Supporting information for:

A Sustainable Synthetic Approach to the Indaceno[1,2-b:5,6-b']dithiophene (IDT) Core through Cascade Cyclization–Deprotection Reactions

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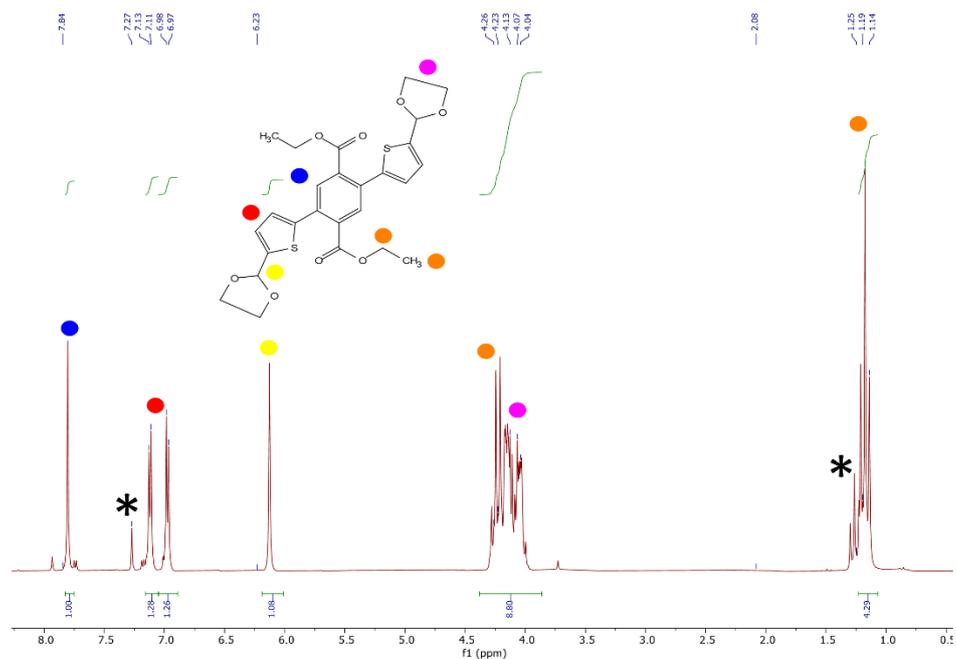
Figure S1. ^{1}H NMR (400 MHz, CDCl₃) of compound **1a**. The asterisks denote residual NMR or other solvent impurities.
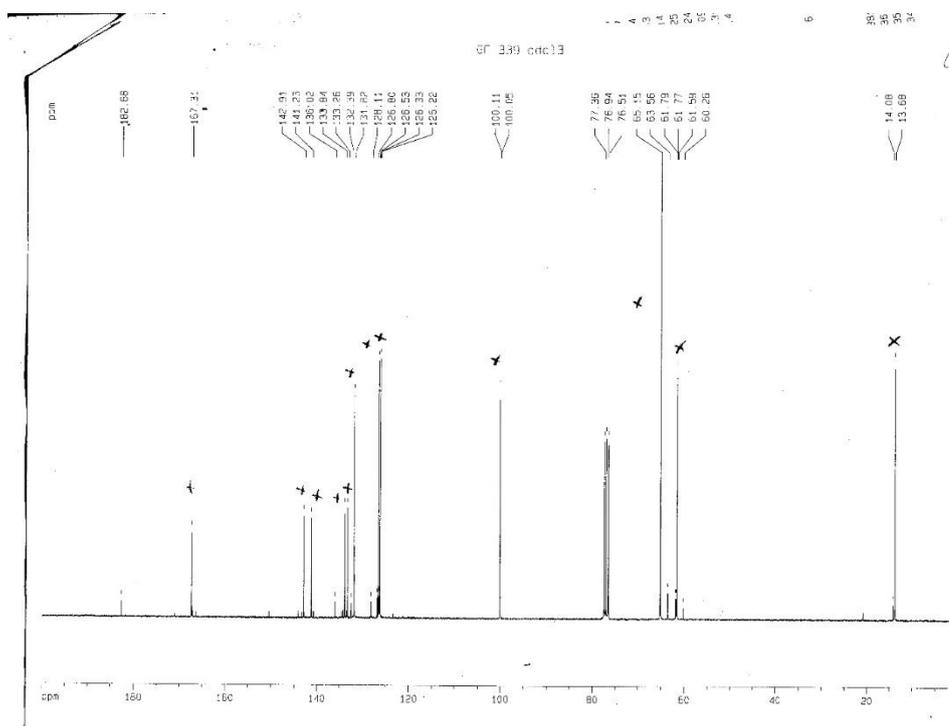

Figure S2. ^{13}C NMR (75 MHz, CDCl₃) of compound **1a**.
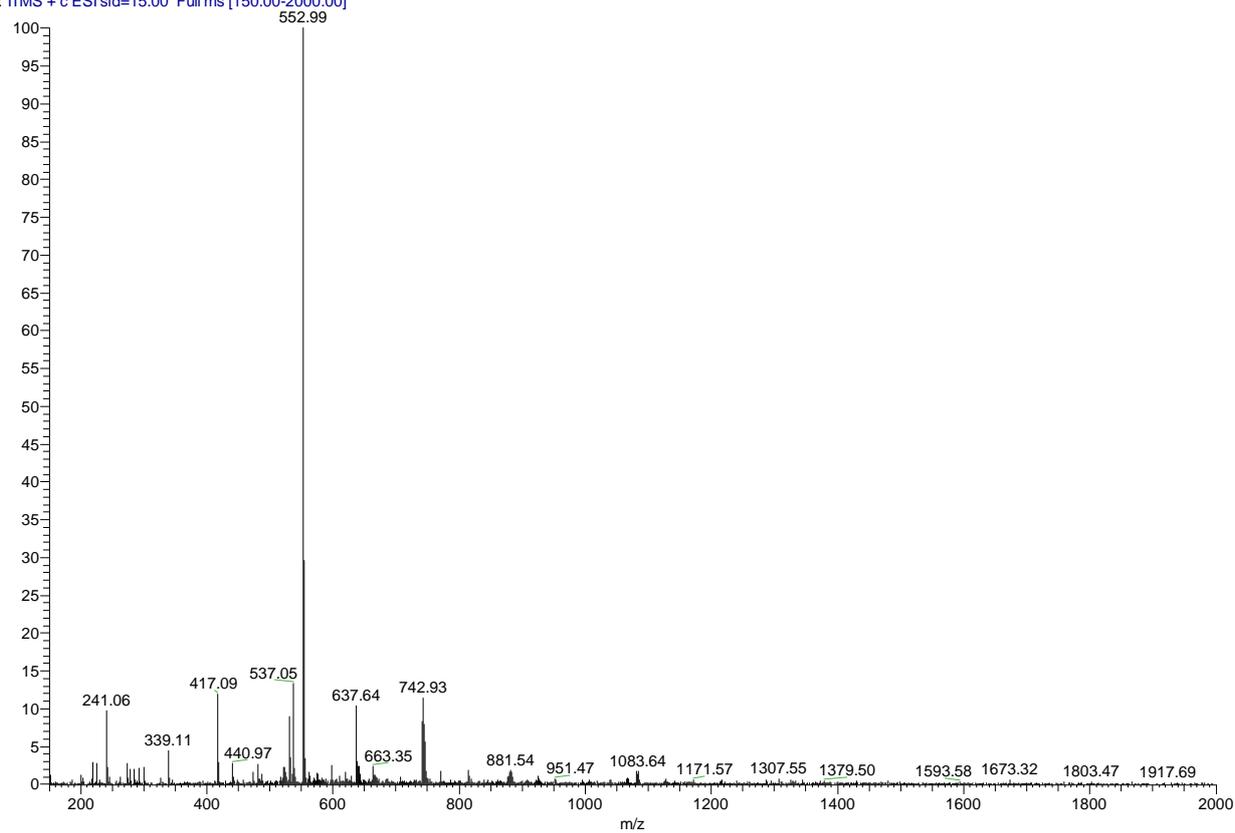
Figure S3. ESI-MS of compound **1a.**
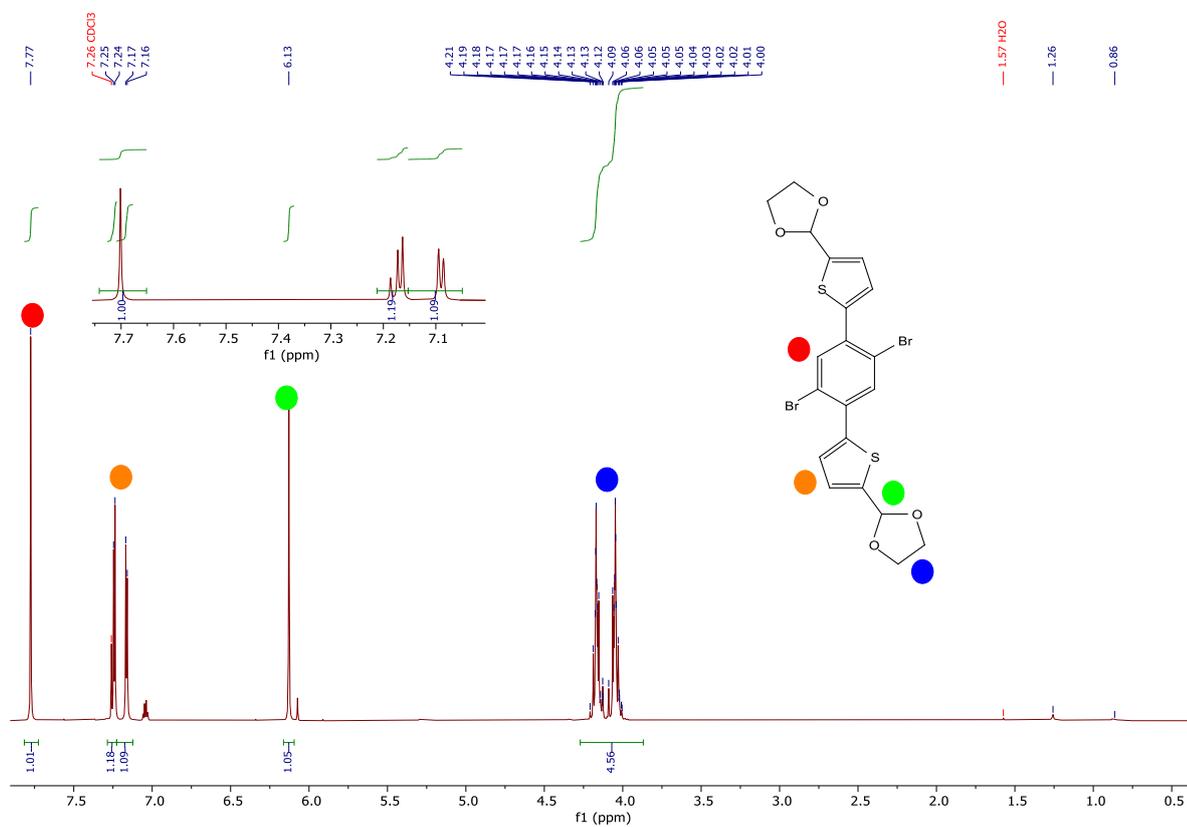
Figure S4. ^{1}H NMR (400 MHz, CDCl₃) of compound **1b**.
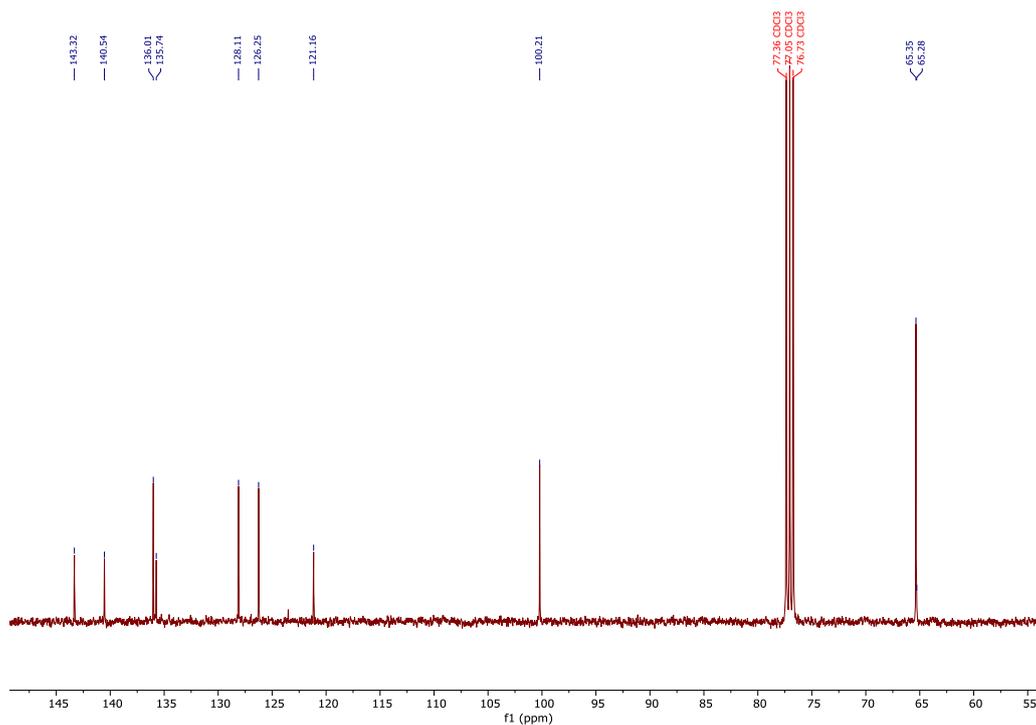
Figure S5. ^{13}C NMR (101 MHz, CDCl$_3$) of compound **1b**.
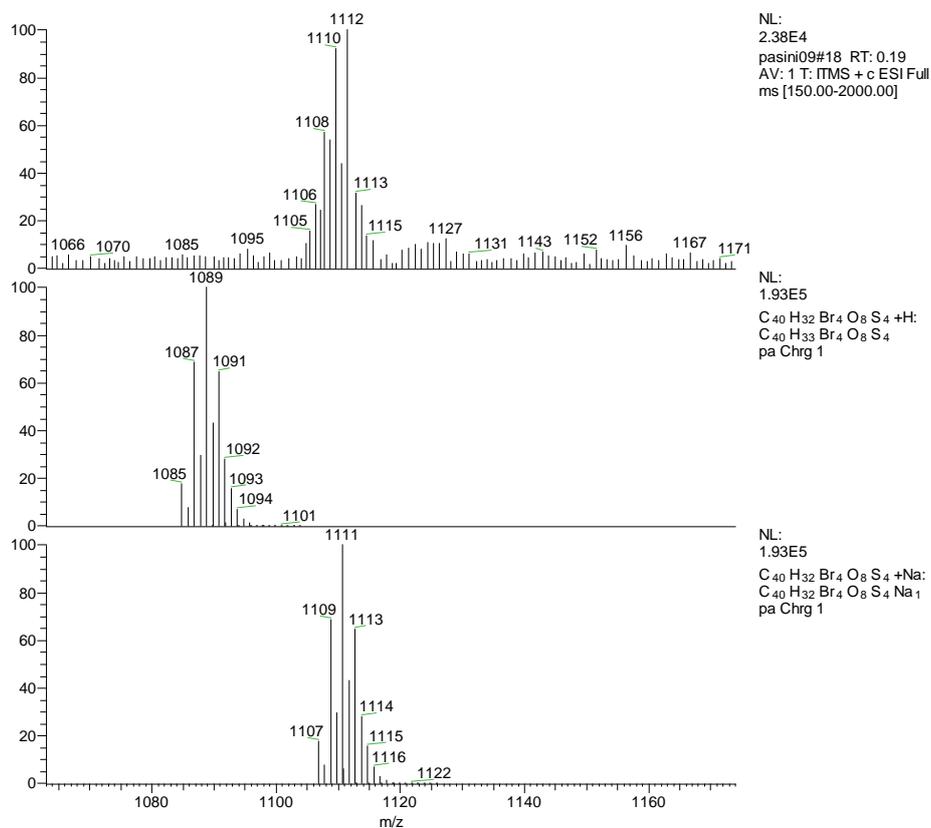
Figure S6. ESI-MS of compound **1b**.
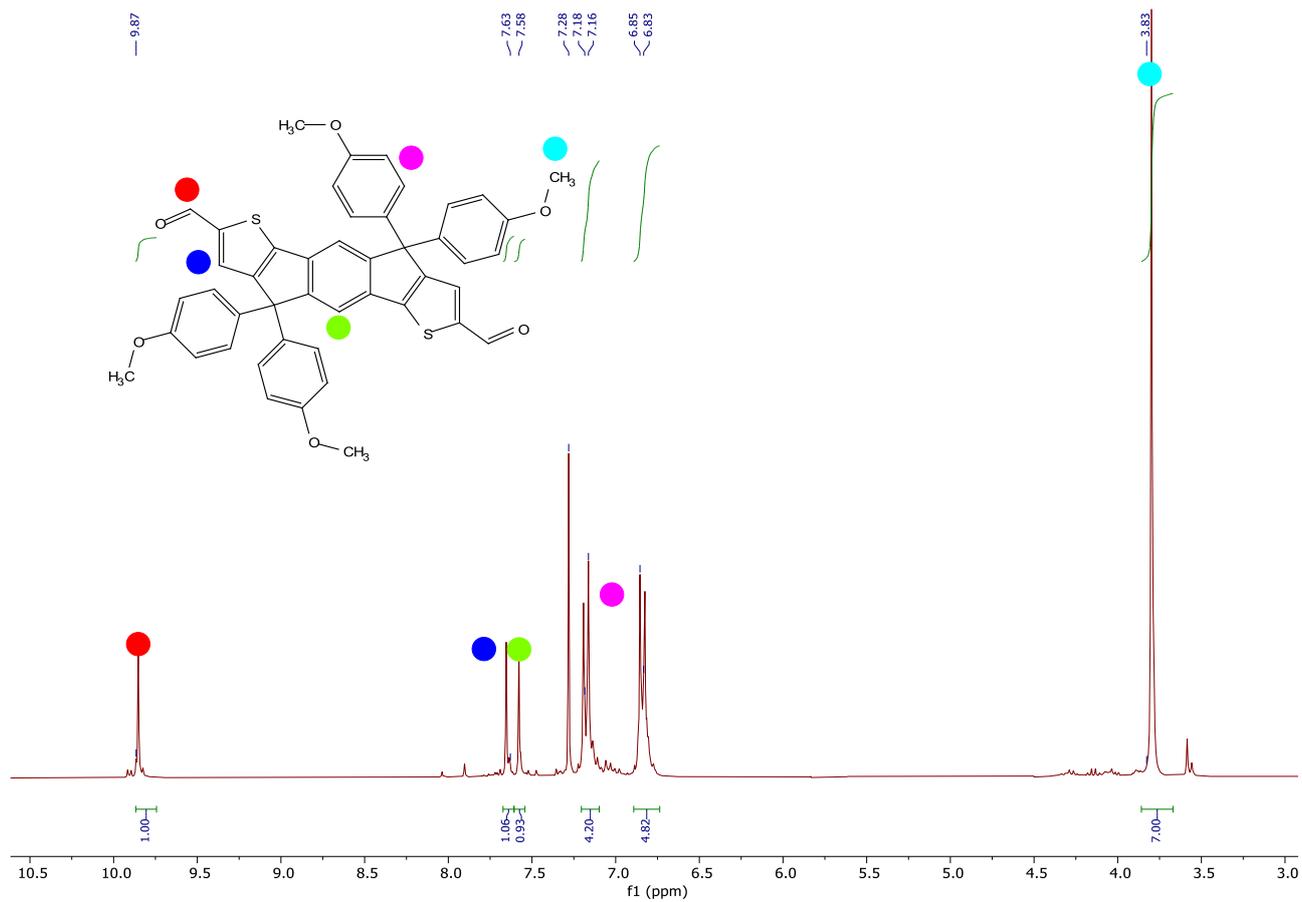
Figure S7. ^{1}H NMR (300 MHz, CDCl$_3$) of compound **2a**.
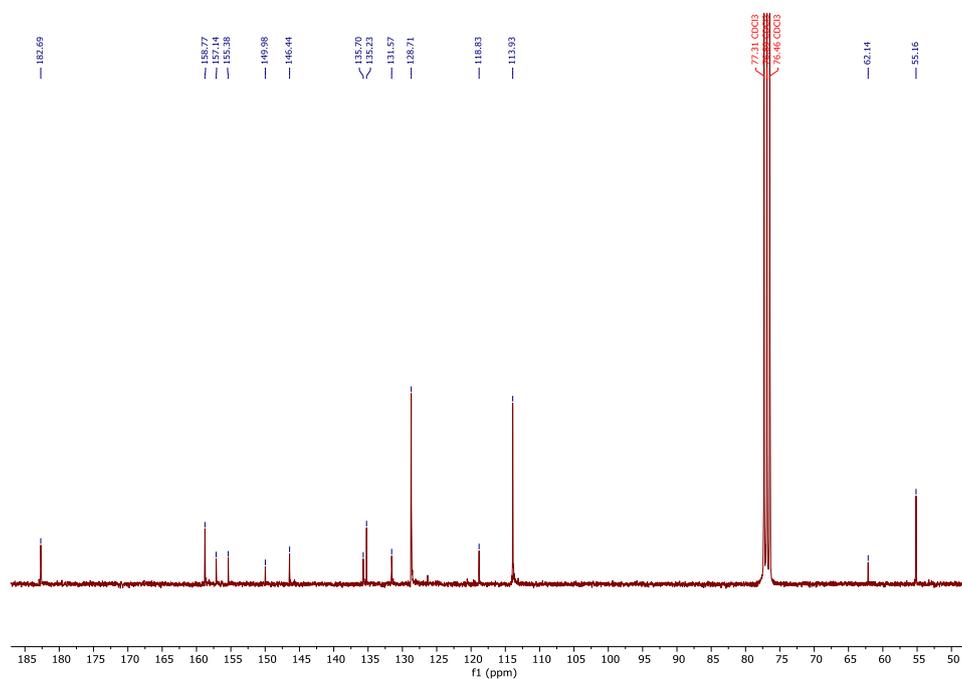
Figure S8. ^{13}C NMR (75 MHz, CDCl$_3$) of compound **2a**.
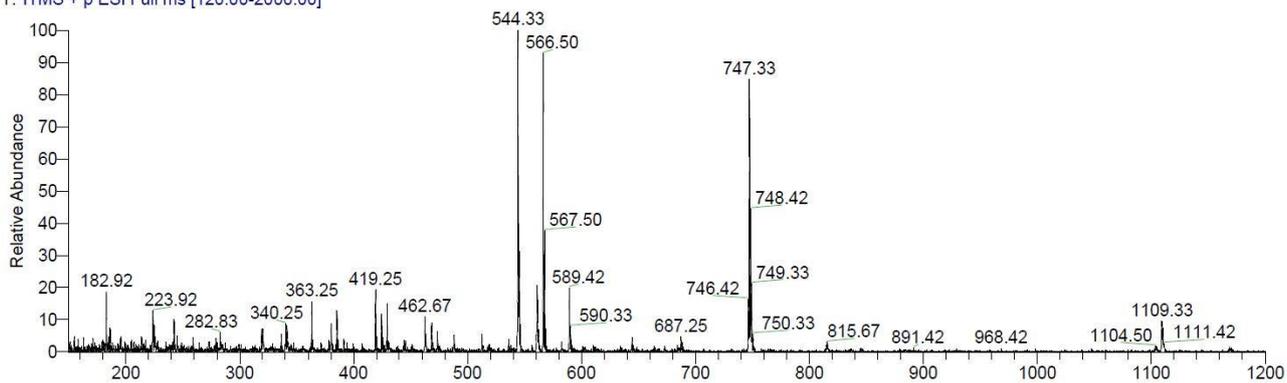
Figure S9. ESI-MS of compound **2a**.
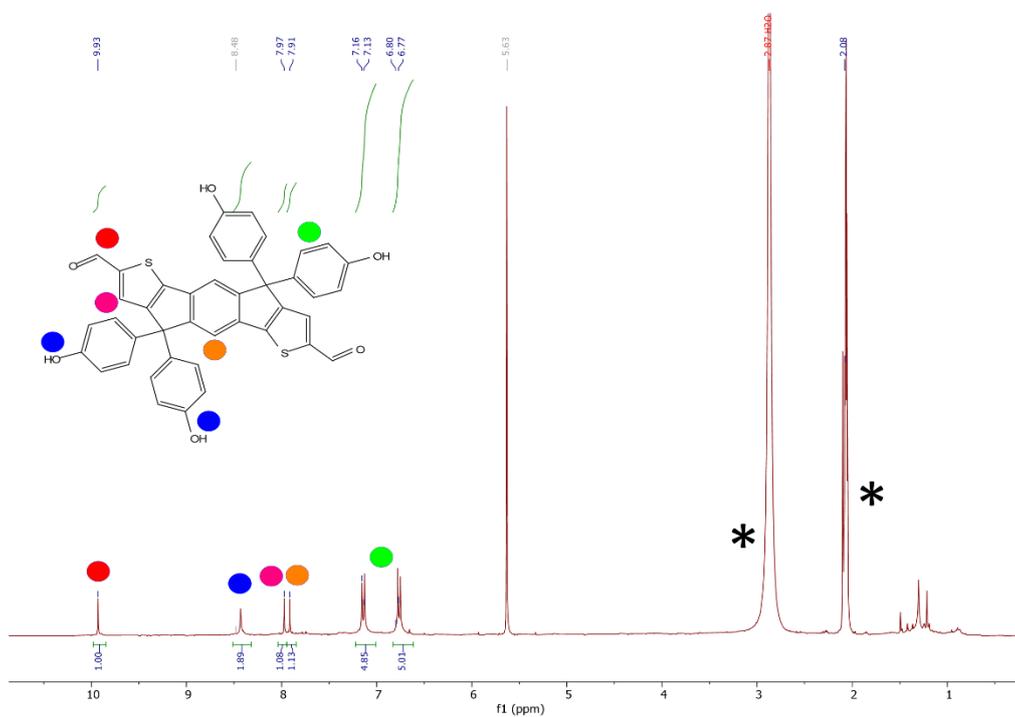
Figure S10. ^{1}H NMR (300 MHz, acetone-d$_6$) of compound **3a**. The asterisks denote residual NMR or other solvent impurities.
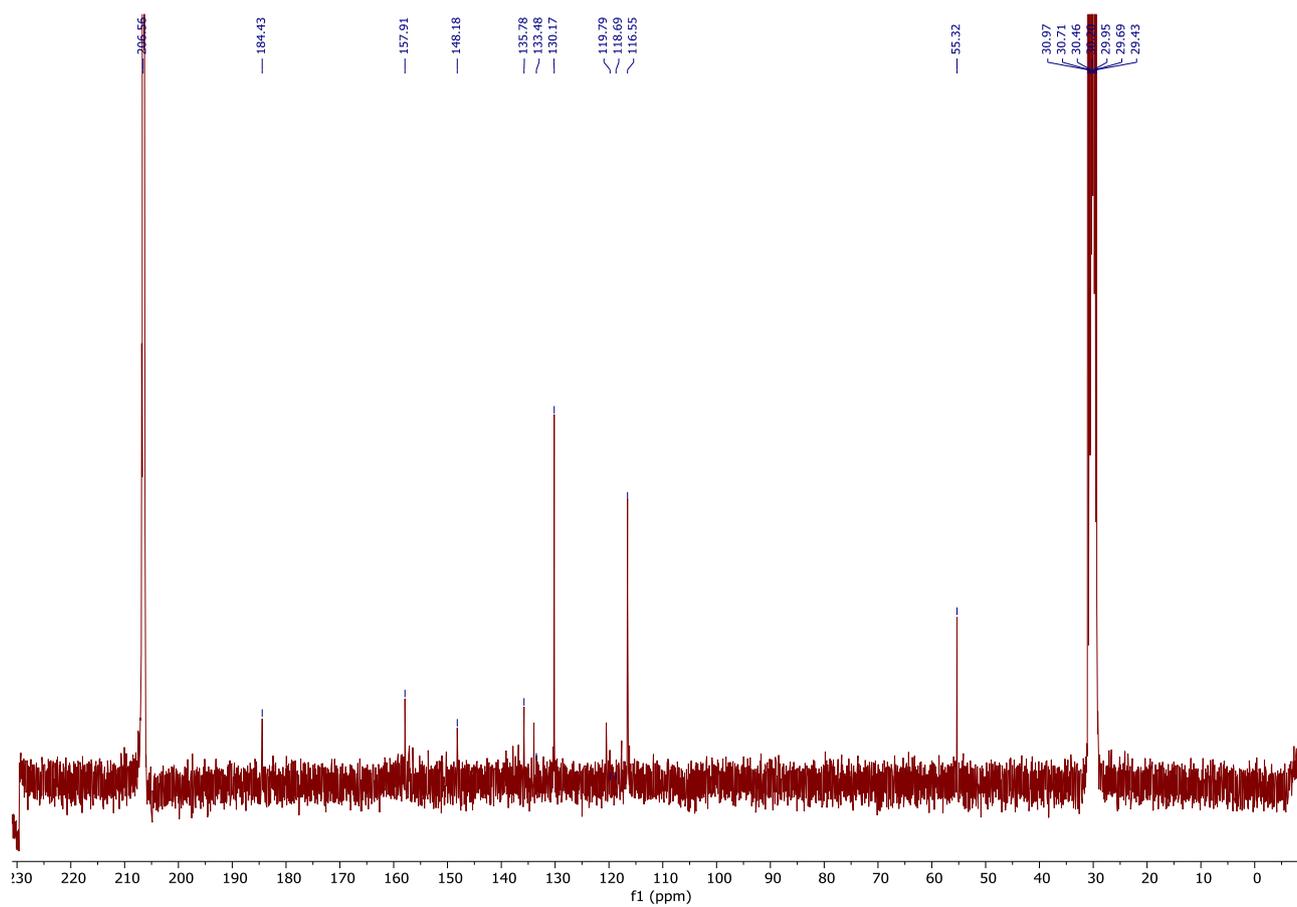
**Figure S11.** ^{13}C NMR (75 MHz, acetone-d$_6$) of compound **3a**.

Table S1. Calculation of E *f*actor for molecule **1a**.

	Amount (g)	Waste (g)
diethyl 2,5-dibromoterephthalate	1	-
(5-(1,3-dioxolan-2-yl)thiophen-2-yl)zinc(II) chloride	1.5	-
Pd(PPh₃)₄	0.122	0.122
NaHCO₃	20	20
Na₂SO₄	5	5
Silica gel	20	20
Total	47.66	45.122

Total waste = 45.122 g; Compound obtained = 1.46 g

E *f*actor = 30.90

Table S2. Calculation of E *f*actor for molecule **2a**.

	Amount (g)	Waste (g)
1a	0.246	0.178
(4-methoxyphenyl) magnesium bromide	0.432	0.311
NaHCO₃	2.5	2.5
Na₂SO₄	2	2
AcOH	5.25	5.25
H₂SO₄	1	1
Silica gel	5	5
Total	16.36	16.239

Total waste = 16.239 g; Compound obtained = 0.095 g

E *f*actor = 170.93

Table S3. Calculation of E *f*actor for reported **IDT** precursor.

	Amount (g)	Waste (g)
diethyl 2,5-dibromoterephthalate	4.48	1.21
2-Bromothiophene	1.66	0.44
Mg °	0.702	0.702
Zinc chloride	3.91	3.91
$Pd(PPh_3)_4$	0.266	0.266
Celite	20	20
Mg_2SO_4	10	10
Silica gel	80	80
Total	121.02	116.53

Total waste = 116.53 g; Compound obtained = 3.3 g

E *f*actor = 35.31

Table S4. Calculation of E *f*actor for reported **IDT** core (4-hexylaryl substituents).

	Amount (g)	Waste (g)
diethyl 2,5-di(thiophen-2-yl)terephthalate	1	0.350
4-bromotoluene	2.64	0.92
Mg °	0.378	0.378
Mg_2SO_4	5	5
AcOH	100	100
H_2SO_4	2	2
Silica	40	40
Total	151.02	148.65

Total waste = 148.65 g; Compound obtained = 1.05 g

E *f*actor = 141.57

Table S5. Calculation of E *f*actor for the IDT dialdehyde core (hexyl substituents).

	Amount (g)	Waste (g)
IDT	0.768	0.261
n-BuLi	0.646	0.646
THF	163	163
DMF	0.257	0.090
Brine	20	20
Silica gel	20	20
Total	204.4	204

Total waste = 204.4 g; Compound obtained =0.530 g

E *f*actor = 385.66

Table S6. E-*f*actor comparison.

Molecule	**E-*Factor* tot**
2a	201.83
IDT core dialdehyde	562.54