Supporting Information

Naphthalene diimide-based non-fullerene acceptors for simple, efficient, and solution-processable bulk-heterojunction devices

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Supporting figures

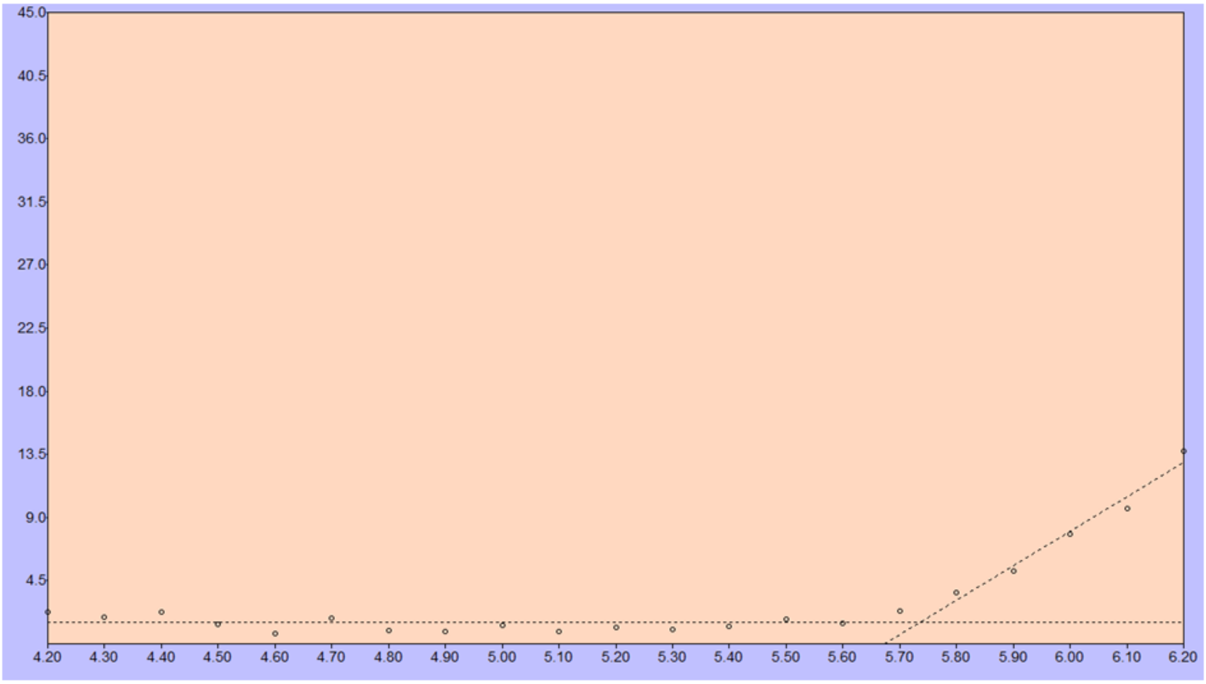


Fig. S1 Photoelectron spectroscopy in air (PESA) curve of **R1.**

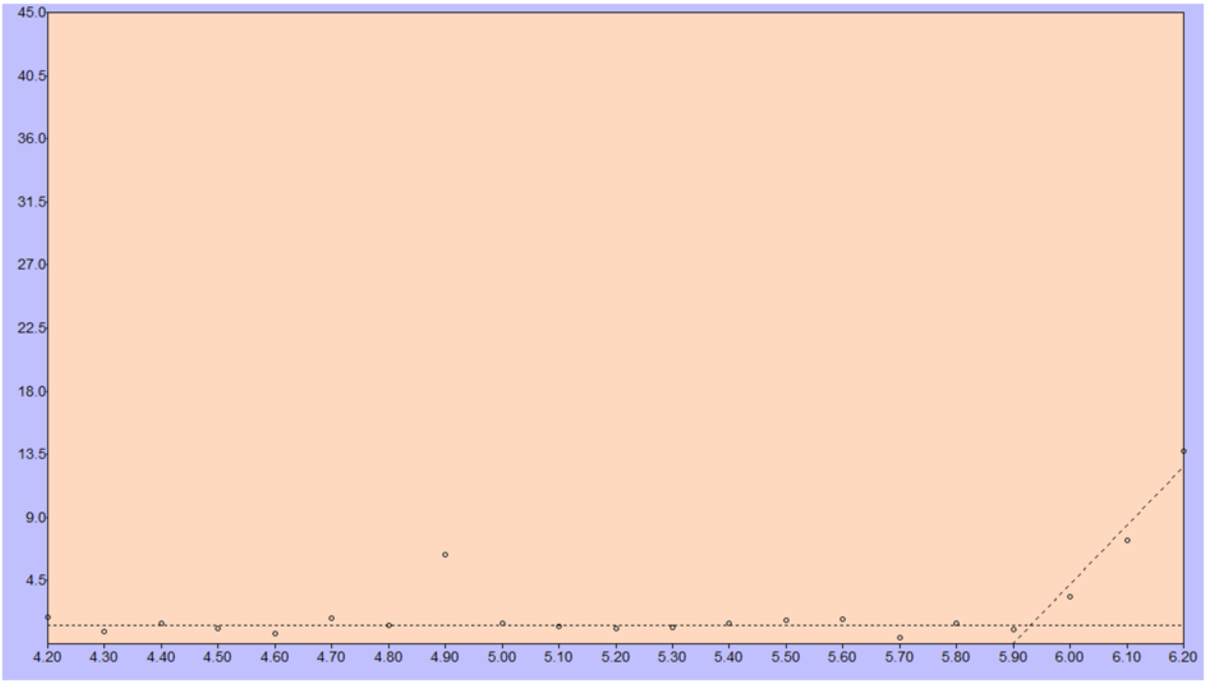


Fig. S2 Photoelectron spectroscopy in air (PESA) curve of **R2**.

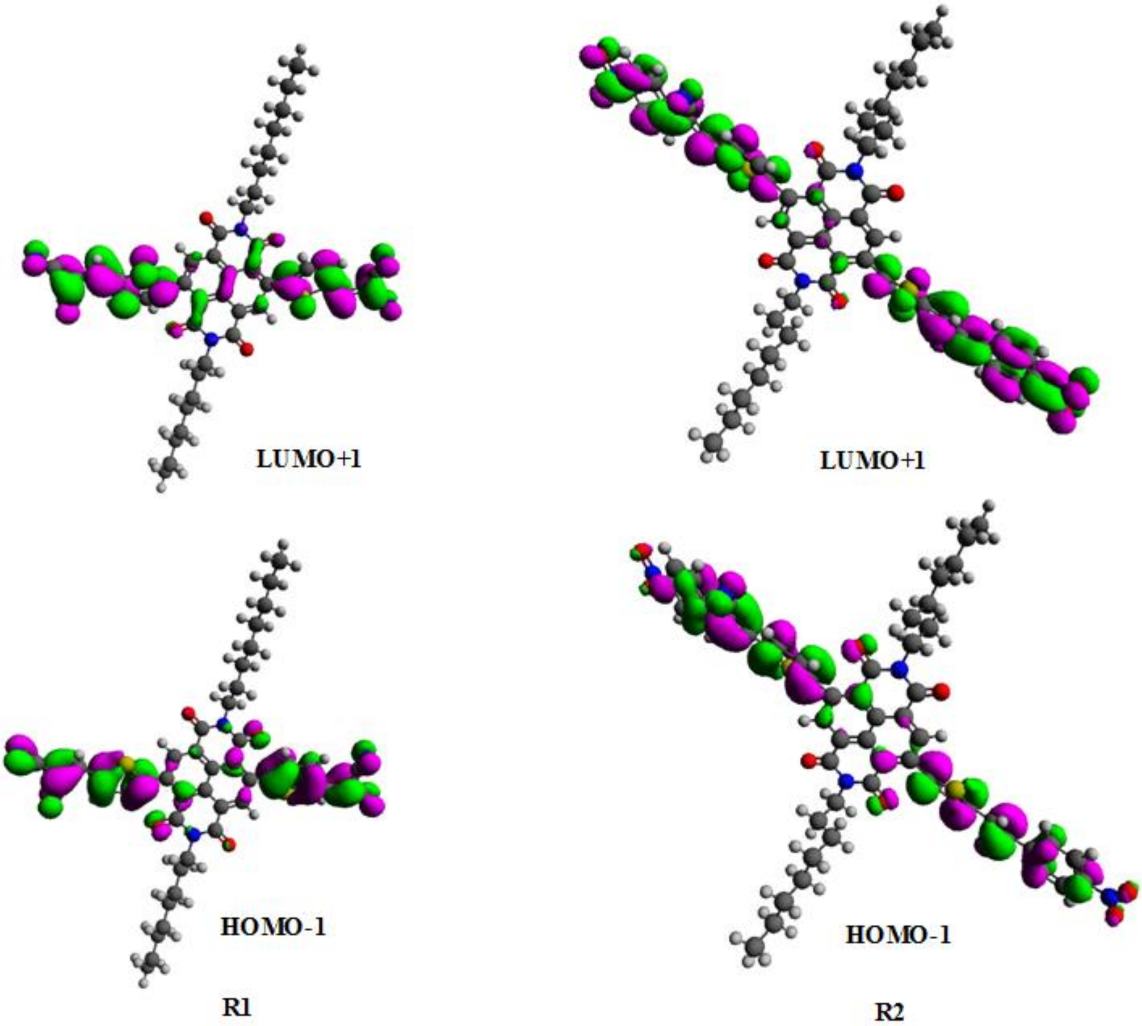
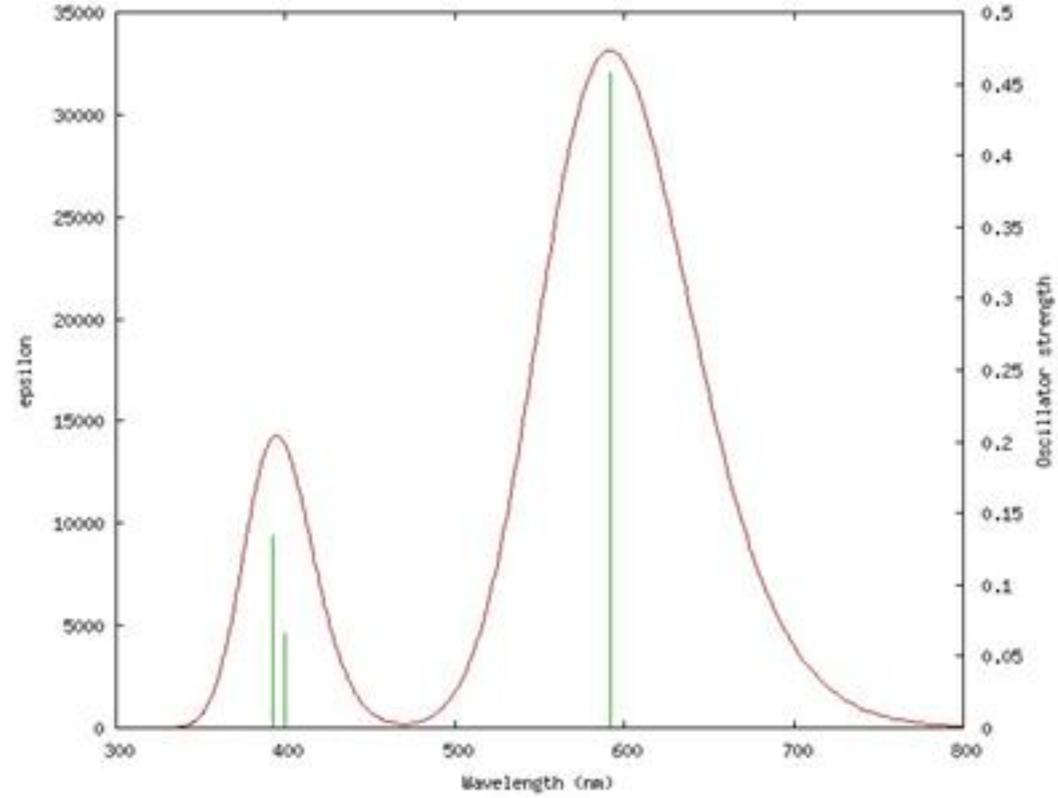


Fig. S3 Theoretical HOMO-1 and LUMO+1 density distributions of **R1** and **R2** indicating the participation of terminal functionalities



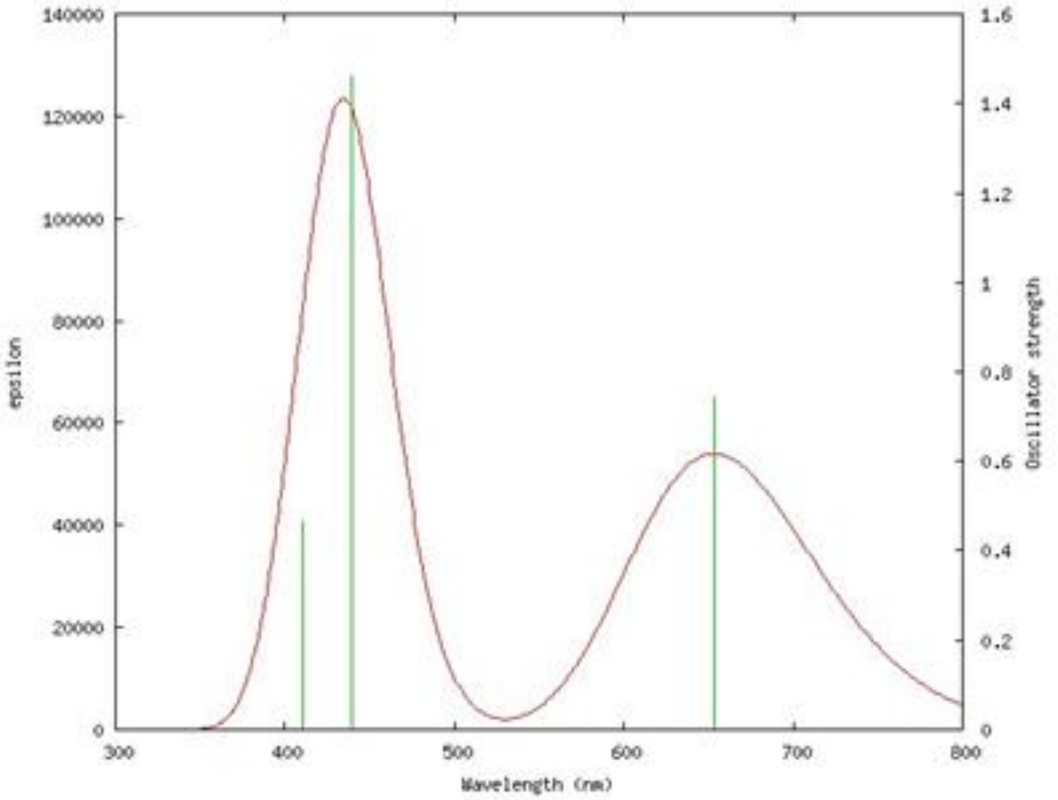


Fig. S4 The computed absorption spectra of **R1** (upper) and **R2** (lower) showing the first transition peaks at 591.58 nm and 653.36 nm respectively.

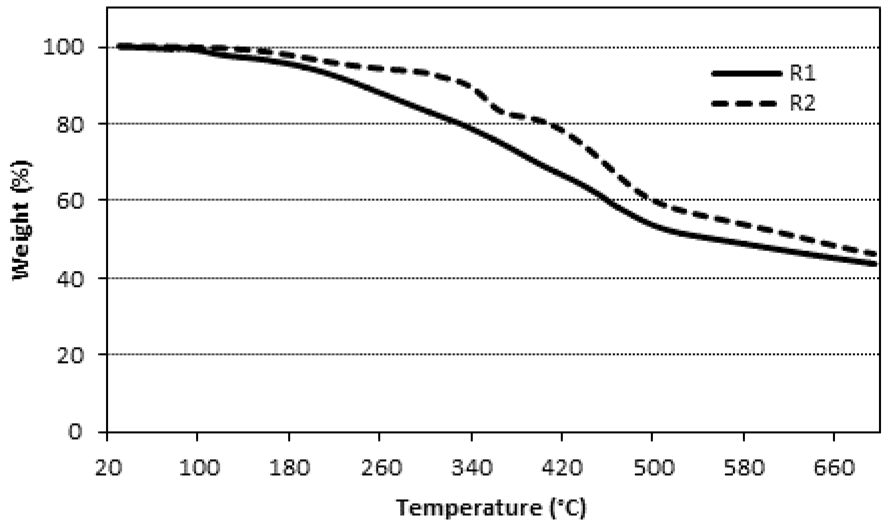


Fig. S5 Thermogravimetric analyses traces of **R1** and **R2**.

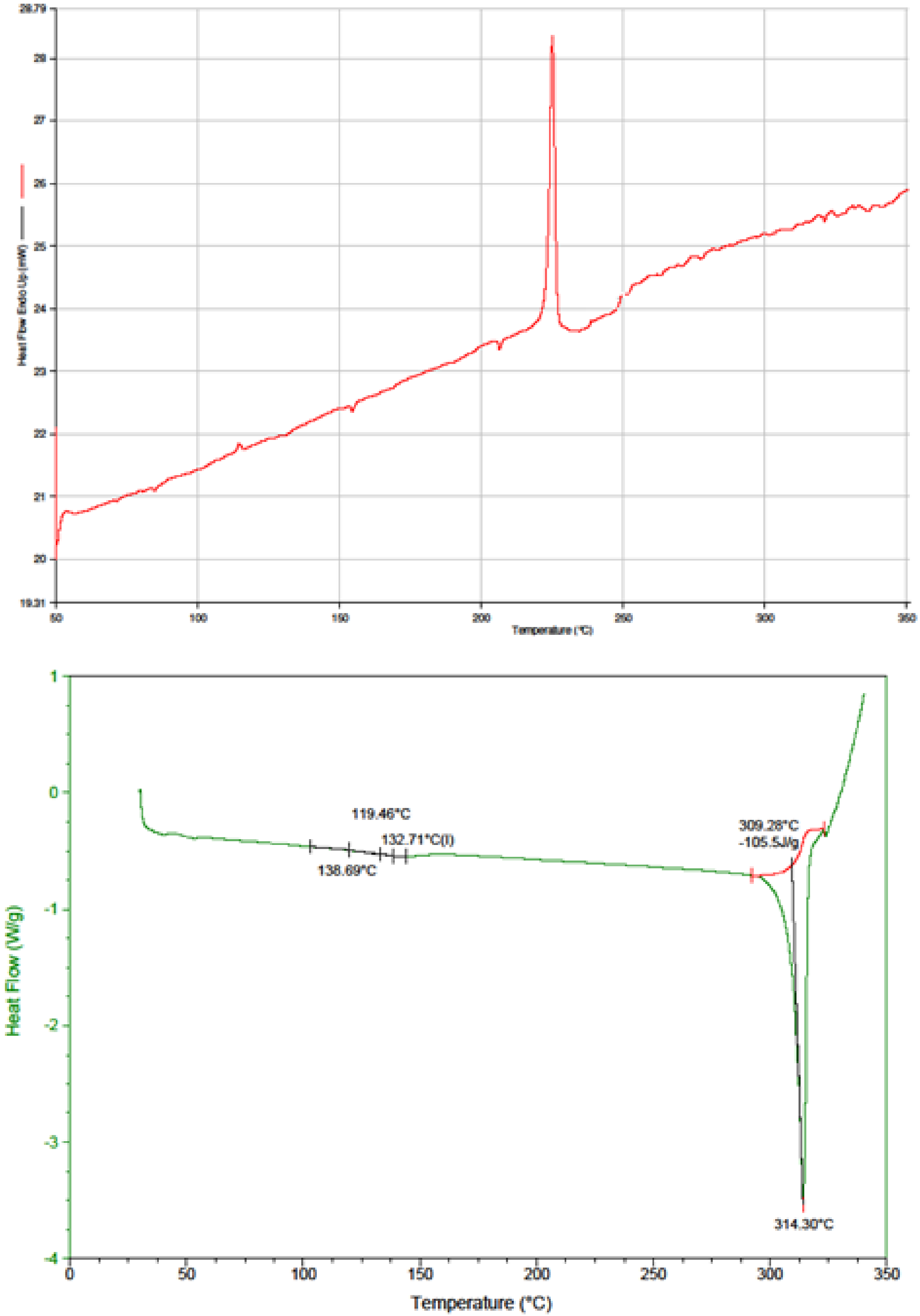


Fig. S6 Differential scanning calorimetry analyses traces of **R1** (above) and **R2** (below).

Table S1 Comparative BHJ device performances

Material	Testing conditions (donor: acceptor)	V_{oc} (mV)	J_{sc} (mA/cm^2)	*FF*	Efficiency (η%)
R1	1:1.2[a]	1020 ±10	2.15 ±0.30	0.36 ± 0.03	0.79 ±0.20
R2	1:1.2[a]	870 ±15	6.77 ±0.25	0.38 ±0.01	2.24 ±0.25
R1	1:1[a]	720 ±20	2.01 ±0.20	0.31 ±0.02	0.46 ±0.20
R2	1:1[a]	640 ±20	7.81 ±0.35	0.35 ±0.03	1.76 ±0.30
R2	1:2[a,b]	700 ±20	6.20 ±0.25	0.32 ±0.04	1.40 ±0.20

[a] BHJ devices with specified weight ratio. Device structure is ITO/PEDOT: PSS (38 nm)/active layer/Ca (20 nm)/Al (100 nm) with an active layer thickness of about 60 nm.

[b] BHJ devices with the weight ratio of 1:2 using **R1** didn't become feasible mainly due to very poor solubility and excess of **R1** in this combination.

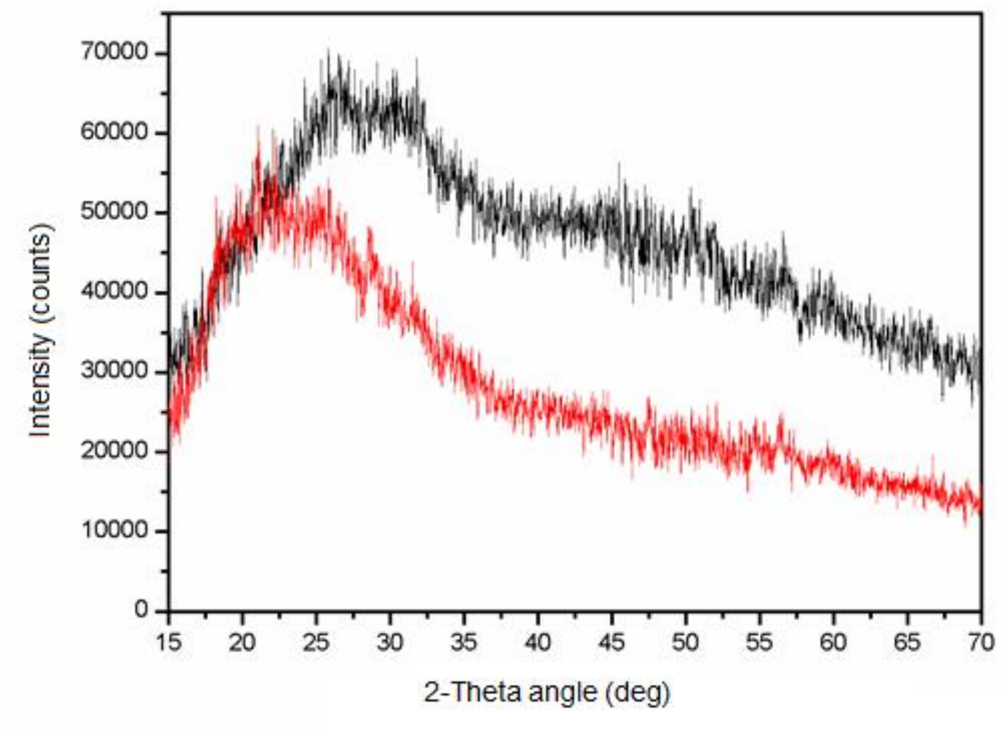


Fig. S7 XRD patterns of **R1** (red curve) and **R2** (black curve).

Spectra of R1 and R2

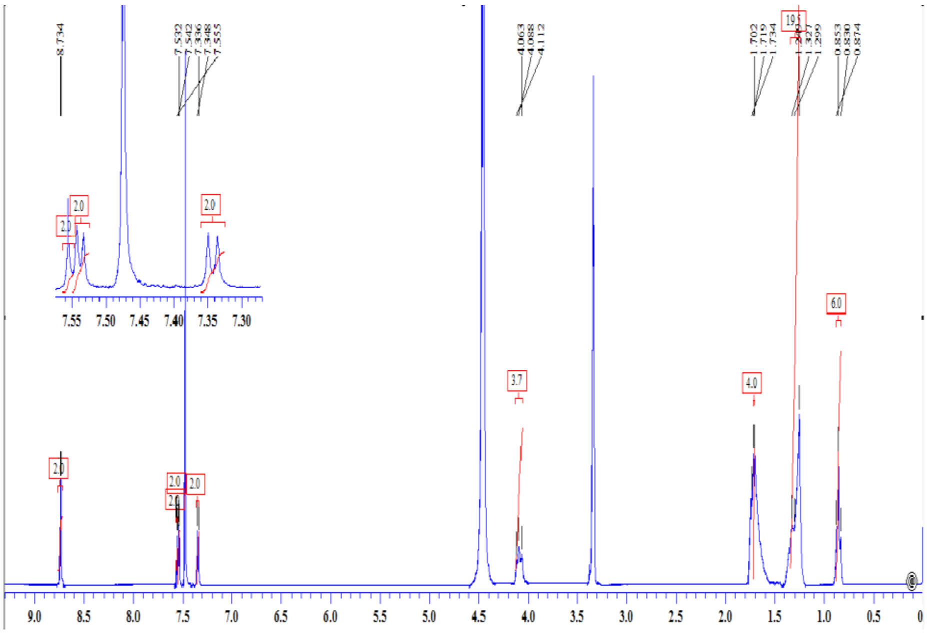


Fig. S8 ^{1}H NMR spectrum of **R1**

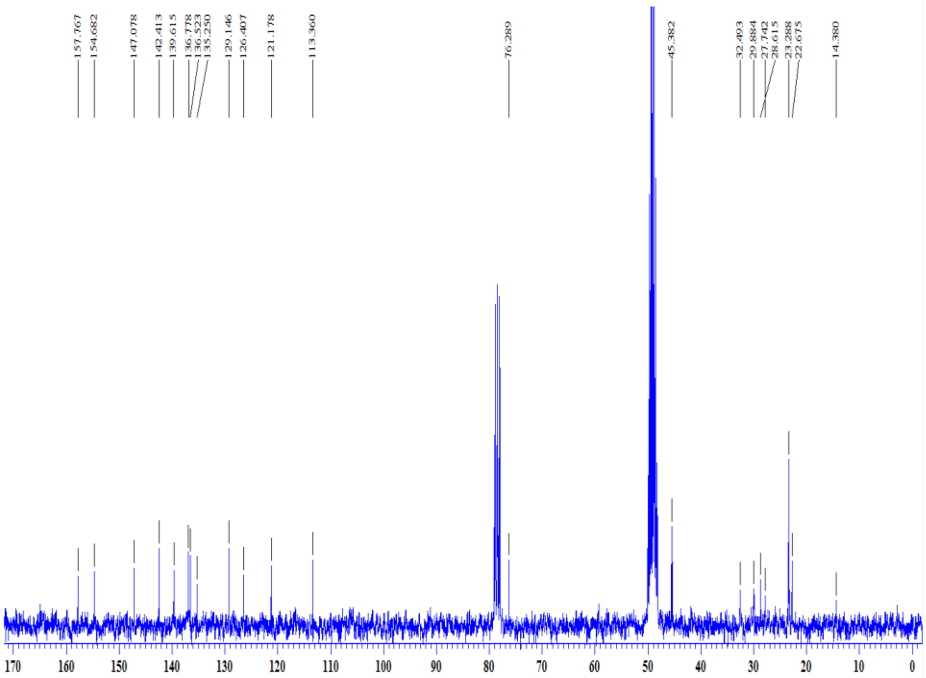


Fig. S9 ^{13}C NMR spectrum of **R1**

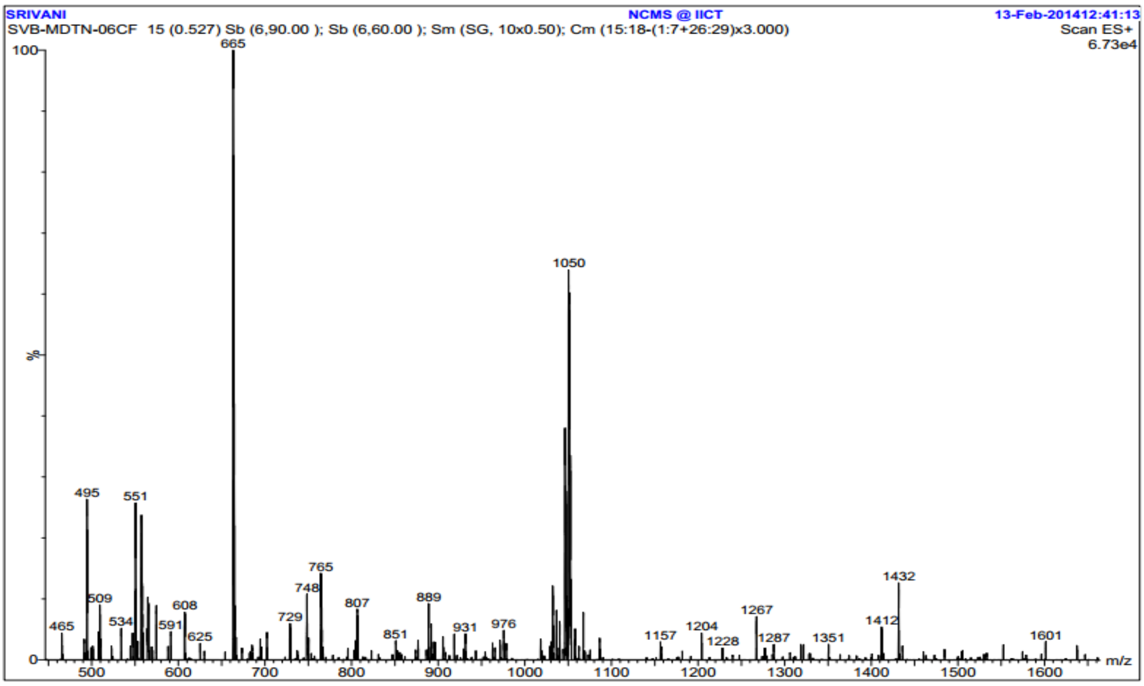
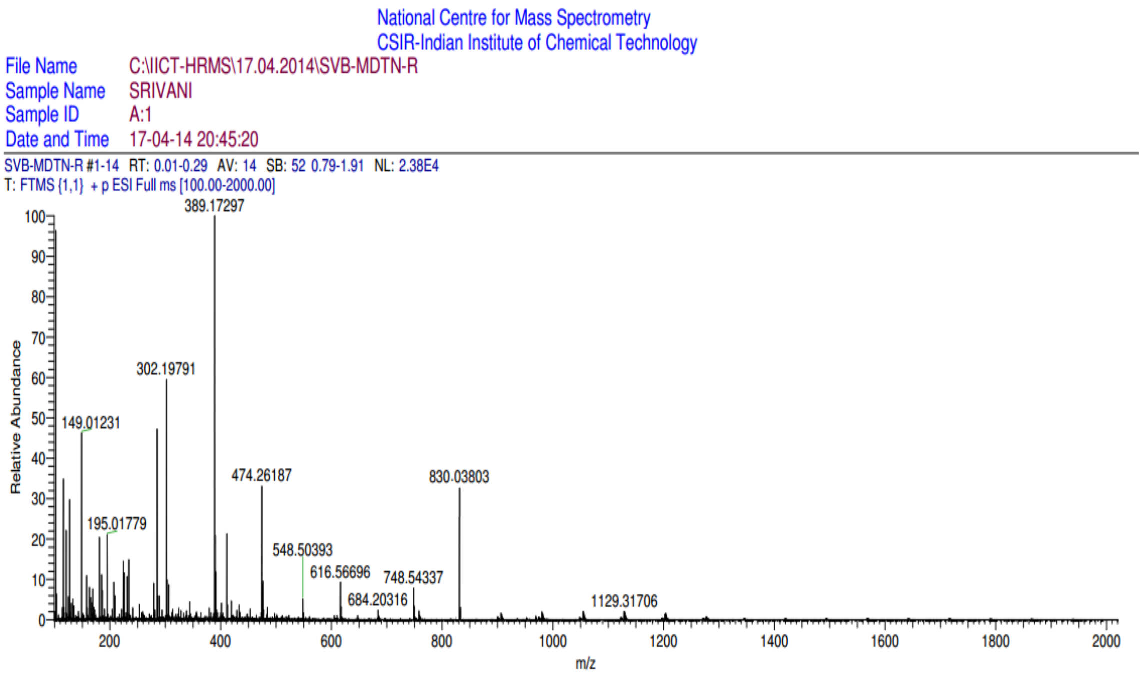


Fig. S10 ESI mass spectrum of **R1**



SVB-MDTN-R#8-30 RT: 0.16-0.64 AV: 23
T: FTMS {1,1} + p ESI Full ms [100.00-2000.00]

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
830.03803	3265.3	100.00				

Fig. S11 HRMS of **R1**

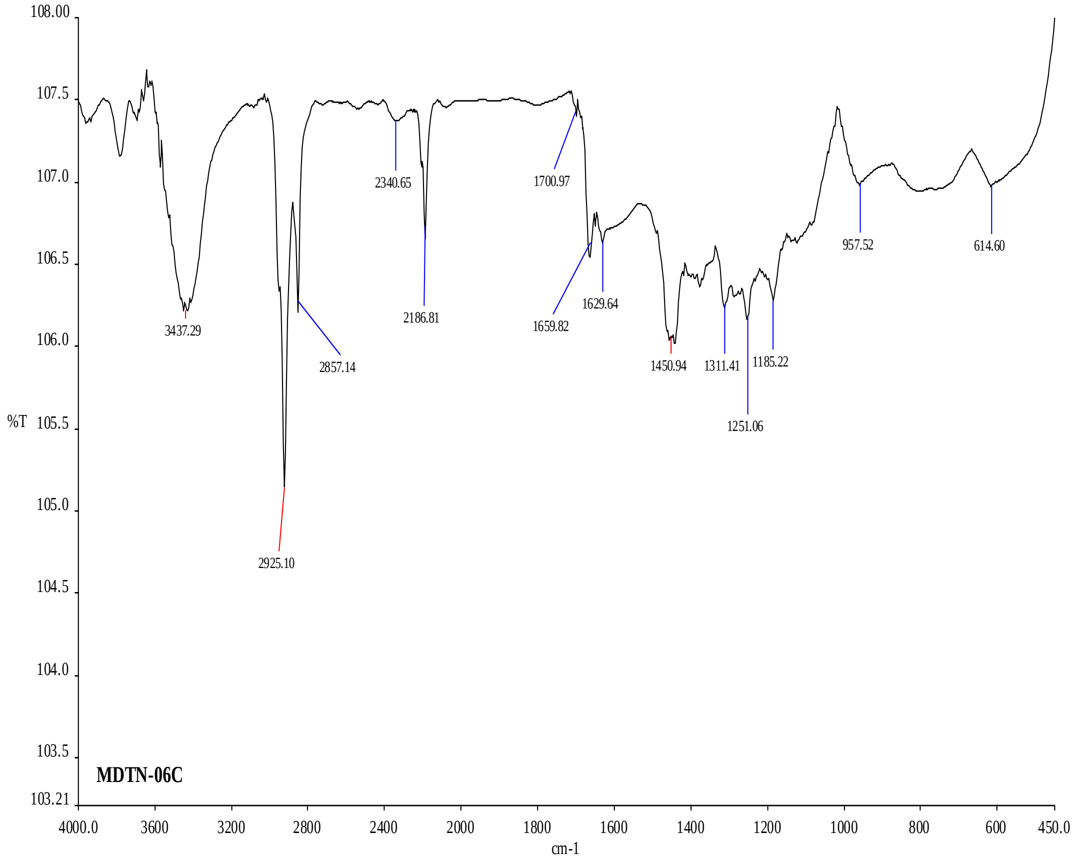


Fig. S12 FT-IRspectrum of **R1**

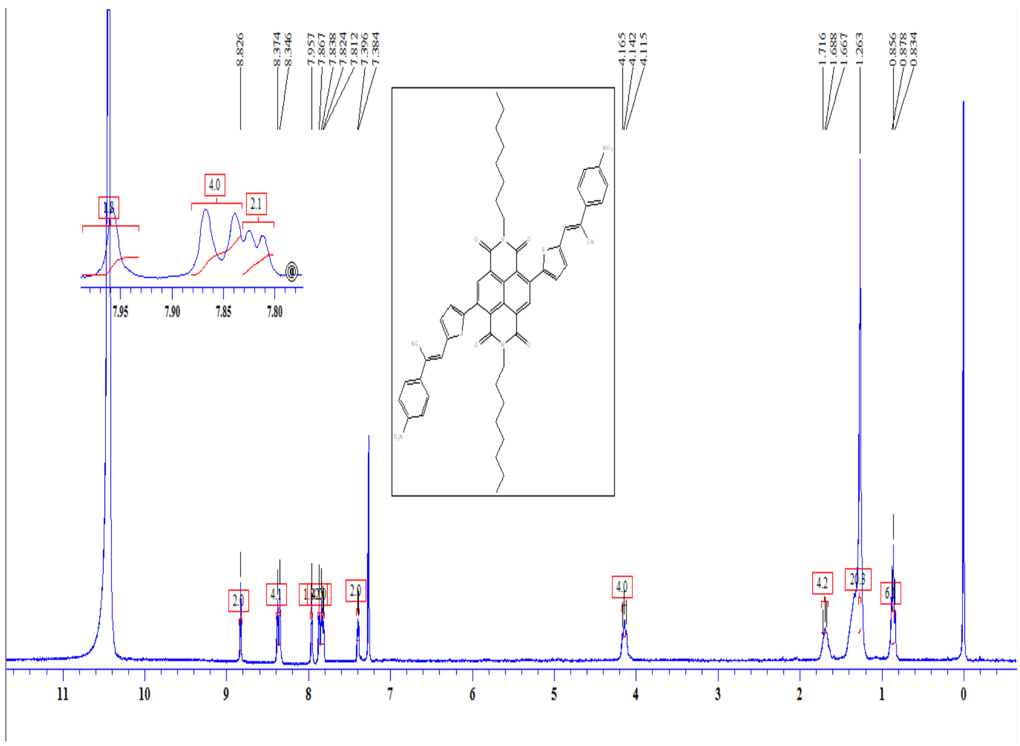


Fig. S13 ^{1}H NMR spectrum of **R2**

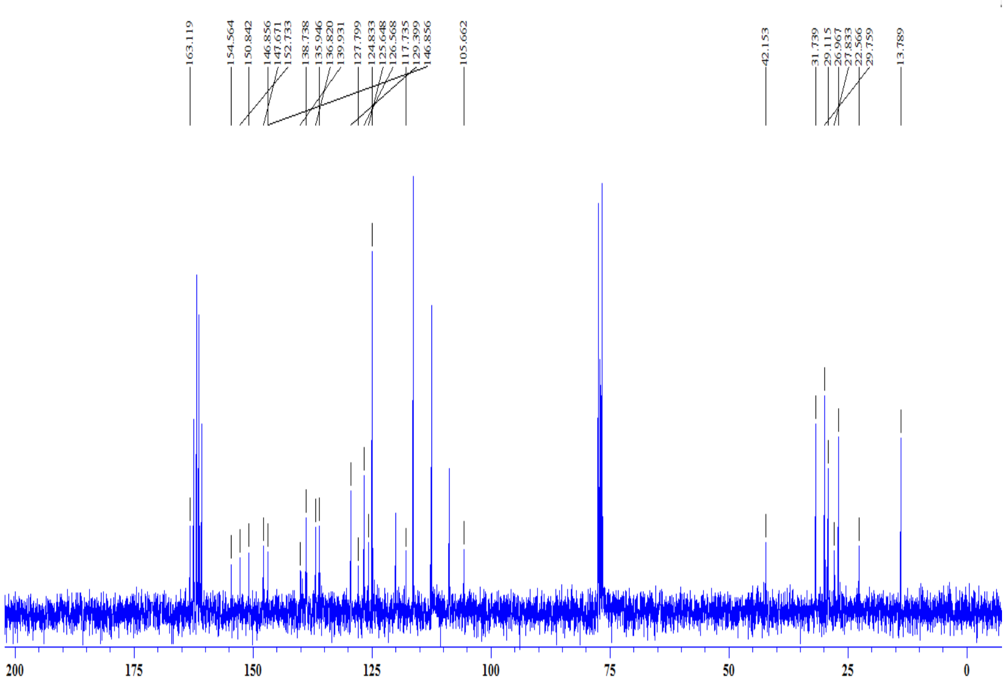


Fig. S14 ^{13}C NMR spectrum of **R2**

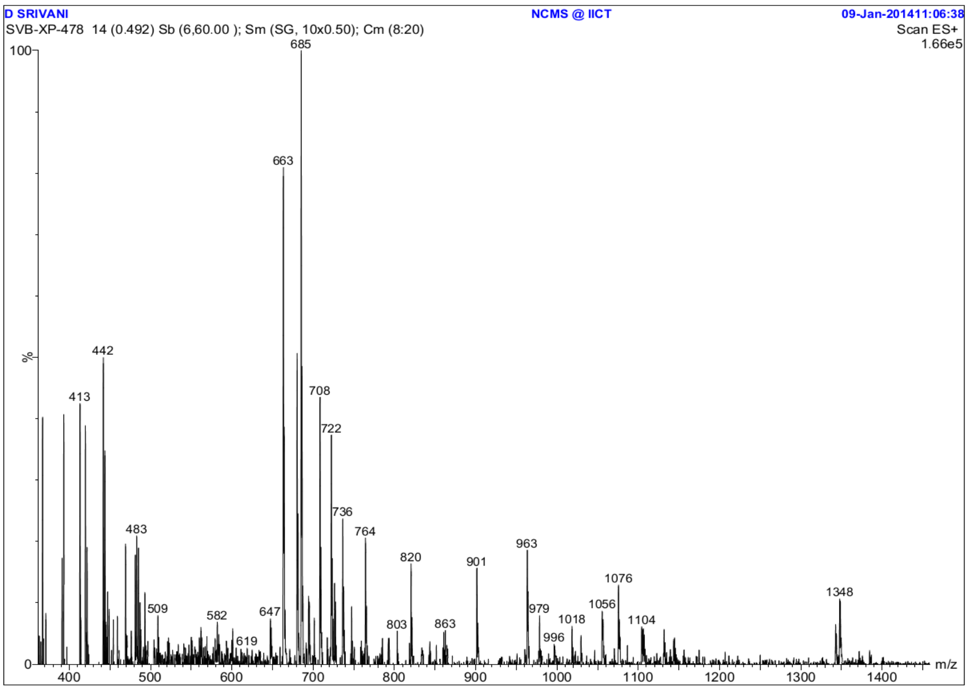


Fig. S15 Mass spectrum of **R2**

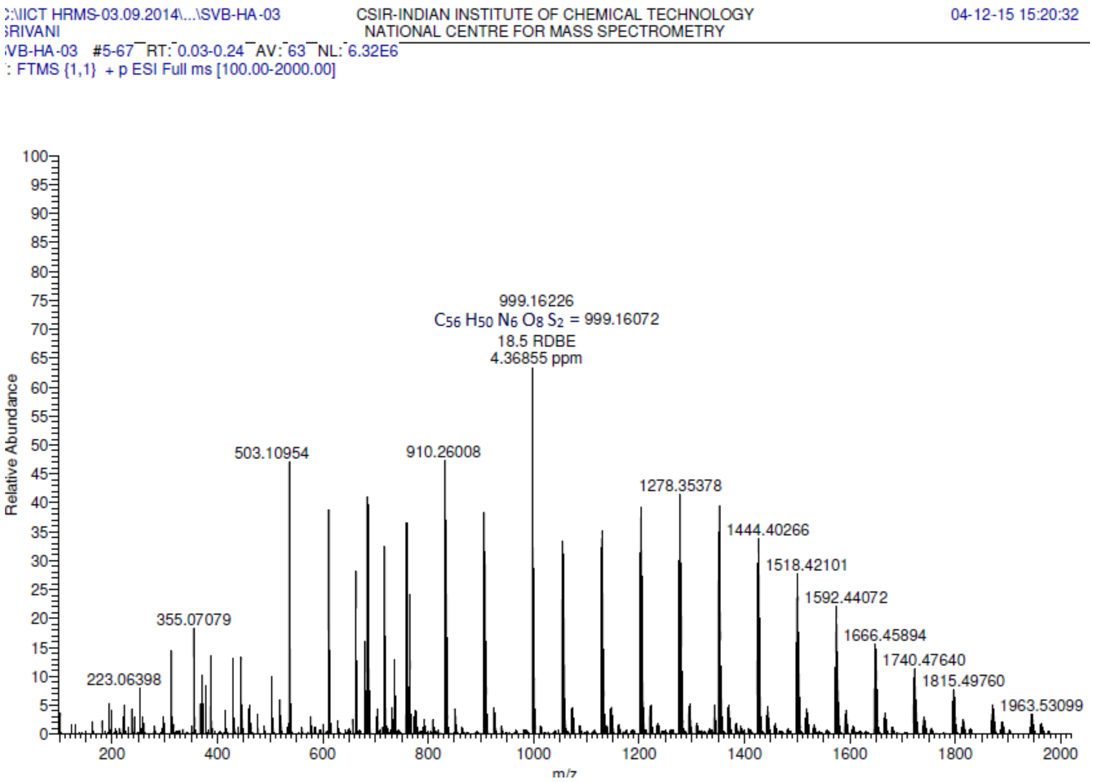


Fig. S16 HRMS of **R2**

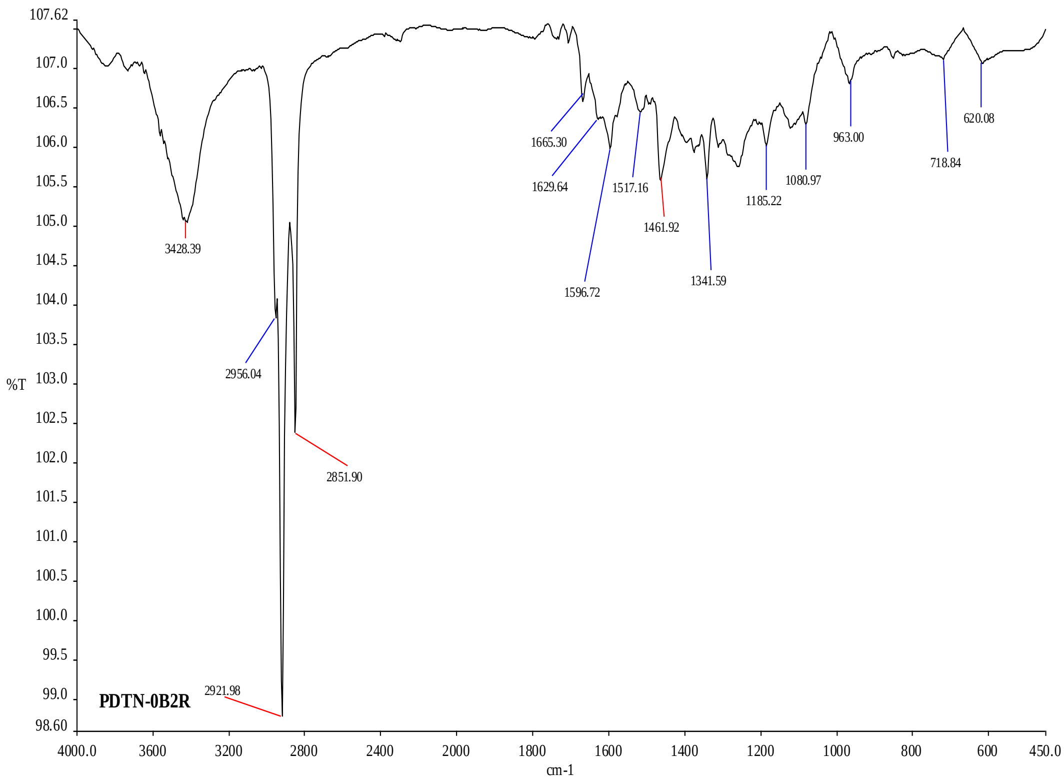


Fig. S17 FT-IR spectrum of **R2**