Electronic Supplementary Information (ESI)

Branched and linear A_2-D-A_1-D-A_2 isoindigo-based solution-processablesmall molecules for organic field-effect transistors and solar cells

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1. ^{1}H NMR spectra of the novel small molecules and precursors

Fig. S1 ^{1}H NMR spectrum of compound **3** ($CDCl_3$).

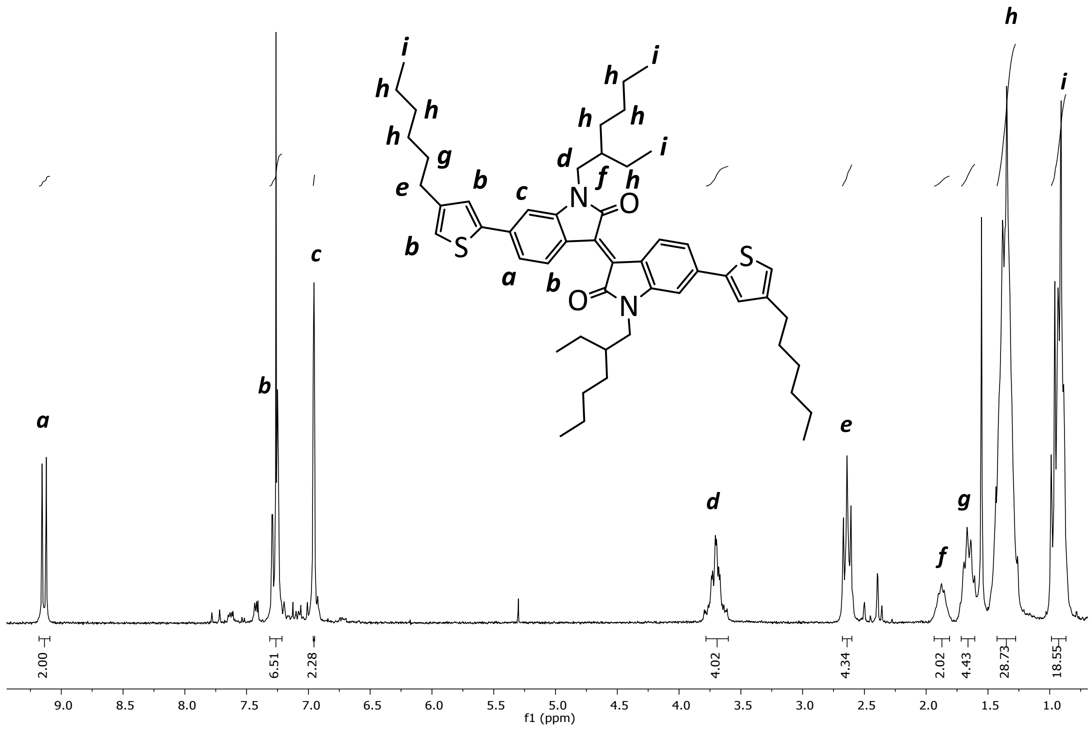


Fig. S2 ^{1}H NMR spectrum of compound **4** ($CDCl_3$).

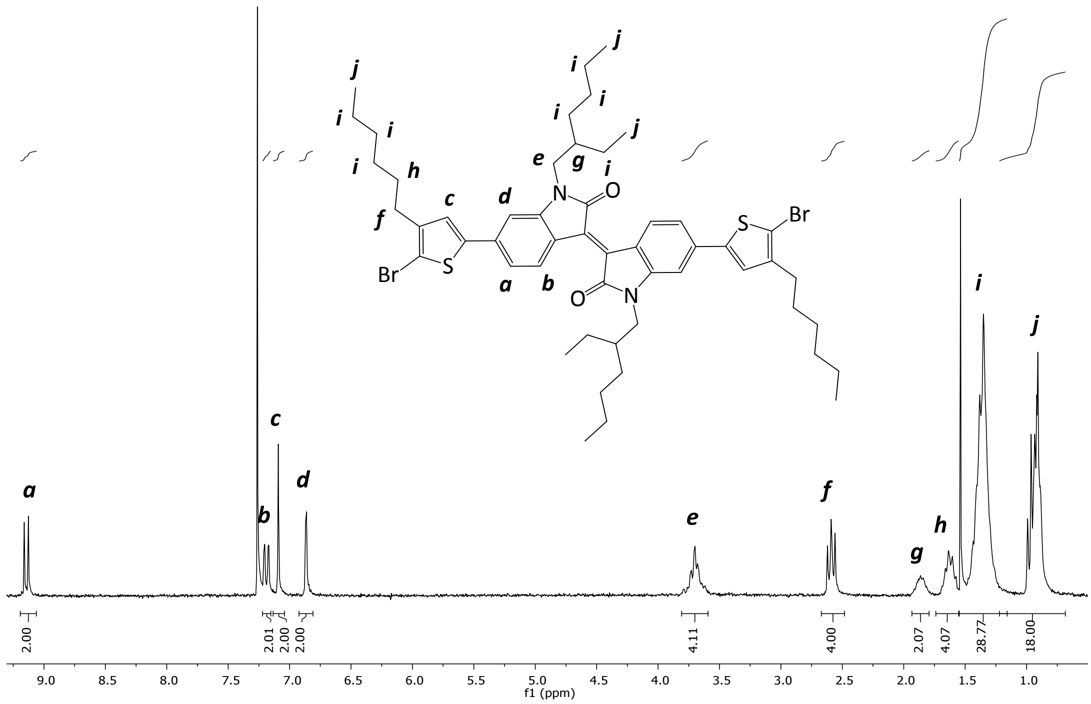


Fig. S3 [1]H NMR spectrum of compound **5** ($CDCl_3$).

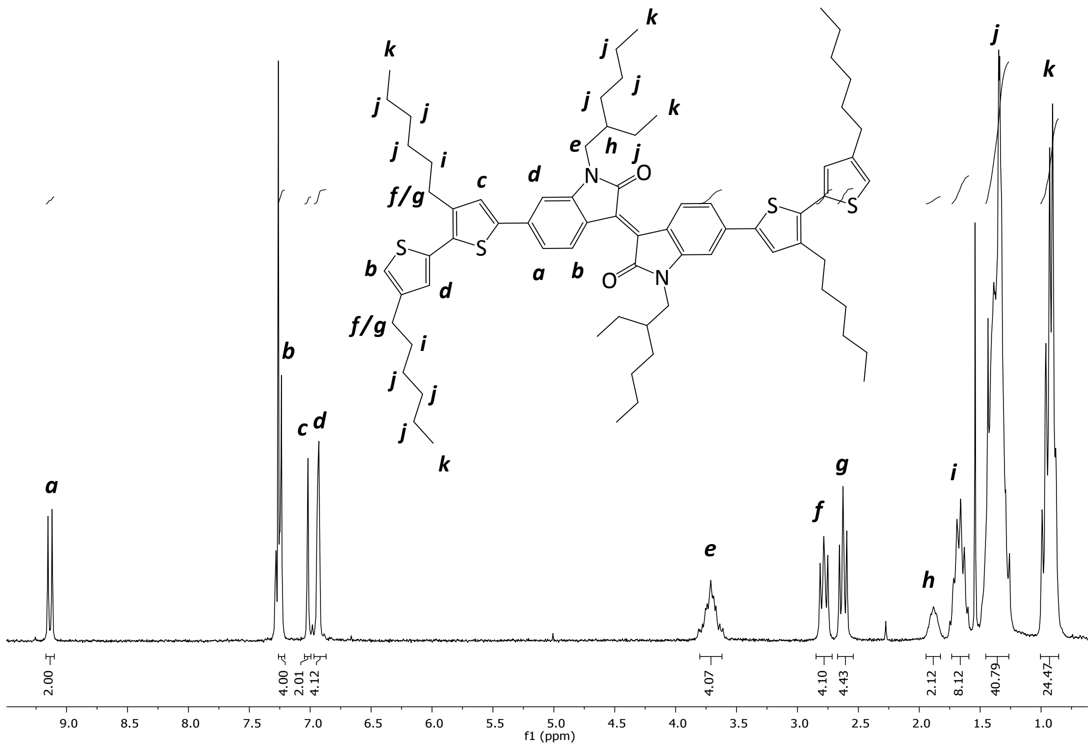


Fig. S4 [1]H NMR spectrum of compound **6** ($CDCl_3$).

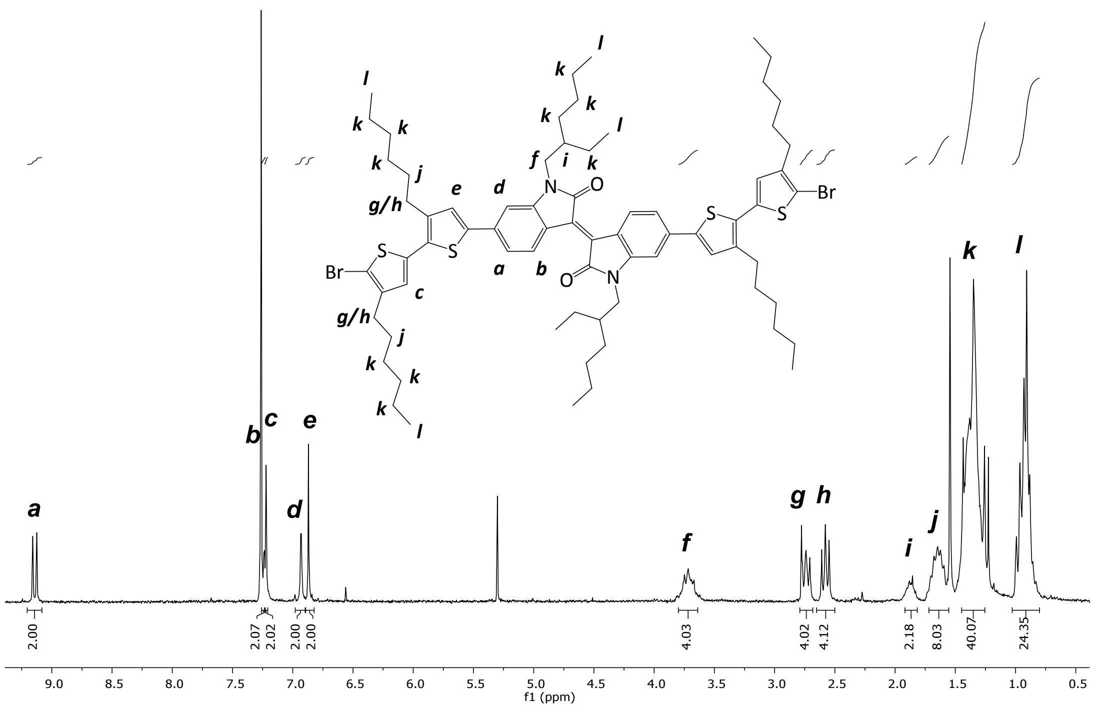


Fig. S5 ^{1}H NMR spectrum of compound **9** ($CDCl_3$).

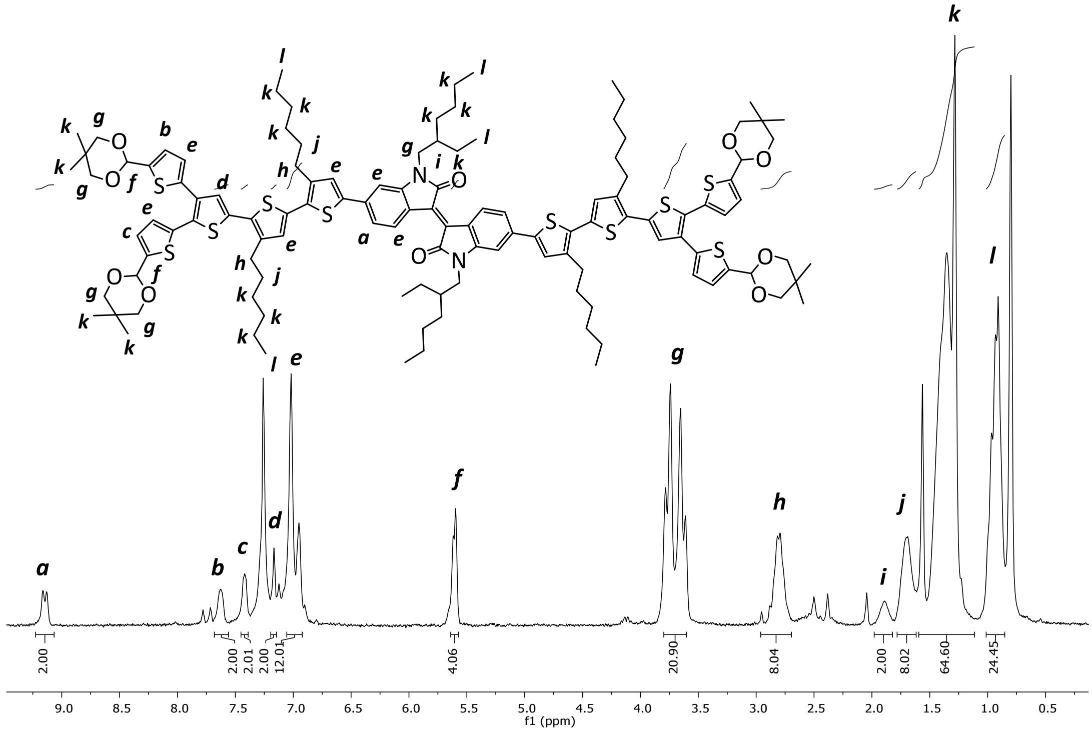


Fig. S6 ^{1}H NMR spectrum of small molecule **CA-5T-IID-5T-CA-*b*** ($CDCl_3$).

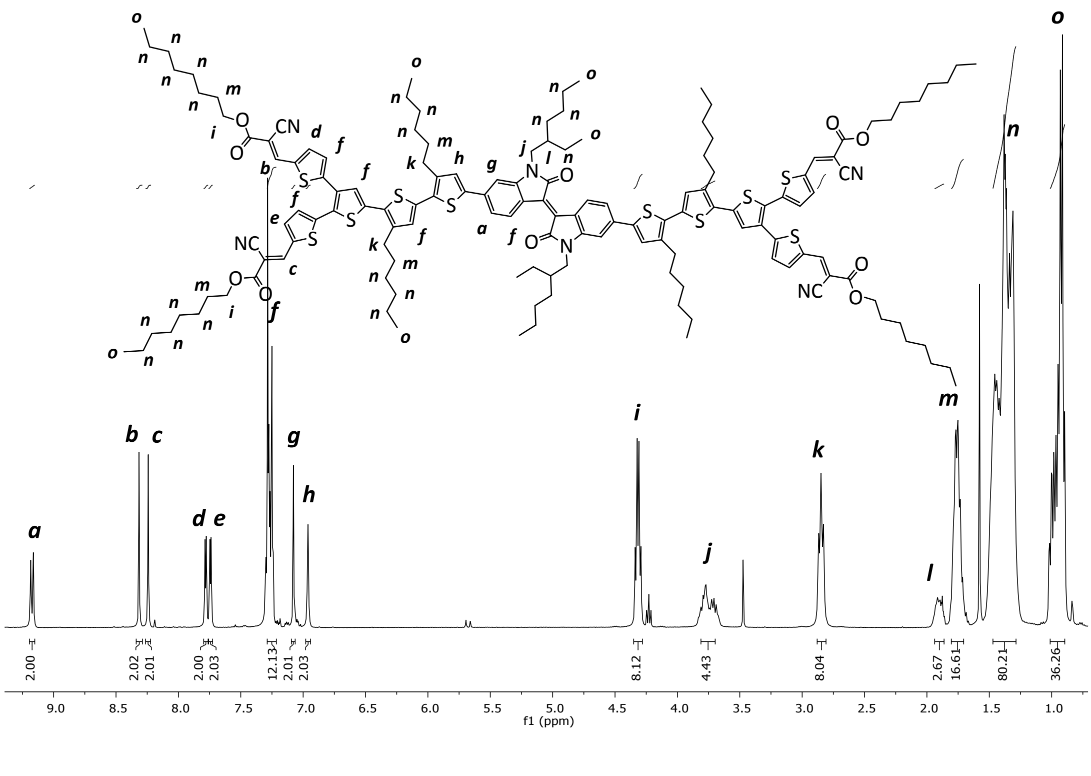


Fig. S7 [1]H NMR spectrum of compound **10** ($CDCl_3$).

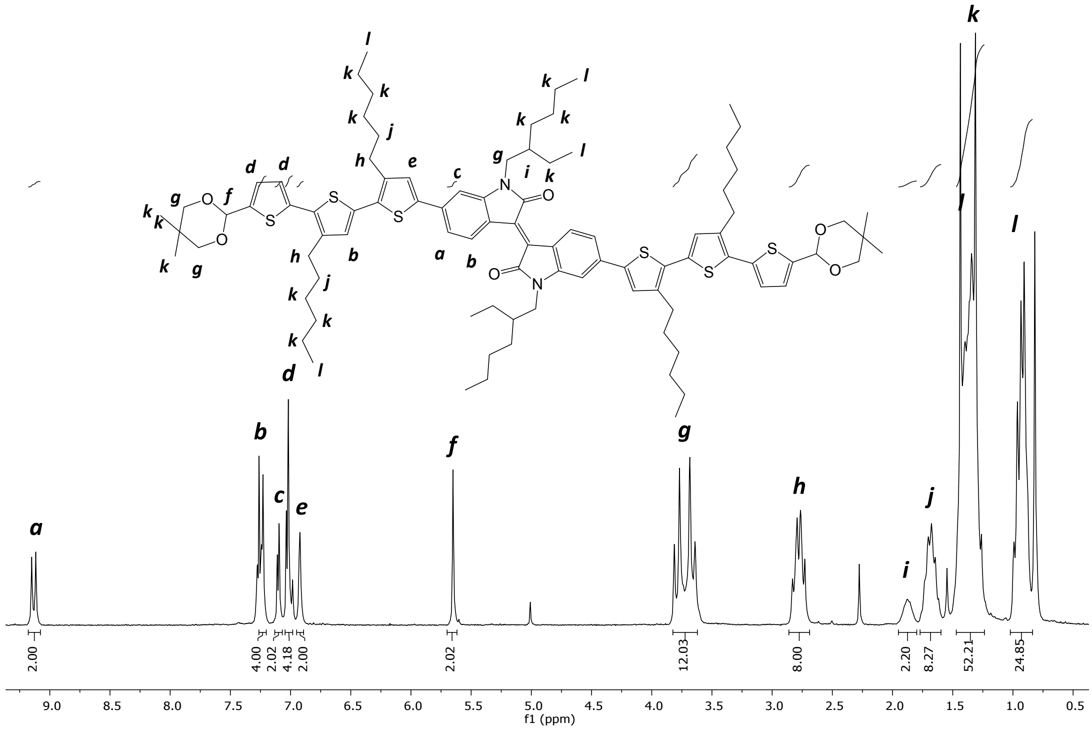
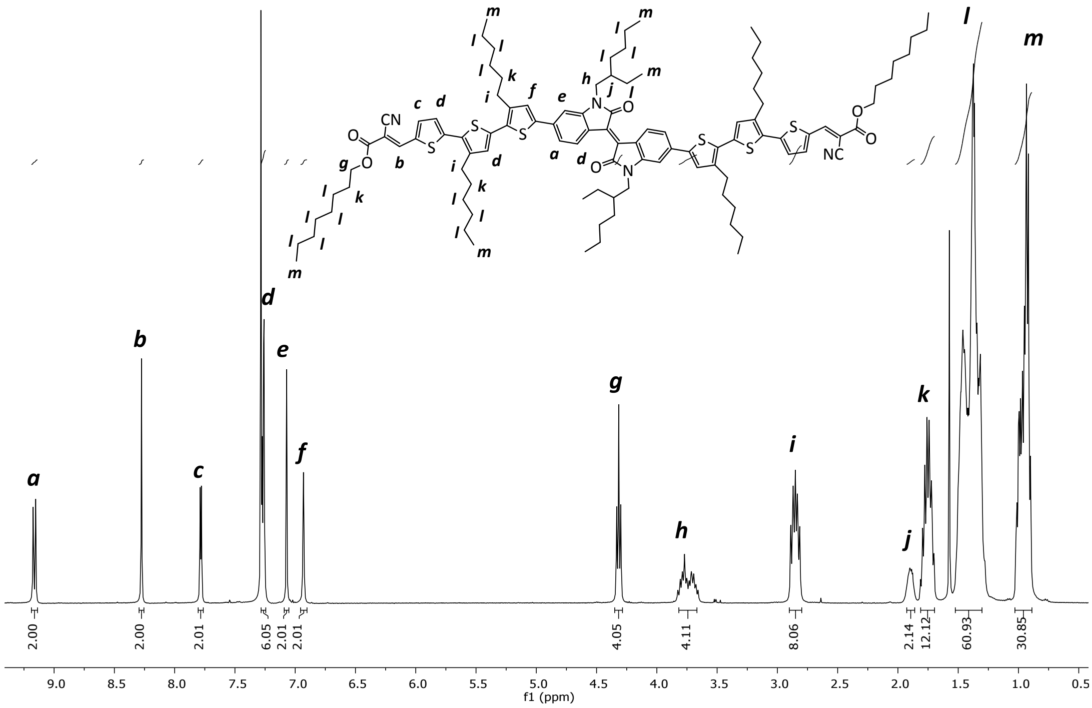


Fig. S8 [1]H NMR spectrum of small molecule **CA-3T-IID-3T-CA-*l*** ($CDCl_3$).



2. ^{13}C APT NMR spectra of the novel small molecules

Fig. S9 ^{13}C APT NMR spectrum of small molecule **CA-5T-IID-5T-CA-*b*** ($CDCl_3$).

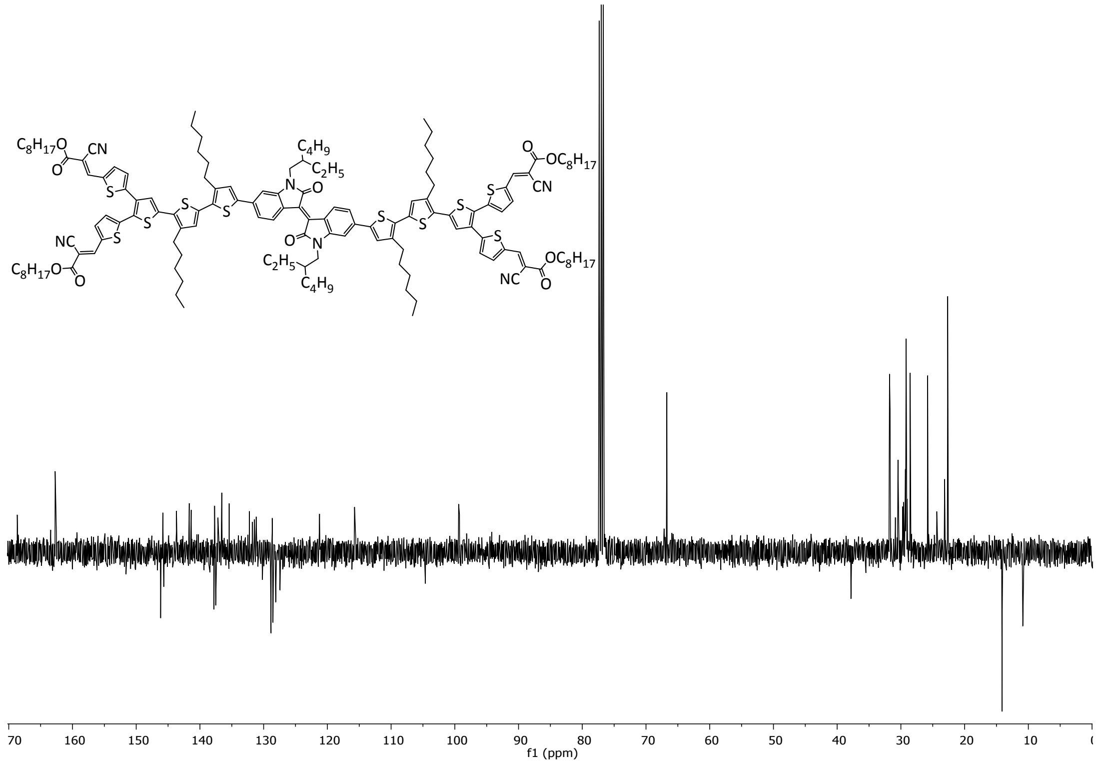
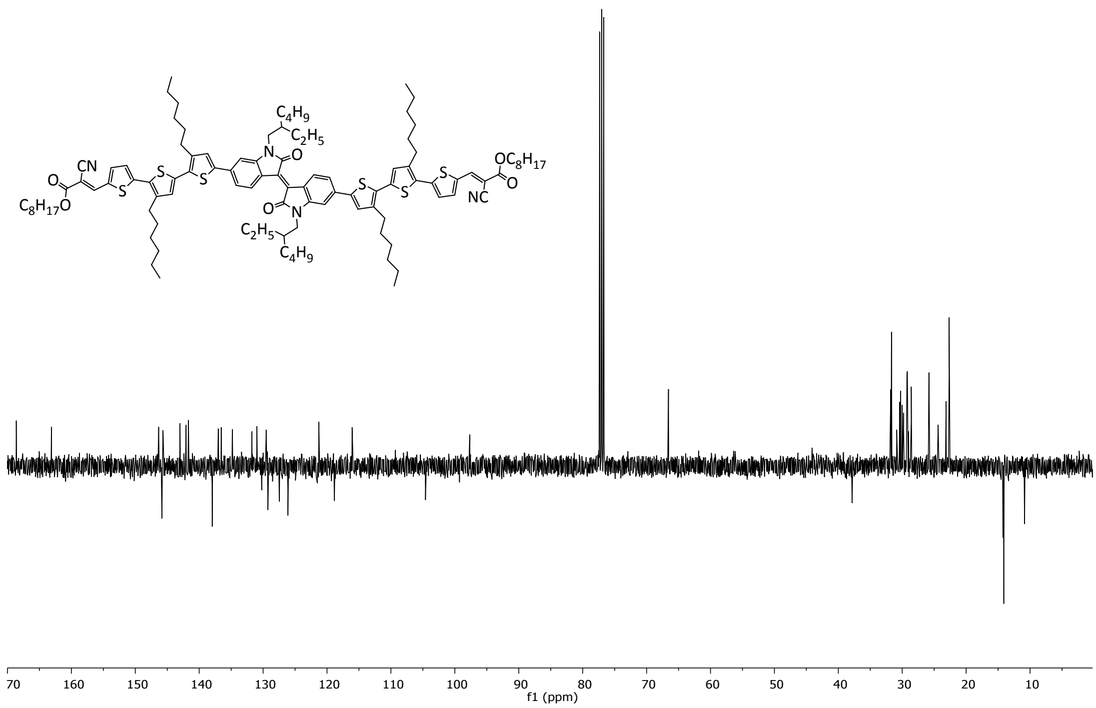


Fig. S10 ^{13}C APT NMR spectrum of small molecule **CA-3T-IID-3T-CA-*l*** ($CDCl_3$).



3. MALDI-TOF mass spectra of the novel small molecules

Fig. S11 MALDI-TOF mass spectrum of small molecule **CA-5T-IID-5T-CA-*b***.

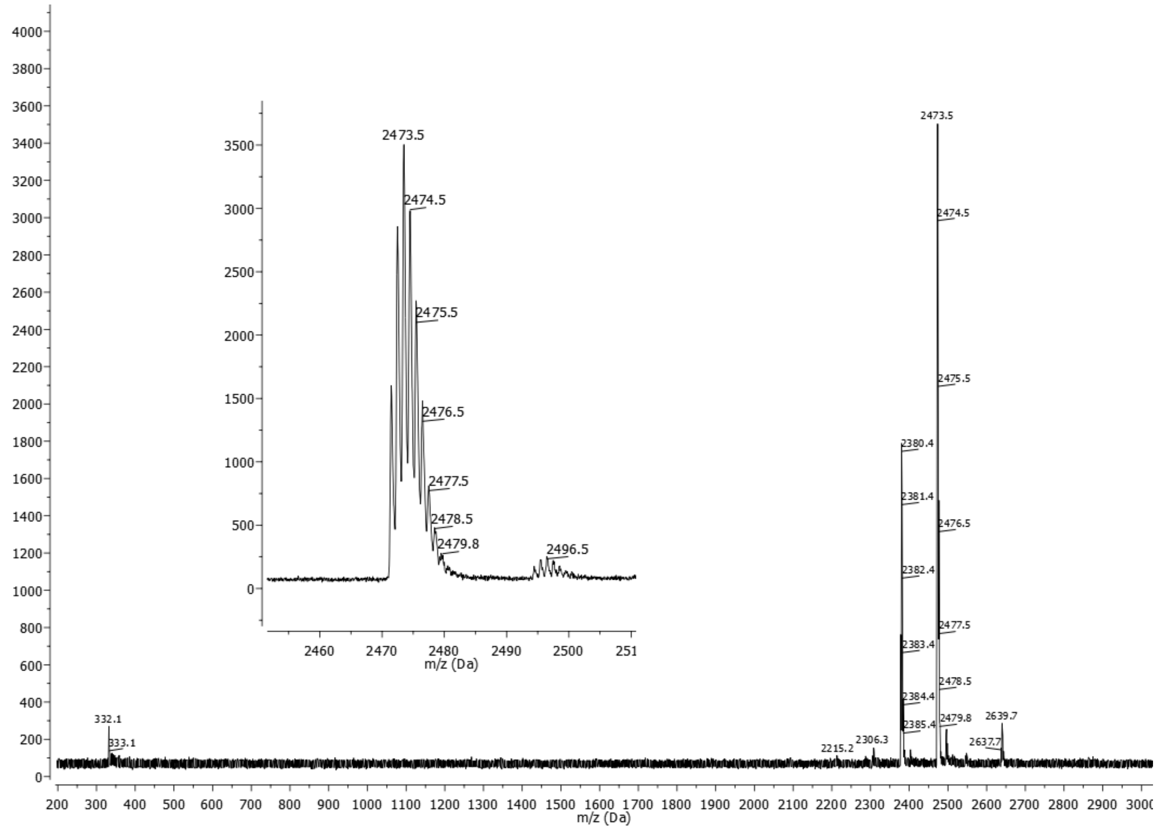
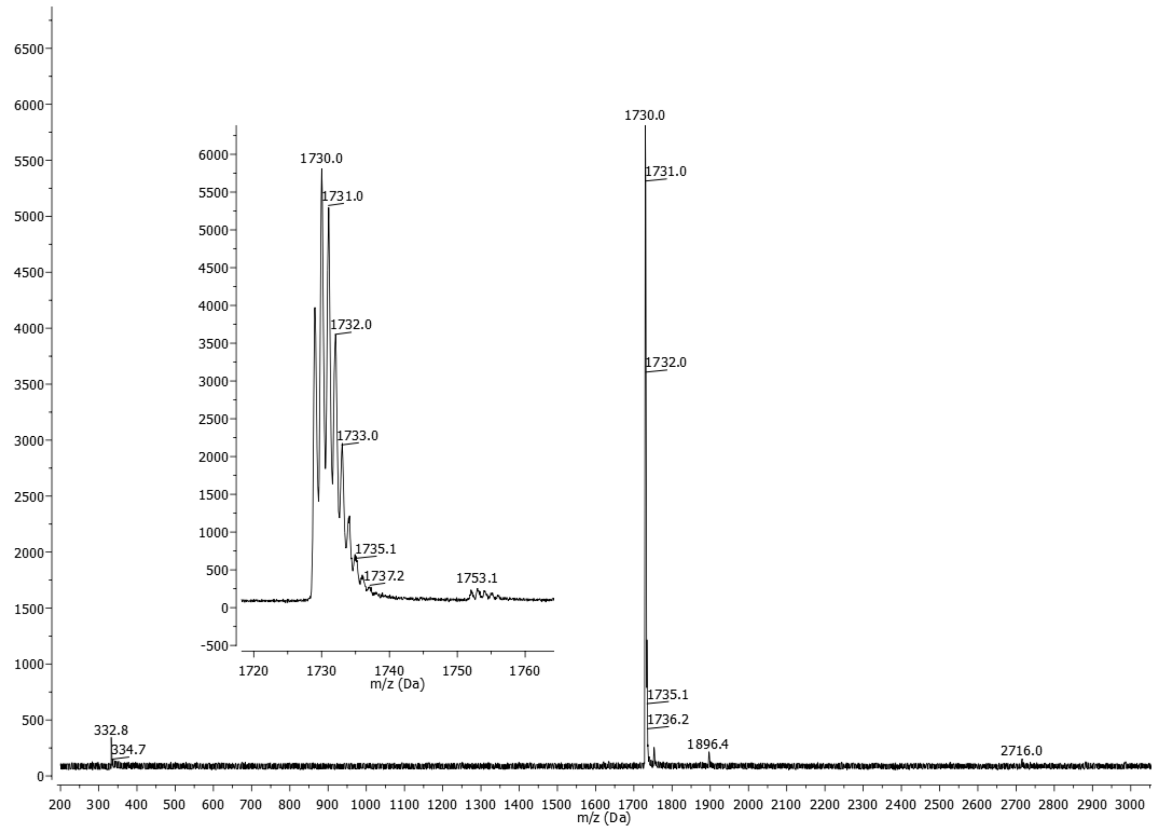
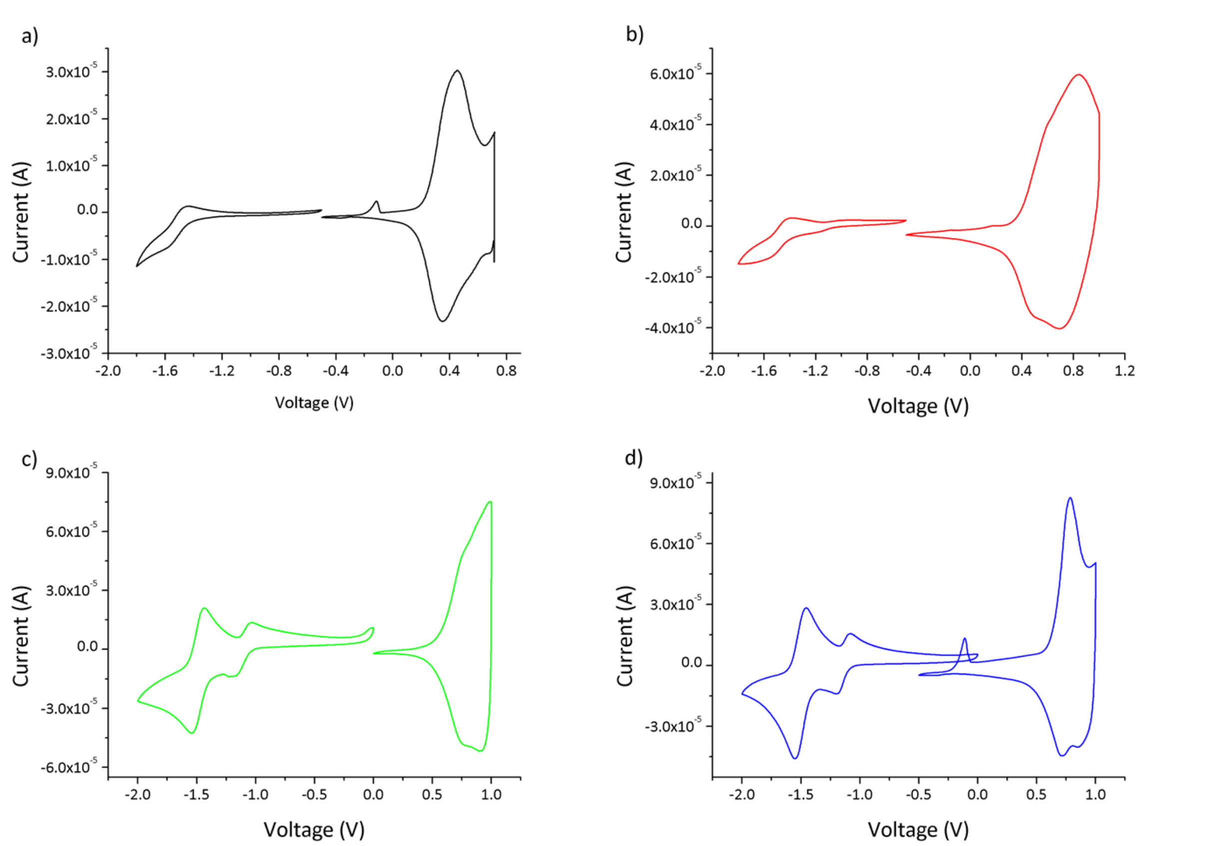


Fig. S12 MALDI-TOF mass spectrum of small molecule **CA-3T-IID-3T-CA-*l***.



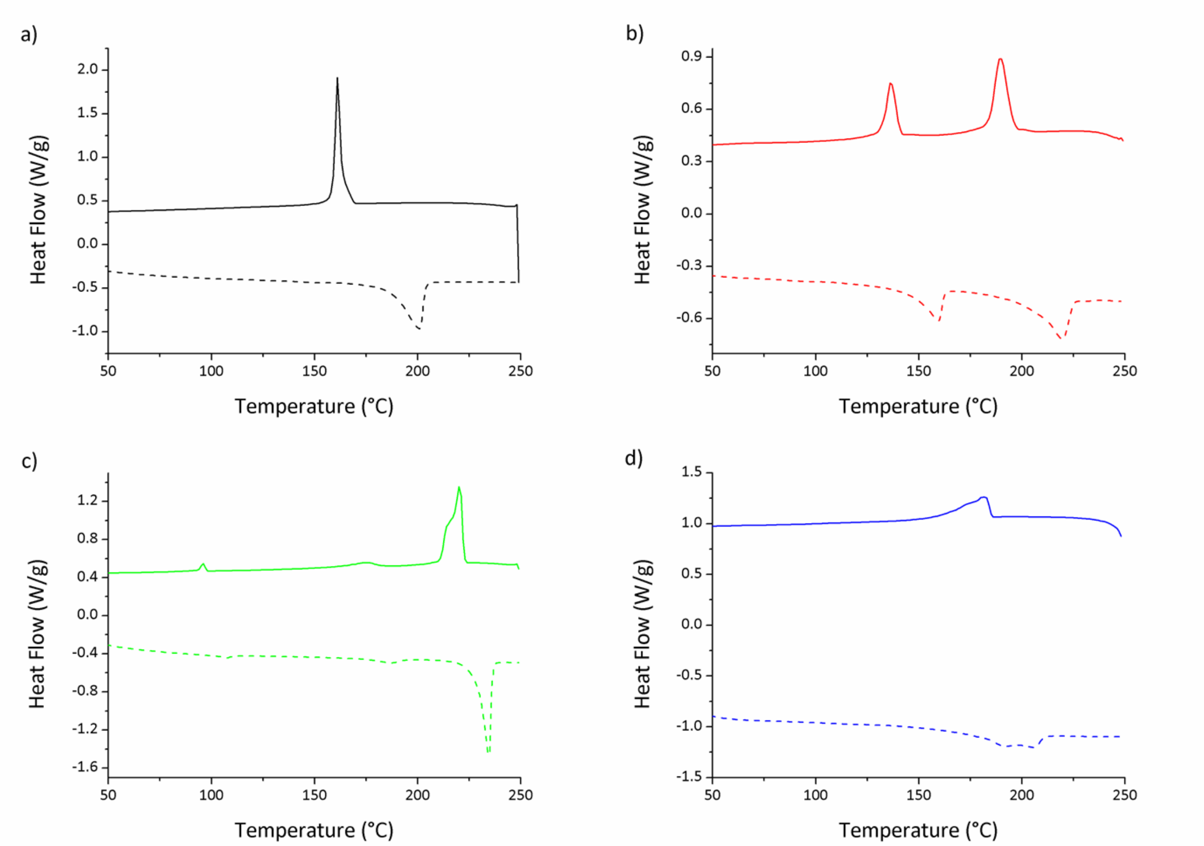
4. Cyclic voltammograms

Fig. S13 Cyclic voltammograms of a) **CA-5T-BT-5T-CA-*b***, b) **CA-5T-IID-5T-CA-*b***, c) **CA-4T-IID-4T-CA-*b*** and d) **CA-3T-IID-3T-CA-*l***.



5. DSC thermograms

Fig. S14 DSC thermograms of a) **CA-5T-BT-5T-CA-*b***, b) **CA-5T-IID-5T-CA-*b***, c) **CA-4T-IID-4T-CA-*b*** and d) **CA-3T-IID-3T-CA-*l***.



6. Organic field-effect transistor characteristics

Fig. S15 Output (a and c) and transfer(b and d) characteristics in the saturated regime of OFETs based on a thin film of **CA-5T-BT-5T-CA-*b*** before and after SVA for 10 s (with a transistor channel width and length of 20000 and 10 μm, respectively).

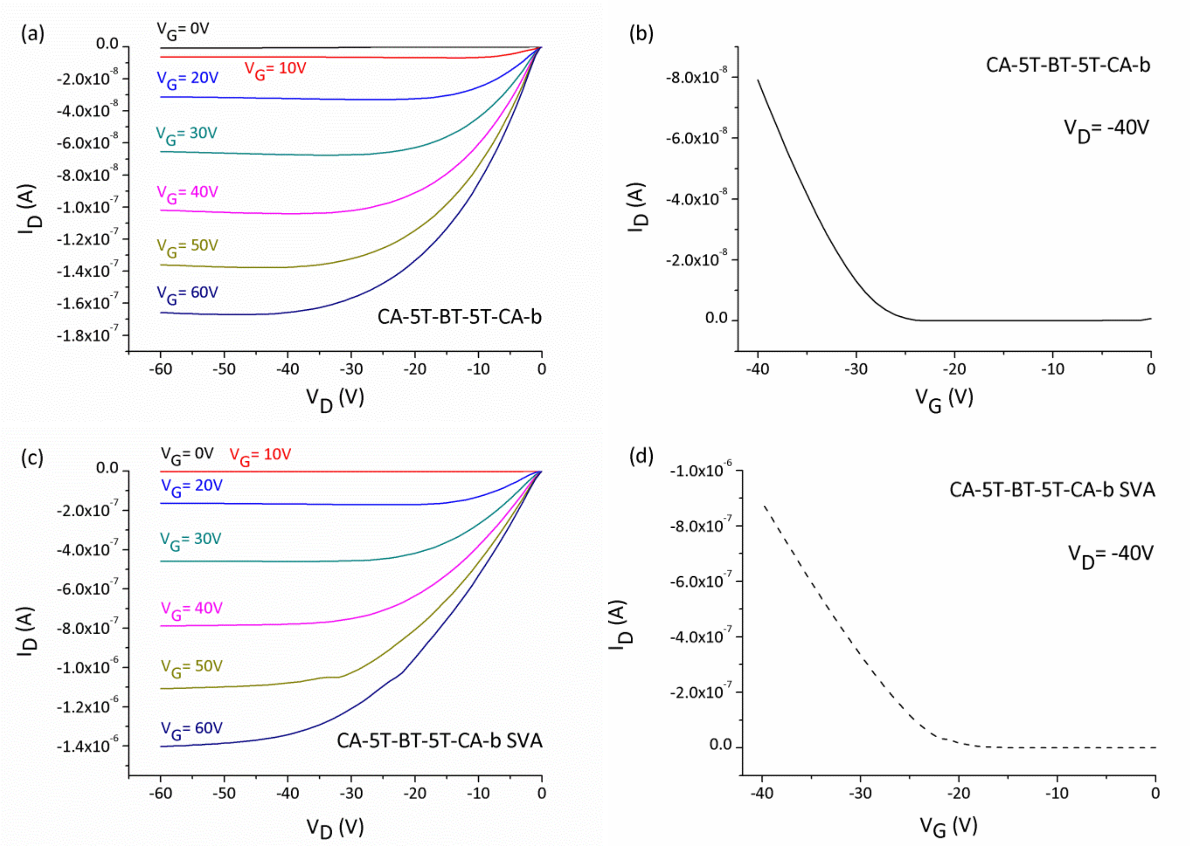


Fig. S16 Output (a and c) and transfer (b and d) characteristics in the saturated regime of OFETs based on a thin film of **CA-5T-IID-5T-CA-*b*** before and after SVA for 10 s (with a transistor channel width and length of 20000 and 10 μm, respectively).

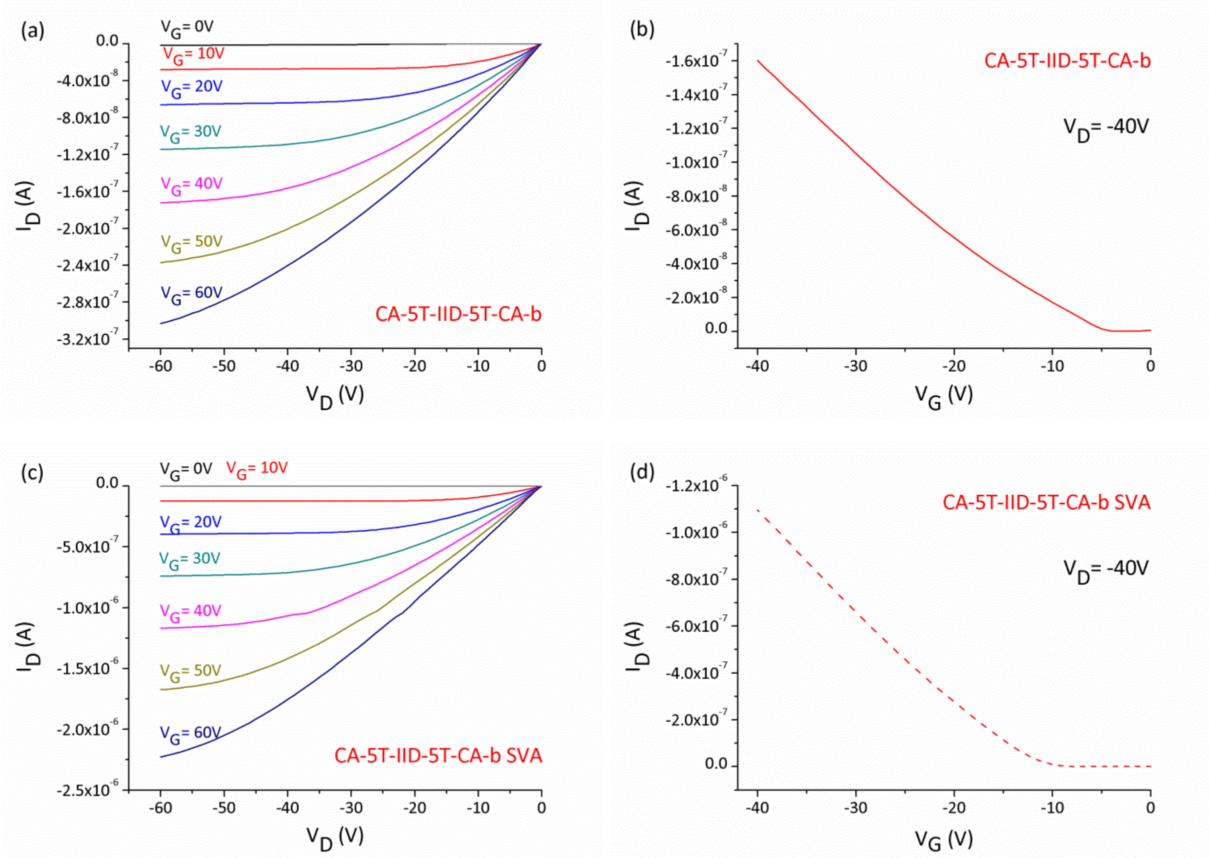


Fig. S17 Output (a and c) and transfer (b and d) characteristics in the saturated regime of OFETs based on a thin film of **CA-4T-IID-4T-CA-*b*** before and after SVA for 10 s (with a transistor channel width and length of 20000 and 10 µm, respectively).

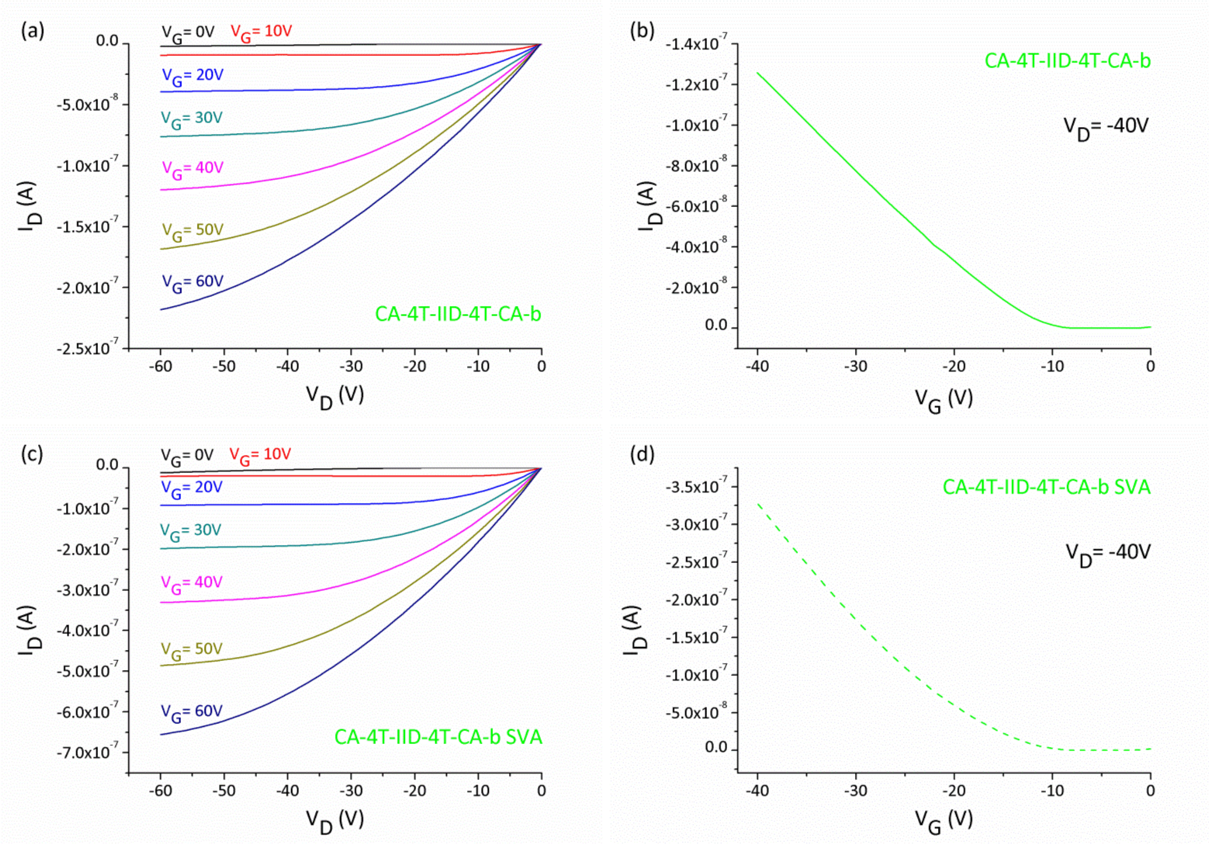
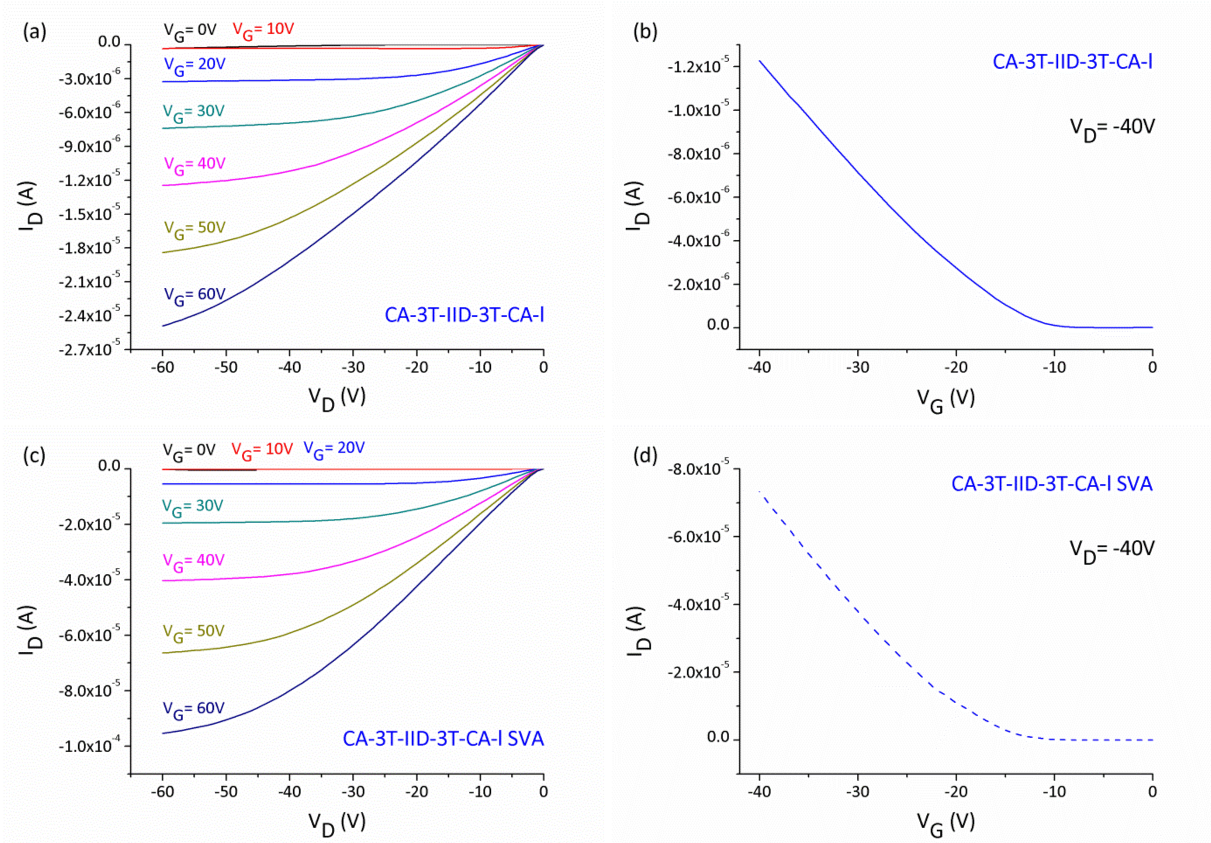


Fig. S18 Output (a and c) and transfer (b and d) characteristics in the saturated regime of OFETs based on a thin film of **CA-3T-IID-3T-CA-*l*** before and after SVA for 10 s (with a transistor channel width and length of 20000 and 10 μm, respectively).



7. Solar cell optimization tables

Table S1 Overview of the organic solar cell optimization studies for the devices based on **CA-5T-BT-5T-CA-*b***:$PC_{71}BM$.[a]

Ratio	Tot. conc. (mg/mL)	SVA[b] (s)	V_{oc} (V)	J_{sc} ($mAcm^{-2}$)	FF (%)	PCE[c] (%)
1:0.5	14	-	0.80	1.34	36	0.39 (0.36)
1:0.5	14	10	0.74	0.93	49	0.34 (0.26)
1:0.8	14	-	0.78	2.42	45	0.85 (0.84)
1:0.8	14	10	0.68	1.14	52	0.40 (0.33)
1:1	14	-	0.72	2.11	51	0.77 (0.74)
1:1	14	10	0.68	1.17	55	0.44 (0.23)
1:1	14	20	0.65	1.17	45	0.34 (0.26)
1:2	14	-	0.61	1.56	38	0.36 (0.24)
1:2	14	-	0.78	1.86	47	0.68 (0.65)
1:2	14	-	0.78	1.45	48	0.54 (0.40)

[a] All processing from $CHCl_3$, no thermal annealing applied. [b] Solvent vapour annealing.
[c] Best efficiencies. Averages over at least 4 devices in parentheses.

Table S2 Overview of the organic solar cell optimization studies for the devices based on **CA-5T-IID-5T-CA-*b***:$PC_{71}BM$.

Ratio	Tot.conc. (mg/mL)	Solvent	$T_{anneal.}$ (°C-min)	SVA[b] (s)	V_{oc} (V)	J_{sc} (mAcm^{-2})	FF (%)	PCE[c] (%)
1:0.5	14	$CHCl_3$	-	-	0.86	1.70	47	0.69 (0.61)
1:0.5	14	$CHCl_3$	-	10	0.77	2.55	37	0.72 (0.69)
1:0.5	14	$CHCl_3$	-	20	0.78	2.21	45	0.78 (0.68)
1:0.5	14	$CHCl_3$	100-5	-	0.86	1.84	51	0.81 (0.72)
1:0.8	14.4	$CHCl_3$	-	-	0.87	1.81	51	0.80 (0.74)
1:0.8	14.4	$CHCl_3$	-	10	0.83	3.29	51	1.39 (1.10)
1:0.8	14	$CHCl_3$	-	-	0.86	1.46	49	0.62 (0.59)
1:0.8	14	$CHCl_3$	-	10	0.82	3.15	50	1.29 (1.19)
1:0.8	14	$CHCl_3$	-	10	0.82	2.88	52	1.23 (1.10)
1:0.8	14	$CHCl_3$	-	15	0.82	2.94	48	1.17 (1.05)
1:0.8	20	CB[a]	-	-	0.85	1.39	44	0.52 (0.50)
1:0.8	20	CB	-	-	0.84	1.11	43	0.40 (0.37)
1:0.8	20	CB	-	10	0.83	2.46	51	1.03 (0.81)
1:0.8	20	CB	-	20	0.83	2.22	52	0.96 (0.89)
1:1	14	$CHCl_3$	-		0.83	1.38	43	0.50 (0.49)
1:1	14	$CHCl_3$	-	10	0.81	2.75	45	1.00 (0.89)
1:1	14	$CHCl_3$	-	20	0.8	2.80	44	0.99 (0.84)
1:1	14	$CHCl_3$	100-5	-	0.83	1.32	44	0.49 (0.33)
1:2	14	$CHCl_3$	-	-	0.84	1.04	45	0.39 (0.31)
1:2	14	$CHCl_3$	-	10	0.72	1.91	37	0.51 (0.42)
1:2	14	$CHCl_3$	-	20	0.79	1.68	44	0.58 (0.42)
1:2	14	$CHCl_3$	100-5	-	0.75	0.94	30	0.22 (0.14)

[a] CB = chlorobenzene. [b] Solvent vapour annealing. [c] Best efficiencies. Averages over at least 4 devices in parentheses.

Table S3 Overview of the organic solar cell optimization studies for the devices based on **CA-4T-IID-4T-CA-*b***:$PC_{71}BM$.[a]

Ratio	Tot. conc. (mg/mL)	SVA[b] (s)	V_{oc} (V)	J_{sc} (mAcm^{-2})	FF (%)	PCE[c] (%)
1:0.5	14	-	0.93	0.98	48	0.44 (0.41)
1:0.5	14	10	0.93	1.69	48	0.76 (0.67)
1:0.8	14.4	-	0.99	0.94	51	0.47 (0.45)
1:0.8	14.4	10	0.98	1.6	50	0.78 (0.70)
1:0.8	14.4	-	0.89	0.76	47	0.32 (0.31)
1:0.8	14.4	10	0.91	1.51	47	0.64 (0.57)
1:0.8	14.4	20	0.57	1.39	32	0.25 (0.22)
1:1	14.4	-	0.92	0.66	50	0.31 (0.28)
1:1	14.4	10	0.91	1.03	50	0.47 (0.43)
1:1	14.4	20	0.85	1.12	48	0.46 (0.35)

[a] All processing from $CHCl_3$, no thermal annealing applied. [b] Solvent vapour annealing. [c] Best efficiencies. Averages over at least 4 devices in parentheses.

Table S4 Overview of the organic solar cell optimization studies for the devices based on **CA-3T-IID-3T-CA-*l***:$PC_{71}BM$.[a]

Ratio	Tot. conc. (mg/mL)	$T_{anneal.}$ (°C-min)	SVA[b] (s)	V_{oc} (V)	J_{sc} (mAcm^{-2})	FF (%)	PCE[c] (%)
1:0.5	14	-	20	0.93	2.04	48	0.91 (0.77)
1:0.5	14	-	-	0.90	1.16	49	0.51 (0.48)
1:0.5	14	-	10	0.93	2.14	54	1.07 (0.96)
1:0.5	14	-	20	0.91	2.26	59	1.20 (1.05)
1:0.5	14	100-5	-	0.38	1.43	27	0.15 (0.11)
1:0.8	14.4	-	-	0.96	1.32	55	0.69 (0.65)
1:0.8	14.4	-	10	0.95	4.46	45	1.92 (1.60)
1:0.8	14.4	-	-	0.93	1.26	53	0.62 (0.53)
1:0.8	14.4	-	10	0.95	2.04	60	1.17 (1.01)
1:0.8	14.4	-	10	0.95	2.89	58	1.60 (1.50)
1:1	14	-	-	0.82	1.21	35	0.35 (0.26)
1:1	14	-	10	0.93	2.06	57	1.09 (0.99)
1:1	14	-	20	0.52	1.60	32	0.27 (0.23)
1:1	14	100-5	-	0.94	1.33	44	0.56 (0.43)
1:2	14	-	-	0.89	1.30	35	0.40 (0.27)
1:2	14	-	10	0.82	1.54	36	0.46 (0.31)
1:2	14	-	20	0.11	1.42	24	0.04 (0.03)
1:2	14	100-5	-	0.91	1.27	39	0.46 (0.36)

[a] All processing from $CHCl_3$. [b] Solvent vapour annealing. [c] Best efficiencies. Averages over at least 4 devices in parentheses.