Supporting Information

Molecular engineering of D-A-π-A sensitizers for highly efficient solid-state dye-sensitized solar cells

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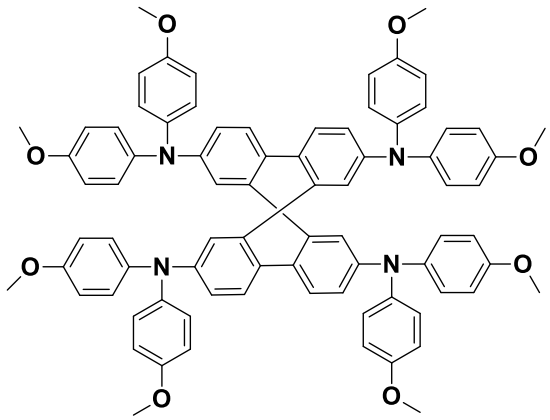


Fig. S1 Molecular structure of HTM Spiro-OMeTAD

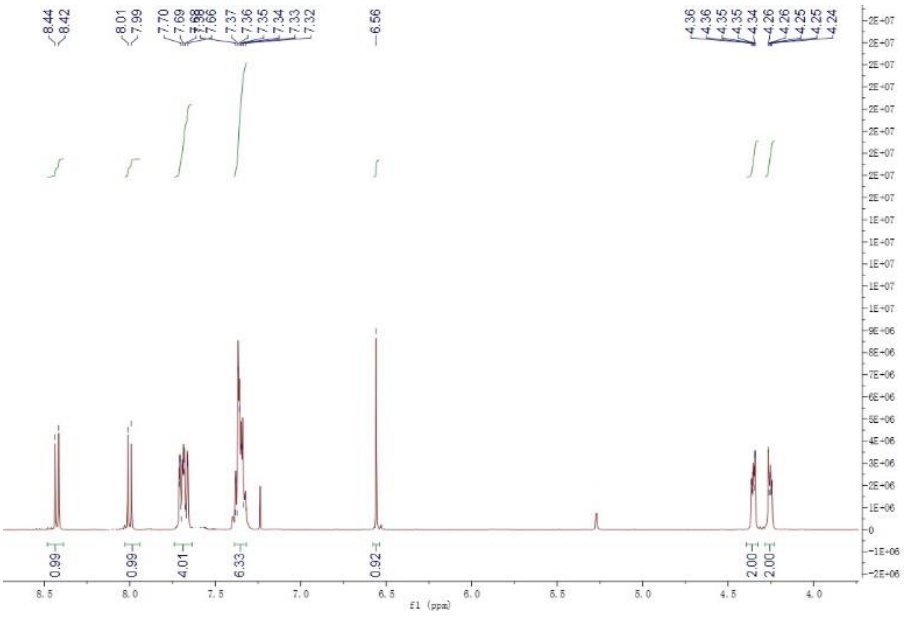


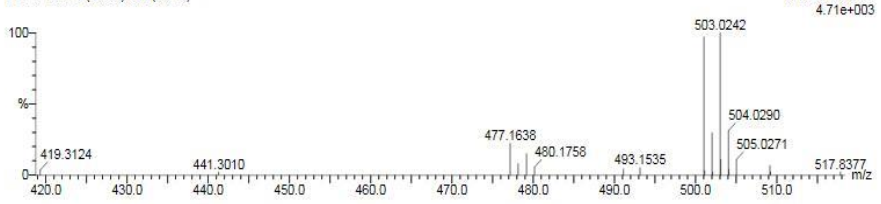
Fig. S2 ^{1}H NRM ($CDCl_3$) spectrum of 2a.

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions
47 formula(e) evaluated with 1 results within limits (up to 1 best isotopic matches for each mass)
Elements Used:
C: 0-26 H: 0-90 N: 0-2 O: 0-2 S: 0-1 Br: 0-1

JL-HUA ECUST institute of Fine Chem 23-Apr-2015 21:14:56
HL-LX-130 31 (0.284) Cm (29:32) 1: TOF MS ES+ 4.71e+003



Minimum:				-1.5			
Maximum:		300.0	50.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
501.0271	501.0272	-0.1	-0.2	18.5	26.0	0.0	C26 H18 N2 O2 S Br

Fig. S3 HR-MS spectrum of 2a.

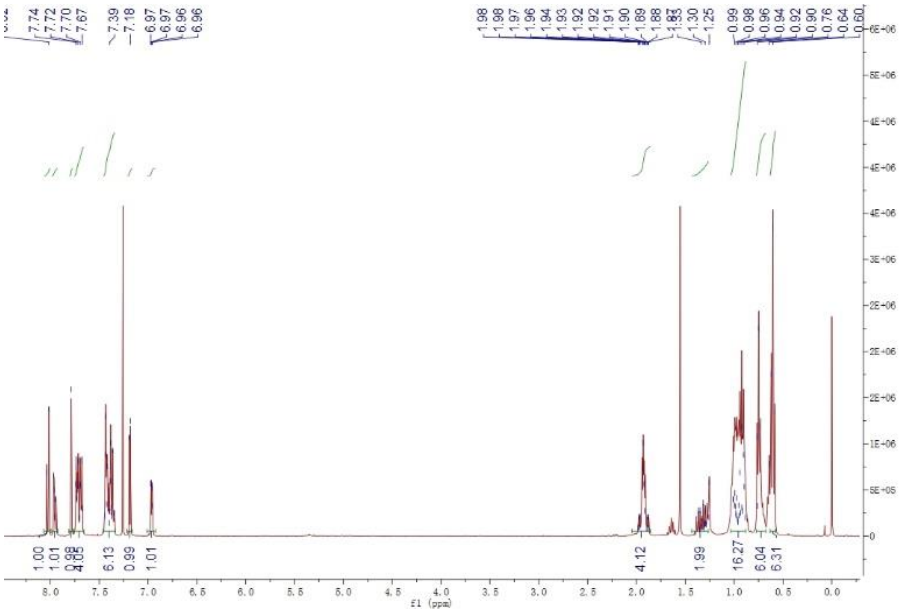


Fig. S4 ^{1}H NRM ($CDCl_3$) spectrum of 2b.

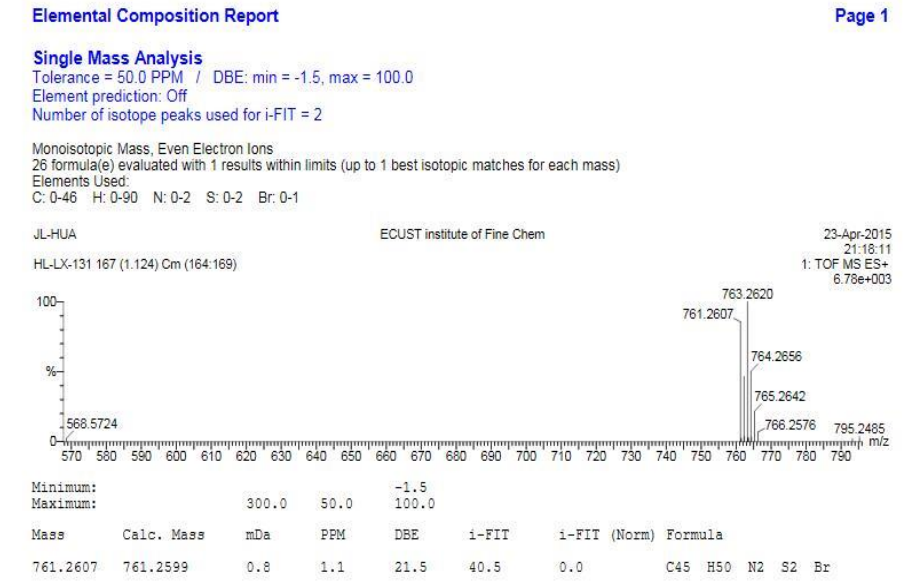


Fig. S5 HR-MS spectrum of 2b.

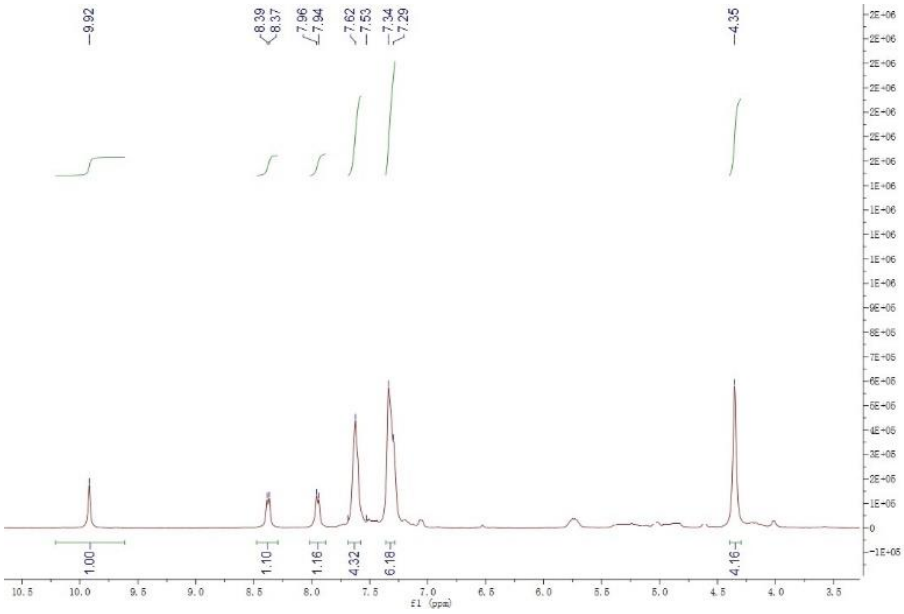
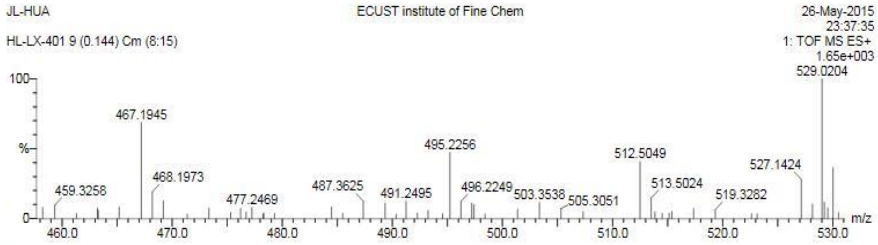


Fig. S6 ^{1}H NRM ($CDCl_3$) spectrum of 3a.

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions
59 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-27 H: 0-70 N: 0-2 O: 0-3 S: 0-1 Br: 0-1



Minimum:				-1.5			
Maximum:		300.0	50.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
529.0204	529.0222	-1.8	-3.4	19.5	29.0	0.0	C27 H18 N2 O3 S Br

Fig. S7 HR-MS spectrum of 3a.

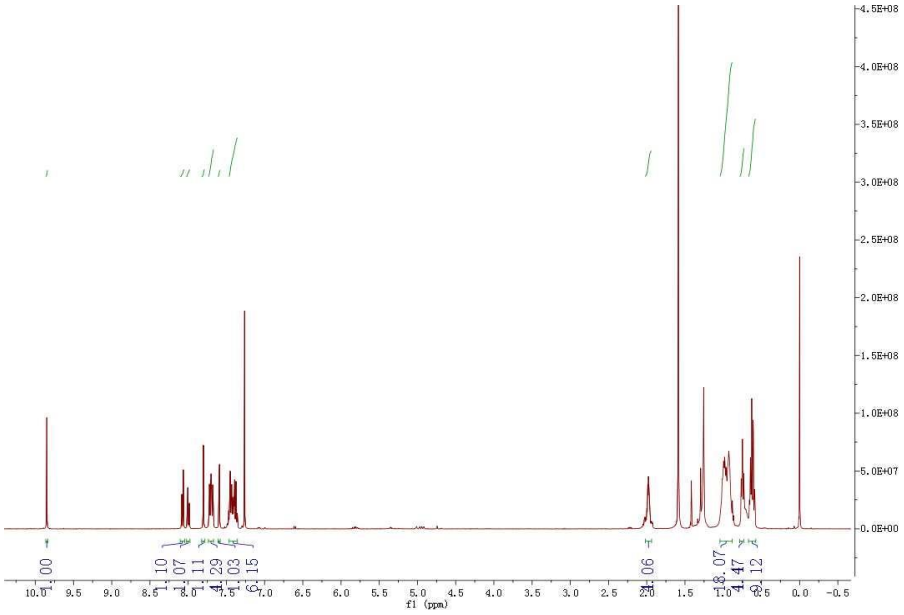


Fig. S8 ^{1}H NRM ($CDCl_3$) spectrum of 3b.

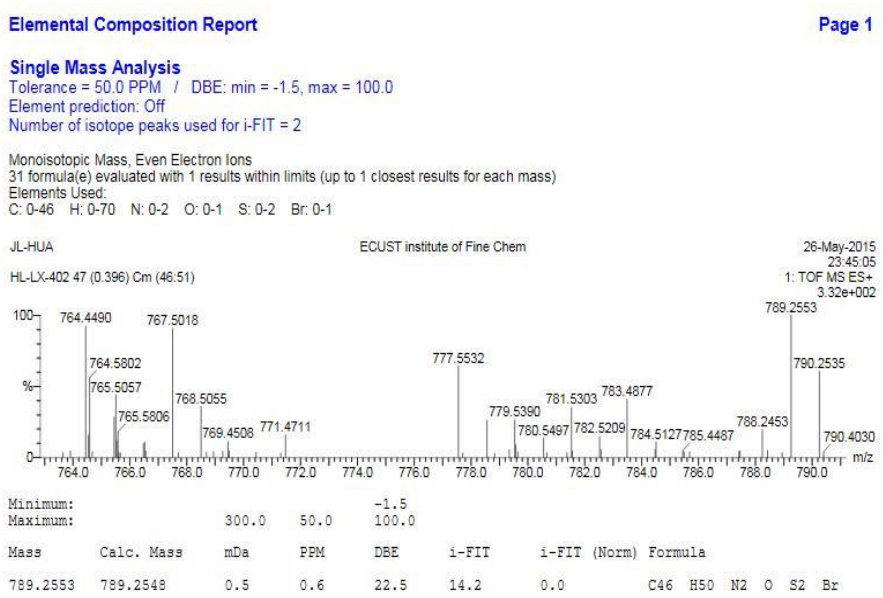


Fig. S9 HR-MS spectrum of 3b.

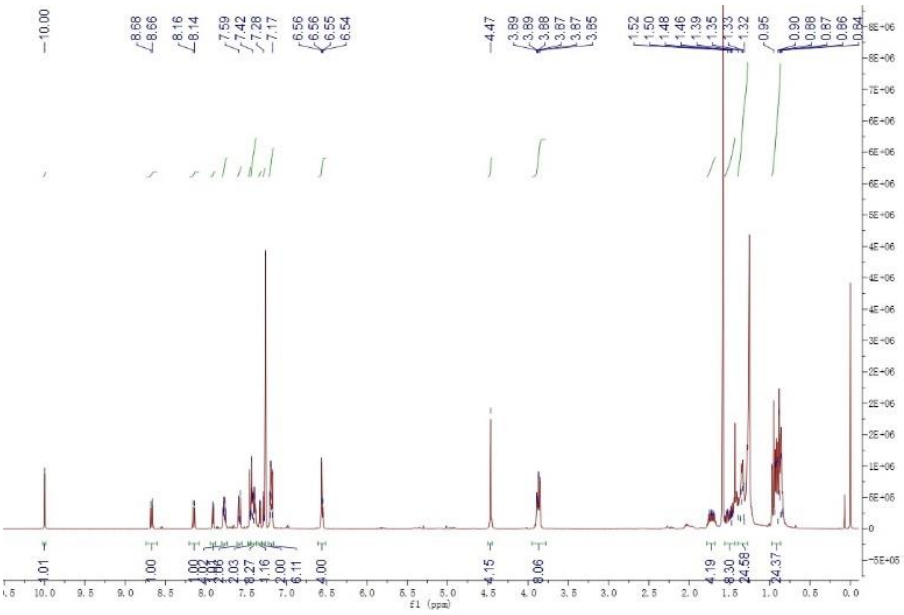


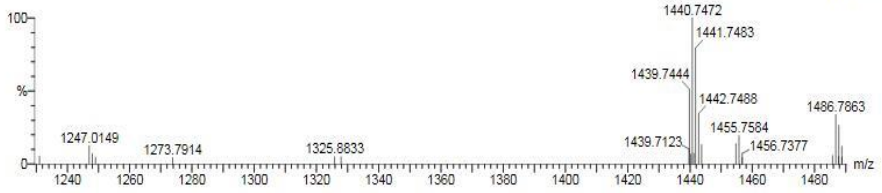
Fig. S10 ^{1}H NRM ($CDCl_3$) spectrum of 5a.

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
58 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-93 H: 0-106 N: 0-3 O: 0-7 S: 0-2

JL-HUA ECUST institute of Fine Chem 20-Mar-2016 20:55:02
HL-LX-409 21 (0.223) Cm (21:25) 1: TOF MS ES+ 1.48e+003



Minimum:				-1.5			
Maximum:		300.0	50.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
1440.7472	1440.7472	0.0	0.0	42.5	27.2	0.0	C93 H106 N3 O7 S2

Fig. S11 HR-MS spectrum of 5a.

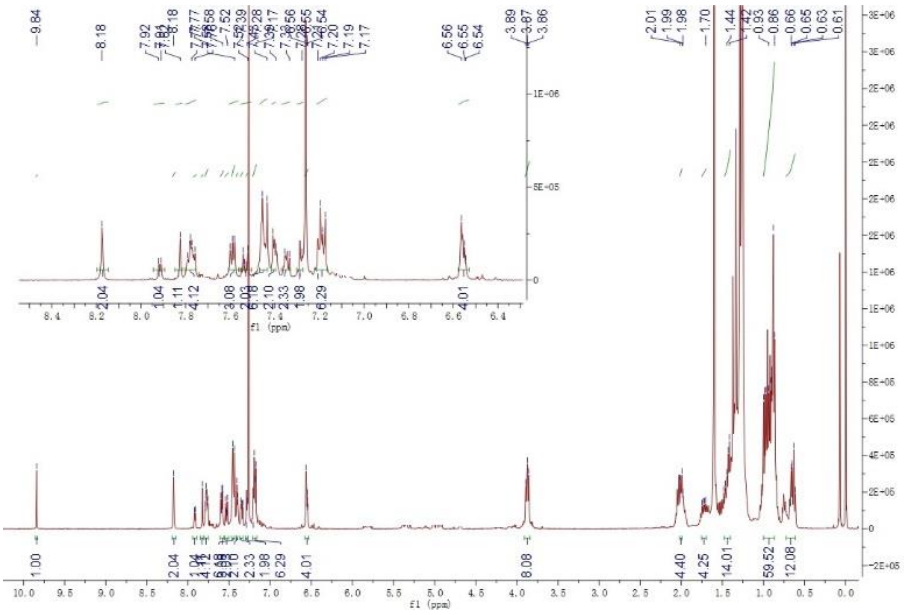


Fig. S12 ^{1}H NRM ($CDCl_3$) spectrum of 5b.

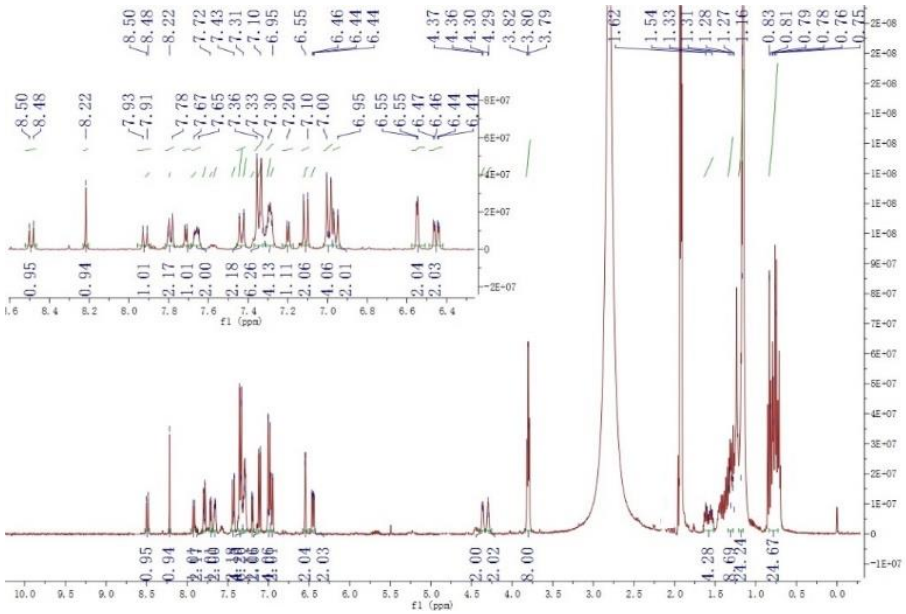


Fig. S13 ^{1}H NRM ($CO(CD_3)_2$-d_6) spectrum of AQ309.

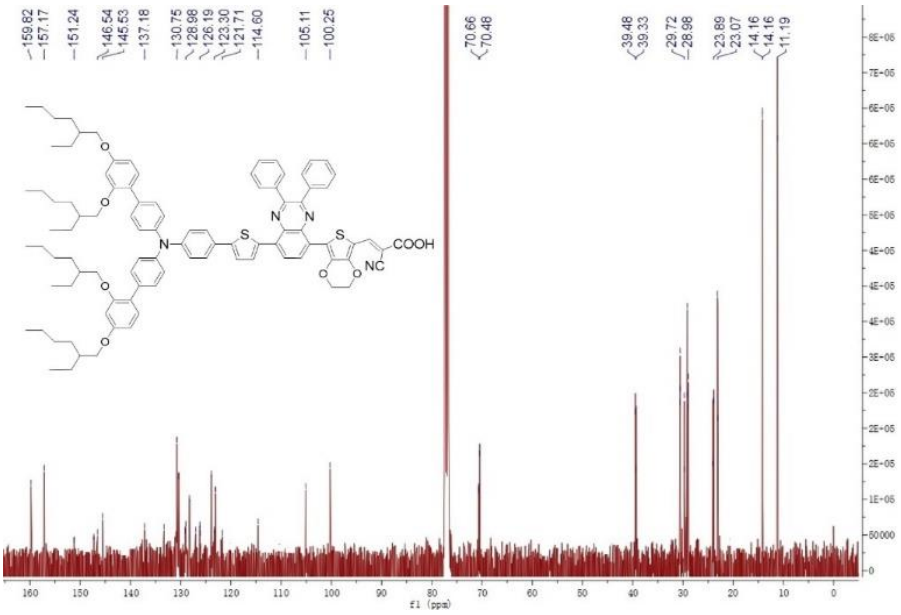


Fig. S14 ^{13}C NRM ($CDCl_3$) spectrum of AQ309.

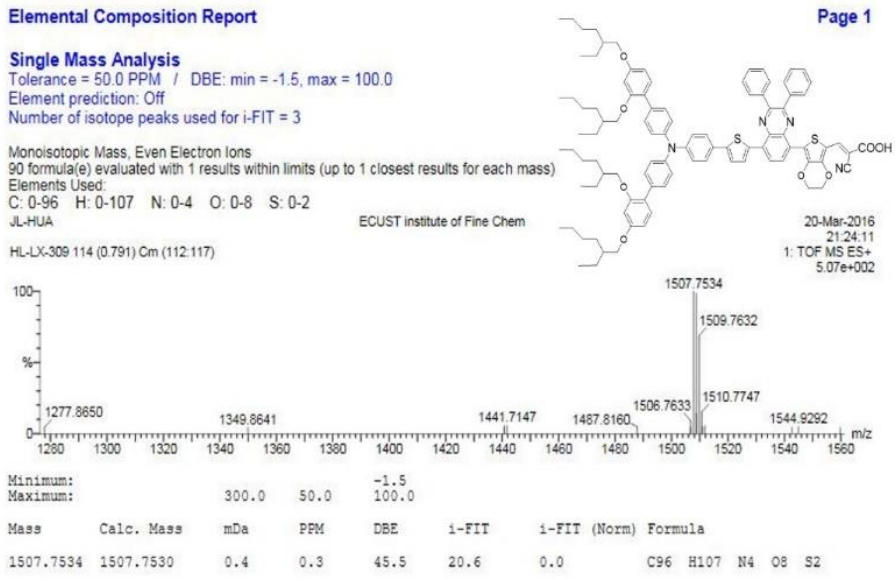


Fig. S15 HR-MS spectrum of AQ309.

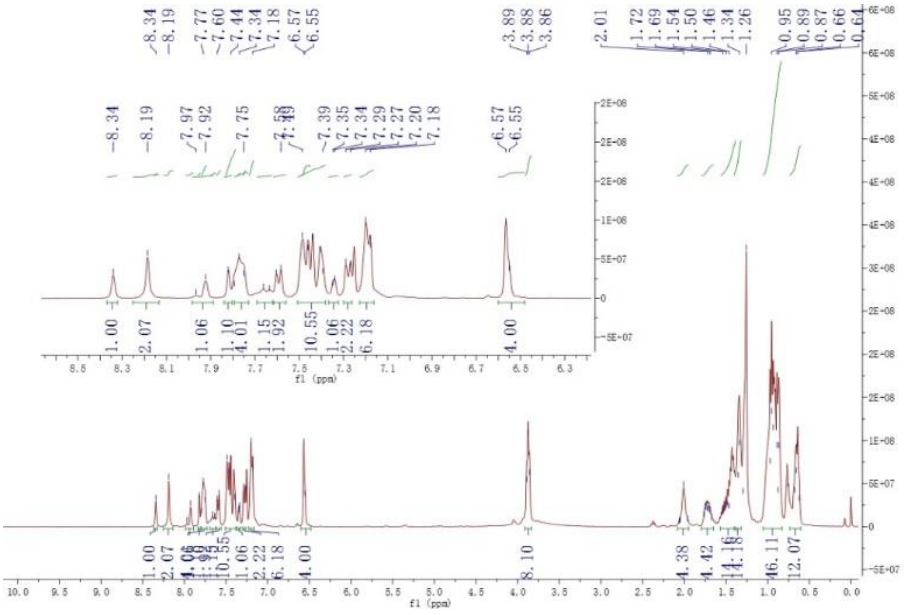


Fig. S16 ^{1}H NRM ($CDCl_3$) spectrum of AQ310.

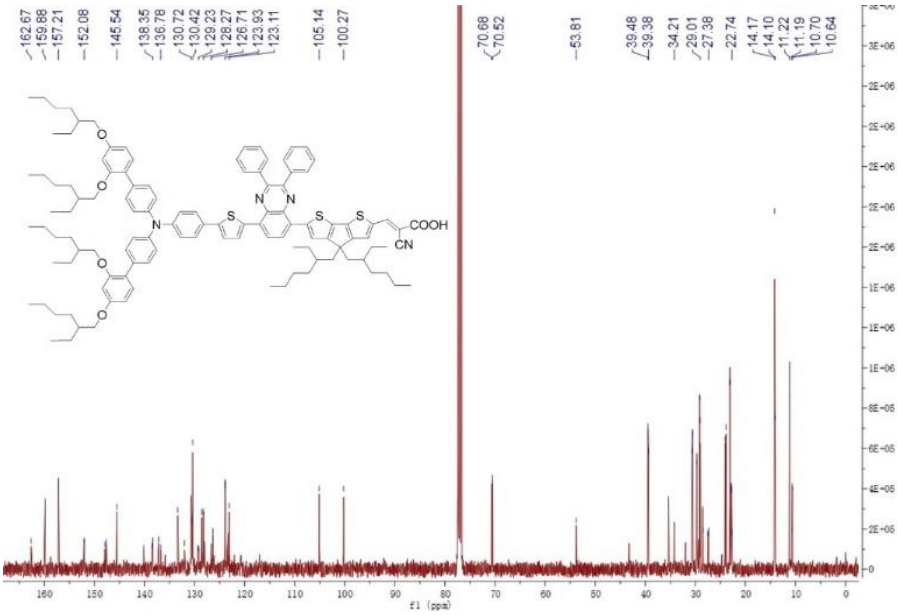


Fig. S17 ^{13}C NRM ($CDCl_3$) spectrum of AQ310.

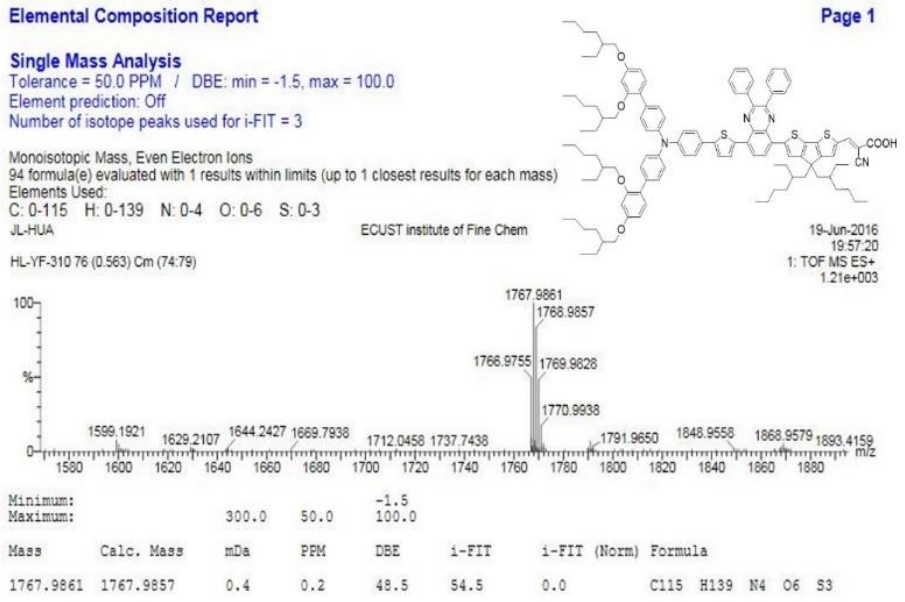
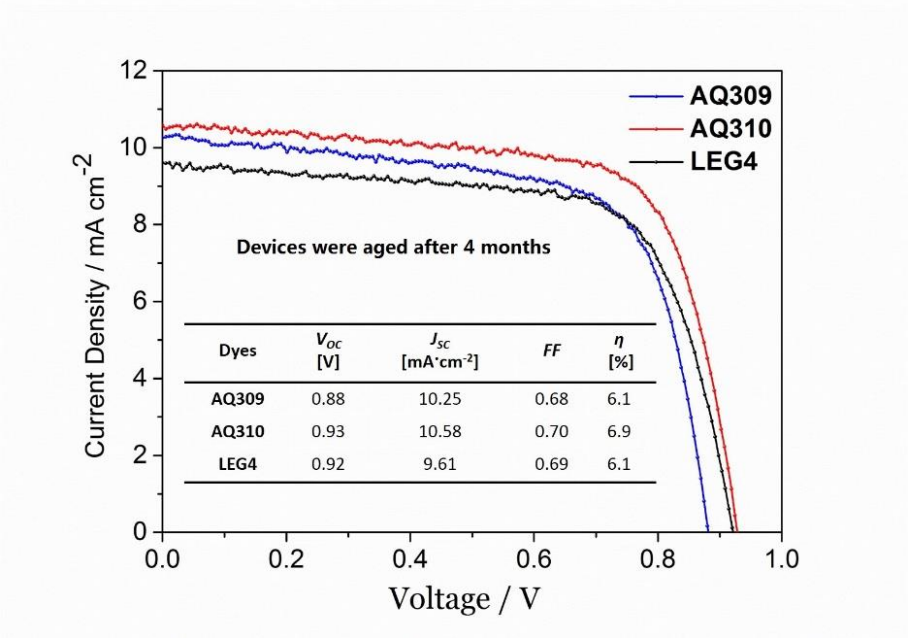


Fig. S18 HR-MS spectrum of AQ310.

Stability Test:



Dyes	V_{OC} [V]	J_{SC} [mA·cm^{-2}]	*FF*	η [%]
AQ309	0.88	10.25	0.68	6.1
AQ310	0.93	10.58	0.70	6.9
LEG4	0.92	9.61	0.69	6.1

Fig. S19 The efficiencies of the devices after four months.