

# Truxene-centered Electron Acceptors for Non-Fullerene Solar Cells Alkyl Chain and Branched Arm Engineering

Kaiwen Lin<sup>a,b\*</sup>, Wenhao Du<sup>a</sup>, Shuqi Shen<sup>a</sup>, Haoshen Liang<sup>a</sup>, Xiaobin Zhang<sup>a</sup>, Manjun Xiao<sup>c</sup> and Yuehui Wang<sup>a</sup>

<sup>a</sup> Department of Materials and Food, University of Electronic Science and Technology of China Zhongshan Institute, Zhongshan 528402, China

<sup>b</sup> School of Optoelectronic Science and Engineering, University of Electronic Science and Technology of China, Chengdu 610054, China

<sup>c</sup> College of Chemistry, Key Lab of Environment-Friendly Chemistry and Application (Ministry of Education), Xiangtan University, Xiangtan 411105, China

\* Correspondence: kevinlin1990@zsc.edu.cn Phone: (+)86-791-88537967. Fax: (+)86-791-83823320.

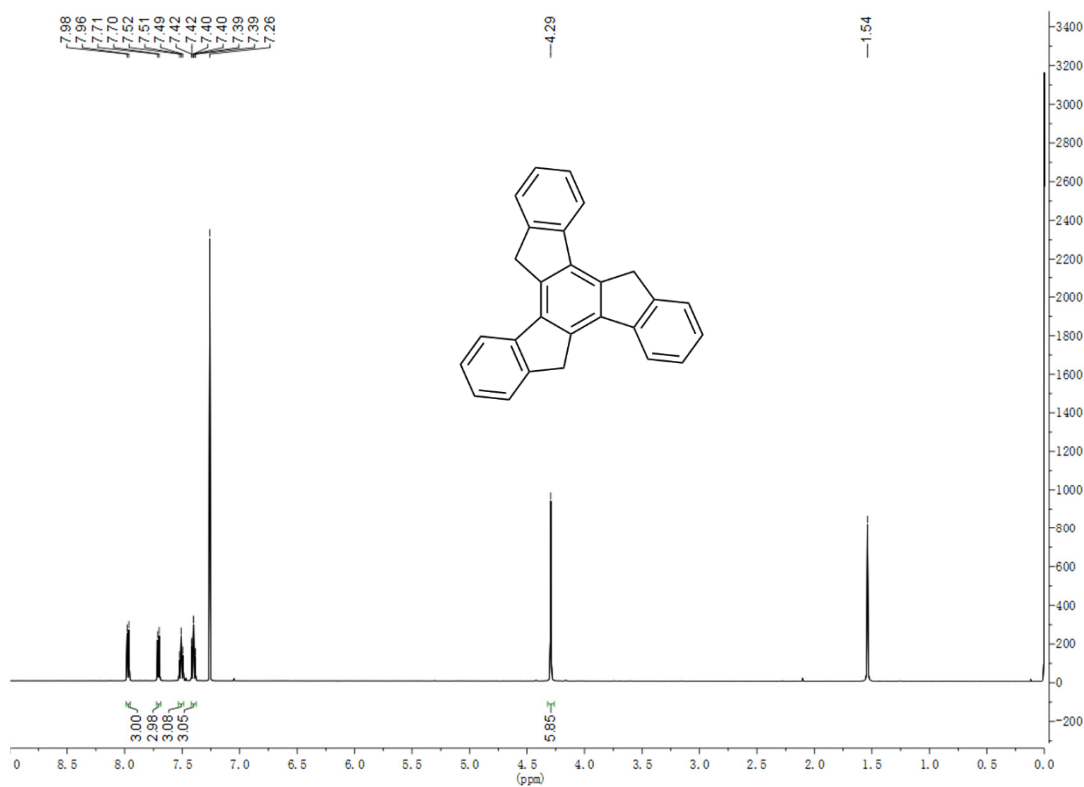


Figure S1. <sup>1</sup>H NMR spectrum of compound 1.

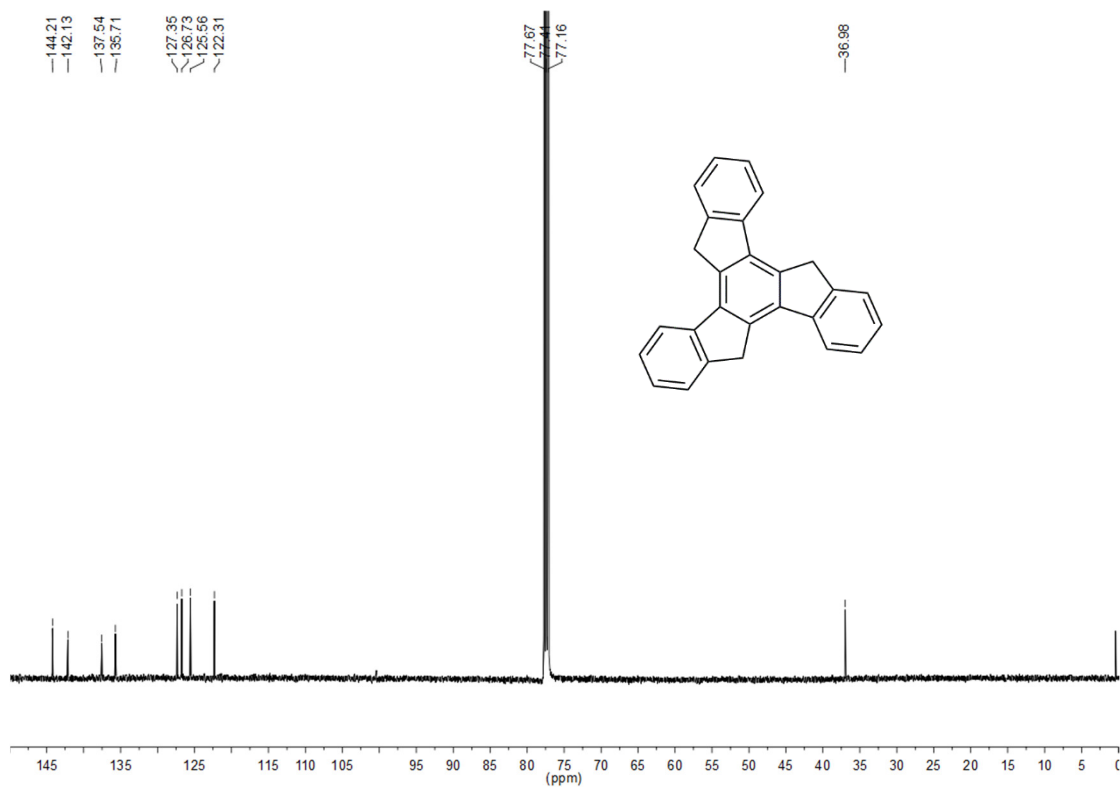


Figure S2. <sup>13</sup>C NMR spectrum of compound 1.

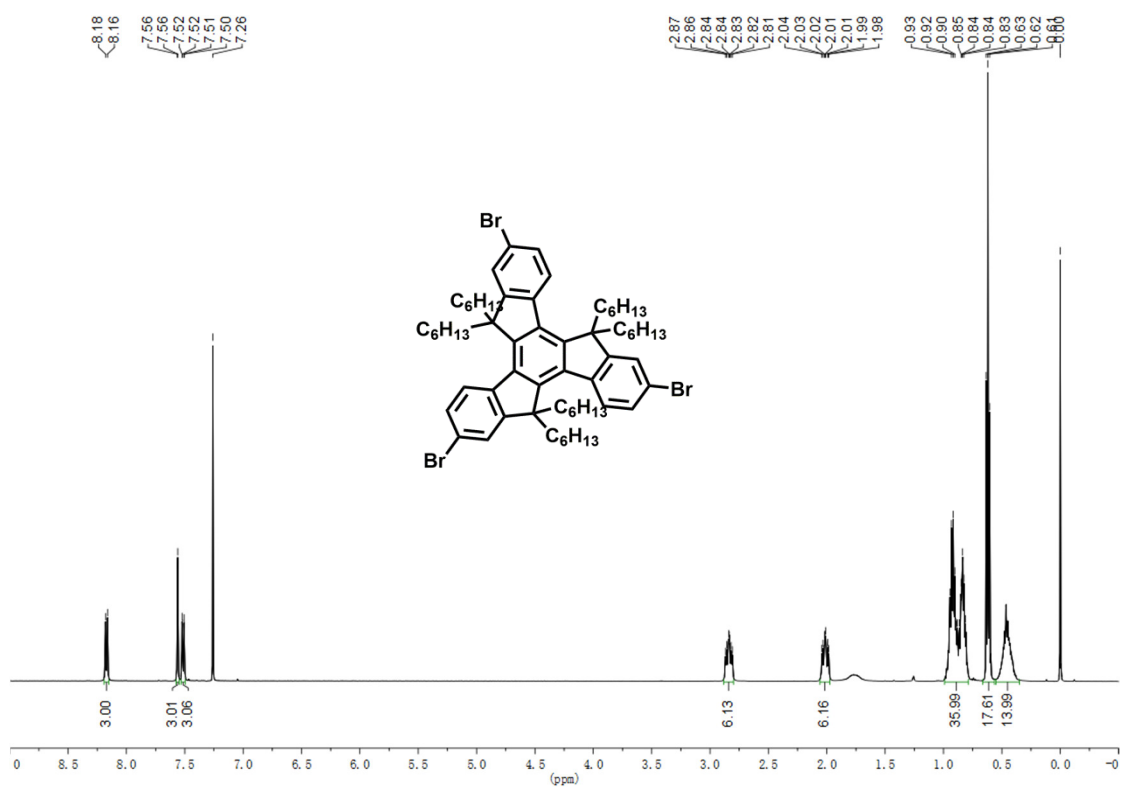


Figure S3. <sup>1</sup>H NMR spectrum of compound **3a**.

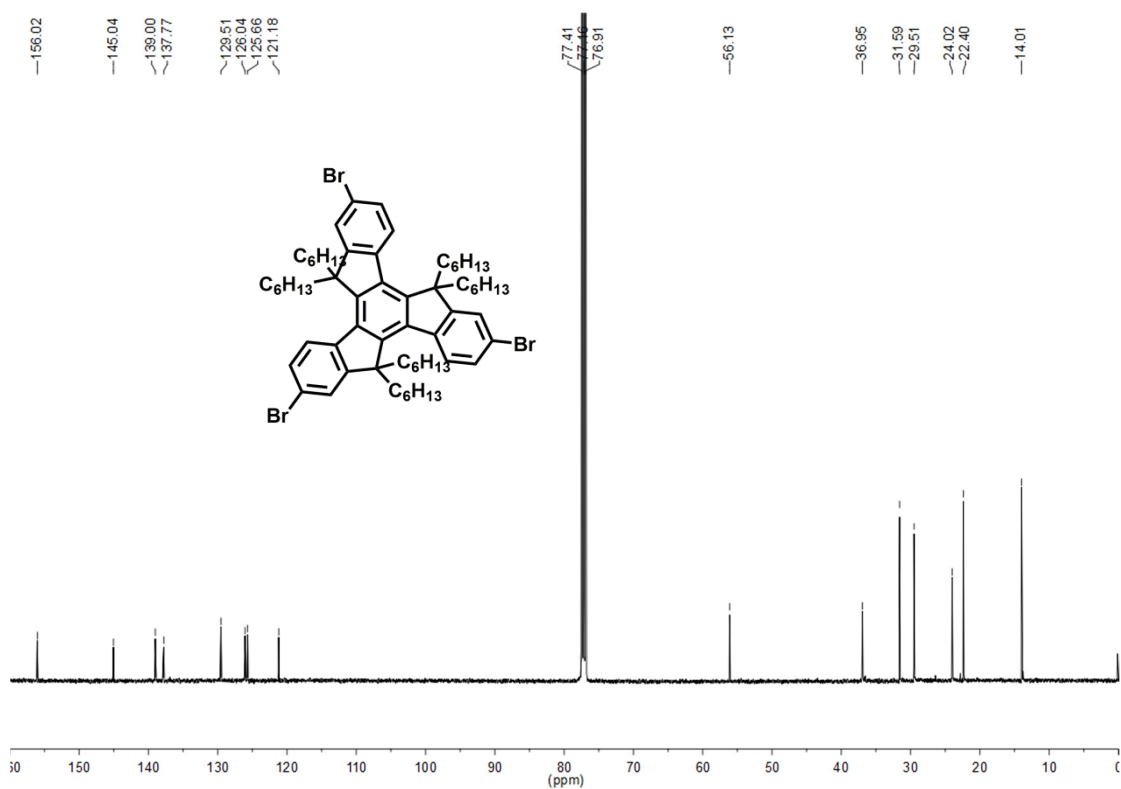


Figure S4. <sup>13</sup>C NMR spectrum of compound **3a**.

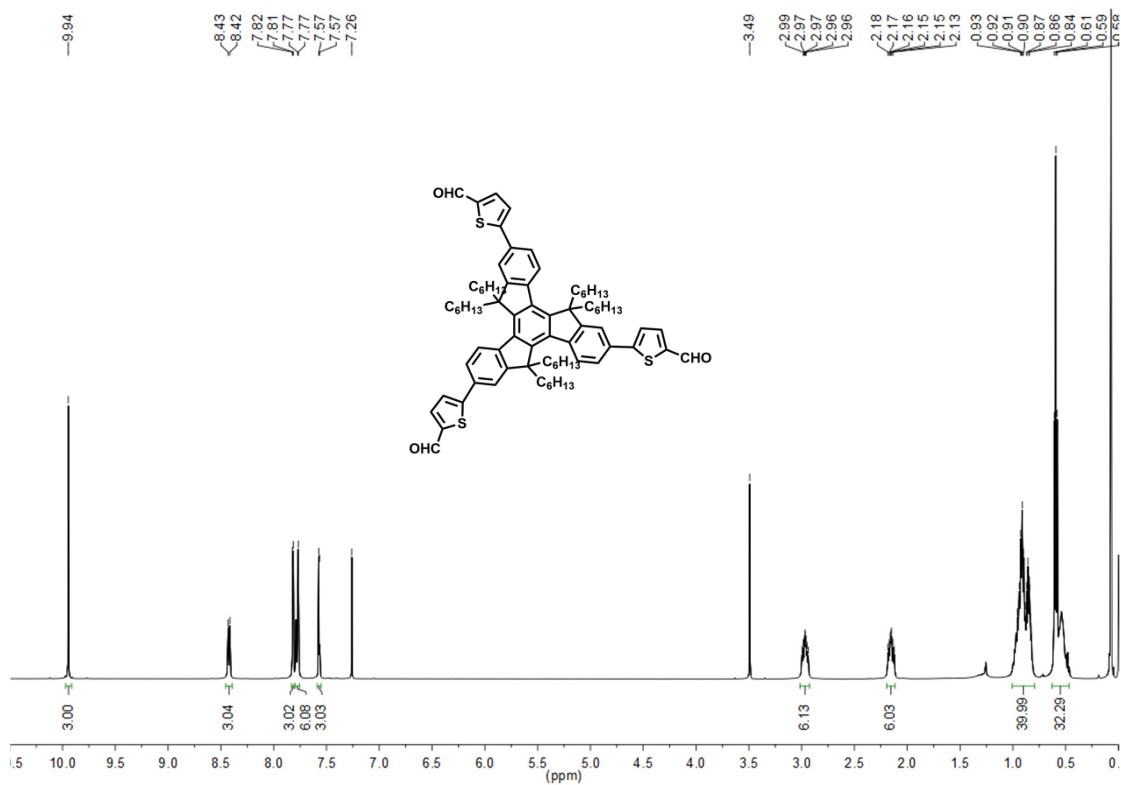


Figure S5 <sup>1</sup>H NMR spectrum of compound 4a

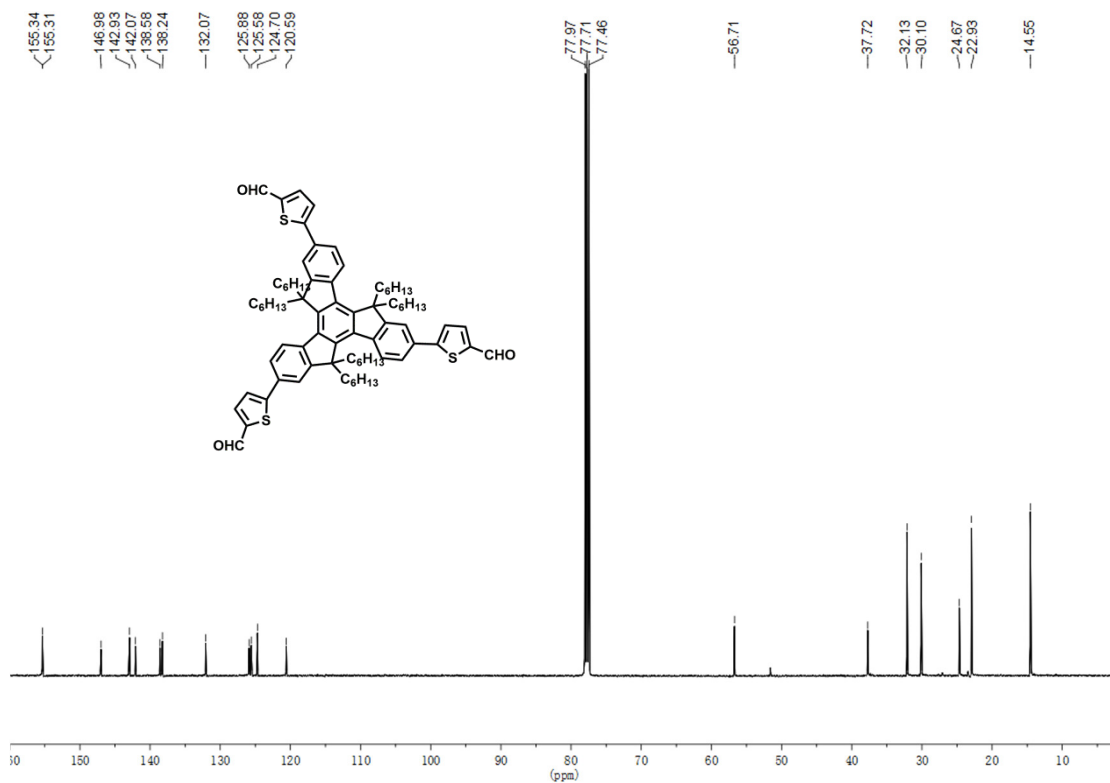


Figure S6 <sup>13</sup>C NMR spectrum of compound 4a

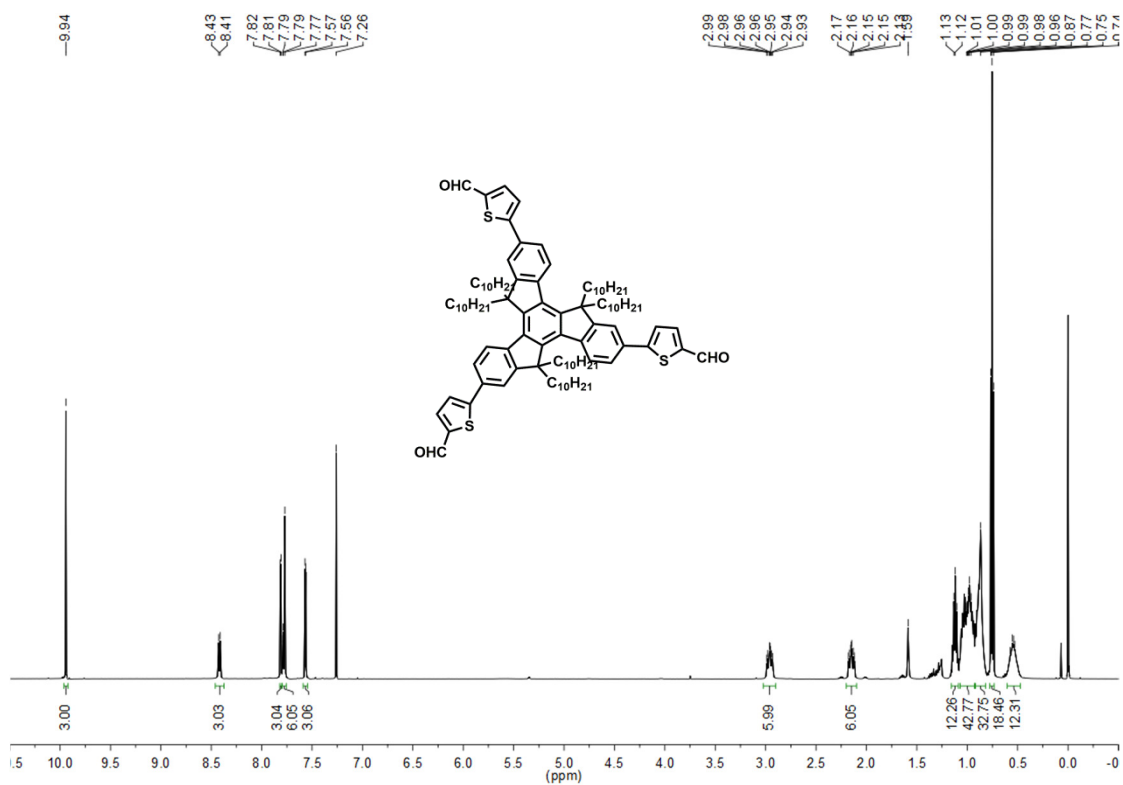


Figure S7 <sup>1</sup>H NMR spectrum of compound 4b

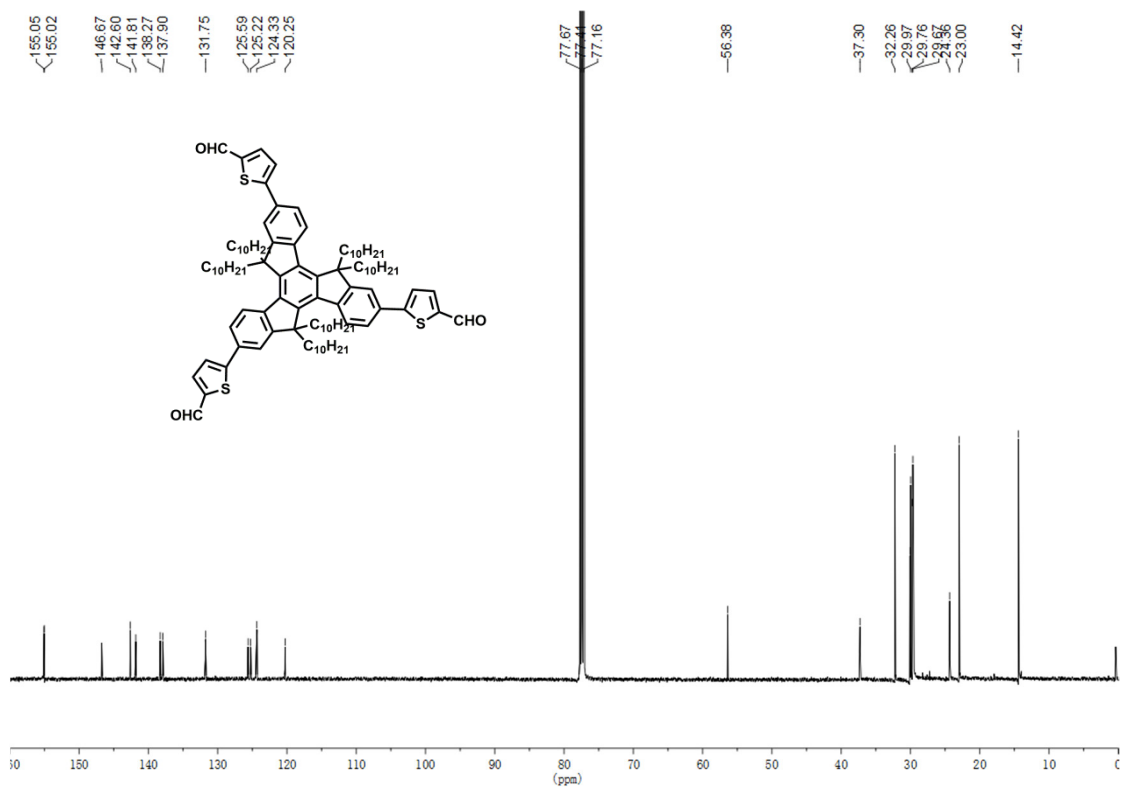


Figure S8 <sup>13</sup>C NMR spectrum of compound 4b

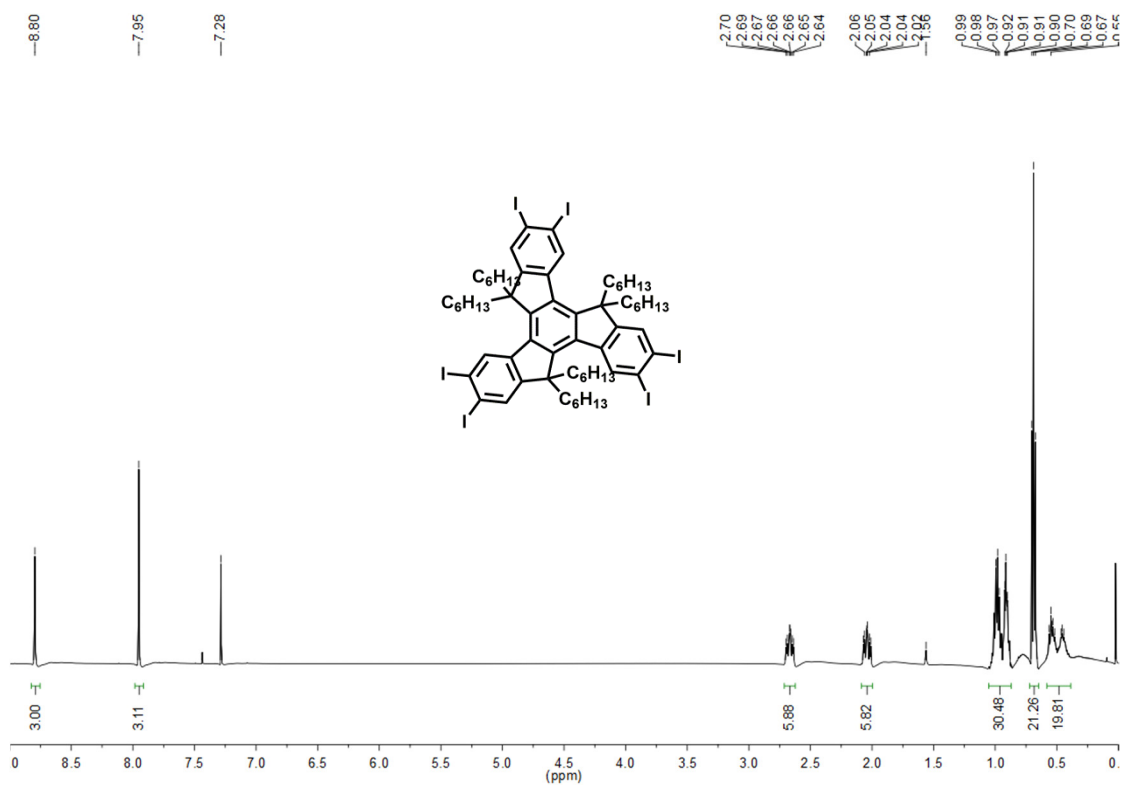


Figure S9 <sup>1</sup>H NMR spectrum of compound 5

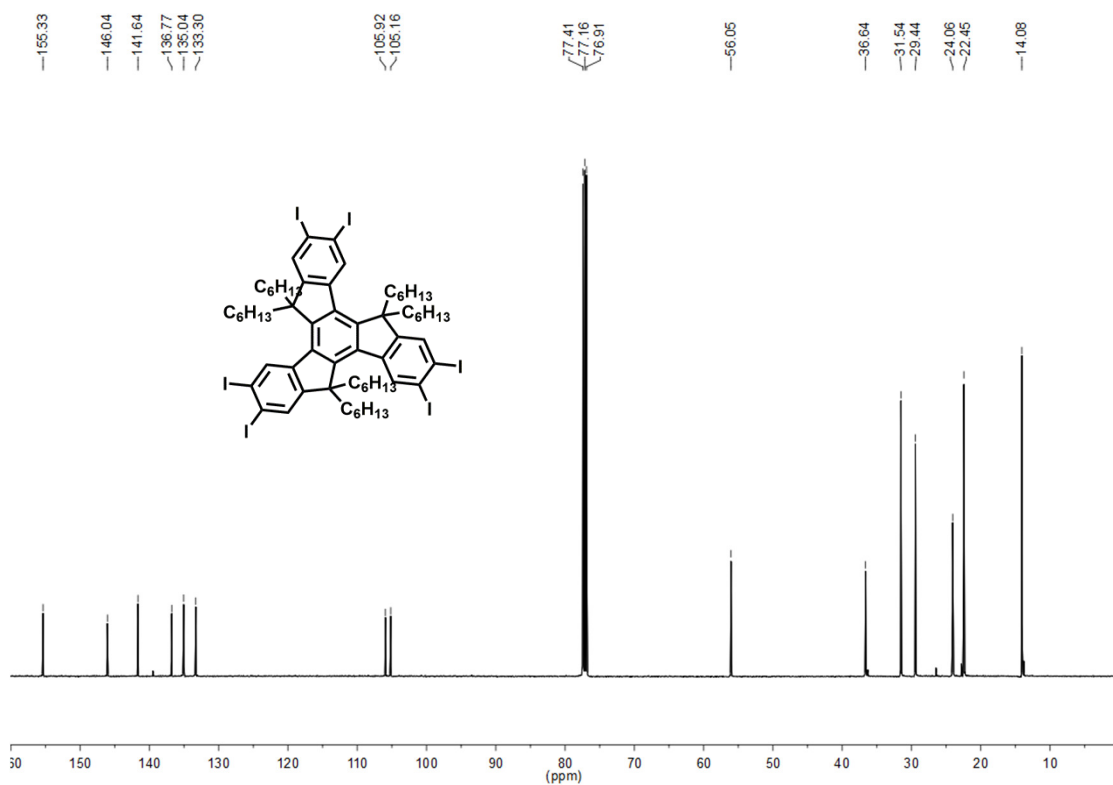


Figure S10 <sup>13</sup>C NMR spectrum of compound 5

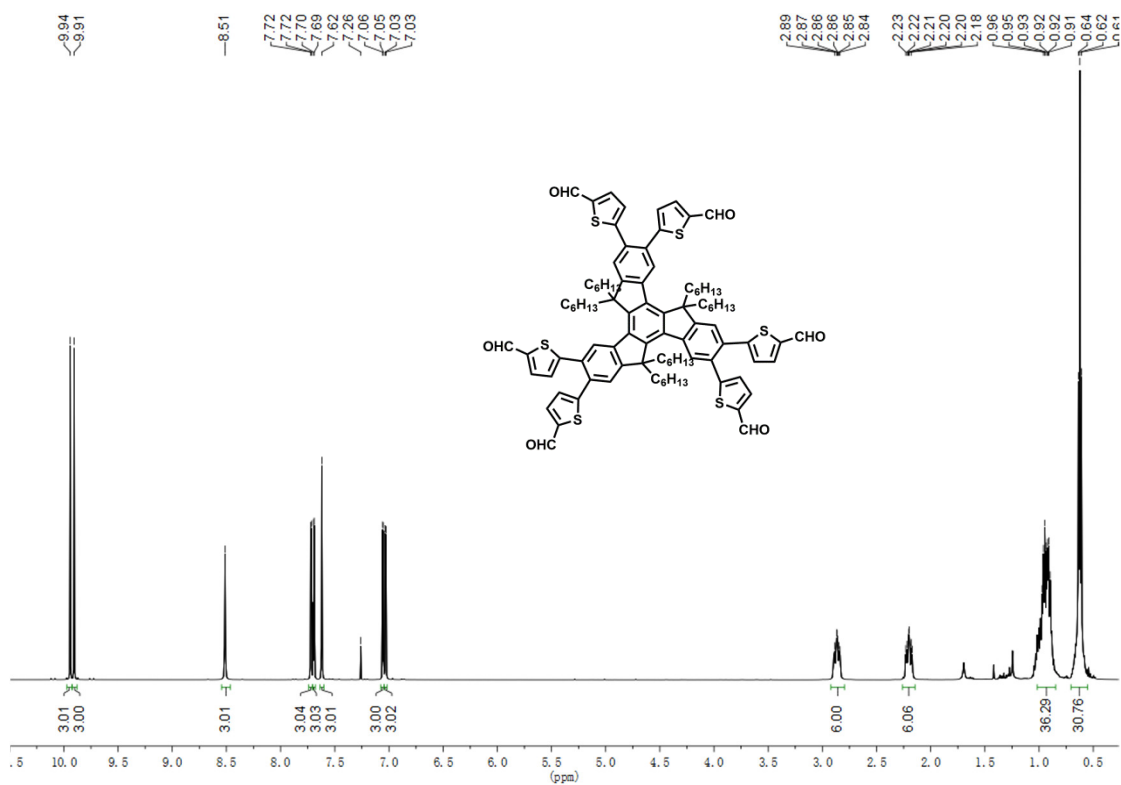


Figure S11 <sup>1</sup>H NMR spectrum of compound **6**

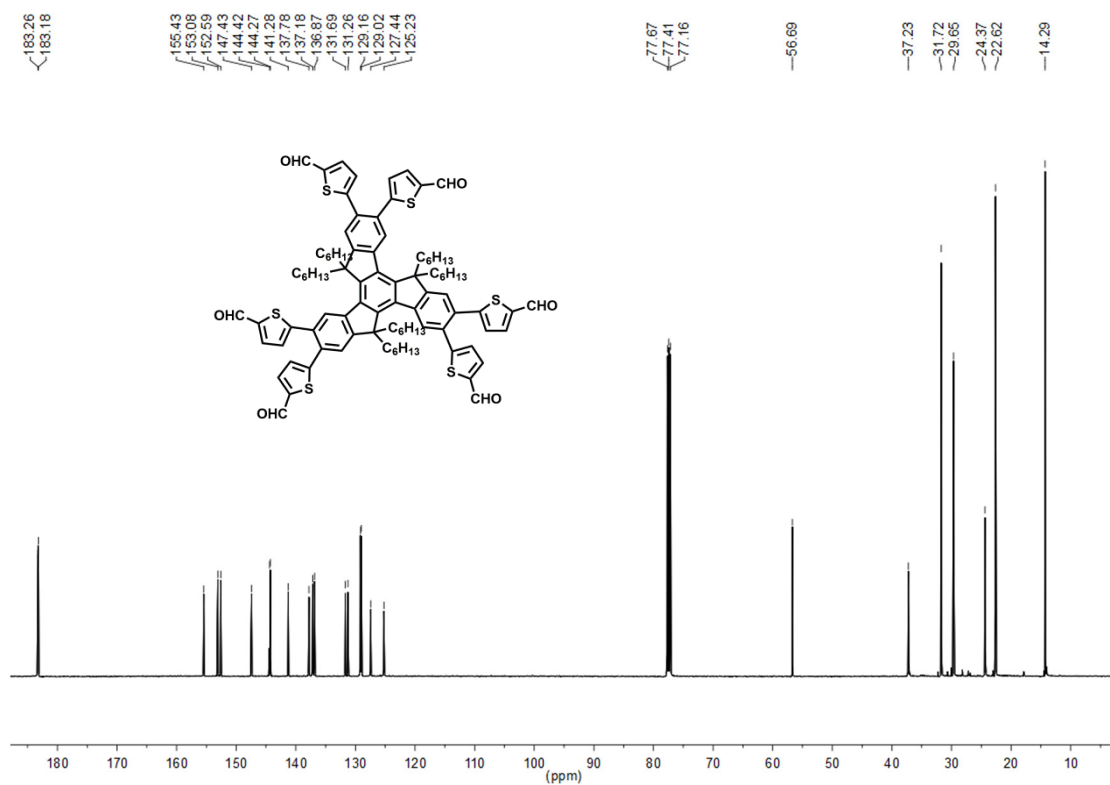
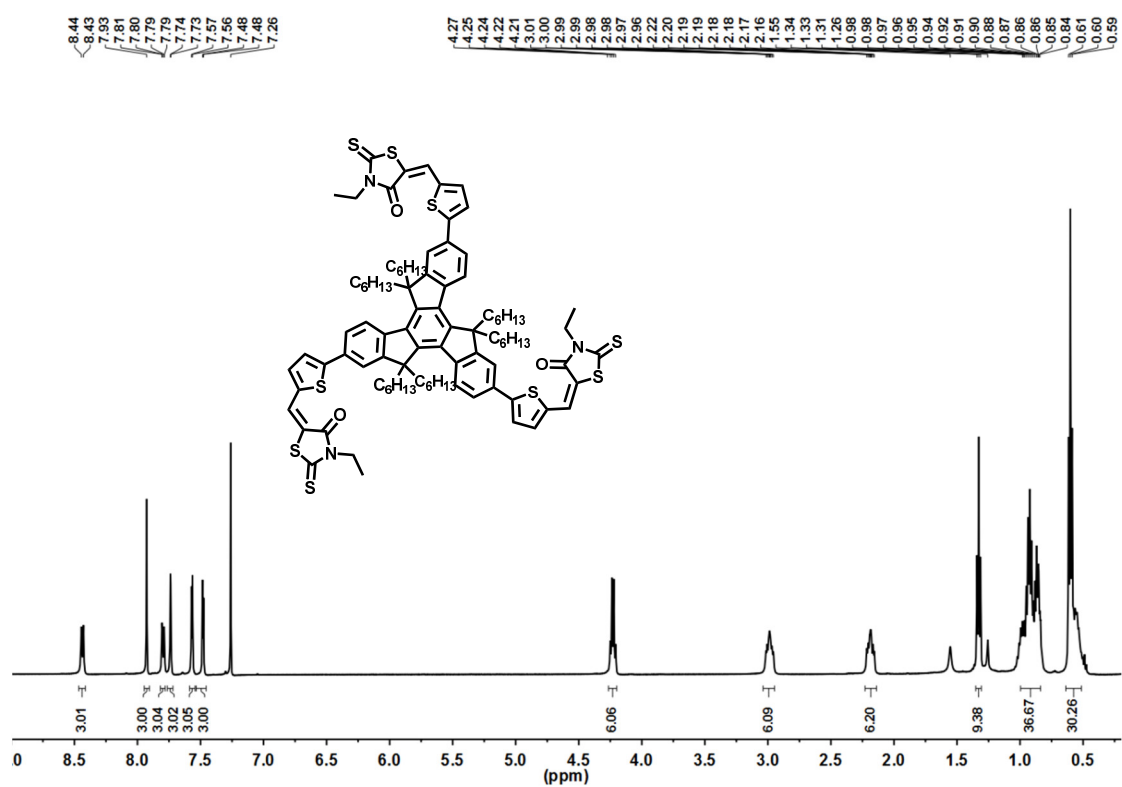
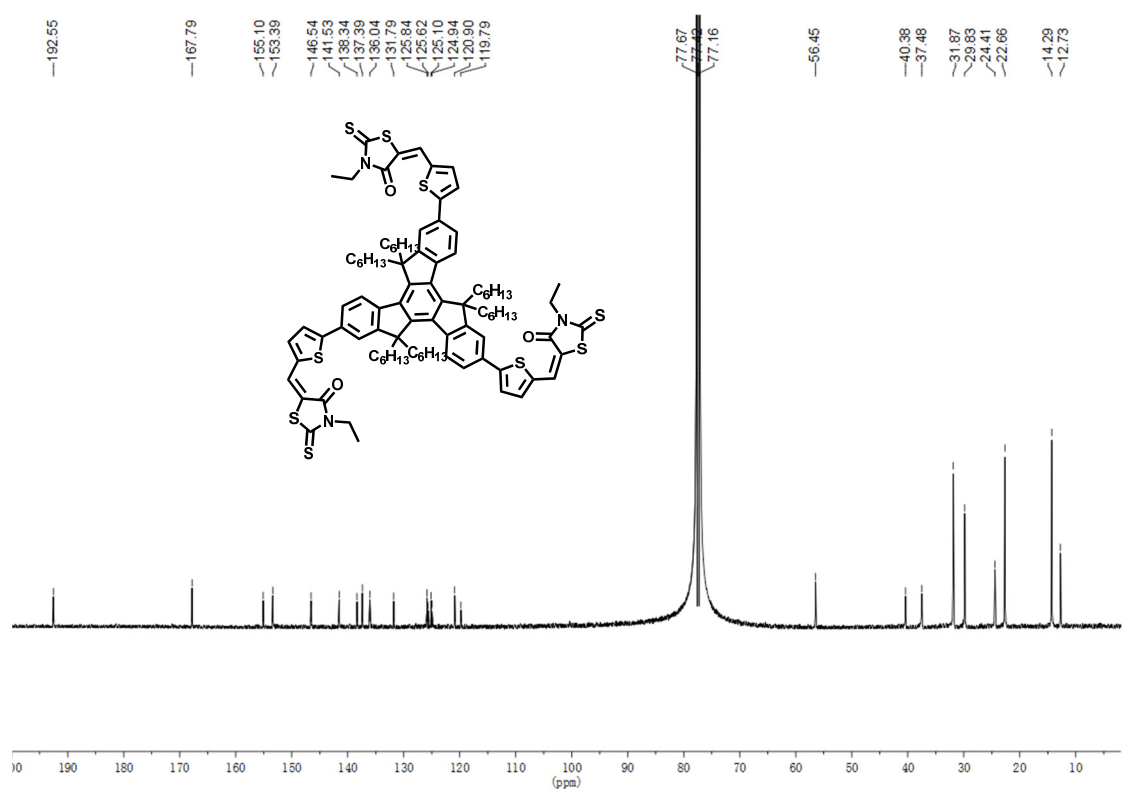


Figure S12 <sup>13</sup>C NMR spectrum of compound **6**

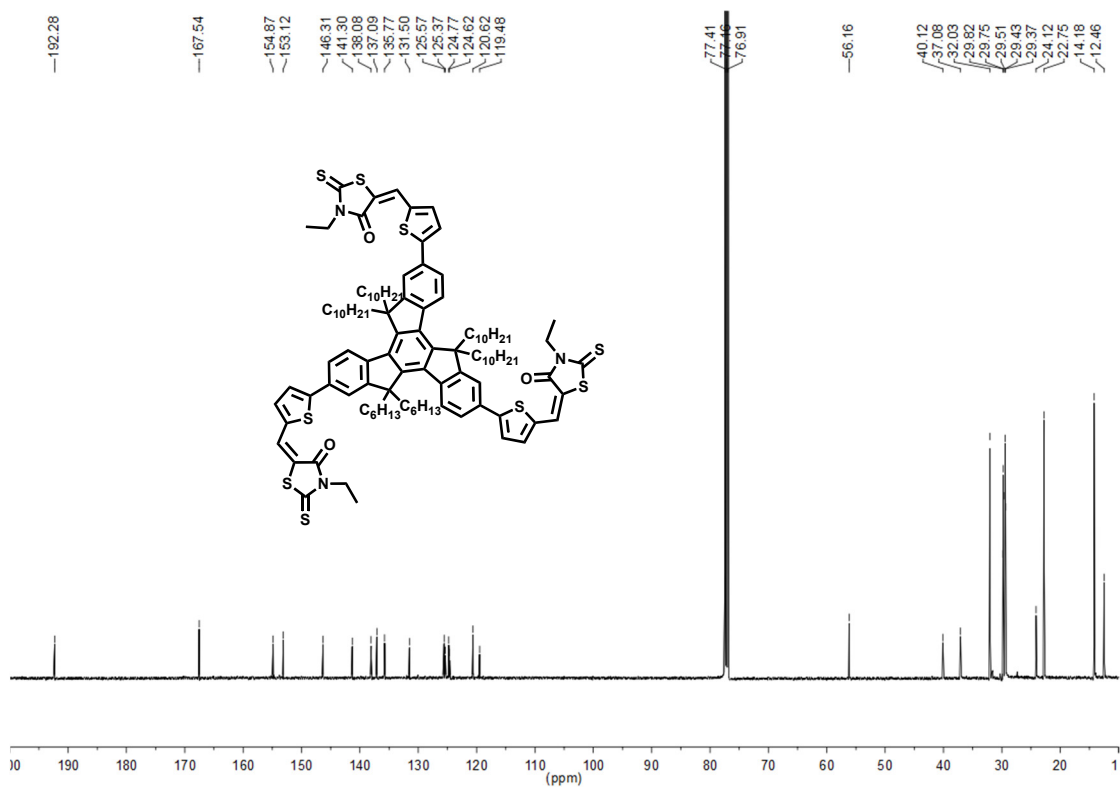
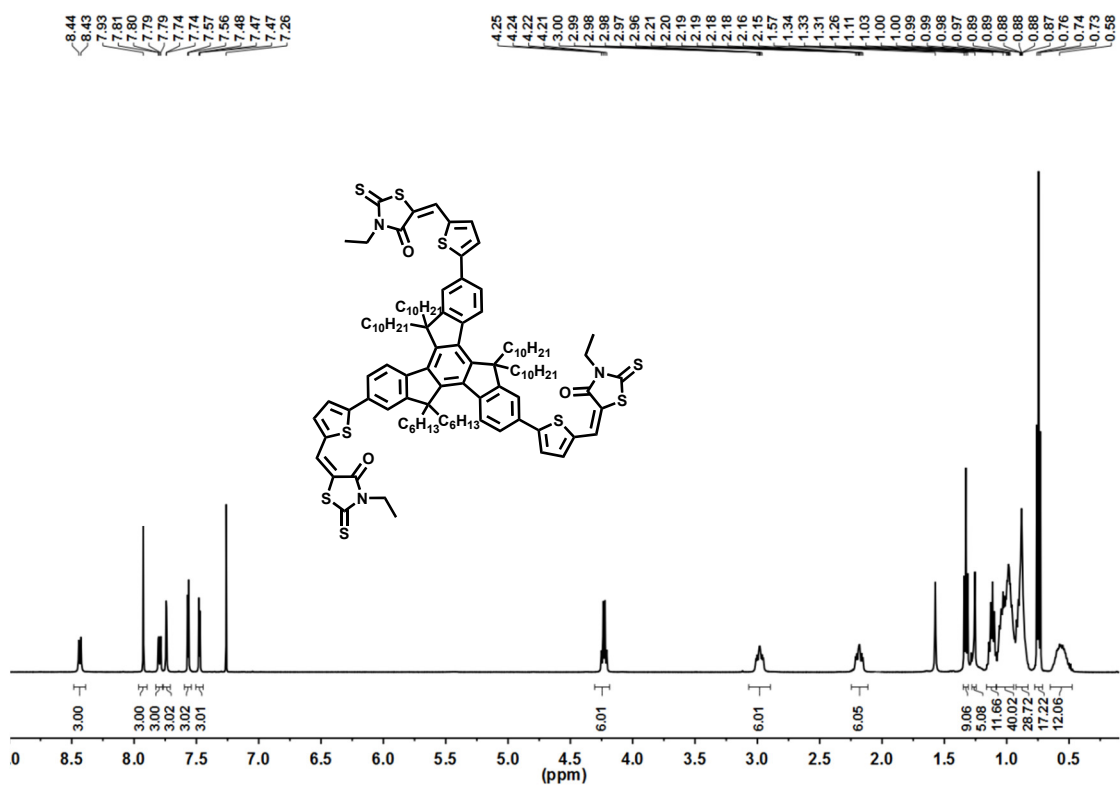


**Figure S13**  $^1\text{H}$  NMR spectrum of  $\text{Tr}(\text{Hex})_6\text{-3RD}$



**Figure S14**  $^{13}\text{C}$  NMR spectrum of  $\text{Tr}(\text{Hex})_6\text{-3RD}$





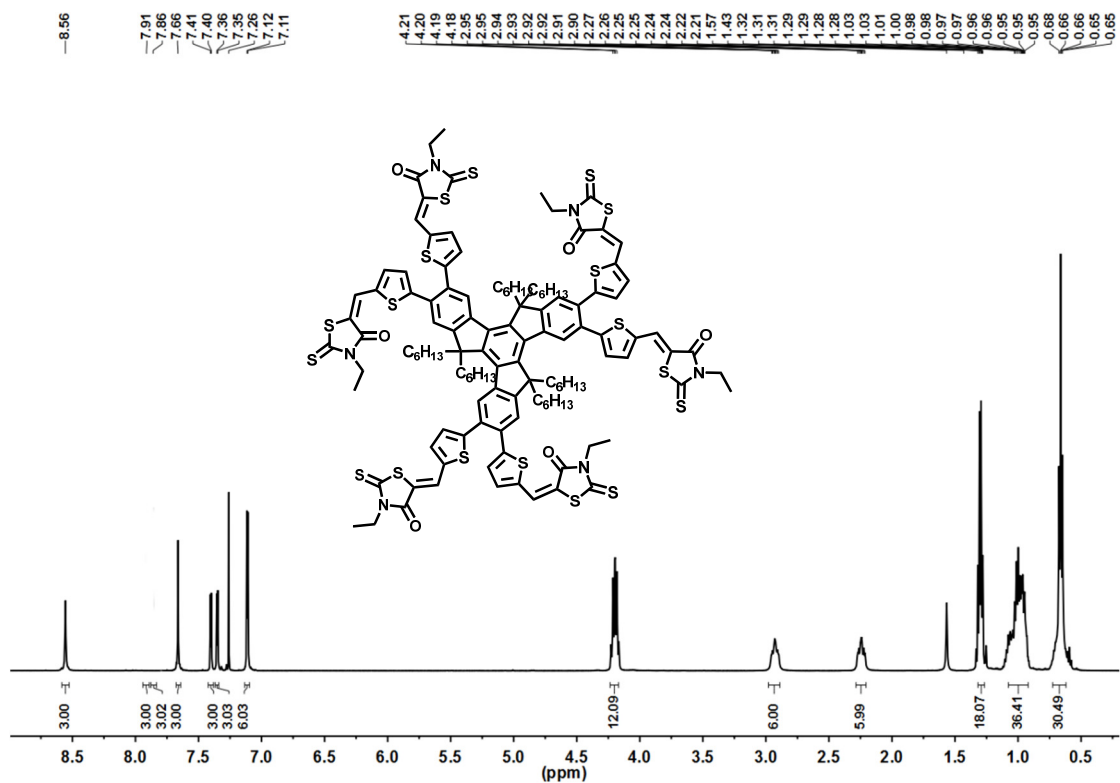


Figure S17 <sup>1</sup>H NMR spectrum of Tr(Hex)<sub>6</sub>-6RD

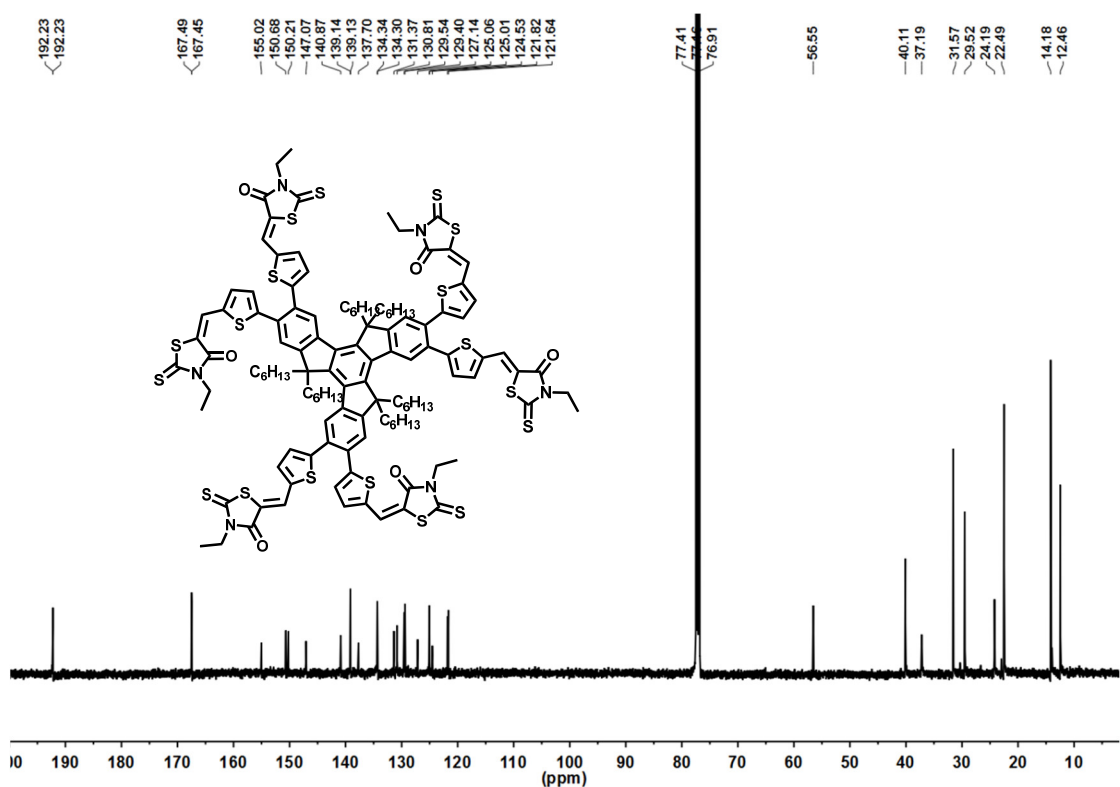
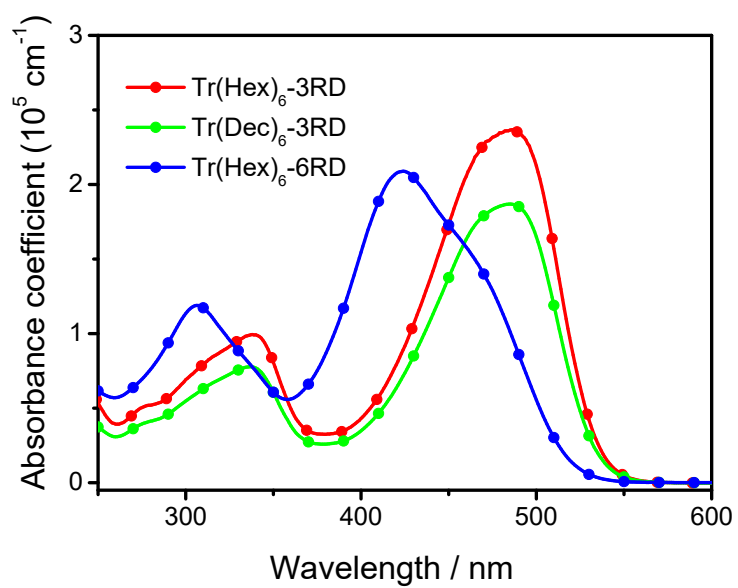
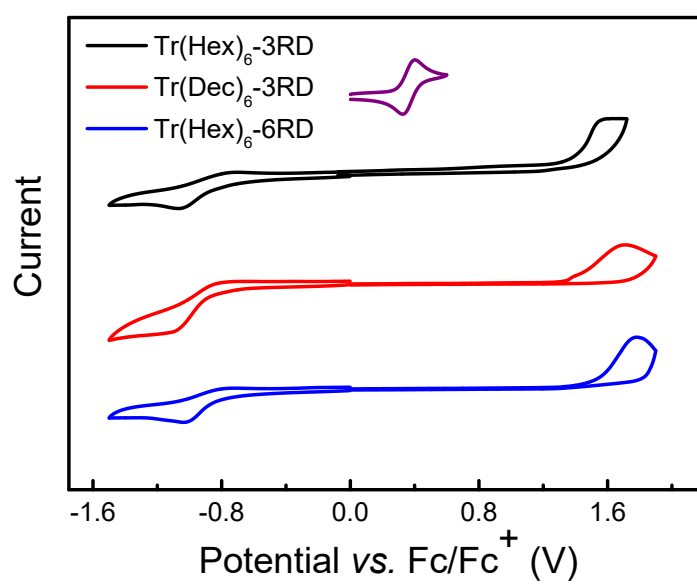


Figure S18 <sup>13</sup>C NMR spectrum of Tr(Hex)<sub>6</sub>-6RD



**Figure S19** UV-vis absorption spectra of truxene-centered acceptors in chloroform solution



**Figure S20** Cyclic voltammograms of truxene-centered acceptors

Table S1. Determined solubilities and thermal parameters of truxene-centered acceptors in chloroform

Acceptors	Solubility (mg/mL)	$T_d$ (°C)	$T_m$ (°C)	$T_c$ (°C)
Tr(Hex) <sub>6</sub> -3RD	80	410	259	203/190
Tr(Dec) <sub>6</sub> -3RD	130	404	178	--
Tr(Hex) <sub>6</sub> -6RD	180	410	--	--

Table S2. Photovoltaic parameters of PTB7-Th: truxene-centered acceptors (weight ratio of 1:1) devices

PTB7-Th: Acceptors	Post-annealing	$V_{oc}$ (V)	$J_{sc}$ (mA cm <sup>-2</sup> )	FF (%)	PCE (%)
PTB7-Th: Tr(Hex) <sub>6</sub> -3RD	60 °C	0.85	0.2	32.9	0.1
	100 °C	0.84	0.2	31.7	0.1
PTB7-Th: Tr(Dec) <sub>6</sub> -3RD	60 °C	0.84	0.2	33.5	0.1
	100 °C	0.85	0.2	32.6	0.1
PTB7-Th: Tr(Hex) <sub>6</sub> -6RD	60 °C	0.84	0.2	31.1	0.1
	100 °C	0.85	0.2	30.1	0.1

Table S3. Photovoltaic parameters of P3HT: Tr(Hex)<sub>6</sub>-6RD (weight ratio of 1:1) devices

Rotational speed	$V_{oc}$ (V)	$J_{sc}$ (mA cm <sup>-2</sup> )	FF (%)	PCE (%)
1200	0.65	0.6	28.4	0.1
1400	0.59	0.6	29.7	0.1
1600	0.55	0.6	27.7	0.1

Table S4. Photovoltaic parameters of PBDB-T: Tr(Hex)<sub>6</sub>-6RD (weight ratio of 1:1) devices

Rotational speed	$V_{oc}$ (V)	$J_{sc}$ (mA cm <sup>-2</sup> )	FF (%)	PCE (%)
1200	1.06	1.2	27.8	0.4
1400	1.09	1.2	28.6	0.4
1600	1.09	1.2	28.7	0.4