

## Supporting Information

*for*

### **Linear, two- and four-armed pyridine-decorated thiazolo[5,4-d]thiazole fluorophores: synthesis, photophysical study and computational investigation**

*by*

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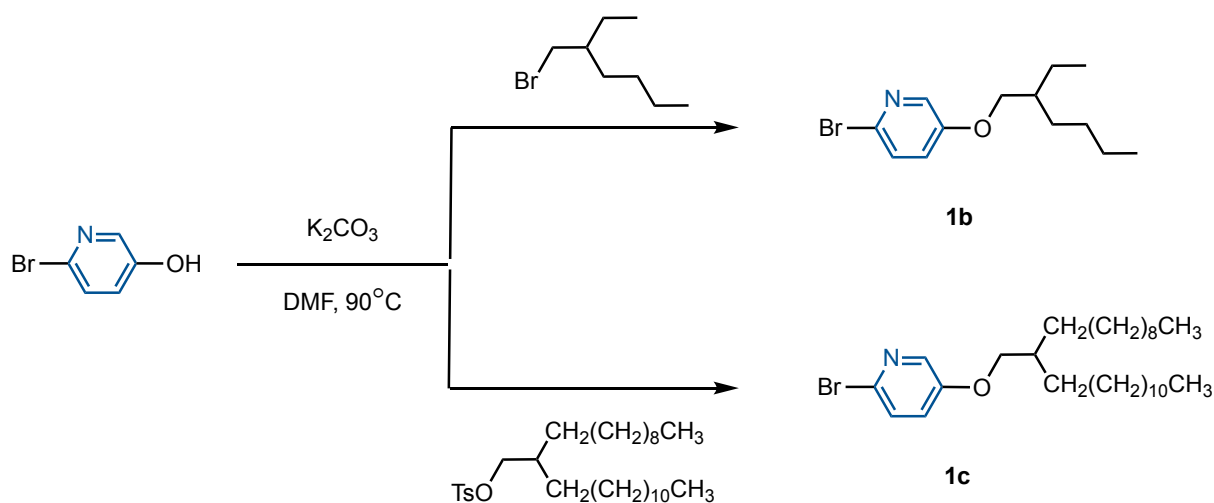
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## 1. Supplementary synthetic procedures

### 1.1. Synthesis of 2-bromo-5-((2-alkyl)oxy)pyridine (1b–c)

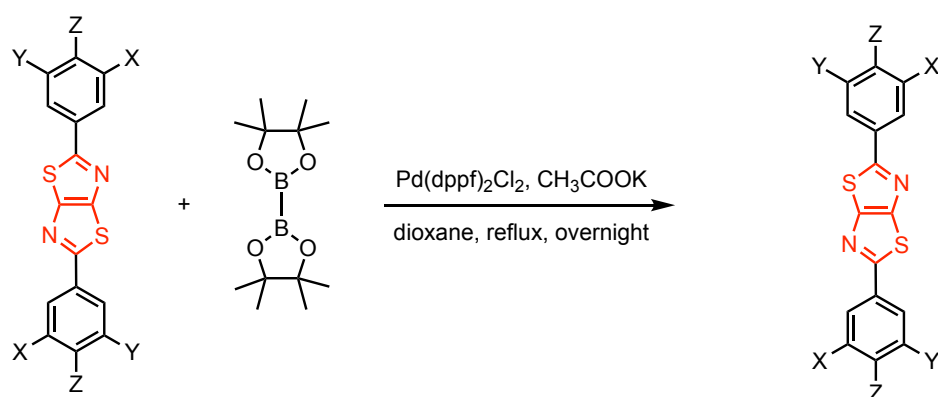


**Compound 1a** and **1b** were synthesized using a similar procedure. To a solution of 2-bromo-5-hydroxypyridine (5.0 g, 28.7 mmol) in DMF (80 mL) under argon,  $K_2CO_3$  (11.8, 3.0 equiv.) and either 2-ethylhexyl bromide (6.66 g, 1.2 equiv.) or 2-decyltetradecyl 4-methylbenzenesulfonate (17.54 g 1.2 equiv.) were added for yielding **1a** and **1b**, respectively.<sup>[S1]</sup> The reaction mixture was allowed to stir overnight at  $90^\circ C$  under an argon atmosphere. After cooling to room temperature, the mixture was filtered through Celite and washed with  $CH_2Cl_2$  and the filtrate was collected and evaporated to dryness under reduced pressure. The resulting residue was purified by short column chromatography ( $SiO_2$ , petroleum ether then  $CH_2Cl_2$ / petroleum ether 1:1) affording the desired compound. **1b** was obtained as colorless oil (7.2 g, yield 87%); **1c** was obtained as pale-yellow oil (13.20 g, yield 90%).

**Compound 1b.**  $^1H$  NMR ( $CDCl_3$ , 500 MHz):  $\delta$  (ppm) 8.04 (d,  $J = 5$  Hz, 1H), 7.33 (d,  $J = 10$  Hz, 1H), 7.08 (dd,  $J_1 = 5$  Hz,  $J_2 = 10$  Hz, 1H), 3.84 (m, 2H), 1.71 (m, 1H), 1.43 (m, 4H), 1.29 (m, 4H), 0.89 (m, 6H).  $^{13}C$  NMR ( $CDCl_3$ , 125 MHz):  $\delta$  (ppm) 155.2, 137.5, 131.7, 128.0, 124.8, 71.2, 39.3, 30.3, 29.0, 25.1, 23.7, 23.0, 14.1, 11.1. HR-MS (ESI):  $m/z$   $[M + H]^+$  calcd for  $C_{13}H_{21}BrNO$   $[M + H]^+$  286.0801; found 286.0805.



### 1.3.Synthesis of compound 5, 6 and 7.



- 2** X = Br, Y = H, Z = H  
**3** X = H, Y = H, Z = Br  
**4** X = Br, Y = Br, Z = H

- 5** X = B(pinacolate), Y = H, Z = H  
**6** X = H, Y = H, Z = B(pinacolate)  
**7** X = B(pinacolate), Y = B(pinacolate), Z = H

To a solution of either **2** or **3** (1.0 g, 2.2 mmol) or **4** (1.0 g, 1.6 mmol) was added bis(pinacolato)diborane (1.4 g, 2.5 equiv.) or (2.0 g, 5.0 equiv. in the case of **4**), respectively, potassium acetate (1.07 g, 5.0 equiv.) or (1.6 g, 10.0 equiv. in the case of **4**), Pd(dppf)<sub>2</sub>Cl<sub>2</sub> (0.04 g), in dried 1,4-dioxane (30 mL) under argon. The reaction mixture was allowed to reflux overnight under an argon atmosphere. The mixture evaporated to dryness under reduced pressure and extracted with CH<sub>2</sub>Cl<sub>2</sub> (2×50 mL). The organic layer was dried with anhydrous MgSO<sub>4</sub> and the solvent was removed under vacuum. The crude product was purified by short column chromatography (SiO<sub>2</sub>), to yield **5** or **6** (eluant: CH<sub>2</sub>Cl<sub>2</sub> then CH<sub>2</sub>Cl<sub>2</sub> with MeOH 0.5%), or **7** (eluant: CH<sub>2</sub>Cl<sub>2</sub> then CH<sub>2</sub>Cl<sub>2</sub>/MeOH 0.5% then CH<sub>2</sub>Cl<sub>2</sub>/MeOH 1%). Final washing with MeOH and then with petroleum ether provided the desired compounds in pure form.

#### **2,5-bis(3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)thiazolo[5,4-d]thiazole (5).**

White solid, 1.1 g, yield: 92%. <sup>1</sup>H NMR (CDCl<sub>3</sub>, 500 MHz): δ (ppm) 8.37 (m, 2H), 8.10 (d, *J* = 7.5 Hz, 2H), 7.89 (d, *J* = 7.5 Hz, 2H), 7.47 (t, *J* = 7.5 Hz, 2H), 1.36 (s, 24H). <sup>13</sup>C NMR (CDCl<sub>3</sub>, 125 MHz): δ (ppm) 169.2, 150.9, 137.0, 133.4, 132.6, 129.1, 128.5, 84.2, 24.9.

HR-MS (ESI): *m/z* [M + H]<sup>+</sup> calcd for C<sub>28</sub>H<sub>33</sub>B<sub>2</sub>N<sub>2</sub>O<sub>4</sub>S<sub>2</sub> [M + H]<sup>+</sup> 547.2072; found 547.2071.

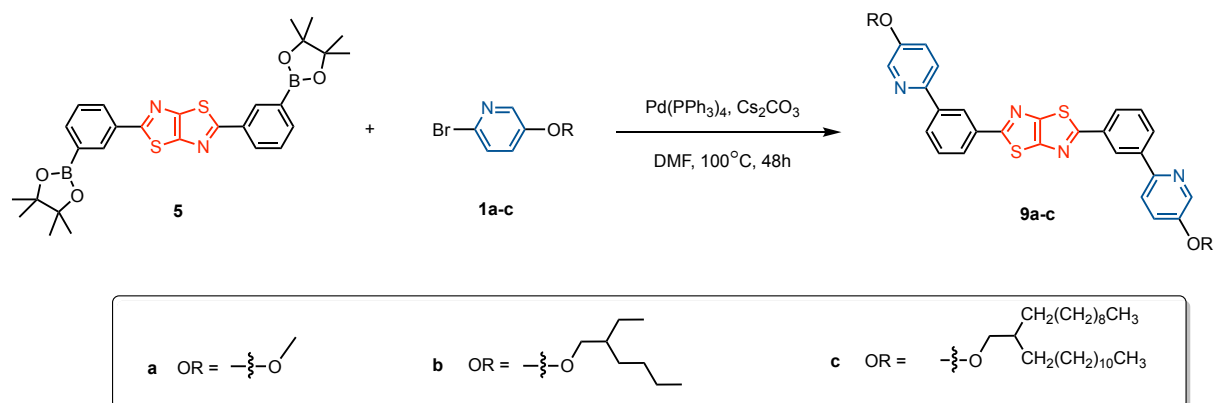


**Compound 8b** and **8c** were synthesized using the same procedures as **8a** and employing the corresponding 2-bromo-5-alkoxy pyridine.

**Compound 8b.** Yellow solid (0.088 g, yield 58%).  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 500 MHz):  $\delta$  (ppm) 8.43 (d,  $J = 2.5$  Hz, 2H), 8.10 (s, 8H), 7.79 (d,  $J = 9$  Hz, 2H), 7.44 (m, 2H), 3.95 (m, 4H), 1.77 (m, 2H), 1.46 (m, 8H), 1.32 (m, 8H), 0.93 (m, 12H).  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  (ppm) 168.6, 155.5, 151.4, 127.5, 127.4, 127.0, 122.2, 122.1, 71.6, 39.3, 30.3, 29.0, 23.7, 23.0, 14.1, 11.1. HR-MS (ESI):  $m/z$   $[\text{M} + \text{H}]^+$  calcd for  $\text{C}_{42}\text{H}_{49}\text{N}_4\text{O}_2\text{S}_2$   $[\text{M} + \text{H}]^+$  705.3291 found 705.3288.

**Compound 8c.** Yellow solid 0.131 g, yield 62%).  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 500 MHz):  $\delta$  (ppm) 8.40 (d,  $J = 2.5$  Hz, 2H), 8.06 (s, 8H), 7.72 (d,  $J = 9$  Hz, 2H), 7.30 (m, 2H), 3.92 (m, 4H), 1.80 (m, 2H), 1.24 (m, 72H), 0.86 (t,  $J = 10$  Hz, 12H).  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  (ppm) 168.8, 155.1, 151.2, 133.6, 132.3, 127.0, 126.8, 121.2, 71.5, 37.9, 31.9, 31.2, 30.0, 29.7, 29.6, 29.4, 29.3, 26.8, 22.7, 14.7. HR-MS (ESI):  $m/z$   $[\text{M} + \text{H}]^+$  calcd for  $\text{C}_{74}\text{H}_{113}\text{N}_4\text{O}_2\text{S}_2$   $[\text{M} + \text{H}]^+$  1153.8299 found 1153.8272.

### 1.5.Synthesis of compound 9a, 9b and 9c.



A DMF solution (30 mL) of compound **5** (0.5 g, 0.91 mmol) and 2-bromo-5-methoxy pyridine (0.37 g, 2.2 equiv.) was degassed with argon for 20 min. Then  $\text{Cs}_2\text{CO}_3$  (0.65 g, 2.2 equiv.) and

$\text{Pd}(\text{PPh}_3)_4$  (0.1 equiv.) were added to the mixture under an argon atmosphere. The reaction media was heated to 90°C for 48 h before it was allowed to reach room temperature. The mixture was filtered through Celite and washed with  $\text{CH}_2\text{Cl}_2$  and the filtrate was collected and evaporated to dryness under reduced pressure. The resulting residue was purified by column chromatography ( $\text{SiO}_2$ ) with  $\text{CH}_2\text{Cl}_2$  then  $\text{CH}_2\text{Cl}_2/\text{MeOH}$  0.5% to yield compounds **4a** as an off-white solid (0.2 g, yield 43%).

**Compound 9a.**  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz):  $\delta$  (ppm) 8.57 (s, 2H), 8.44 (d,  $J = 3$  Hz, 2H), 8.07 (d,  $J = 8$  Hz, 2H), 8.01 (d,  $J = 8$  Hz, 2H), 7.81 (d,  $J = 8$  Hz, 2H), 7.55 (t,  $J = 8$  Hz, 2H), 7.36 (dd,  $J_1 = 3$  Hz,  $J_2 = 8$  Hz, 2H), 3.93 (m, 4H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  (ppm) 169.1, 160.9, 155.3, 151.0, 140.0, 134.5, 129.7, 128.7, 126.3, 124.4, 123.3, 121.0, 121.1, 55.8. HR-MS (ESI):  $m/z$   $[\text{M} + \text{H}]^+$  calcd for  $\text{C}_{28}\text{H}_{21}\text{N}_4\text{O}_2\text{S}_2$   $[\text{M} + \text{H}]^+$  509.1100 found 509.1101.

Compound **9b** and **9c** were synthesized using the same procedures as **9a**, employing **1b** and **1c**, respectively, instead of **1a**.

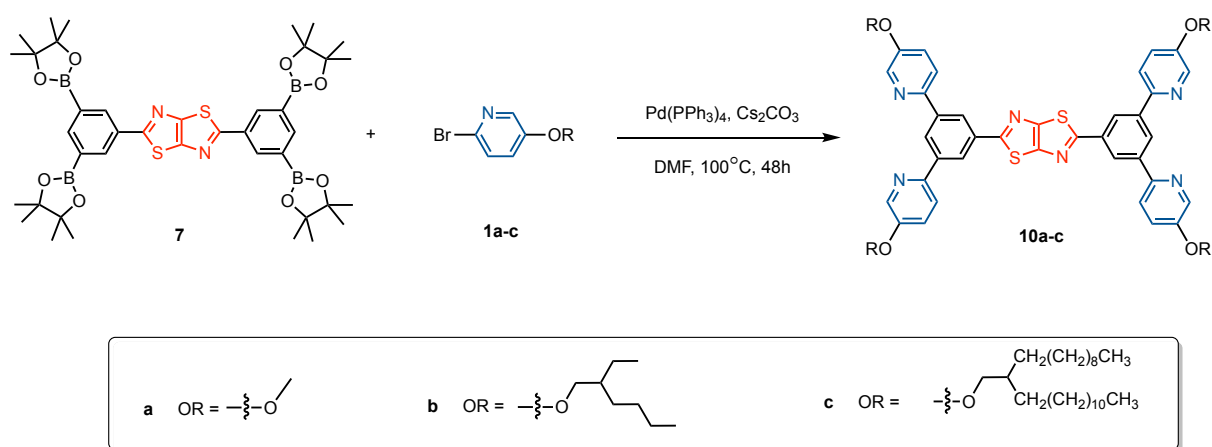
**Compound 9b.** Off-white solid (0.4 g, yield 62%).  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz):  $\delta$  (ppm) 8.54 (s, 2H), 8.4 (d,  $J = 3$  Hz, 2H), 8.03 (d,  $J = 8$  Hz, 2H), 7.98 (d,  $J = 8$  Hz, 2H), 7.75 (d,  $J = 8$  Hz, 2H), 7.54 (t,  $J = 8$  Hz, 2H), 7.28 (dd,  $J_1 = 3$  Hz,  $J_2 = 8$  Hz, 2H), 3.93 (m, 4H), 1.75 (m, 2H), 1.46 (m, 8H), 1.33 (m, 8H), 0.92 (m, 12H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  (ppm) 169.2, 155.0, 151.0, 148.6, 140.2, 137.8, 134.4, 129.5, 128.6, 126.0, 124.3, 121.8, 121.0, 71.0, 39.3, 30.4, 29.1, 23.8, 23.0, 14.1, 11.1. HR-MS (ESI):  $m/z$   $[\text{M} + \text{H}]^+$  calcd for  $\text{C}_{42}\text{H}_{49}\text{N}_4\text{O}_2\text{S}_2$   $[\text{M} + \text{H}]^+$  705.3291 found 705.3287.

**Compound 9c.** Off-white solid (0.25 g, yield 59%).  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz):  $\delta$  (ppm) 8.55 (1s, 2H), 8.4 (d,  $J = 3$  Hz, 2H), 8.03 (d,  $J = 8$  Hz, 2H), 7.98 (d,  $J = 8$  Hz, 2H), 7.75 (d,  $J = 8$  Hz, 2H), 7.54 (t,  $J = 8$  Hz, 2H), 7.28 (dd,  $J_1 = 3$  Hz,  $J_2 = 8$  Hz, 2H), 3.93 (d,  $J = 5.5$  Hz, 4H), 1.80 (m, 2H), 1.26 (m, 80H), 0.85 (m, 12H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  (ppm) 169.2, 155.0,



151.0, 148.6, 140.2, 137.8, 134.4, 129.5, 128.6, 126.0, 124.3, 121.8, 121.0, 71.4, 37.9, 31.9, 31.2, 30.0, 29.7, 29.6, 29.4, 26.8, 22.7, 14.1 HR-MS (ESI):  $m/z$   $[M + H]^+$  calcd for  $C_{74}H_{113}N_4O_2S_2$   $[M + H]^+$  1153.8299 found 1153.8300.

### 1.6.Synthesis of compound 10a, 10b and 10c.



A DMF solution (30 mL) of compound **7** (0.5g, 0.62 mmol) with 2-bromo-5-methoxypyridine (0.70 g, 6 equiv.) was degassed with argon for 20 min. To the mixture,  $\text{Cs}_2\text{CO}_3$  (1.22 g, 6 equiv.) and  $\text{Pd}(\text{PPh}_3)_4$  (0.1 equiv.) were added under an argon atmosphere. The reaction mixture was heated to  $90^\circ\text{C}$  for 72 h, before it was allowed to reach room temperature. The mixture was filtered through Celite and washed with  $\text{CH}_2\text{Cl}_2$  and the filtrate was collected and evaporated to dryness under reduced pressure. The resulting residue was purified by column chromatography ( $\text{SiO}_2$ ), eluant,  $\text{CH}_2\text{Cl}_2$  then  $\text{CH}_2\text{Cl}_2/\text{MeOH}$  0.5% then  $\text{CH}_2\text{Cl}_2/\text{MeOH}$  1% to yield compounds **10a** as an off-white solid (0.22 g, yield 31%).

**Compound 10a.**  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz):  $\delta$  (ppm) 8.68 (t,  $J = 1.5$  Hz, 2H), 8.56 (d,  $J = 1.5$  Hz, 4H), 8.45 (d,  $J = 2.5$  Hz, 4H), 7.88 (d,  $J = 9$  Hz, 4H), 7.31 (dd,  $J_1 = 2.5$  Hz,  $J_2 = 9$  Hz, 4H), 3.93 (s, 12H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  (ppm) 169.1, 155.2, 151.1, 148.9, 140.5,

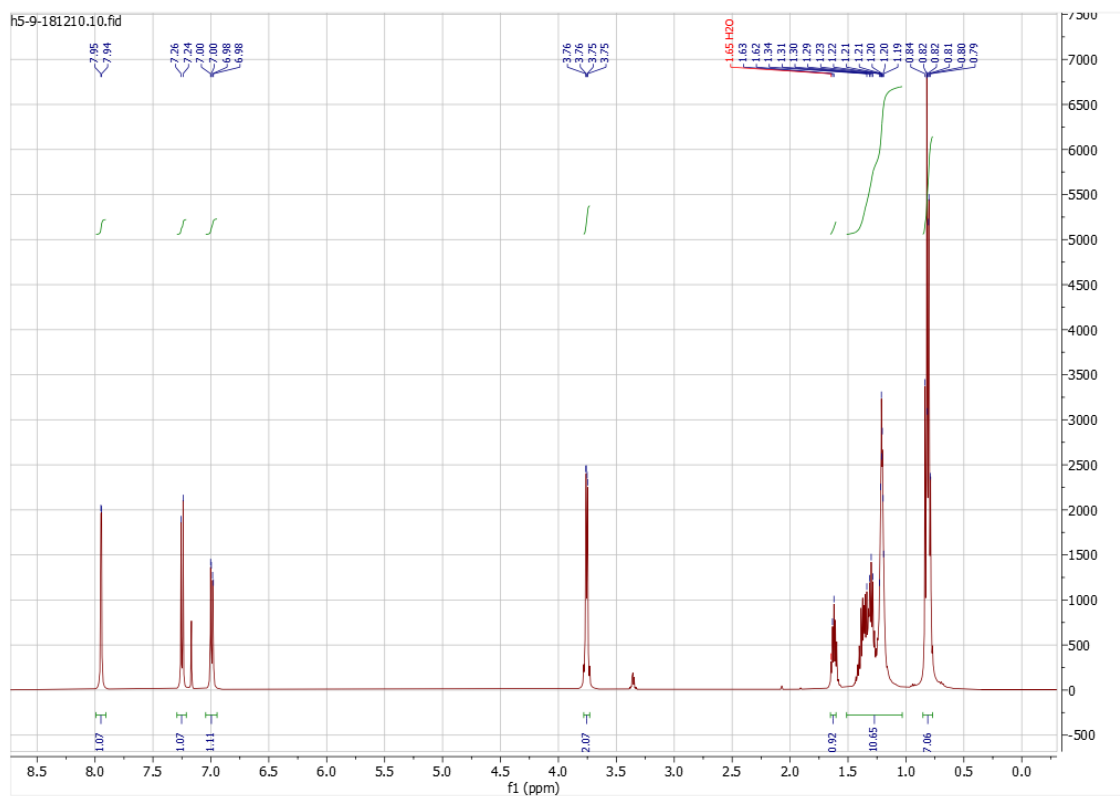
137.3, 134.9, 126.5, 123.9, 121.2, 55.7. HR-MS (ESI):  $m/z$   $[M + H]^+$  calcd for  $C_{40}H_{31}N_6O_4S_2$   
 $[M + H]^+$  723.1843 found 723.1843.

Compound **10b** and **10c** were synthesized using the same procedures as for **10a**.

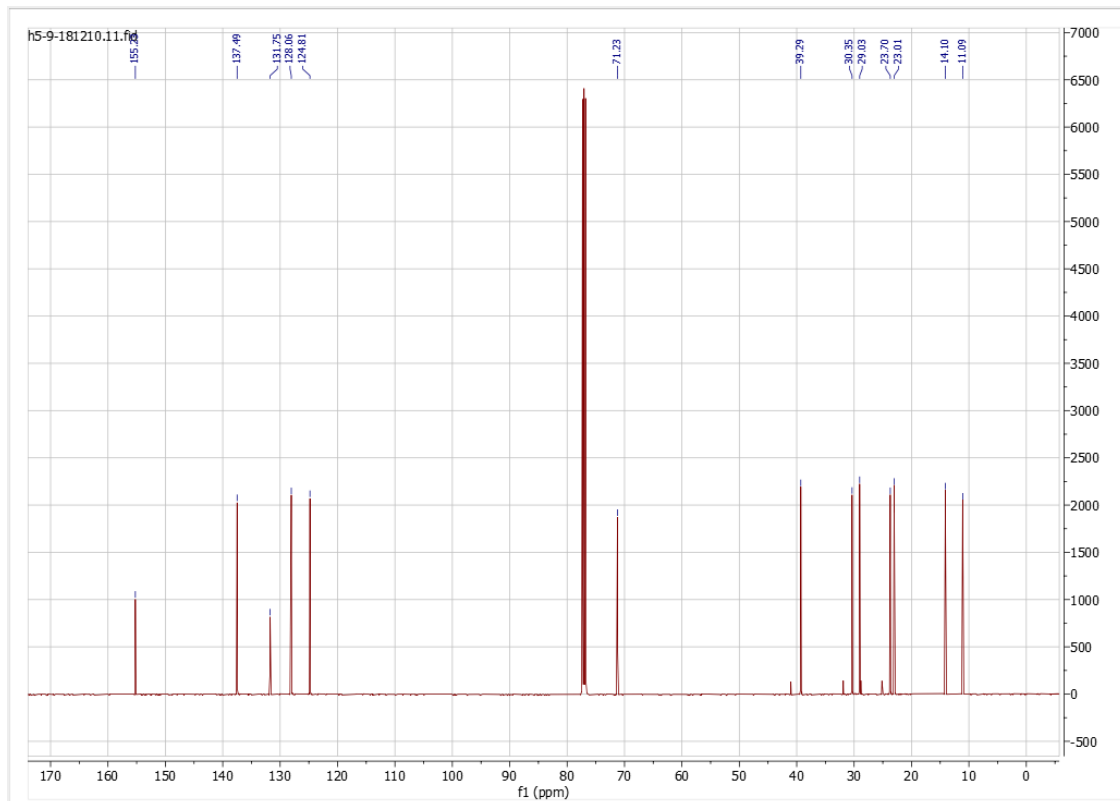
**Compound 10b** Light brown oil (0.4 g, yield 57%).  $^1H$  NMR ( $CDCl_3$ , 500 MHz):  $\delta$  (ppm) 8.62 (t,  $J$  = 1.5 Hz, 2H), 8.57 (d,  $J$  = 1.5 Hz, 4H), 8.42 (d,  $J$  = 2.5 Hz, 4H), 7.86 (d,  $J$  = 8.5 Hz, 4H), 7.30 (dd,  $J_1$  = 2.5 Hz,  $J_2$  = 8.5 Hz, 4H), 3.94 (m, 8H), 1.75 (m, 4H), 1.46 (m, 16H), 1.32 (m, 16H), 0.92 (m, 24H).  $^{13}C$  NMR ( $CDCl_3$ , 125 MHz):  $\delta$  (ppm) 169.2, 155.1, 151.0, 148.6, 140.6, 137.8, 134.8, 126.4, 123.8, 121.7, 121.2, 71.0, 39.4, 30.4, 29.1, 23.8, 23.0, 14.1, 11.1. HR-MS (ESI):  $m/z$   $[M + H]^+$  calcd for  $C_{68}H_{87}N_6O_4S_2$   $[M + H]^+$  1115.6225 found 1115.6168.

**Compound 10c**. Light brown oil (0.15 g, yield 30%).  $^1H$  NMR ( $CDCl_3$ , 500 MHz):  $\delta$  (ppm) 8.62 (t,  $J$  = 1.5 Hz, 2H), 8.57 (d,  $J$  = 1.5 Hz, 4H), 8.42 (d,  $J$  = 2.5 Hz, 4H), 7.86 (d,  $J$  = 8.5 Hz, 4H), 7.30 (dd,  $J_1$  = 2.5 Hz,  $J_2$  = 8.5 Hz, 4H), 3.94 (m, 8H), 1.81 (m, 4H), 1.24 (m, 160H), 0.85 (m, 24H).  $^{13}C$  NMR ( $CDCl_3$ , 125 MHz):  $\delta$  (ppm) 169.3, 155.1, 151.0, 148.6, 140.6, 137.8, 134.9, 126.4, 123.8, 121.7, 121.2, 71.5, 38.0, 31.9, 31.2, 30.0, 29.7, 29.6, 29.4, 26.8, 22.7, 14.1. HR-MS data are not available most likely due to decomposition of the compound during MS experiment.

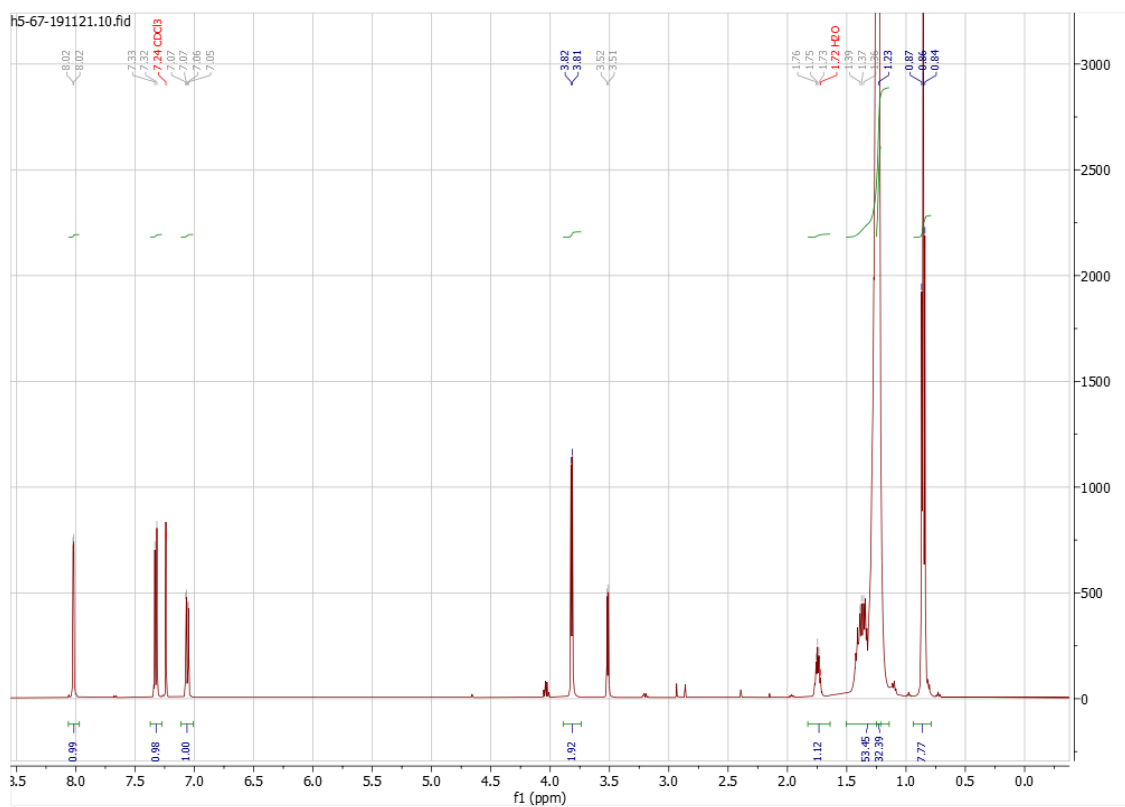
## 2. NMR spectra



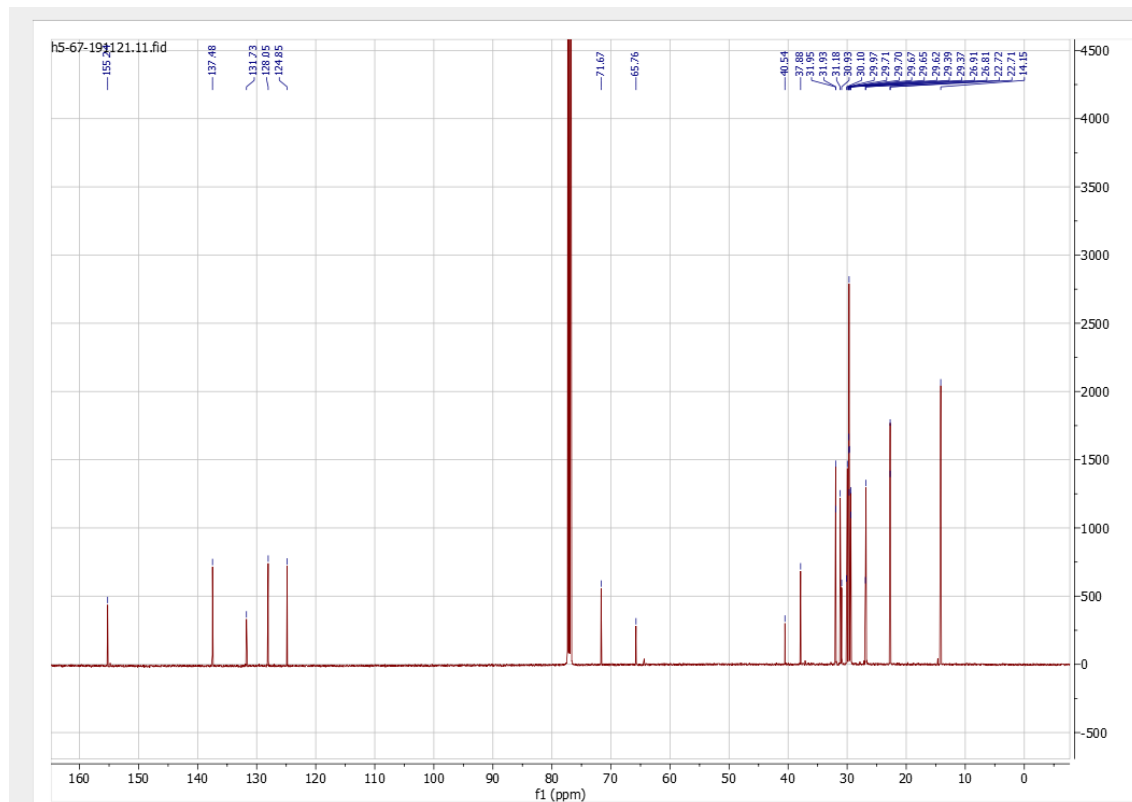
**Figure S1.**  $^1\text{H}$  NMR (500 MHz, 298K) spectrum of compound **1b** in  $\text{CDCl}_3$ .



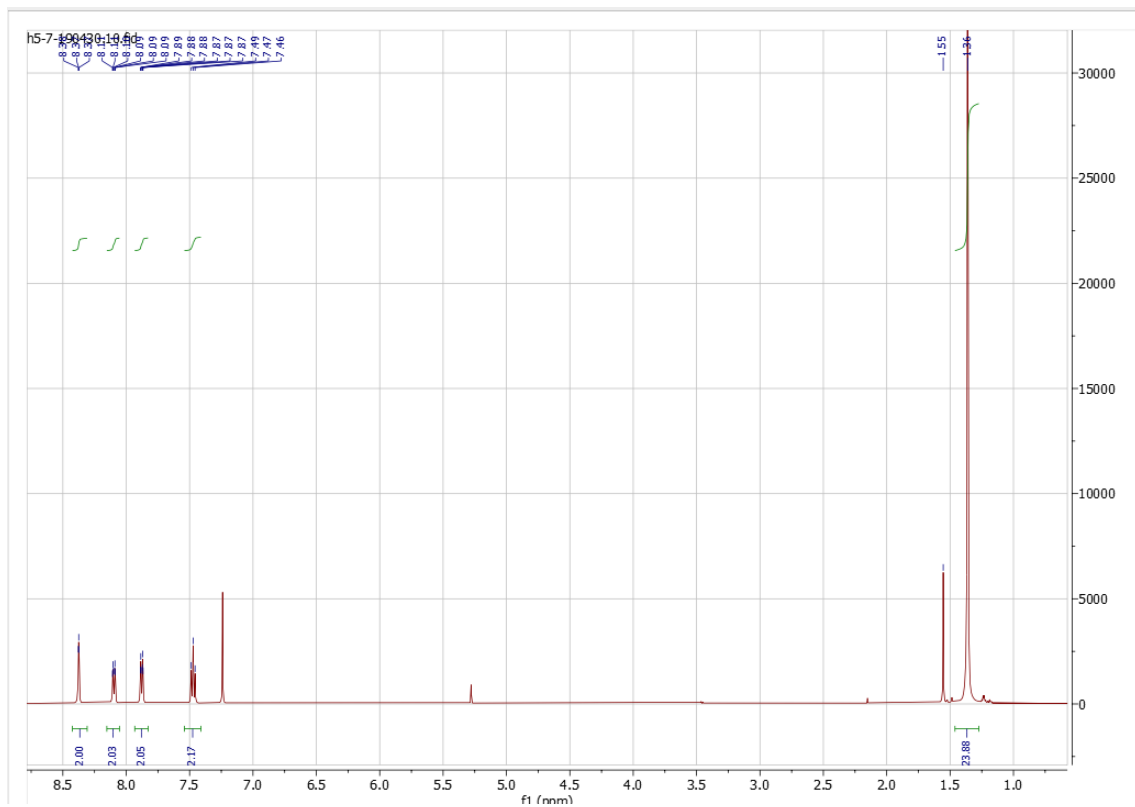
**Figure S2.**  $^{13}\text{C}$  NMR (125 MHz, 298K) spectrum of compound **1b** in  $\text{CDCl}_3$ .



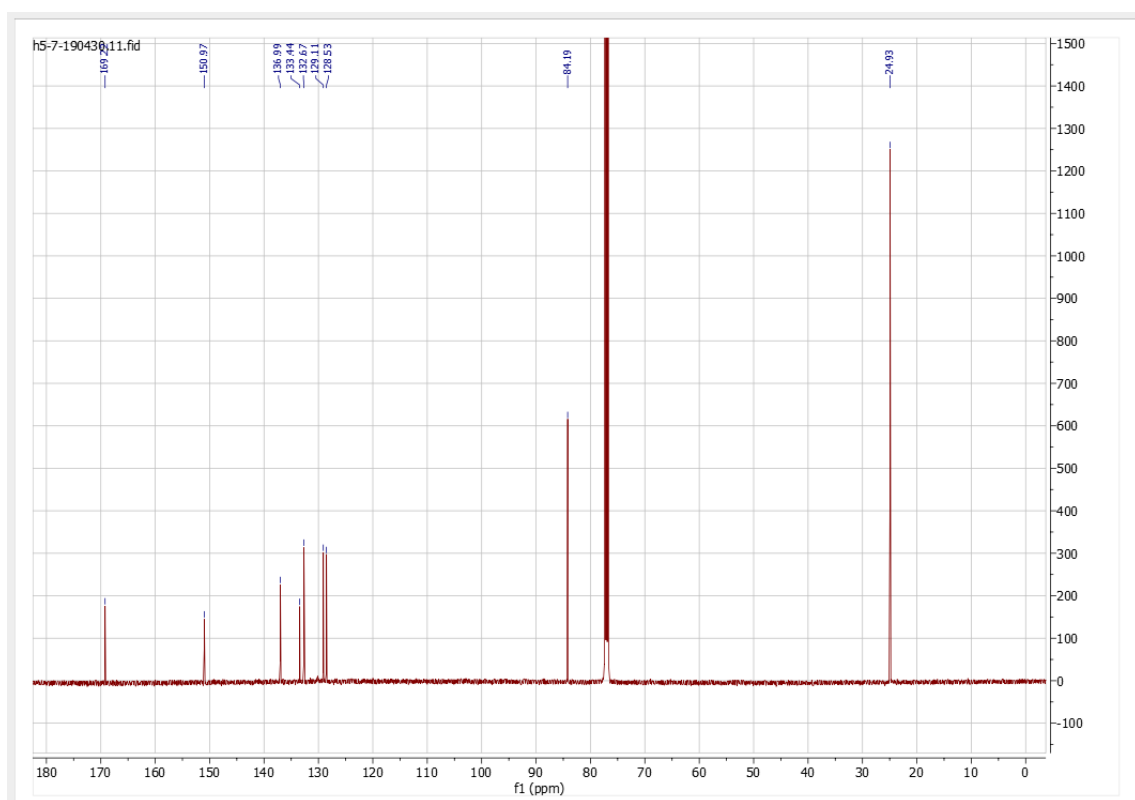
**Figure S3.**  $^1\text{H}$  NMR (500 MHz, 298K) spectrum of compound **1c** in  $\text{CDCl}_3$ .



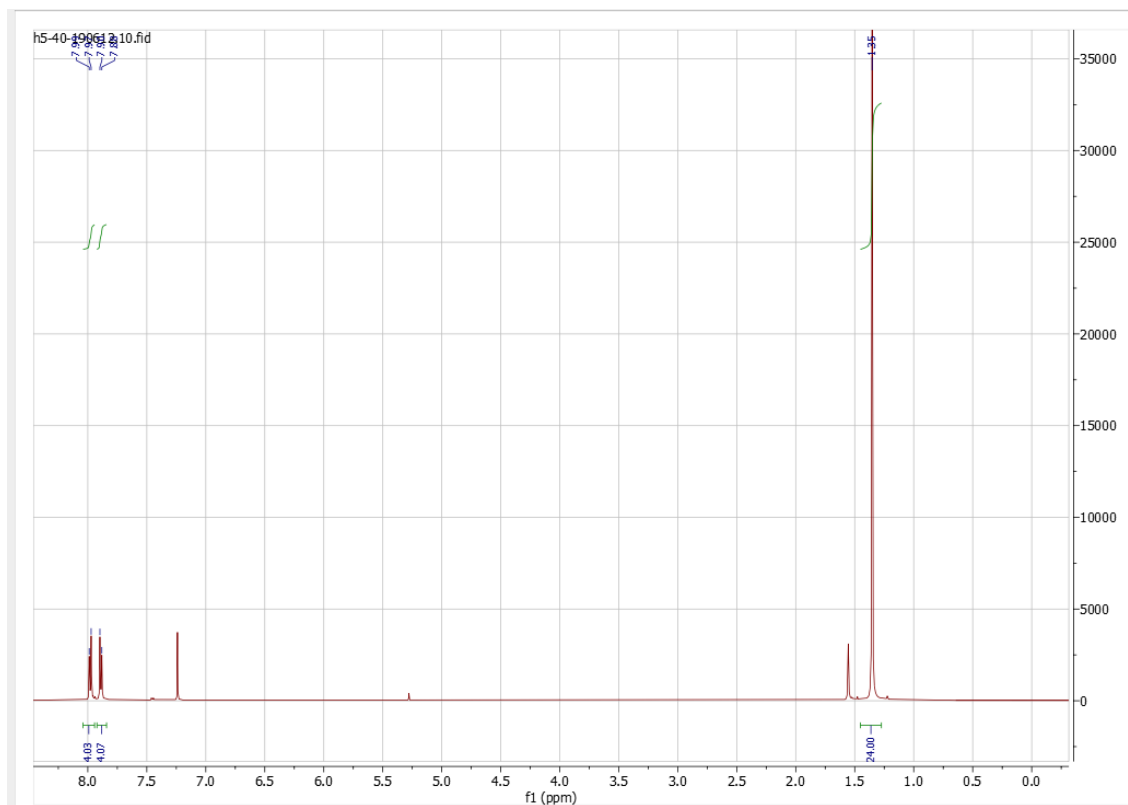
**Figure S4.**  $^{13}\text{C}$  NMR (125 MHz, 298K) spectrum of compound **1b** in  $\text{CDCl}_3$ .



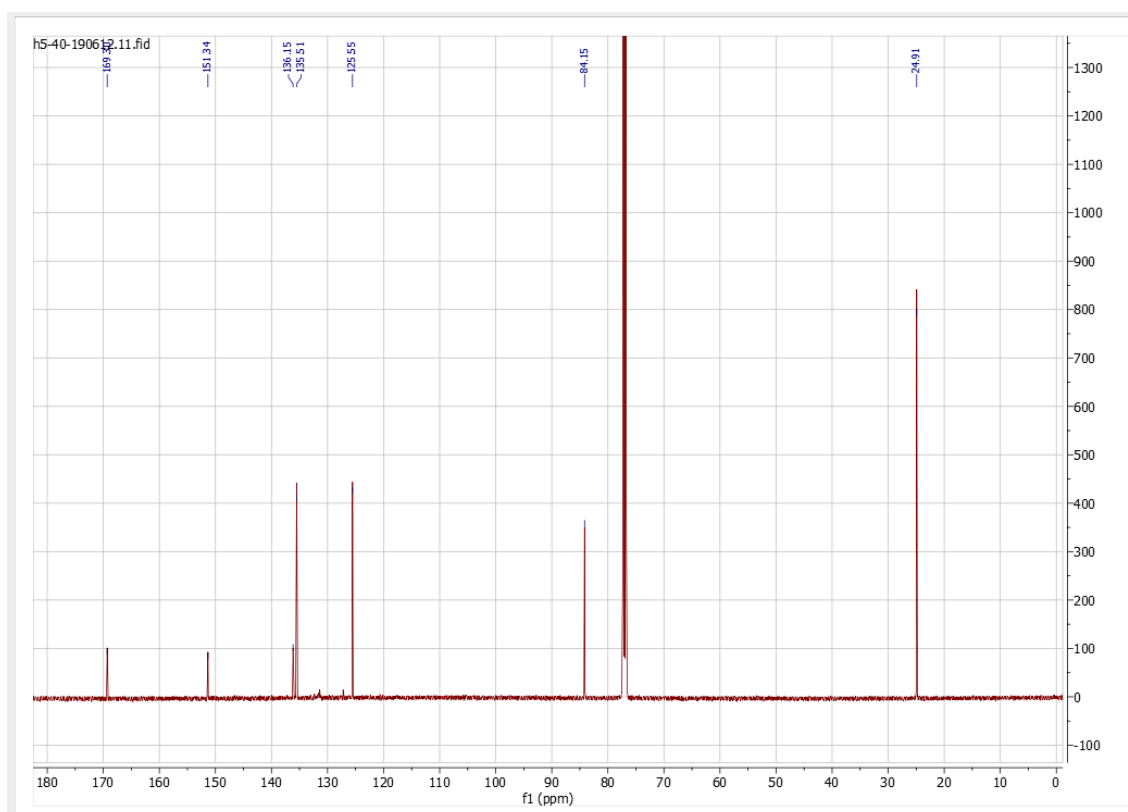
**Figure S5.**  $^1\text{H}$  NMR (500 MHz, 298K) spectrum of compound **5** in  $\text{CDCl}_3$ .



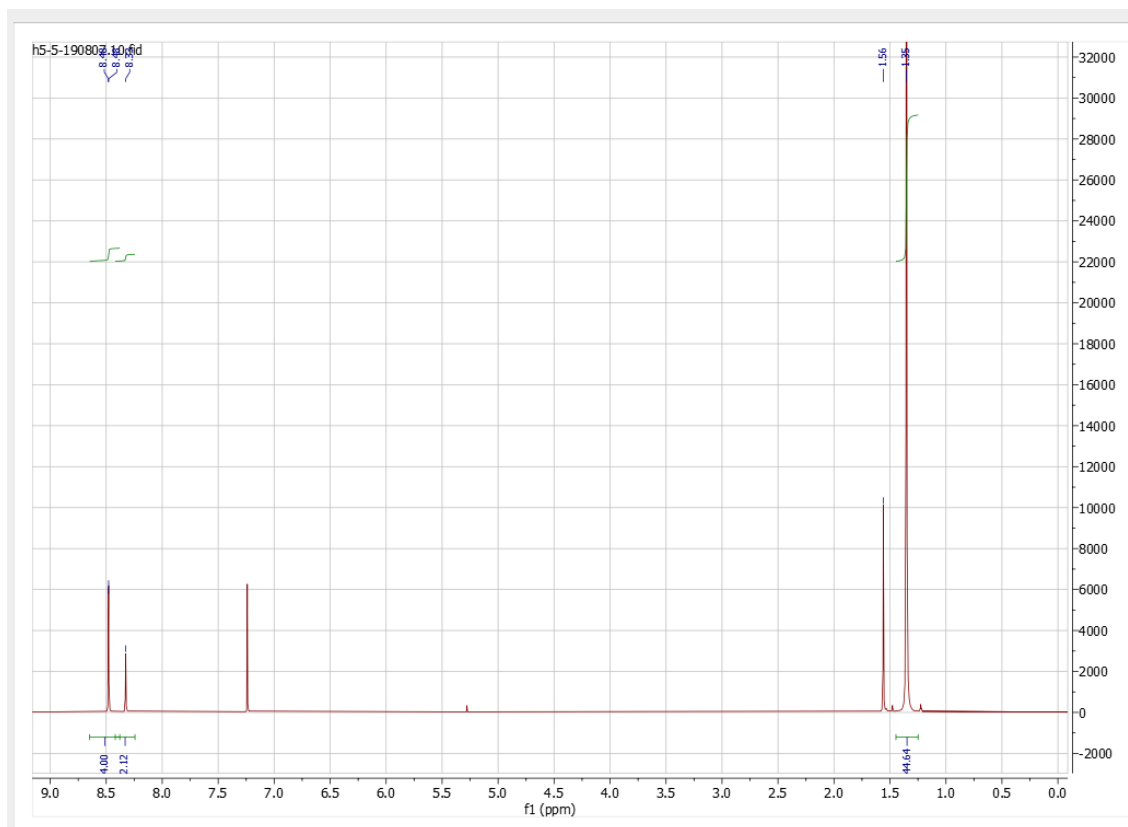
**Figure S6.**  $^{13}\text{C}$  NMR (125 MHz, 298K) spectrum of compound **5** in  $\text{CDCl}_3$ .



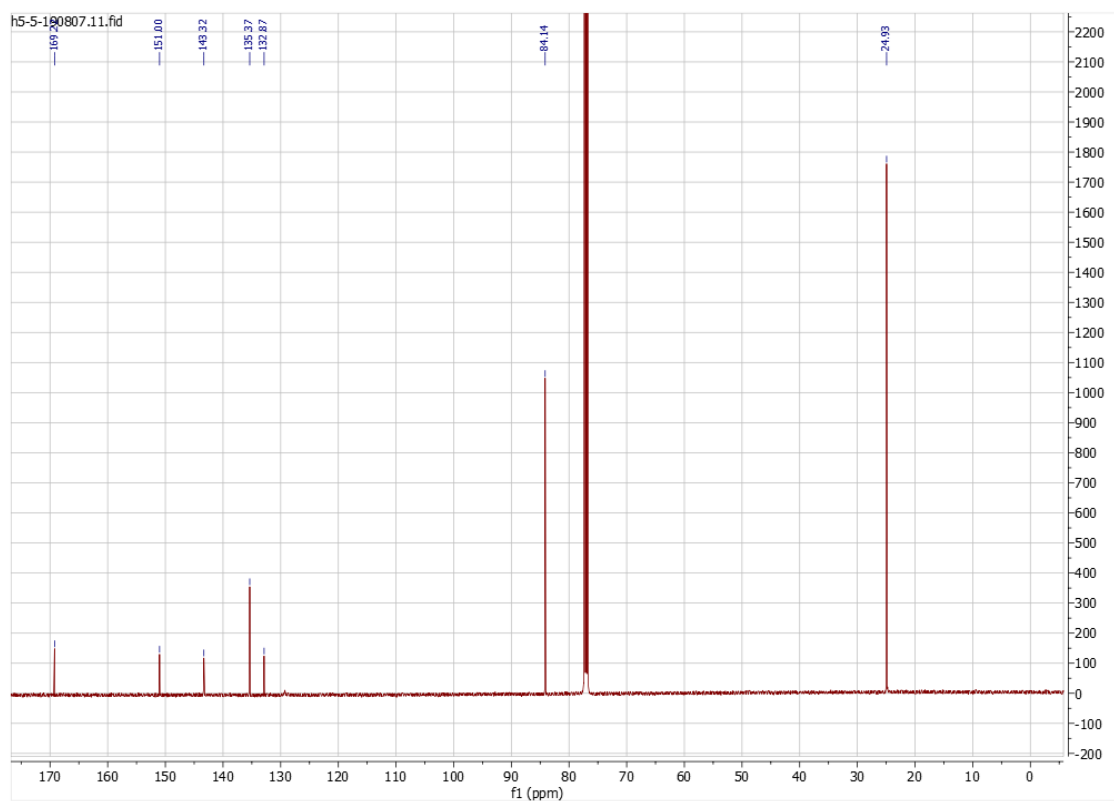
**Figure S7.**  $^1\text{H}$  NMR (500 MHz, 298K) spectrum of compound **6** in  $\text{CDCl}_3$ .



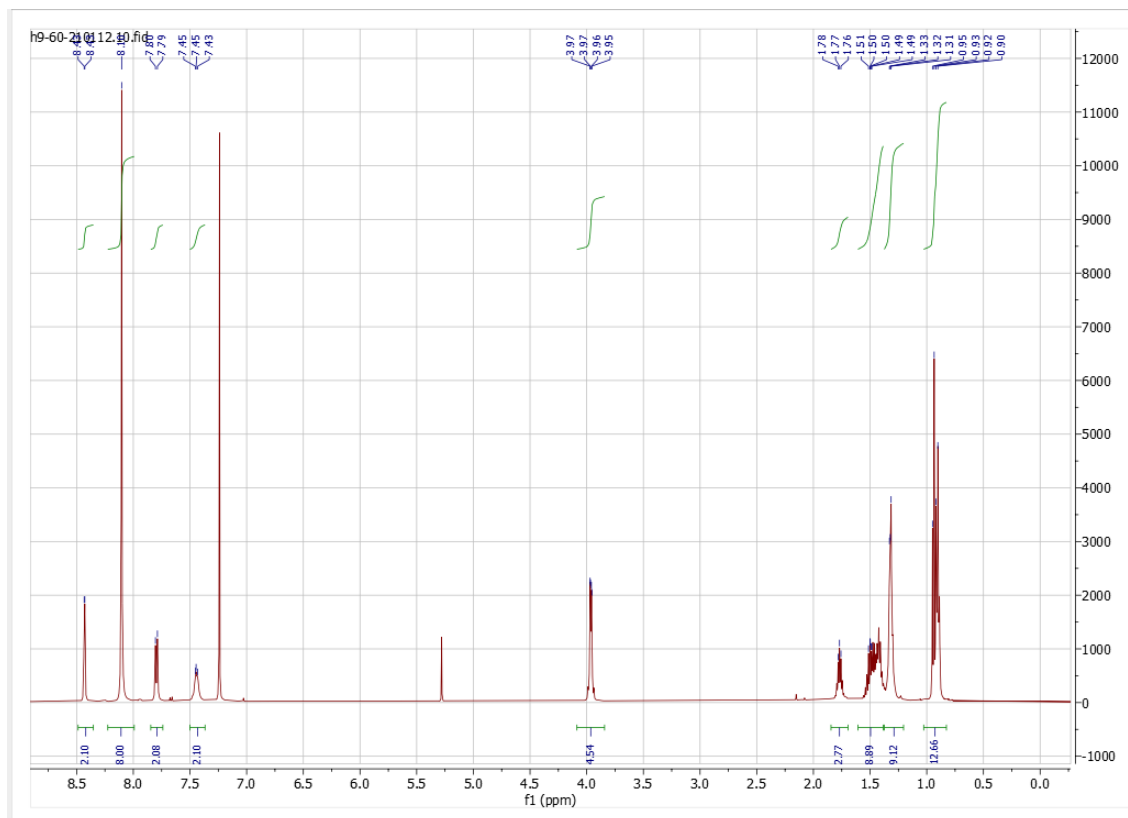
**Figure S8.**  $^{13}\text{C}$  NMR (125 MHz, 298K) spectrum of compound **6** in  $\text{CDCl}_3$ .



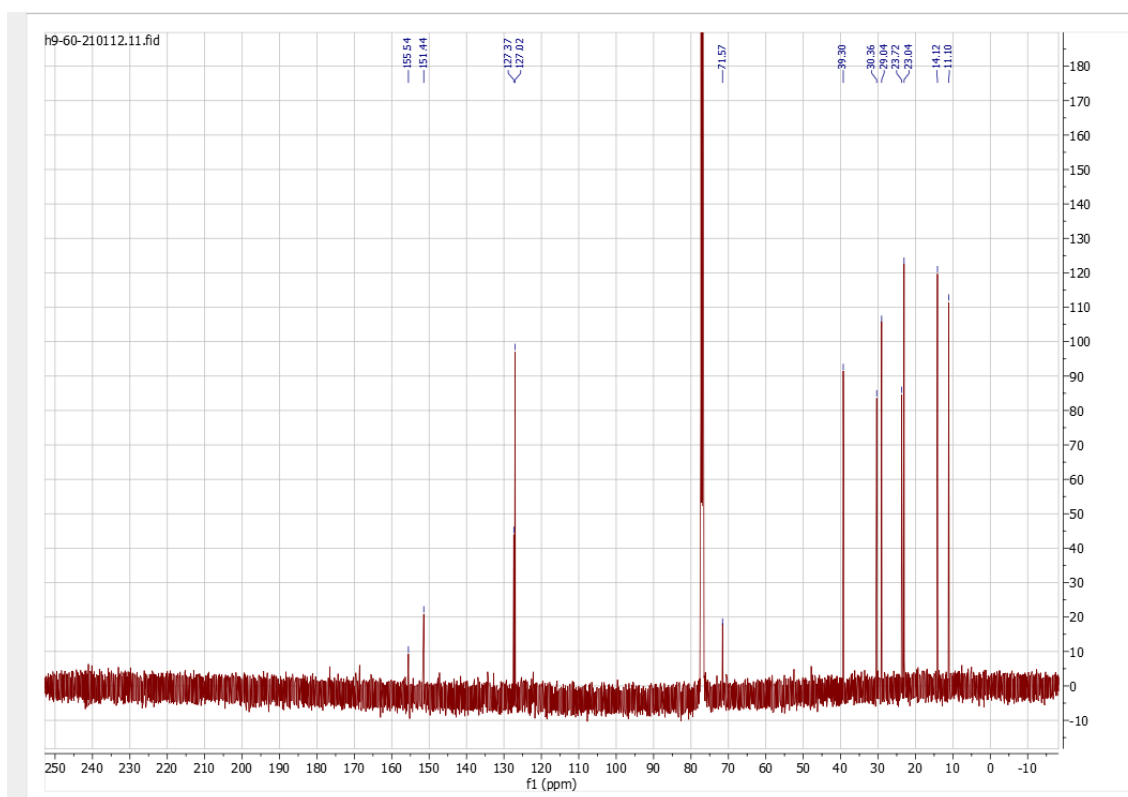
**Figure S9.**  $^1\text{H}$  NMR (500 MHz, 298K) spectrum of compound **7** in  $\text{CDCl}_3$ .



**Figure S10.**  $^{13}\text{C}$  NMR (125 MHz, 298K) spectrum of compound **7** in  $\text{CDCl}_3$ .



**Figure S11.**  $^1\text{H}$  NMR (500 MHz, 298K) spectrum of compound **8b** in  $\text{CDCl}_3$ .



**Figure S12.**  $^{13}\text{C}$  NMR (125 MHz, 298K) spectrum of compound **8b** in  $\text{CDCl}_3$ .



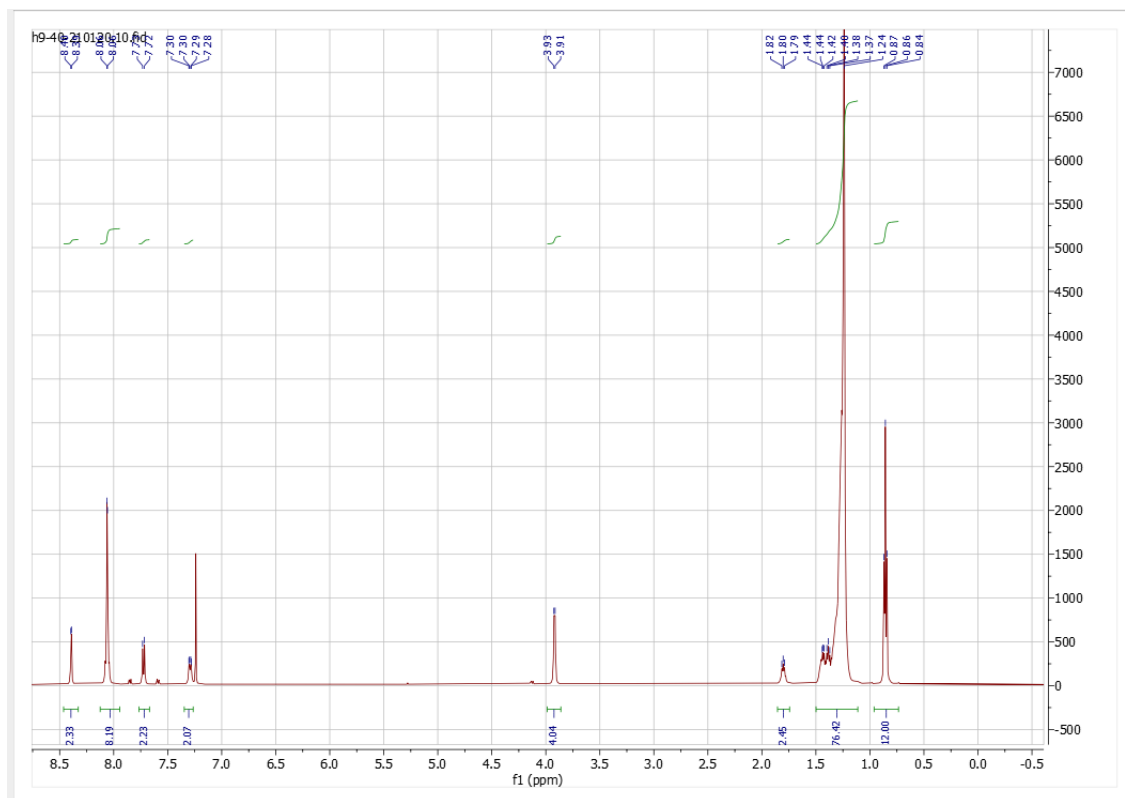


Figure S13.  $^1\text{H}$  NMR (500 MHz, 298K) spectrum of compound **8c** in  $\text{CDCl}_3$ .

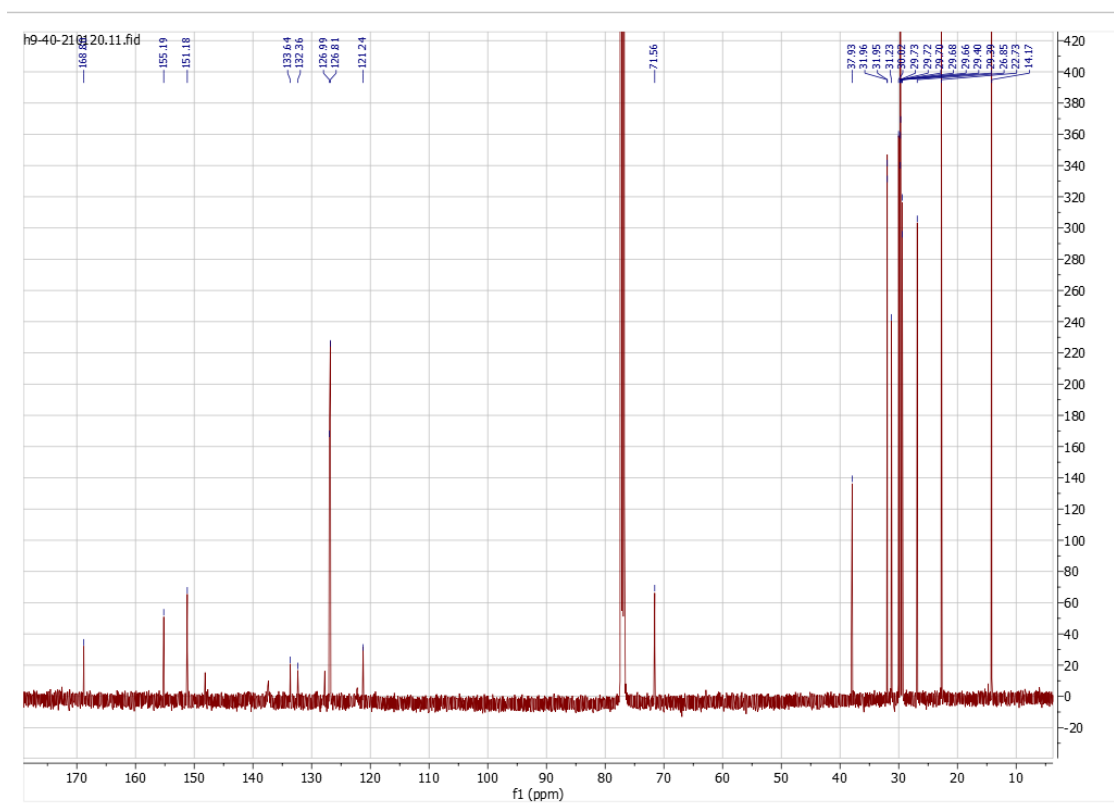
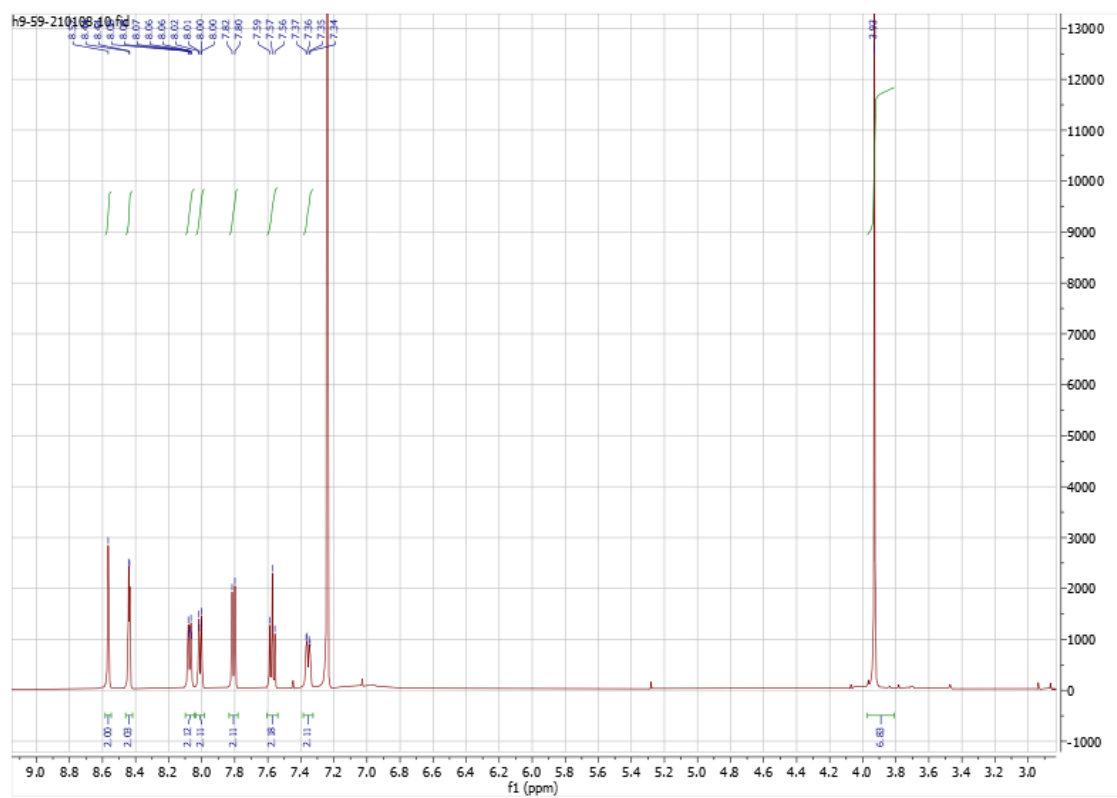
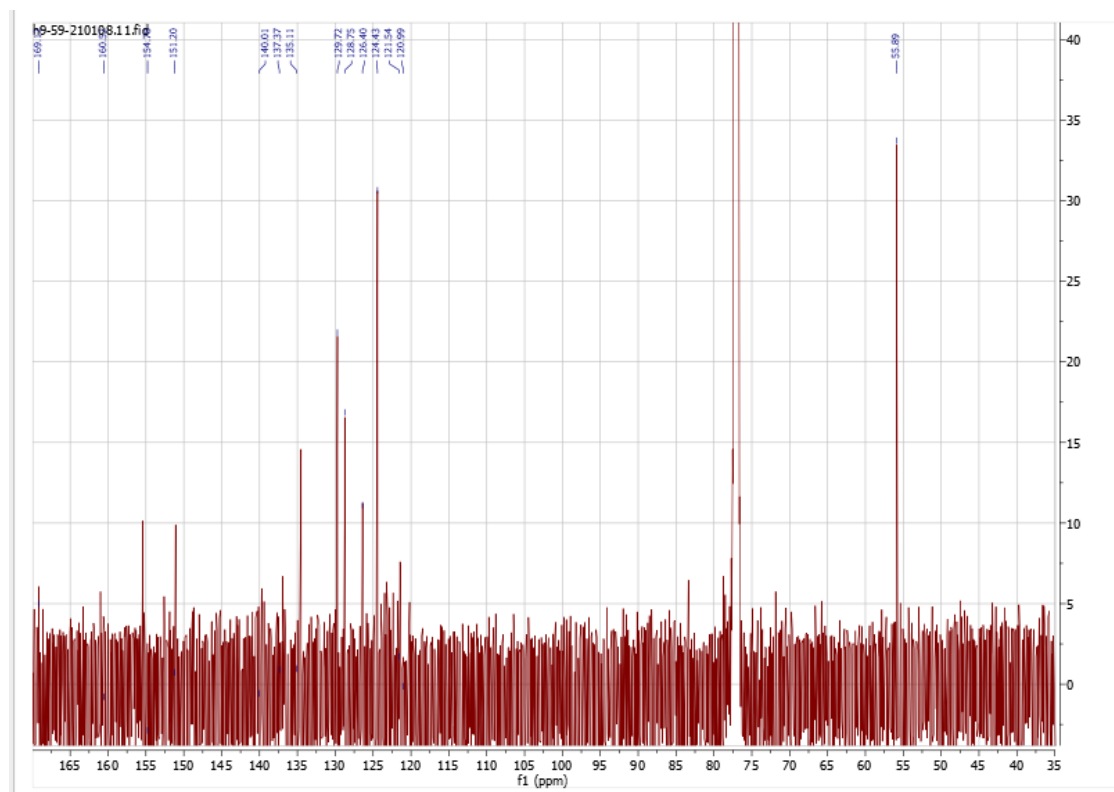


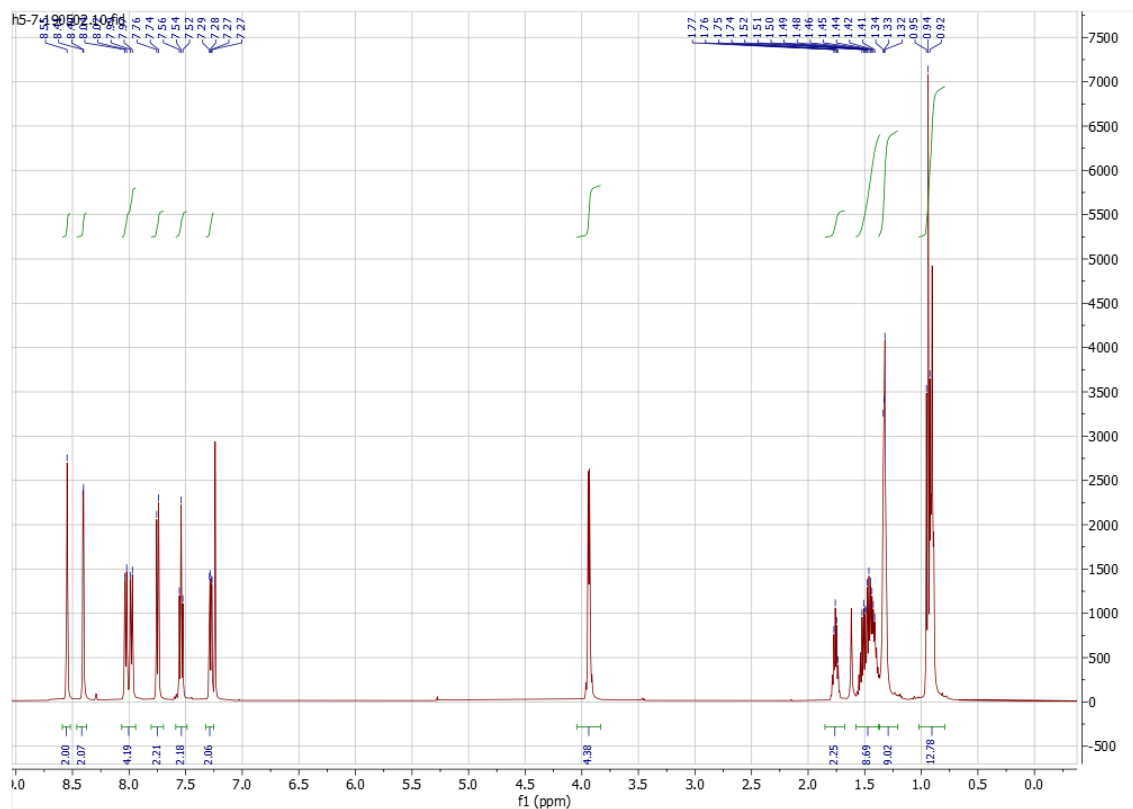
Figure S14.  $^{13}\text{C}$  NMR (125 MHz, 298K) spectrum of compound **8c** in  $\text{CDCl}_3$ .



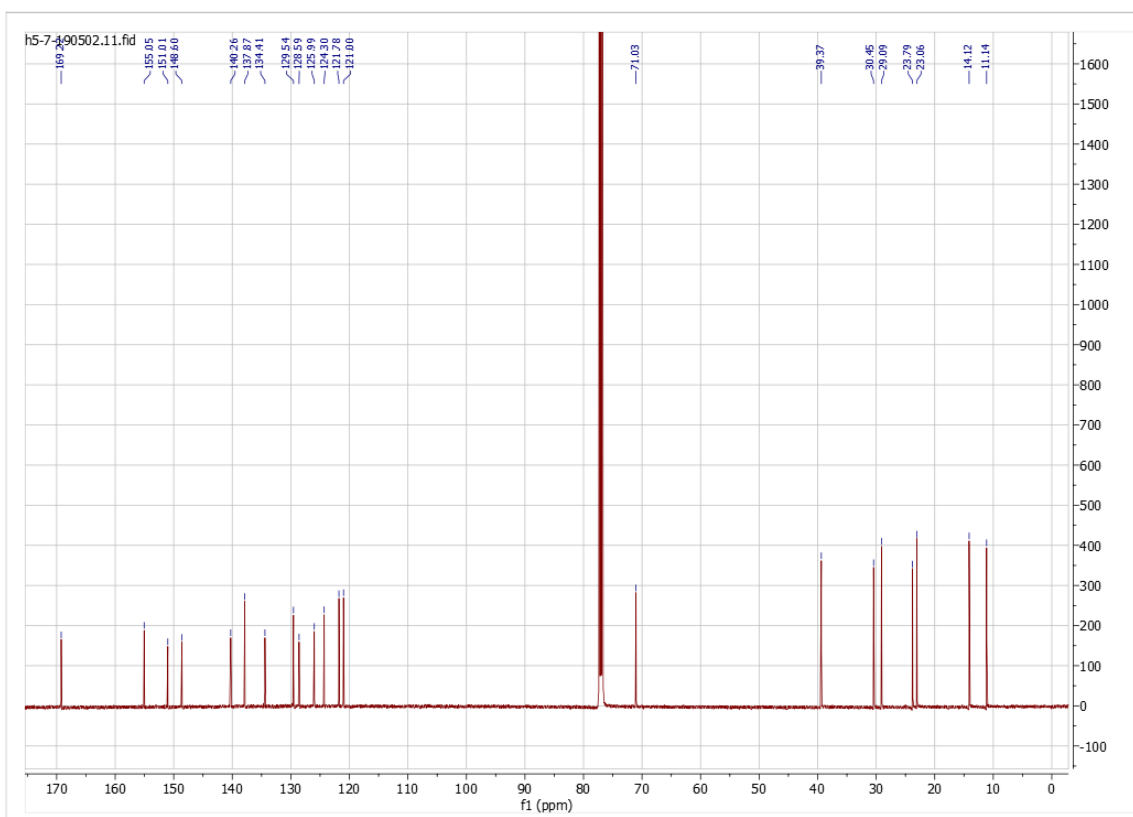
**Figure S15.**  $^1\text{H}$  NMR (500 MHz, 298K) spectrum of compound **9a** in  $\text{CDCl}_3$ .



**Figure S16.**  $^{13}\text{C}$  NMR (125 MHz, 298K) spectrum of compound **9a** in  $\text{CDCl}_3$ .



**Figure S17.**  $^1\text{H}$  NMR (500 MHz, 298K) spectrum of compound **9b** in  $\text{CDCl}_3$ .



**Figure S18.**  $^{13}\text{C}$  NMR (125 MHz, 298K) spectrum of compound **9b** in  $\text{CDCl}_3$ .

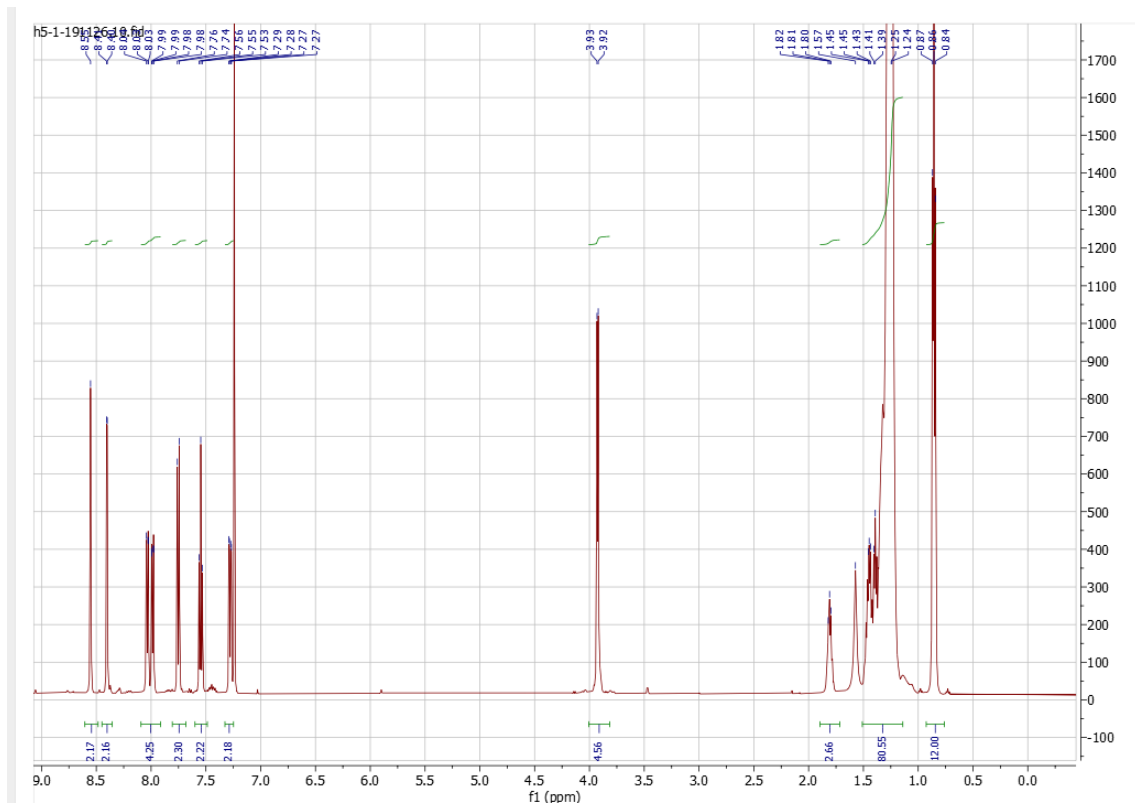


Figure S19.  $^1\text{H}$  NMR (500 MHz, 298K) spectrum of compound **9c** in  $\text{CDCl}_3$ .

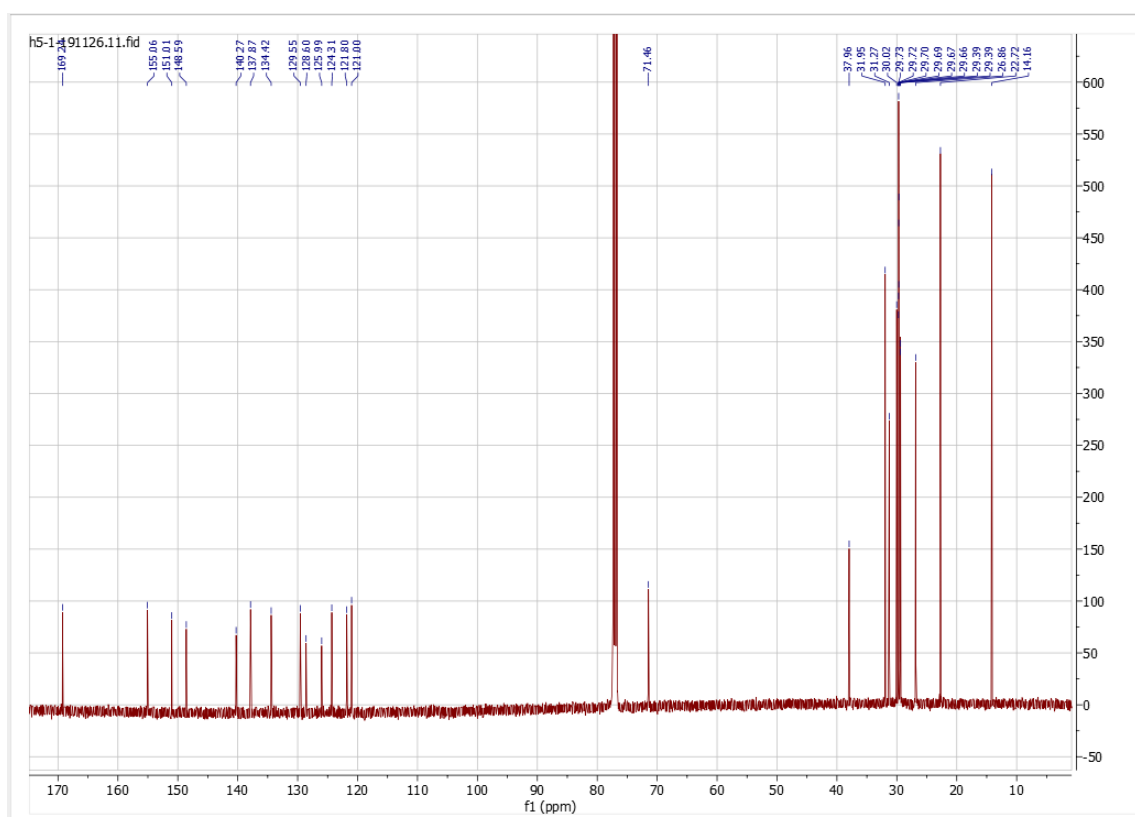


Figure S20.  $^{13}\text{C}$  NMR (125 MHz, 298K) spectrum of compound **9c** in  $\text{CDCl}_3$ .

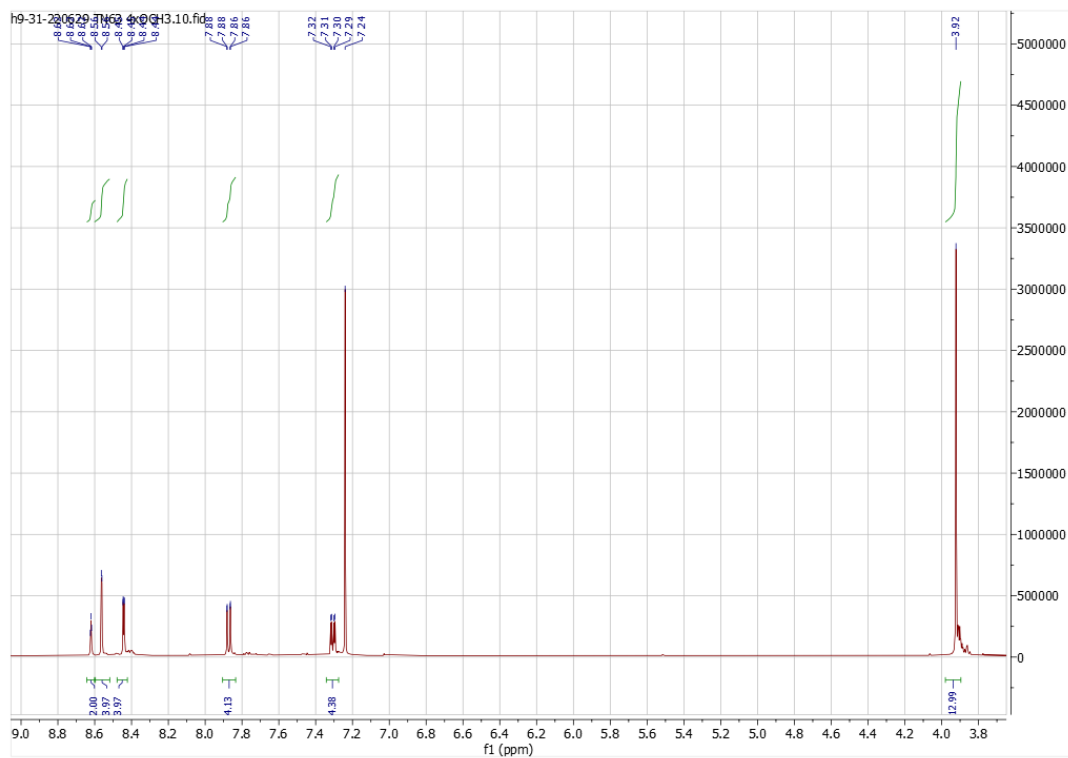


Figure S21.  $^1\text{H}$  NMR (500 MHz, 298K) spectrum of compound **10a** in  $\text{CDCl}_3$ .

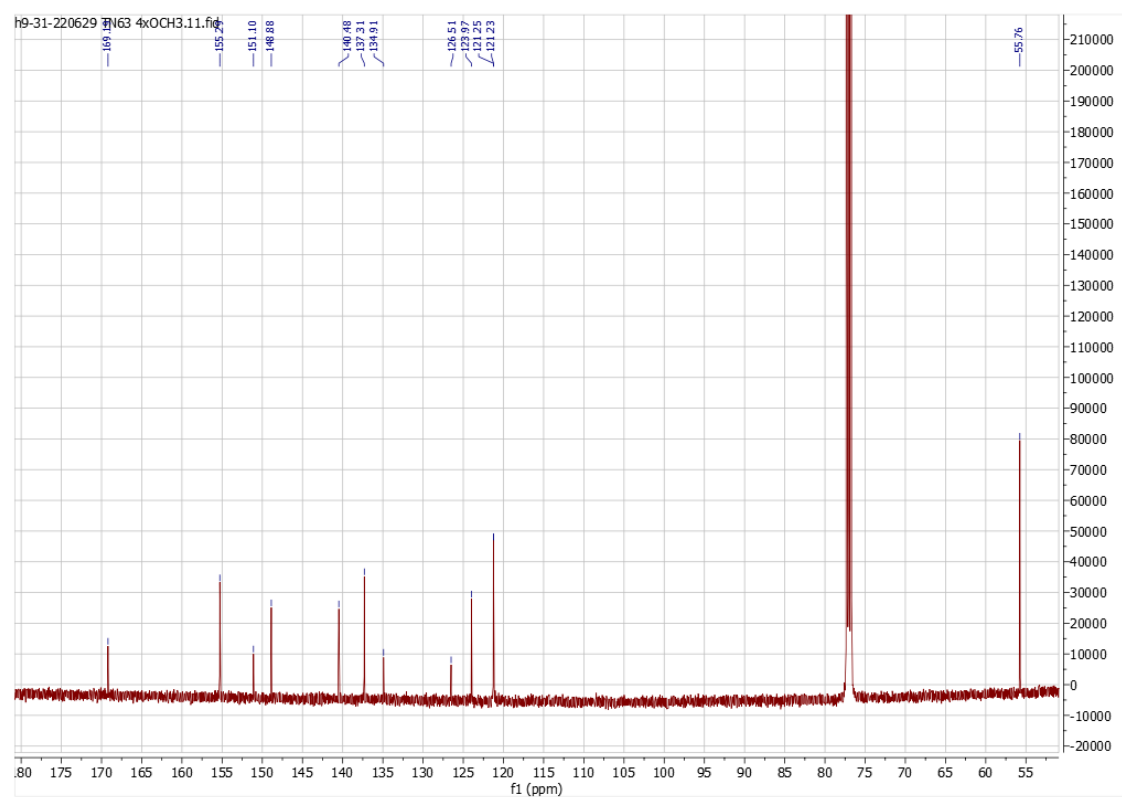


Figure S22.  $^{13}\text{C}$  NMR (125 MHz, 298K) spectrum of compound **10a** in  $\text{CDCl}_3$ .

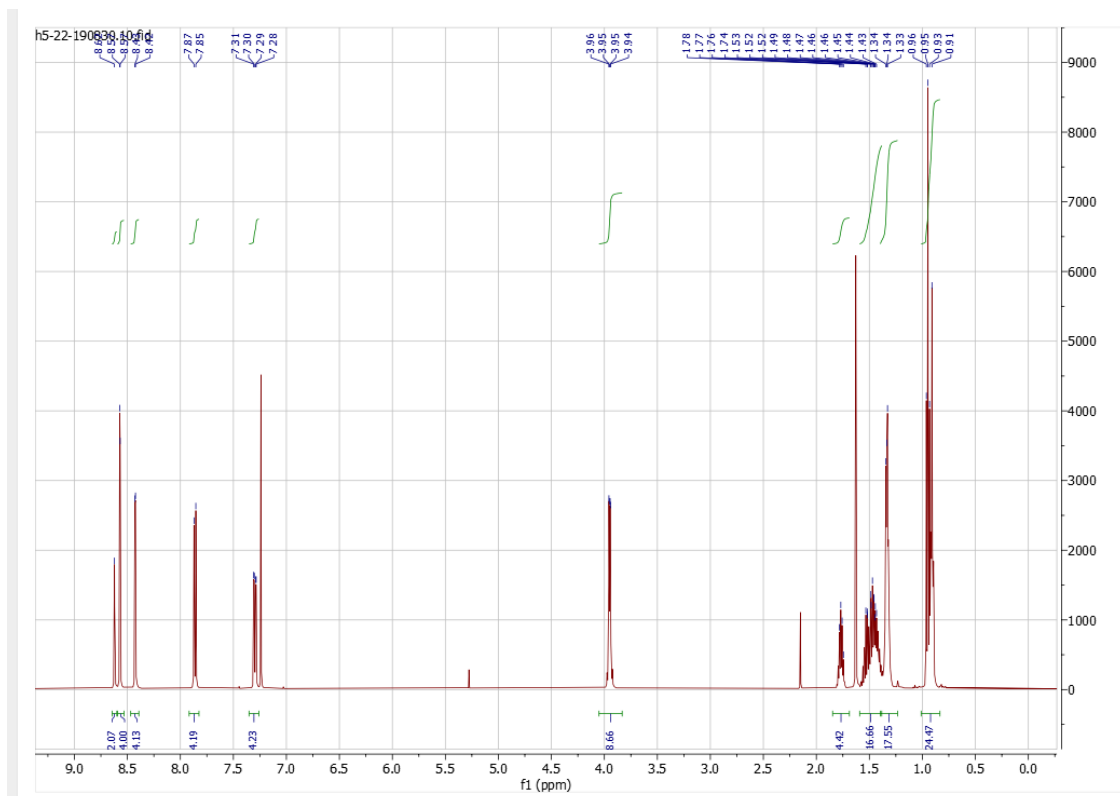


Figure S23.  $^1\text{H}$  NMR (500 MHz, 298K) spectrum of compound **10b** in  $\text{CDCl}_3$ .

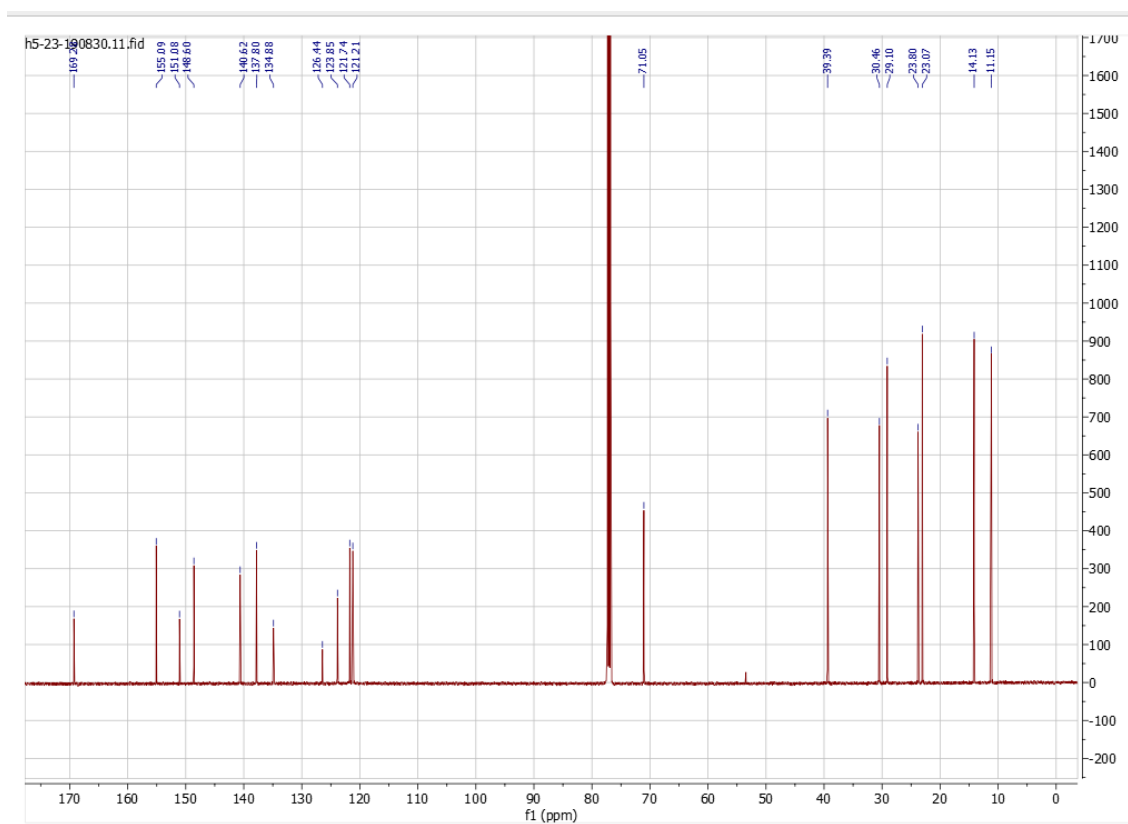


Figure S24.  $^{13}\text{C}$  NMR (125 MHz, 298K) spectrum of compound **10b** in  $\text{CDCl}_3$ .

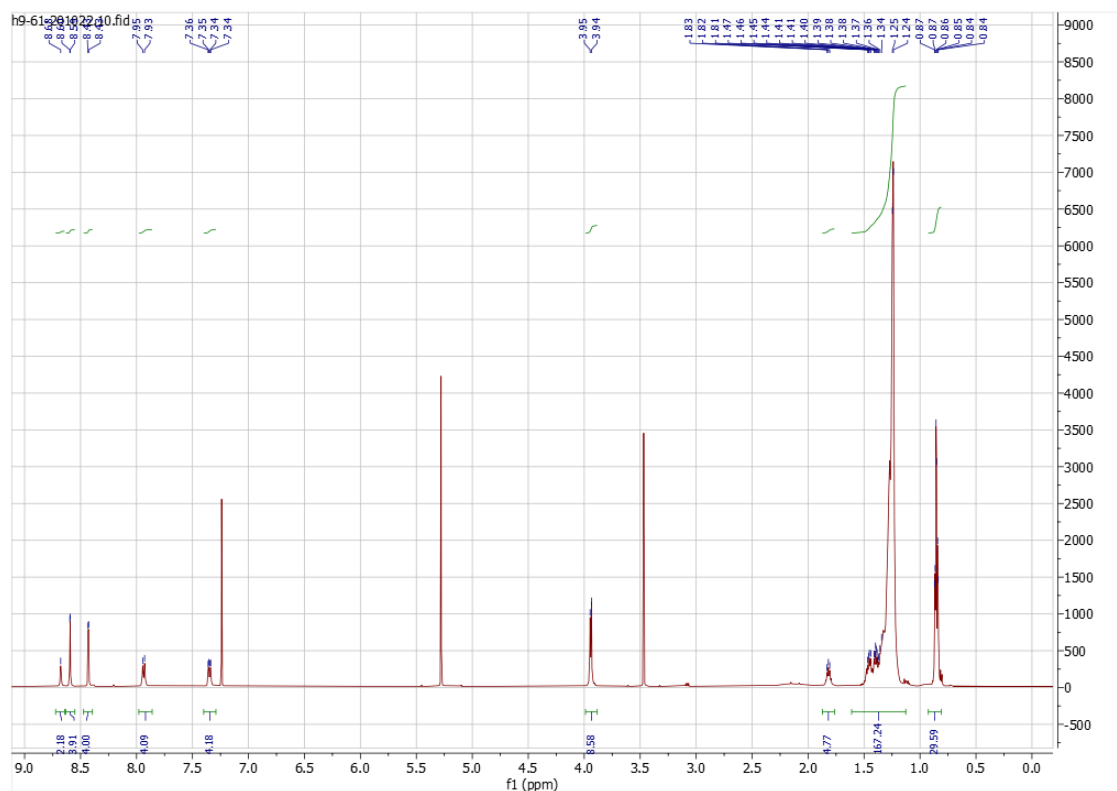


Figure S25.  $^1\text{H}$  NMR (500 MHz, 298K) spectrum of compound **10c** in  $\text{CDCl}_3$ .

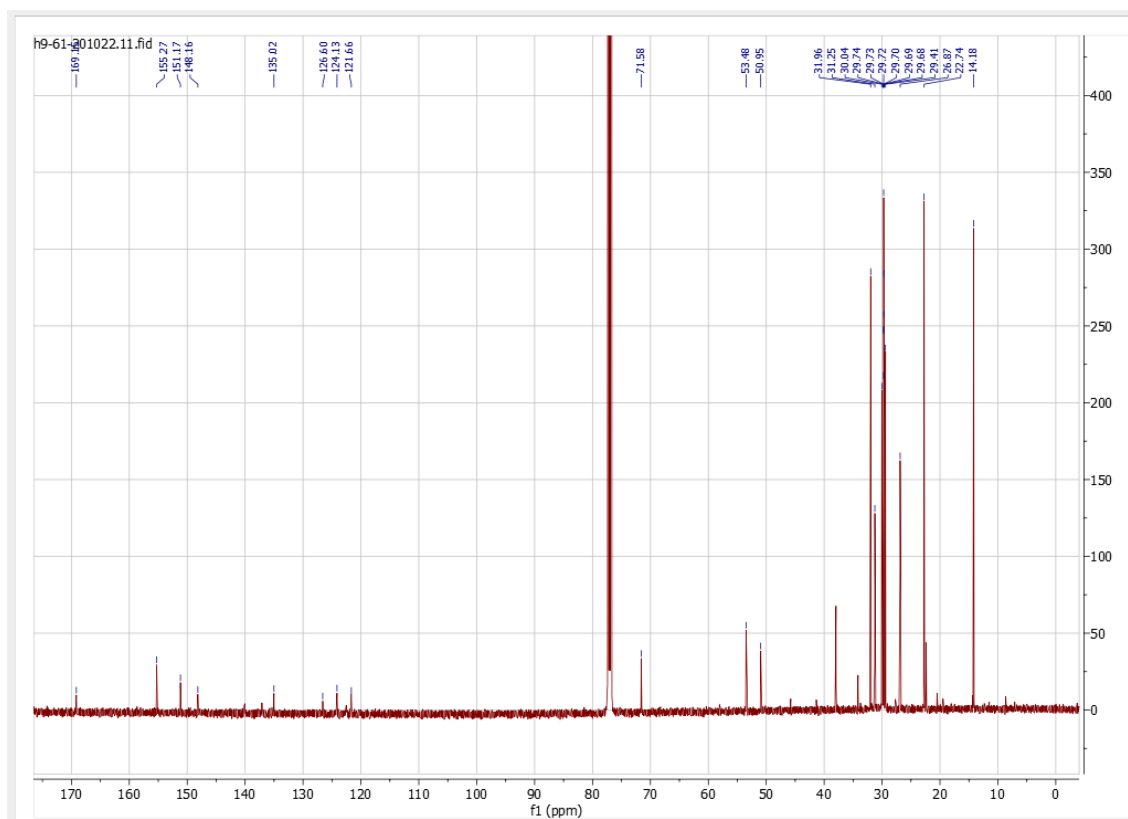
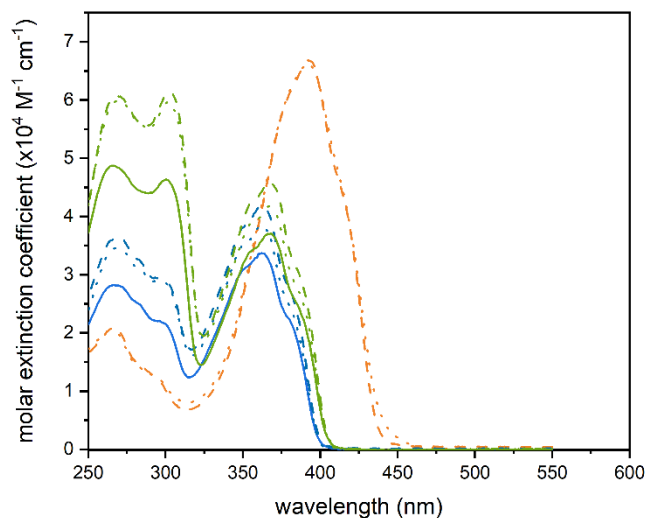
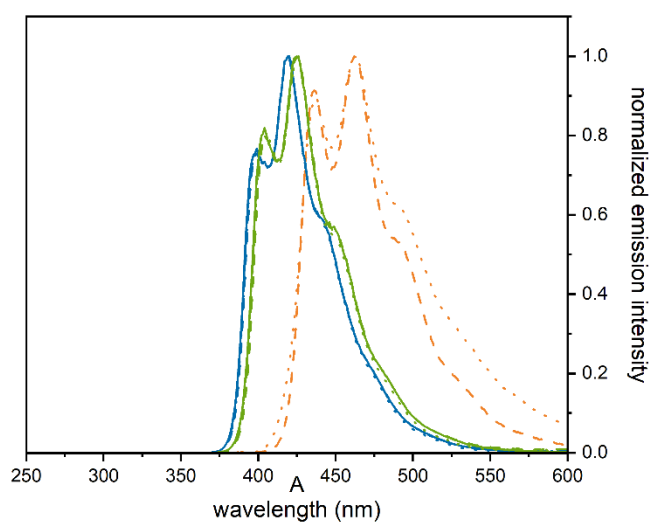


Figure S26.  $^{13}\text{C}$  NMR (125 MHz, 298K) spectrum of compound **10c** in  $\text{CDCl}_3$ .

### 3. Supplementary photophysical data



**Figure S27.** Comparison of the electronic absorption spectra of compound of series **8** (orange traces), **9** (blue traces), and **10** (green traces) in CH<sub>2</sub>Cl<sub>2</sub> at concentration of 5×10<sup>-6</sup>M. Series **a**, **b**, and **c** are displayed as solid, dashed and dotted line, respectively.



**Figure S28.** Comparison of the photoluminescence spectra of compound of series **8** (orange traces), **9** (blue traces), and **10** (green traces) in CH<sub>2</sub>Cl<sub>2</sub> at concentration of 5×10<sup>-6</sup>M. Series **a**, **b**, and **c** are displayed as solid, dashed and dotted line, respectively. Samples were excited upon  $\lambda_{\text{exc}} = 350$  nm.



#### 4. References

- [S1] B. Wang, R. Sun, D. D. Günbaş, H. Zhang, F. C. Grozema, K. Xiao, S. Jin, *Chem. Commun.*, 2015, **51**, 11837-11840.
- [S2] F. J. Rizzuto, T. B. Faust, B. Chan, C. Hua, D. M. D'Alessandro, C. J. Kepert, *Chem. Eur. J.* 2014, 20, 17597 – 17605.
- [S3] A. Dessi, M. Calamante, A. Mordini, L. Zani, M. Taddei, G. Reginato, *RSC Adv.*, **2014**, 4, 1322–1328.