Supporting Information for:

Synthesis and Characterization of Two Unsymmetrical Indenofluorene Analogues: Benzo[5,6]-*s*-indaceno[1,2-*b*]thiophene and Benzo[5,6]-*s*-indaceno[2,1-*b*]thiophene

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Cyclic Voltammetry

General remarks. All electrochemical experiments were conducted in a traditional 3-electrode geometry using a potentiostat. Electrolyte solutions (0.1 M) were prepared from HPLC grade CH_2Cl_2 and anhydrous Bu_4NBF_4, and the solutions were degassed via freeze-pump-thaw (3×) prior to analysis. The working electrode was a glassy carbon electrode (3-mm diameter), with a Pt-coil counter electrode and Ag wire pseudo reference. The ferrocene/ferrocenium (Fc/Fc^+) couple was used as an internal standard following each experiment. Potential values were re-referenced to SCE using a value of 0.46 (V vs. SCE) for the Fc/Fc^+ couple in CH_2Cl_2. When necessary, potentials were re-referenced to NHE using SCE = –0.24 (V vs. NHE). LUMO and HOMO levels were approximated using SCE = –4.68 eV vs. vacuum.[1] Cyclic voltammetry experiments were conducted in an N_2-filled drybox at sweep rates of 50 (reported), 75, 100, 125 and 150 mV s^{-1}. All scan rates show quasi-reversible kinetics with no alteration of peak splitting with scan rate. $E_{1/2}$ values were calculated assuming $E^{o'} \approx E_{1/2} = (E_{anodic} + E_{cathodic})/2$ based on these observations for reversible couples. The $E_{a,c}$ peak splitting of the Fc/Fc^+ couple was similar to that of the analyte (~100 mV). The anodic peak current increases linearly with the square root of the scan rate in the range 50 to 150 mV s^{-1}, indicating a diffusion-controlled process. Analyte concentrations were ca. 1-5 mM.

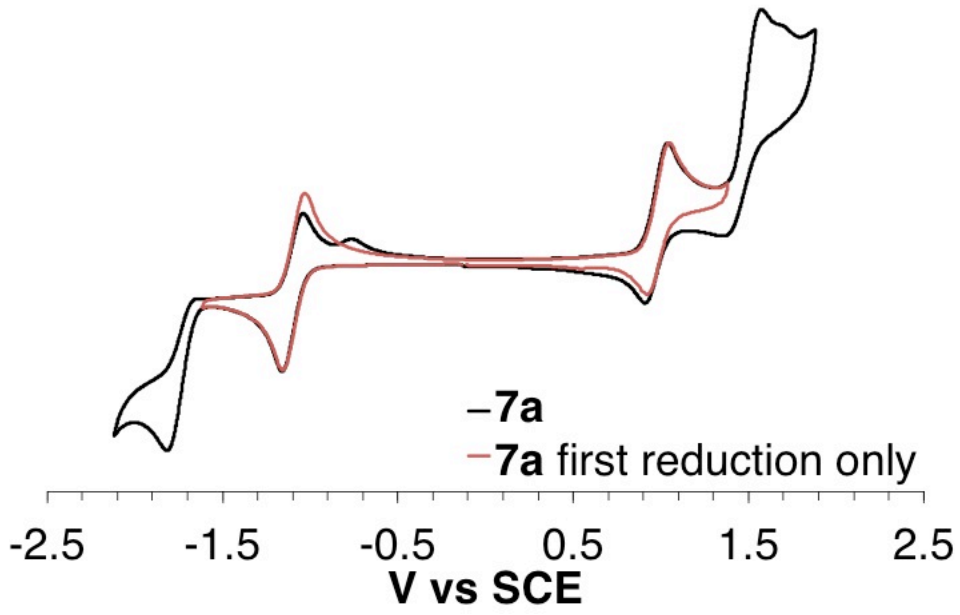


Figure S1. Cyclic voltammogram of *anti*-BIT **7a** showing first reduction only versus first and second reduction.

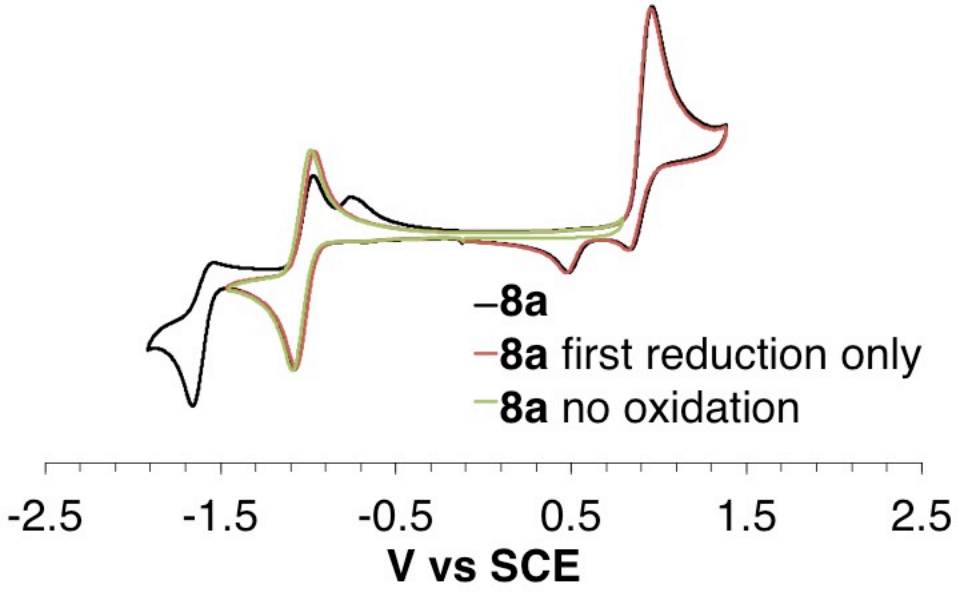


Figure S2. Cyclic voltammogram of *syn*-BIT **8a** showing first reduction only versus first and second reduction.

X-ray Crystallography

General remarks. Diffraction intensities for **7a-b**, **8a-c** and **15** were collected at 223 K (**8b** and **8c**) and 173 K on a diffractometer using MoKα (**7a**) and CuKα radiations (all others), λ= 0.71073 Å and 1.54178 Å, respectively. Space groups were determined based on systematic absences. Absorption corrections were applied by SADABS.[2] Structures were solved by direct methods and Fourier techniques and refined on F^2 using full matrix least-squares procedures. All non-H atoms were refined with anisotropic thermal parameters. All H atoms in **8a** and H atoms in the aromatic parts of **7a** and **7b** were found from the residual density map and refined with isotropic thermal parameters. H atoms in the terminal Me groups in **7a** and **7b** and all H atoms in **8b**, **8c** and **15** were refined in calculated positions in a rigid group model. H atoms in solvent CH_3CN molecules in **8b** were not found and not taken into consideration. One of the H...H contacts between the Me groups in **8b** and **8c** is slightly short, 1.98 Å, showing that the real orientation of these Me groups seems to be slightly different versus the calculated positions of the H atoms. It was found that the molecules of **7a**, **8a** and **15** are disordered in the crystal structures over two centro-symmetrical positions corresponding two opposite orientations; thus, the five-membered S-cycle and six-membered C-cycle share the same positions in the crystal structures in the ratio 1:1. The solvent hexane molecule in **8b** highly disordered over an inversion center was treated by SQUEEZE.[3] Corrections of the X-ray data by SQUEEZE (100 electron per cell) is the same as the required value of 100 electron per cell for two hexane molecules in the full unit cell. The diffraction data for **8b** at the high angles were very weak even when using a strong *Incoatec IμS* Cu source; thus, only reflections up to $2\theta_{max} = 120°$, have been using in the final refinement of **8b**. All calculations were performed by the Bruker SHELXL-2013 package.[4]

Crystallographic Data for **7a**: $C_{36}H_{30}S$, M = 494.66, 0.16 × 0.13 × 0.02 mm, T = 173 K, Monoclinic, space group $P2_1/c$, a = 14.422(3) Å, b = 7.1233(15) Å, c = 13.738(3) Å, β = 109.229(4)°, V = 1332.6(5) Å^3, Z = 2, D_c = 1.233 Mg/m^3, μ(Mo) = 0.145 mm^{-1}, F(000) = 524, $2\theta_{max}$ = 50.0°, 16075 reflections, 2360 independent reflections [R_{int} = 0.0492], R1 = 0.0496, wR2 = 0.1058 and GOF = 1.024 for 2360 reflections (209 parameters) with I>2σ(I), R1 = 0.0842, wR2 = 0.1202 and GOF = 1.024 for all reflections, max/min residual electron density +0.217/–0.213 eÅ^3.

Crystallographic Data for **7b**: $C_{40}H_{38}S$, M = 550.76, 0.19 × 0.09 × 0.03 mm, T = 173 K, Monoclinic, space group $P2_1/n$, a = 17.8322(5) Å, b = 8.1594(2) Å, c = 21.3798(6) Å, β =

98.114(2)°, V = 3079.62(14) Å^3, Z = 4, D_c = 1.188 Mg/m^3, μ(Cu) = 1.116 mm^{-1}, F(000) = 1176, $2\theta_{max}$ = 133.3°, 23074 reflections, 5437 independent reflections [R_{int} = 0.0372], R1 = 0.0484, wR2 = 0.1303 and GOF = 1.035 for 5437 reflections (438 parameters) with I>2σ(I), R1 = 0.0626, wR2 = 0.1404 and GOF = 1.035 for all reflections, max/min residual electron density +0.377/–0.316 eÅ^3.

Crystallographic Data for **8a**: $C_{36}H_{30}S$, M = 494.66, 0.13 × 0.10 × 0.02 mm, T = 173 K, Monoclinic, space group $P2_1/c$, a = 14.4257(4) Å, b = 7.1547(2) Å, c = 13.5478(5) Å, β = 108.148(2)°, V = 1328.73(7) Å^3, Z = 2, D_c = 1.236 Mg/m^3, μ(Cu) = 1.238 mm^{-1}, F(000) = 524, $2\theta_{max}$ = 133.1°, 7749 reflections, 2336 independent reflections [R_{int} = 0.0264], R1 = 0.0427, wR2 = 0.1132 and GOF = 1.033 for 2336 reflections (245 parameters) with I>2σ(I), R1 = 0.0507, wR2 = 0.1202 and GOF = 1.033 for all reflections, max/min residual electron density +0.241/–0.160 eÅ^3.

Crystallographic Data for **8b**: $C_{47}H_{46}NS$, $C_{45}H_{43}S$ (CH_3CN), M = 656.91, 0.15 × 0.11 × 0.01 mm, T = 223 K, Monoclinic, space group $P2_1/c$, a = 7.9020(8) Å, b = 26.050(2) Å, c = 36.307(3) Å, β = 92.155(7)°, V = 7468.2(12) Å^3, Z = 8, Z'=2, D_c = 1.168 Mg/m^3, μ(Cu) = 1.007 mm^{-1}, F(000) = 2808, $2\theta_{max}$ = 120.0°, 44858 reflections, 11013 independent reflections [R_{int} = 0.0831], R1 = 0.0909, wR2 = 0.2383 and GOF = 1.030 for 11013 reflections (883 parameters) with I>2σ(I), R1 = 0.1436, wR2 = 0.2823 and GOF = 1.030 for all reflections, max/min residual electron density +0.369/–0.378 eÅ^3.

Crystallographic Data for **8c**: $C_{78}H_{72}S_2$, $C_{75}H_{65}S_2$ 0.5(C_6H_{14}), M = 1073.47, 0.13 × 0.10 × 0.01 mm, T = 223 K, Monoclinic, space group $P2_1/c$, a = 12.4687(11) Å, b = 8.0770(8) Å, c = 30.391(7) Å, β = 98.391(7)°, V = 3039.9(5) Å^3, Z = 2, D_c = 1.173 Mg/m^3, μ(Cu) = 1.118 mm^{-1}, F(000) = 1144, $2\theta_{max}$ = 133.7°, 20006 reflections, 5361 independent reflections [R_{int} = 0.0419], R1 = 0.0586, wR2 = 0.1677 and GOF = 1.035 for 5361 reflections (334 parameters) with I>2σ(I), R1 = 0.0796, wR2 = 0.1791 and GOF = 1.035 for all reflections, max/min residual electron density +0.339/–0.276 eÅ^3.

Crystallographic Data for **15**: $C_{18}H_8O_2S$, M = 288.30, 0.19 × 0.02 × 0.01 mm, T = 173 K, Monoclinic, space group $P2_1/c$, a = 10.6449(9) Å, b = 3.7919(3) Å, c = 15.6497(14) Å, β = 101.161(6)°, V = 619.74(9) Å^3, Z = 2, D_c = 1.545 Mg/m^3, μ(Cu) = 2.324 mm^{-1}, F(000) = 296, $2\theta_{max}$ = 133.2°, 6103 reflections, 1088 independent reflections [R_{int} = 0.0415], R1 = 0.0504, wR2 = 0.1175 and GOF = 1.037 for 1088 reflections (109 parameters) with I>2σ(I), R1 = 0.0633,

wR2 = 0.1242 and GOF = 1.037 for all reflections, max/min residual electron density +0.191/ –0.192 eÅ^3.

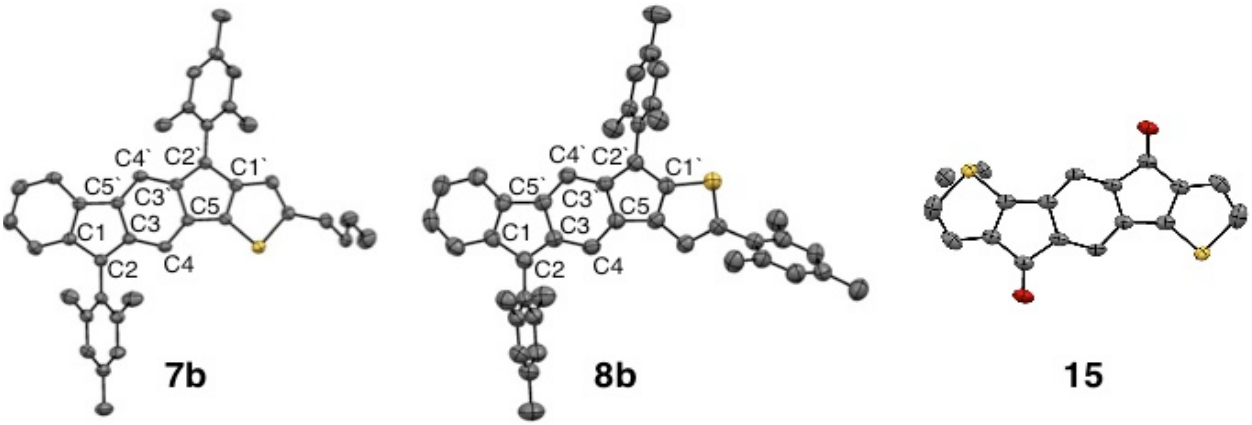
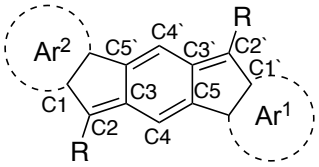


Figure S3. ORTEPs of compounds **7b**, **8b** and **15** with bond numbering scheme; ellipsoids at 50%.

Table S1. Select bond lengths (Å) for compounds **7b**, **8b**, and **8c**



	anti/*syn*-BIT			IF, *anti*/*syn*-IDT[b]		
bond[a]	**7b**	**8b**[a]	**8c**	**1b (mes)**	**2a**	**3a**
C1–C2	1.466(3)	1.481(8)/1.450(7)	1.4648	1.471(3)	1.460(2)	1.447(3)
C2–C3	1.379(3)	1.392(7)/1.368(7)	1.3888	1.380(2)	1.388(2)	1.398(3)
C3–C4	1.429(3)	1.438(7)/1.425(7)	1.4301	1.433(3)	1.431(2)	1.418(3)
C4–C5	1.360(3)	1.357(7)/1.361(6)	1.3616	1.356(2)	1.360(2)	1.363(3)
C5–C3`	1.470(3)	1.457(8)/1.476(7)	1.4649	1.467(3)	1.469(2)	1.456(3)
C3–C5`	1.459(3)	1.446(8)/1.460(7)	1.4527	1.467(3)	1.469(2)	1.456(3)
C1`–C2`	1.466(3)	1.456(7)/1.451(7)	1.4341	1.471(3)	1.460(2)	1.447(3)
C2`–C3`	1.387(3)	1.394(7)/1.383(7)	1.3913	1.380(2)	1.388(2)	1.398(3)
C3`–C4`	1.434(3)	1.442(7)/1.429(7)	1.4190	1.433(3)	1.431(2)	1.418(3)
C4`–C5`	1.363(3)	1.372(7)/1.367(7)	1.3679	1.356(2)	1.360(2)	1.363(3)

[a] Compound **8b** contained two crystallographically independent molecules per unit cell.

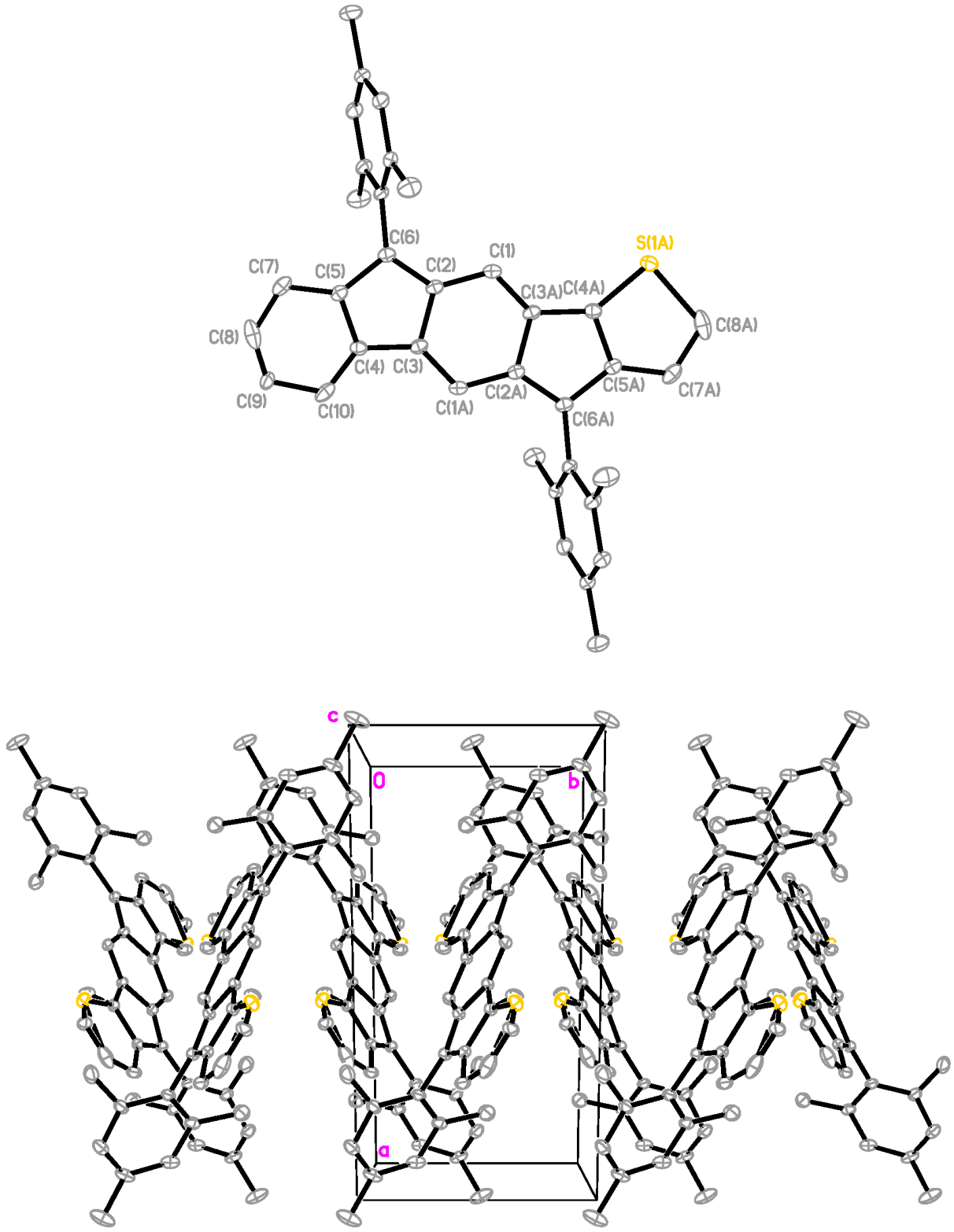


Figure S4. ORTEP and molecular packing of **7a** (generated from CIF mh143); ellipsoids at 30%.

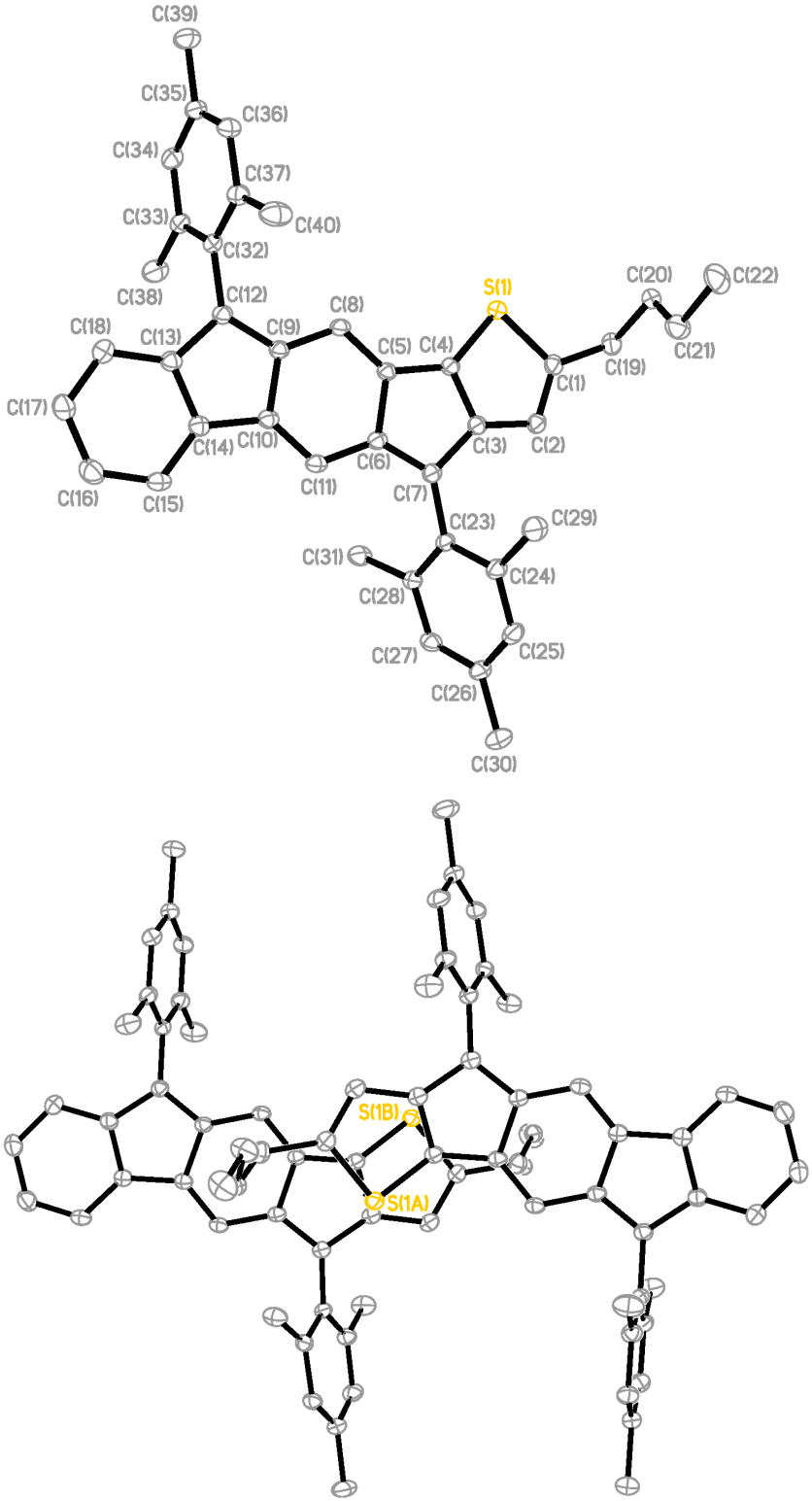


Figure S5. ORTEP and packing of **7b** (generated from CIF mh141); ellipsoids at 30%.

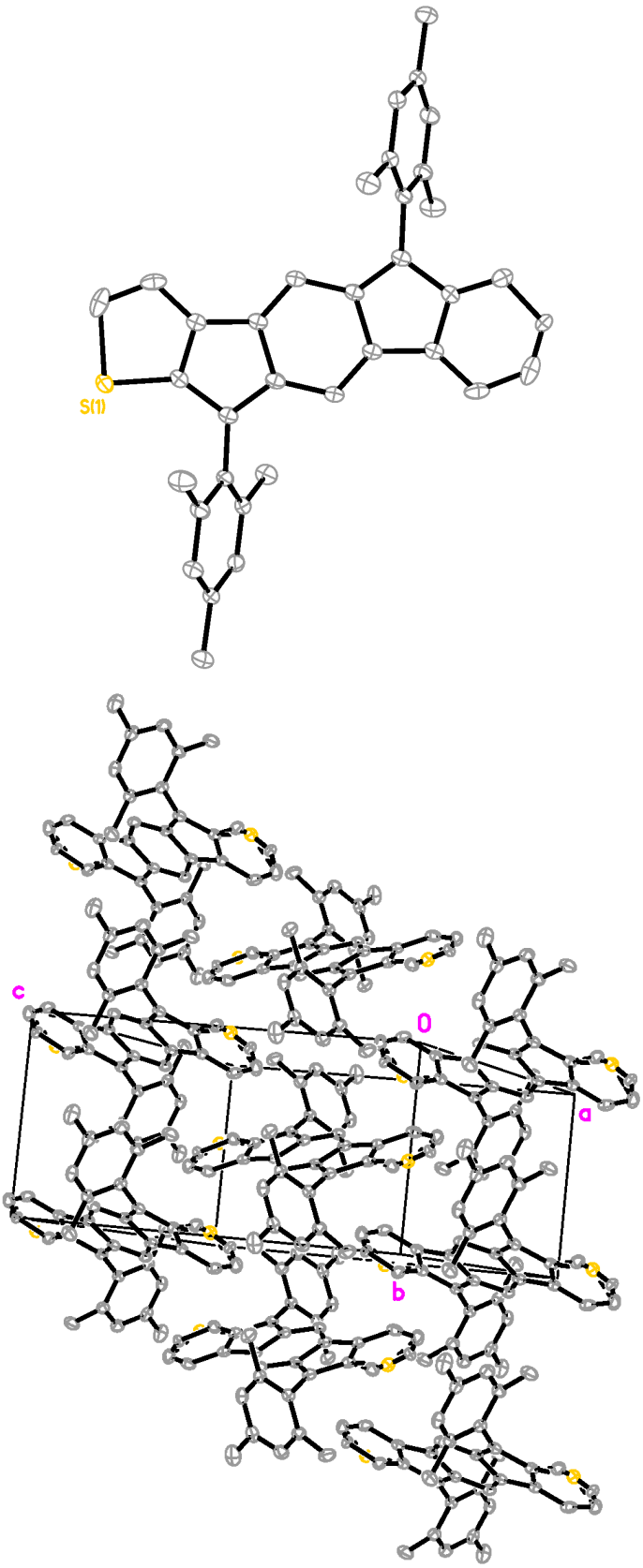


Figure S6. ORTEP and molecular packing of **8a** (generated from CIF mh171); ellipsoids at 30%.

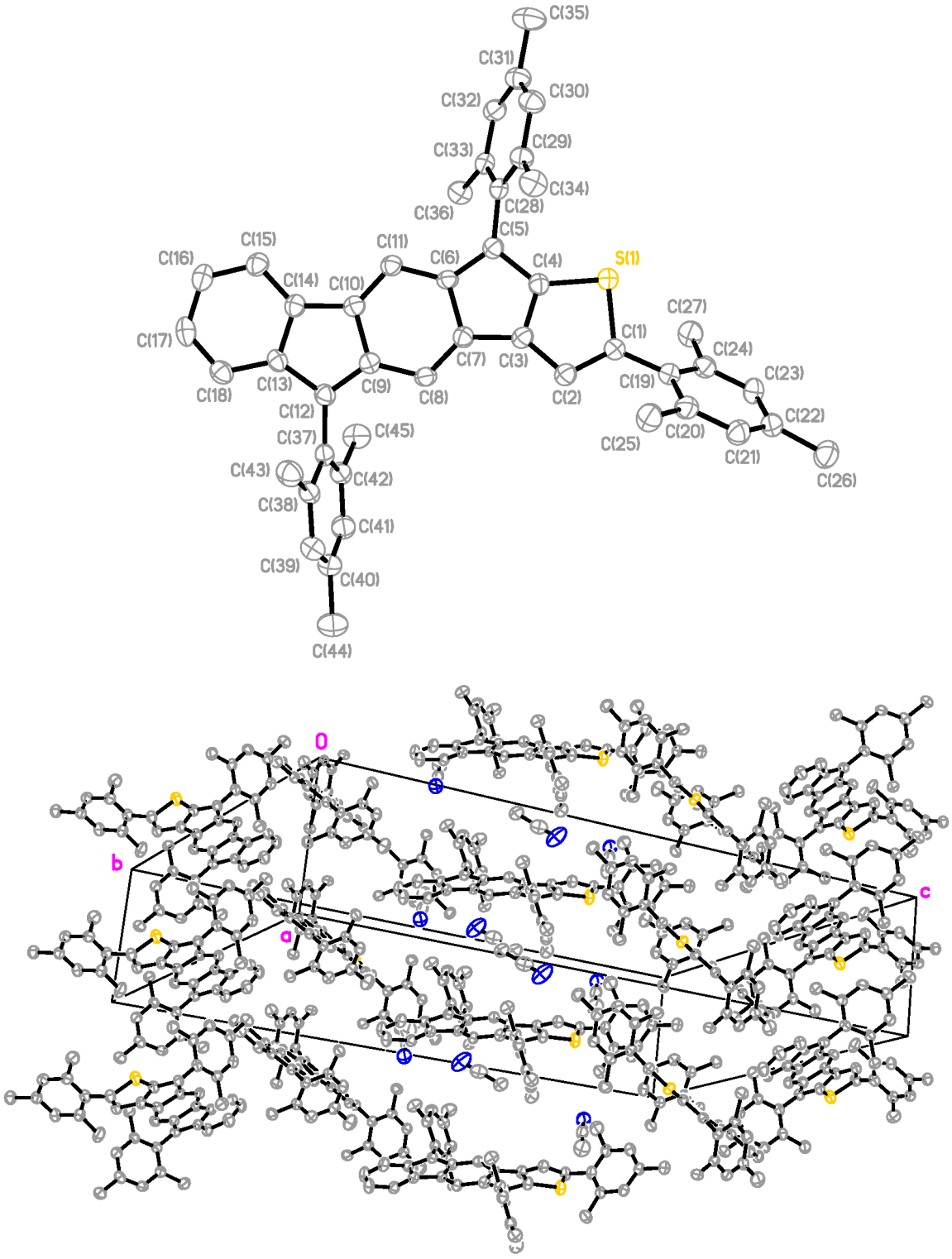


Figure S7. ORTEP and molecular packing of **8b** (generated from CIF mh169); ellipsoids at 30%.

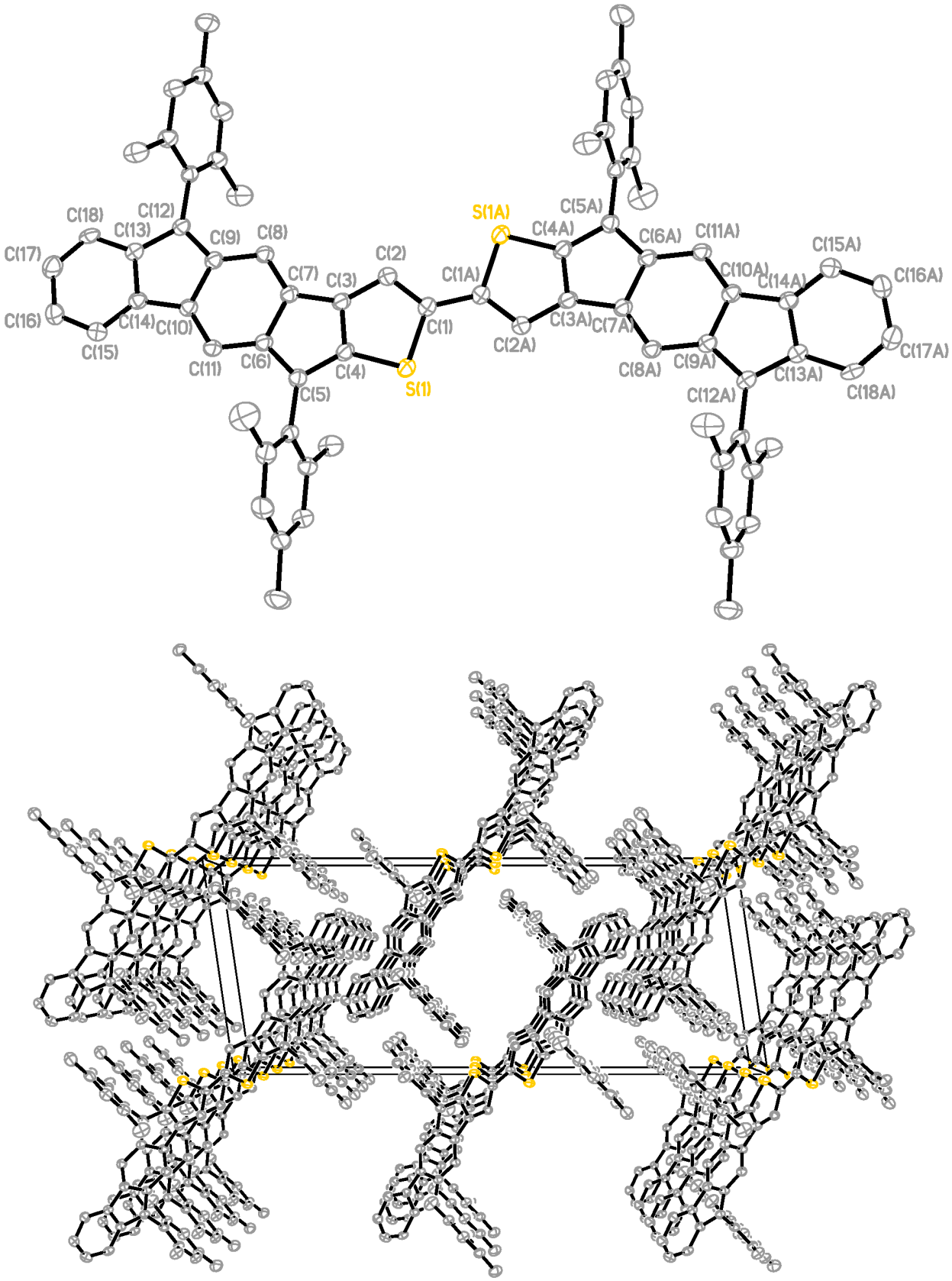


Figure S8. ORTEP and molecular packing of **8c** (generated from CIF mh170); ellipsoids at 30%.

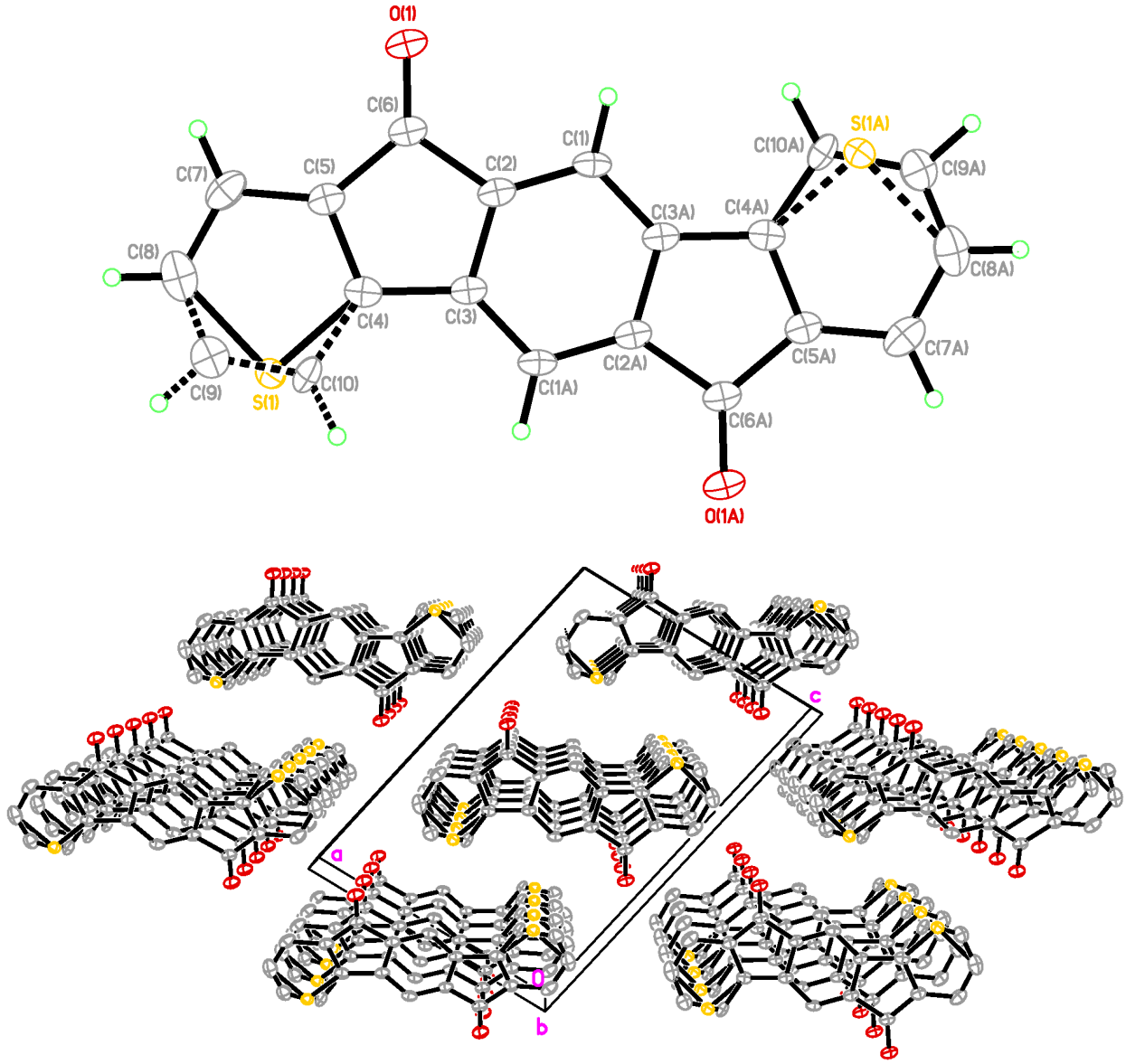


Figure S9. ORTEP and molecular packing of **15** (generated from CIF mh145); ellipsoids at 30%.

References

1. Reiss, H.; Heller, A. *J. Phys. Chem.* **1985**, *89*, 4207-4213.

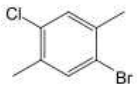
2. Sheldrick, G. M. *Bruker/Siemens Area Detector Absorption Correction Program*, Bruker AXS, Madison, WI, 1998.

3. Van der Sluis, P.; Spek, A. L. *Acta Cryst., Sect. A* **1990**, *A46*, 194-201.

4. Sheldrick, G. M. *Acta Cryst., Sect. A* **2008**, *A64*, 112-122.

Copies of NMR Spectra

^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.38 (s, 1H), 7.20 (s, 1H), 2.33 (s, 3H), 2.31 (s, 3H).



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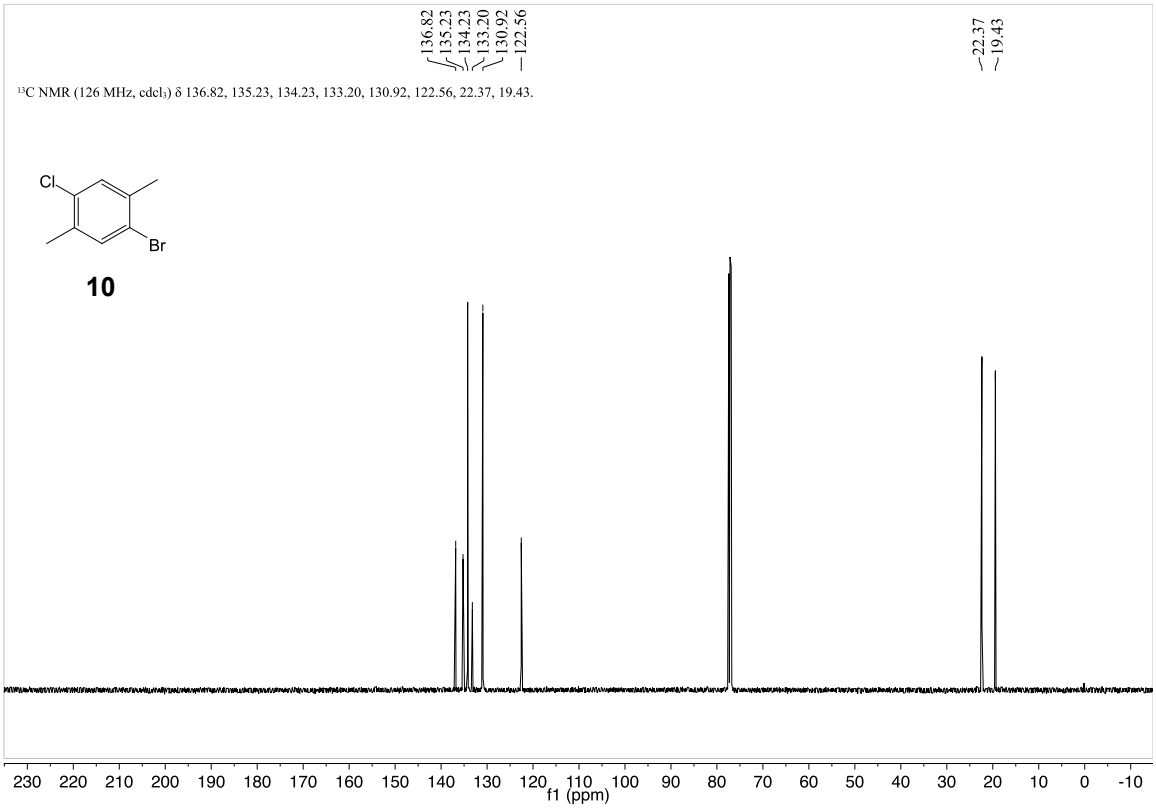
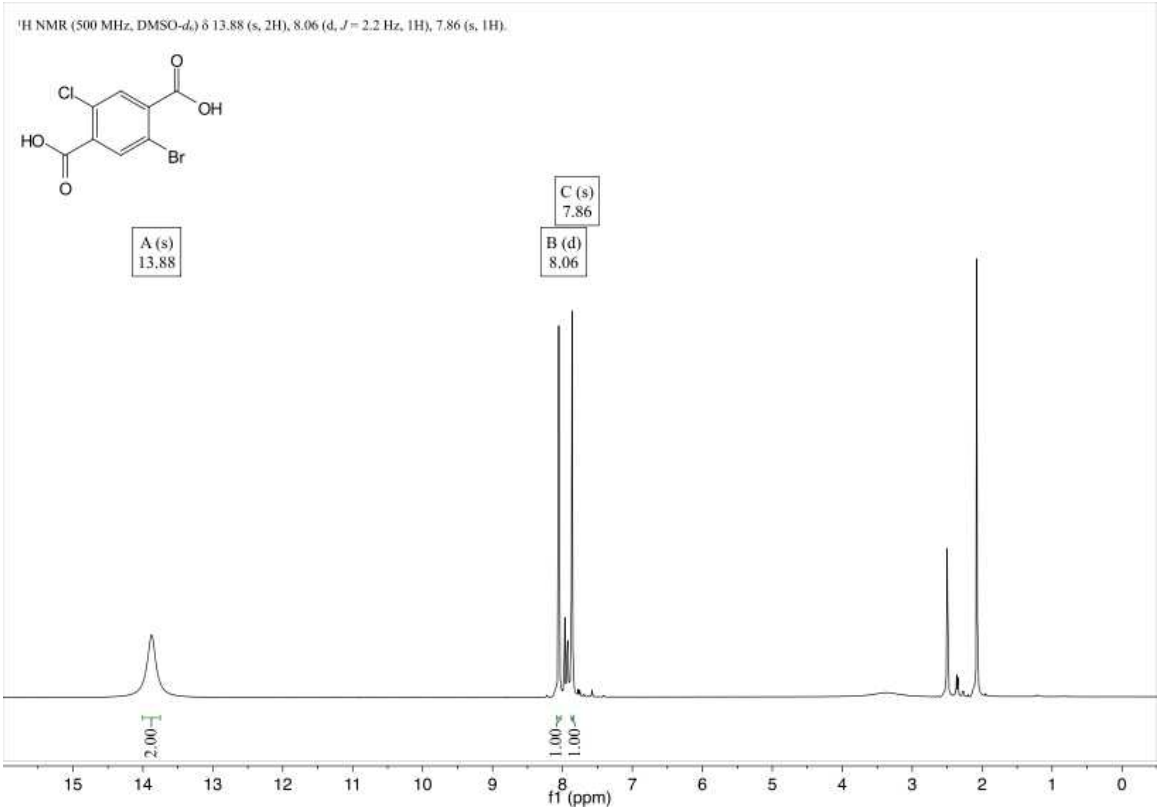
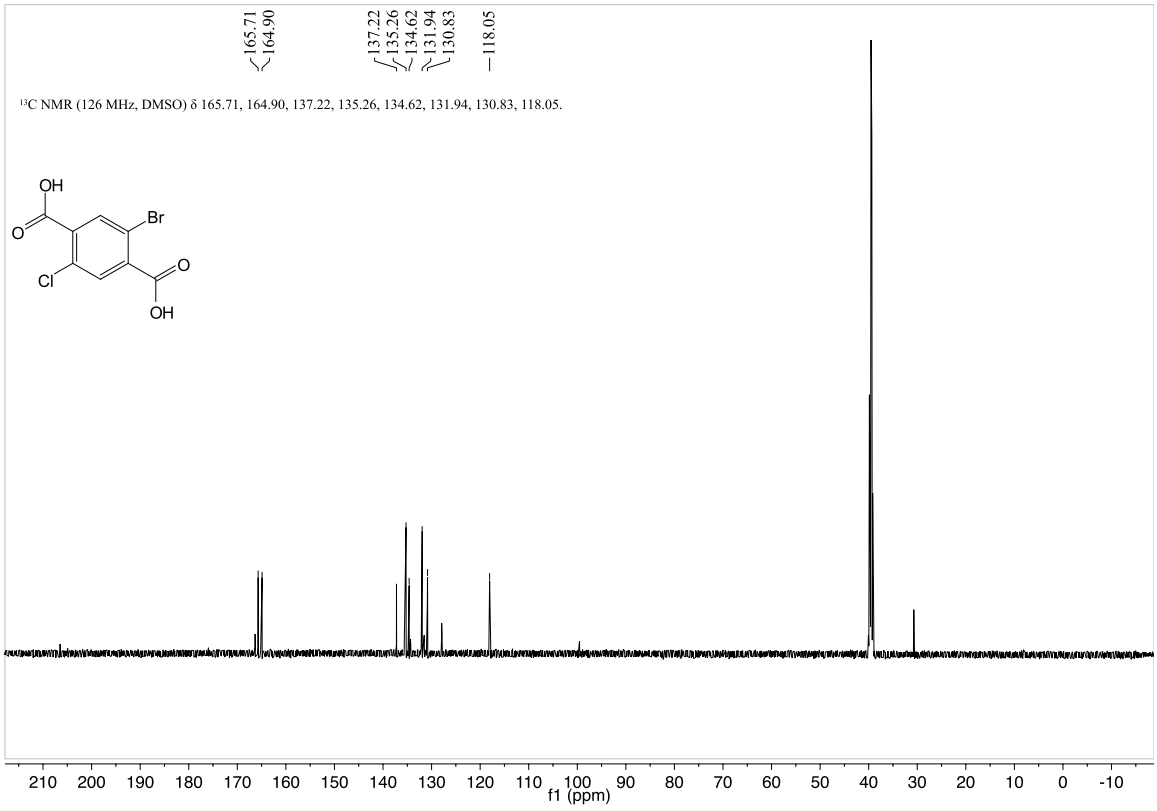
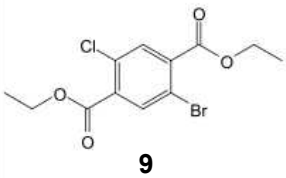


^{13}C NMR (126 MHz, cdcl$_3$) δ 136.82, 135.23, 134.23, 133.20, 130.92, 122.56, 22.37, 19.43.


¹H NMR (500 MHz, DMSO-d₆) δ 13.88 (s, 2H), 8.06 (d, J = 2.2 Hz, 1H), 7.86 (s, 1H).
Cl
O
OH
HO
Br
O
A (s)
13.88
B (d)
8.06
C (s)
7.86
2.00
1.00
1.00
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0
f1 (ppm)


165.71
164.90
137.22
135.26
134.62
131.94
130.83
118.05
¹³C NMR (126 MHz, DMSO) δ 165.71, 164.90, 137.22, 135.26, 134.62, 131.94, 130.83, 118.05.
OH
O
Br
Cl
O
OH
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.07 (s, 1H), 7.83 (s, 1H), 4.41 (q, *J* = 7.2 Hz, 4H), 1.41 (t, *J* = 7.2 Hz, 6H).



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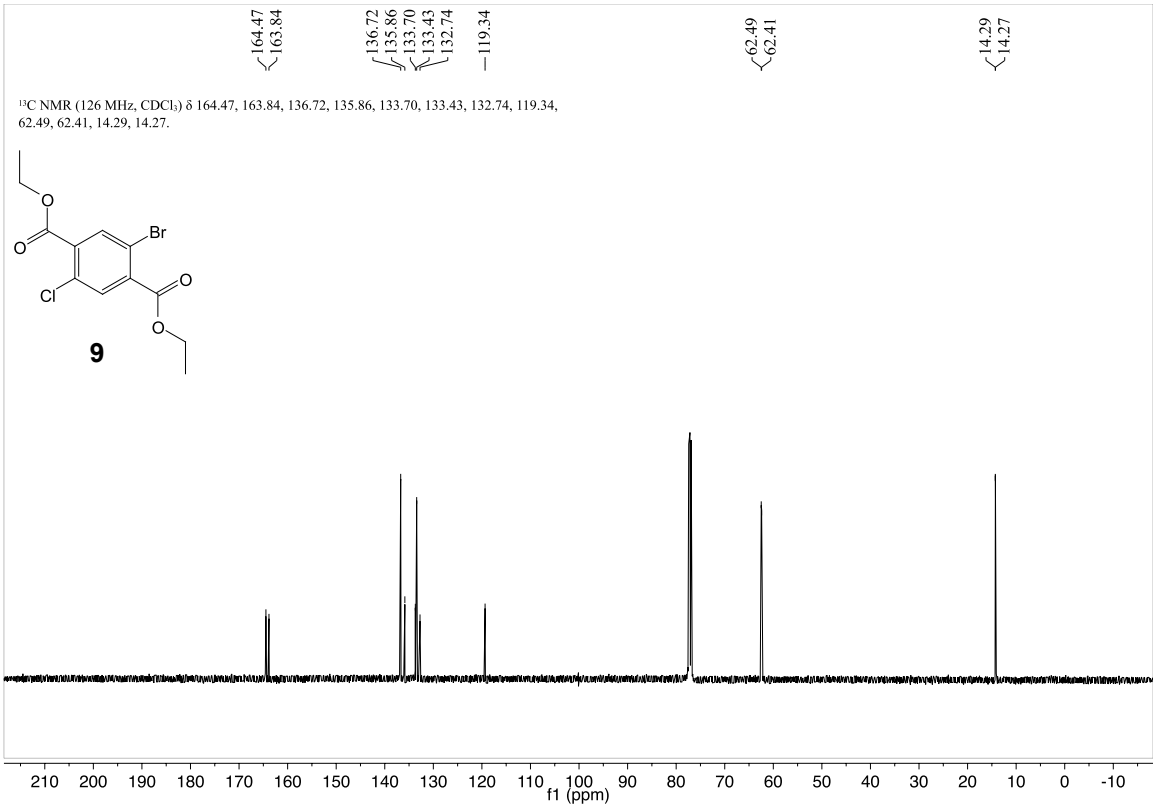

^{13}C NMR (126 MHz, $CDCl_3$) δ 164.47, 163.84, 136.72, 135.86, 133.70, 133.43, 132.74, 119.34, 62.49, 62.41, 14.29, 14.27.

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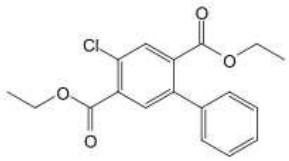
^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.88 (s, 1H), 7.80 (s, 1H), 7.43 – 7.37 (m, 3H), 7.32 – 7.27 (m, 2H), 4.42 (q, *J* = 7.1 Hz, 2H), 4.11 (q, *J* = 7.1 Hz, 2H), 1.40 (t, *J* = 7.2 Hz, 3H), 1.01 (t, *J* = 7.2 Hz, 3H).



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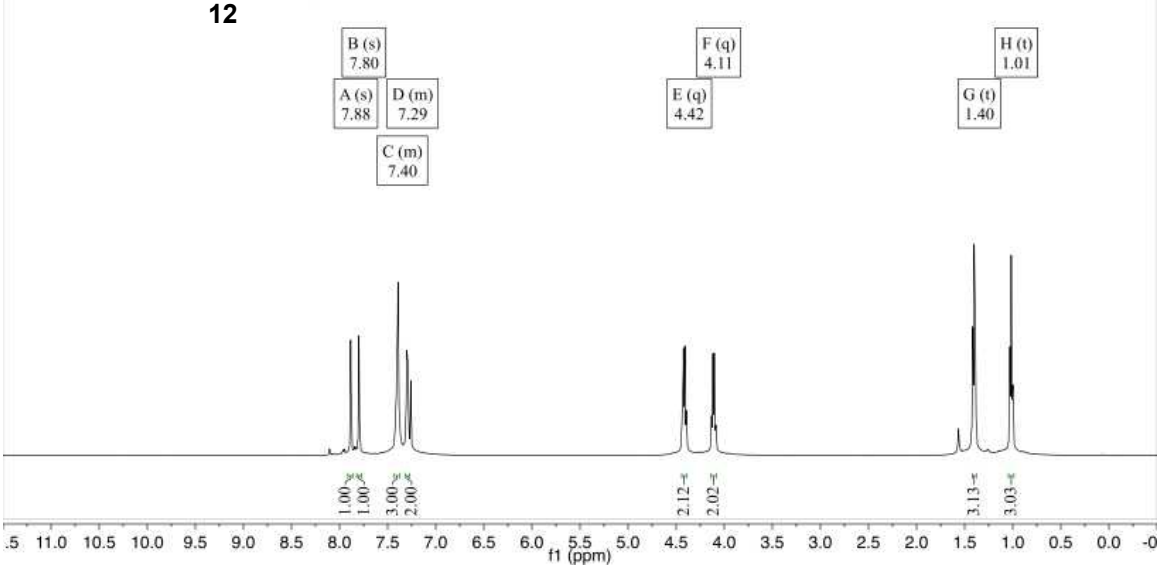

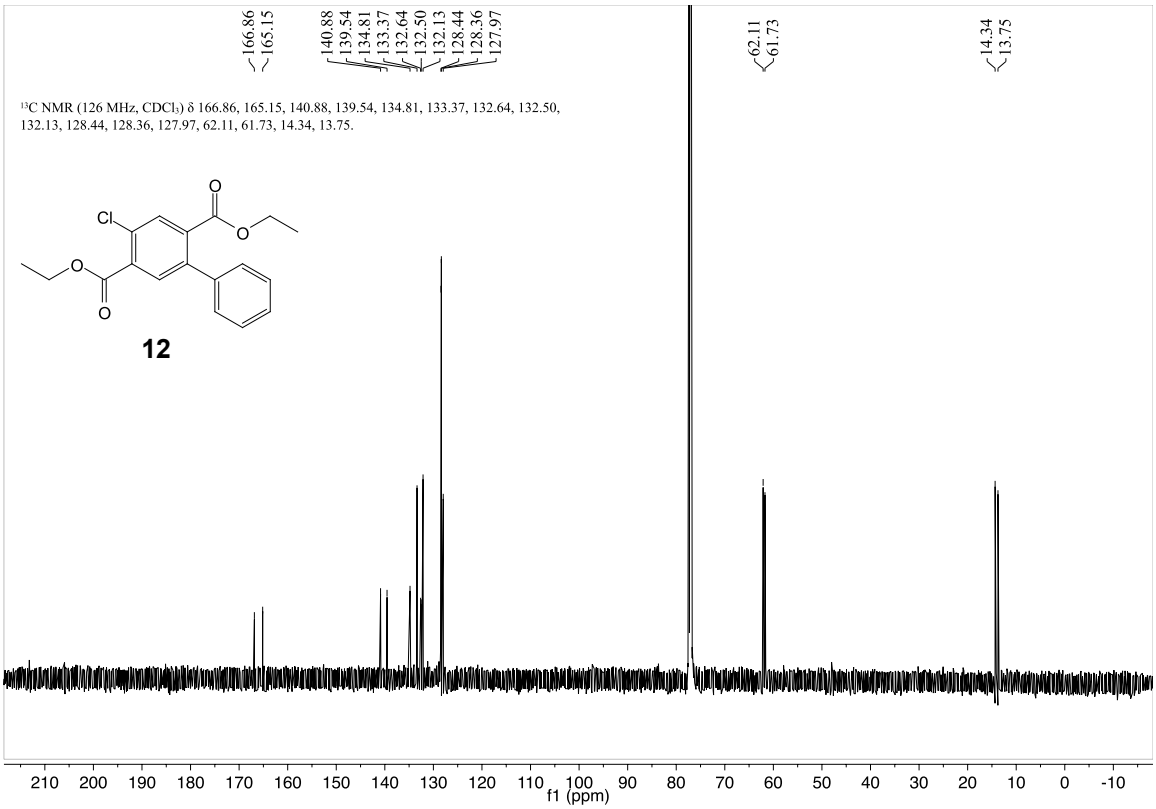

^{13}C NMR (126 MHz, $CDCl_3$) δ 166.86, 165.15, 140.88, 139.54, 134.81, 133.37, 132.64, 132.50, 132.13, 128.44, 128.36, 127.97, 62.11, 61.73, 14.34, 13.75.

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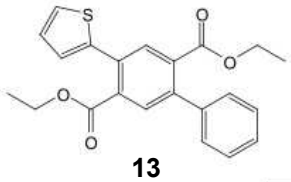
^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.92 (s, 1H), 7.72 (s, 1H), 7.44 – 7.36 (m, 4H), 7.36 – 7.31 (m, 2H), 7.11 (dd, *J* = 3.5, 1.3 Hz, 1H), 7.08 (dd, *J* = 5.0, 3.7 Hz, 1H), 4.22 (d, *J* = 7.2 Hz, 2H), 4.11 (q, *J* = 7.2 Hz, 2H), 1.15 (t, *J* = 7.2 Hz, 3H), 1.00 (t, *J* = 7.2 Hz, 3H).



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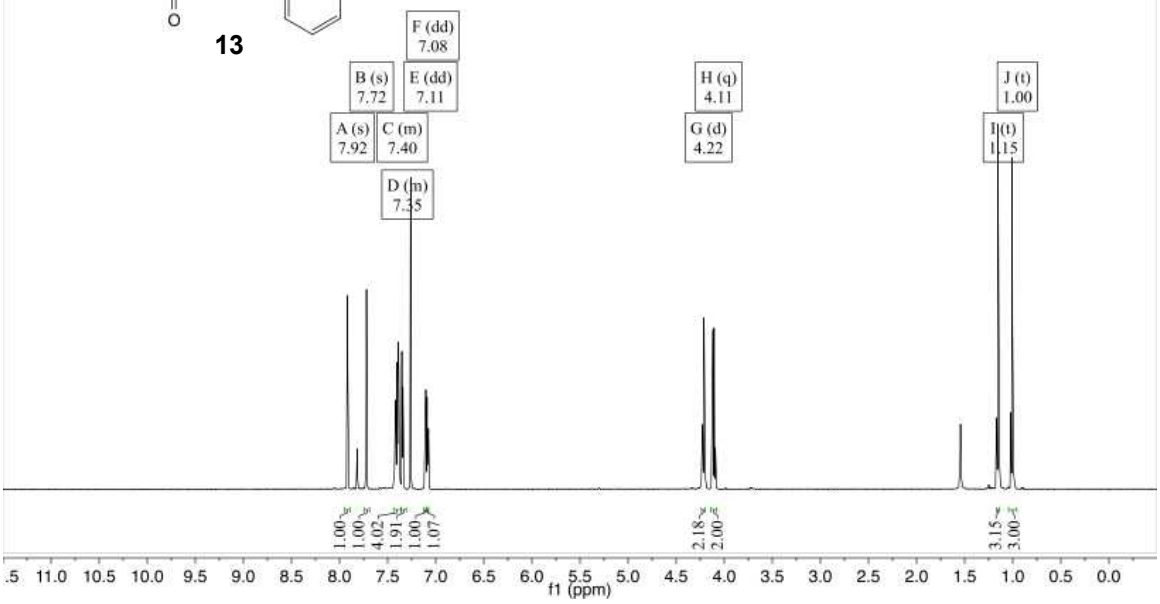

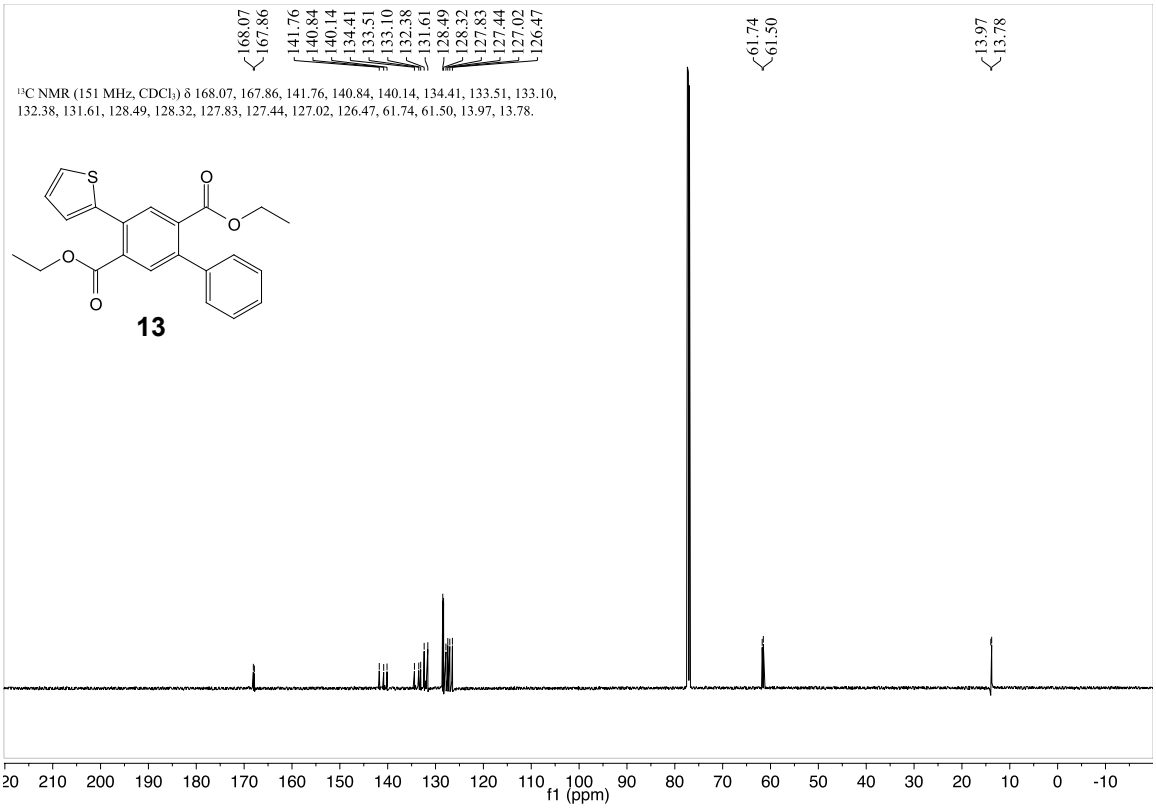

^{13}C NMR (151 MHz, $CDCl_3$) δ 168.07, 167.86, 141.76, 140.84, 140.14, 134.41, 133.51, 133.10, 132.38, 131.61, 128.49, 128.32, 127.83, 127.44, 127.02, 126.47, 61.74, 61.50, 13.97, 13.78.

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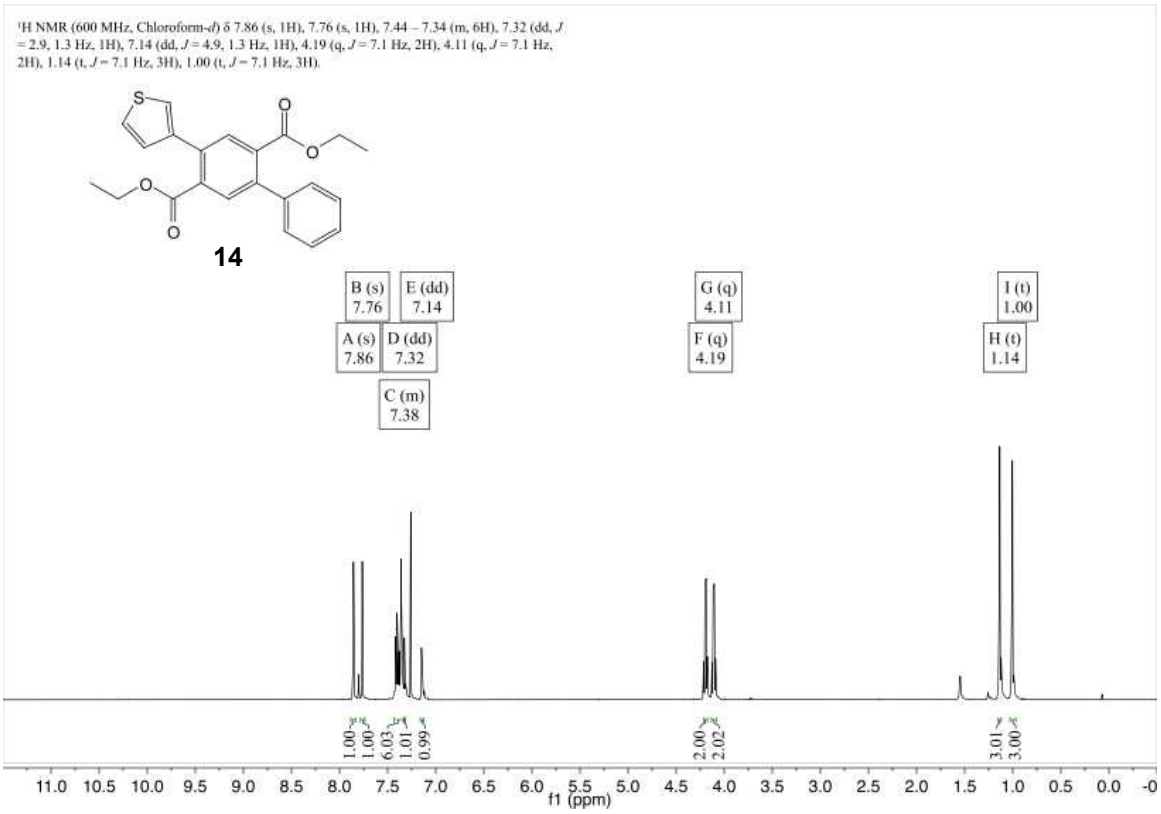
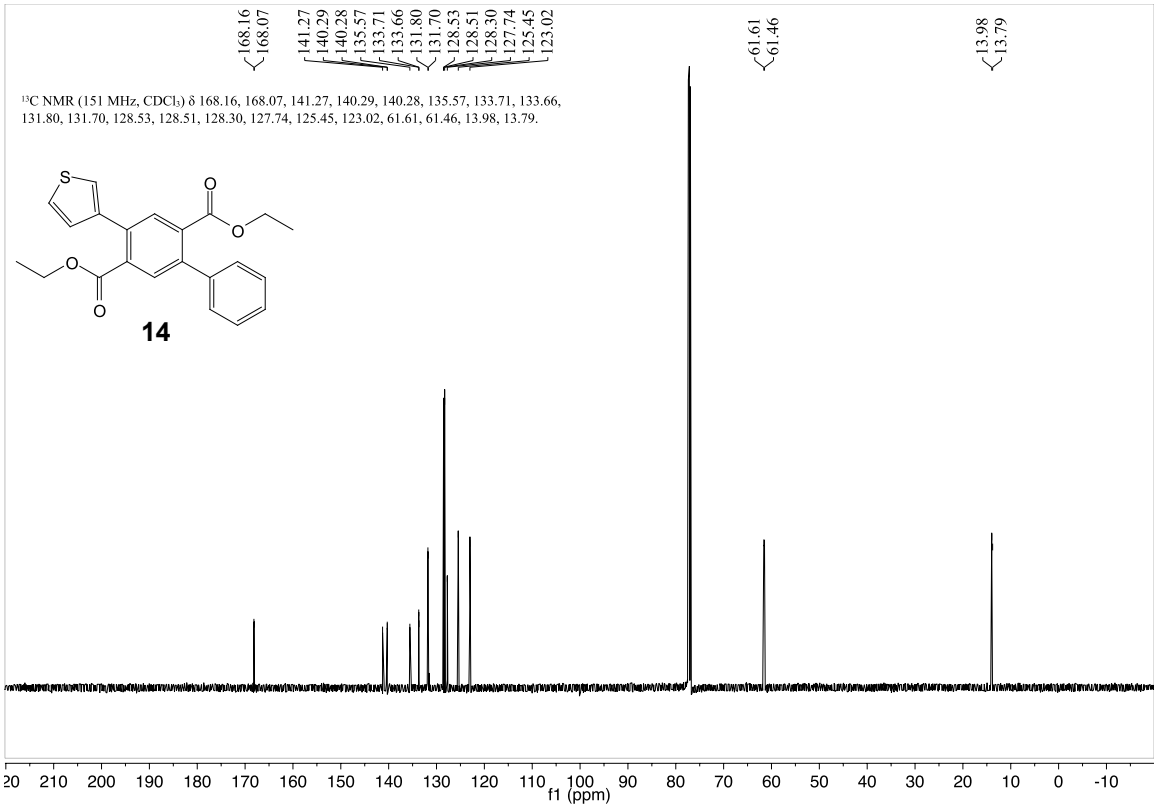
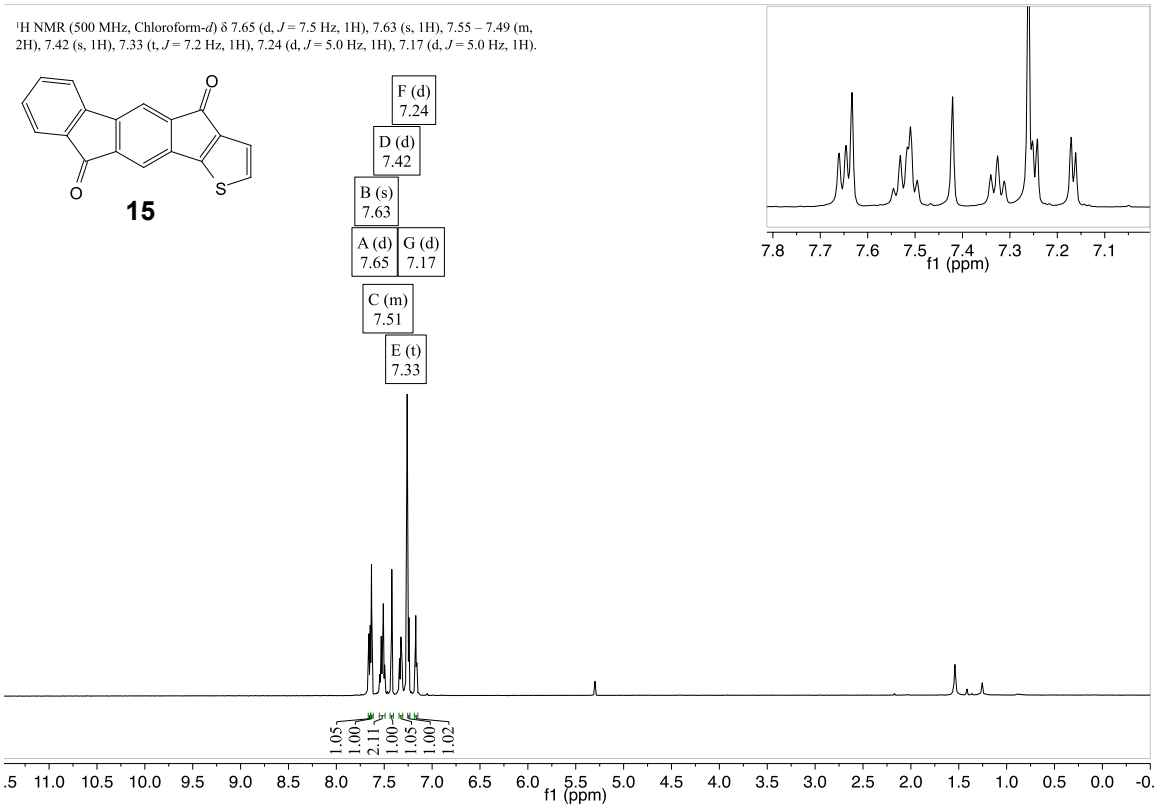
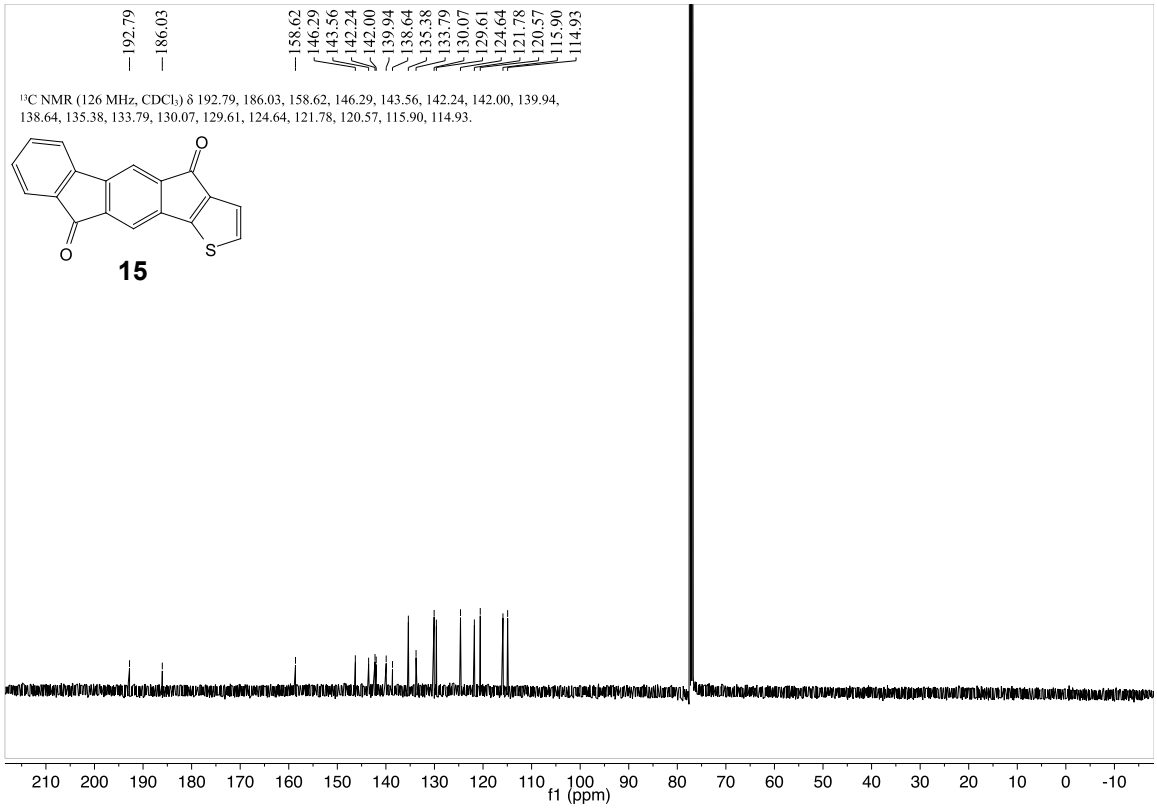
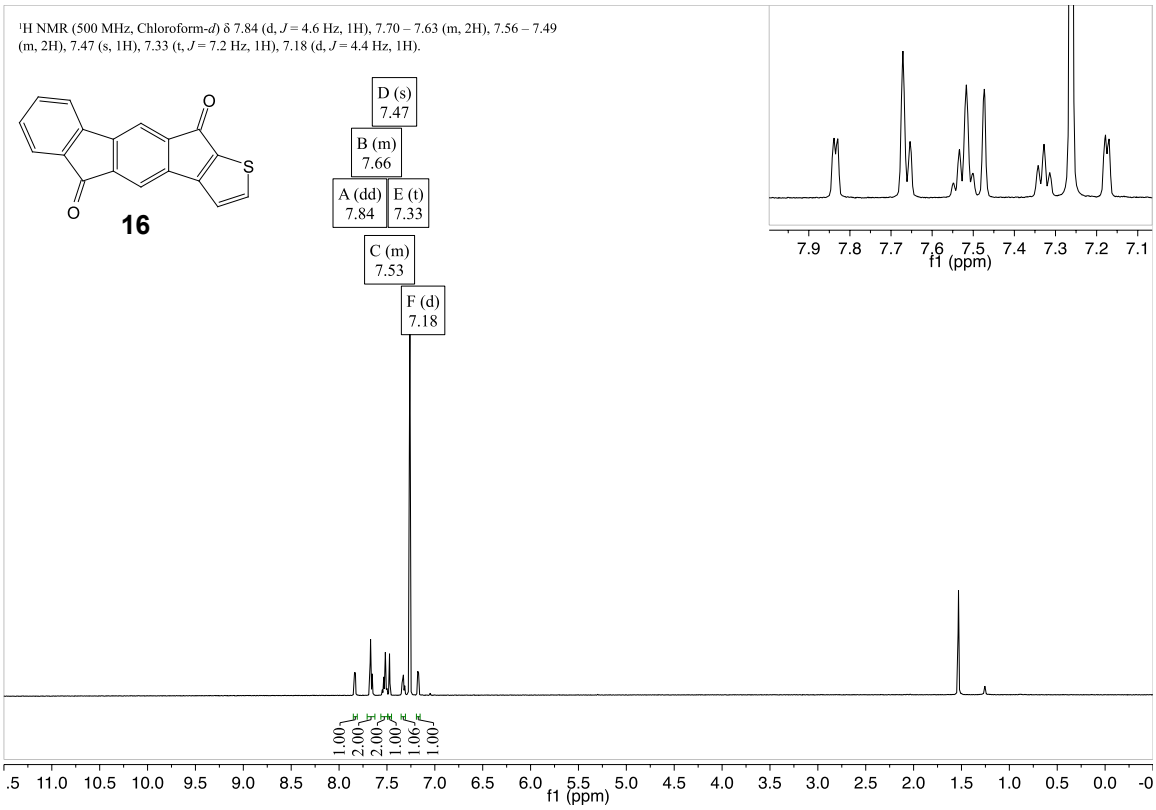
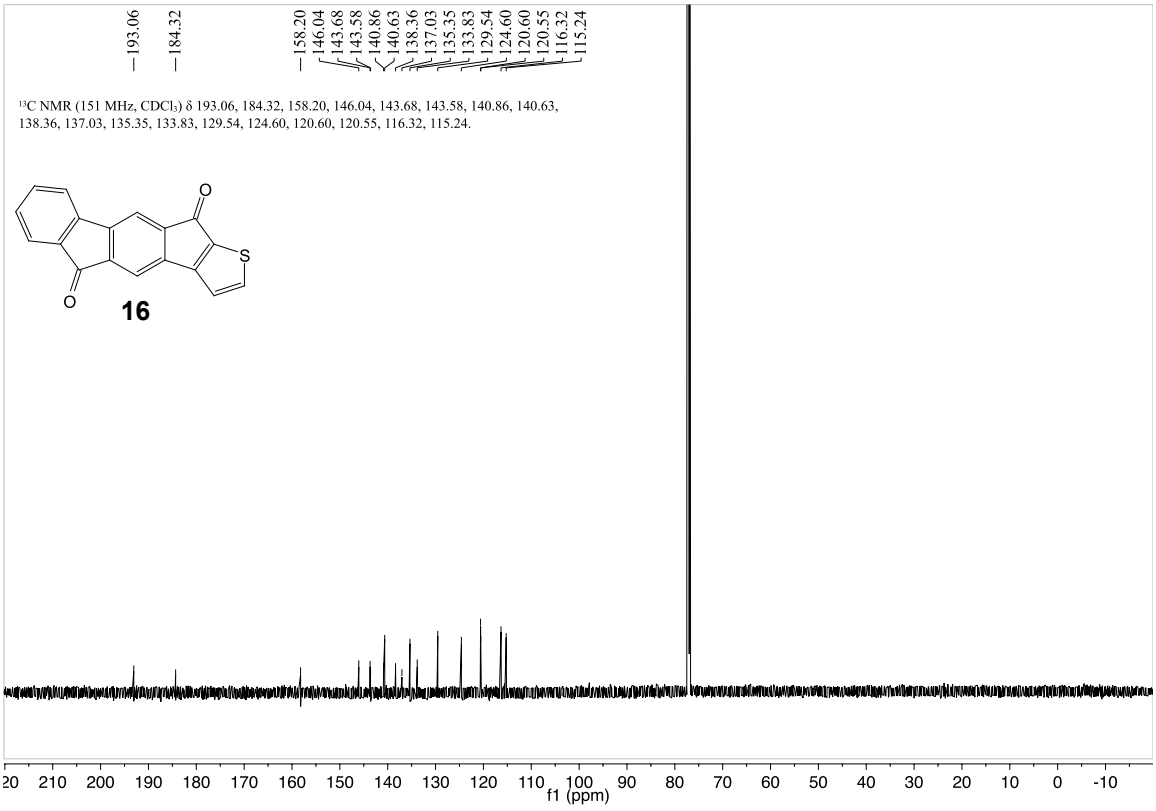

1H NMR (600 MHz, Chloroform-d) δ 7.86 (s, 1H), 7.76 (s, 1H), 7.44 – 7.34 (m, 6H), 7.32 (dd, J = 2.9, 1.3 Hz, 1H), 7.14 (dd, J = 4.9, 1.3 Hz, 1H), 4.19 (q, J = 7.1 Hz, 2H), 4.11 (q, J = 7.1 Hz, 2H), 1.14 (t, J = 7.1 Hz, 3H), 1.00 (t, J = 7.1 Hz, 3H).
14
B (s) 7.76
E (dd) 7.14
A (s) 7.86
D (dd) 7.32
C (m) 7.38
G (q) 4.11
F (q) 4.19
I (t) 1.00
H (t) 1.14
1.00
1.00
6.03
1.01
0.99
2.00
2.02
3.01
3.00
f1 (ppm)

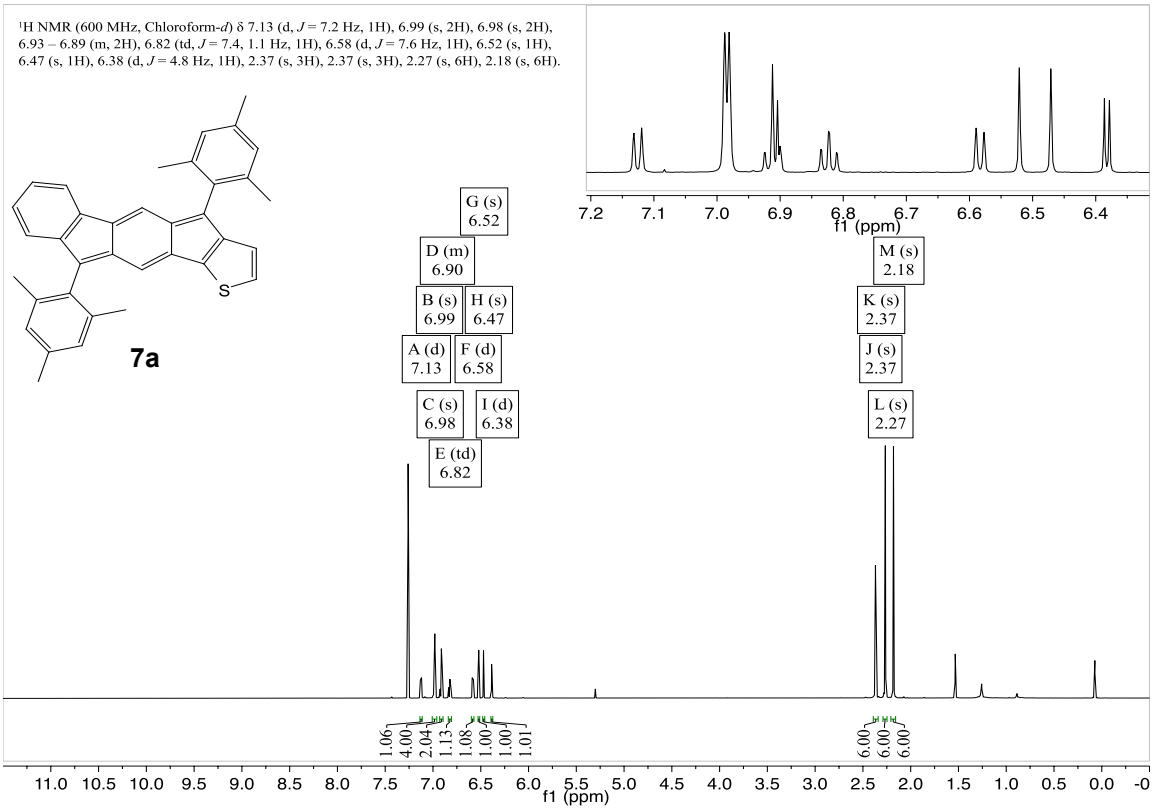

168.16
168.07
141.27
140.29
140.28
135.57
133.71
133.66
131.80
131.70
128.53
128.51
128.30
127.74
125.45
123.02
61.61
61.46
13.98
13.79
13C NMR (151 MHz, CDCl3) δ 168.16, 168.07, 141.27, 140.29, 140.28, 135.57, 133.71, 133.66, 131.80, 131.70, 128.53, 128.51, 128.30, 127.74, 125.45, 123.02, 61.61, 61.46, 13.98, 13.79.
14
f1 (ppm)

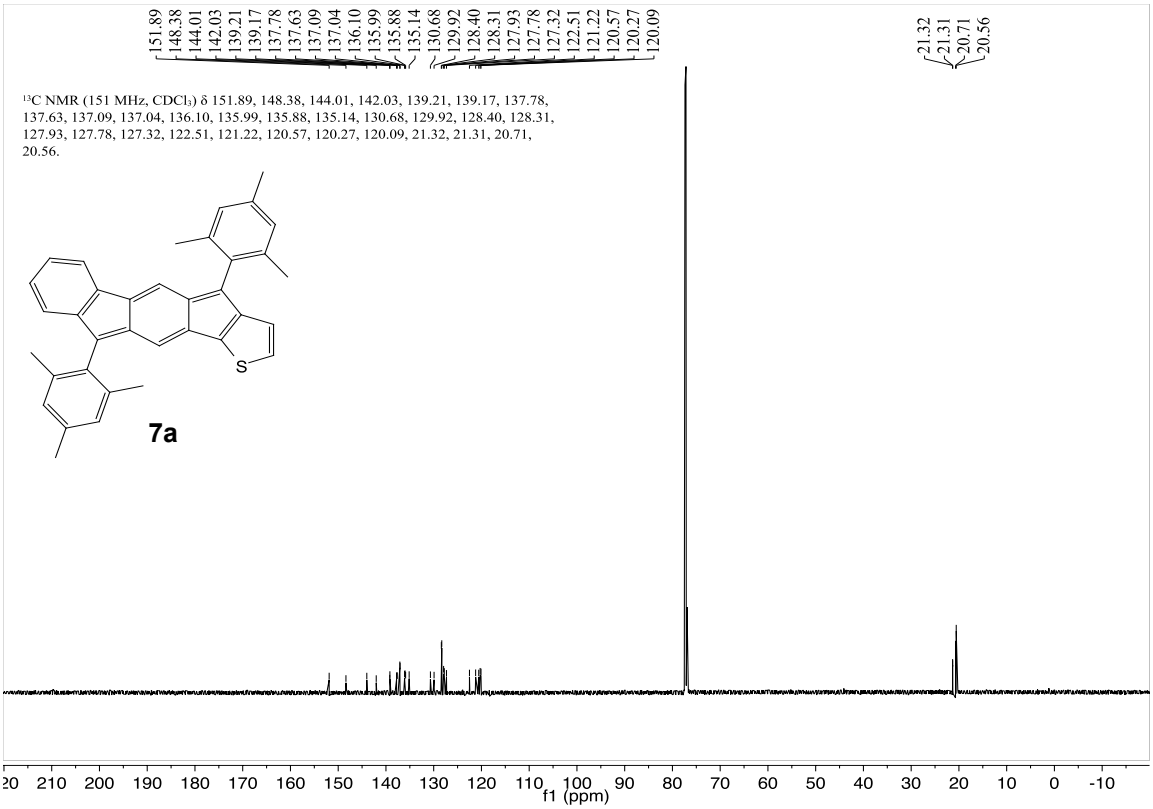

[1]H NMR (500 MHz, Chloroform-d) δ 7.65 (d, J = 7.5 Hz, 1H), 7.63 (s, 1H), 7.55 – 7.49 (m, 2H), 7.42 (s, 1H), 7.33 (t, J = 7.2 Hz, 1H), 7.24 (d, J = 5.0 Hz, 1H), 7.17 (d, J = 5.0 Hz, 1H).
15
F (d) 7.24
D (d) 7.42
B (s) 7.63
A (d) 7.65
G (d) 7.17
C (m) 7.51
E (t) 7.33
1.05
1.00
2.11
1.00
1.05
1.00
1.02
f1 (ppm)

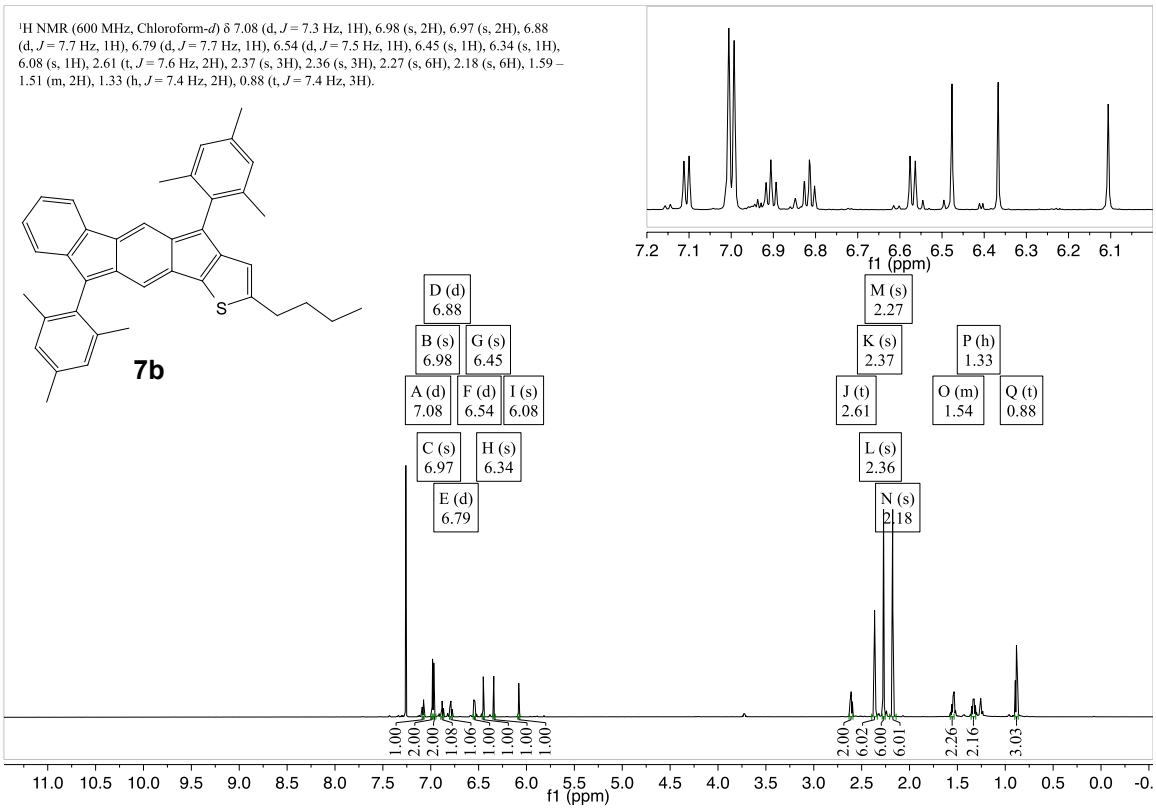

192.79
186.03
158.62
146.29
143.56
142.24
142.00
139.94
138.64
135.38
133.79
130.07
129.61
124.64
121.78
120.57
115.90
114.93
[13]C NMR (126 MHz, CDCl3) δ 192.79, 186.03, 158.62, 146.29, 143.56, 142.24, 142.00, 139.94, 138.64, 135.38, 133.79, 130.07, 129.61, 124.64, 121.78, 120.57, 115.90, 114.93.
15
f1 (ppm)

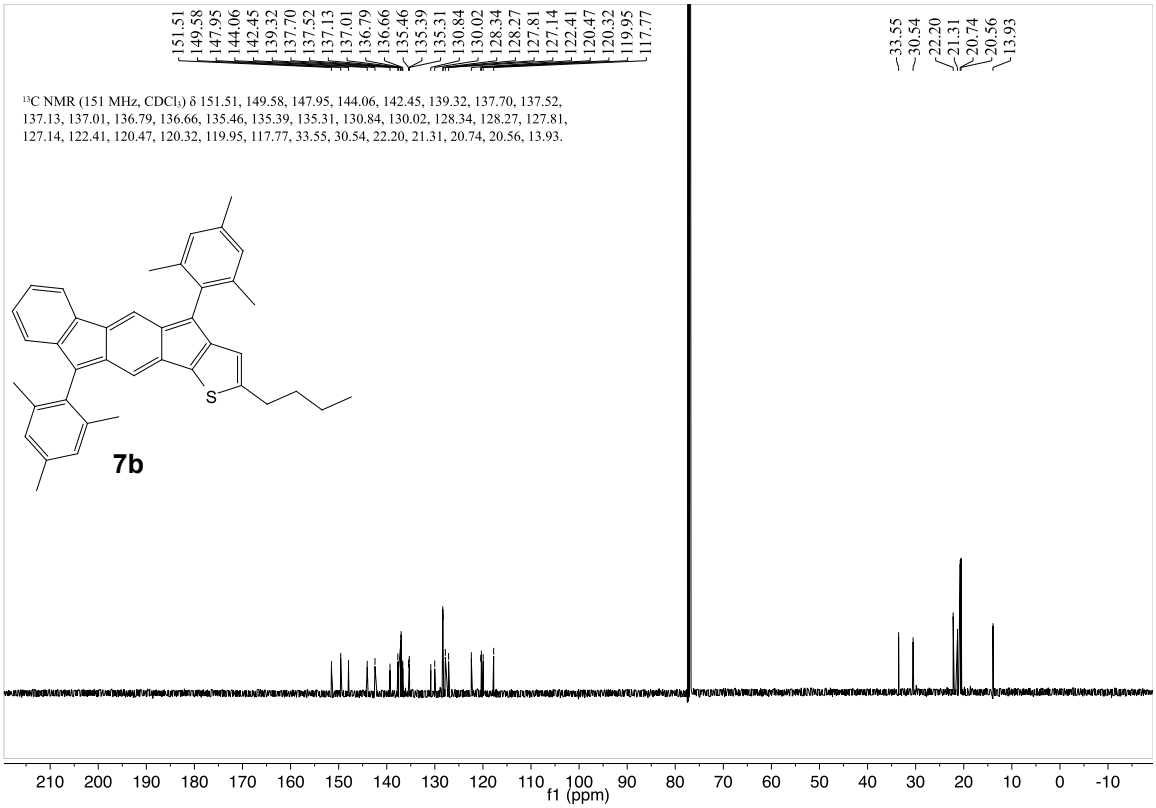

[1]H NMR (500 MHz, Chloroform-d) δ 7.84 (d, J = 4.6 Hz, 1H), 7.70 – 7.63 (m, 2H), 7.56 – 7.49 (m, 2H), 7.47 (s, 1H), 7.33 (t, J = 7.2 Hz, 1H), 7.18 (d, J = 4.4 Hz, 1H).
O
S
O
16
D (s) 7.47
B (m) 7.66
A (dd) 7.84
E (t) 7.33
C (m) 7.53
F (d) 7.18
1.00
2.00
2.00
1.00
1.06
1.00
f1 (ppm)

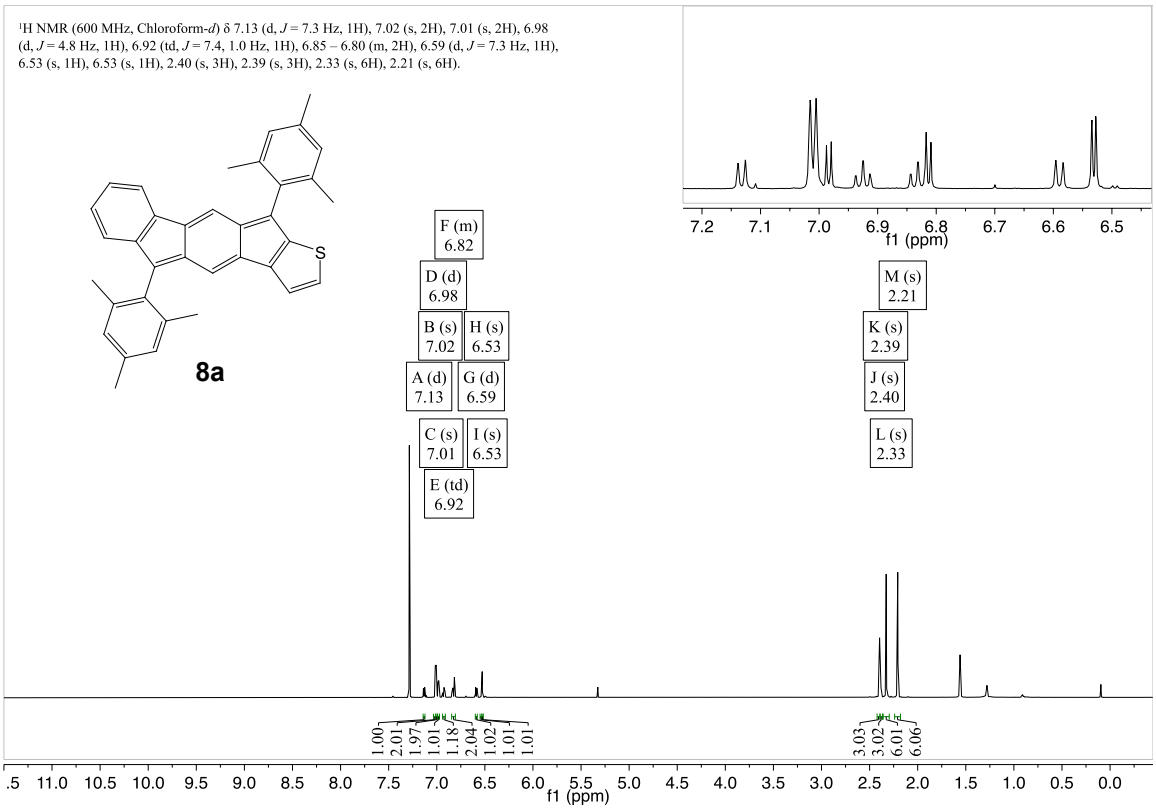

193.06
184.32
158.20
146.04
143.68
143.58
140.86
140.63
138.36
137.03
135.35
133.83
129.54
124.60
120.60
120.55
116.32
115.24
[13]C NMR (151 MHz, CDCl3) δ 193.06, 184.32, 158.20, 146.04, 143.68, 143.58, 140.86, 140.63, 138.36, 137.03, 135.35, 133.83, 129.54, 124.60, 120.60, 120.55, 116.32, 115.24.
O
S
O
16
f1 (ppm)

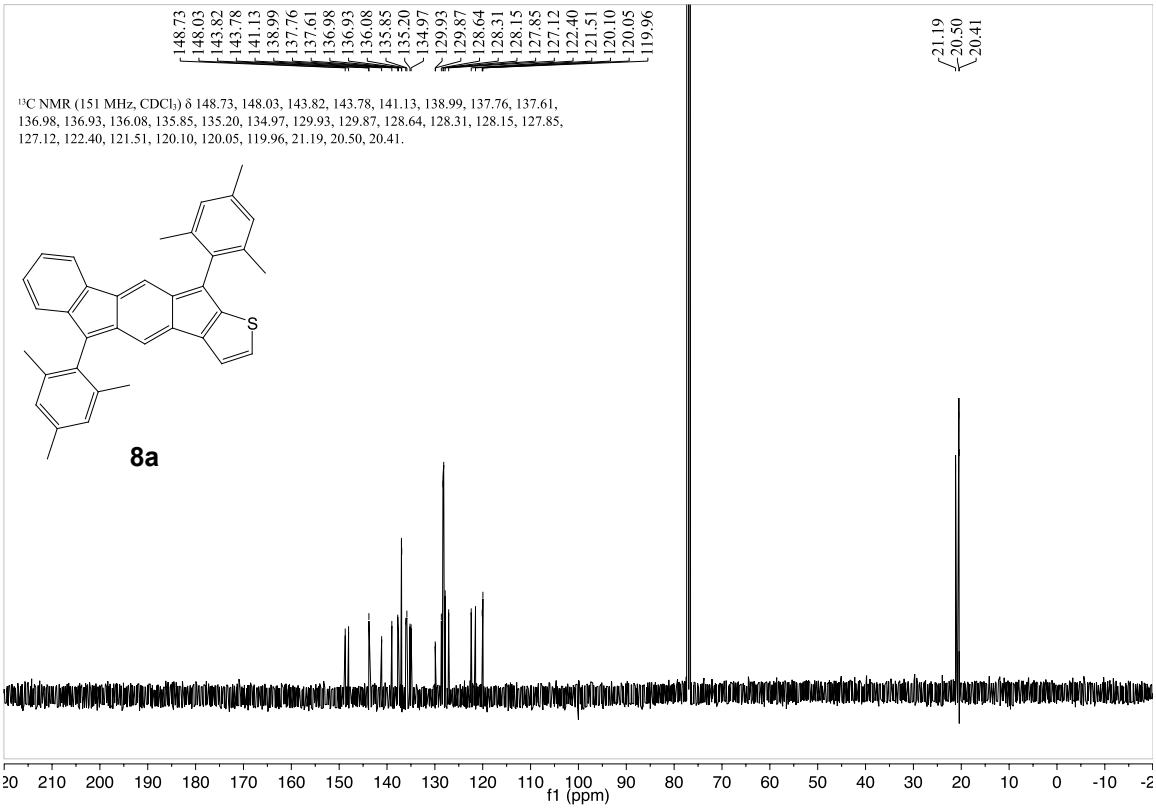

1H NMR (600 MHz, Chloroform-d) δ 7.13 (d, J = 7.2 Hz, 1H), 6.99 (s, 2H), 6.98 (s, 2H), 6.93 – 6.89 (m, 2H), 6.82 (td, J = 7.4, 1.1 Hz, 1H), 6.58 (d, J = 7.6 Hz, 1H), 6.52 (s, 1H), 6.47 (s, 1H), 6.38 (d, J = 4.8 Hz, 1H), 2.37 (s, 3H), 2.37 (s, 3H), 2.27 (s, 6H), 2.18 (s, 6H).
S
7a
G (s) 6.52
D (m) 6.90
B (s) 6.99
H (s) 6.47
A (d) 7.13
F (d) 6.58
C (s) 6.98
I (d) 6.38
E (td) 6.82
M (s) 2.18
K (s) 2.37
J (s) 2.37
L (s) 2.27
1.06 4.00 2.04 1.13 1.08 1.00 1.00 1.01
6.00 6.00 6.00
f1 (ppm)

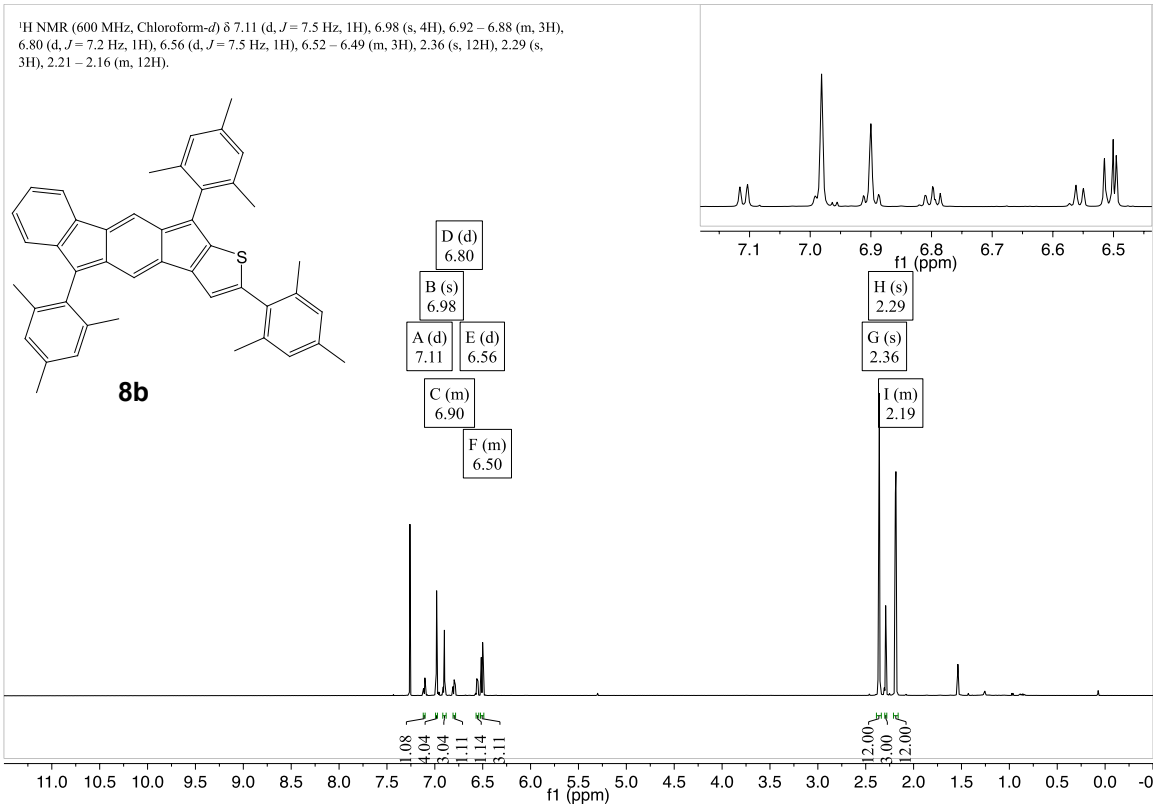

151.89 148.38 144.01 142.03 139.21 139.17 137.78 137.63 137.09 137.04 136.10 135.99 135.88 135.14 130.68 129.92 128.40 128.31 127.93 127.78 127.32 122.51 121.22 120.57 120.27 120.09
21.32 21.31 20.71 20.56
13C NMR (151 MHz, CDCl3) δ 151.89, 148.38, 144.01, 142.03, 139.21, 139.17, 137.78, 137.63, 137.09, 137.04, 136.10, 135.99, 135.88, 135.14, 130.68, 129.92, 128.40, 128.31, 127.93, 127.78, 127.32, 122.51, 121.22, 120.57, 120.27, 120.09, 21.32, 21.31, 20.71, 20.56.
S
7a
f1 (ppm)

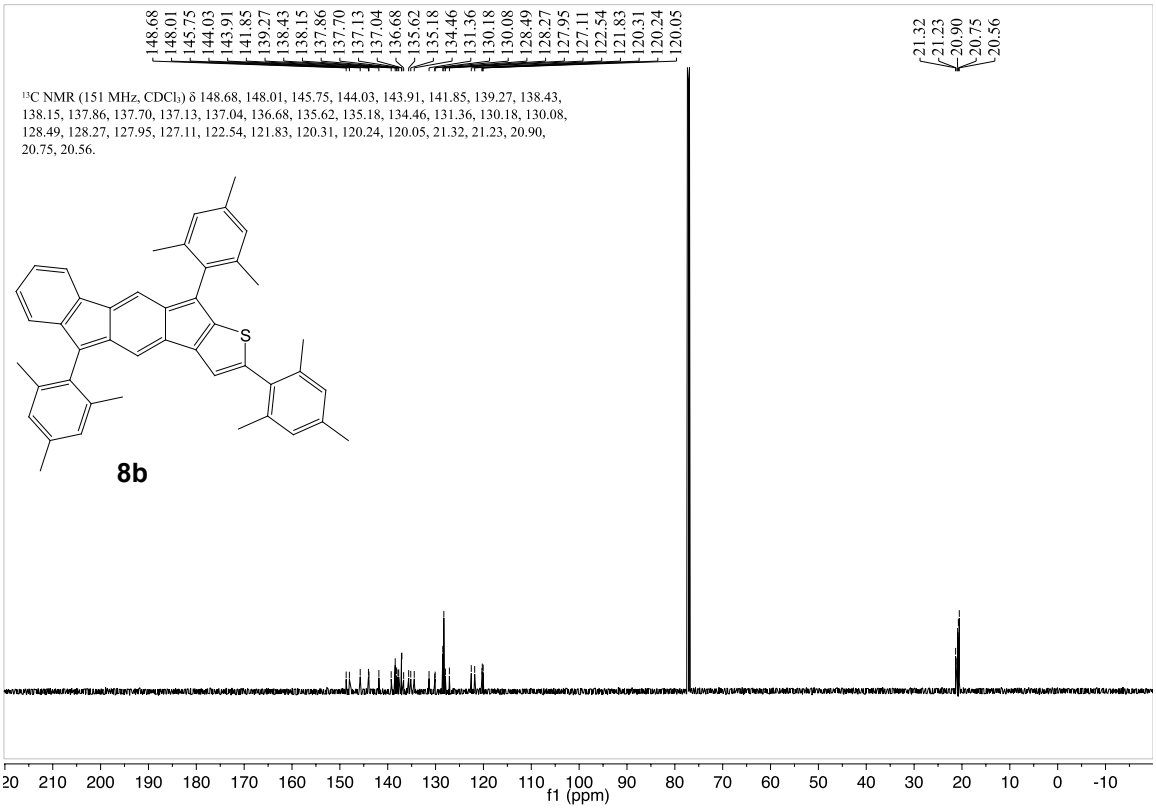

[1]H NMR (600 MHz, Chloroform-d) δ 7.08 (d, J = 7.3 Hz, 1H), 6.98 (s, 2H), 6.97 (s, 2H), 6.88 (d, J = 7.7 Hz, 1H), 6.79 (d, J = 7.7 Hz, 1H), 6.54 (d, J = 7.5 Hz, 1H), 6.45 (s, 1H), 6.34 (s, 1H), 6.08 (s, 1H), 2.61 (t, J = 7.6 Hz, 2H), 2.37 (s, 3H), 2.36 (s, 3H), 2.27 (s, 6H), 2.18 (s, 6H), 1.59 – 1.51 (m, 2H), 1.33 (h, J = 7.4 Hz, 2H), 0.88 (t, J = 7.4 Hz, 3H).
S
7b
D (d) 6.88
B (s) 6.98
G (s) 6.45
A (d) 7.08
F (d) 6.54
I (s) 6.08
C (s) 6.97
H (s) 6.34
E (d) 6.79
M (s) 2.27
K (s) 2.37
P (h) 1.33
J (t) 2.61
O (m) 1.54
Q (t) 0.88
L (s) 2.36
N (s) 2.18
1.00 2.00 2.00 1.08 1.06 1.00 1.00 1.00 1.00
2.00 6.02 6.00 6.01 2.26 2.16 3.03
f1 (ppm)

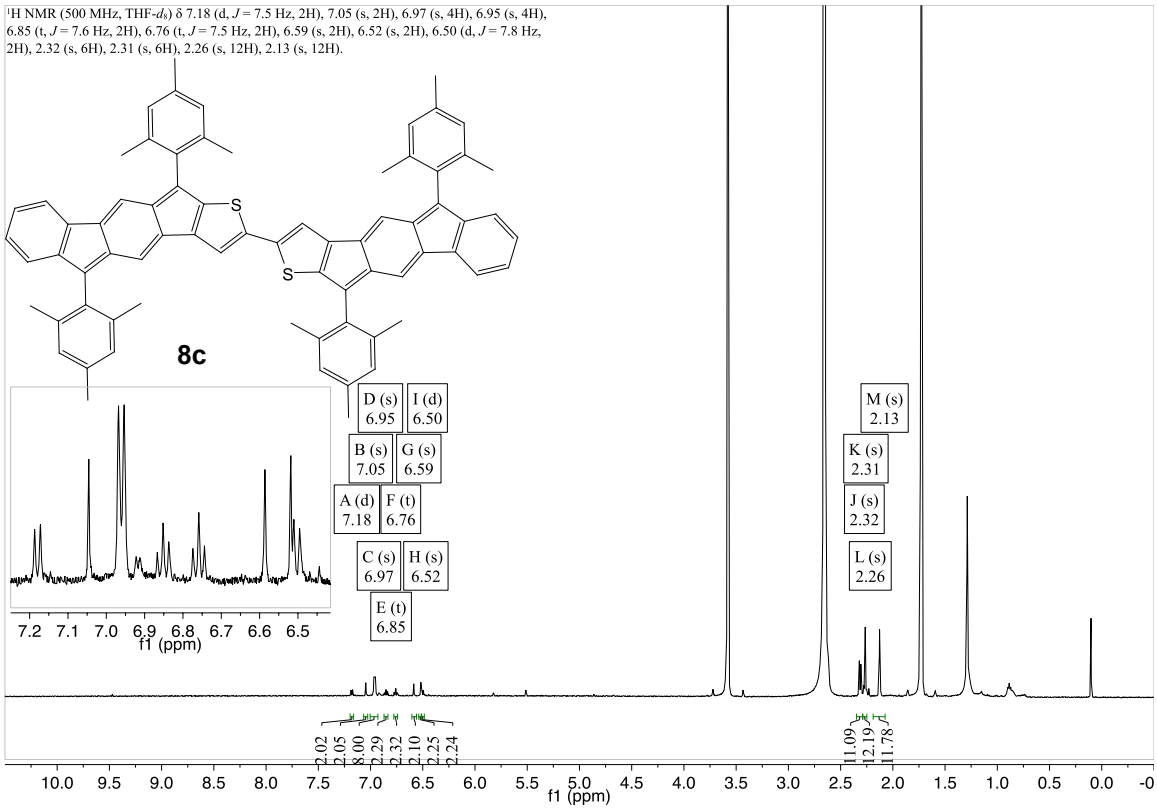

151.51 149.58 147.95 144.06 142.45 139.32 137.70 137.52 137.13 137.01 136.79 136.66 135.46 135.39 135.31 130.84 130.02 128.34 128.27 127.81 127.14 122.41 120.47 120.32 119.95 117.77
33.55 30.54 22.20 21.31 20.74 20.56 13.93
[13]C NMR (151 MHz, CDCl3) δ 151.51, 149.58, 147.95, 144.06, 142.45, 139.32, 137.70, 137.52, 137.13, 137.01, 136.79, 136.66, 135.46, 135.39, 135.31, 130.84, 130.02, 128.34, 128.27, 127.81, 127.14, 122.41, 120.47, 120.32, 119.95, 117.77, 33.55, 30.54, 22.20, 21.31, 20.74, 20.56, 13.93.
S
7b
f1 (ppm)


[1]H NMR (600 MHz, Chloroform-d) δ 7.13 (d, J = 7.3 Hz, 1H), 7.02 (s, 2H), 7.01 (s, 2H), 6.98 (d, J = 4.8 Hz, 1H), 6.92 (td, J = 7.4, 1.0 Hz, 1H), 6.85 – 6.80 (m, 2H), 6.59 (d, J = 7.3 Hz, 1H), 6.53 (s, 1H), 6.53 (s, 1H), 2.40 (s, 3H), 2.39 (s, 3H), 2.33 (s, 6H), 2.21 (s, 6H).
8a
F (m) 6.82
D (d) 6.98
B (s) 7.02
H (s) 6.53
A (d) 7.13
G (d) 6.59
C (s) 7.01
I (s) 6.53
E (td) 6.92
M (s) 2.21
K (s) 2.39
J (s) 2.40
L (s) 2.33
1.00 2.01 1.97 1.01 1.18 2.04 1.02 1.01 1.01
3.03 3.02 6.01 6.06
f1 (ppm)


148.73 148.03 143.82 143.78 141.13 138.99 137.76 137.61 136.98 136.93 136.08 135.85 135.20 134.97 129.93 129.87 128.64 128.31 128.15 127.85 127.12 122.40 121.51 120.10 120.05 119.96
21.19 20.50 20.41
[13]C NMR (151 MHz, CDCl3) δ 148.73, 148.03, 143.82, 143.78, 141.13, 138.99, 137.76, 137.61, 136.98, 136.93, 136.08, 135.85, 135.20, 134.97, 129.93, 129.87, 128.64, 128.31, 128.15, 127.85, 127.12, 122.40, 121.51, 120.10, 120.05, 119.96, 21.19, 20.50, 20.41.
8a
f1 (ppm)


1H NMR (600 MHz, Chloroform-d) δ 7.11 (d, J = 7.5 Hz, 1H), 6.98 (s, 4H), 6.92 – 6.88 (m, 3H), 6.80 (d, J = 7.2 Hz, 1H), 6.56 (d, J = 7.5 Hz, 1H), 6.52 – 6.49 (m, 3H), 2.36 (s, 12H), 2.29 (s, 3H), 2.21 – 2.16 (m, 12H).
8b
D (d) 6.80
B (s) 6.98
A (d) 7.11
E (d) 6.56
C (m) 6.90
F (m) 6.50
H (s) 2.29
G (s) 2.36
I (m) 2.19
1.08
4.04
3.04
1.11
1.14
3.11
12.00
3.00
12.00
f1 (ppm)


148.68
148.01
145.75
144.03
143.91
141.85
139.27
138.43
138.15
137.86
137.70
137.13
137.04
136.68
135.62
135.18
134.46
131.36
130.18
130.08
128.49
128.27
127.95
127.11
122.54
121.83
120.31
120.24
120.05
21.32
21.23
20.90
20.75
20.56
13C NMR (151 MHz, CDCl3) δ 148.68, 148.01, 145.75, 144.03, 143.91, 141.85, 139.27, 138.43, 138.15, 137.86, 137.70, 137.13, 137.04, 136.68, 135.62, 135.18, 134.46, 131.36, 130.18, 130.08, 128.49, 128.27, 127.95, 127.11, 122.54, 121.83, 120.31, 120.24, 120.05, 21.32, 21.23, 20.90, 20.75, 20.56.
8b
f1 (ppm)


^{1}H NMR (500 MHz, THF-d_8) δ 7.18 (d, J = 7.5 Hz, 2H), 7.05 (s, 2H), 6.97 (s, 4H), 6.95 (s, 4H), 6.85 (t, J = 7.6 Hz, 2H), 6.76 (t, J = 7.5 Hz, 2H), 6.59 (s, 2H), 6.52 (s, 2H), 6.50 (d, J = 7.8 Hz, 2H), 2.32 (s, 6H), 2.31 (s, 6H), 2.26 (s, 12H), 2.13 (s, 12H).
S
S
8c
D (s) 6.95
I (d) 6.50
B (s) 7.05
G (s) 6.59
A (d) 7.18
F (t) 6.76
C (s) 6.97
H (s) 6.52
E (t) 6.85
M (s) 2.13
K (s) 2.31
J (s) 2.32
L (s) 2.26
7.2 7.1 7.0 6.9 6.8 6.7 6.6 6.5
f1 (ppm)
2.02 2.05 8.00 2.29 2.32 2.10 2.25 2.24
11.09 12.19 11.78
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0
f1 (ppm)