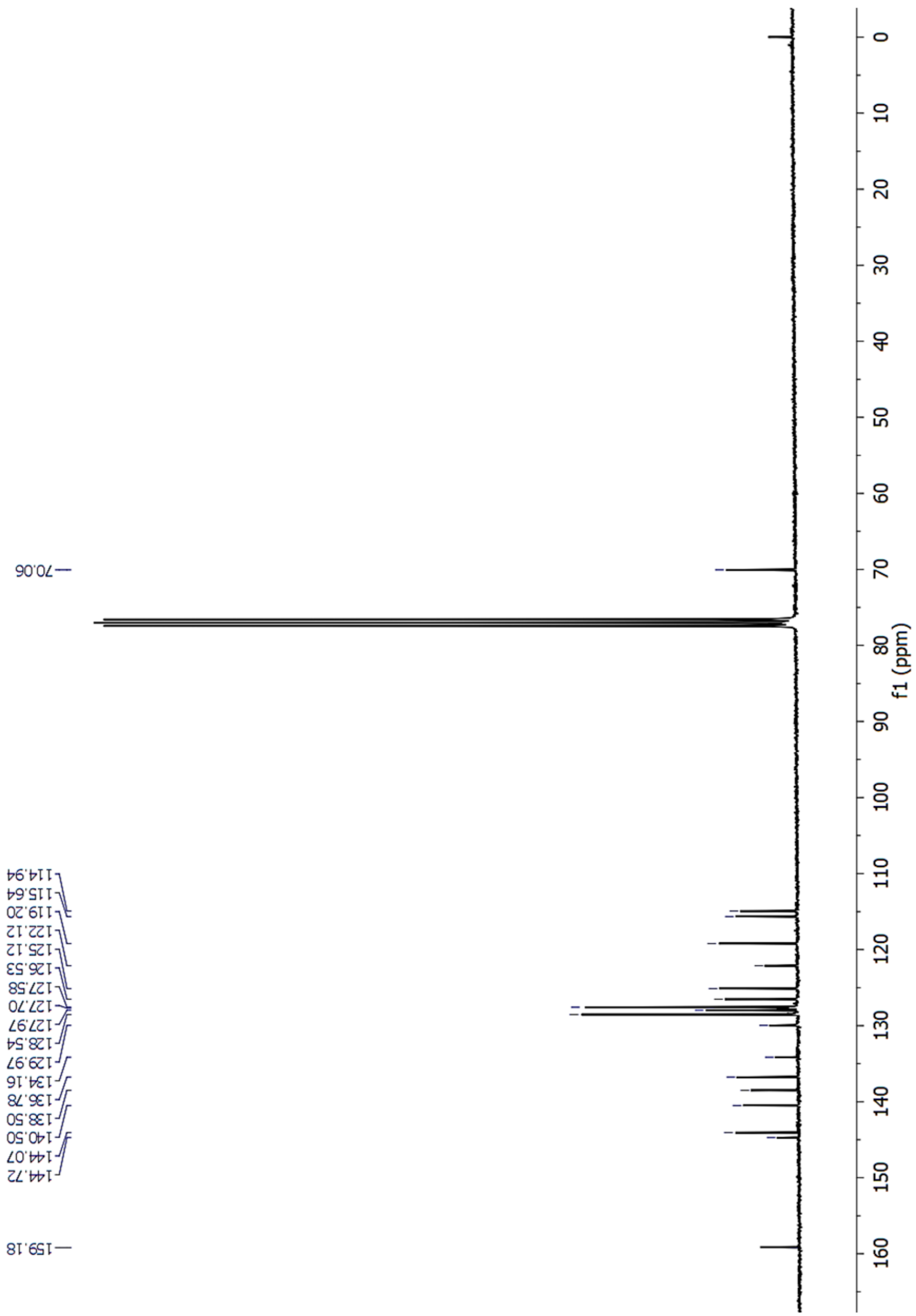


Fig. S-10 ^{13}CNMR (75 MHz, $CDCl_3$) of compound **8b.**

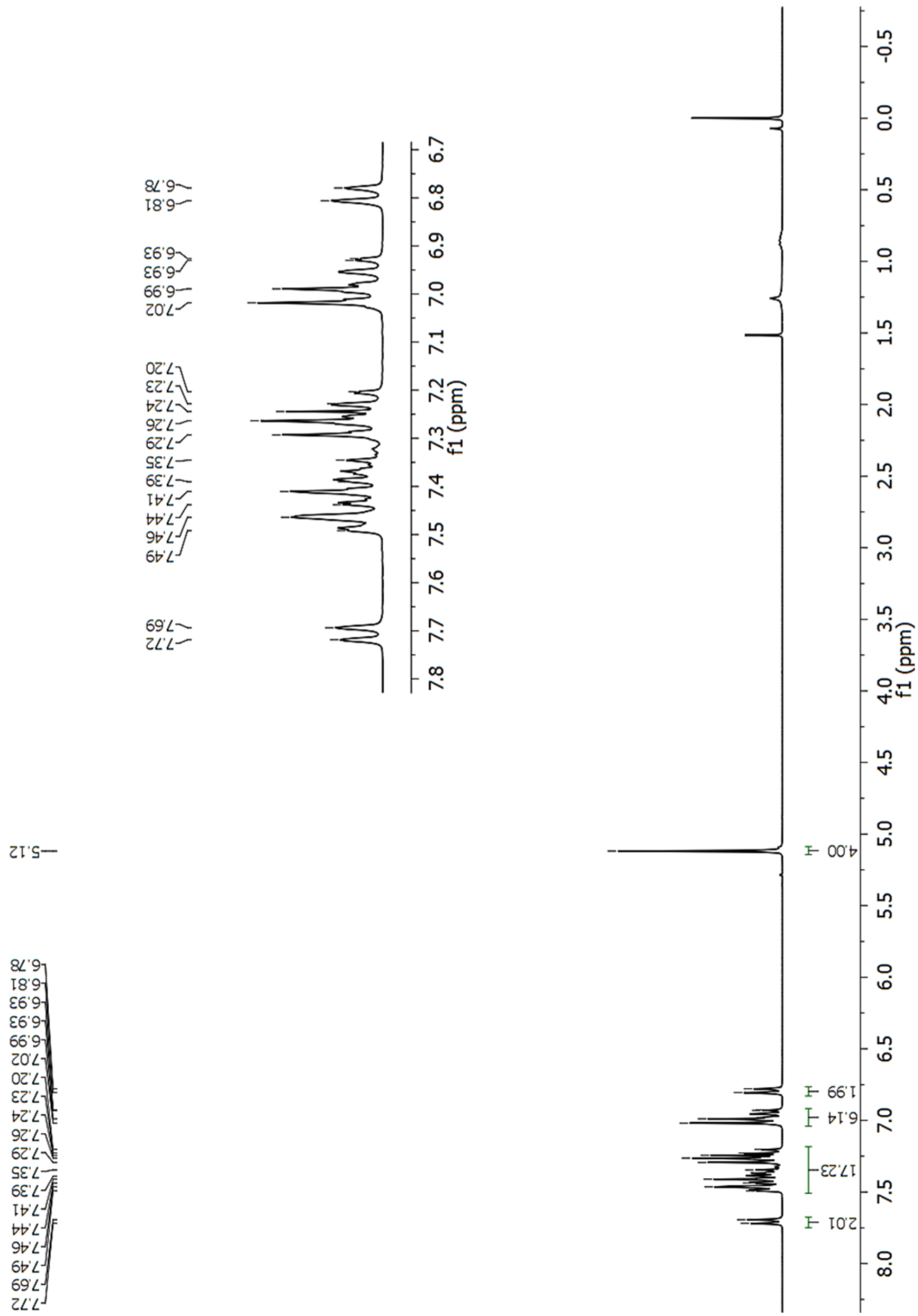


Fig. S-11 ^{1}HNMR (300 MHz, $CDCl_3$) of compound **8c.**

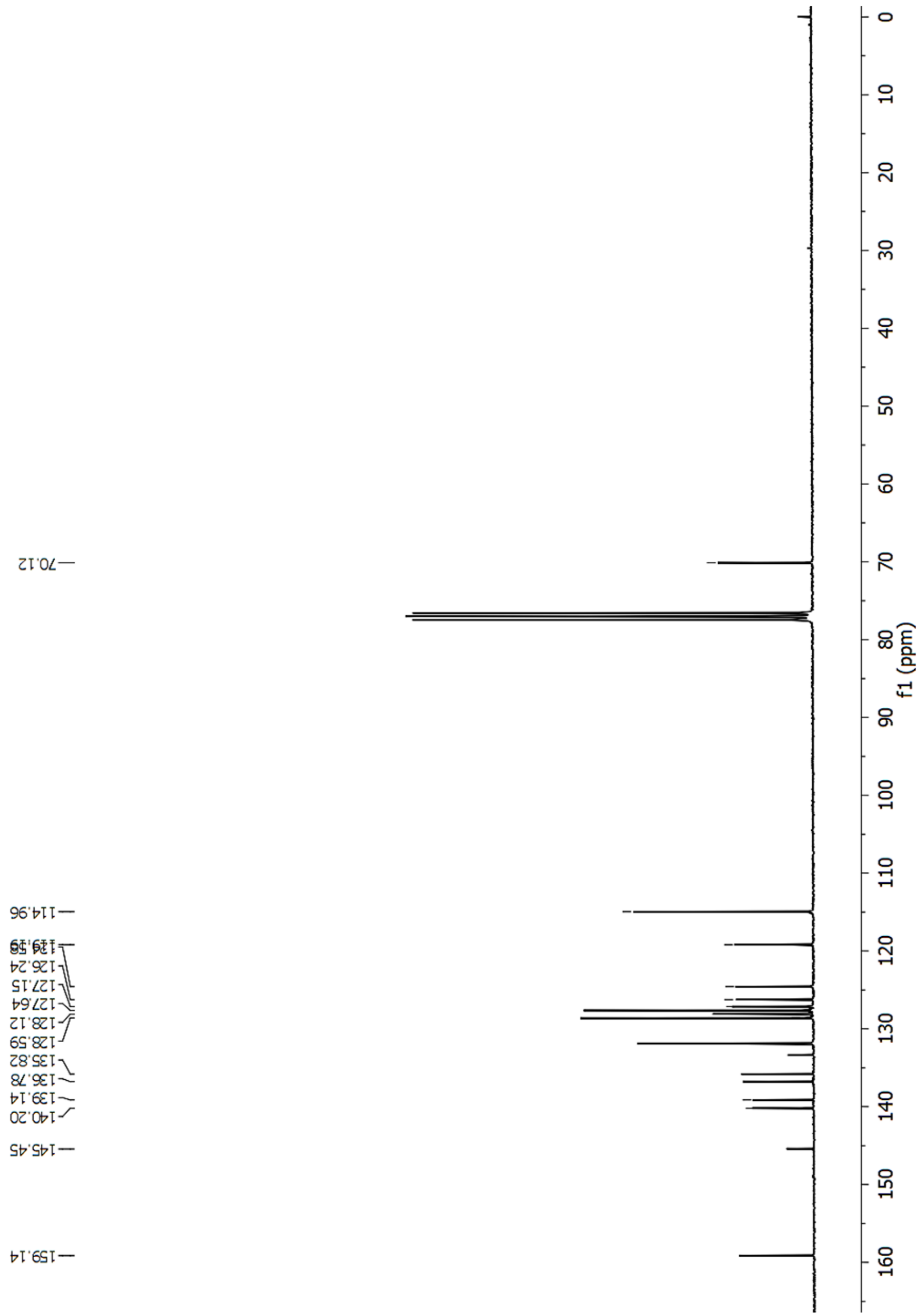


Fig. S-12 ^{13}CNMR (75 MHz, $CDCl_3$) of compound **8c.**

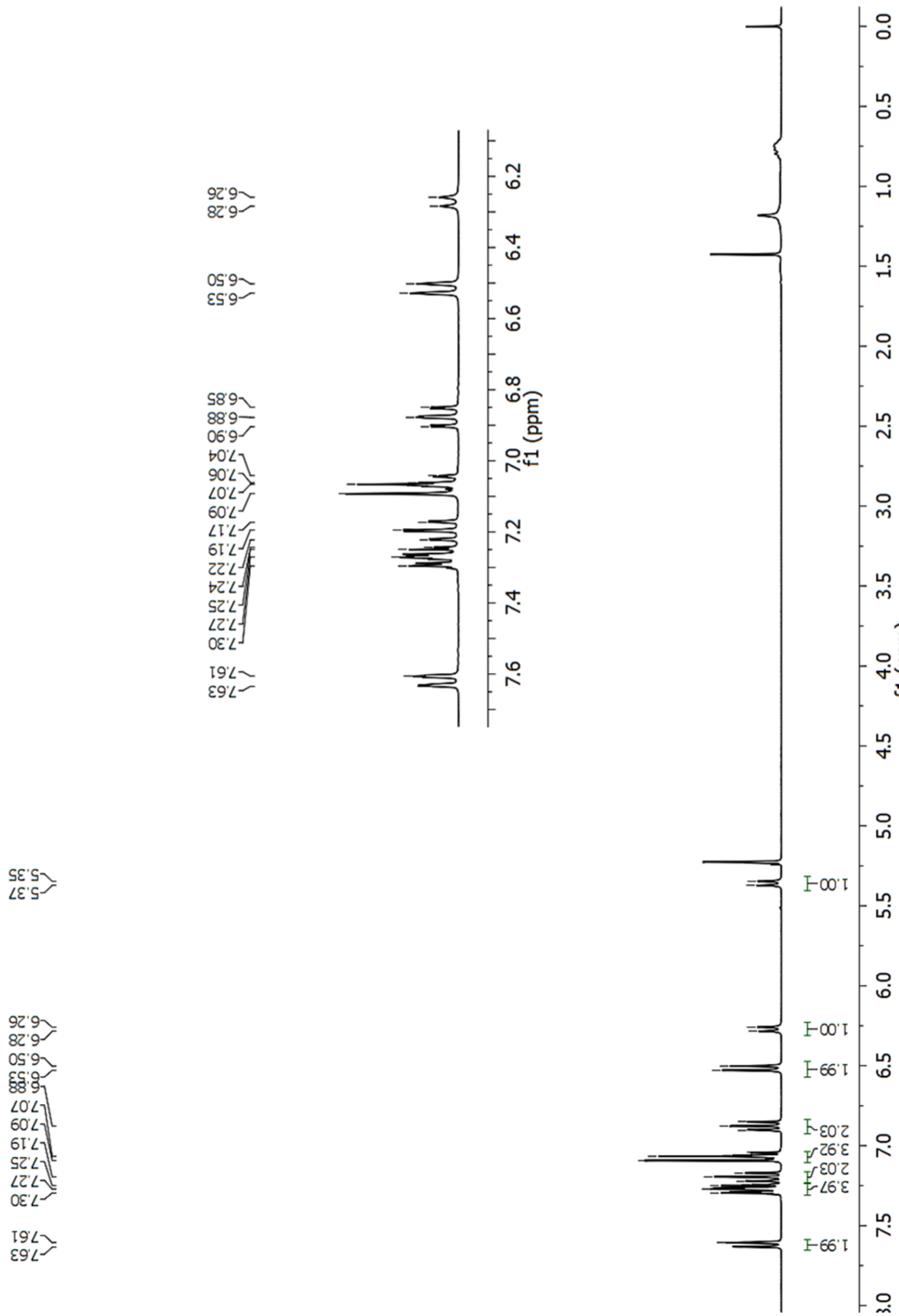


Fig. S-13 [1]HNMR (300 MHz, CD_2Cl_2) of compound **9.**

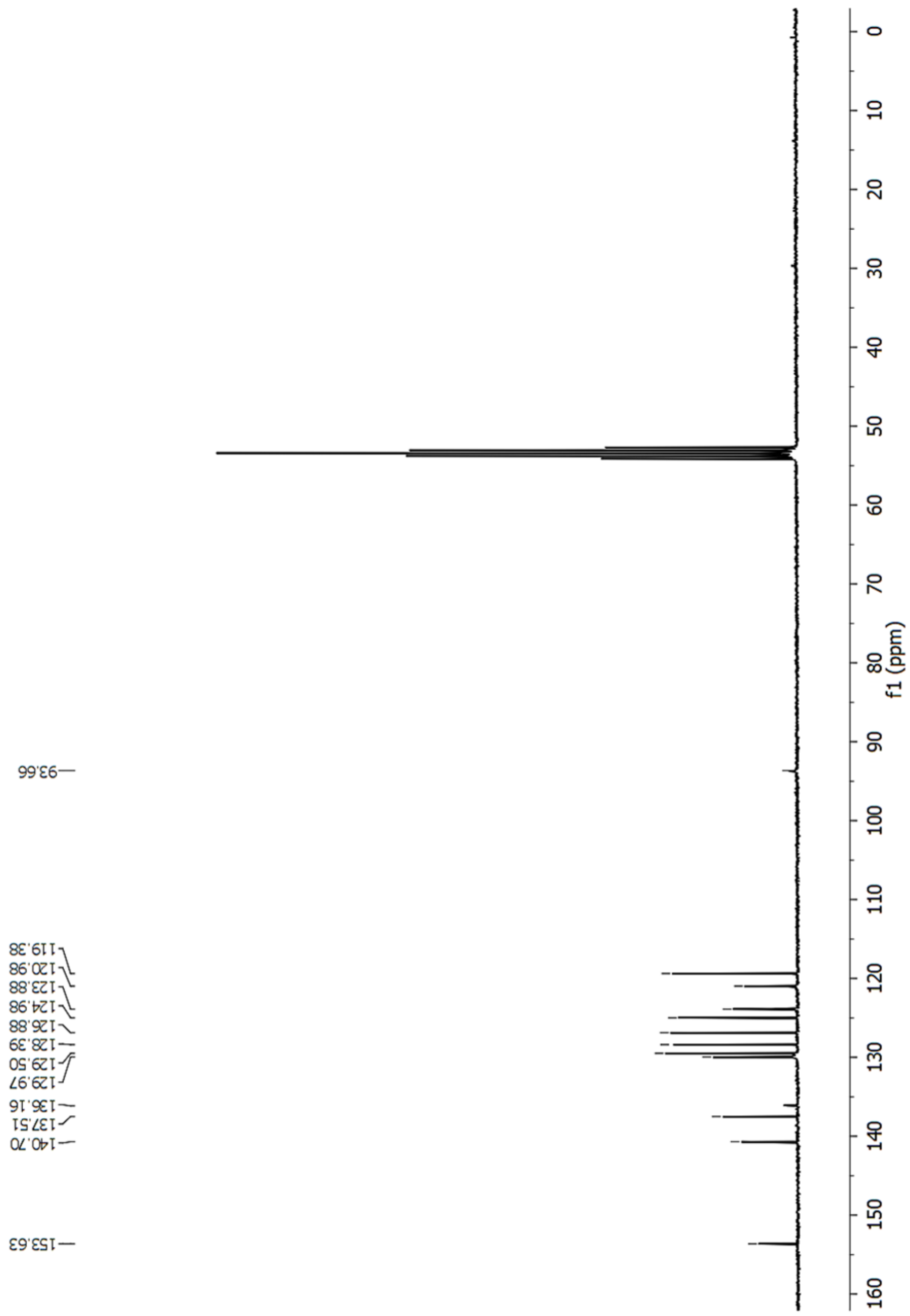


Fig. S-14 ^{13}CNMR (75 MHz, CD_2Cl_2) of compound **9.**

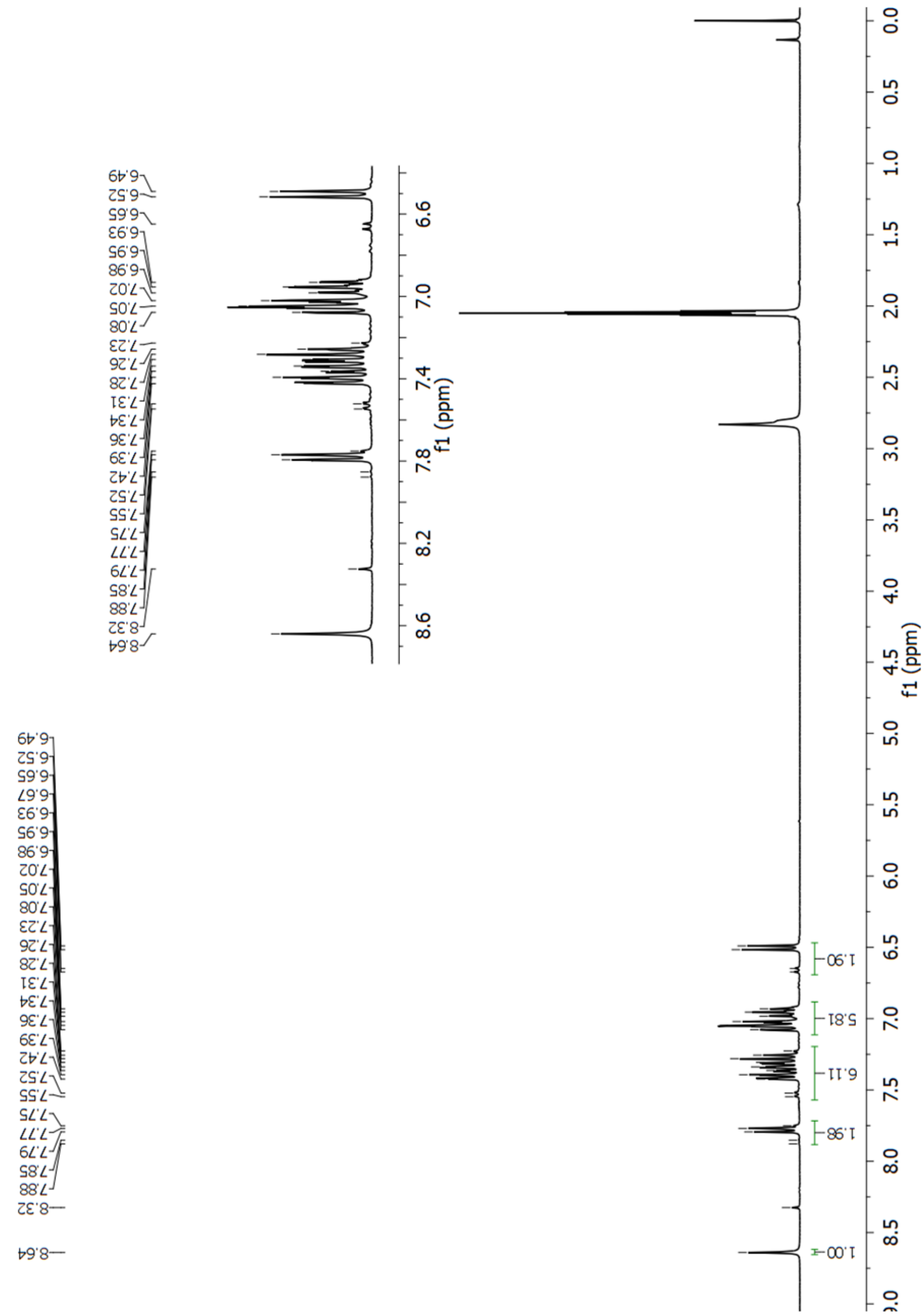


Fig. S-15 ^{1}HNMR (300 MHz, acetone-d_6) of compound **12a.**

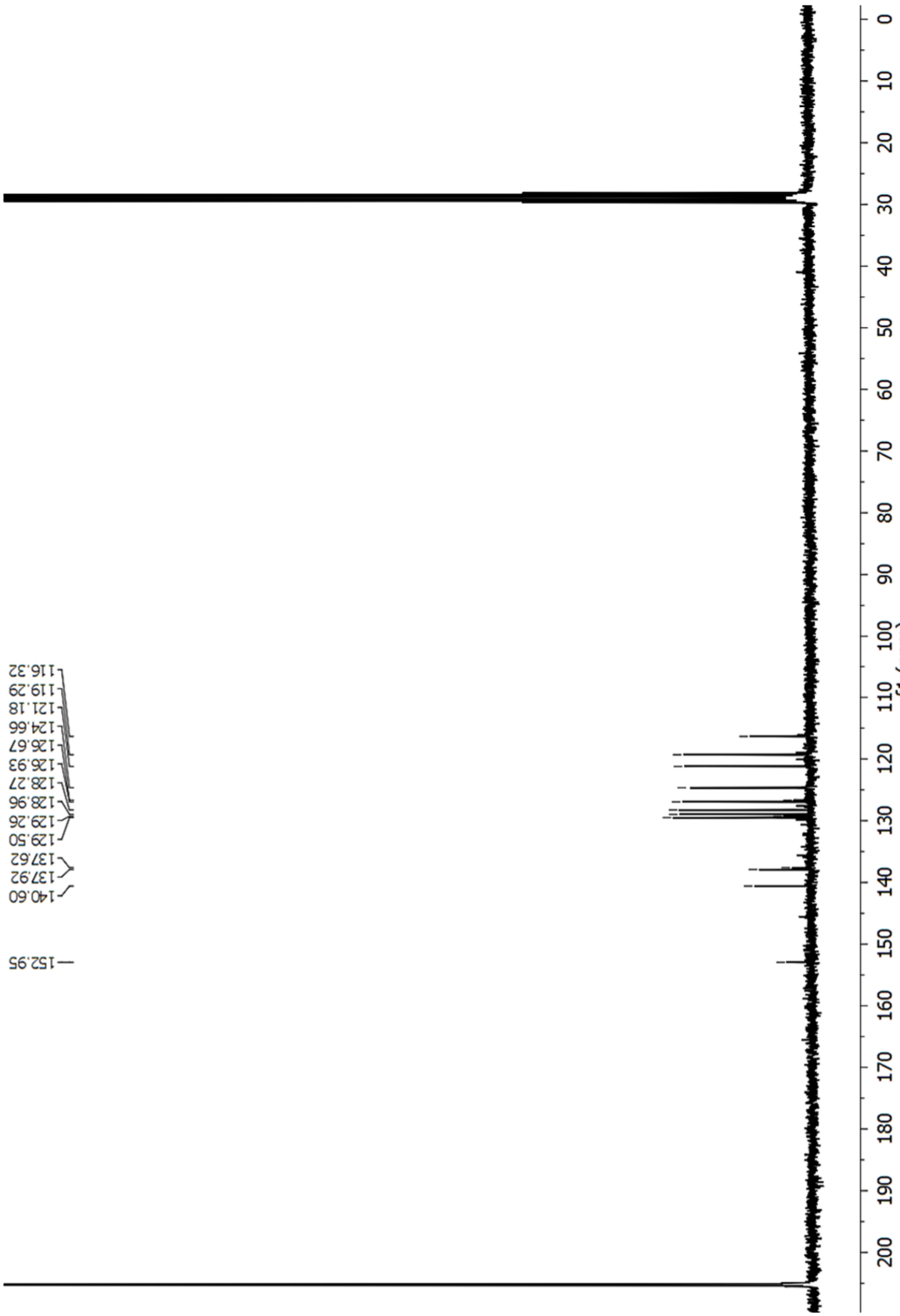


Fig. S-16 ^{13}CNMR (75 MHz, acetone-d_6) of compound **12a.**

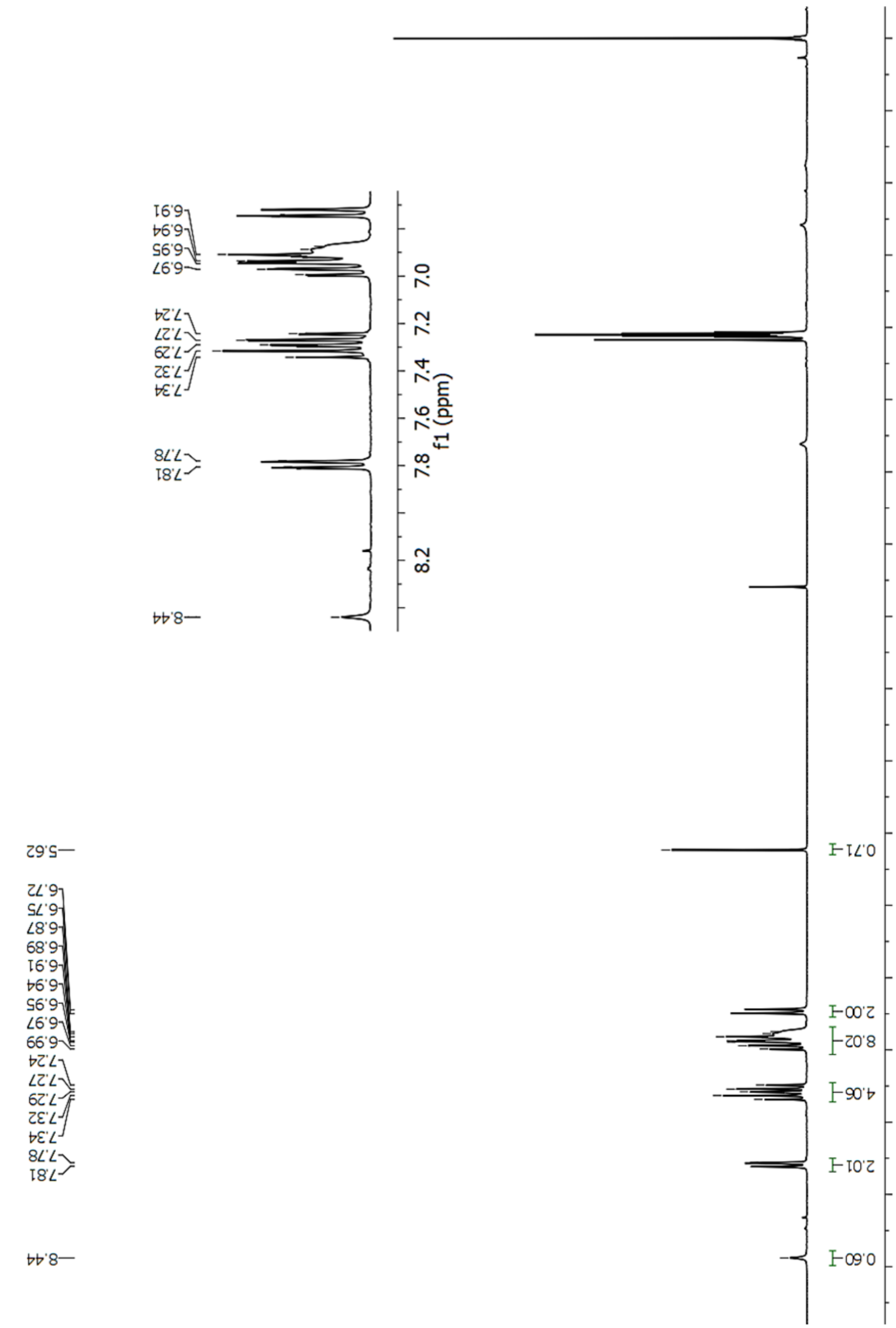


Fig. S-17 ^{1}HNMR (300 MHz, acetone-d_6) of compound **12b.**

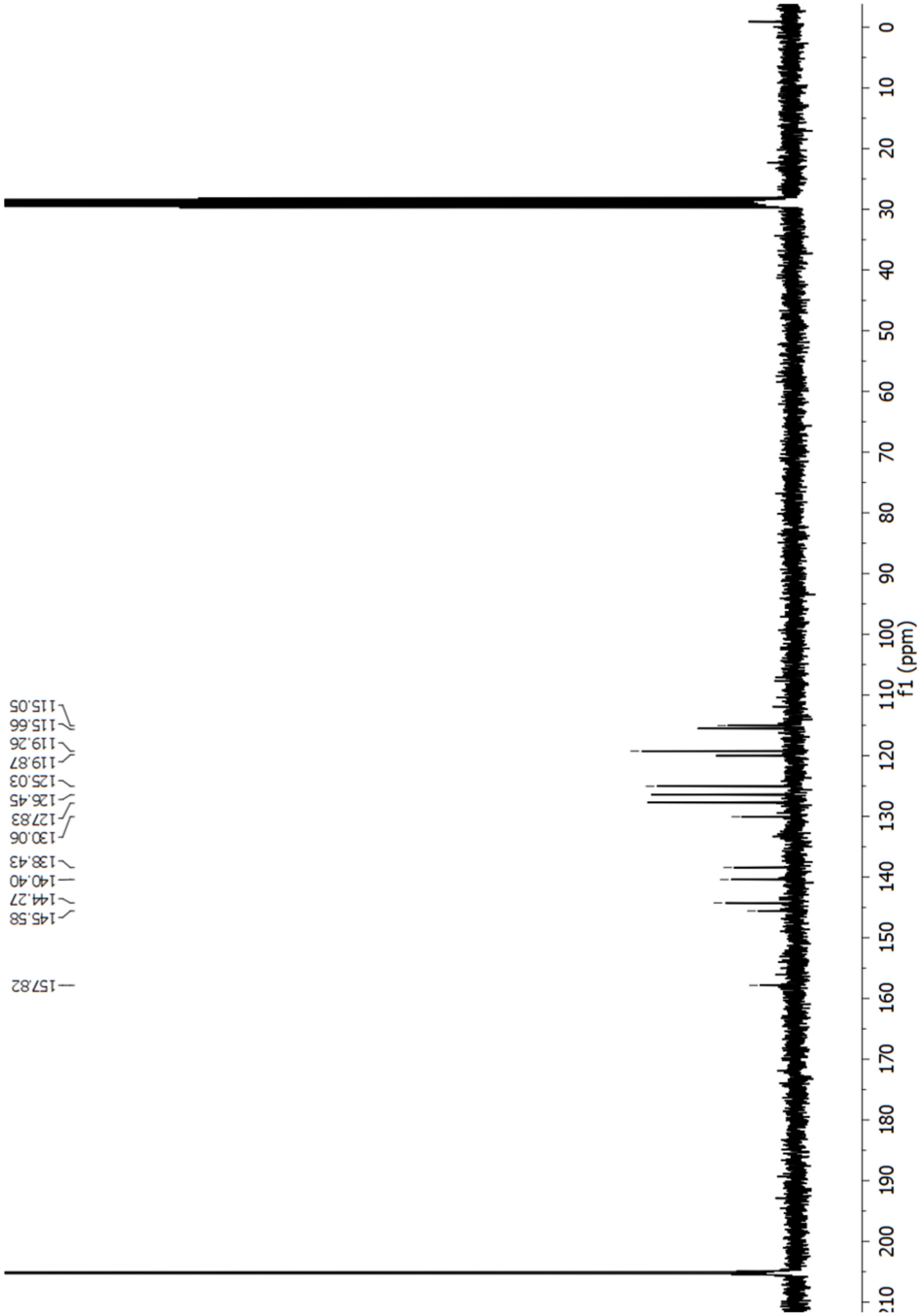


Fig. S-18 ^{13}CNMR (75 MHz, acetone-d_6) of compound **12b.**

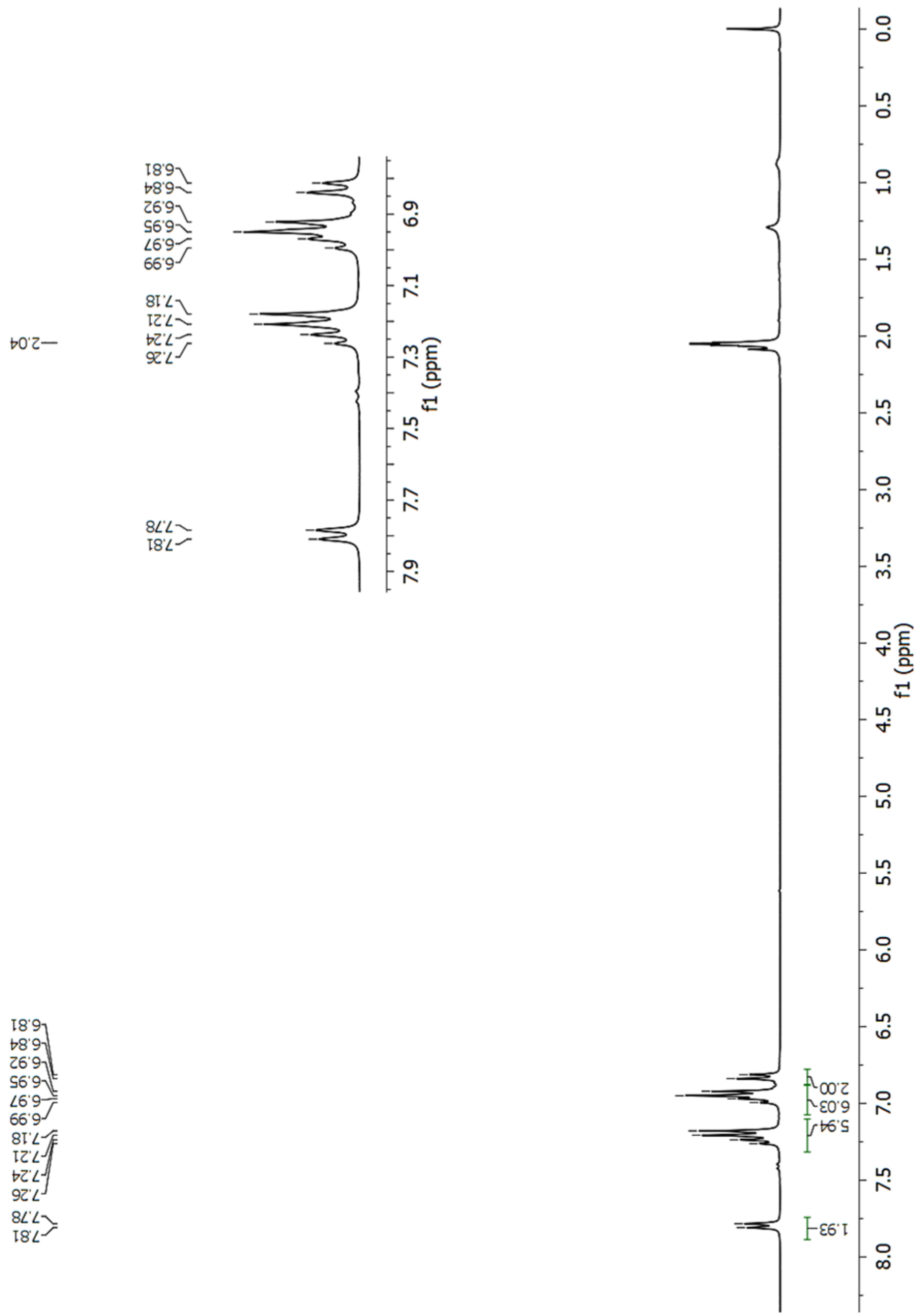


Fig. S-19 ^{1}HNMR (300 MHz, acetone-d_6) of compound **12c.**

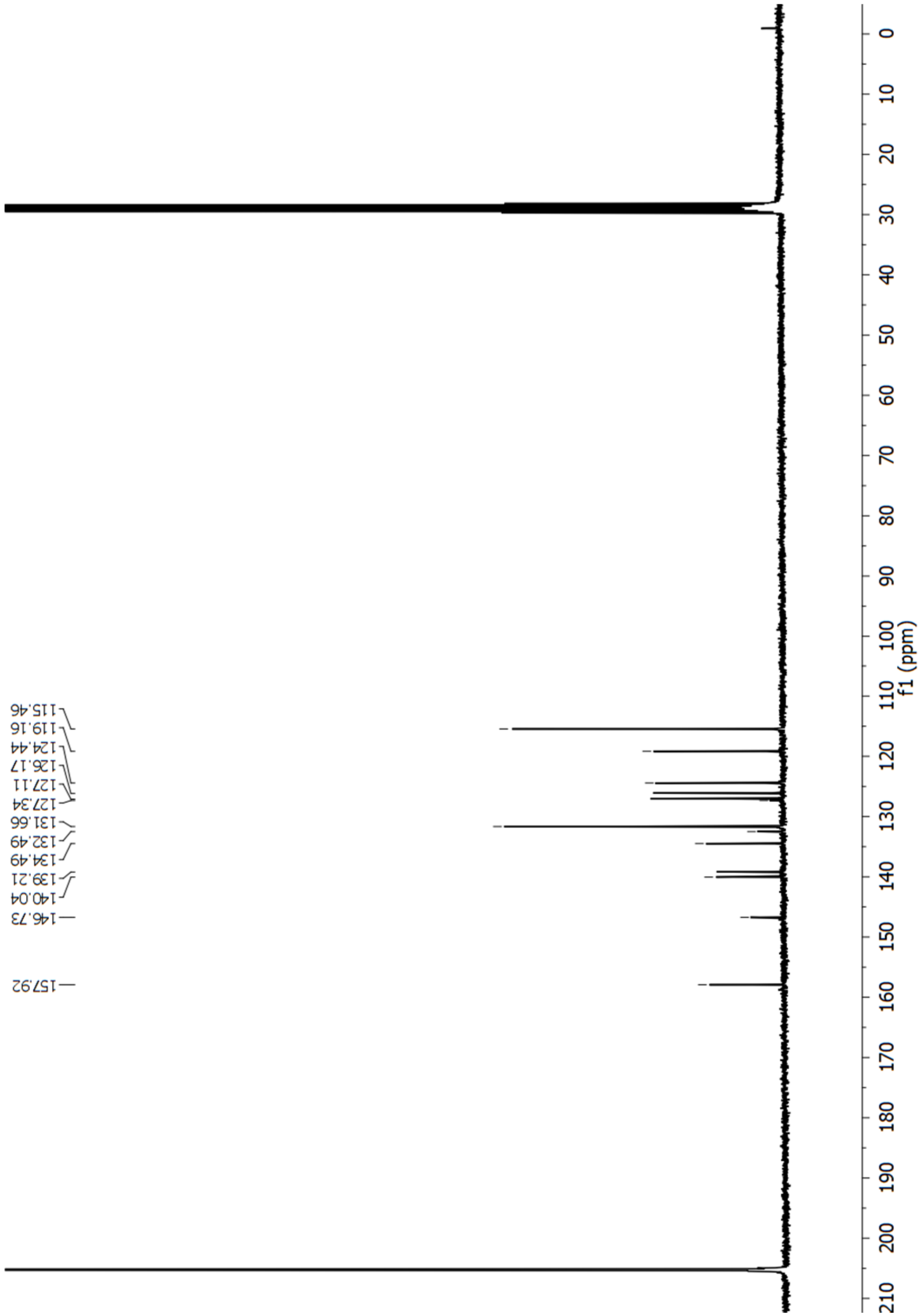


Fig. S-20 ^{13}CNMR (75 MHz, acetone-d_6) of compound **12c.**

3. Solid-State UV-Vis and Fluorescence Spectral Analysis

3.1 Experimental conditions

Solid-state UV-Vis absorption spectra of **5a**-**c**, **8a**-**c**, and **9** were measured from their solid thin films prepared by drop-casting on their CH_2Cl_2 solutions on a quartz substrate. Solid-state fluorescence spectra of **5a**-**c**, **8a**-**c**, and **9** were recorded on the FLS980 series of fluorescence spectrometer (Edinburgh Instruments, EI) at room temperature. B. The samples were measured in both the crystalline and grounded powdery forms. Luminescence lifetimes (τ) of the crystals of **5a**-**c** and **9** were also measured with the FLS980 series of fluorescence spectrometer. The measured emission decays were fit to a multi-exponential function using the standard convolute-and-compare nonlinear least-squares procedure. Emission absolute quantum yields (Φ_f) in the solid state were determined at room temperature.

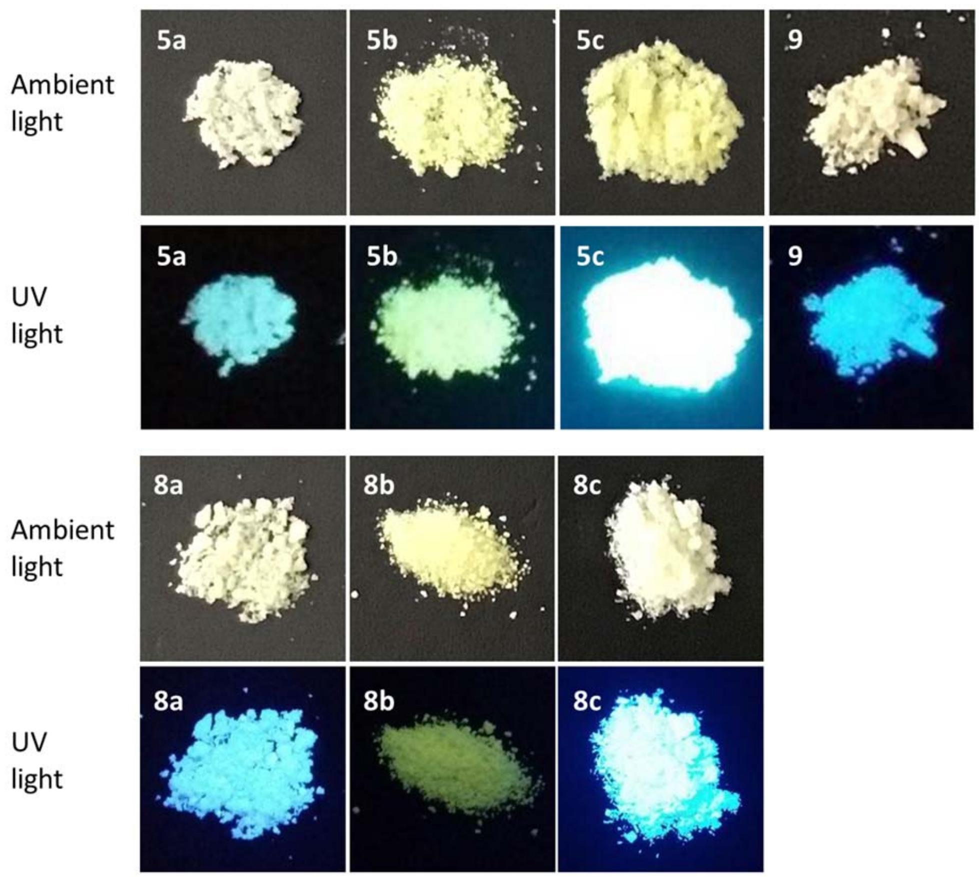


Fig. S-21 Photographic images of the grounded powders of **5a**-**c**, **8a**-**c**, and **9** under ambient light and UV light irradiation**.**

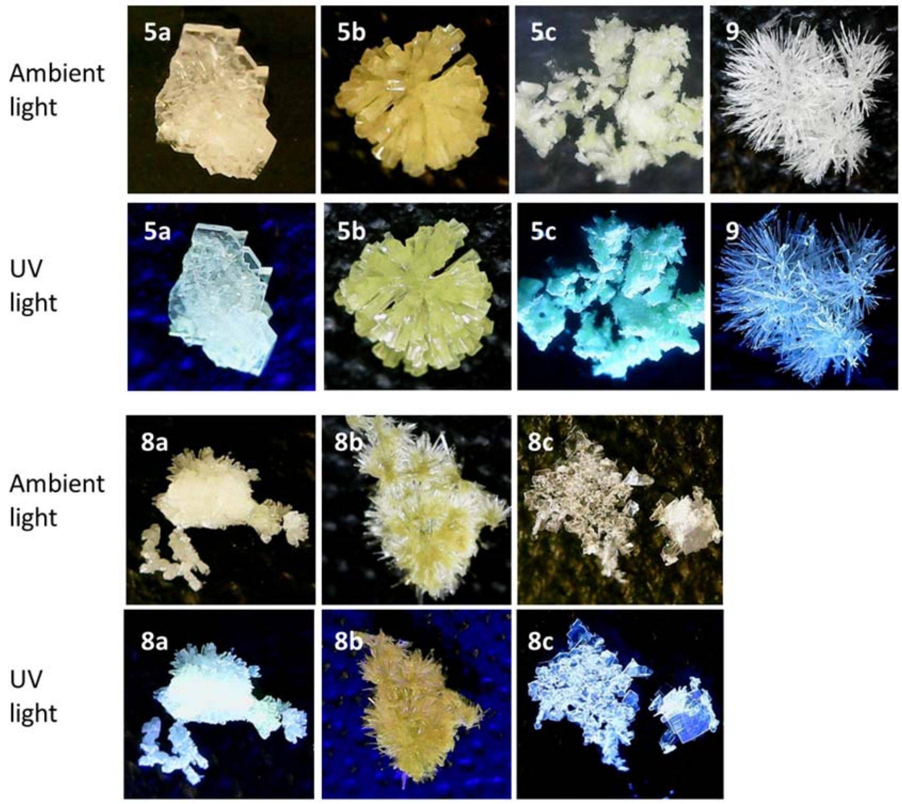


Fig. S-22 Photographic images of the crystals of **5a-c**, **8a-c**, and **9** under ambient light and UV light irradiation**.**

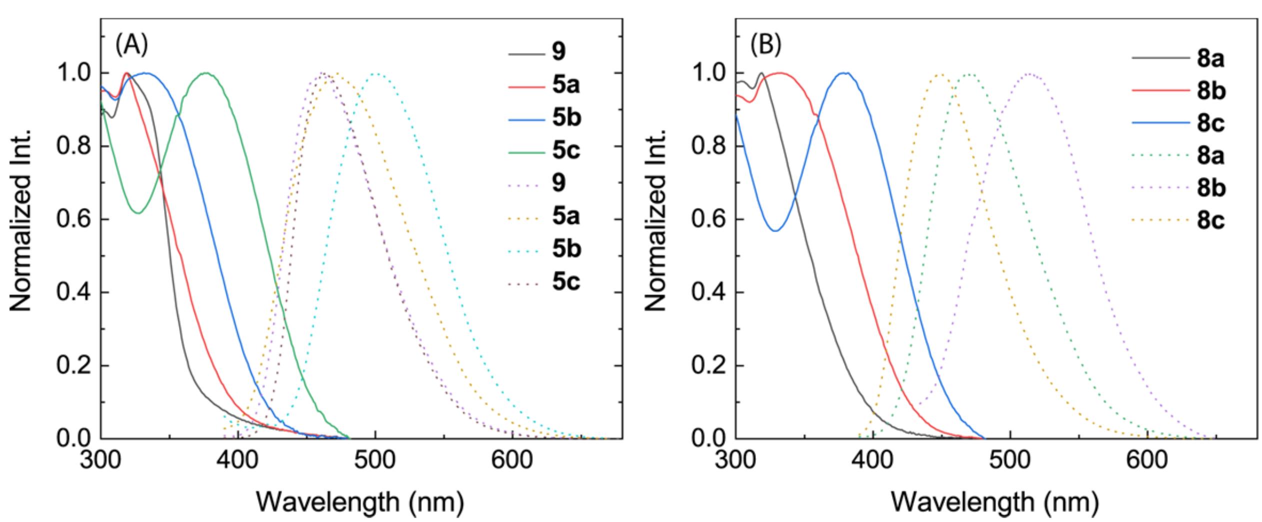


Fig. S-23 Solid-state UV-Vis absorption spectra (solid lines, measured from solid thin films cast on a quartz substrate) and fluorescence spectra (dotted lines, measured in the crystalline state) for the compounds **5a-c**, **8a-c**, and **9.**

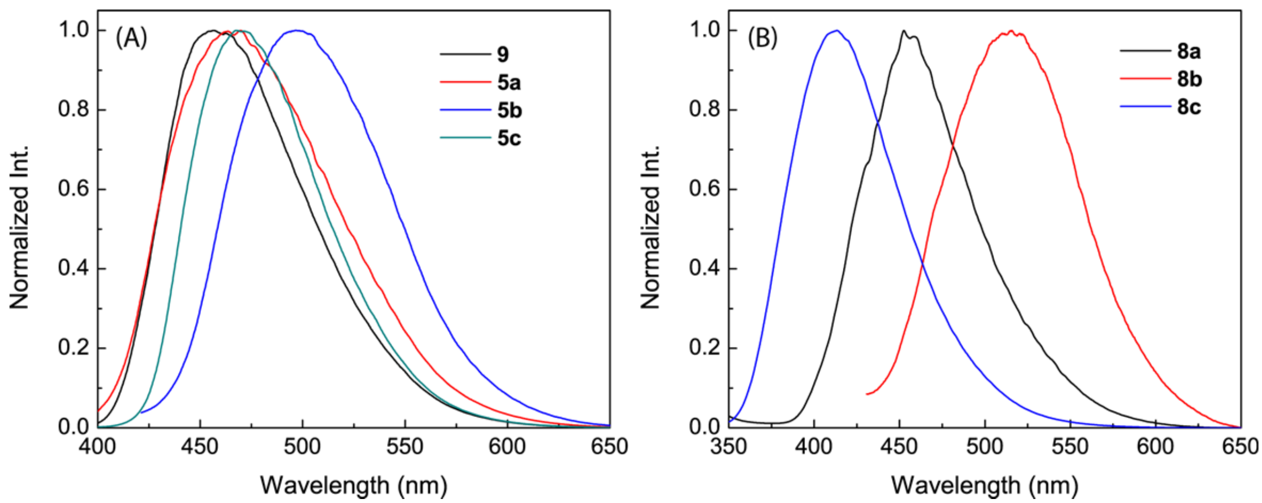


Fig. S-24 Solid-state fluorescence spectra for the grounded powders of **5a-c**, **8a-c**, and **9.**

Table S-1 Summary of solid-state fluorescence properties of **5a-c**, **8a-c**, and **9**

Entry		λ_{em} (nm)	Lifetime (ns)	Φ_f (%)
5a	powder	466	-	16.21
	crystal	473	5.988 14.42	1.44
5b	powder	497	-	1.8
	crystal	507	3.539 14.47	4.22
5c	powder	468	-	66.59
	crystal	461	12.62	89.81
9	powder	457	-	23.51
	crystal	459	11.40 27.20	17.63
8a	powder	454	-	10.94
	crystal	471	-	27.89
8b	powder	515	-	1.59
	crystal	514	-	2.95
8c	powder	413	-	74.26
	crystal	449	-	86.01

4. Electronic Absorption Properties

4.1 Experimental conditions

UV-Vis absorption spectra were measured on a Cary 6000i spectrophotometer. Samples were dissolved in chloroform and measured at room temperature.

4.2 Time-dependent density functional theory (TD-DFT) calculations

Molecular geometries of **DP-DBF**s **5a-c**, **8a-c**, and **9** were optimized at the M06-2X/Def2SVP level of theory using the *Gaussian 16* software package.[2] The optimized geometries were subjected to TD-DFT calculations at the TD-B3LYP/6-311+G(d,p) level to compute the vertical electronic transition energies (only singlet-to-singlet transitions were considered, nstates = 20).

Table S-2 Summary of electronic absorption properties of **DP-DBF**s **5a-c**, **8a-c**, and **9**

Entry	$\lambda_{S0\rightarrow S1}$ (cald) (nm)	$\lambda^{abs}_{1/2}$ (exp) (nm)	λ_{max} (exp) (nm)	*f*
5a	378 (*cis*) 355 (*trans*)	351	316	0.0783 (*cis*) 0.0063 (*trans*)
5b	384 (*cis*) 384 (*trans*)	374	331	0.0028 (*cis*) 0.0024 (*trans*)
5c	399	407	368	0.4097
8a	360	343	316	0.0135
8b	390	373	328	0.0027
8c	397	407	368	0.4775
9	371	343	315	0.0048

$\lambda_{S0\rightarrow S1}$ is the wavelength corresponding to the vertical transition from the ground state (S_0) to the first-excited state (S_1) calculated at the TD-B3LYP/6-311+G(d,p) level.
$\lambda^{abs}_{1/2}$ is the half-height wavelength of the lowest-energy absorption band.
f is calculated oscillator strength.

[2] Gaussian 16, Revision B.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.

5. Crystallographic Analysis

Single crystals of compounds **5a-c**, **8a-c**, and **9** suitable for X-ray diffraction analysis were grown by slow diffusion of hexane into their chloroform solutions at room temperature. Single-crystal X-ray diffraction data was collected at 100(2) K on a XtaLAB Synergy-S, Dualflex, HyPix-6000HE diffractometer using Cu *K*α radiation (λ = 1.5406 Å). Crystal was mounted on nylon CryoLoops with Paraton-N. The data collection and reduction were processed within *CrysAlisPro* (Rigaku OD, 2019). A Gaussian absorption correction was applied to the collected reflections. Using Olex[2,3] the structure was solved with the ShelXT[4] structure solution program using Intrinsic Phasing and refined with the ShelXL[5] refinement package using Least Squares minimization. All non-hydrogen atoms were refined anisotropically. The organic hydrogen atoms were generated geometrically.

For *ortho*-OMe substituted **5a**, two different conformations, namely *cis* and *trans*, were grown as a single crystal at ratio of 49:51. Molecular structures of the two conformers are depicted in Fig. S-25.

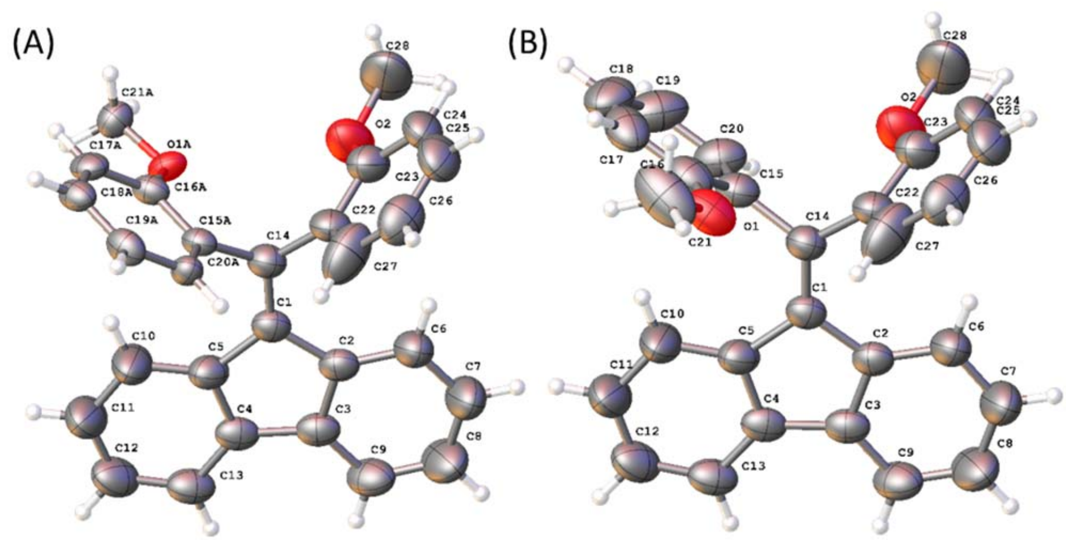


Fig. S-25 ORTEP drawings (50% probability level) of two different conformations, (A) *cis* and (B) *trans*, showed in the same single crystal of **5a** (CCDC 1980233).

3 Dolomanov, O.V., Bourhis, L.J., Gildea, R.J, Howard, J.A.K. & Puschmann, H. (2009), *J. Appl. Cryst*. 42, 339-341.
4 Sheldrick, G.M. (2015). *Acta Cryst*. A71, 3-8.
5 Sheldrick, G.M. (2015). *Acta Cryst*. C71, 3-8.

For *meta*-OMe substituted **5b**, two types of single crystals were obtained during the crystallization process. As shown in Fig. S-26A. the *cis* single crystal structure shows two OMe groups on the same side with respect to the fluorene plane, and this crystal is a minor product (ca. 20%). The *trans* single crystal (Figure S-26B) is the major product (ca. 80%).

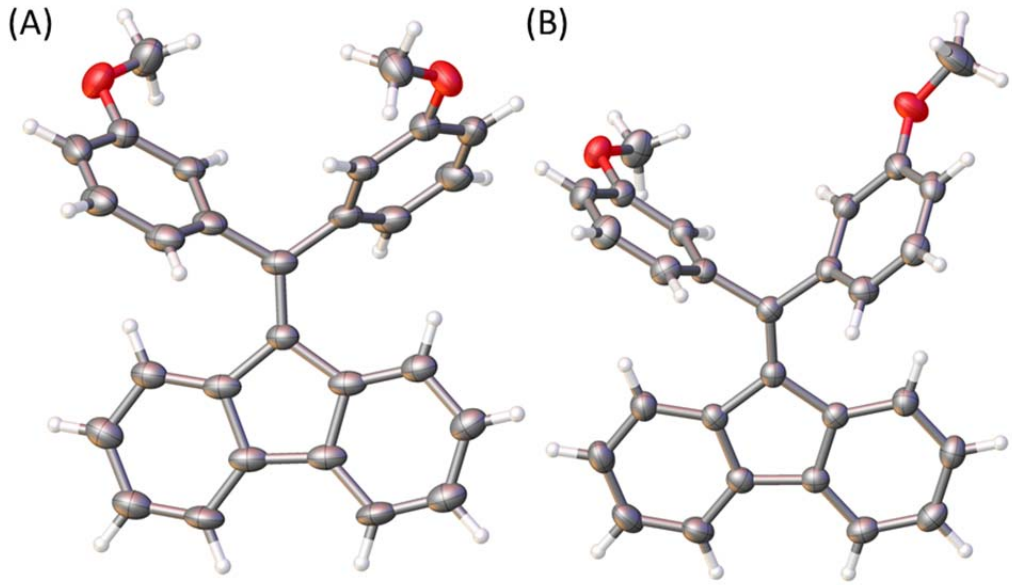


Fig. S-26 ORTEP drawings (50% probability level) of two single crystal structures, (A) *cis* (CCDC 2017099) and (B) *trans* (CCDC 2016939), of **5b**.

Crystallographic data for the **DP-DBP** derivatives reported in this work have been deposited with the Cambridge Crystallographic Data Centre (CCDC). CCDC numbers: 1980233 (**5a**), 2016939 (**5b** *trans*), 2017099 (**5b** *cis*), 2016946 (**5c**), 2016948 (**8a**), 2016952 (**8b**), 2016953 (**8c**), 2016933 (**9**).

6. DFT Optimized Molecular Geometries

Cartesian coordinates and energies of optimized ground-state geometries of **5a**-***cis*****/*****trans***, **5b**-***cis/trans***, **5c**, **8a**-**c**, and **9** (at the M06-2X/Def2SVP level) are provided below.

5a-*cis*: (*E* = -1229.256629 Hartree)

C	-0.80720584	0.27140254	0.31749552
C	-1.91218323	-0.71693089	0.44442364
C	-1.92446077	-2.06564299	0.81120125
C	-3.13784267	-0.05975101	0.20449024
C	-4.35347156	-0.73453333	0.28522825
C	-2.86268692	1.35028631	-0.09703685
C	-1.46874724	1.56606005	-0.01836476
C	-3.74050274	2.37412455	-0.44198537
C	-0.95998432	2.82975654	-0.33398343
C	0.52292052	0.04323282	0.45370730
C	-4.35002996	-2.08690830	0.62331798
C	-3.14400614	-2.74031897	0.89213721
C	-3.22201035	3.63639798	-0.72792138
C	-1.84296866	3.85419464	-0.68182994
H	0.10906386	3.03280065	-0.31912760
H	-4.81494258	2.18947570	-0.49684960
H	-3.89292524	4.45305124	-0.99877952
H	-1.44409537	4.84075407	-0.92269712
H	-1.00465343	-2.59750299	1.05018387
H	-5.29278396	-0.21216337	0.09464269
H	-5.29151620	-2.63416208	0.69136686
H	-3.15287930	-3.79370319	1.17683278
C	1.13364296	-1.31206990	0.53325730
C	1.50469784	1.15239152	0.58150019
C	0.92658732	-2.27136621	-0.48459488

C	1.98493970	-1.63291782	1.59050287
C	2.58982117	-2.88744671	1.68896052
C	2.35921757	-3.82907379	0.69354525
C	1.53594357	-3.52592395	-0.39409174
H	2.82464951	-4.81449341	0.74982318
H	1.37622166	-4.27271462	-1.17026775
O	0.12045327	-1.90861526	-1.49881565
H	2.16301850	-0.87689505	2.35829947
H	3.23544542	-3.12070183	2.53575844
C	2.53712317	1.28654543	-0.37075610
C	3.48572314	2.30471245	-0.23626164
C	3.41275055	3.18100216	0.84919332
C	2.40771495	3.05085964	1.80225256
C	1.46103338	2.03475315	1.66073137
O	2.51591306	0.40266169	-1.38805353
H	2.35784524	3.73296882	2.65112331
H	0.65659843	1.91926822	2.39033799
H	4.27950885	2.42455678	-0.97204748
H	4.15870545	3.97172879	0.94399943
C	-0.27505625	-2.87678469	-2.43161649
C	3.54012086	0.44505066	-2.34426524
H	3.34472454	-0.37291603	-3.04617468
H	4.52980163	0.29724605	-1.88146359
H	3.53926832	1.40063767	-2.89431632
H	-0.98633961	-2.38772404	-3.10592322
H	-0.77271396	-3.72758230	-1.93655863
H	0.58058727	-3.25091177	-3.01863073

5a-*trans*: (E = -1229.257114 Hartree)

C	2.64498514	-3.44847766	0.18400567
C	1.56913811	-2.55824867	0.14738380

C	1.82364091	-1.18479734	0.09253613
C	3.16091466	-0.73327167	0.05080946
C	4.23045527	-1.62349045	0.08852640
C	3.96426165	-2.99029961	0.16080950
H	2.44685273	-4.52035597	0.23073055
H	0.55373949	-2.94985556	0.16085598
C	0.92168207	-0.00027149	-0.00055618
C	3.16126246	0.73166723	-0.05107842
H	5.25871024	-1.25871456	0.05586729
H	4.78823131	-3.70484232	0.19218218
C	1.82420793	1.18382123	-0.09355731
C	-0.42993868	0.00002414	-0.00038634
C	4.23125360	1.62134428	-0.08846840
C	1.57043152	2.55738173	-0.14900497
C	3.96578009	2.98826863	-0.16126825
C	2.64674194	3.44707235	-0.18533740
H	2.44914435	4.51902772	-0.23255874
H	0.55524589	2.94951121	-0.16322081
H	5.25930800	1.25605858	-0.05519003
H	4.79011482	3.70240117	-0.19237847
C	-1.23454991	-1.22031455	0.28738870
C	-1.23400888	1.22088348	-0.28758171
C	-1.32814133	1.73272088	-1.58051667
C	-1.93038020	1.85990509	0.75678996
C	-2.68857405	3.00538512	0.49458750
C	-2.75778421	3.50592787	-0.80729283
C	-2.08404717	2.87487576	-1.84829432
O	-1.78564511	1.31456981	1.98481014
H	-3.22144952	3.51502352	1.29584965
H	-0.78870928	1.21677227	-2.37618059
H	-2.14417599	3.26752200	-2.86361356

H	-3.35086116	4.40124665	-1.00073165
C	-1.93247604	-1.85880402	-0.75626602
C	-1.32774117	-1.73212248	1.58042989
C	-2.69128252	-3.00370965	-0.49327034
C	-2.75955484	-3.50419615	0.80867473
C	-2.08425136	-2.87367607	1.84898899
H	-2.14363029	-3.26629837	2.86436187
H	-0.78707116	-1.21658325	2.37552571
O	-1.78855578	-1.31363901	-1.98445498
H	-3.22539907	-3.51292518	-1.29397270
H	-3.35312838	-4.39905424	1.00272173
C	-2.48736383	1.87966155	3.05964964
C	-2.49108609	-1.87876267	-3.05873871
H	-3.57896614	-1.86403967	-2.88114813
H	-2.17165321	-2.91681184	-3.24826557
H	-2.26266808	-1.26775570	-3.93892306
H	-3.57532412	1.86569579	2.88250379
H	-2.16719223	2.91742532	3.24949566
H	-2.25896157	1.26812471	3.93947265

5b-*cis*: (*E* = -1229.255077 Hartree)

C	-0.72341565	0.85901617	0.16178296
C	-2.19683020	0.69863762	0.32291302
C	0.23351263	-0.08471224	0.35595319
C	-0.52071206	2.27599198	-0.25411801
C	0.62087419	2.98002772	-0.64919541
C	-1.78234655	2.90391450	-0.34218168
C	-2.81707422	1.93506523	0.03911457
C	-1.90815472	4.22403584	-0.76722182
C	-2.97720695	-0.36505325	0.78589701
C	-4.19366058	2.10307333	0.16552012

C	-4.35642962	-0.19257474	0.91362401
C	-4.96485041	1.02520337	0.59741126
C	0.49093808	4.30236957	-1.07680520
C	-0.75875110	4.92621514	-1.12656004
H	1.60600231	2.51654333	-0.63640282
H	-2.89008138	4.69656685	-0.82959806
H	1.38191198	4.85412809	-1.38011772
H	-0.83568097	5.96166088	-1.46174165
H	-2.53095504	-1.32143256	1.05309895
H	-4.65889416	3.06468568	-0.05854347
H	-4.96652697	-1.02429473	1.26897390
H	-6.04525337	1.13569229	0.70185960
C	-0.07289053	-1.53892132	0.43095565
C	1.67366581	0.25447478	0.51679710
C	-0.72645898	-2.16391984	-0.62927153
C	0.33643997	-2.29859231	1.53937398
C	-1.00317225	-3.53709940	-0.58629912
C	-0.62408274	-4.28681175	0.53222680
C	0.04459628	-3.65515212	1.58534283
H	0.34400395	-4.24566368	2.45267406
H	0.86965569	-1.81333697	2.35825772
H	-1.04655983	-1.59446834	-1.50312962
O	-1.63730361	-4.04914513	-1.66349911
H	-0.83230856	-5.35394463	0.59082983
C	2.63376859	-0.35772424	-0.28630260
C	3.99235074	-0.05023024	-0.13323352
C	4.39246454	0.85641148	0.85461035
C	3.42619983	1.44243956	1.67764811
C	2.07781176	1.15273782	1.51918760
H	2.34781450	-1.07779331	-1.05474193
O	4.84185253	-0.67655424	-0.97642401

H	1.32446472	1.62179693	2.15362143
H	5.44304262	1.10416512	0.99782670
H	3.74345058	2.13922793	2.45511899
C	-1.93701159	-5.41891457	-1.67293156
C	6.21297012	-0.40365246	-0.86732610
H	6.71524082	-1.00226146	-1.63501690
H	6.60455096	-0.68688685	0.12392393
H	6.42834716	0.66336782	-1.04419493
H	-2.44082316	-5.62439791	-2.62365141
H	-2.60953932	-5.69189875	-0.84259649
H	-1.02352007	-6.03339472	-1.60853681

5b-*trans*: (*E* = -1229.254842 Hartree)

C	1.07936162	1.79896772	0.49275457
C	-0.00002800	0.89631735	-0.00006690
C	-1.07940940	1.79903215	-0.49280113
C	-0.00004377	-0.46149364	-0.00006185
C	-0.66213018	3.13637656	-0.31662598
C	-2.28436213	1.54223531	-1.15374732
C	0.66212386	3.13633704	0.31664425
C	-1.44712833	4.20436816	-0.74367905
C	2.28433661	1.54210783	1.15363761
C	1.44715628	4.20428633	0.74373241
C	-3.06768182	2.61490514	-1.58269004
C	-2.66197366	3.93562530	-1.37213397
C	3.06769545	2.61474108	1.58260888
C	2.66201170	3.93548056	1.37214589
H	-2.62040559	0.52448875	-1.34508489
H	-1.11160172	5.23298335	-0.59976097
H	-3.29224976	4.75815845	-1.71358675
H	-4.01102604	2.41509598	-2.09298867

H	4.01106132	2.41487680	2.09284623
H	3.29231568	4.75797949	1.71362990
H	2.62040061	0.52434870	1.34487248
H	1.11164726	5.23291533	0.59987383
C	1.23824280	-1.26738186	0.17876739
C	-1.23825225	-1.26749516	-0.17876430
C	1.31271892	-2.25119958	1.17866399
C	2.31506561	-1.08150805	-0.68626665
C	2.47631831	-2.99513464	1.32211004
C	3.56688763	-2.80361548	0.46820727
C	3.48100300	-1.84647397	-0.54845327
C	-2.31524686	-1.08133689	0.68599695
C	-1.31248683	-2.25178090	-1.17823498
C	-2.47599341	-2.99587147	-1.32154919
C	-3.56673201	-2.80406238	-0.46791877
C	-3.48109805	-1.84646468	0.54832525
H	0.46029379	-2.41317378	1.84009384
O	4.46663264	-1.59228030	-1.43663239
H	2.27568823	-0.32822345	-1.47458037
H	2.54596507	-3.74728339	2.10955332
H	4.46396141	-3.40686277	0.59837824
H	-2.27606909	-0.32772182	1.47400508
H	-0.45992964	-2.41398346	-1.83943894
H	-2.54544747	-3.74837716	-2.10866776
O	-4.46689974	-1.59196430	1.43622466
H	-4.46373936	-3.40743213	-0.59798412
C	5.65642419	-2.32830557	-1.34248543
C	-5.65653257	-2.32827161	1.34230007
H	6.31216249	-1.97047896	-2.14367128
H	5.47649536	-3.40781757	-1.47866013
H	6.15474157	-2.16971255	-0.37152662

H	-6.31239337	-1.97027077	2.14330794
H	-5.47638984	-3.40769336	1.47890969
H	-6.15482428	-2.17016699	0.37124726

5c: (*E* = -1229.257396 Hartree)

C	-1.12290669	2.00787332	-0.37858657
C	-0.00003021	1.10609446	-0.00003674
C	0.00009336	-0.25746135	-0.00006077
C	1.12262372	2.00808141	0.37862754
C	0.68982870	3.34657199	0.24804584
C	2.38669768	1.75238710	0.92178846
C	1.51342001	4.41433462	0.59883669
C	-0.69030162	3.34644393	-0.24811393
C	-1.51406441	4.41406982	-0.59890999
C	-2.38698795	1.75197296	-0.92163765
C	-3.20731141	2.82342593	-1.27528676
C	-2.78371019	4.14541410	-1.10594129
C	3.20685008	2.82397029	1.27543559
C	2.78306657	4.14588884	1.10597883
H	-2.73977734	0.73363537	-1.07855165
H	-4.19469322	2.62299287	-1.69407093
H	-1.16542432	5.44280190	-0.49077131
H	-3.44409458	4.96747351	-1.38607685
H	2.73960091	0.73409261	1.07874843
H	1.16463486	5.44301055	0.49063154
H	3.44330916	4.96806062	1.38611877
H	4.19423173	2.62370488	1.69429982
C	-1.25261783	-1.05068289	0.02497337
C	1.25284303	-1.05058031	-0.02505687
C	1.44685923	-2.13480447	0.84916649
C	2.25247647	-0.77277317	-0.96207622

C	3.42959679	-1.51811424	-1.01563326
C	3.62090363	-2.57217891	-0.11422311
C	2.61676595	-2.87577530	0.81854288
H	0.66581708	-2.38353058	1.57068435
H	4.18296377	-1.27216586	-1.76232272
H	2.78643776	-3.70672986	1.50351229
O	4.72314537	-3.34867958	-0.07827397
H	2.10707351	0.05423083	-1.66008830
C	-2.25204666	-0.77318999	0.96228712
C	-3.42918473	-1.51852355	1.01578625
C	-3.62068659	-2.57223835	0.11401720
C	-2.61673414	-2.87551045	-0.81906072
C	-1.44680822	-2.13456615	-0.84962243
H	-2.10651052	0.05358947	1.66053694
H	-2.78656268	-3.70620246	-1.50430963
H	-0.66589761	-2.38304151	-1.57137029
H	-4.18242664	-1.27279744	1.76267443
O	-4.72298375	-3.34866186	0.07793058
C	5.75646087	-3.08612185	-0.99087075
C	-5.75560889	-3.08720744	0.99162454
H	5.41481107	-3.20408708	-2.03244622
H	6.54789402	-3.81575323	-0.78828822
H	6.16071434	-2.06868891	-0.86054133
H	-5.41290852	-3.20552450	2.03281287
H	-6.54680100	-3.81719329	0.78937739
H	-6.16060396	-2.06994853	0.86222534

8a: (*E* = -1690.844965 Hartree)

C	-1.52448631	0.24115022	1.25817578
C	-0.38321393	0.04168276	0.32160045
C	0.04704589	1.41252228	-0.07996531

C	0.09590028	-1.13455795	-0.14297008
C	1.07493476	1.87241819	-0.90958616
C	-0.83338823	2.34668966	0.51016107
C	-1.80784251	1.62197841	1.33446389
C	-0.70725496	3.71227819	0.27550408
C	-2.85607903	2.10675679	2.10963489
C	-2.27080910	-0.65274823	2.02948230
C	-3.32001261	-0.16234084	2.81236679
C	-3.62200023	1.20091988	2.84366378
H	-2.04635050	-1.71840935	2.04384535
H	-3.90538422	-0.85887432	3.41505909
H	-3.07476536	3.17556446	2.14393166
H	-4.45035928	1.55975650	3.45659114
C	1.20259000	3.24625052	-1.13663158
C	0.32066886	4.15999709	-0.55495373
H	1.78513430	1.19080991	-1.37608736
H	2.00773365	3.60507473	-1.77990759
H	-1.40240262	4.41971698	0.73143069
H	0.43806439	5.22716349	-0.74960263
C	1.24871050	-1.21253386	-1.08717551
C	2.55890192	-1.37782905	-0.61528049
C	1.02413010	-1.15922306	-2.46701708
C	2.08830379	-1.21925180	-3.36339780
C	3.39140904	-1.35314083	-2.88328148
C	3.62690768	-1.44017638	-1.51297302
O	2.78407042	-1.52604113	0.72986286
H	4.63532605	-1.56183535	-1.11721870
H	1.90046968	-1.16588179	-4.43640628
H	4.23034843	-1.40150979	-3.57889962
C	-0.55773944	-2.44219890	0.14317202
H	-0.00358889	-1.06045589	-2.82379167

C	0.09194235	-3.44674988	0.86337173
C	-0.55414654	-4.65107923	1.14604923
C	-1.85122095	-4.86466507	0.68488863
C	-2.50161402	-3.88822493	-0.07081212
C	-1.85550814	-2.68334416	-0.34859061
H	-3.50691028	-4.06183751	-0.45729817
O	-2.42454713	-1.70343976	-1.09170045
H	-0.04345858	-5.42007231	1.72631054
H	-2.36180658	-5.80460382	0.90009583
H	1.10622153	-3.25388109	1.21924376
C	-3.78446245	-1.37978457	-0.89248912
C	-3.96448718	0.11404633	-1.02659407
H	-4.10650949	-1.69962945	0.11313501
H	-4.40759814	-1.91046709	-1.63530182
C	-5.05733668	0.73987298	-0.42131146
C	-3.04564579	0.88593343	-1.74314092
C	-3.21586175	2.26510677	-1.84730901
C	-4.30884007	2.88528231	-1.24259317
C	-5.23195986	2.11814380	-0.53236949
H	-5.76836958	0.14647093	0.15910695
H	-2.17531969	0.40293370	-2.18863065
H	-2.47727938	2.85943722	-2.38868229
H	-6.08481069	2.59686043	-0.04798684
H	-4.43847070	3.96610411	-1.32032793
C	2.94887230	-0.32265516	1.47310493
C	4.26518370	0.36058430	1.18898307
H	2.89609553	-0.63110212	2.52668954
H	2.11313720	0.36702871	1.27659300
C	4.31065797	1.70848055	0.82993826
C	5.53444640	2.33039503	0.57298660
C	6.71931337	1.60473226	0.66578701

C	6.68050118	0.25391776	1.02097166
C	5.46055865	-0.36240303	1.28268624
H	3.37914069	2.27416492	0.74664984
H	7.60728613	-0.31728979	1.09660432
H	5.42146849	-1.42031904	1.55352027
H	5.55872897	3.38481686	0.29328775
H	7.67562874	2.08871740	0.46144654

8b: (*E* = -1690.836081 Hartree)

C	-3.58552411	1.83943640	-0.51355385
C	-2.96747238	0.60088976	0.03902325
C	-4.10833383	-0.24502917	0.49267607
C	-1.64366294	0.30304428	0.10764630
C	-5.31252449	0.43647621	0.21070174
C	-4.16445527	-1.54725807	0.99892460
C	-6.55239166	-0.14177814	0.47057281
C	-4.98816387	1.73679785	-0.38826816
C	-3.02789811	3.03191832	-0.98465505
C	-3.87355843	4.07487663	-1.36577117
C	-5.26244961	3.94932664	-1.27249651
C	-5.82919548	2.77835374	-0.77160675
H	-6.91186345	2.68457877	-0.66993707
H	-1.94944968	3.16560745	-1.05345868
H	-3.43956381	5.00375733	-1.73862500
H	-5.90391711	4.77697498	-1.57887086
C	-6.59442796	-1.42810274	1.00590846
C	-5.40887899	-2.12476699	1.25609886
H	-7.47472082	0.39773622	0.24795987
H	-3.25932942	-2.12078481	1.19219502
H	-7.55563483	-1.89868330	1.21794447
H	-5.45281621	-3.13846266	1.65696130

C	-1.10790364	-0.77266044	0.98442384
C	-1.38043996	-0.76303530	2.35416717
C	-0.27802147	-1.76615521	0.44079958
C	0.23982174	-2.76866245	1.26361633
C	-0.05188055	-2.76511589	2.63605032
C	-0.84918923	-1.76333790	3.17138200
H	-2.01677243	0.02017649	2.76849900
H	-1.06070334	-1.75913254	4.24167101
H	-0.05945942	-1.73693317	-0.62633441
O	1.03039709	-3.77418024	0.82492905
H	0.37084373	-3.55608262	3.25585382
C	-0.61663231	1.02365566	-0.69297054
C	-0.74527067	1.11196902	-2.08967379
C	0.23497278	1.75833691	-2.83041017
C	1.35254032	2.32556869	-2.21084631
C	1.48966045	2.22322406	-0.82221950
C	0.51022123	1.55971992	-0.07197108
H	-1.62279455	0.68191921	-2.57463746
H	0.13695054	1.82909342	-3.91479450
H	2.10389340	2.83066254	-2.81539915
O	2.53120507	2.72836637	-0.12340022
H	0.64464363	1.48124441	1.00810936
C	1.37862521	-3.81276140	-0.53508469
C	2.28450791	-4.98897809	-0.79969927
H	1.89217230	-2.87532642	-0.81936612
H	0.47113381	-3.89194743	-1.16081155
C	2.86312827	-5.71694932	0.24053821
C	2.56816831	-5.34210921	-2.12310457
C	3.71694687	-6.78400677	-0.04175733
C	4.00062399	-7.12997322	-1.36094808
C	3.42286642	-6.40449090	-2.40369210

H	2.11288323	-4.77990672	-2.94258021
H	2.63490412	-5.44350073	1.27006474
H	4.16290605	-7.34908970	0.77832349
H	4.66823754	-7.96491591	-1.57844506
H	3.63576586	-6.67071886	-3.44014943
C	3.55357725	3.39349563	-0.81808138
C	4.61550951	3.85421376	0.14888157
H	3.14341601	4.26283311	-1.36389199
H	4.00313831	2.71650169	-1.56859432
C	5.62944721	4.70109593	-0.31094121
C	6.63916302	5.12585132	0.54792884
C	6.64301760	4.71034092	1.88021832
C	5.63276140	3.87009924	2.34236083
C	4.62173106	3.44104301	1.48143350
H	5.62708565	5.03290174	-1.35255115
H	5.62832980	3.54357768	3.38351069
H	3.82765128	2.78600398	1.83782117
H	7.42436141	5.78684681	0.17784913
H	7.43179772	5.04420392	2.55584674

8c: (*E* = -1690.837263 Hartree)

C	-0.00006486	2.73662912	0.00000684
C	1.13534500	3.63849806	0.33937468
C	0.69838858	4.97694283	0.22351245
C	2.41760080	3.38246819	0.83711206
C	1.53396346	6.04442574	0.54430709
C	-0.69864935	4.97688076	-0.22368472
C	-1.53427937	6.04428841	-0.54458014
C	-1.13552729	3.63839865	-0.33943030
C	-2.41776352	3.38225600	-0.83715694
C	-0.00001059	1.37350530	0.00004929

C	-3.25096146	4.45377525	-1.16012831
C	-2.82155400	5.77539319	-1.00565905
C	3.25074245	4.45406107	1.15997747
C	2.82125686	5.77564185	1.00539493
H	2.77620893	2.36461000	0.98278278
H	4.25286396	4.25358836	1.54194392
H	1.18187345	7.07316525	0.44843982
H	3.49145781	6.59777596	1.26082545
H	-2.77632445	2.36436813	-0.98273964
H	-1.18224387	7.07305439	-0.44879736
H	-3.49179728	6.59746719	-1.26117157
H	-4.25306570	4.25320737	-1.54209038
C	1.25250276	0.58063480	-0.06126675
C	-1.25249159	0.58057258	0.06140105
C	-1.47365829	-0.49530771	-0.80298520
C	-2.64707503	-1.24806248	-0.74530878
C	-3.61503553	-0.94298156	0.21826007
C	-3.39156063	0.11299612	1.11523794
C	-2.22866541	0.86005303	1.03438013
H	-0.71575461	-0.74314842	-1.54912947
H	-2.79091910	-2.06608990	-1.44907410
H	-2.06226372	1.68609563	1.72867413
O	-4.77874779	-1.61292159	0.36357866
H	-4.15139930	0.32117853	1.86872766
C	2.22868725	0.86015535	-1.03423191
C	3.39160097	0.11313689	-1.11508027
C	3.61509781	-0.94285109	-0.21811074
C	2.64714321	-1.24796206	0.74544800
C	1.47369959	-0.49524036	0.80311429
H	2.06227017	1.68620410	-1.72851541
H	4.15145798	0.32135911	-1.86854068

O	4.77882890	-1.61275135	-0.36344656
H	2.79100374	-2.06598428	1.44921628
H	0.71580212	-0.74311076	1.54925545
C	-5.05730162	-2.68237418	-0.50238325
C	5.05751834	-2.68209111	0.50262780
C	6.39871207	-3.28336660	0.16406916
H	5.05991736	-2.33226059	1.55127482
H	4.27127164	-3.45483710	0.41598869
C	6.89466890	-4.31952276	0.96269443
C	8.12330814	-4.90688369	0.67562841
C	8.87205849	-4.46198318	-0.41510347
C	8.38214053	-3.42953666	-1.21105125
C	7.14946811	-2.84053311	-0.92491871
H	6.76192738	-2.03196893	-1.54332947
H	6.31215815	-4.66938529	1.81909204
H	8.49973541	-5.71396476	1.30597036
H	9.83589526	-4.92014749	-0.64128604
H	8.96296818	-3.07591445	-2.06442413
C	-6.39848066	-3.28372097	-0.16388604
H	-4.27102022	-3.45506612	-0.41566121
H	-5.05967903	-2.33262187	-1.55106522
C	-6.89273439	-4.32221377	-0.96053817
C	-7.15101135	-2.83850366	0.92289668
C	-8.38376733	-3.42745578	1.20879915
C	-8.87200954	-4.46218978	0.41480249
C	-8.12147300	-4.90947927	-0.67373164
H	-6.76474461	-2.02819216	1.53981320
H	-8.49655966	-5.71840551	-1.30250528
H	-6.30878131	-4.67400778	-1.81516427
H	-8.96597322	-3.07199054	2.06046754
H	-9.83590484	-4.92031514	0.64081265

9: (E = -1188.809008 Hartree)

C	1.63945921	-1.27716397	0.02824641
C	0.77976307	-0.07047828	-0.15212269
C	-0.56775188	-0.03578837	-0.27634701
C	1.71645453	1.09169496	-0.15096060
C	3.03753997	0.59795364	-0.06860059
C	1.50875599	2.47280180	-0.21820733
C	4.13601373	1.45139264	-0.07648689
C	2.98941138	-0.86475317	0.05448029
C	4.02395663	-1.77825218	0.23277499
C	1.33378651	-2.62450730	0.24011497
C	3.70782923	-3.12493247	0.41224037
C	2.37404216	-3.53775172	0.42909053
C	2.61492187	3.32675837	-0.21911985
C	3.91661352	2.82654256	-0.15590305
H	0.30495175	-2.97852149	0.26676293
H	5.06325250	-1.44543577	0.24696868
H	4.50448131	-3.85650896	0.55508130
H	2.13585259	-4.58959519	0.59311138
H	0.51056743	2.90285438	-0.26326649
H	4.76390420	3.51380892	-0.16164635
H	2.45244690	4.40431738	-0.26854522
H	5.15030959	1.05297596	-0.01601215
C	-1.42504189	-1.24113419	-0.43482881
C	-1.32394432	1.24877305	-0.33905164
C	-1.48727026	1.89082600	-1.57353696
C	-1.85918098	1.84670256	0.80974404
C	-2.47681216	3.09900199	0.72065265
C	-2.10715595	3.13141838	-1.66540290
C	-2.58814613	3.74302850	-0.50510955

H	-1.08034529	1.40785605	-2.46450837
O	-1.79435794	1.30519835	2.05821646
H	-2.86684894	3.53873532	1.63870248
H	-2.20907407	3.62267586	-2.63332169
H	-3.06984183	4.72041086	-0.55815242
C	-1.24118761	-2.09030157	-1.53639971
C	-2.09198854	-3.16253030	-1.77628485
C	-3.15890026	-3.40061897	-0.90689787
C	-3.36436211	-2.56952706	0.18777081
C	-2.51161574	-1.48726374	0.42127689
H	-4.18756705	-2.72812713	0.88454189
O	-2.82133285	-0.70015234	1.49198199
H	-0.40349107	-1.88718608	-2.20682111
H	-1.92879234	-3.80604144	-2.64106042
H	-3.83572639	-4.23789433	-1.08263549
C	-1.81870792	-0.08187712	2.24622402
H	-2.07543137	-0.20980385	3.30489177
H	-0.84201397	-0.54497287	2.04018769