Electronic Supplementary Material (ESI) for Materials Chemistry Frontiers.

Electronic Supplementary Information

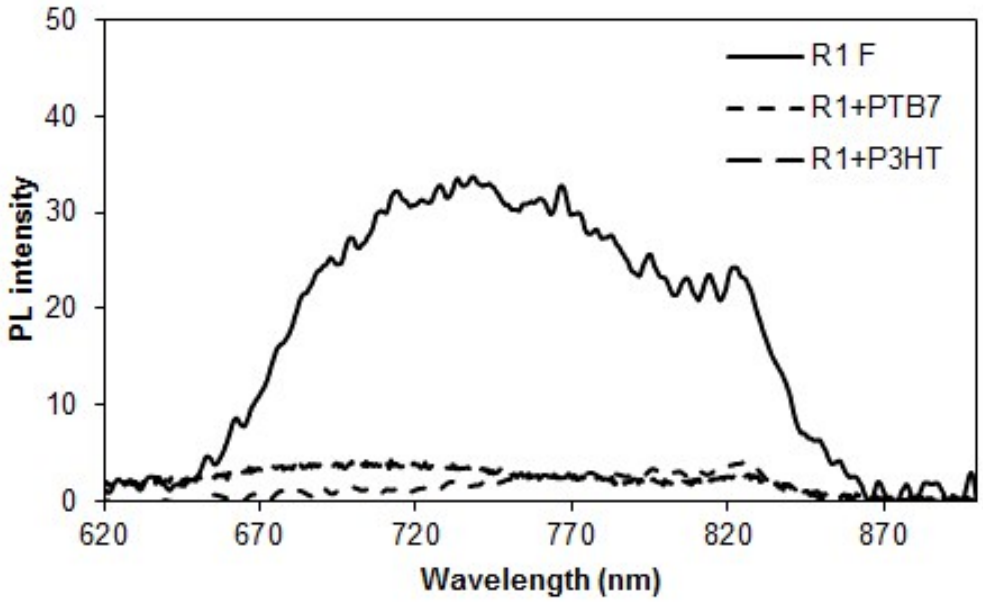


Fig. S1. Fluorescence spectra of pristine and blend films (D: A 1: 1.2 *w*/*w*) of **R1**; (excitation wavelength = 590 nm).

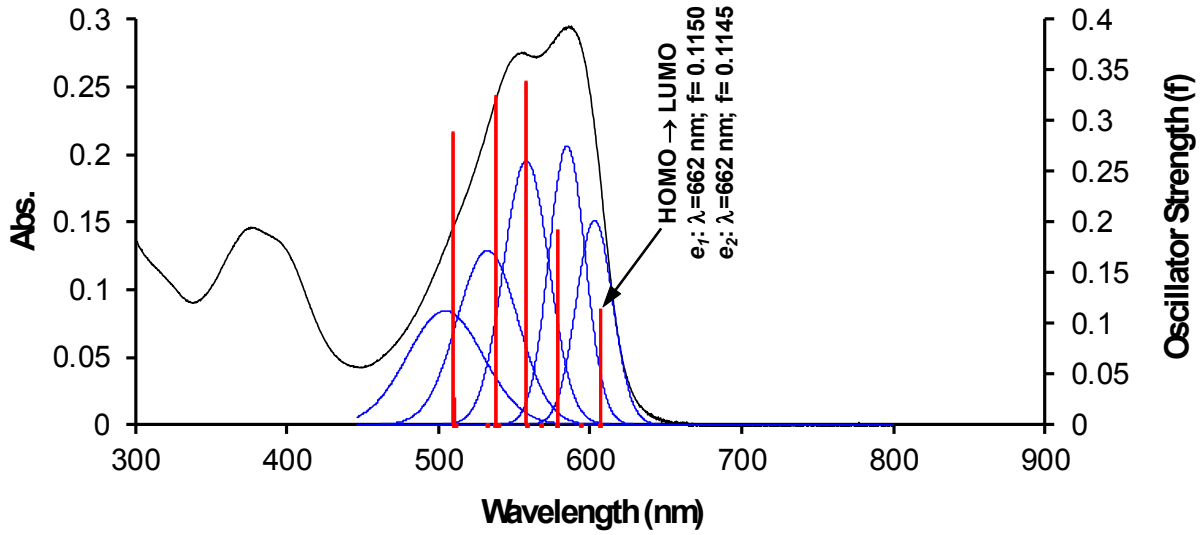


Fig. S2. The UV-vis spectrum of **R1** and the singlet electronic transitions as calculated using the TD-DFT at the B3LYP/6-311+G(d,p)//B3LYP/6-31G level of theory *in vacuo*.

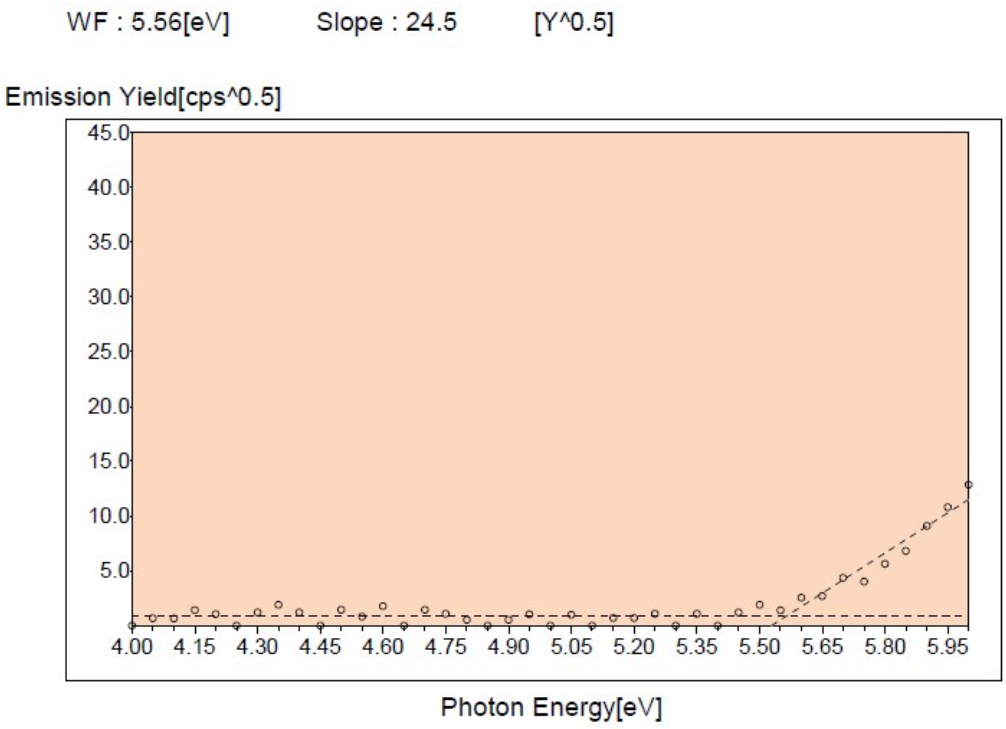


Fig. S3. PESA spectrum of thin film of **R1**. The dashed-lines show the fits to extract ionisation potential (-5.56 eV) which corresponds to the HOMO energy level.

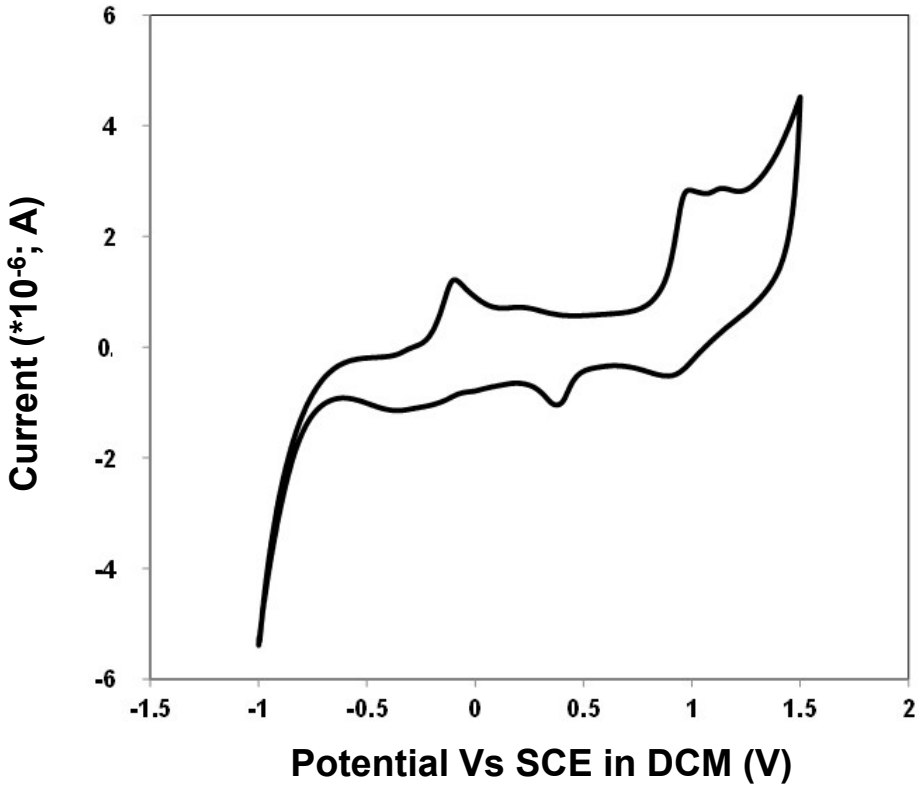


Fig. S4. Cyclic voltammogram of **R1**, run in dichloromethane at a sweep rate of 50 mV sec^{-1}.

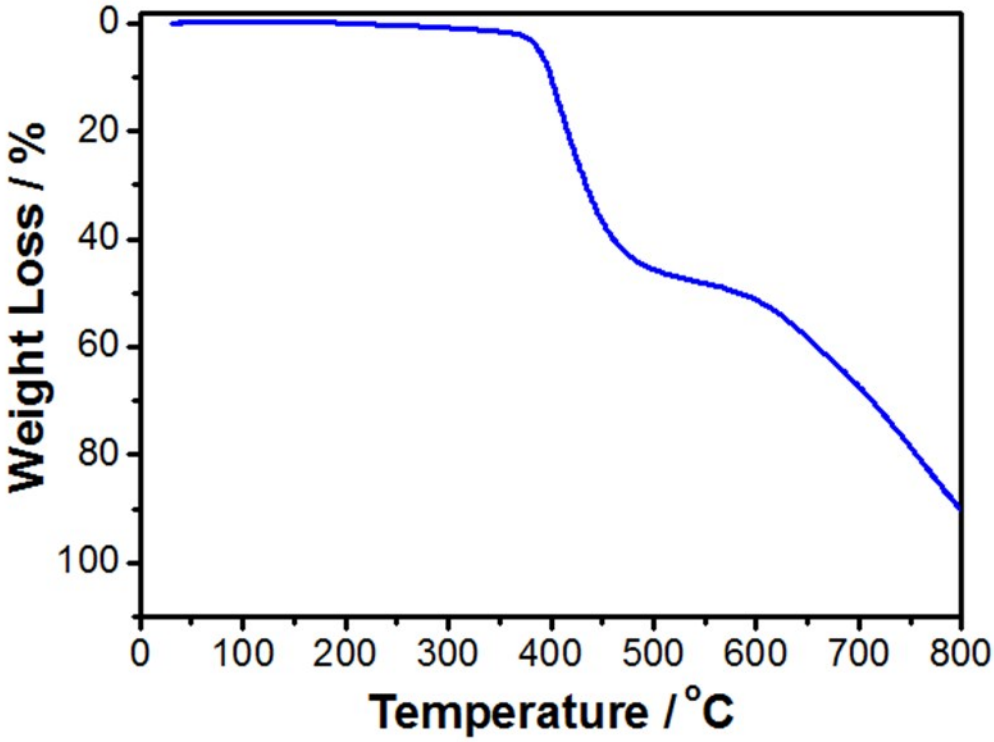


Fig. S5. TGA curve showing thermal stability of **R1**.

Table S1. Photovoltaic cell parameters for **R1** blends

Acceptor	**Donor**	**Testing conditions (D: A)[a]**	V_{oc} **(V)**	J_{sc} **(mA/cm^2)**	***FF***	**Best PCE (%)**	**Average PCE (%) (± std dev)**
R1	PTB7	1: 1.2 (no annealing)	1.00	13.01	0.60	7.89	7.82 (± 0.06)
R1	PTB7	1: 1.2 (annealed)	1.02	15.20	0.61	9.33	9.29 (± 0.03)
R1	P3HT	1: 1.2 (no annealing)	0.90	9.81	0.60	5.32	5.26 (± 0.06)
R1	P3HT	1: 1.2 (annealed)	0.91	10.20	0.61	5.62	5.53 (± 0.09)
$PC_{61}BM$	P3HT	1: 1.2[b]	0.57	8.28	0.64	3.05	3.03 (± 0.02)

[a] BHJ devices with specified weight ratio. Device structure = ITO/PEDOT: PSS (38 nm)/active layer (~75 nm)/Ca (20 nm)/Al (100 nm); [b] A standard P3HT: $PC_{61}BM$ device afforded 3.05% efficiency when tested under alike annealing conditions.

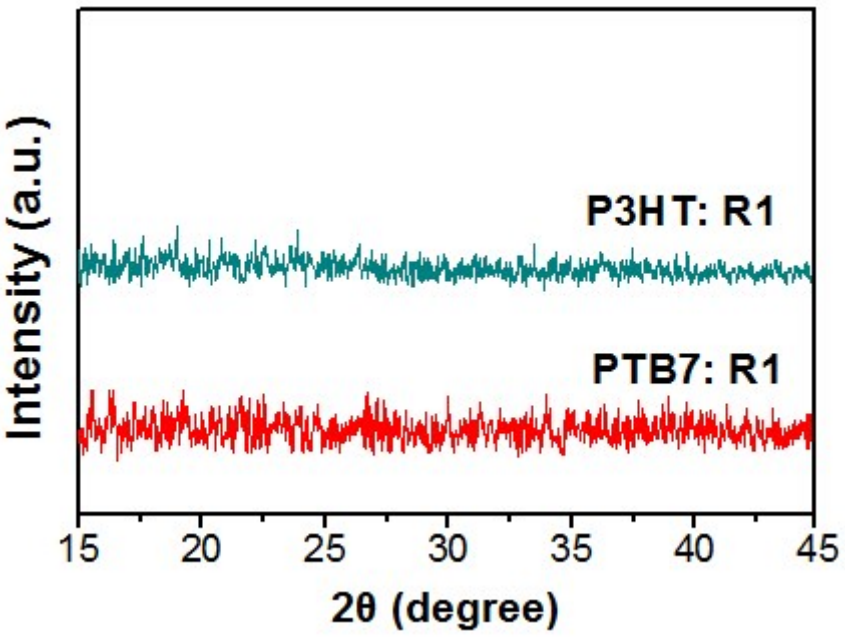


Fig. S6. XRD spectra for the active blend surfaces of **R1**. The XRD spectra indicate the blend surfaces to be amorphous.

Experimental Spectra

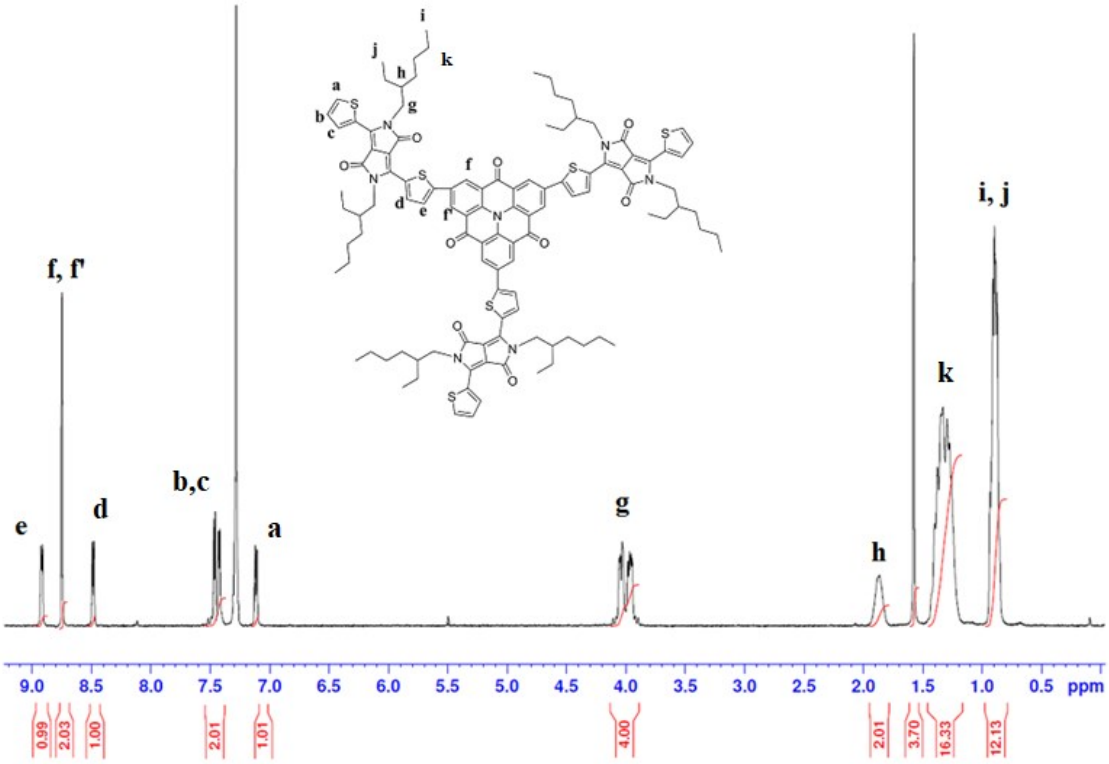


Fig. S7. ^{1}H NMR spectrum.

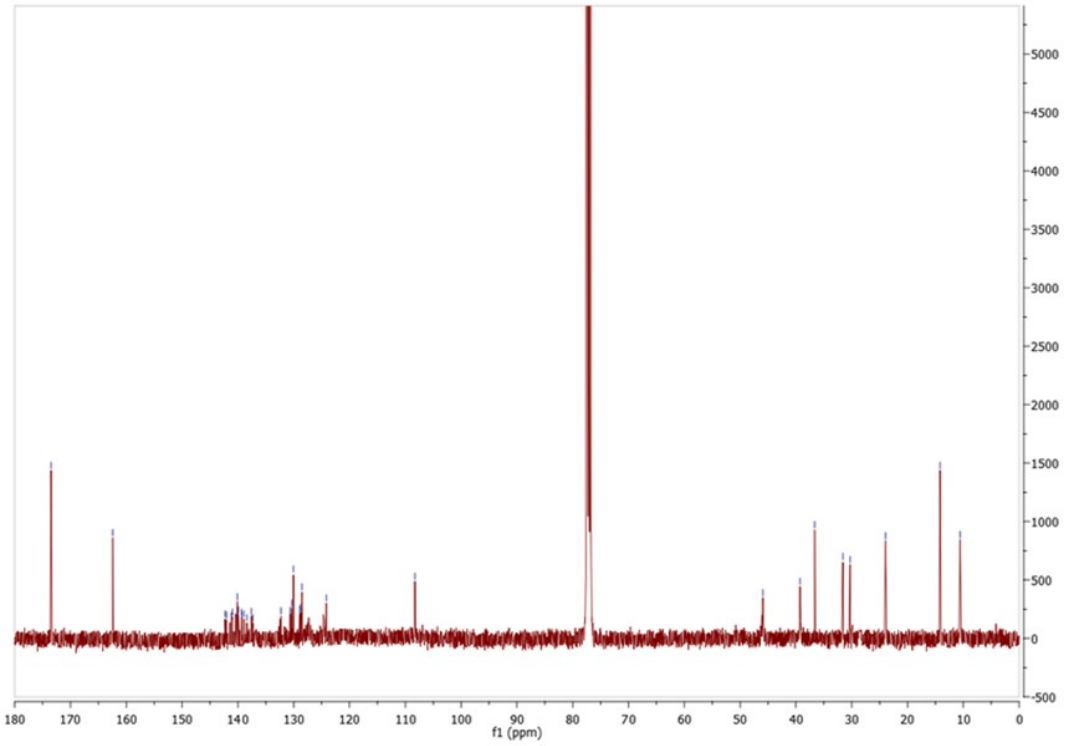
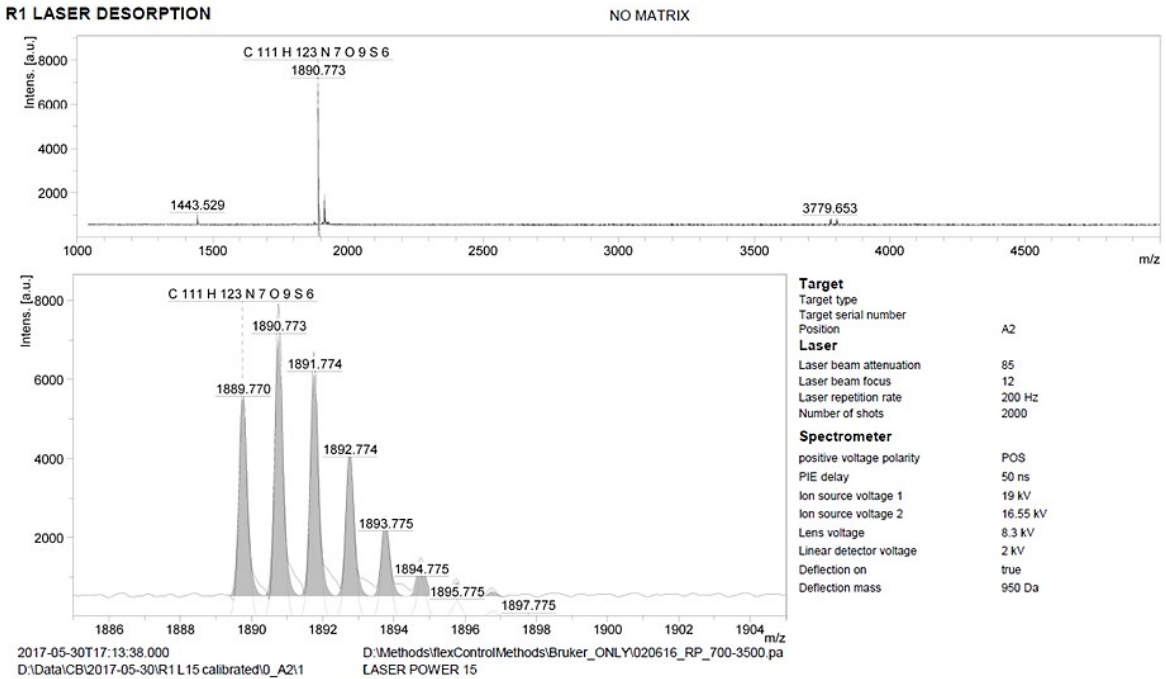


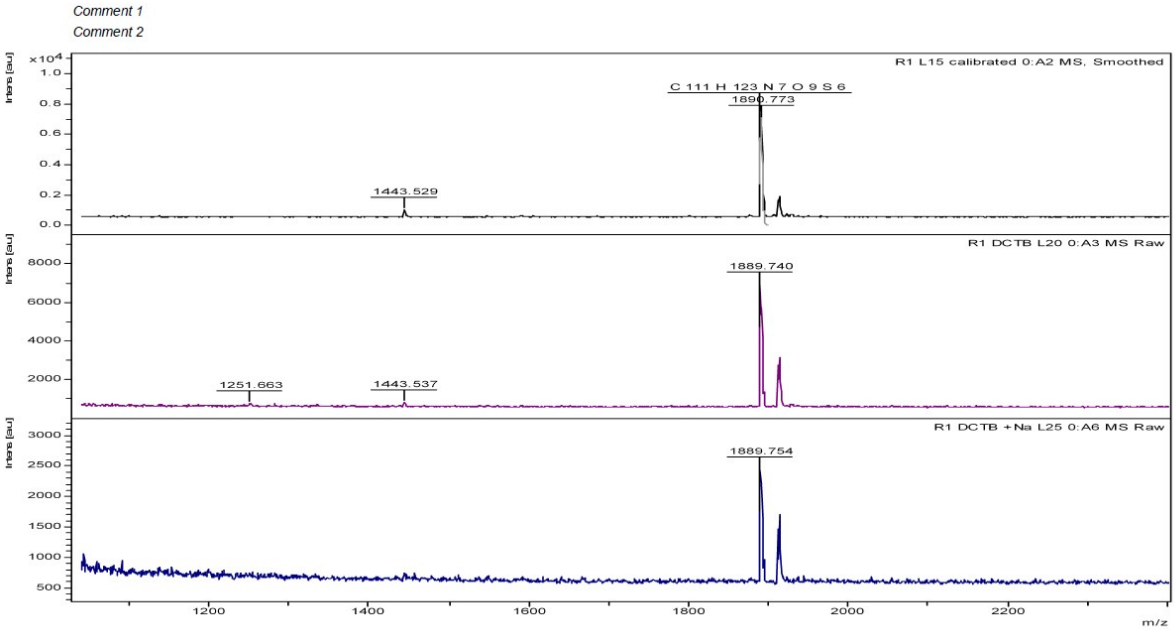
Fig. S8. ^{13}C NMR spectrum.

Autoflex III smart beam vertical matrix-assisted laser desorption-ionization/time-of-flight (**MALDI-TOF**): Without matrix: $[M]^+$ found for $C_{111}H_{123}N_7O_9S_6$ = 1889.770; With matrix, {trans-2-[3-(4-tert-Butylphenyl)-2-methyl-2-propenylidene]malononitrile (commonly known as DCTB)}: $[M]^+$ found for $C_{111}H_{123}N_7O_9S_6$ = 1889.740.

Mass spectrum without matrix:



Mass spectrum with matrix:



HRMS R1 (ESI): Calculated for $C_{111}H_{123}N_7O_9S_6$ = 1889.7741; found 1889.7701