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ELECTRONIC SUPPLEMENTARY INFORMATION

Carbo[5]helicene versus Planar Phenanthrene as a Scaffold for Organic Materials in OLEDs: Electroluminescence of Anthracene-Functionalized Emissive Materials

Samik Jhulki,[a] Abhaya Kumar Mishra, [a] Tahsin J. Chow, [b,] and Jarugu Narasimha Moorthy[a,]**

[a]Department of Chemistry, Indian Institute of Technology, Kanpur 208016, INDIA
[b]Institute of Chemistry, Academia Sinica, Taipei, Taiwan 115, Republic of China
Email: chowtj@gate.sinica.edu.tw; moorthy@iitk.ac.in

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General aspects. ^{1}H NMR spectra were recorded on JEOL (400/500 MHz) spectrometers in $CDCl_3$ as a solvent. ^{13}C NMR spectra were recorded on JEOL-Lambda (100/125 MHz) spectrometers with complete proton decoupling. ESI and EI mass spectra analyses were carried out on Waters ^{Q}TOF and GCT premier mass spectrometers, respectively. Melting points were determined with a JSGW melting point apparatus. IR spectra were recorded on a Bruker Vector 22 FT-IR spectrophotometer. The TGA and DSC measurements were carried out using Mettler-Toledo and SDT Q600 instruments, respectively, at 10 ºC/min under a nitrogen gas atmosphere. UV-vis absorption spectra were recorded on a Shimadzu UV-1800 spectrophotometer. PL measurements in solution and solid state were carried out using FluoroMax-4; FM4-3000 spectrofluorimeter, Horiba Scientific. Cyclic voltammetry measurements were performed using CHI610E electrochemical work-station (CH instruments, Texas, USA). All solvents were distilled prior to use, and HPLC grade solvents used for UV-vis and PL measurements were procured from Merck. Column chromatography was conducted with a silica gel of 100-200μ mesh.

Materials. ITO-coated glass slides (thickness 0.7 mm; resistance 11 Ω) and NPB, TPBI, BCP, TmPyPB, LiF and Al, and HPLC grade solvents employed for cleaning of the ITO-coated glasses, and carrying out other measurements such as Uv-vis, fluorescence, CV, etc. were procured from commercial sources. Device fabrications and photophysical, thermal, electrochemical and electroluminescence characterizations were carried out as described elsewhere.[S1-S2]

Details of Single Crystal X-Ray Structure Determination

The X-ray diffraction intensity data collection for the single crystals of **PDANT** was carried out with APEX-II CCD detector system equipped with Mo-sealed Siemens ceramic diffraction tube (λ = 0.7107 Å) and a highly oriented graphite monochromator operating at 50 kV and 30 mA. The data were collected in a hemisphere mode and processed with Bruker's SAINT program. The structures were solved by direct methods using SHELXL package and refined by full matrix least-squares method based on F^2 using SHELXL-2014 program (Sheldrick, 2014). The hydrogens were fixed geometrically, treated as riding on their nonhydrogens, and refined isotropically, while all nonhydrogens were subjected to anisotropic refinement. CCDC-1574102 (**PDANT**) contains the supplementary X-ray crystallographic data for this paper. These data can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Table S1. Crystal data of **PDANT**.

parameters	**PDANT**
Empirical formula	$C_{54}H_{34}\bullet 3CHCl_3$
Formula weight	1040.99
Temperature (K)	100(2)
Wavelength (Å)	0.71073
Solvent of crystallization	$CHCl_3$/hexane
Crystal habit	Block
Crystal color	Colorless
Crystal system	Monoclinic
Space group	$P2_1/n$
a (Å)	9.325 (4)
b (Å)	16.641 (3)
c (Å)	31.414 (5)
α (deg)	90.000
β (deg)	93.589 (3)
γ (deg)	90.000
Volume ($Å^3$)	4865.7 (13)
Z	4
Calculated density (mg/m^3)	1.421
Absorption coefficient (mm^{-1})	0.557
F(000)	2128
θ range for data collection (°)	1.785 to 28.303
Index ranges	$-12\leq h\leq 12$
	$-15\leq k\leq 21$
	$-40\leq l\leq 41$
Refinement method	Full-matrix least-squares on F^2
Goodness-of-fit on F^2	1.032
Final R indices [I>2sigma(I)]	$R_1 = 0.0884$,
	$wR_2 = 0.1860$
R indices (all data)	$R_1 = 0.1961$,
	$wR_2 = 0.2471$
CCDC deposition number	1574102

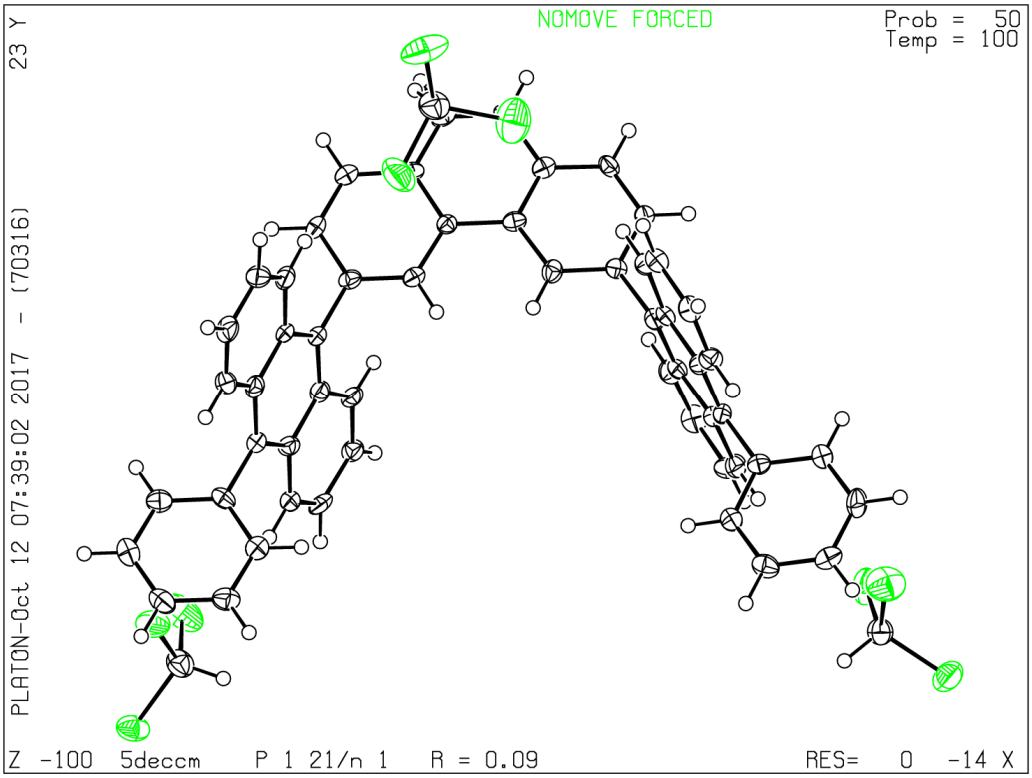


Fig. S1 Ortep plot (drawn at 50% probability) of the structures of the **PDANT** along with three chloroform guest molecules (in green) found in the asymmetric unit.

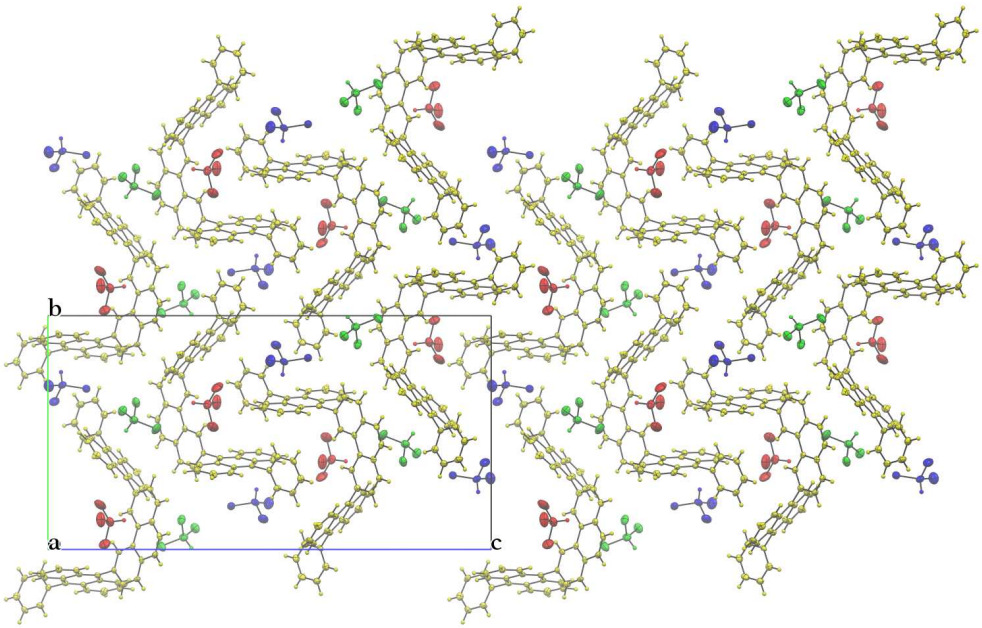


Fig. S2 Crystal packing diagram of **PDANT** down a-axis. Notice that three guest chloroform molecules found for each **PDANT** are shown in different colors.

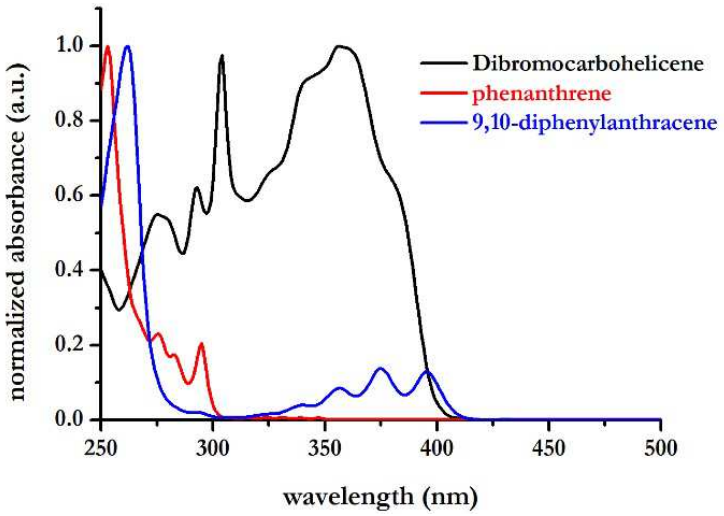


Fig. S3 UV-vis profiles of 2,13-dibromocarbohelicene, phenanthrene and 9,10-diphenylanthracene.

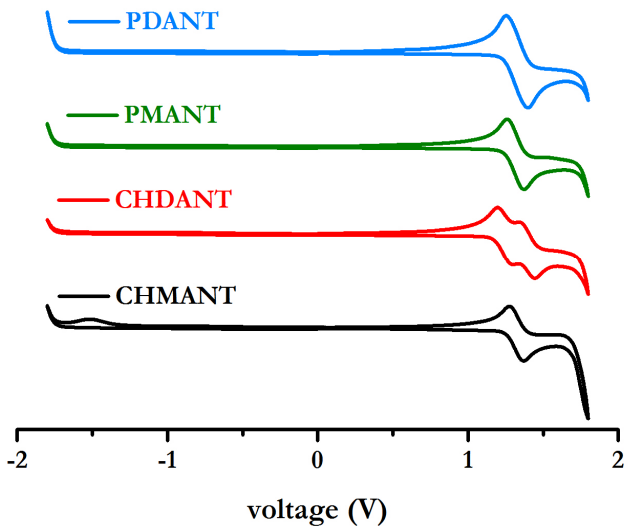


Fig. S4 CV profiles of **CHMANT**, **CHDANT**, **PMANT** and **PDANT**.

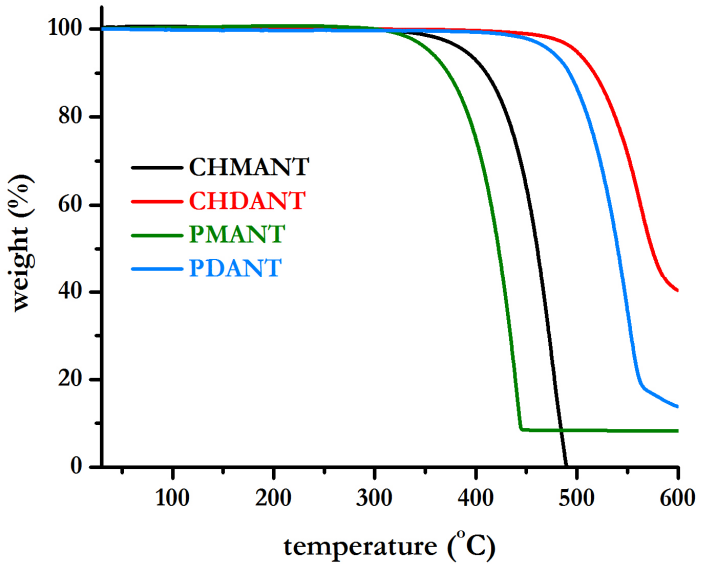


Fig. S5 TGA profiles of **CHMANT**, **CHDANT**, **PMANT** and **PDANT**.

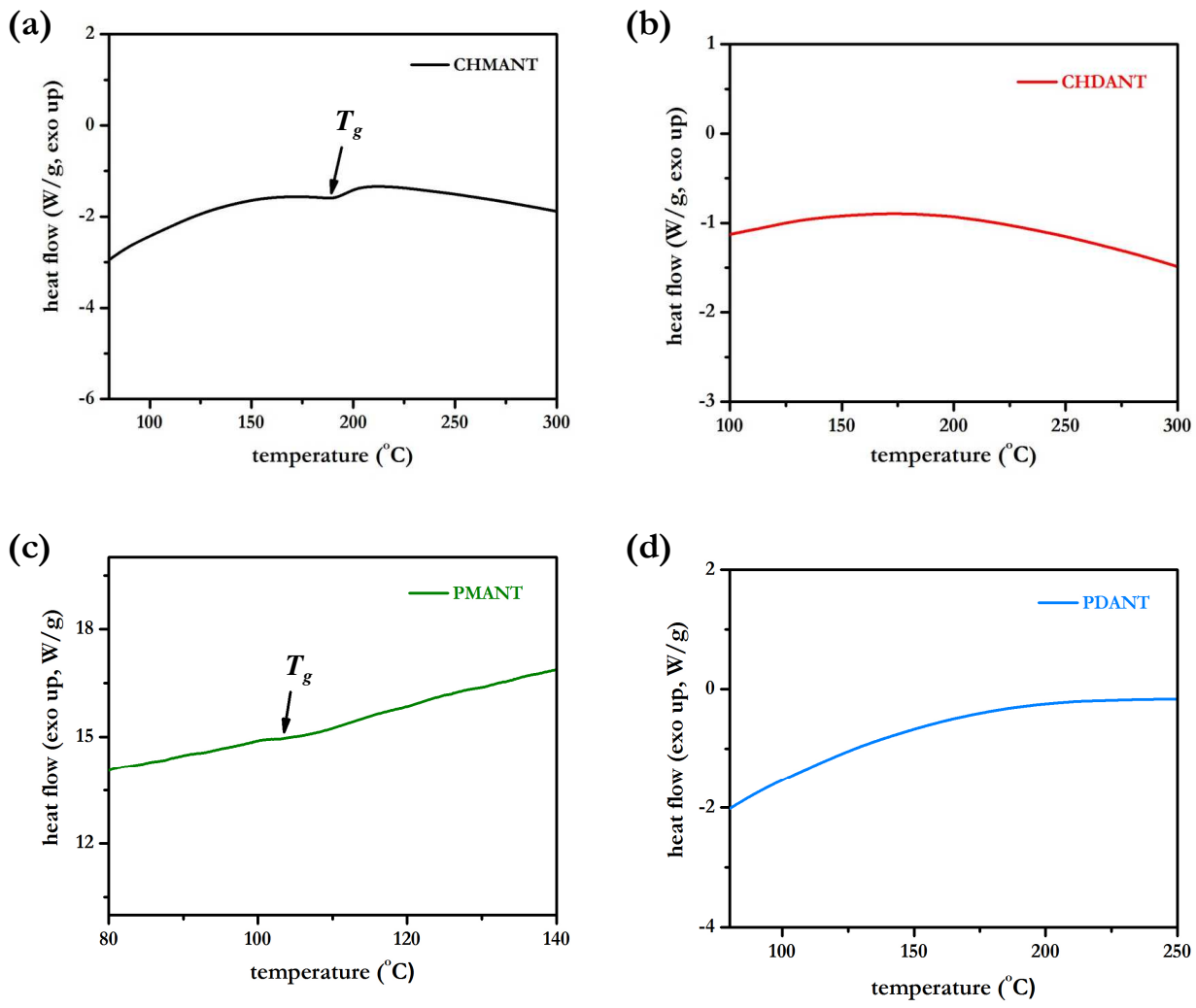


Fig. S6 DSC profiles of **CHMANT**, **CHDANT**, **PMANT** and **PDANT**.

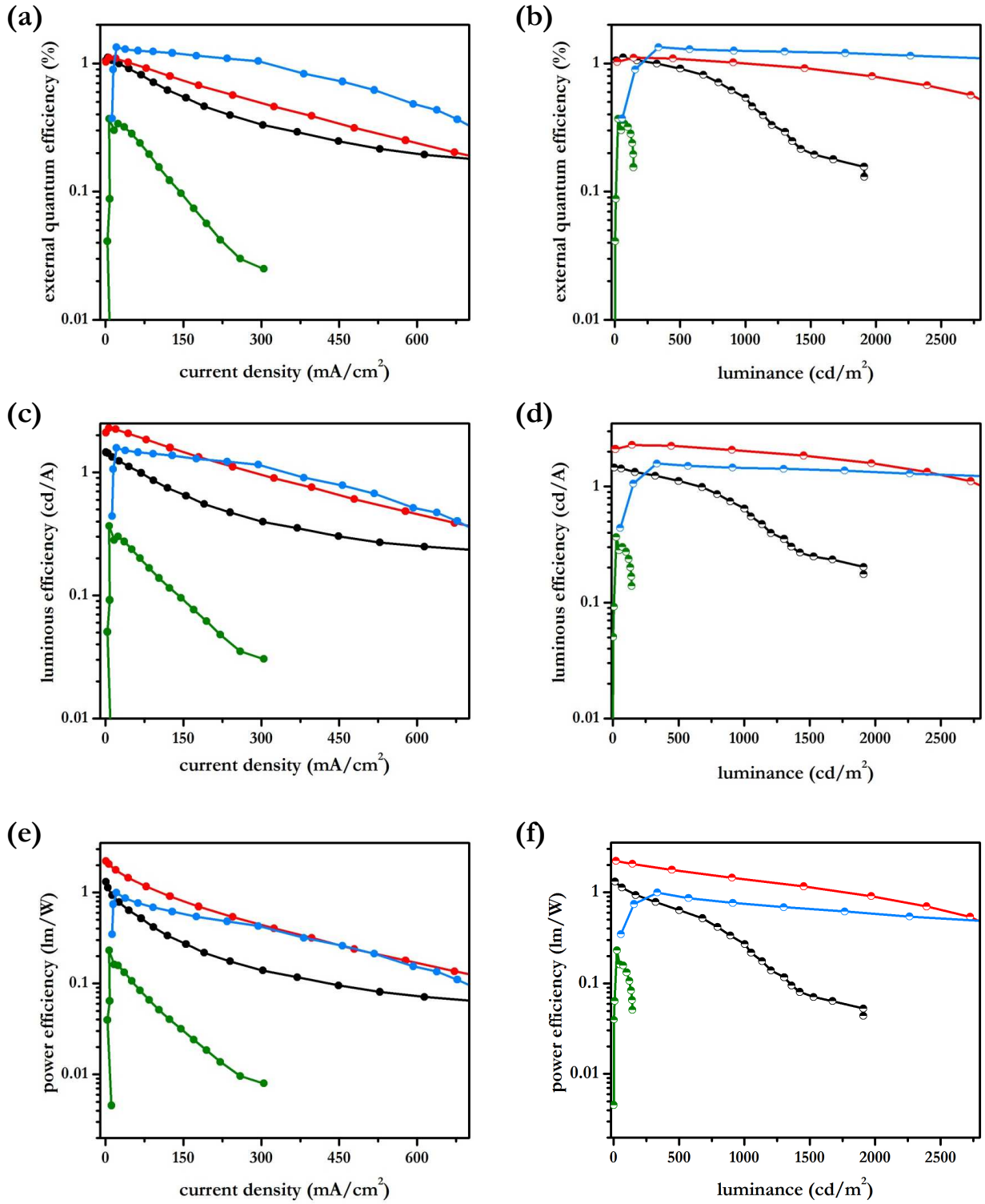


Fig. S7 Plots of external quantum efficiency vs current density (a), external quantum efficiency vs luminance (b), luminous efficiency vs current density (c), luminous efficiency vs luminance (d), power efficiency vs current density (e) and power efficiency vs luminance (f) for the devices of configuration A fabricated with **CHMANT** (black), **CHDANT** (red), **PMANT** (olive) and **PDANT** (sky blue), refer to text.

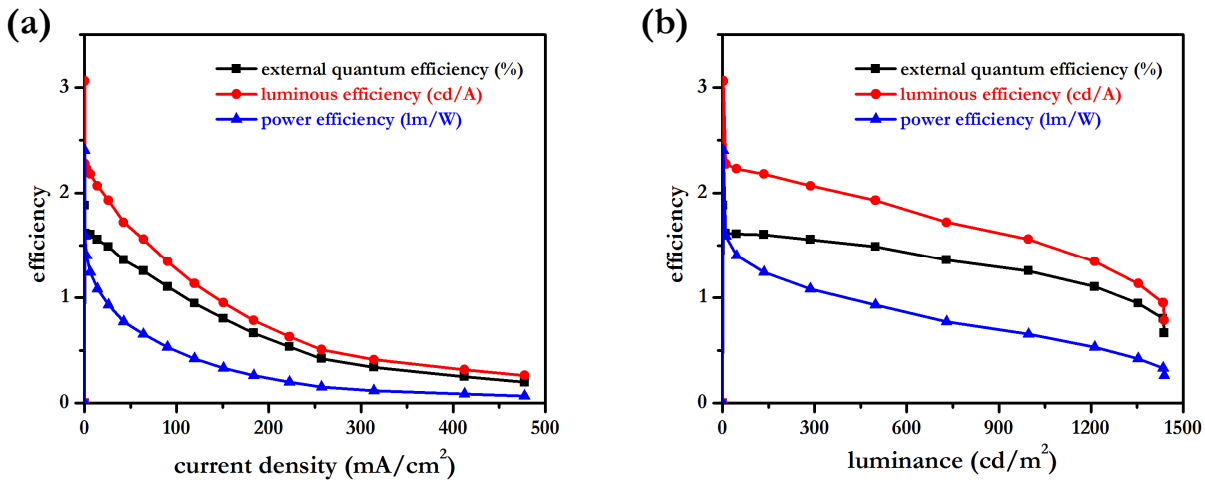
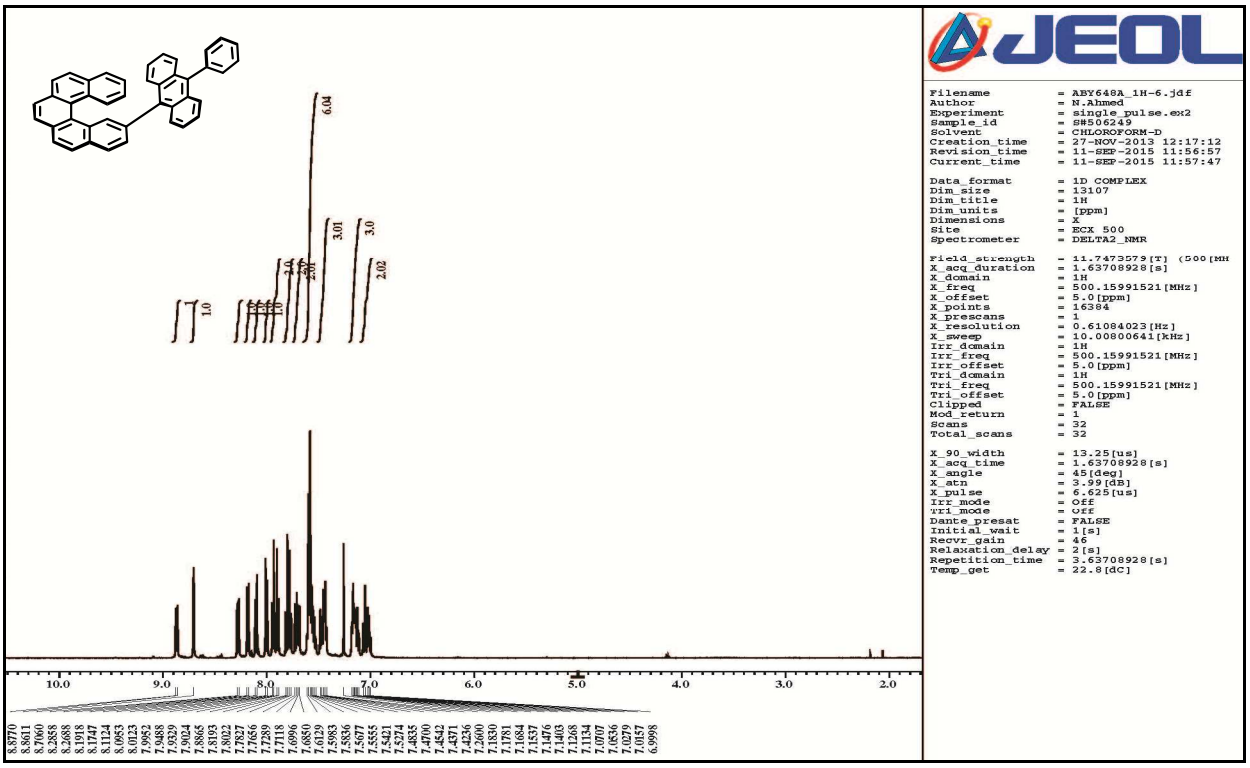


Fig. S8 Plots of external quantum efficiency, luminous efficiency and power efficiency vs current density (a), and luminance (b) for the devices in which **CHTPA** doped in **CHMANT** serves as the emissive layer.



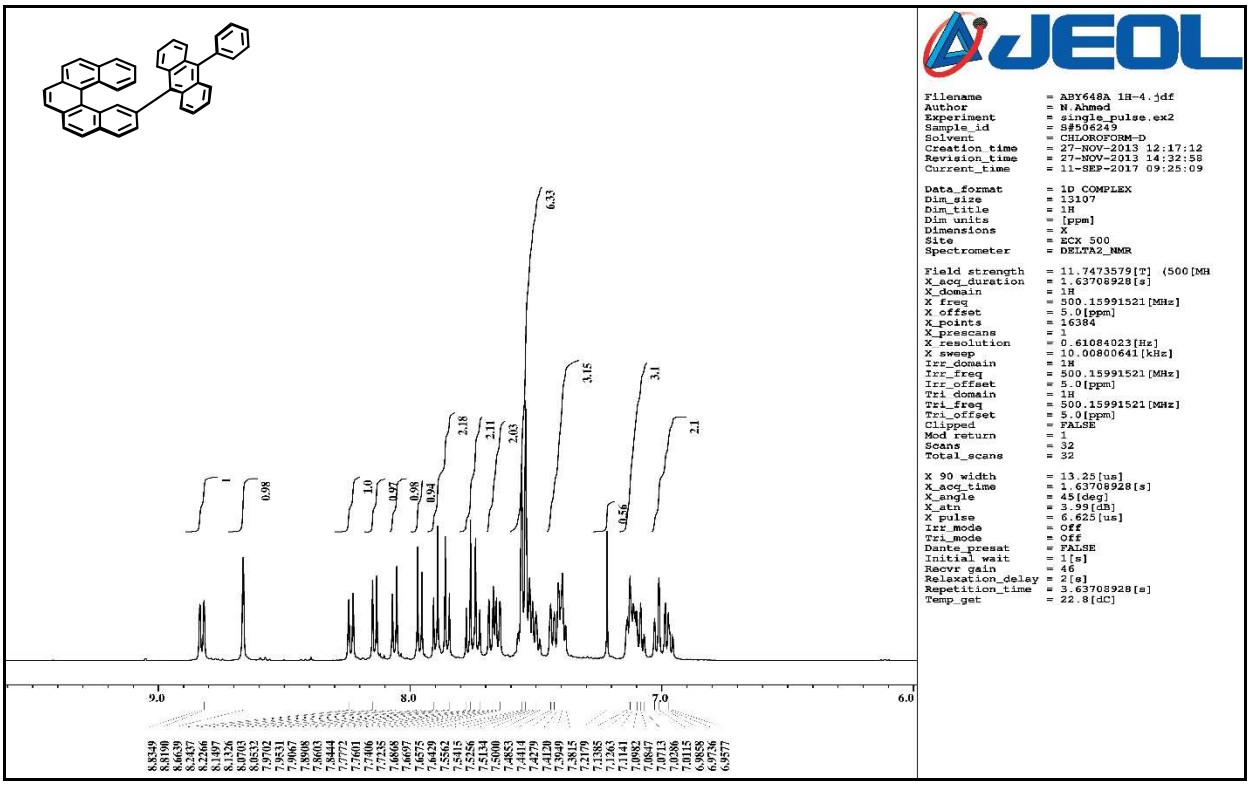
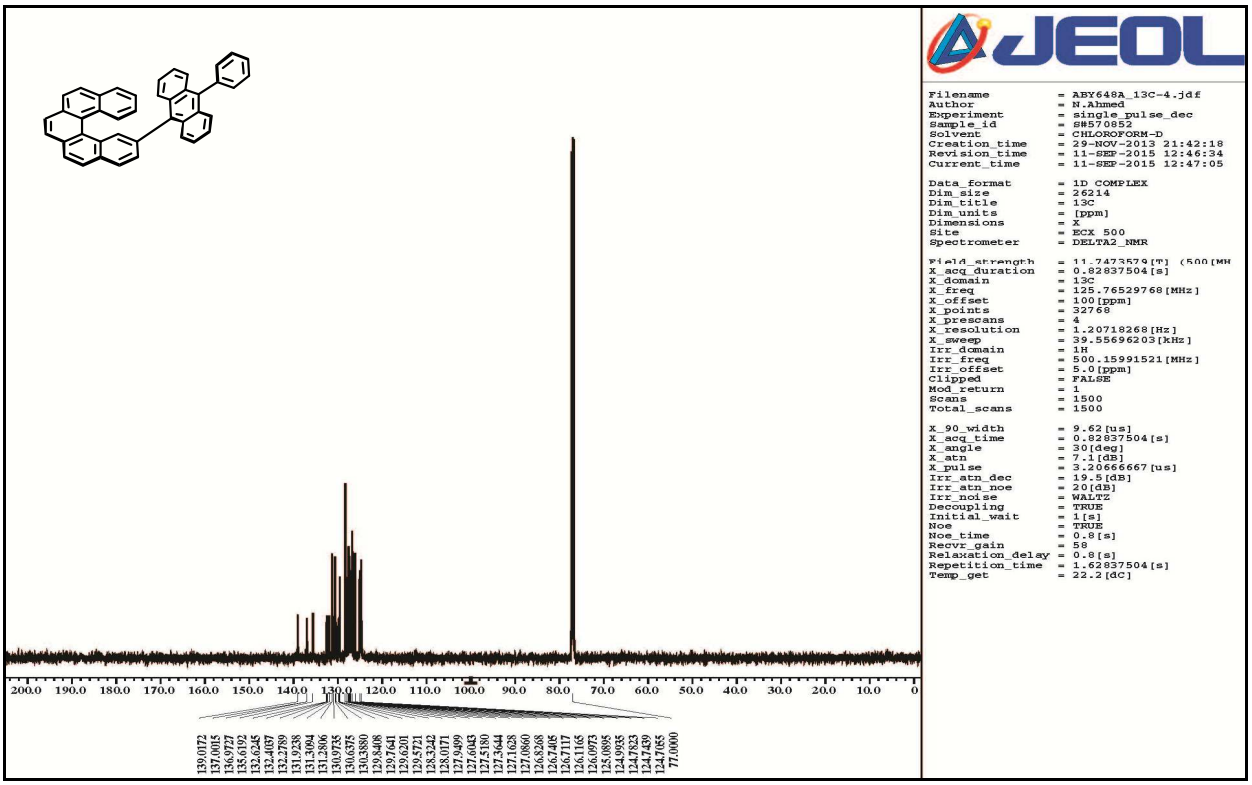


Fig. S9 ^{1}H (500 MHz) NMR spectra (full scale: top, expanded: below) of **CHMANT** in $CDCl_3$.



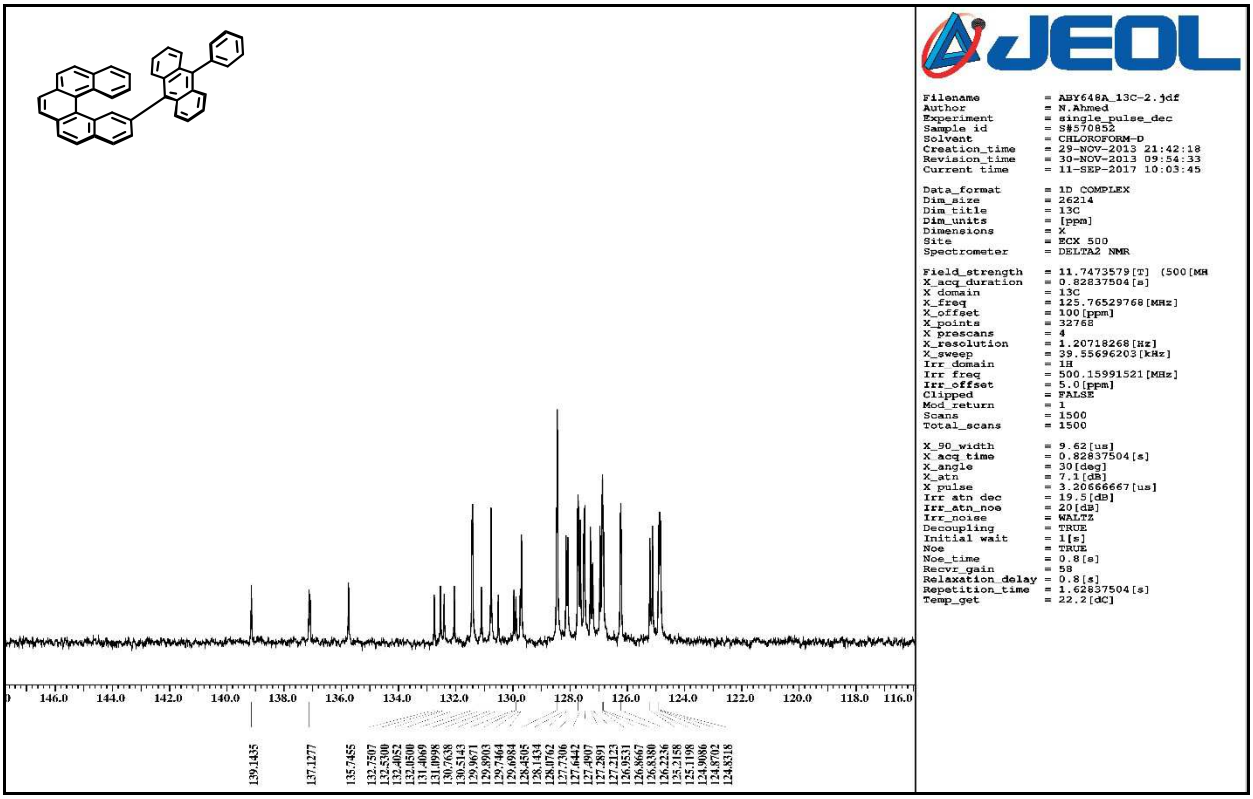


Fig. S10 ^{13}C (125 MHz) NMR spectra (full scale: top, expanded: below) of **CHMANT** in $CDCl_3$.

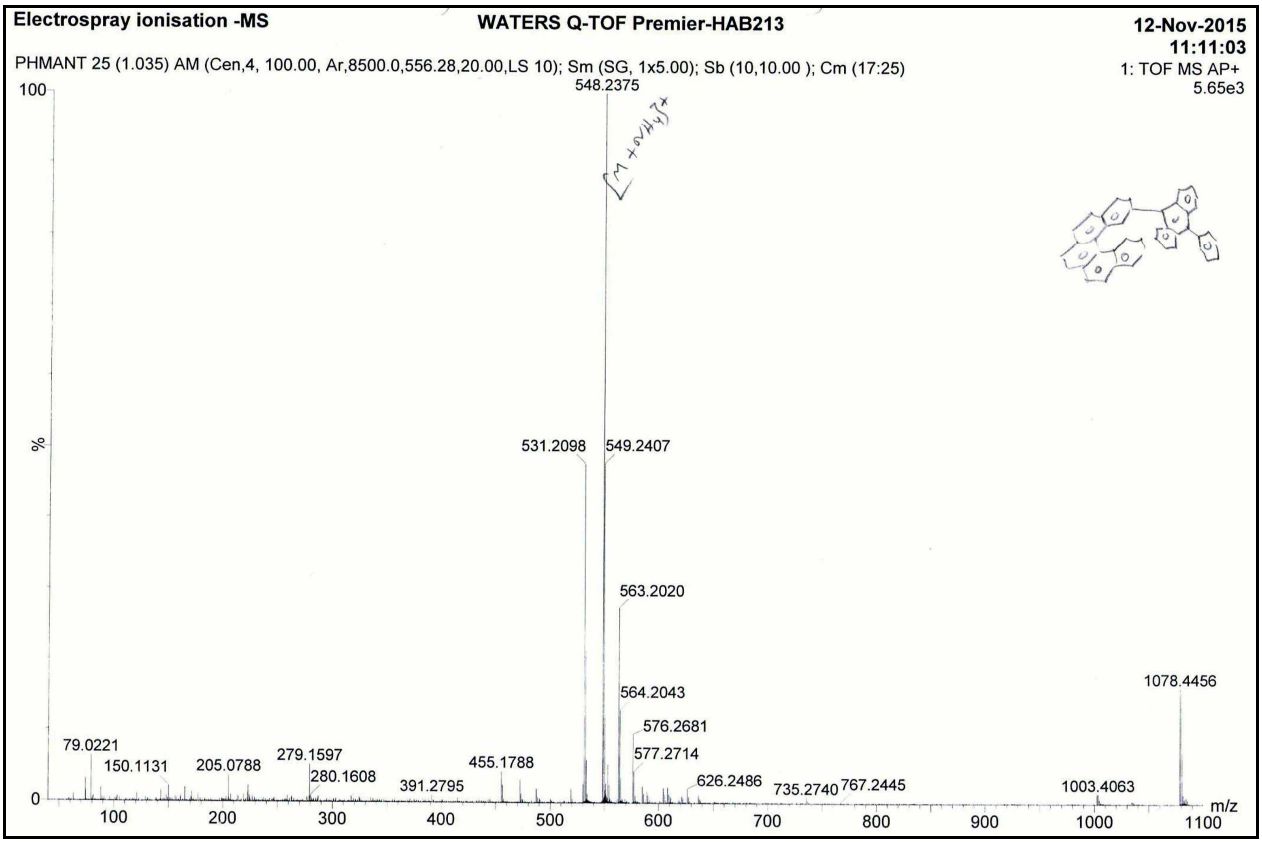


Fig. S11 ESI Mass spectrum of **CHMANT**.

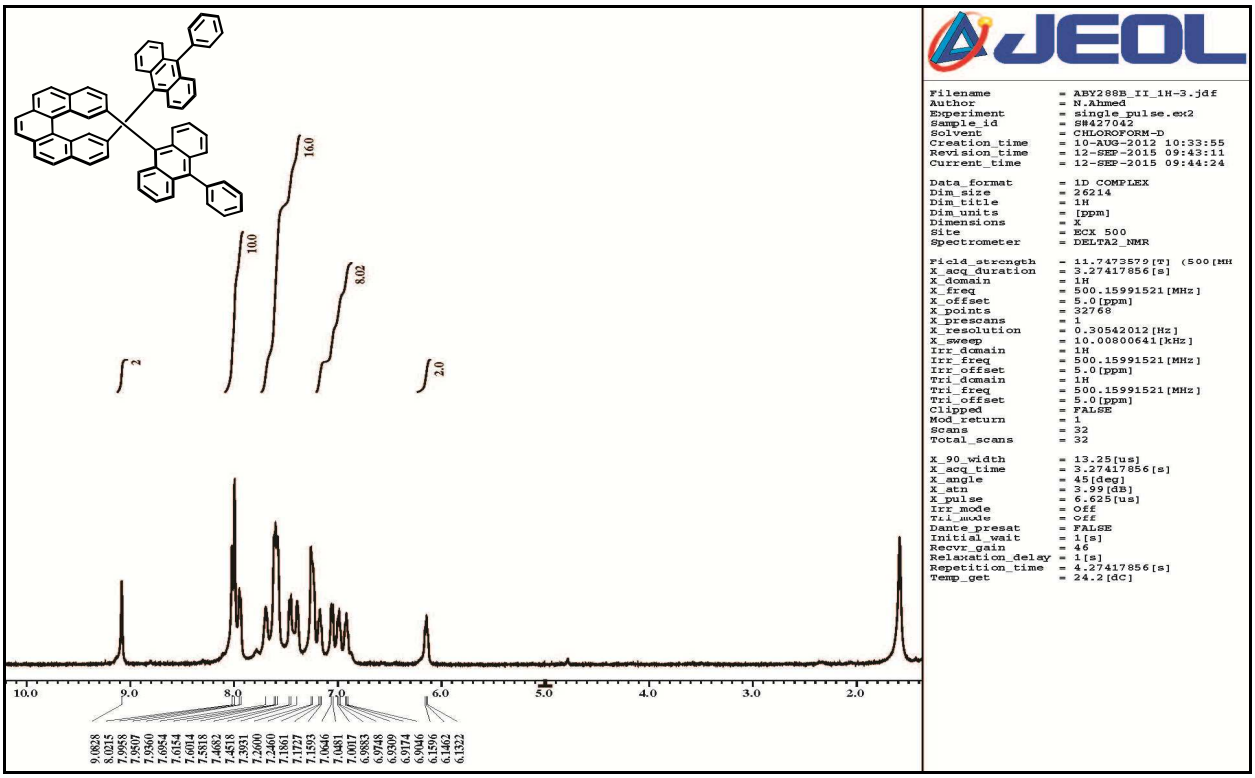


Fig. S12 ^{1}H (500 MHz) NMR spectra (full scale: top, expanded: below) of **CHDANT** in $CDCl_3$.

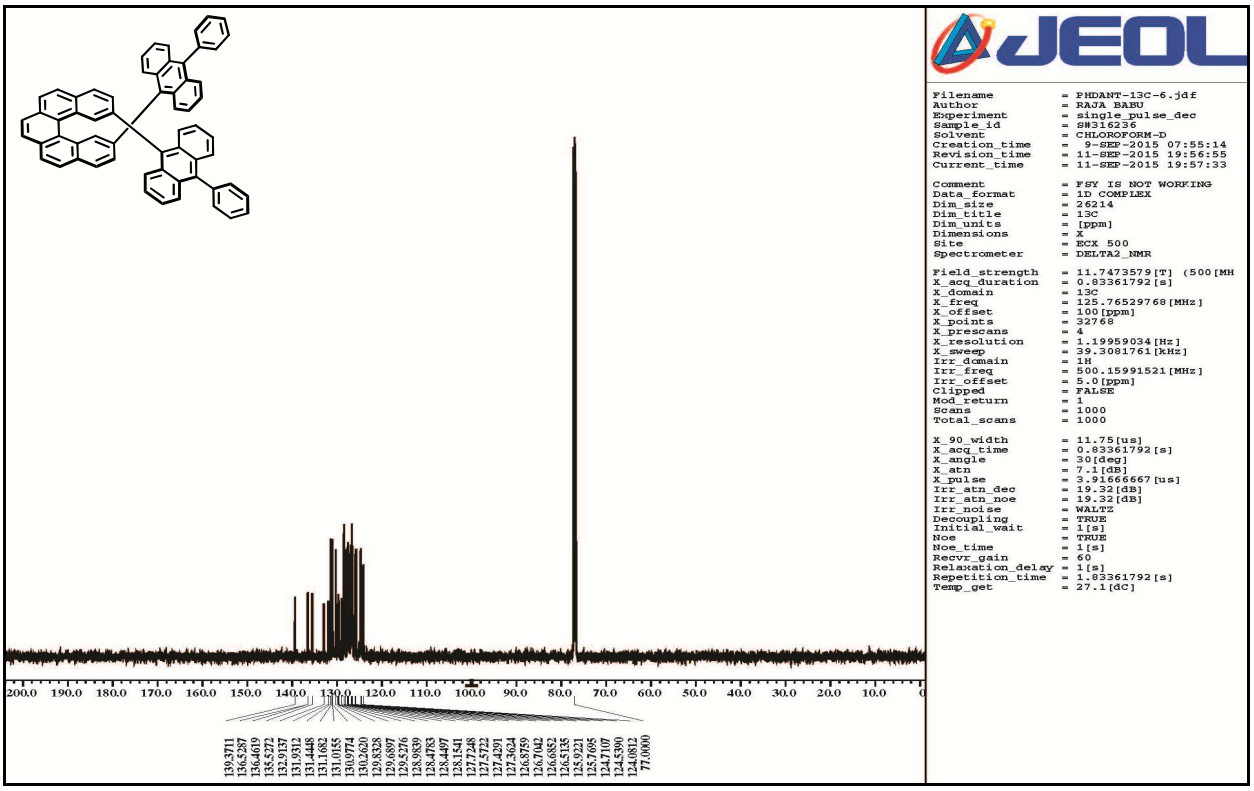


Fig. S13 ^{13}C (125 MHz) NMR spectra (full scale: top, expanded: below) of **CHDANT** in $CDCl_3$.

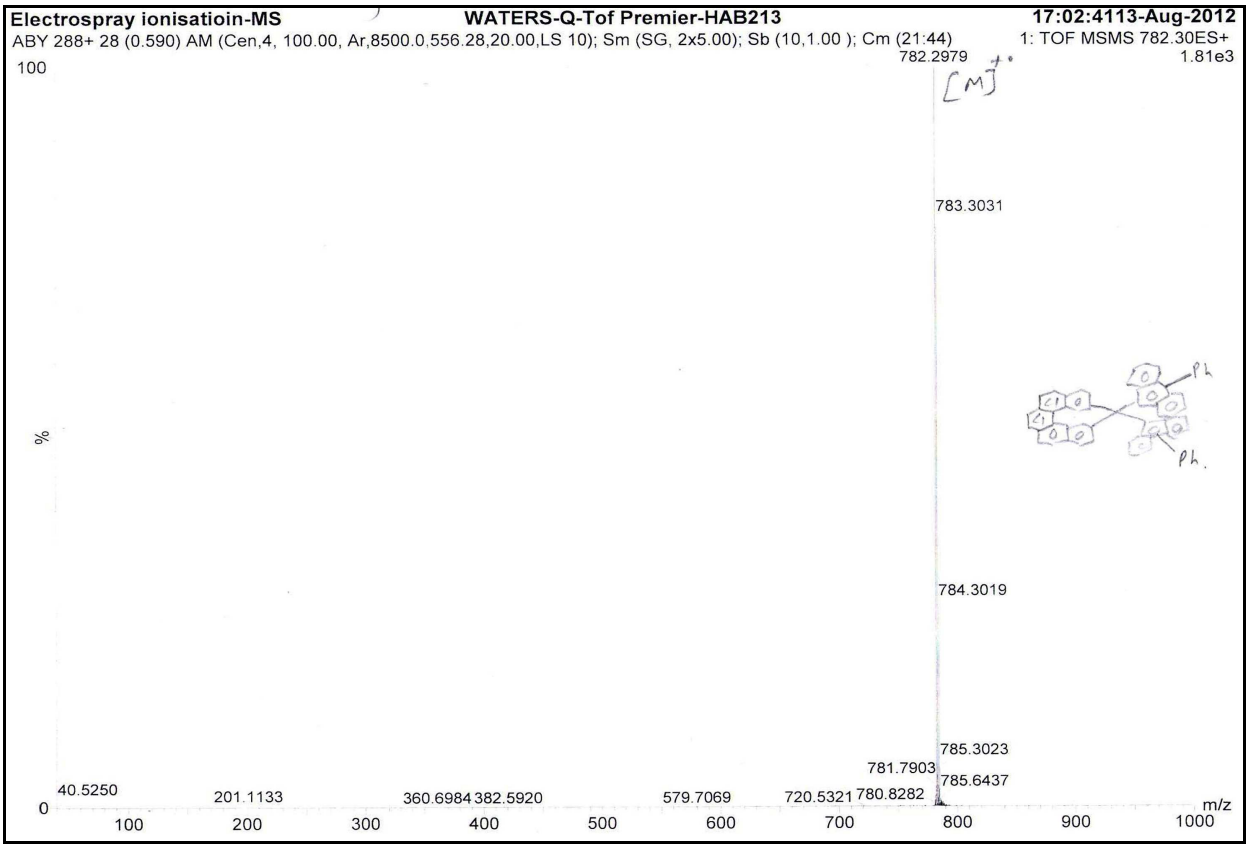
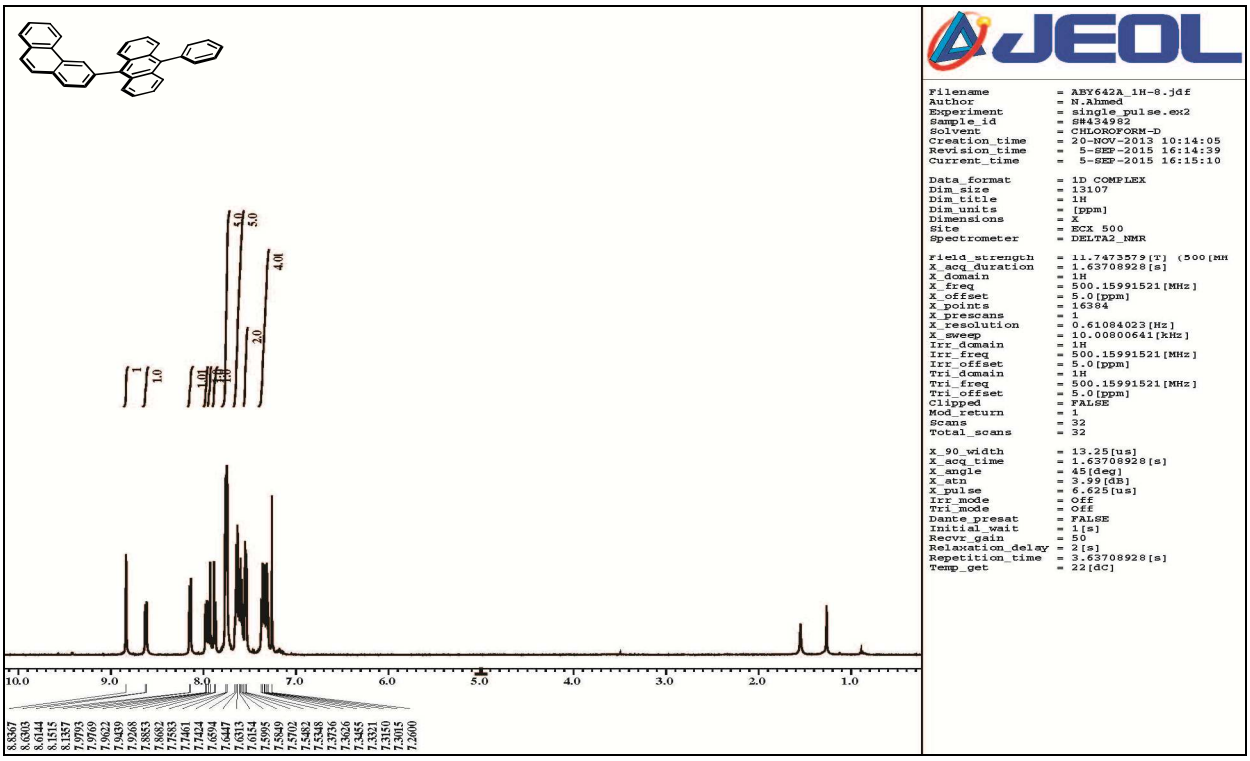


Fig. S14 ESI Mass spectrum of **CHDANT**.



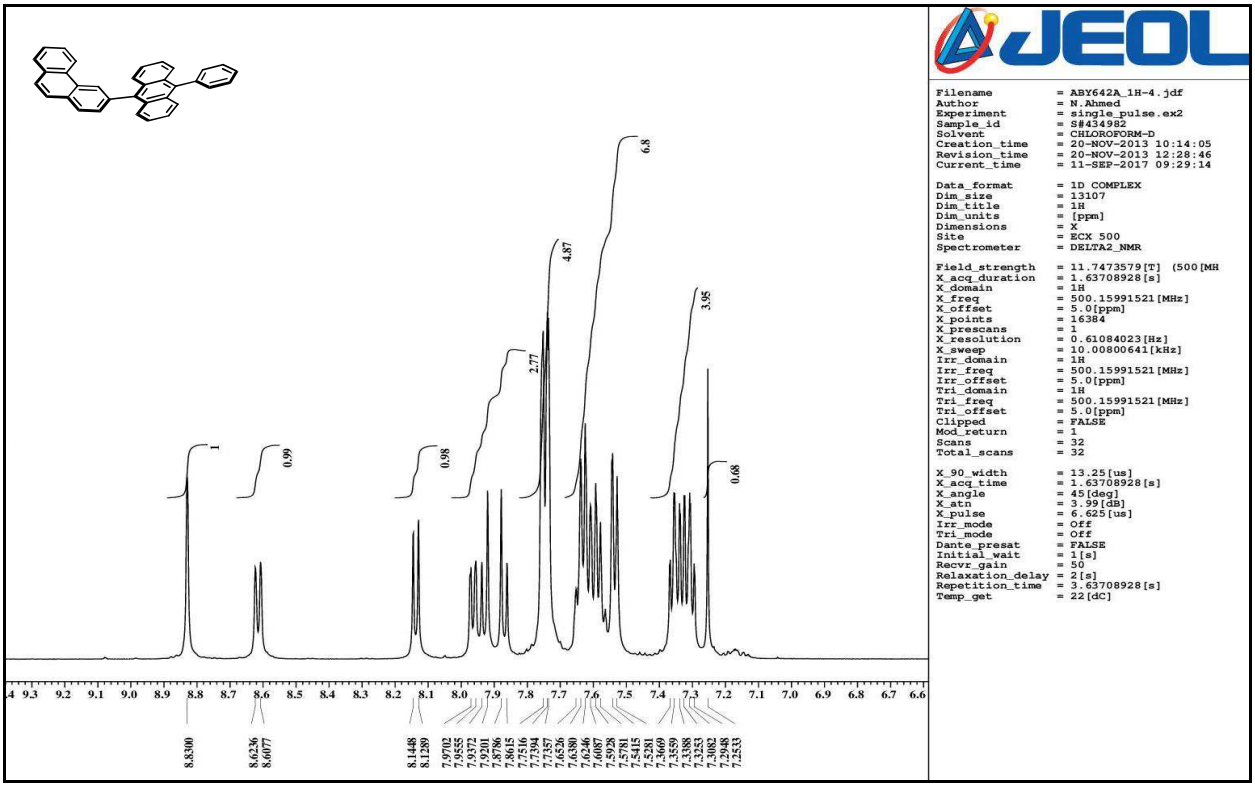
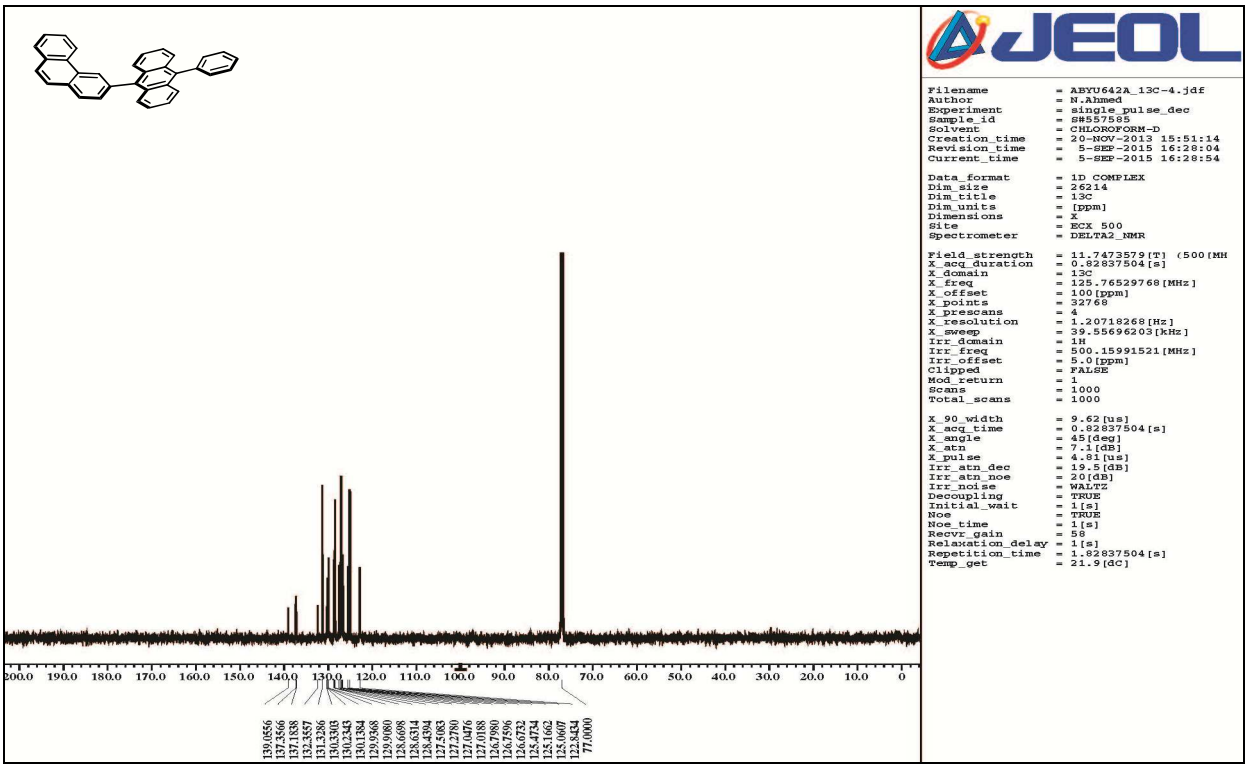


Fig. S15 ^{1}H (500 MHz) NMR spectra (full scale: top, expanded: below) of **PMANT** in $CDCl_3$.



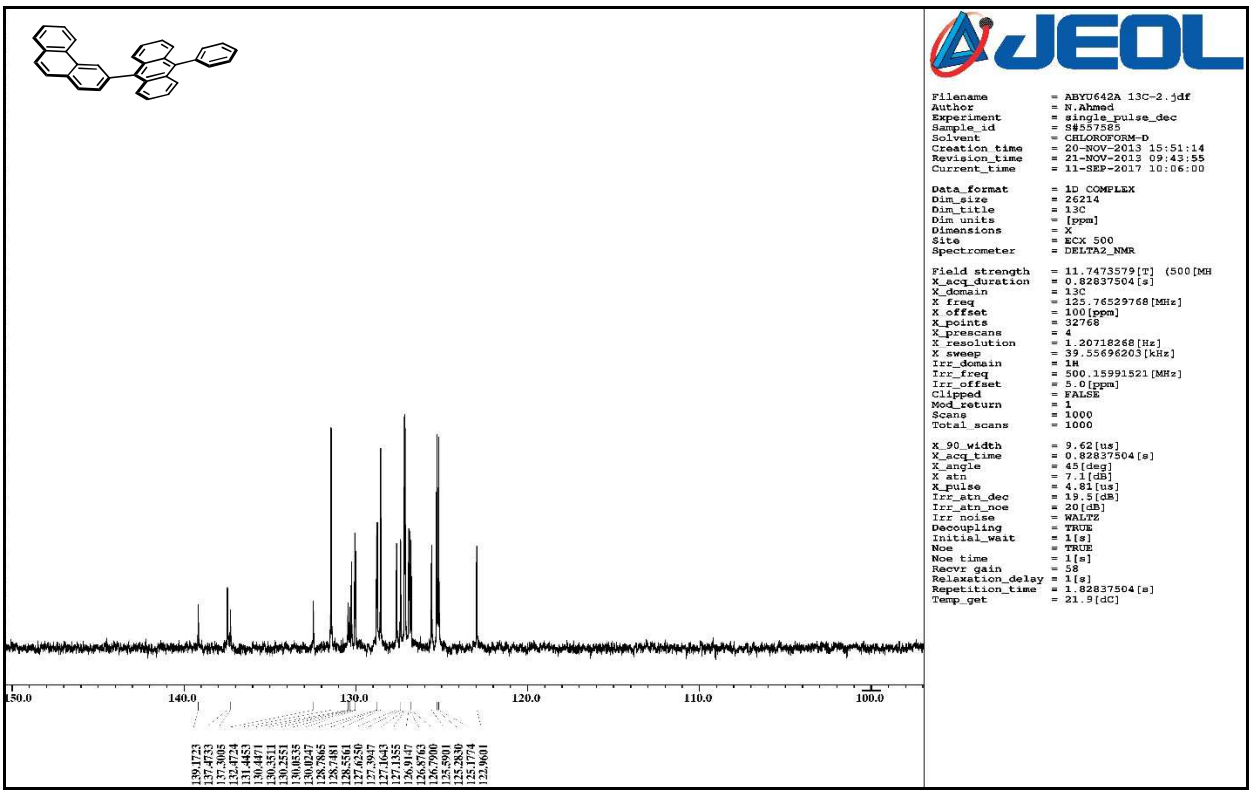


Fig. S16 ^{13}C (125 MHz) NMR spectra (full scale: top, expanded: below) of **PMANT** in $CDCl_3$.

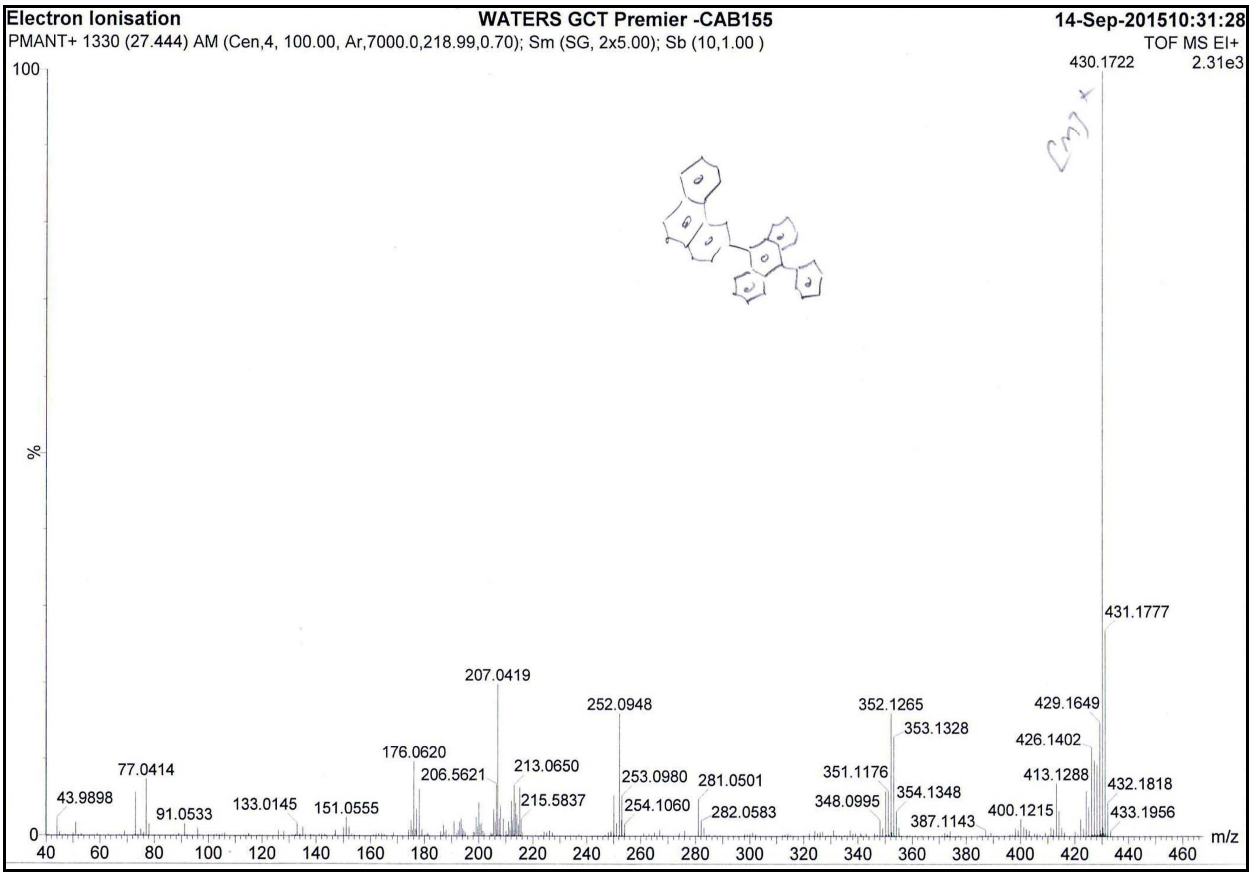


Fig. S17 EI Mass spectrum of **PMANT**.

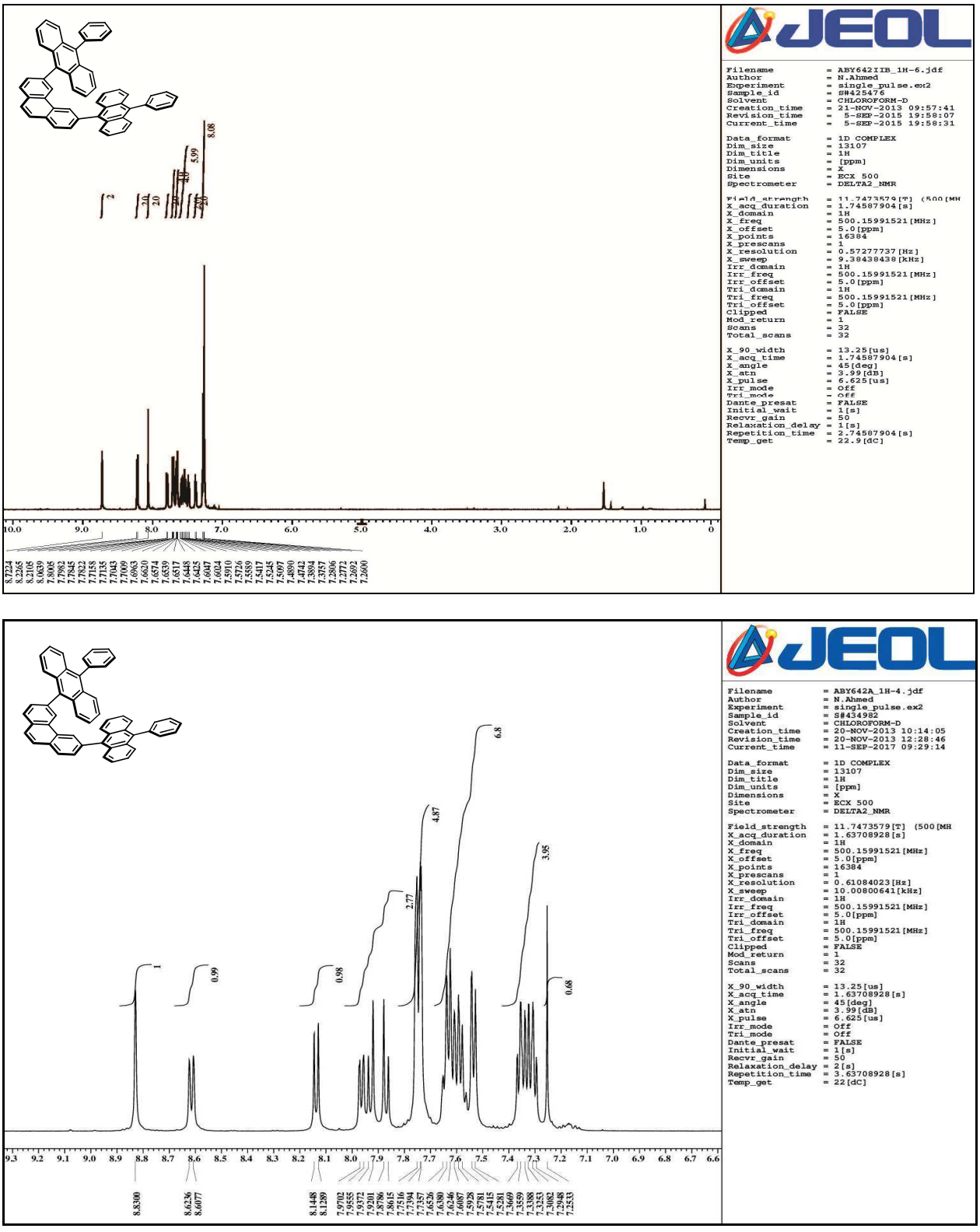
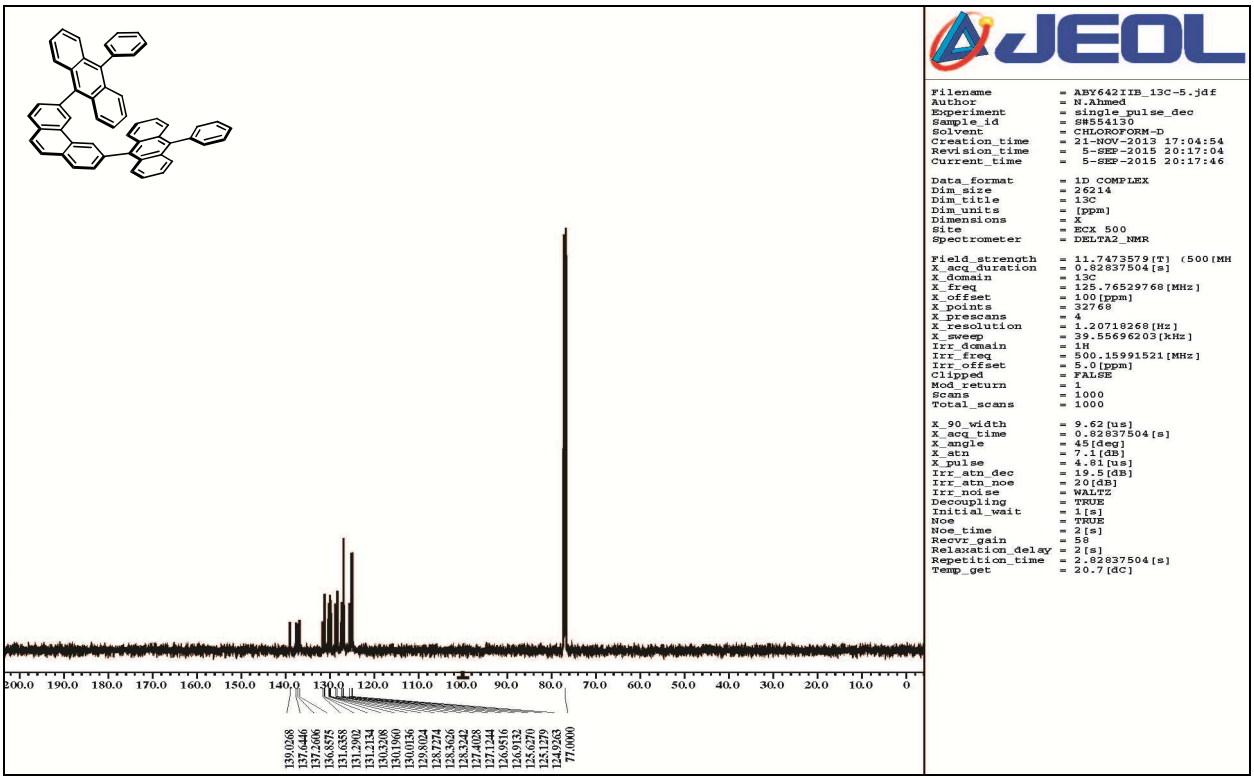


Fig. S18 ^{1}H (500 MHz) NMR spectra (full scale: top, expanded: below) of **PDANT** in $CDCl_3$.



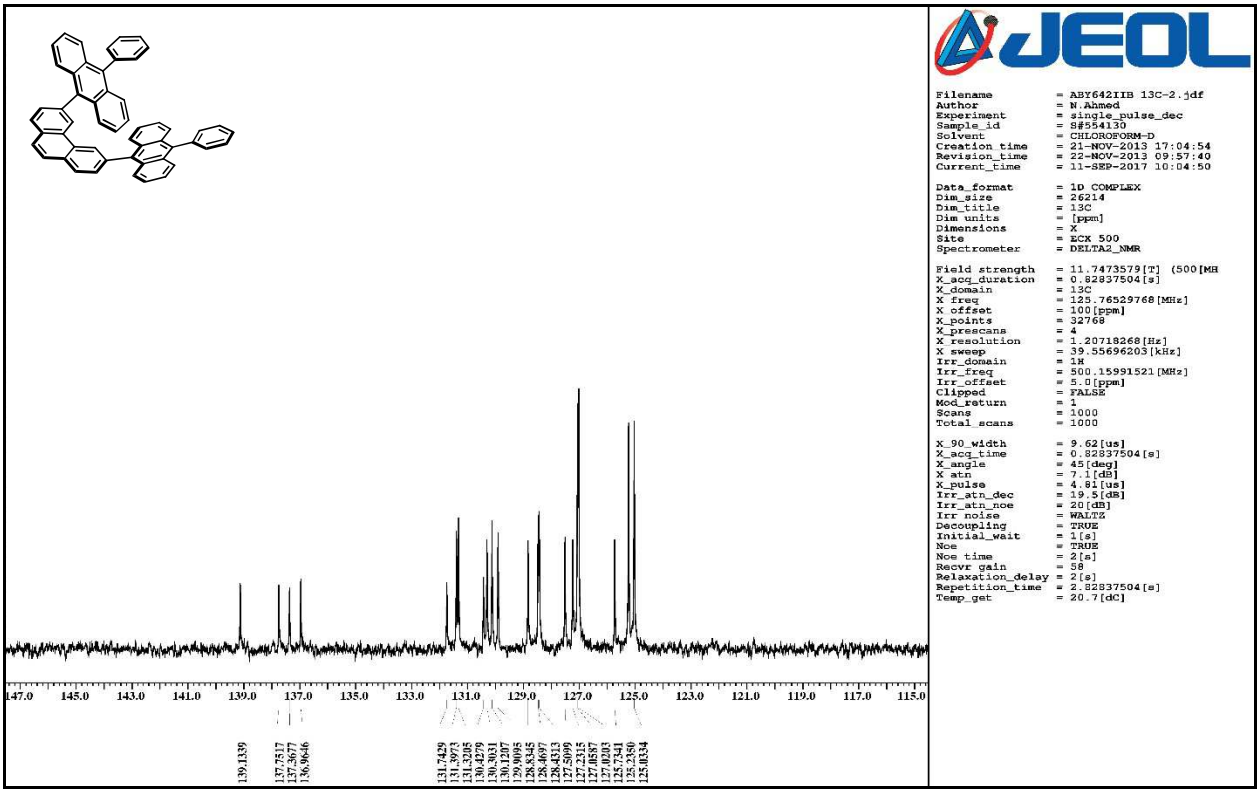


Fig. S19 ^{13}C (125 MHz) NMR spectra (full scale: top, expanded: below) of **PDANT** in $CDCl_3$.

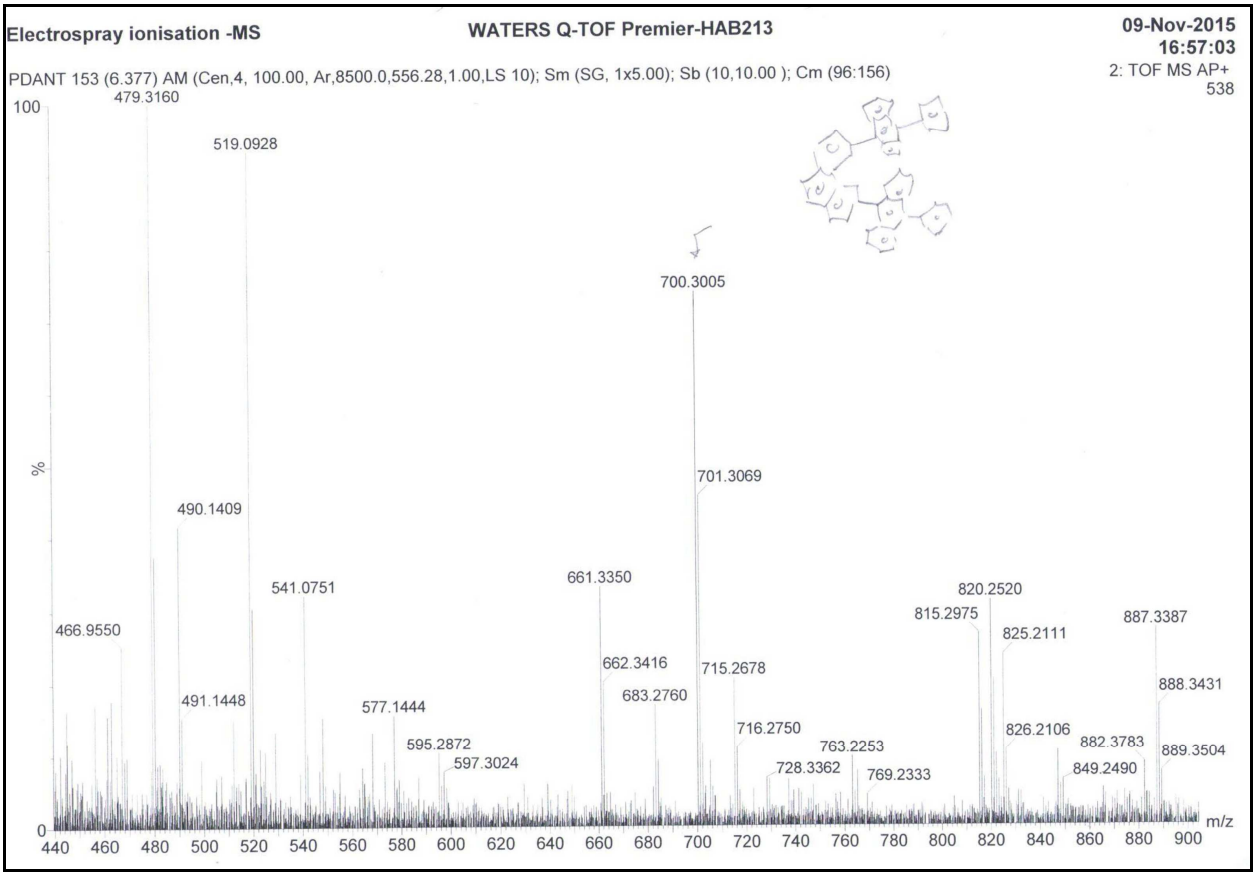


Fig. S20 ESI Mass spectrum of **PDANT**.

References

S1 I. Neogi, S. Jhulki, A. Ghosh, T. J. Chow and J. N. Moorthy, *Org. Electron.*, 2014, **15**, 3766−3772.

S2 S. Jhulki, A. K. Mishra, A. Ghosh, T. J. Chow and J. N. Moorthy, *J. Mater. Chem. C*, 2016, **4**, 9310–9315.