Supporting Information

Length-Dependent Conductance of Oligothiophenes

Brian Capozzi,[1,§] Emma J. Dell,[2,§] Timothy C. Berkelbach,[2] David R. Reichman,[2] Latha Venkataraman,[*,1] Luis M. Campos.[*,2]

[1]Department of Applied Physics and Mathematics, and [2]Department of Chemistry, Columbia University, New York, NY 10027, USA.

Contents:

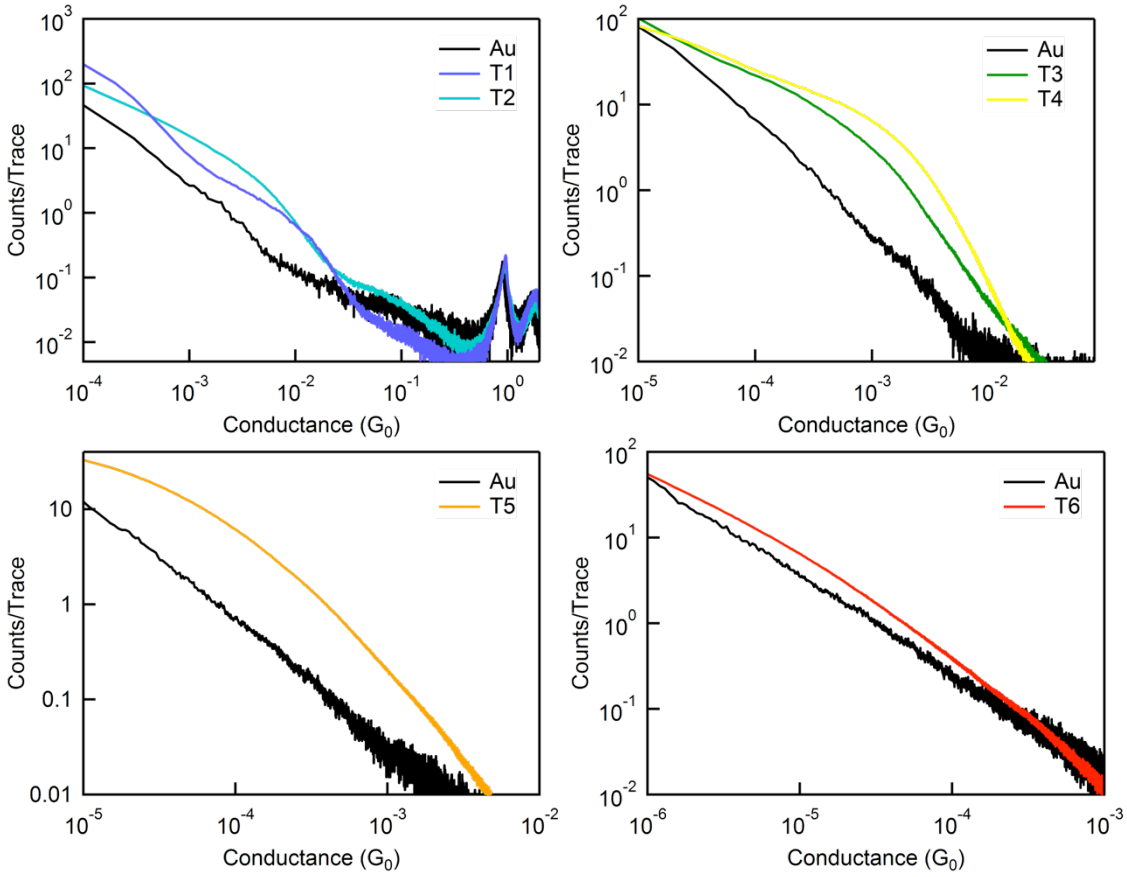


Figure S1. Linear-binned conductance histograms for T1-T6.

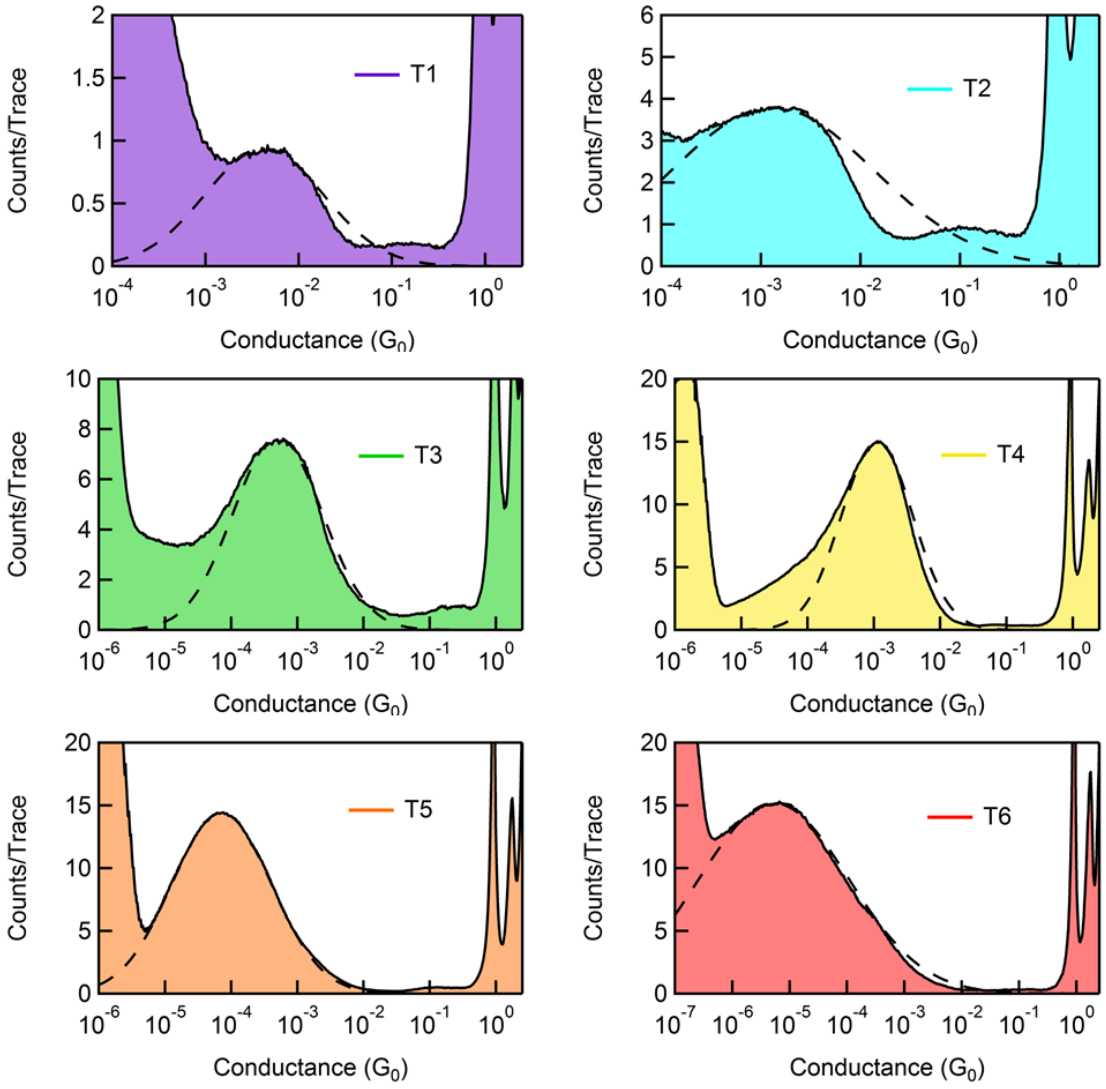


Figure S2. Logarithmically binned conductance histograms for T1-T6.

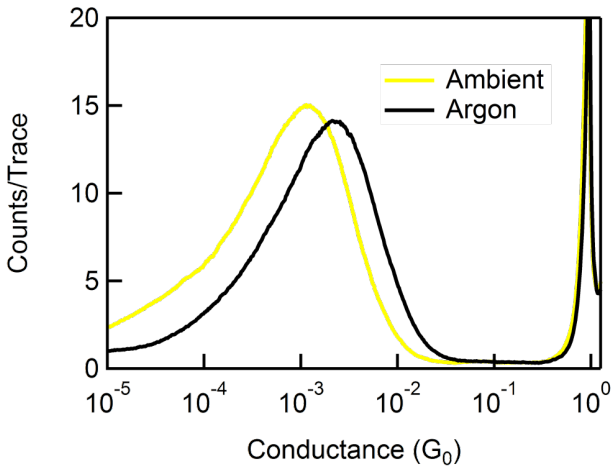


Figure S3. T4 conductance under argon and in ambient conditions.

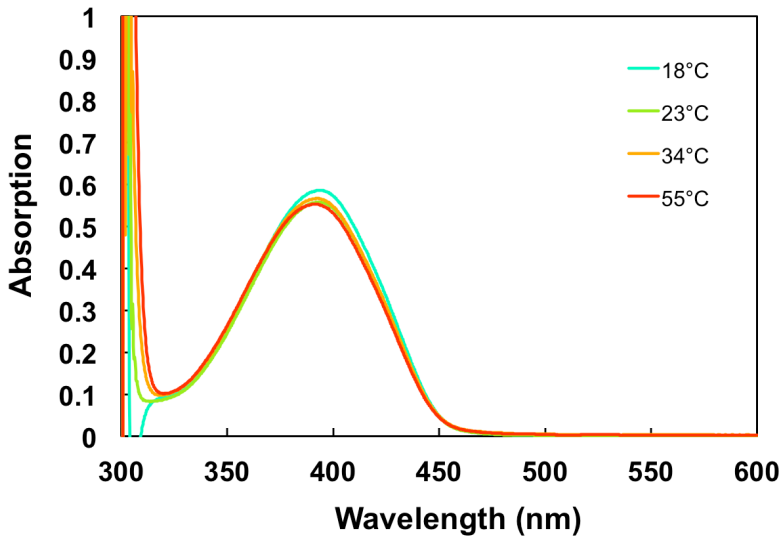


Figure S4. UV-vis absorption data taken in 1,2,4 trichlorobenzene for T3 at temperatures from 18°C to 55°C.

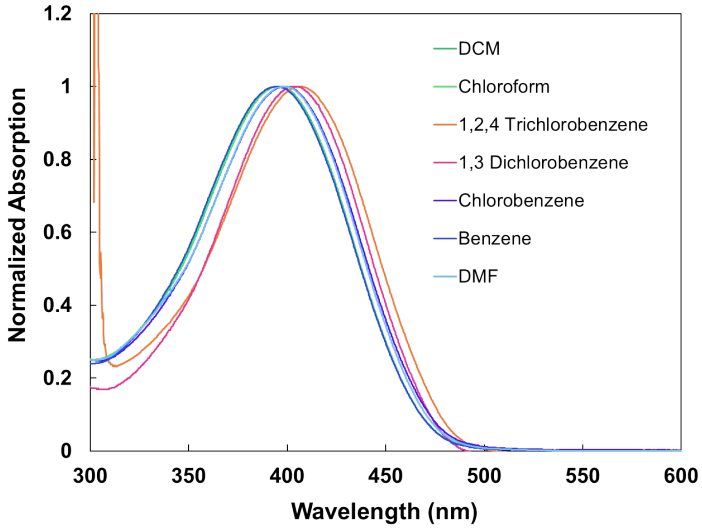


Figure S5. UV-vis absorption data taken in various solvents for T4

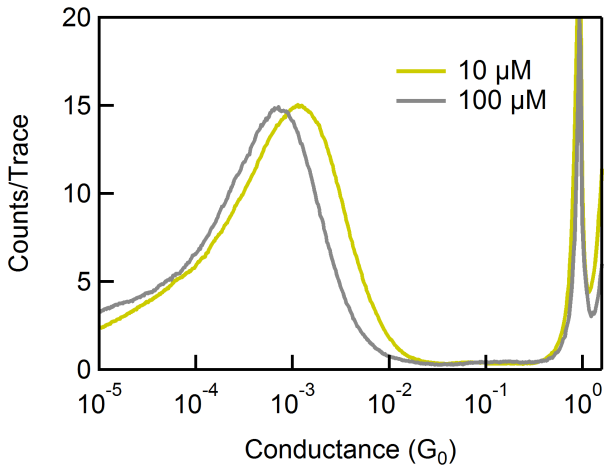


Figure S6. Logarithmically binned conductance histograms for T4 in 1,2,4-trichlorobenzne at two concentrations.

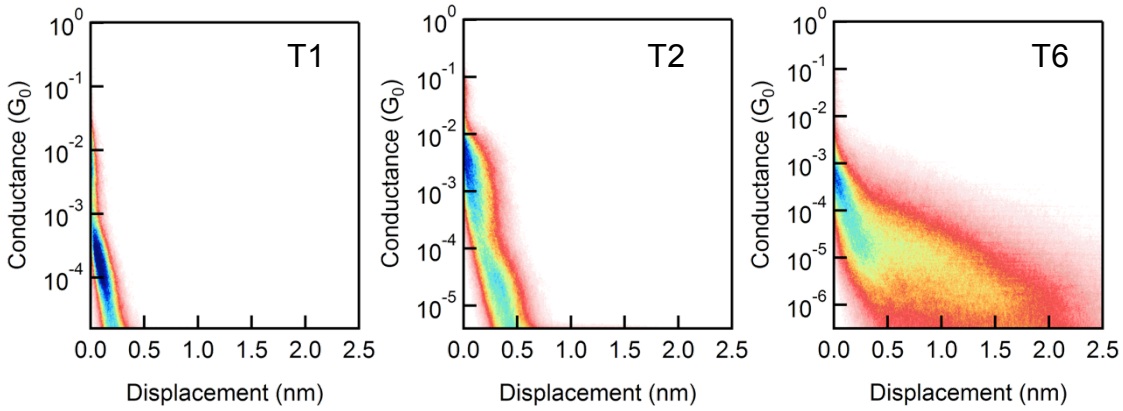
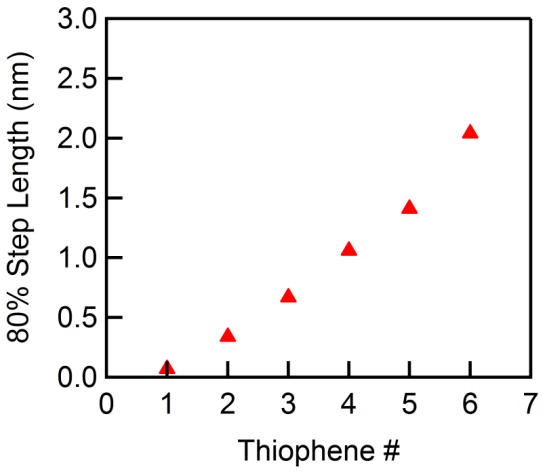


Figure S7. 2D conductance histograms for T1, T2 and T6.

Figure S8. The relationship between the number of thiophene units and the observed step length. Step-lengths are computed by integrating all counts in the conductance feature, and creating a 1D line profile. The plotted step-length is then obtained by finding where the line profile falls to 20% of its peak value.



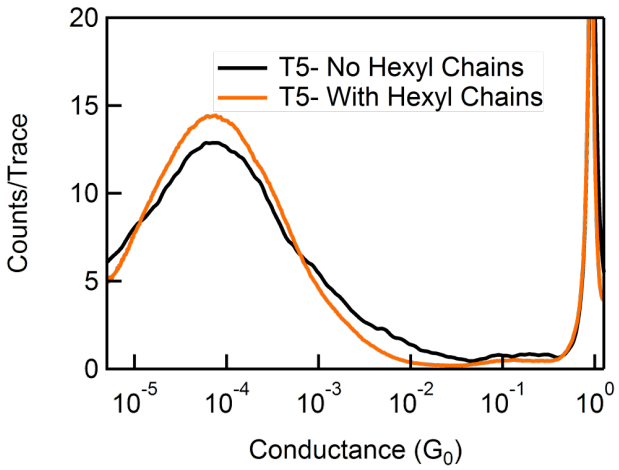


Figure S9. Logarithmically binned conductance histograms for a T5 molecule with and without hexyl chains.

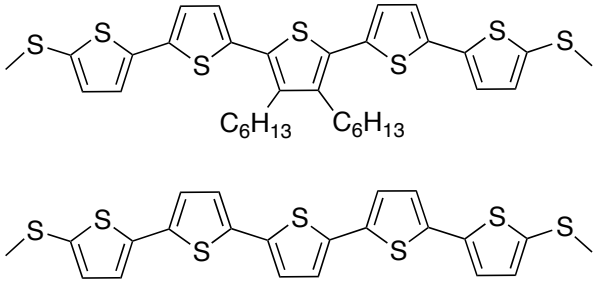
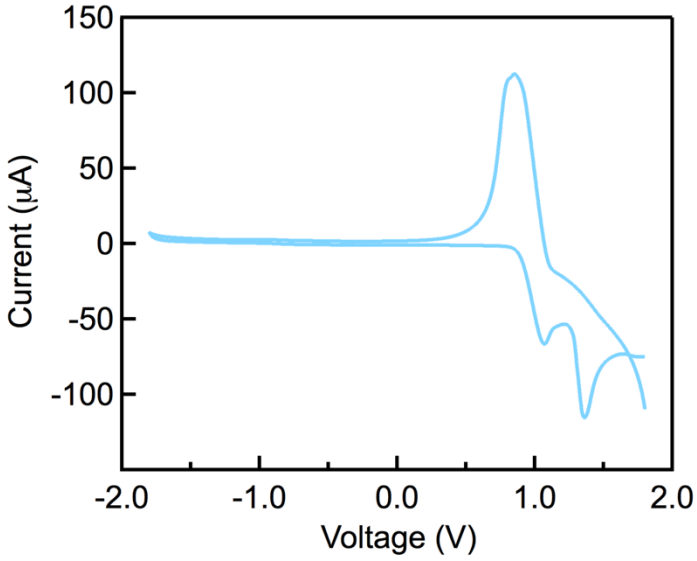
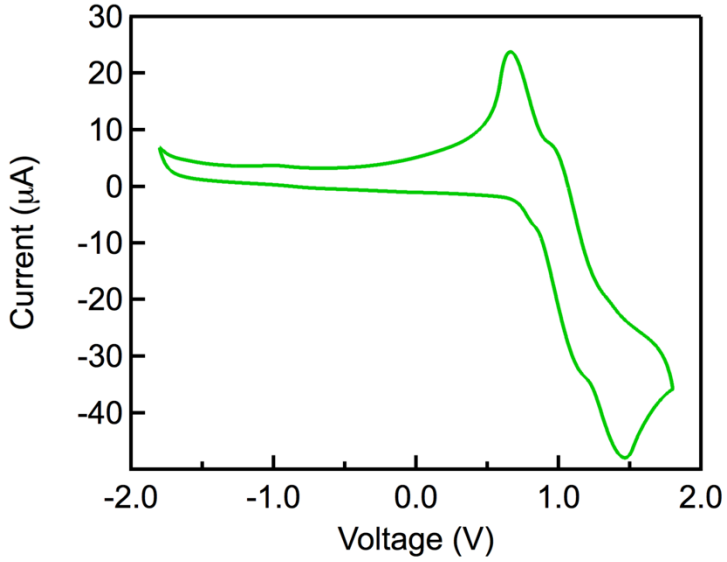


Figure S10.
Cyclic voltammograms performed in dichloromethane (DCM) with Ag/AgCl reference electrode, 0.1M tetrabutyl ammonium hexafluorophosphate as the electrolyte and a scan rate of 50 mVs^{-1} for T2 to T6

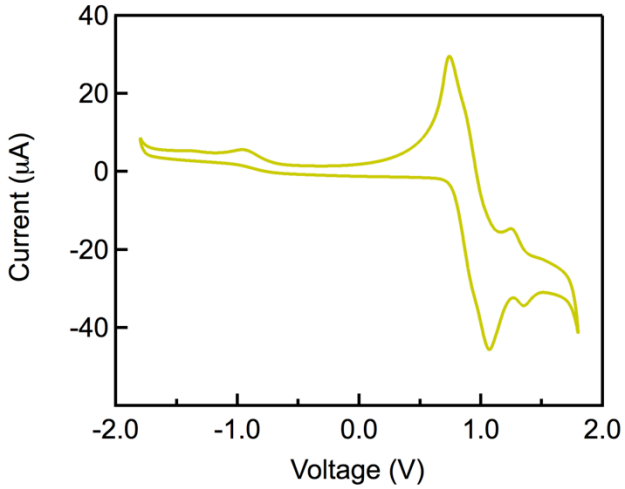
T2



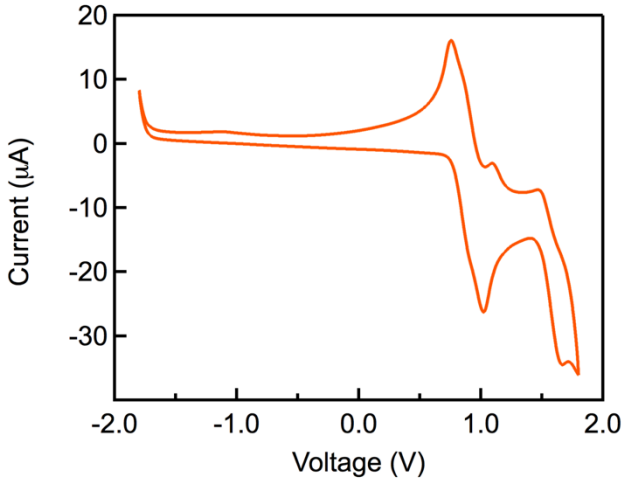
T3



T4


40
20
0
-20
-40
Current (μA)
-2.0
-1.0
0.0
1.0
2.0
Voltage (V)

T5


20
10
0
-10
-20
-30
Current (μA)
-2.0
-1.0
0.0
1.0
2.0
Voltage (V)

T6

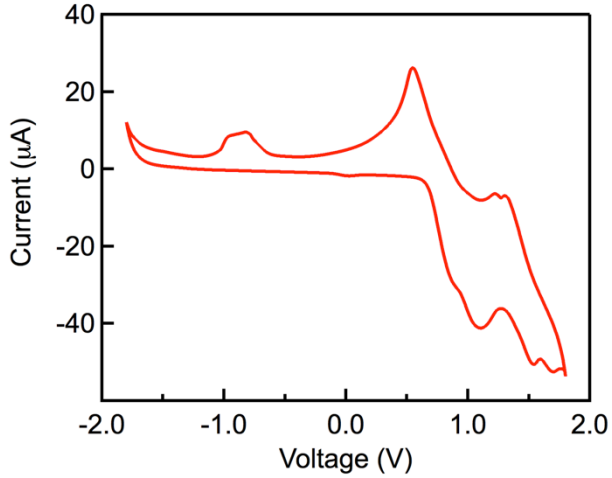
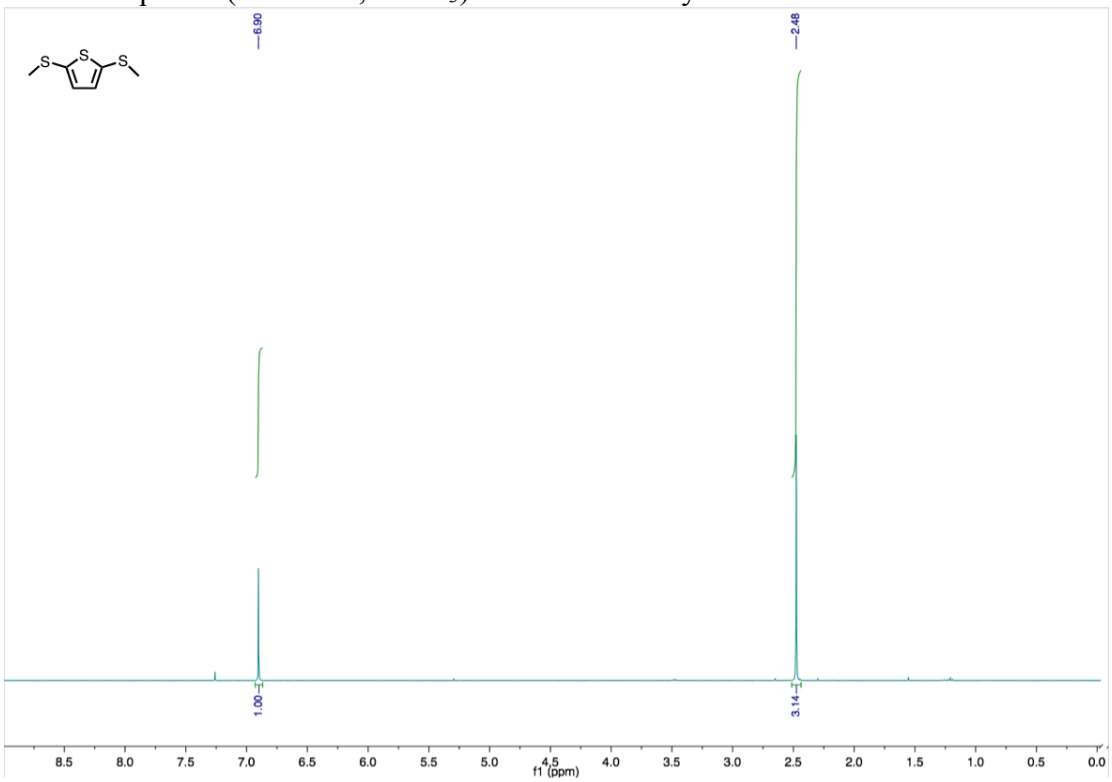
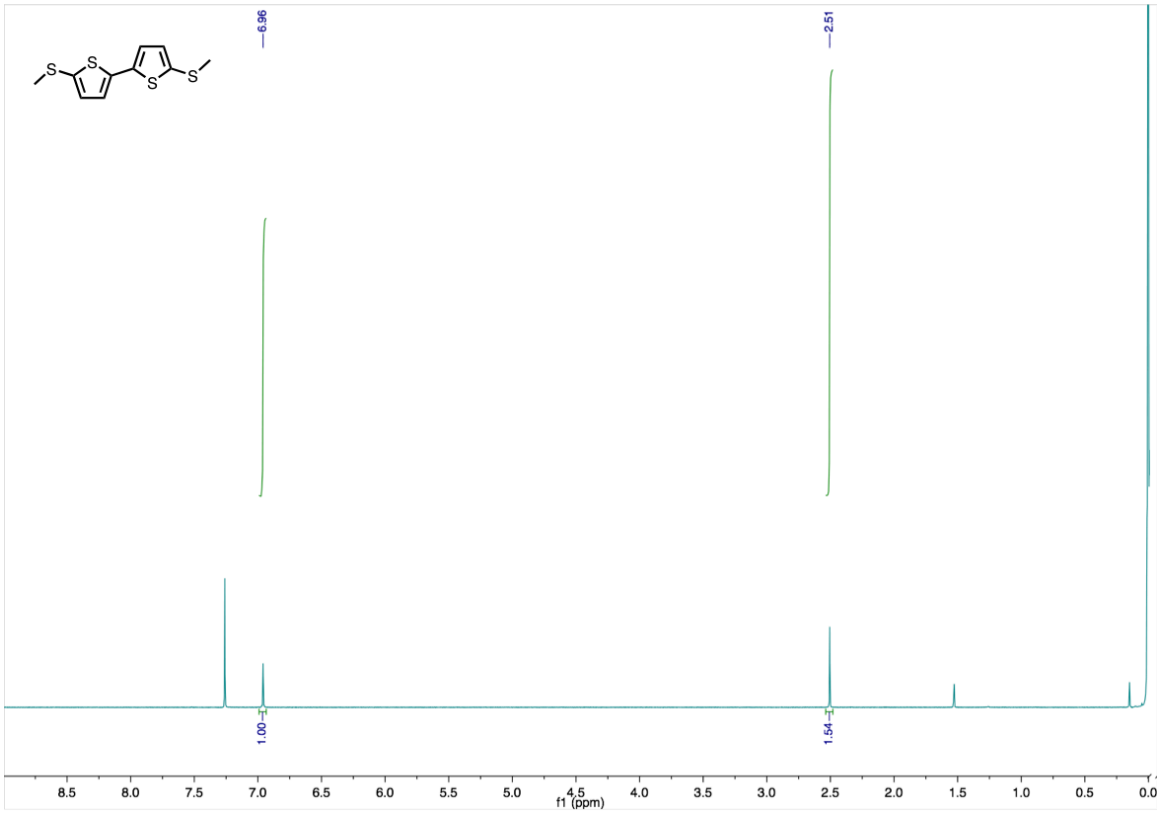
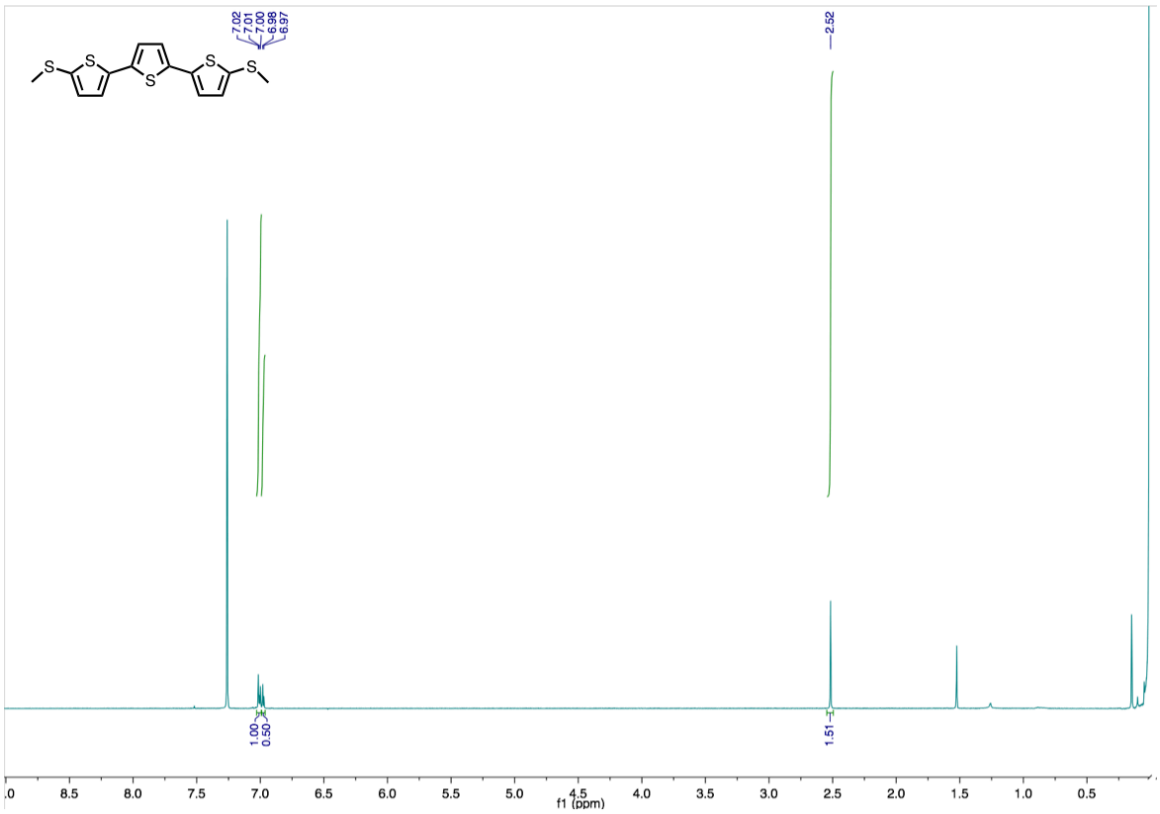
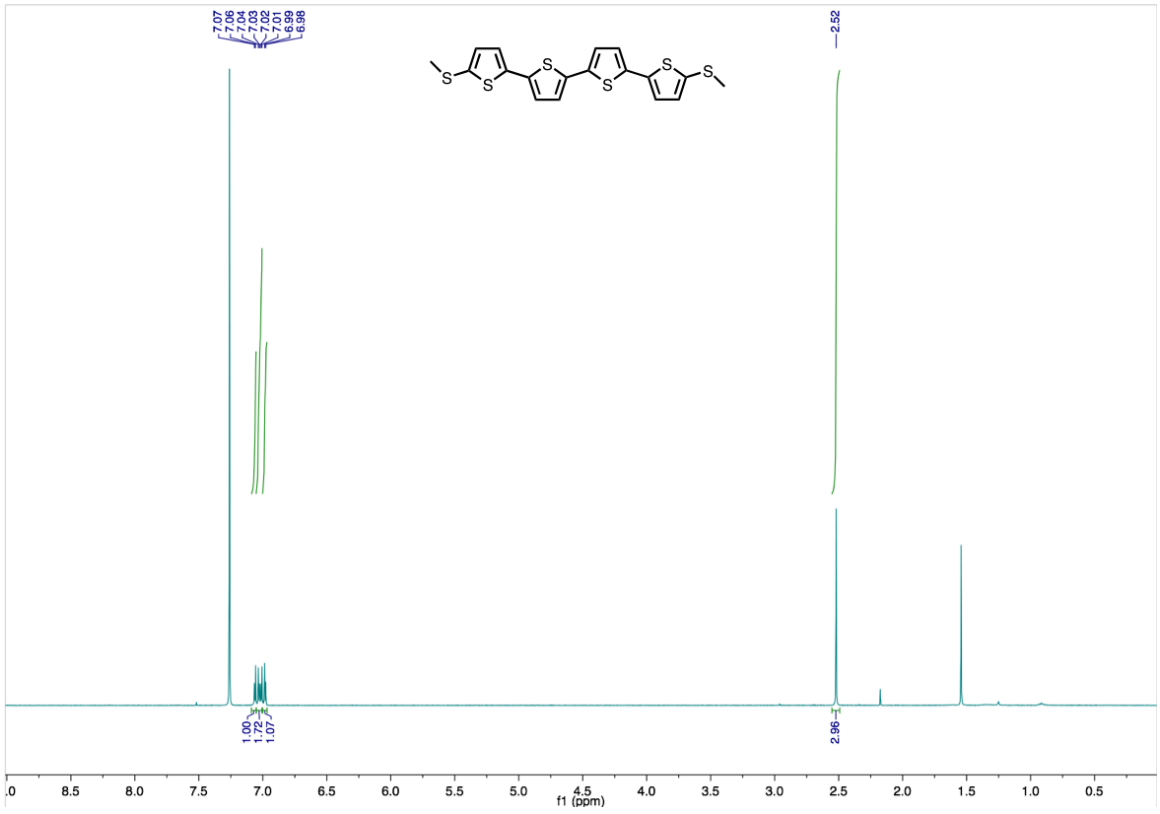

40
20
0
-20
-40
Current (μA)
-2.0
-1.0
0.0
1.0
2.0
Voltage (V)

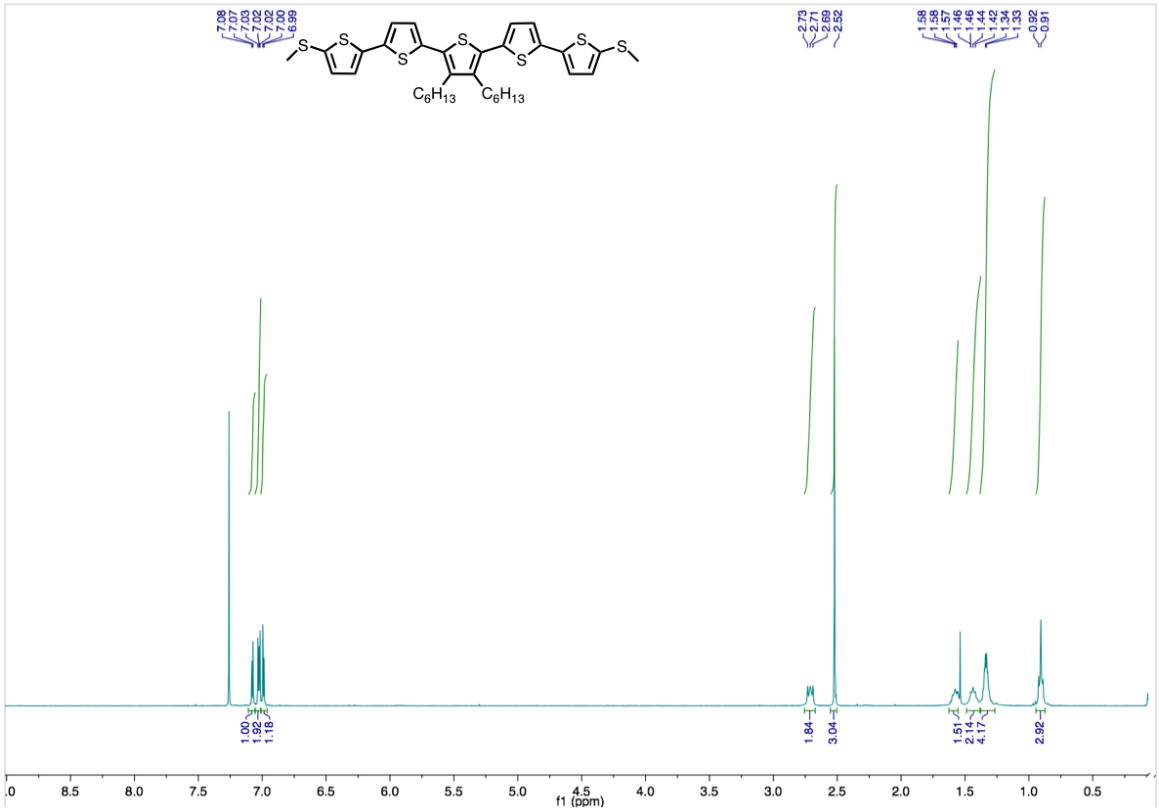
Figure S11.
^{1}H NMR spectra (400 MHz, $CDCl_3$) for the Tn family

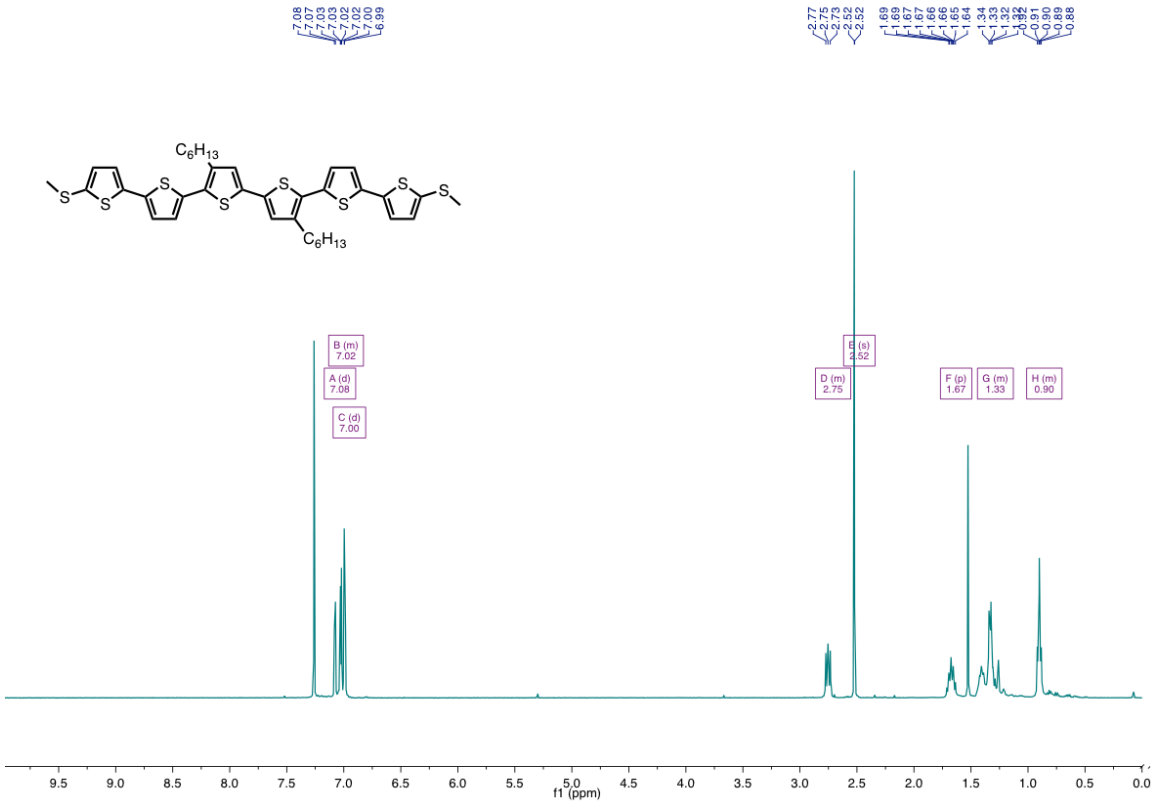




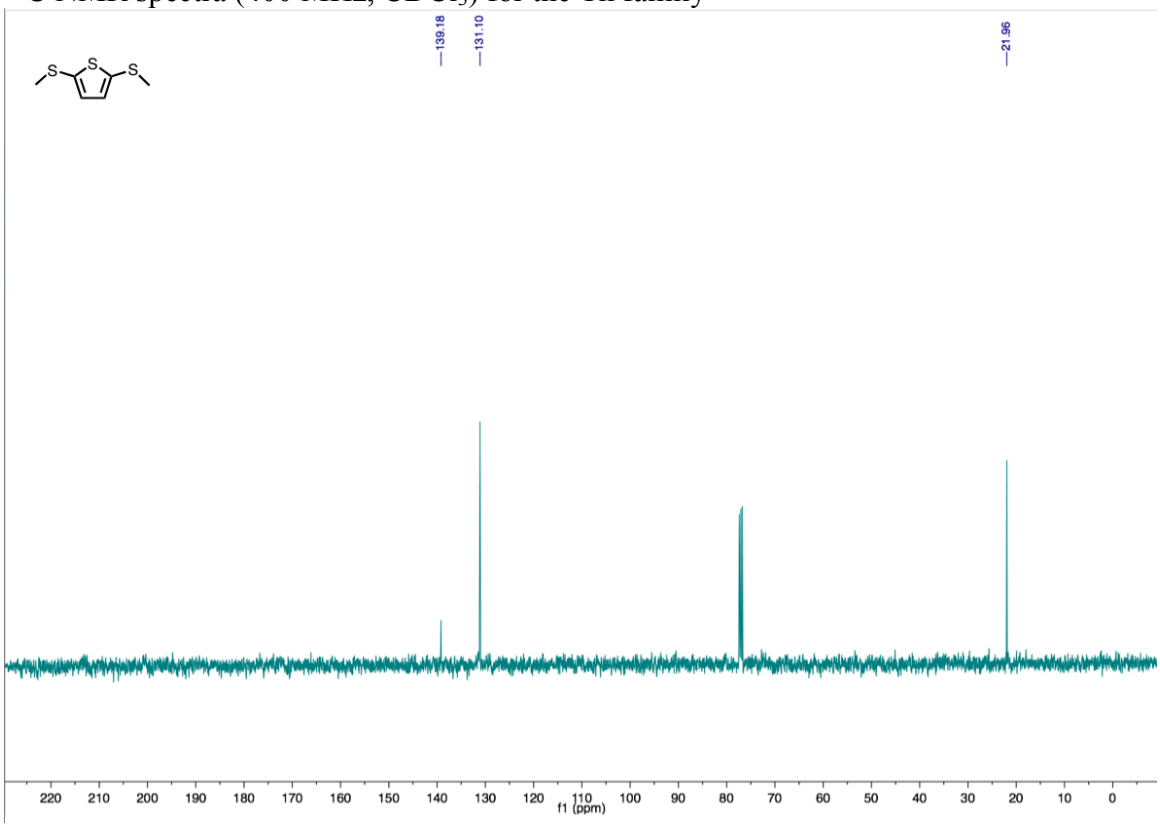

7.02
7.01
7.00
6.98
6.97
2.52
1.00
0.50
1.51
f1 (ppm)

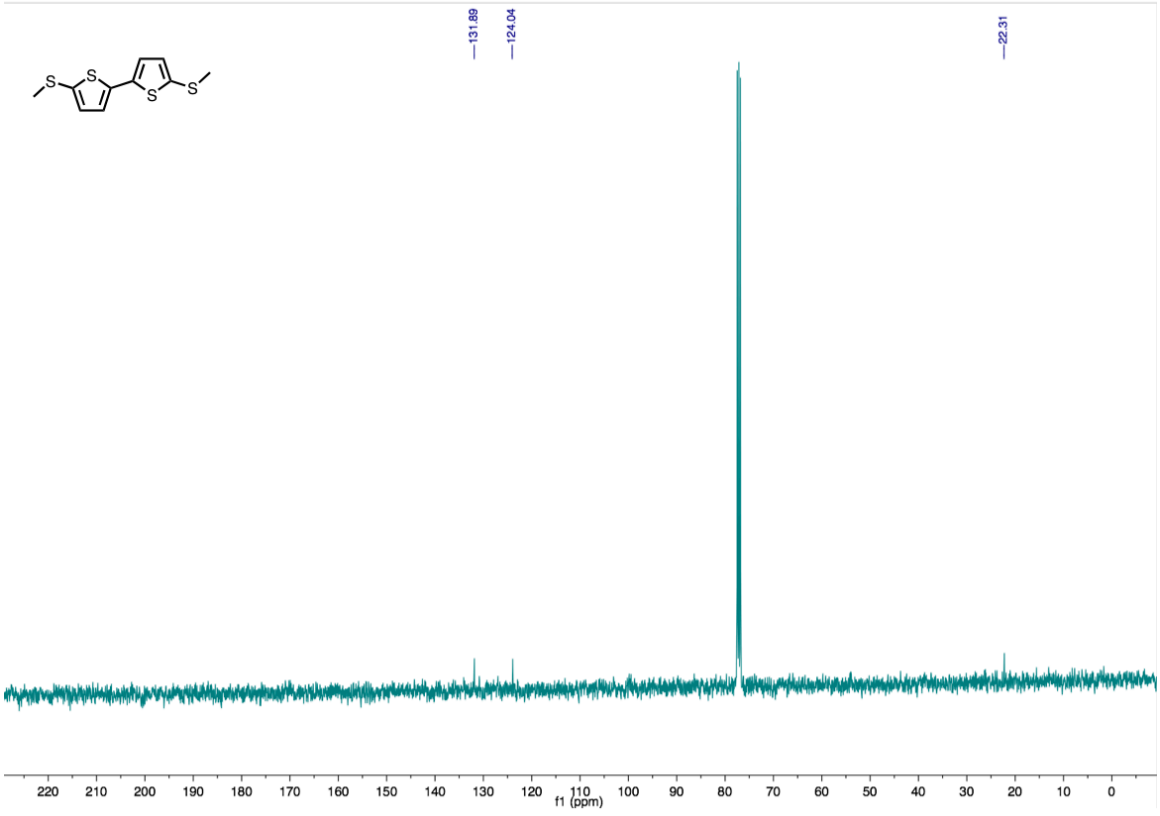

7.07
7.06
7.04
7.03
7.02
7.01
6.99
6.98
2.52
1.00
1.72
1.07
2.96
f1 (ppm)

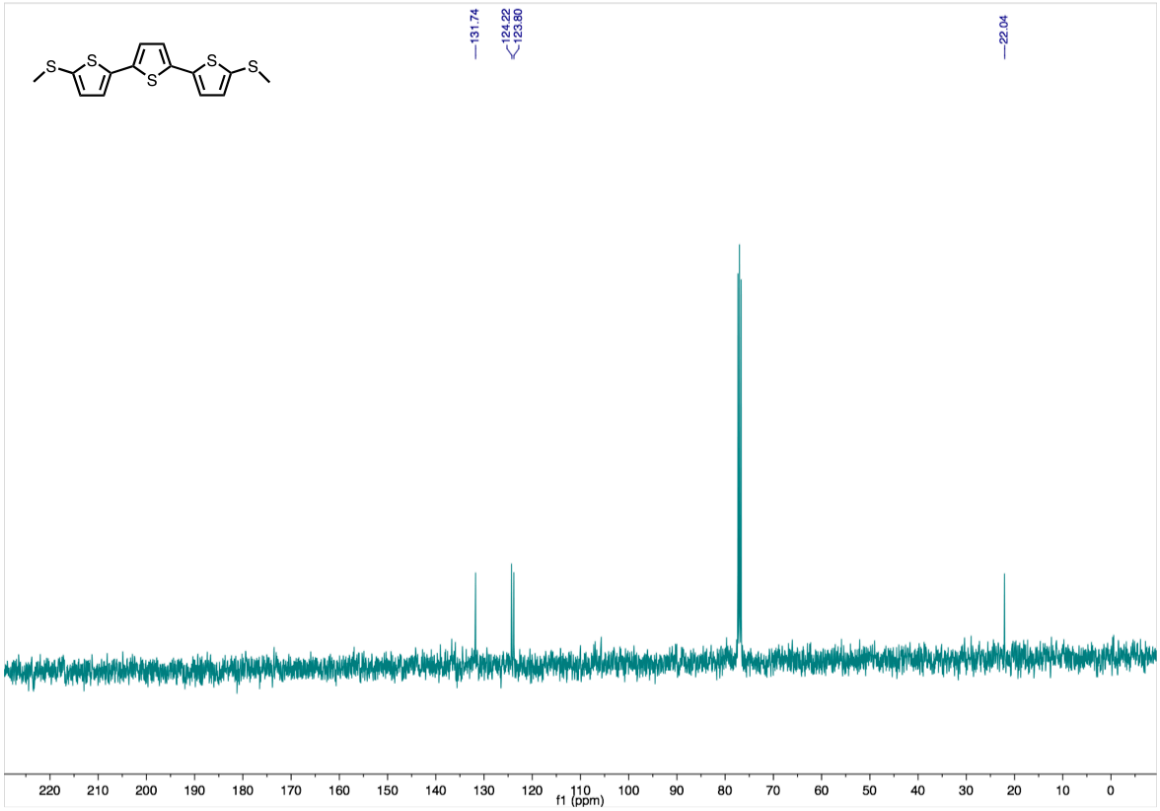

7.08
7.07
7.03
7.02
7.02
7.00
6.99
2.73
2.71
2.69
2.52
1.58
1.58
1.57
1.46
1.46
1.44
1.42
1.34
1.33
0.92
0.91
C_6H_{13}
C_6H_{13}
1.00
1.92
1.18
1.84
3.04
1.51
2.14
4.17
2.92
f1 (ppm)

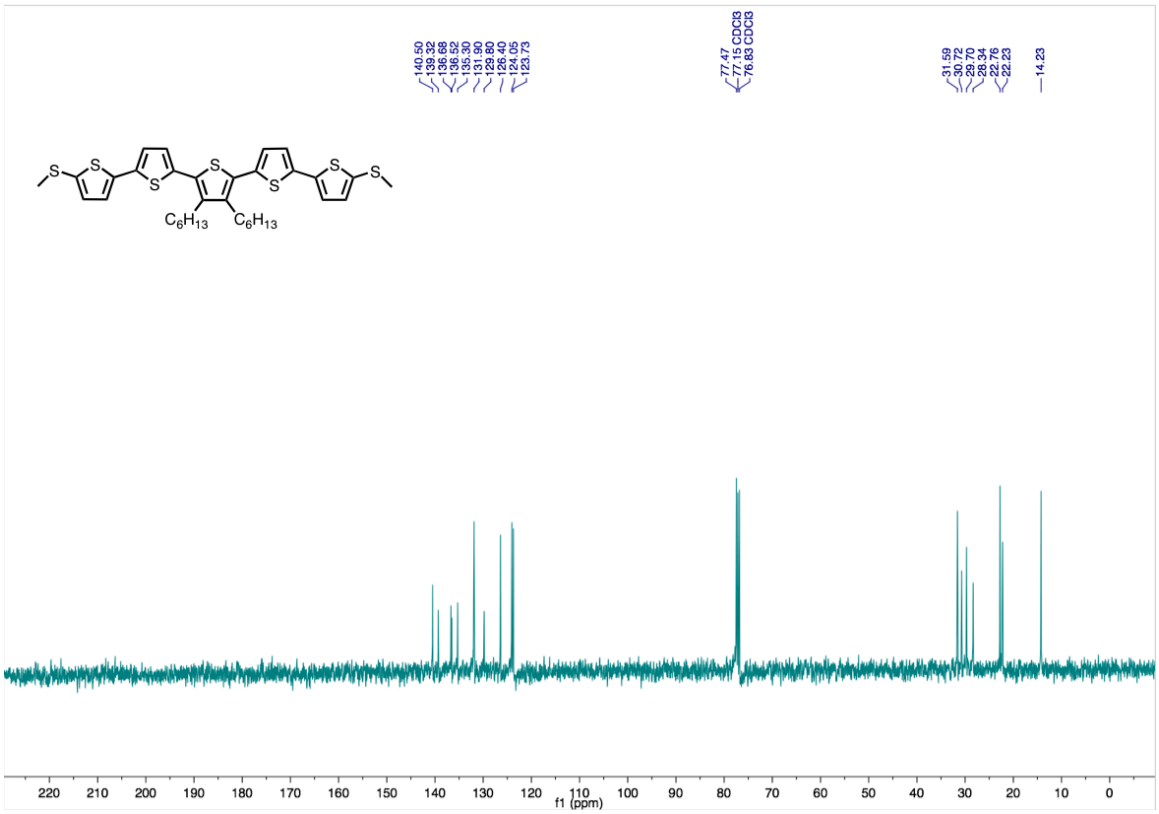

7.08
7.07
7.03
7.02
7.02
7.00
6.99
2.77
2.75
2.73
2.52
2.52
1.69
1.69
1.67
1.67
1.66
1.66
1.65
1.64
1.34
1.33
1.32
0.91
0.90
0.89
0.88
C_6H_{13}
C_6H_{13}
B (m)
7.02
A (d)
7.08
C (d)
7.00
E (s)
2.52
D (m)
2.75
F (p)
1.67
G (m)
1.33
H (m)
0.90
f1 (ppm)

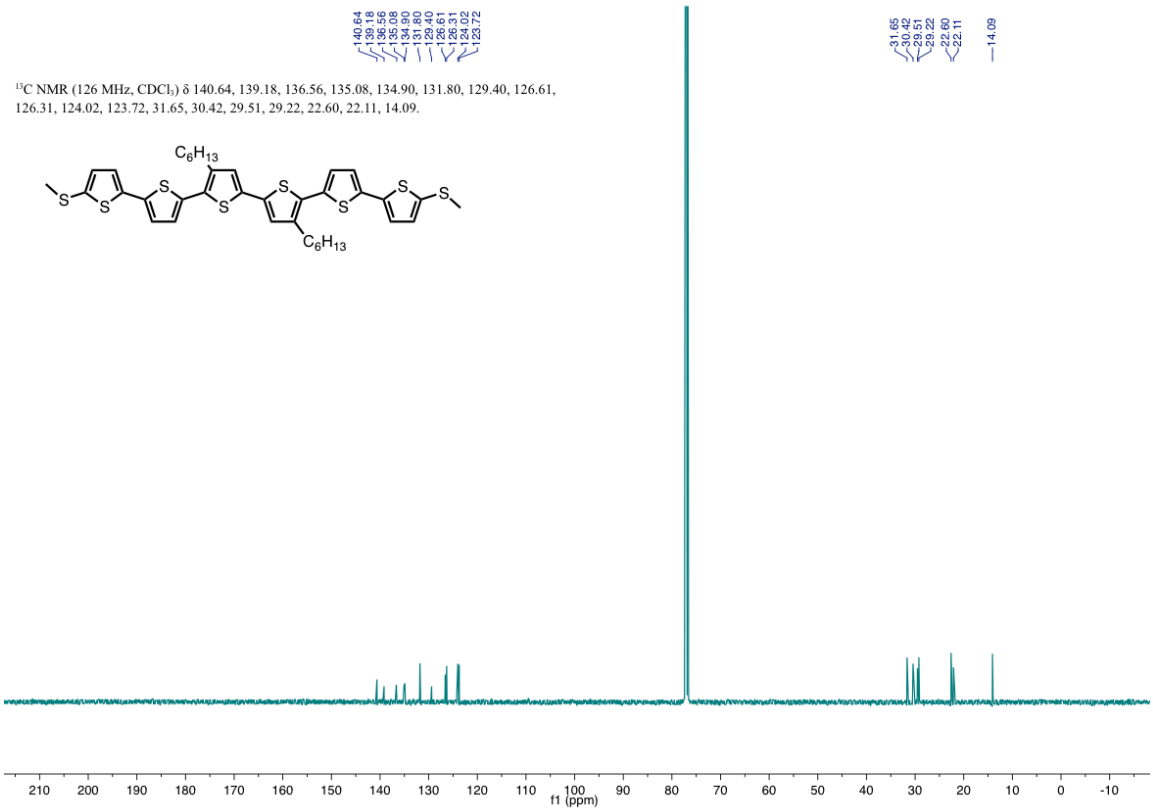
^{13}C NMR spectra (400 MHz, $CDCl_3$) for the Tn family






131.74
124.22
123.60
22.04
f1 (ppm)


140.50
139.32
136.68
136.52
135.30
131.90
129.80
126.40
124.05
123.73
77.47
77.15 CDCl3
76.83 CDCl3
31.59
30.72
29.70
29.34
28.76
22.23
14.23
C6H13
C6H13
f1 (ppm)



^{13}C NMR (126 MHz, $CDCl_3$) δ 140.64, 139.18, 136.56, 135.08, 134.90, 131.80, 129.40, 126.61, 126.31, 124.02, 123.72, 31.65, 30.42, 29.51, 29.22, 22.60, 22.11, 14.09.