

Performance enhancement of dye-sensitized solar cell by peripheral aromatic and heteroaromatic functionalization in di-branched organic sensitizers

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Electronic Supplementary Information

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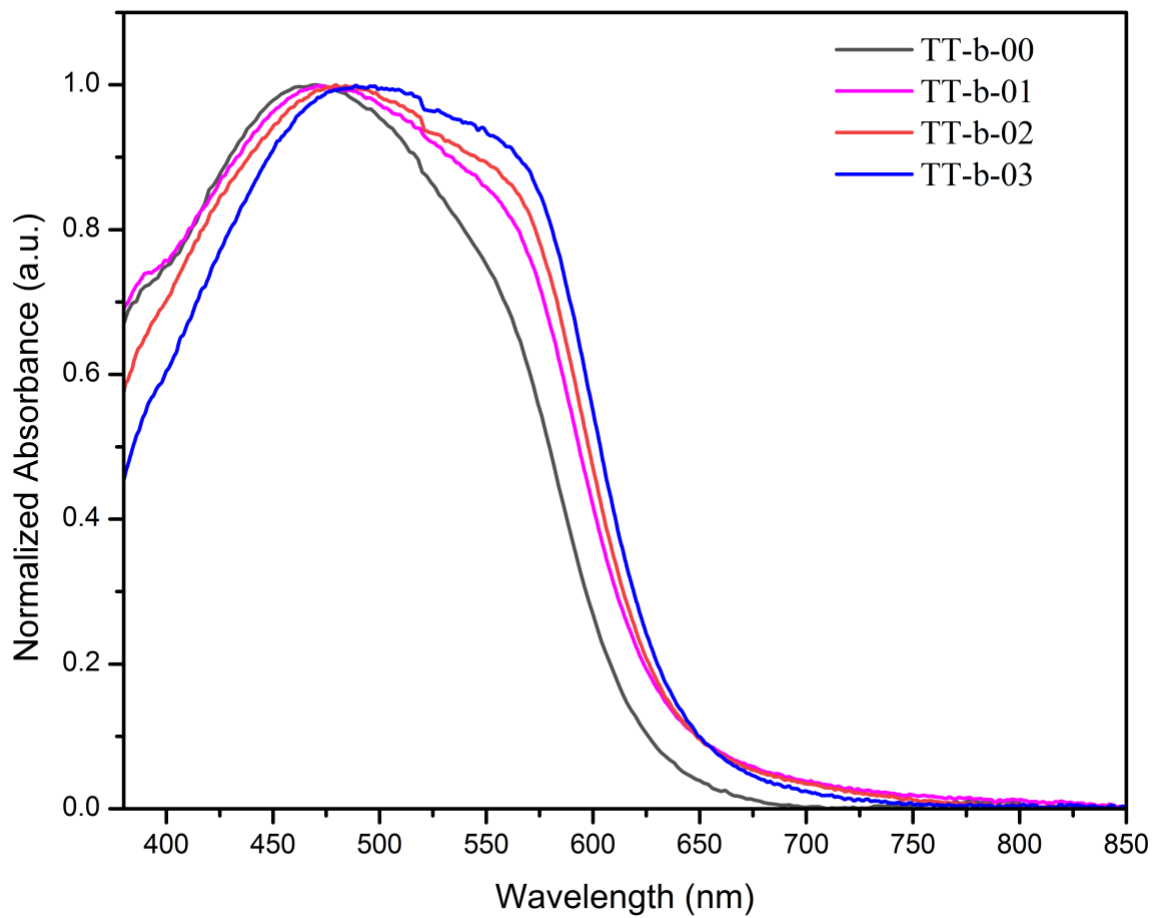


Figure S1. Normalized absorption (spectra of the investigated dyes adsorbed onto a 2.5 μm transparent TiO_2 film).

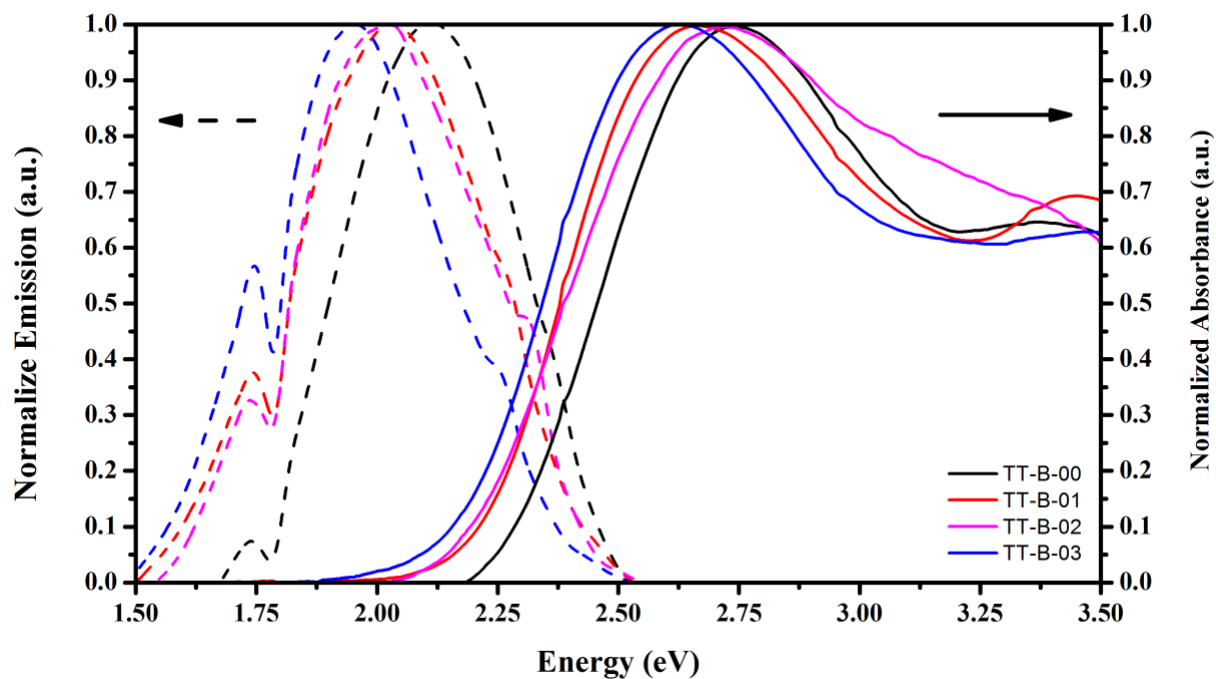


Figure S2. Normalized absorption (solid line) and emission (dashed line) spectra of the investigated dyes in EtOH solution.

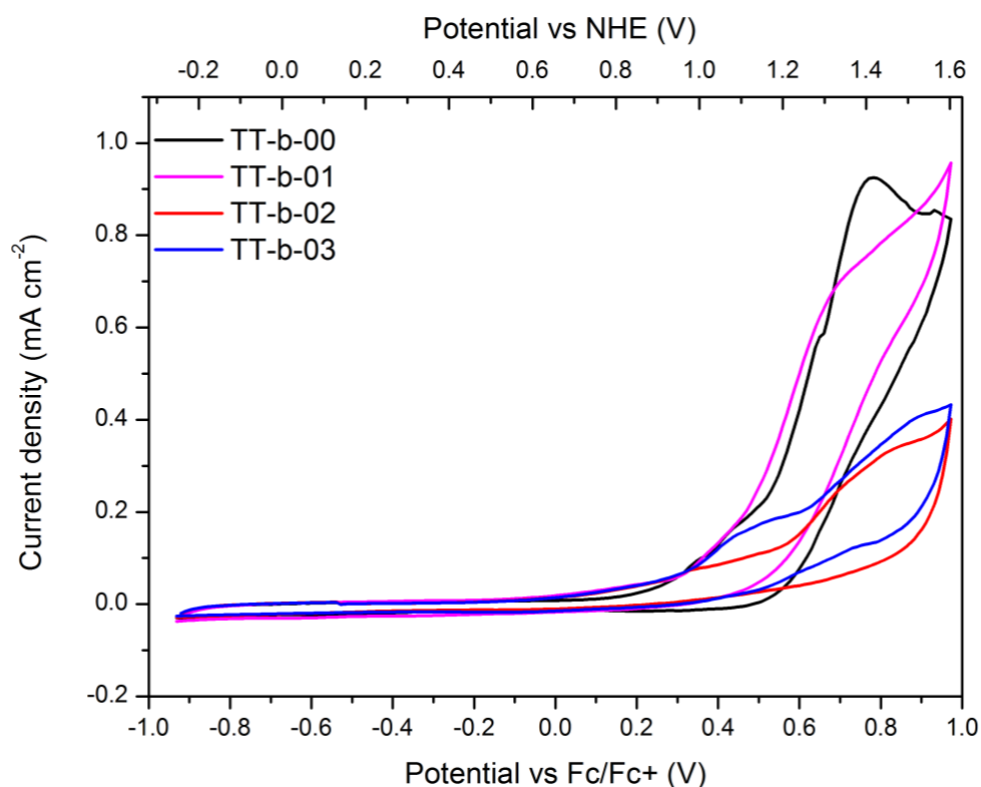


Figure S3. Cyclic voltammetry (CV) plots of the investigated dyes in TBABF₄ 0.1 M in DMF solution.

Table S1: Main photovoltaic parameters of DSSCs based on the di-branched sensitizer **TT-b-02**, varying the electrolyte and the chenodeoxycholic acid (**CDCA**) amount in the 2×10^{-4} M dye solution.

Electrolyte	CDCA (M)	J_{sc} (mA cm ⁻²)	V_{oc} (mV)	FF	PCE (%)
Z959 ^a	0	14.0	624	0.70	6.1
Z960 ^b	0	12.7	664	0.68	5.7
Z959 ^a	2×10^{-4}	15.9	663	0.59	6.2
Z960 ^b	2×10^{-4}	15.6	645	0.62	6.3
Z959 ^a	2×10^{-3}	12.9	628	0.71	5.8
Z960 ^b	2×10^{-3}	12.8	678	0.70	6.1
Z959 ^a	2×10^{-2}	12.6	619	0.72	5.6
Z960 ^b	2×10^{-2}	12.9	678	0.71	6.2

^a 1.0 M DMII, 0.03 M I₂, 0.1 M GSCN, 0.5 M TBP in ACN/VN=85/15; ^b 1.0 M DMII, 0.03 M I₂, 0.05 LiI, 0.1 M GSCN, 0.5 M TBP in ACN/VN=85/15.

Table S2: Main photovoltaic parameters of DSSCs based on the di-branched sensitizers recorded at different time.

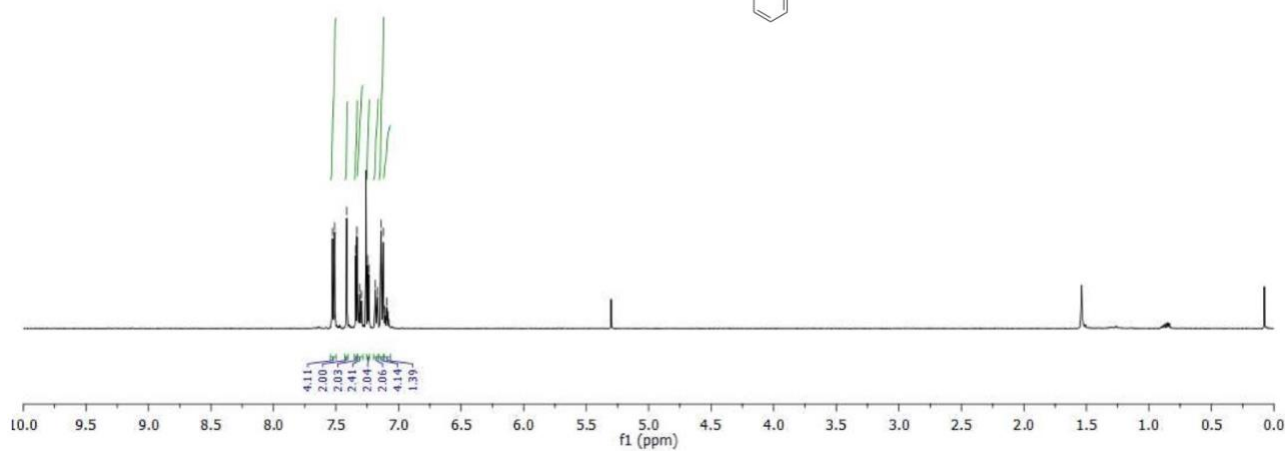
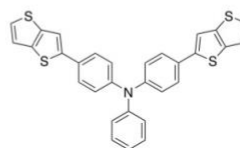
Dye ^a	Time	J _{sc} (mA cm ⁻²)	V _{oc} (mV)	FF	PCE (%)
TT-b-00	3 h	11.5	625	0.60	4.3
	24 h	11.3	629	0.60	4.3
	7 days	10.9	631	0.58	4.0
TT-b-01	3 h	14.3	628	0.62	5.6
	24 h	14.2	630	0.63	5.6
	7 days	13.8	633	0.64	5.6
TT-b-02	3 h	15.6	645	0.62	6.2
	24 h	15.5	644	0.63	6.3
	7 days	14.8	650	0.64	6.2
TT-b-03	3 h	12.5	627	0.71	5.6
	24 h	12.4	625	0.70	5.4
	7 days	11.9	630	0.71	5.3

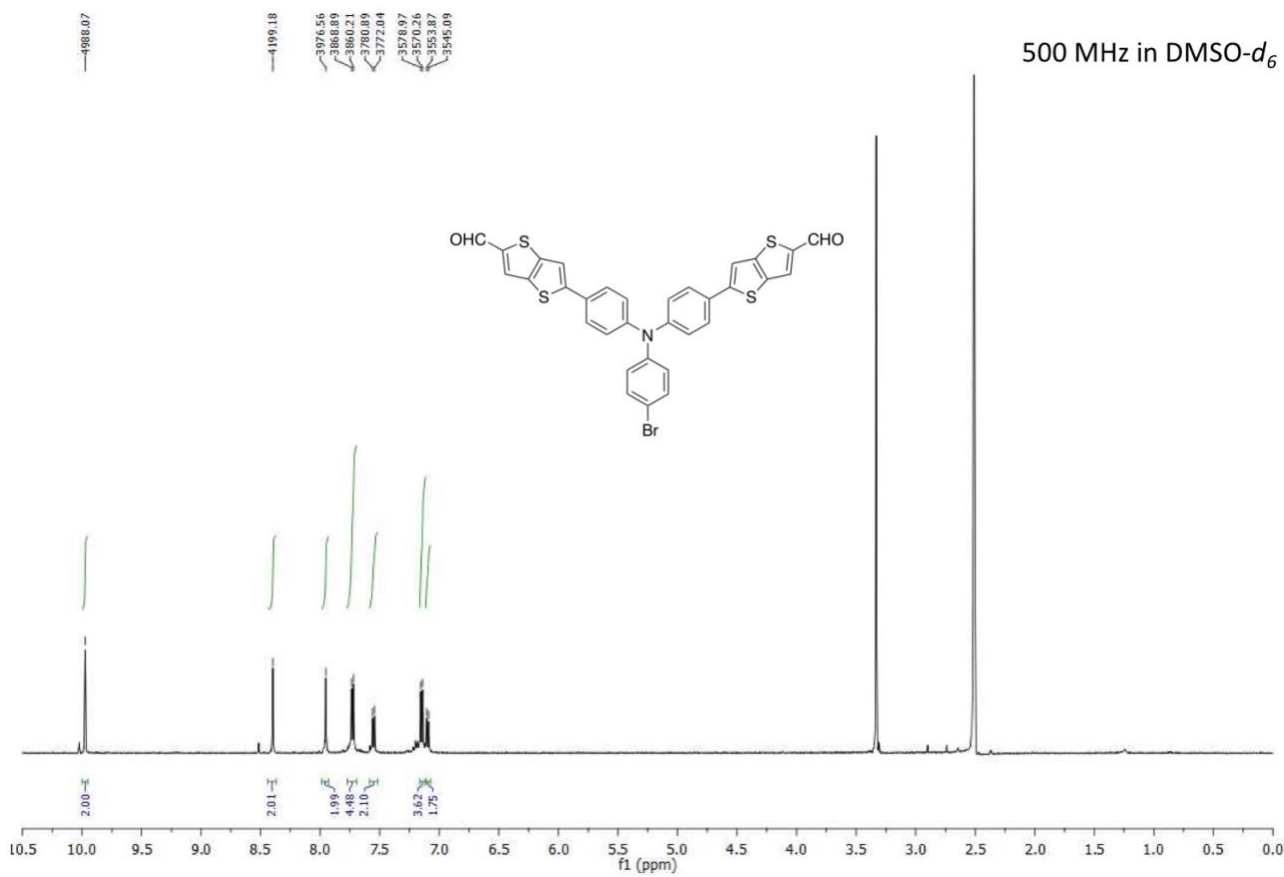
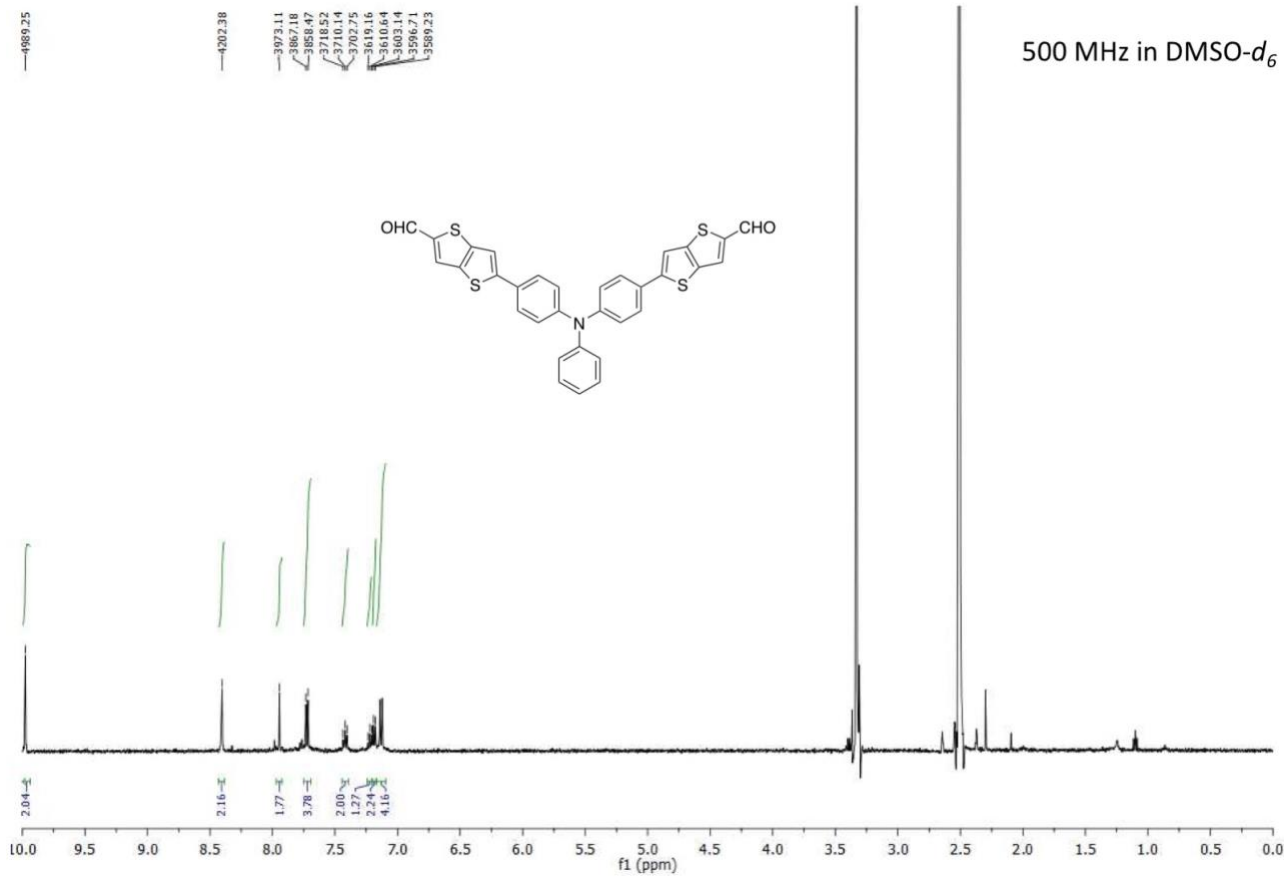
^aDye solution: 2 x 10⁻⁴ M in EtOH + 2 x 10⁻⁴ M CDCA

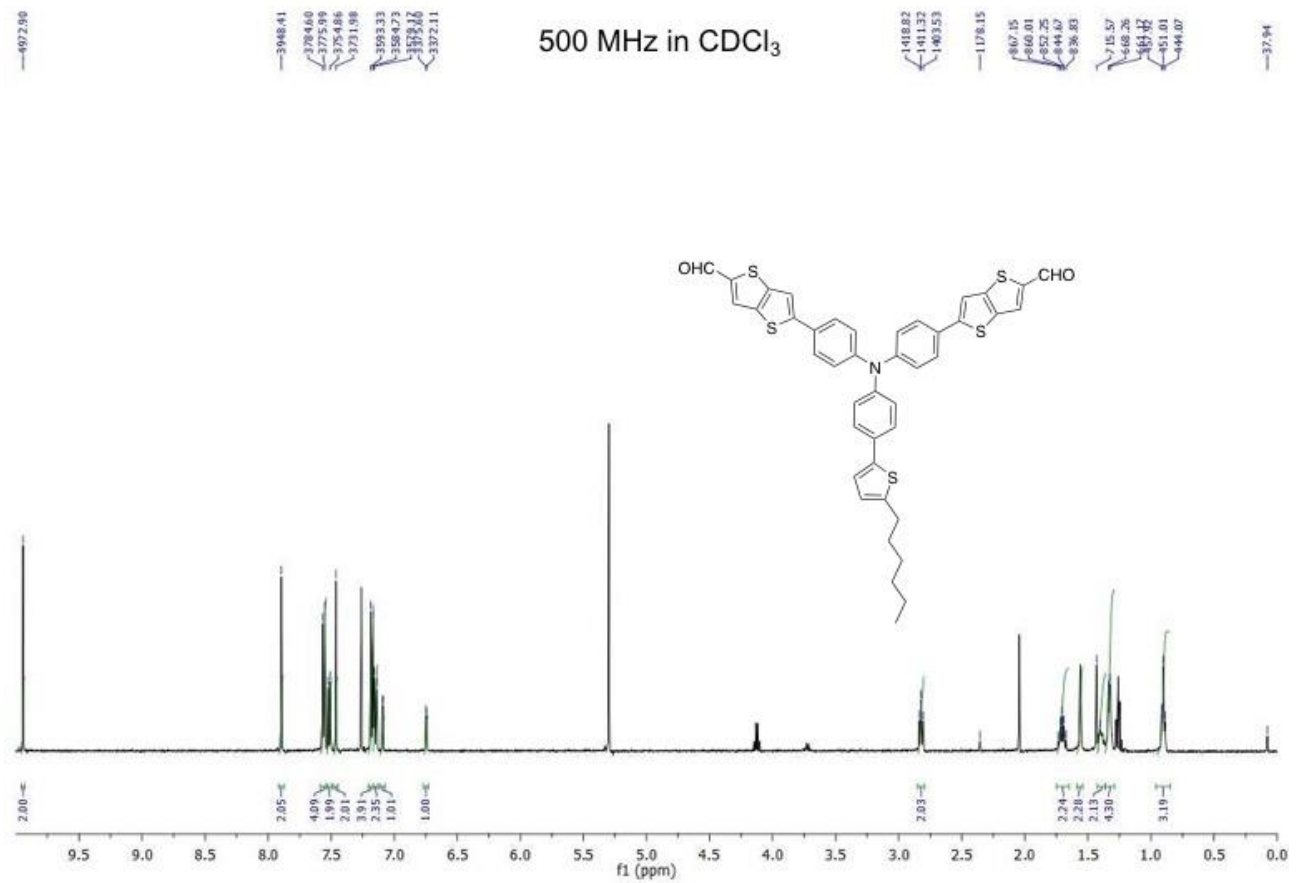
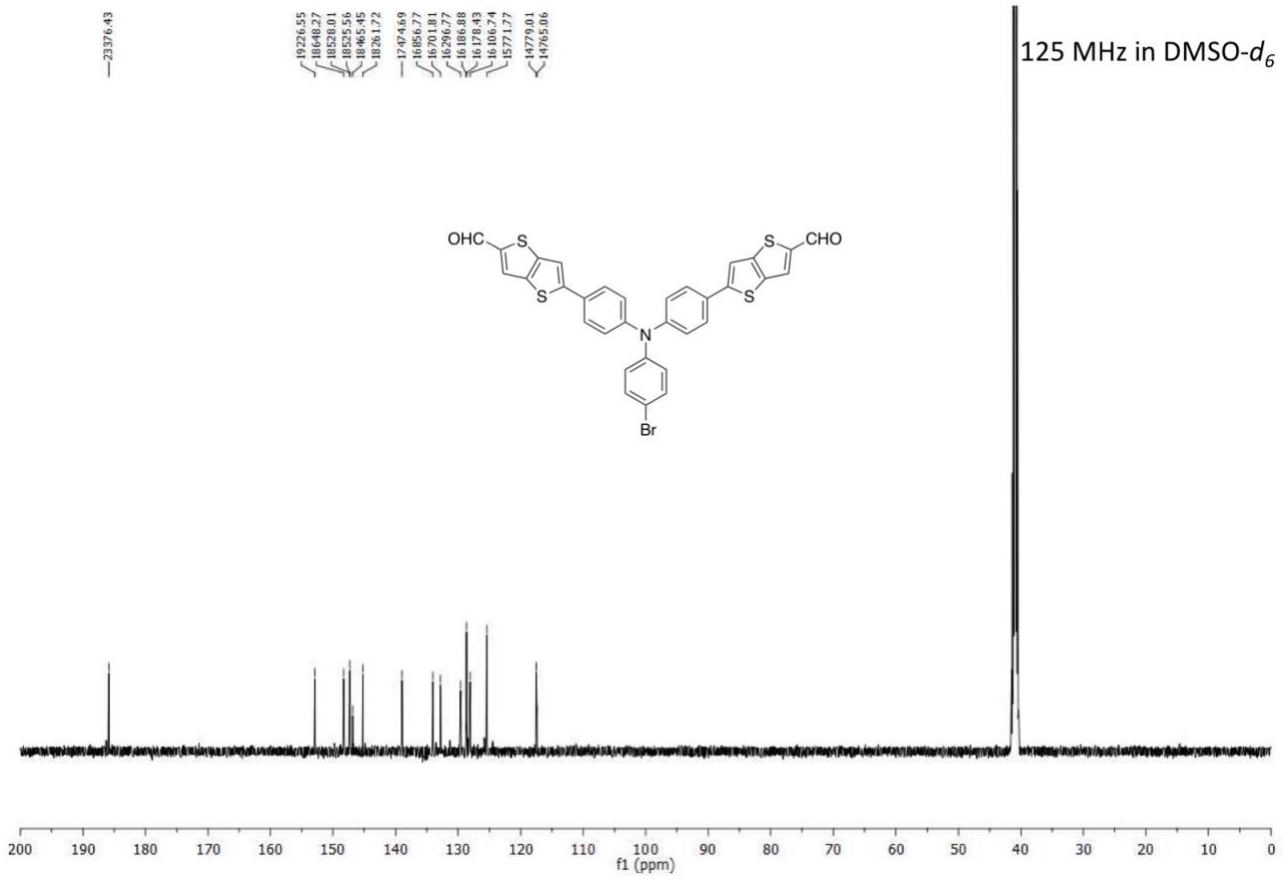
¹H and ¹³C NMR spectra

3764.75
3256.08
3207.91
3071.67
2666.66
2664.39
3056.03
3048.50
3024.46
3619.33
3593.12
3585.56
3571.00
3562.35
3555.50
3548.25
3541.77

500 MHz in CDCl₃



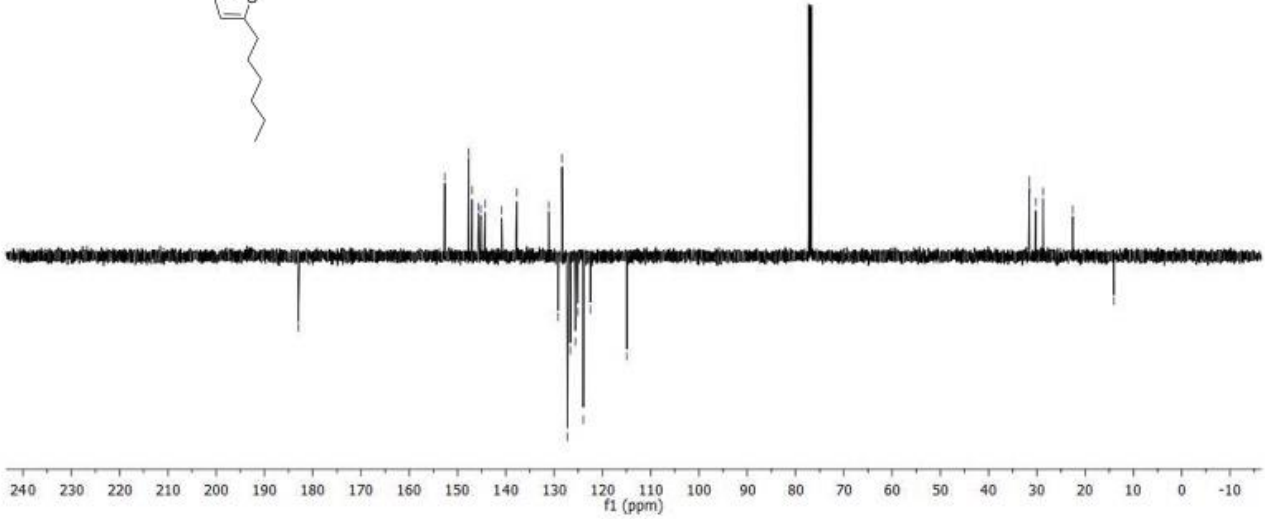
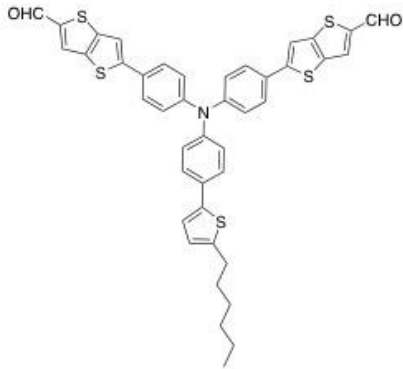




125 MHz in CDCl₃

182.99
152.63
147.68
147.01
145.73
144.30
140.84
137.74
128.34
127.23
126.62
125.60
113.95

31.58
31.56
30.25
28.74
22.55
14.05

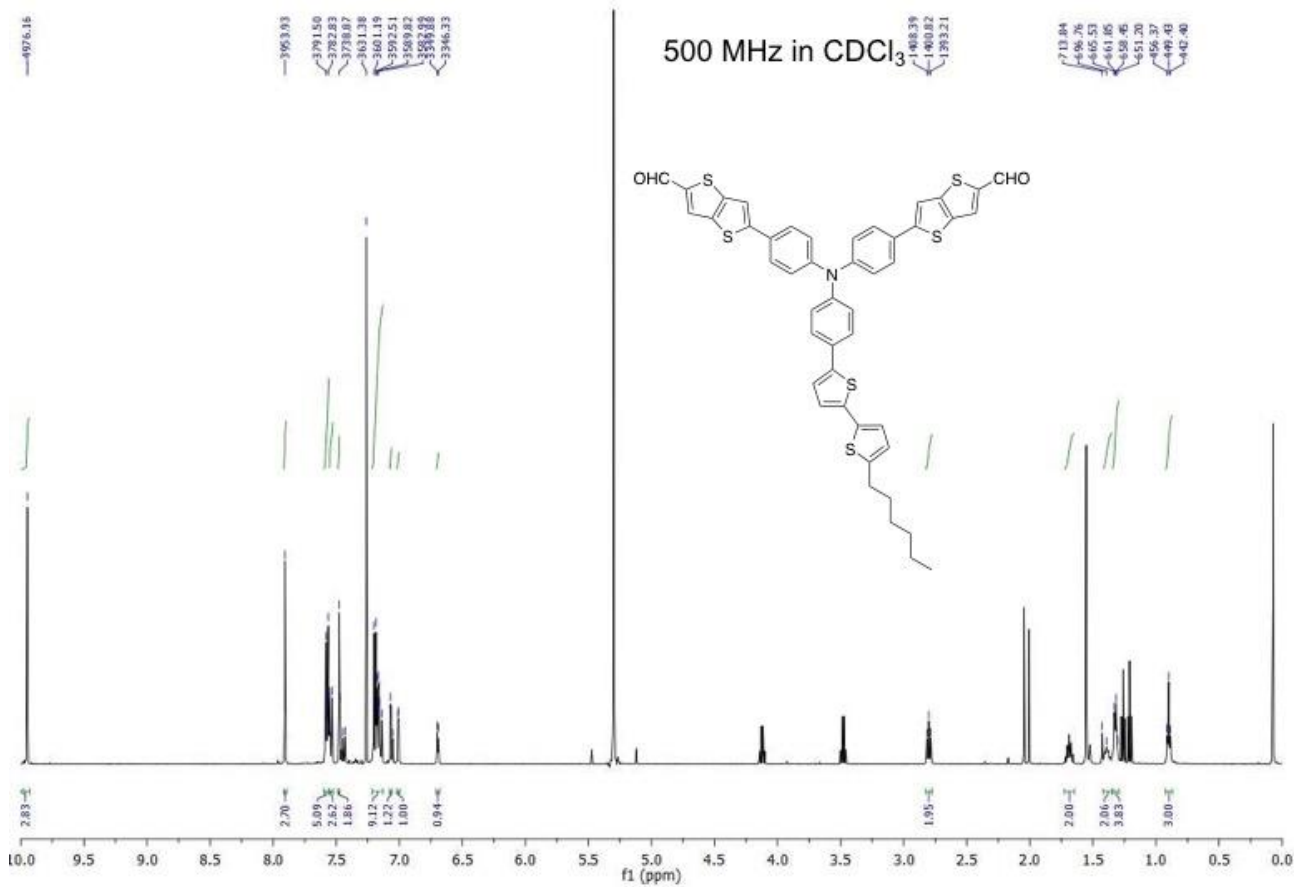
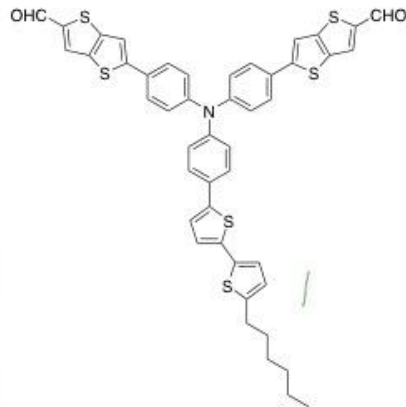


500 MHz in CDCl₃

9976.15
3953.93
3291.50
3282.83
3278.87
3031.38
3001.19
3002.51
3009.82
3002.88
3002.88
3006.33

1.983.39
1.90.82
1.393.21

7.13.84
6.96.76
6.65.53
6.61.85
6.58.46
6.51.20
6.56.37
6.49.43
6.40.40



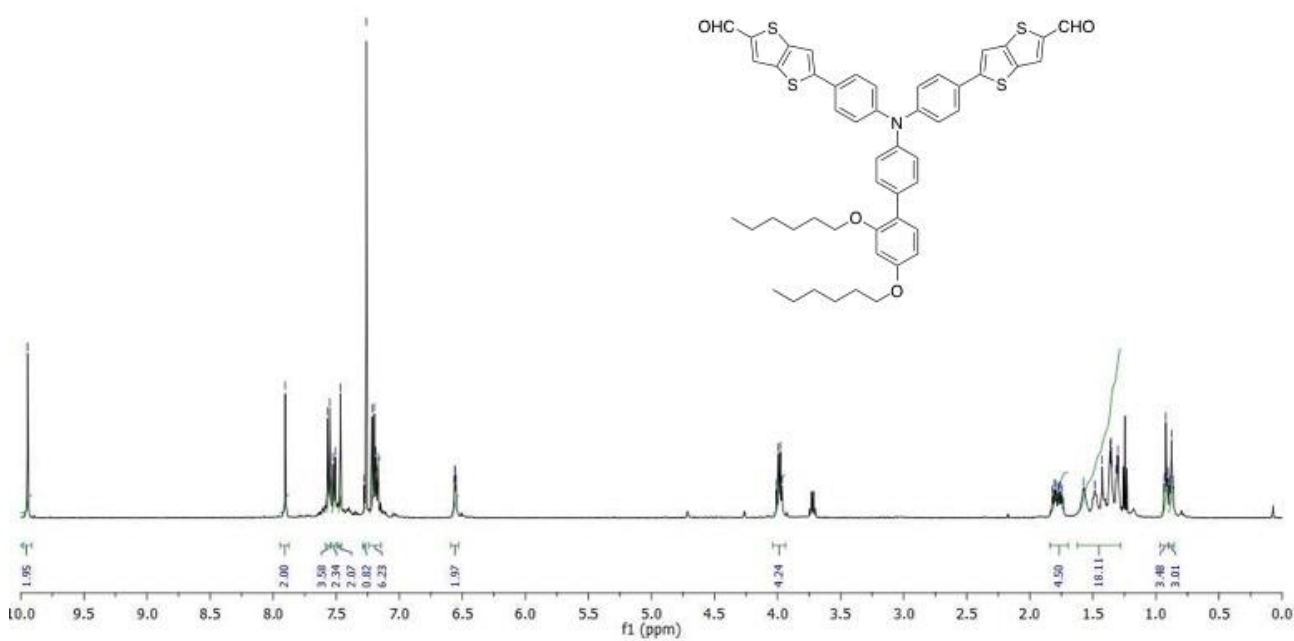
9.95

7.90
7.57
7.52
7.51
7.47
7.26
7.22
7.20
7.18
6.58
6.56
6.55

500 MHz in CDCl₃

3.00
3.98
3.97

1.82
1.79
1.78
1.76
1.75
1.73
1.57
1.48
1.43
1.36
1.35
1.32
1.31
1.30
0.93
0.92
0.89
0.88
0.86



4288.87
4164.00
3991.50
3866.41
3857.72
3718.77
3710.52
3703.07
3616.41
3610.01
3605.86
3598.99
3593.25
3571.91
3562.77

500 MHz in DMSO-d₆

