Supporting Information

Effect of end group functionalisation of small molecules featuring the fluorene-thiophene-benzothiadiazole motif as emitters in solution-processed red and orange organic light-emitting diodes†

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† Supporting data are accessible from http://dx.doi.org/10.5525/gla.researchdata.622

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Cyclic voltammetry (CV) of Compound 1

Recorded using glassy carbon, platinum wire and Ag wire as the working, counter and pseudo-reference electrodes respectively, with (nBu)$_4$PF$_6$ as the electrolyte in dichloromethane solution (0.1 M) at a scan rate of 100 mV s^{-1}. The data were referenced to the Fc/Fc$^+$ redox couple, which has a HOMO of -4.8 eV.

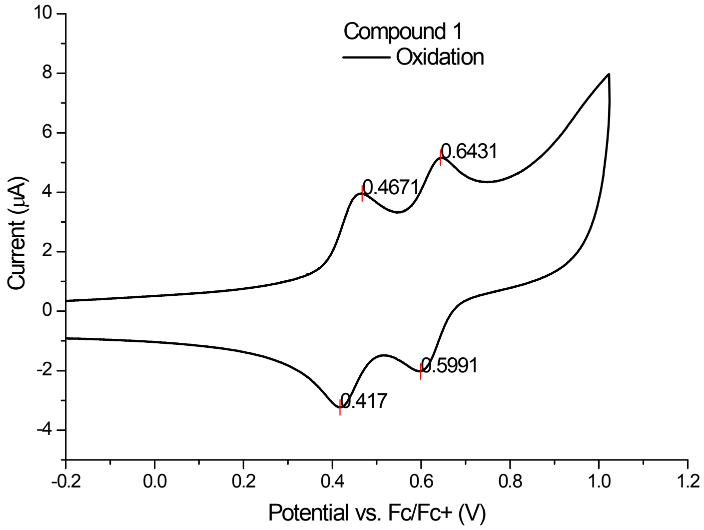


Figure S1a: Oxidation CV cycle of compound **1**.

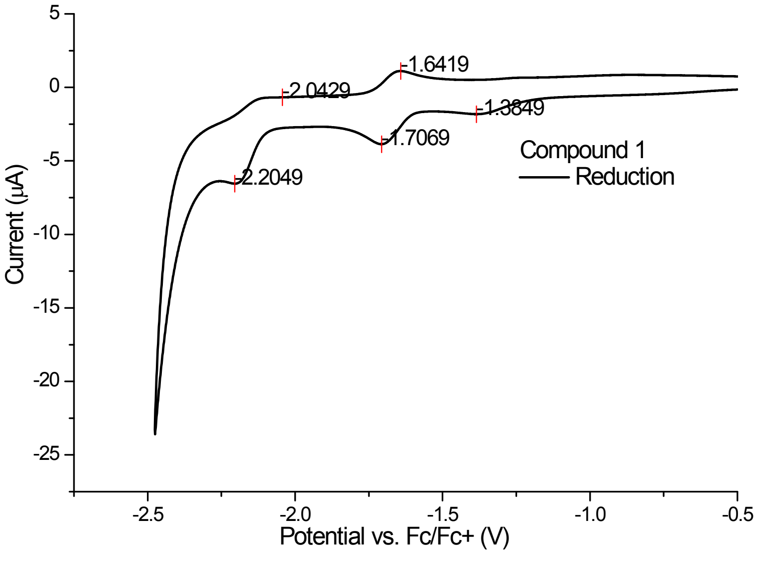


Figure S1b: Reduction CV cycle of compound **1**.

Cyclic voltammetry (CV) of Compound 2

Recorded using glassy carbon, platinum wire and Ag wire as the working, counter and pseudo-reference electrodes respectively, with $(n\mathrm{Bu})_4\mathrm{PF}_6$ as the electrolyte in dichloromethane solution (0.1 M) at a scan rate of 100 mV s^{-1}. The data were referenced to the Fc/Fc⁺ redox couple, which has a HOMO of -4.8 eV.

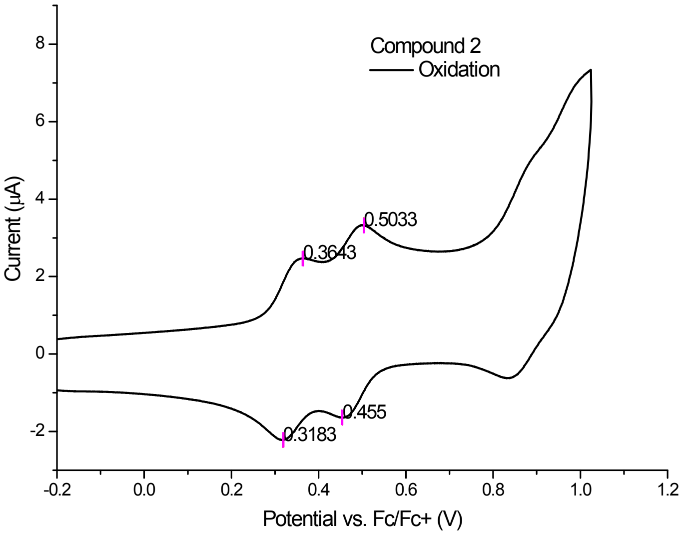


Figure S2a: Oxidation CV cycle of compound **2**.

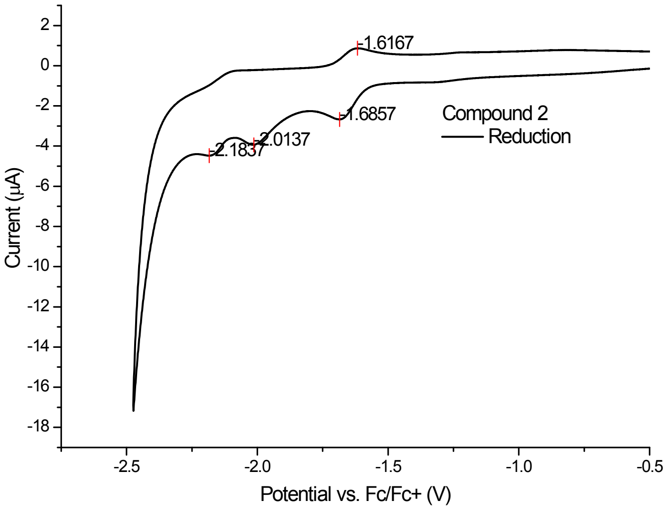
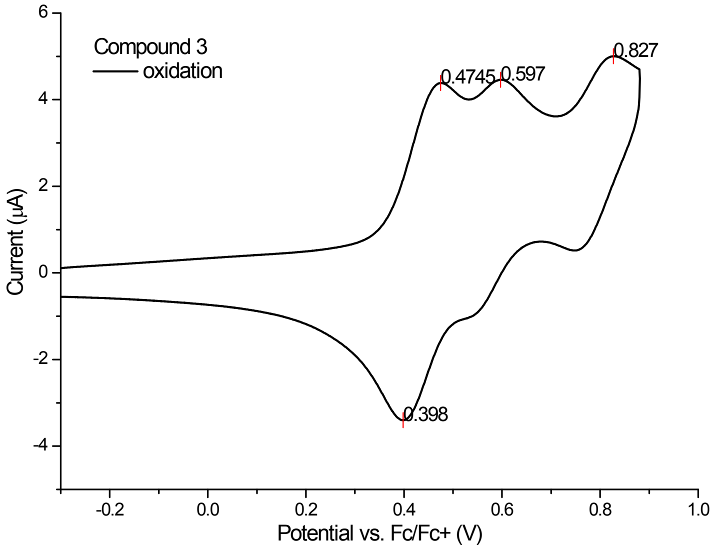


Figure S2b: Reduction CV cycle of compound **2**.

Cyclic voltammetry (CV) of Compound 3

Recorded using glassy carbon, platinum wire and Ag wire as the working, counter and pseudo-reference electrodes respectively, with (nBu)$_4$PF$_6$ as the electrolyte in dichloromethane solution (0.1 M) at a scan rate of 100 mV s^{-1}. The data were referenced to the Fc/Fc$^+$ redox couple, which has a HOMO of -4.8 Ev



.Figure S3a: Oxidation CV cycle of compound **3**.

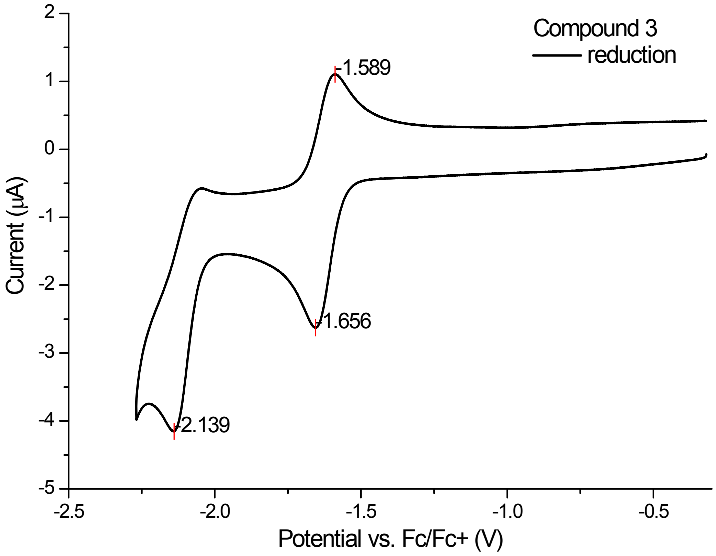


Figure S3b: Reduction CV cycle of compound **3**.

Cyclic voltammetry (CV) of Compound 4

Recorded using glassy carbon, platinum wire and Ag wire as the working, counter and pseudo-reference electrodes respectively, with $(n\mathrm{Bu})_4\mathrm{PF}_6$ as the electrolyte in dichloromethane solution (0.1 M) at a scan rate of 100 mV s^{-1}. The data were referenced to the Fc/Fc$^+$ redox couple, which has a HOMO of -4.8 eV.

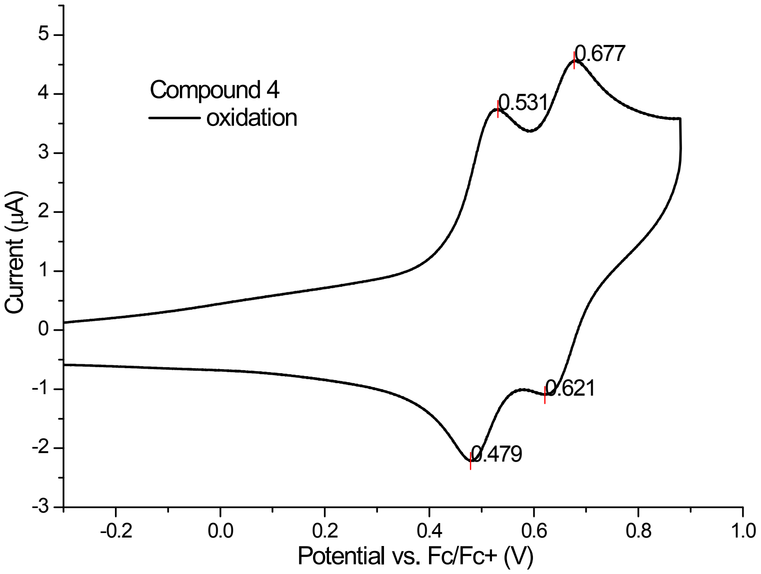


Figure S4a: Oxidation CV cycle of compound **4**.

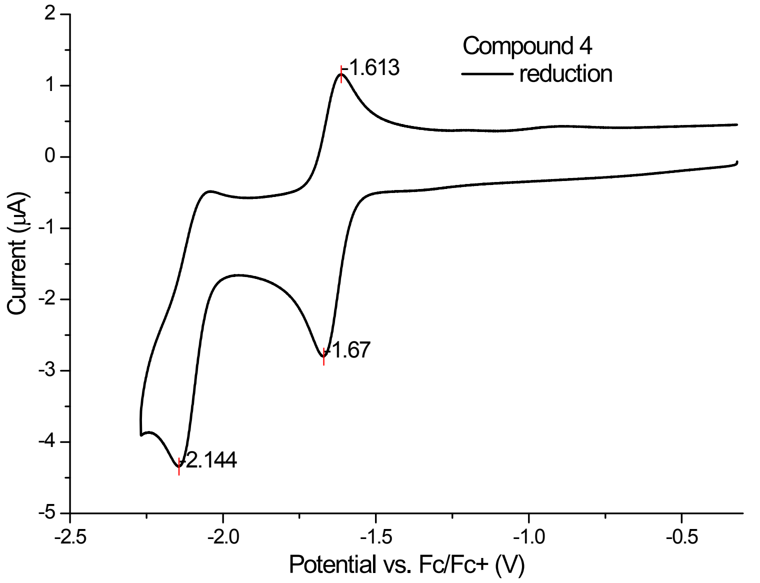
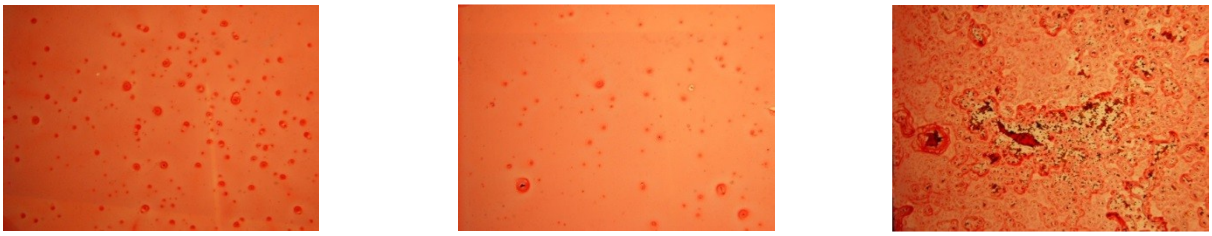


Figure S4b: Reduction CV cycle of compound **4**.

AFM and Optical Images



1

2

3 (unfiltered)

4

3 (filtered)

Figure S5: Optical microscope images of spin-coated films of compounds **1**-**4** All materials were spin-coated at 800 RPM from 20 mg ml^{-1} toluene solutions.

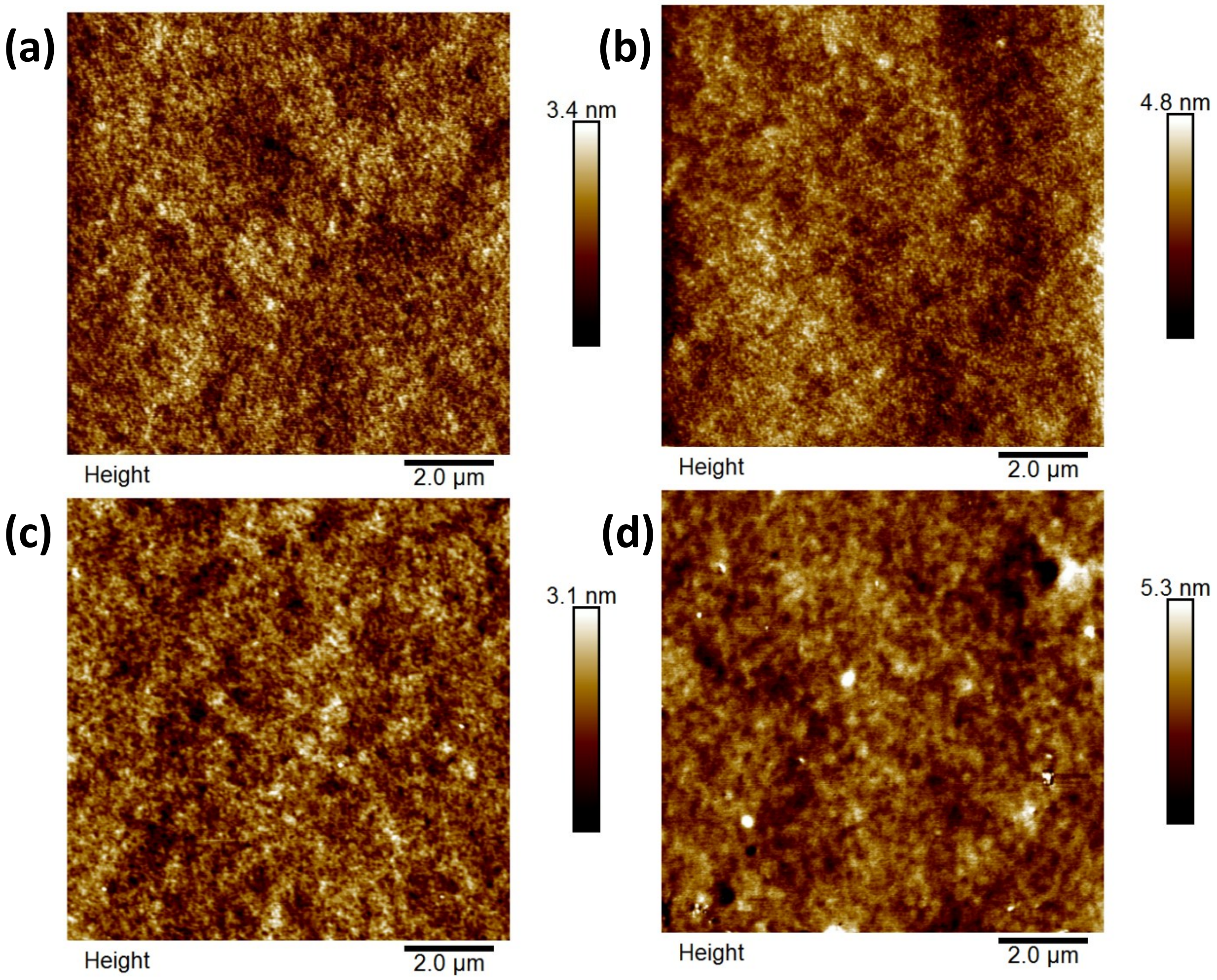


Figure S6: AFM topography images for films of compounds (a) **1** (RMS roughness = 0.49 nm) (b) **2** (RMS roughness = 0.67 nm) (c) **3**, filtered (RMS roughness = 0.45 nm) and (d) **4** (RMS roughness = 0.74 nm), deposited using 20 mg ml^{-1} solutions with no annealing treatment.

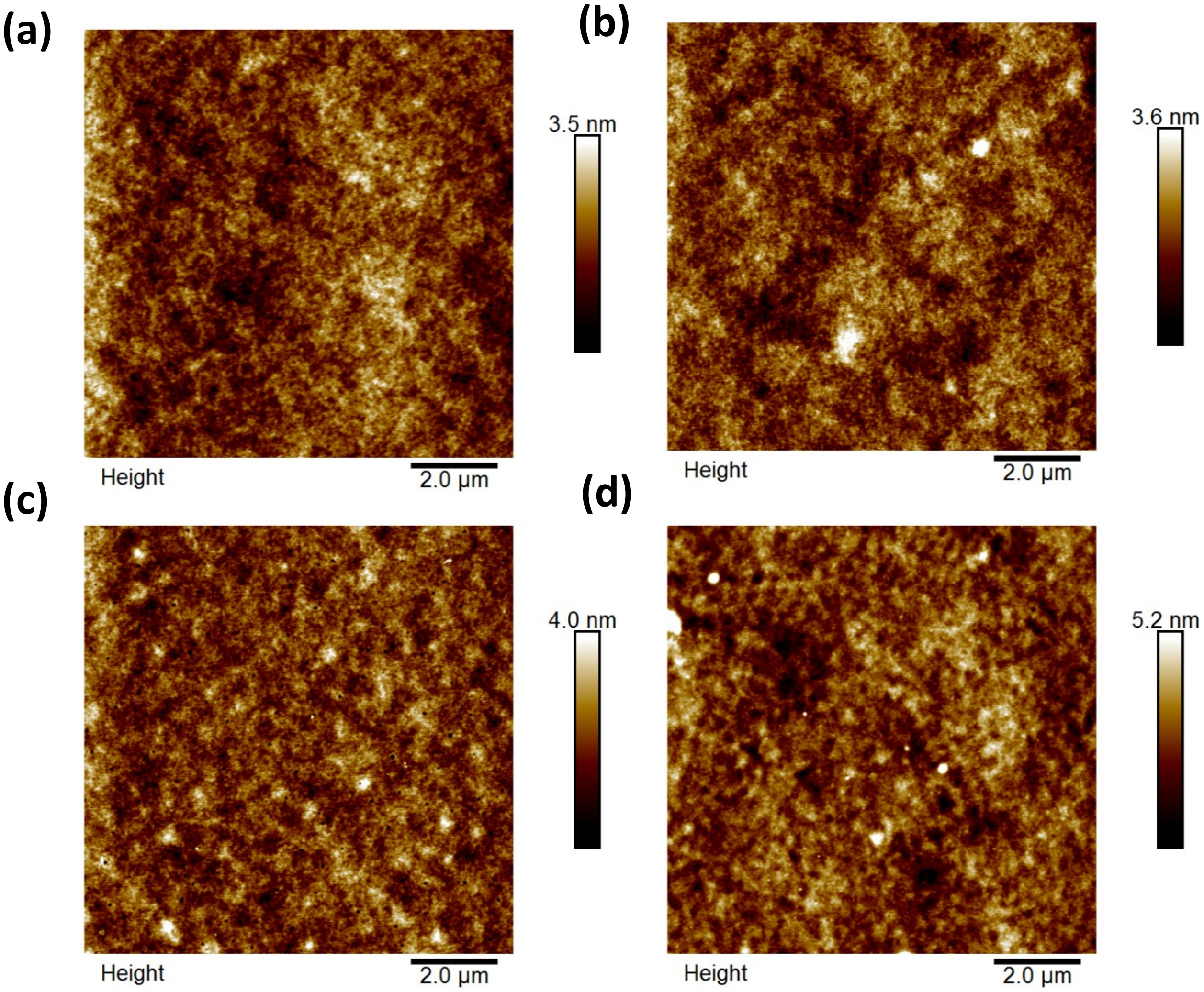


Figure S7: AFM topography images for films of compounds (a) **1** (RMS roughness = 0.50 nm) (b) **2** (RMS roughness = 0.52 nm) (c) **3**, filtered (RMS roughness = 0.58 nm) and (d) **4** (RMS roughness = 0.75 nm), deposited using 20 mg ml^{-1} solutions with films annealed at 80°C for 10 minutes.

OLED optimisation

Table S1: OLED data for compounds **1**, **2**, **3** and **4** at various annealing temperatures. All devices were prepared from toluene solutions at 20 mg ml^{-1} concentration. Average values are in parentheses.

Compound	**Annealing (°C)**	**Turn on voltage (V) (at 100 cd m^{-2})**	**Luminance (cd m^{-2})**	**Current efficiency (cd A^{-1})**	**Maximum EQE (%)**
1	r.t	2.7 (2.8)[a]	854 @ 7 V (708 @ 7 V)[a]	0.10 (0.093)[a]	0.22 (0.19)[a]
	40	3.6 (4.2)[a]	440 @ 11V (382 @ 11 V)[a]	0.079 (0.072)[a]	0.17 (0.15)[a]
	60	3.8 (4.0)[b]	429 @10V (348 @ 10 V)[b]	0.072 (0.060)[b]	0.15 (0.13)[b]
	80	3.8 (4.2)[d]	245 @ 8V (199 @ 10 V)[d]	0.060 (0.045)[d]	0.12 (0.07)[d]
2	r.t	2.9 (3.0)[d]	1561 @ 8 V (1410 @ 8 V)[d]	0.15 (0.14)[d]	0.25 (0.23)[d]
	40	3.0 (3.1)[b]	1609 @ 9V (1367 @ 9V)[b]	0.19 (0.16)[b]	0.32 (0.29)[b]
	60	3.1 (3.3)[d]	1409 @ 9V (1146 @ 10V)[d]	0.17 (0.16)[d]	0.31 (0.26)[b]
	80	3.1 (3.2)[c]	1362 @ 9V (1169 @ 9V)[c]	0.16 (0.15)[c]	0.27 (0.25)[c]
	100	3.4 (3.5)[e]	1295 @ 9V (1076 @ 9V)[e]	0.15 (0.13)[e]	0.24 (0.23)[e]
3 (filtered)	r.t	2.3 (2.5)[a]	2135 @ 8.8 V (1915 @ 9 V)[a]	0.086 (0.070)[a]	0.16 (0.14)[a]
	40	2.6 (2.7)[c]	1802 @ 8V (1640 @ 8V)[c]	0.091 (0.067)[c]	0.15 (0.13)[c]
	60	2.7 (2.8)[c]	1665 @ 8V (1521 @ 8V)[c]	0.080 (0.059)[c]	0.14 (0.12)[c]
	80	2.5 (2.7)[f]	1790 @ 8V (1699 @ 8V)[f]	0.086 (0.070)[f]	0.14 (0.13)[f]
4	r.t	2.5 (2.9)[d]	1498 @ 7 V (1079 @ 6.7 V)[d]	0.081 (0.064)[d]	0.17 (0.13)[a]
	40	2.4 (2.6)[d]	1339 @ 6.9 V (1168 @ 6.7 V)[d]	0.076 (0.074)[d]	0.16 (0.15)[d]
	60	2.3 (2.4)[d]	990 @ 7.6 V (715 @ 6.9 V)[d]	0.06 (0.044)[d]	0.12 (0.09)[d]
	80	2.4 (2.5)[d]	909 @ 9.5 V (713 @ 8.2 V)[d]	0.040 (0.031)[d]	0.08 (0.06)[d]

[a] recorded as an average over 8 devices; [b] recorded as an average over 7 devices; [c] recorded as an average over 4 devices; [d] recorded as an average over 6 devices; [e] recorded as an average over 5 devices; [f] recorded as an average over 3 devices. The best turn on voltages were achieved with the devices 'annealed' at room temperature (r.t).

NMR spectra

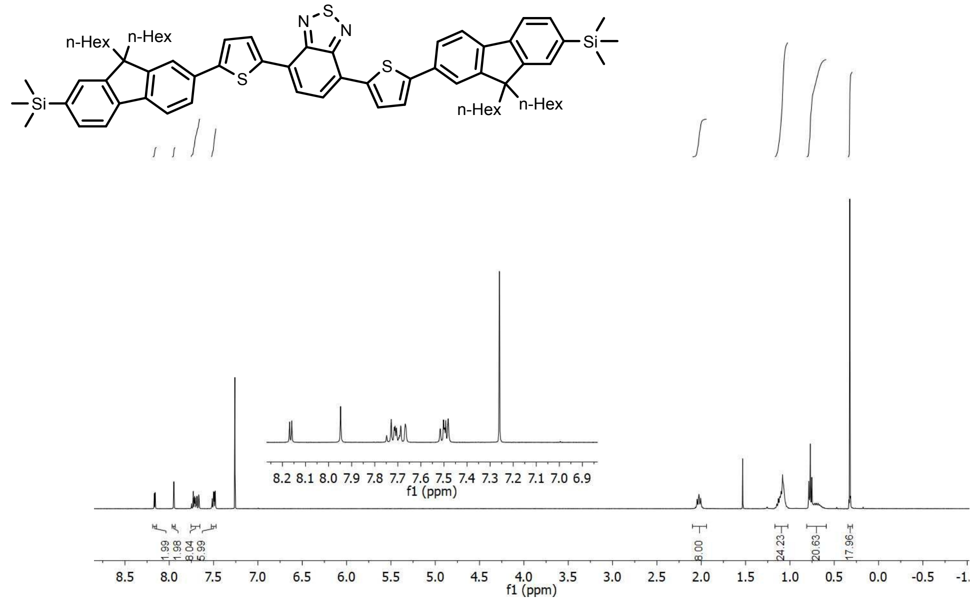
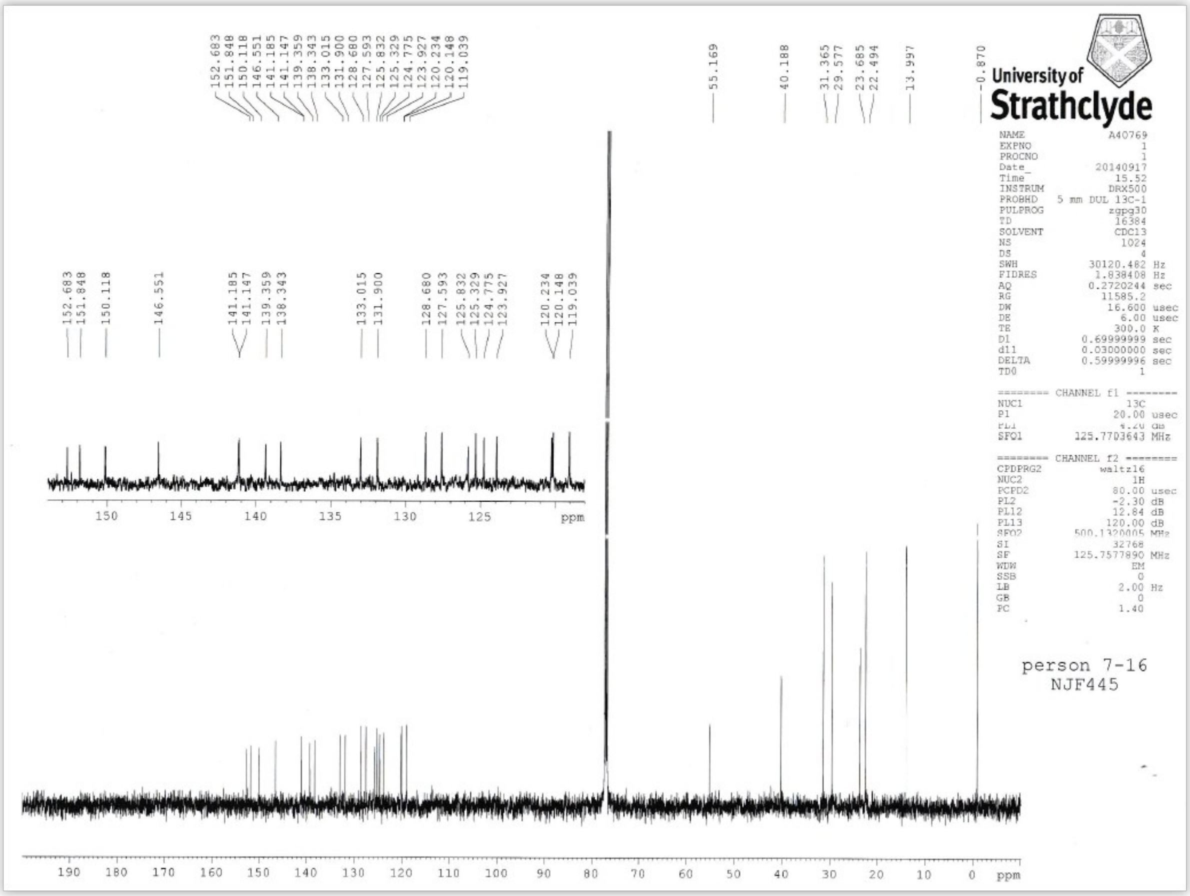


Figure S8: ^{1}H-NMR of compound **1** in $CDCl_3$.



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PROCNO                   1
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PULPROG            zgpg30
TD                   16384
SOLVENT              CDCl3
NS                    1024
DS                       4
SWH             30120.482 Hz
FIDRES           1.838408 Hz
AQ              0.2720244 sec
RG                 11585.2
DW                  16.600 usec
DE                    6.00 usec
TE                   300.0 K
D1              0.69999999 sec
d11             0.03000000 sec
DELTA           0.59999996 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                   20.00 usec
PL1                   4.20 dB
SFO1       125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                    1H
PCPD2                80.00 usec
PL2                  -2.30 dB
PL12                 12.84 dB
PL13                120.00 dB
SFO2       500.1320005 MHz
SI                   32768
SF         125.7577890 MHz
WDW                     EM
SSB                      0
LB                    2.00 Hz
GB                       0
PC                    1.40
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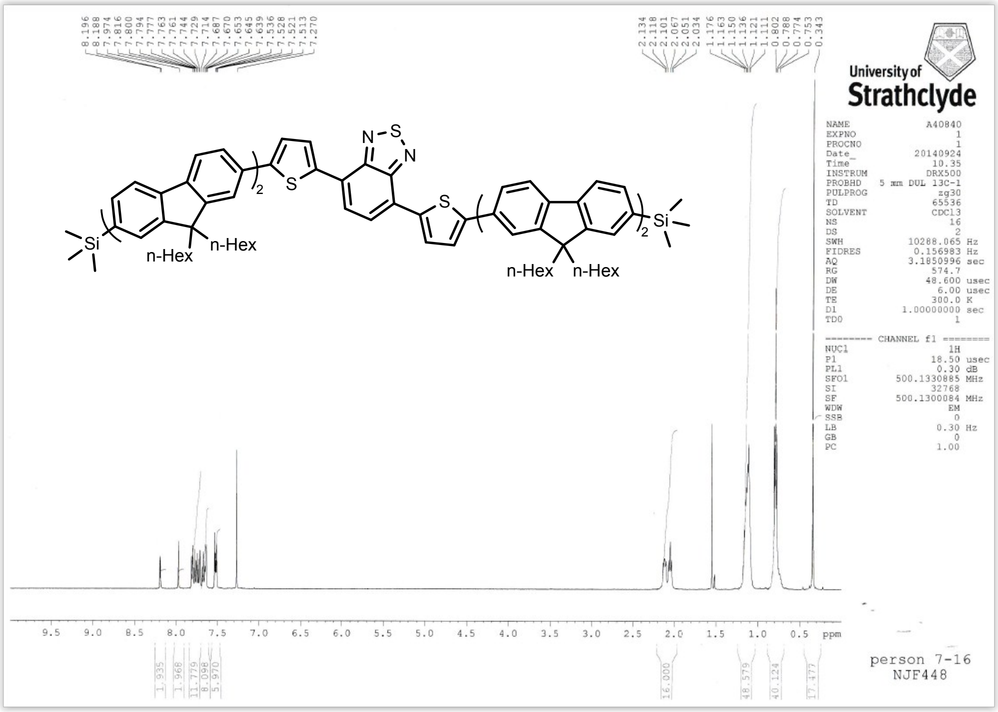
Figure S9: ^{13}C-NMR of compound **1** in $CDCl_3$.



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TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH            10288.065 Hz
FIDRES          0.156983 Hz
AQ             3.1850996 sec
RG                 574.7
DW                48.600 usec
DE                  6.00 usec
TE                 300.0 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 18.50 usec
PL1                 0.30 dB
SFO1         500.1330885 MHz
SI                 32768
SF           500.1300084 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
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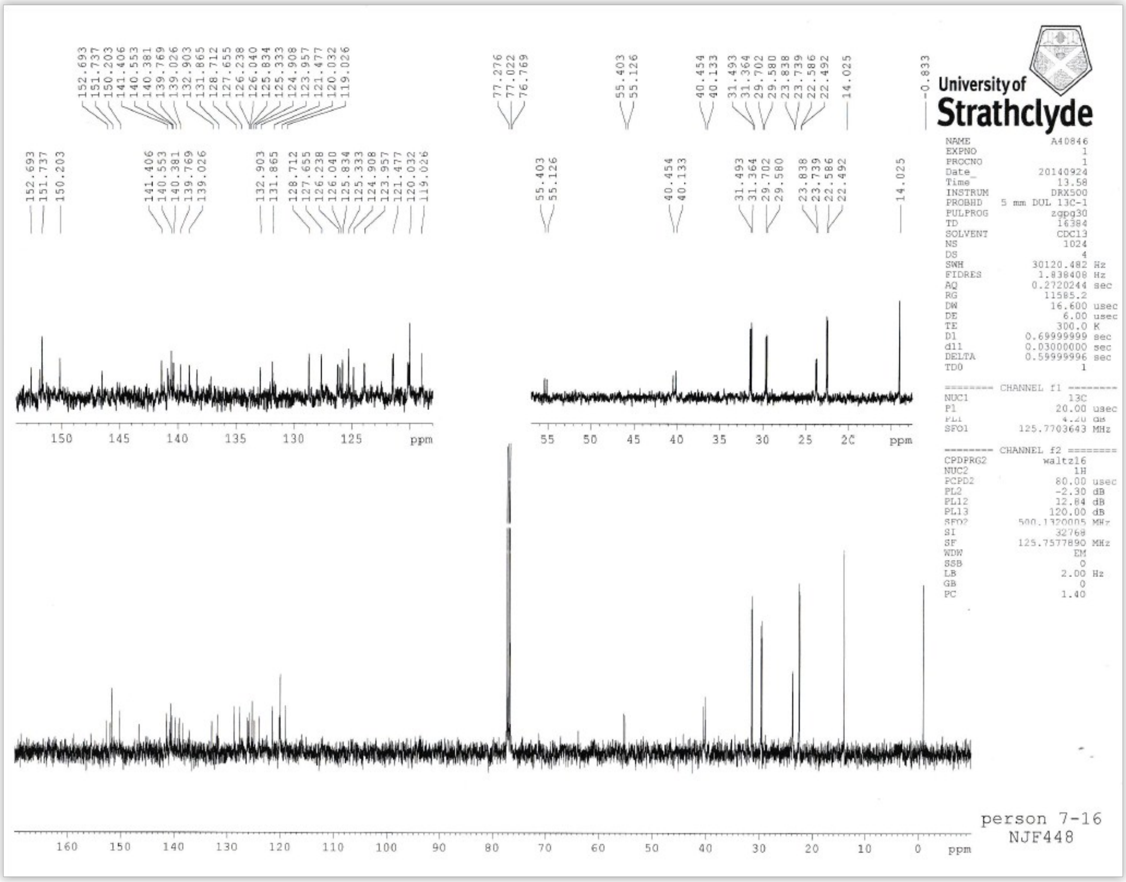
Figure S10: ${}^{1}H$-NMR of compound **2** in $CDCl_3$.



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PROCNO                 1
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TD                 16384
SOLVENT            CDCl3
NS                  1024
DS                     4
SWH            30120.482 Hz
FIDRES          1.838408 Hz
AQ             0.2720244 sec
RG               11585.2
DW                16.600 usec
DE                  6.00 usec
TE                 300.0 K
D1            0.69999999 sec
d11           0.03000000 sec
DELTA         0.59999996 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                 20.00 usec
PL1                 4.20 dB
SFO1         125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                -2.30 dB
PL12               12.84 dB
PL13              120.00 dB
SFO2         500.1320005 MHz
SI                 32768
SF           125.7577890 MHz
WDW                   EM
SSB                    0
LB                  2.00 Hz
GB                     0
PC                  1.40
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Figure S11: ${}^{13}C$-NMR of compound **2** in $CDCl_3$.

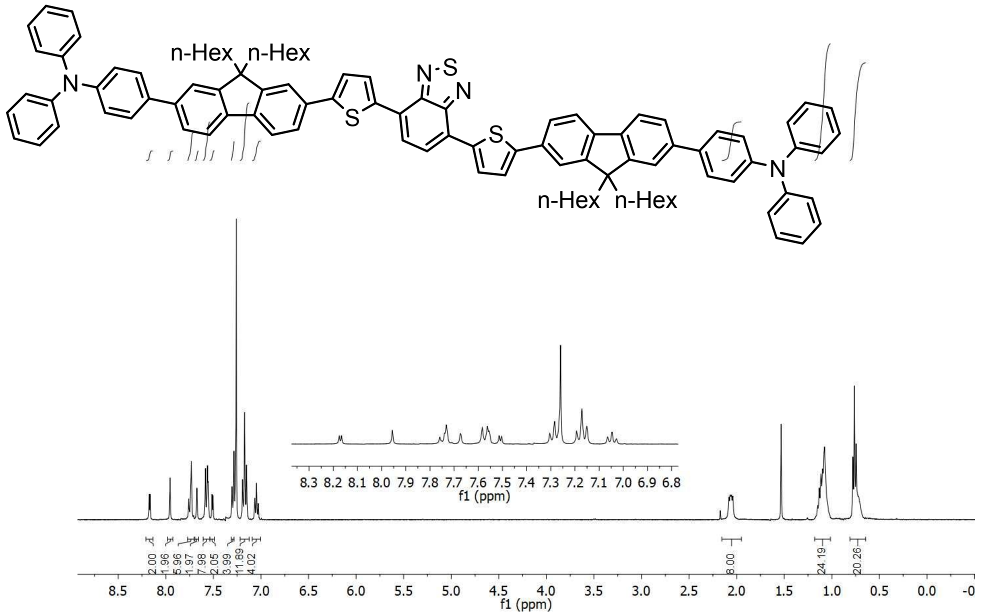

Figure S12: ^{1}H-NMR of compound **3** in $CDCl_3$.

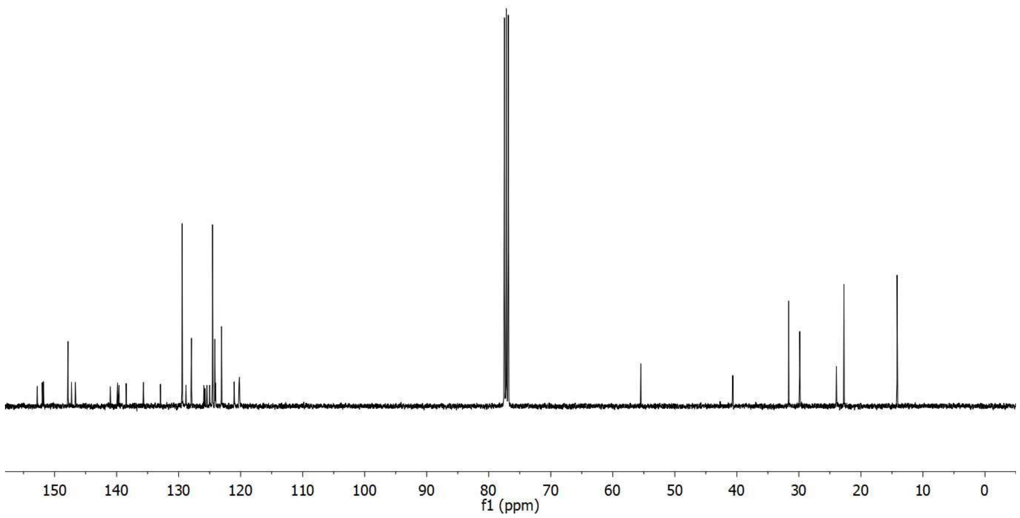

Figure S13: ^{13}C-NMR of compound **3** in $CDCl_3$.

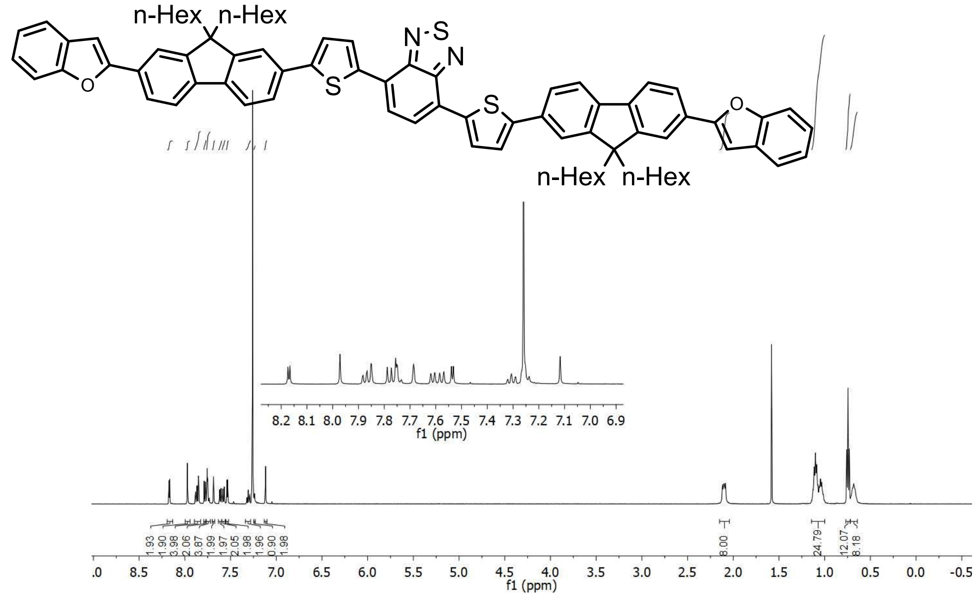

Figure S14: ^{1}H-NMR of compound **4** in $CDCl_3$.

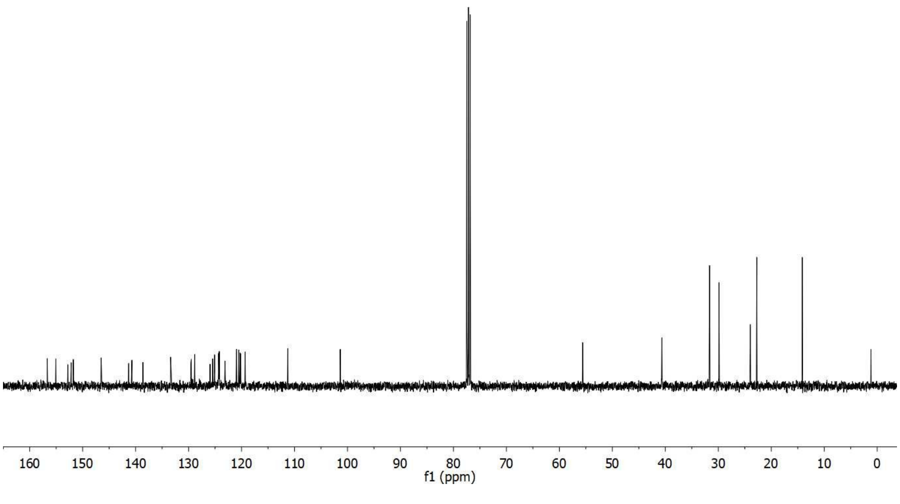

Figure S15: ^{13}C-NMR of compound **4** in $CDCl_3$.