Electronic Supplementary Material (ESI) for Dalton Transactions
This journal is © The Royal Society of Chemistry 2012

Supporting Information

Triphenylene Derivatives: Chemosensors for Sensitive Detection of Nitroaromatic Explosives.

Vandana Bhalla*, Harshveer Arora, Hardev Singh and Manoj Kumar

Department of Chemistry, UGC Centre for Advanced Studies.
Guru Nanak Dev University, Amritsar, INDIA- 143005

Page No.	Contents
S2	Spectral overlaps for compound 3 and 5
S3	Fluorescence spectra of compound 5 in different solvents
S4-S5	Fluorescence response of compound 3 with other nitroaromatic derivatives
S6- S7	Fluorescence response of compound 5 with other nitroaromatic derivatives
S8	Calculated Stern-Volmer constants for compounds 3 and 5 with various nitroaromatic derivatives
S9	^{1}H NMR of compound 3
S10	^{13}C NMR of compound 3
S11	MALDI-TOF mass spectrum of compound 3
S12	^{1}H NMR of compound 5
S13	^{13}C NMR of compound 5
S14	FAB Mass Spectrum of compound 5
S15	Comparison of derivative 5 with previous reports

Spectral overlaps for compound 3 and 5.

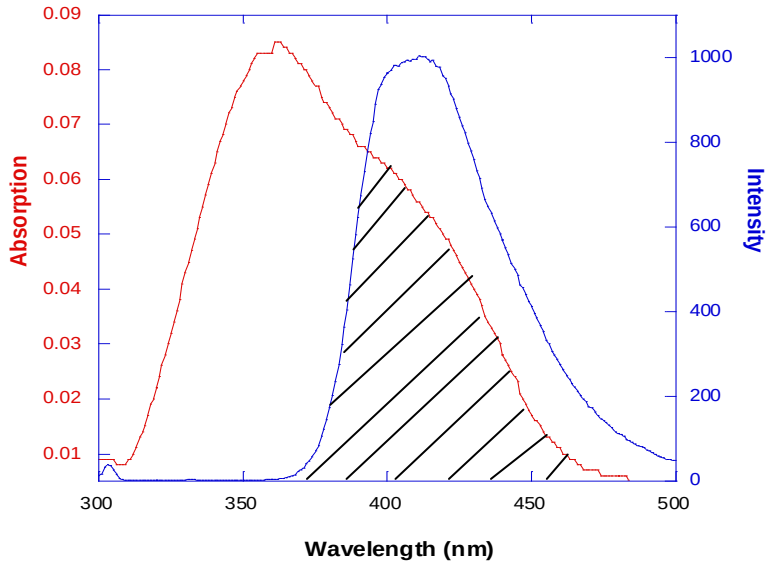


Figure S1: Spectral overlap of the absorption spectrum of picric acid (red line) with the emission spectrum of compound **3** (blue line).

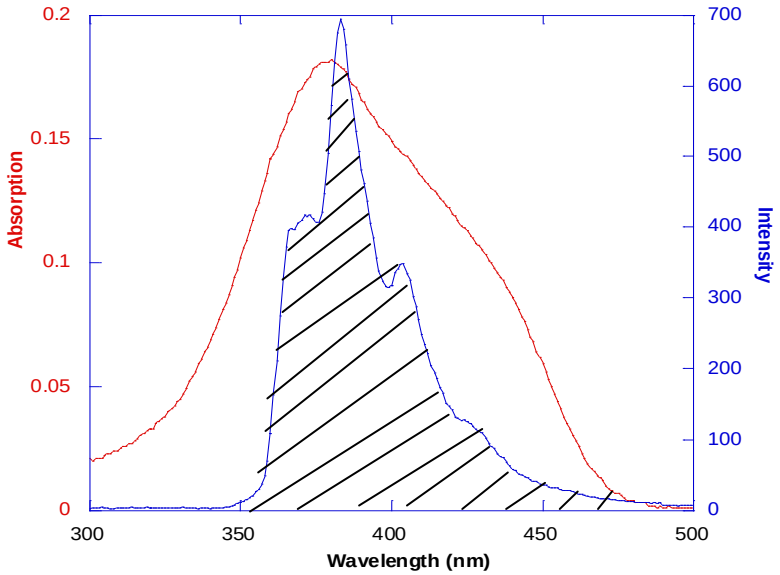
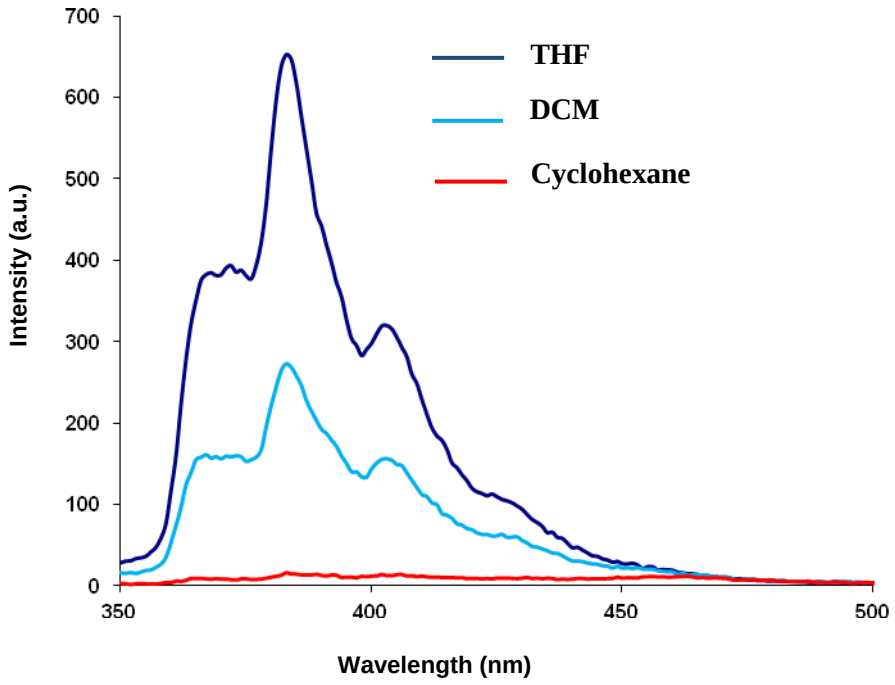


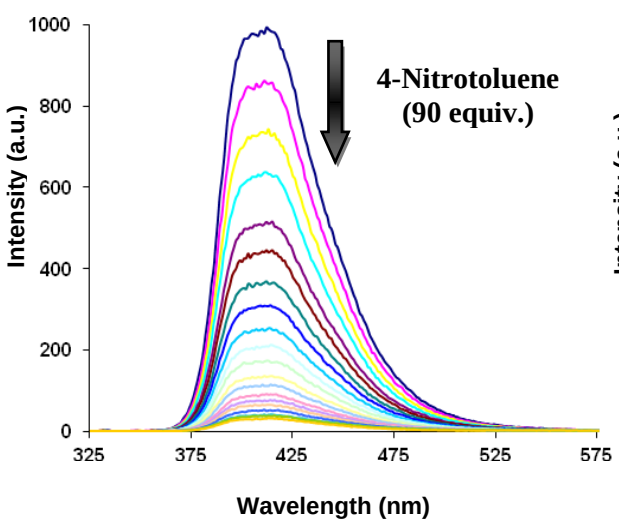
Figure S2: Spectral overlap of the absorption spectrum of picric acid (red line) with the emission spectrum of compound **5** (blue line)

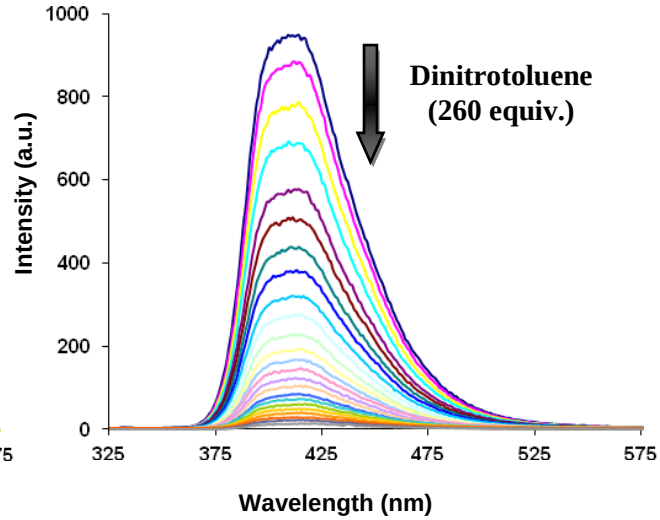
This journal is © The Royal Society of Chemistry 2012

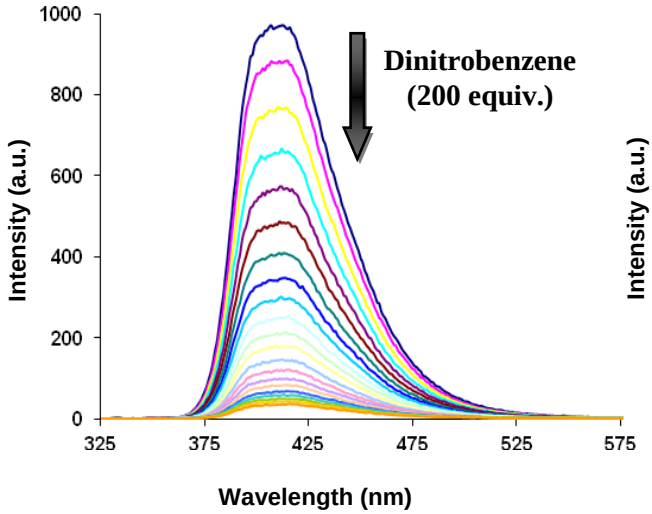
Fluorescence spectra of compound 5 in different solvents

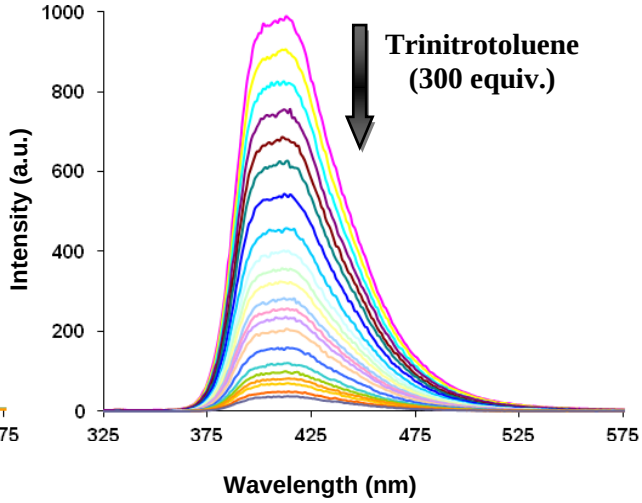


Fluorescence response of derivative 3 with other nitroaromatic derivatives

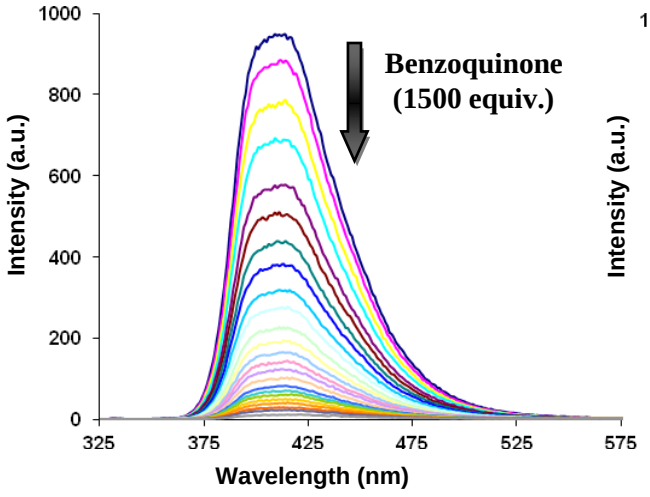


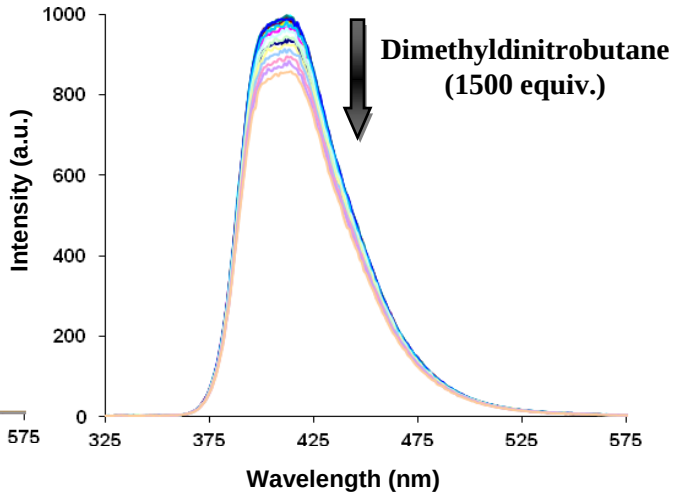


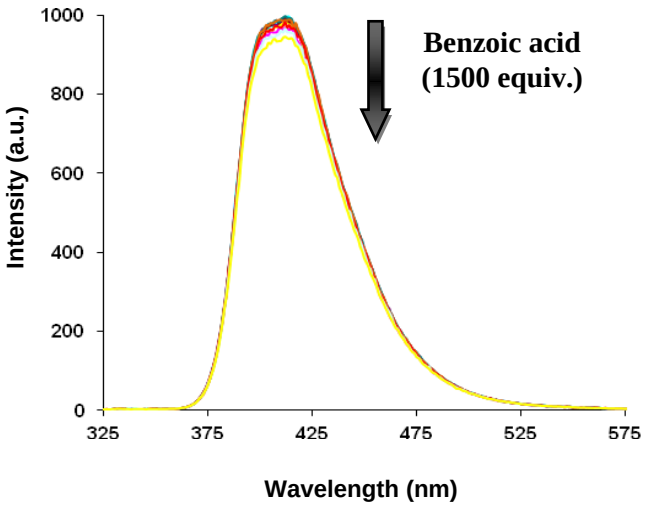




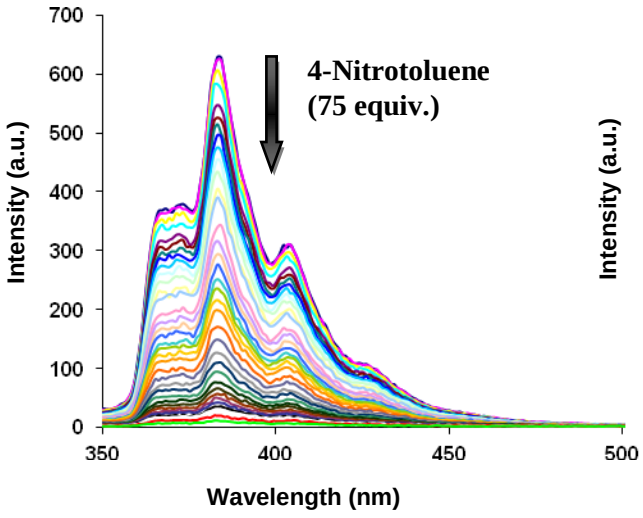
Fluorescence response of derivative 3 with other nitroaromatic derivatives

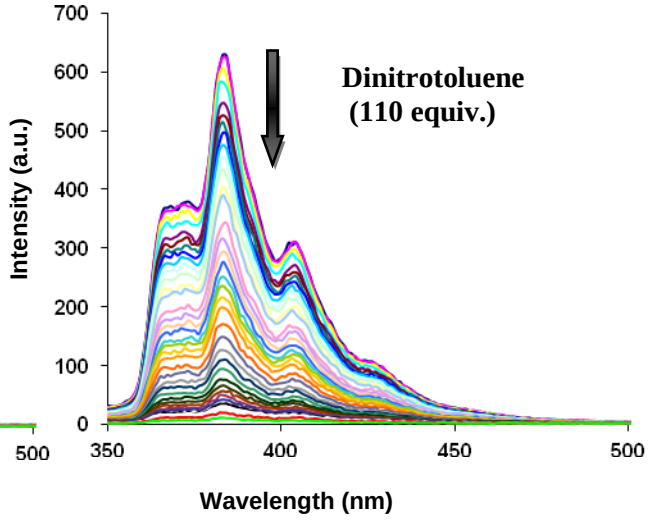


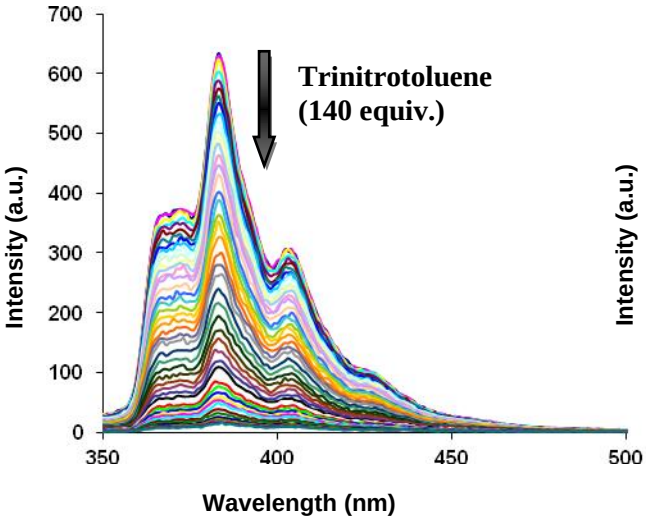


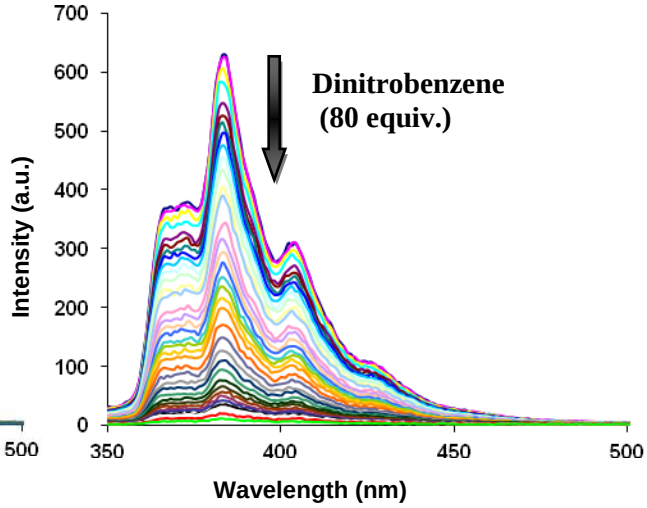


Fluorescence response of derivative 5 with other nitroaromatic derivatives

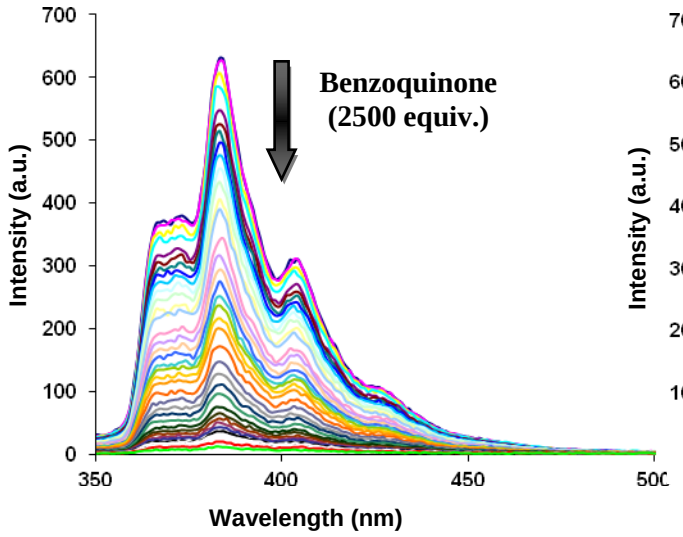


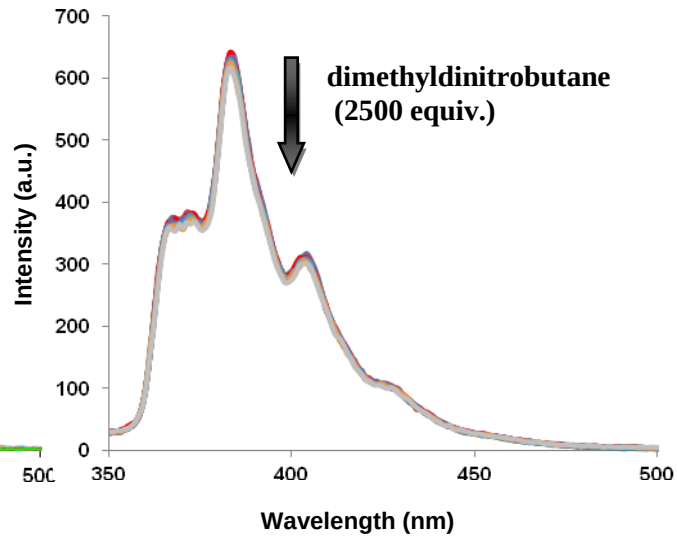


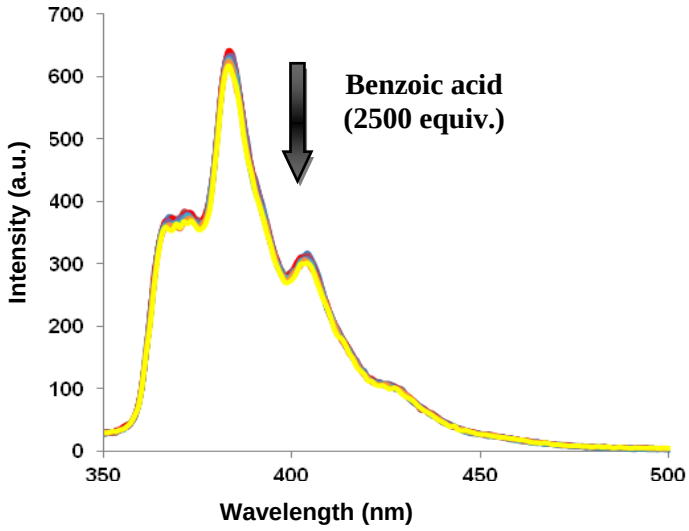




Fluorescence response of derivative 5 with other nitroaromatic derivatives







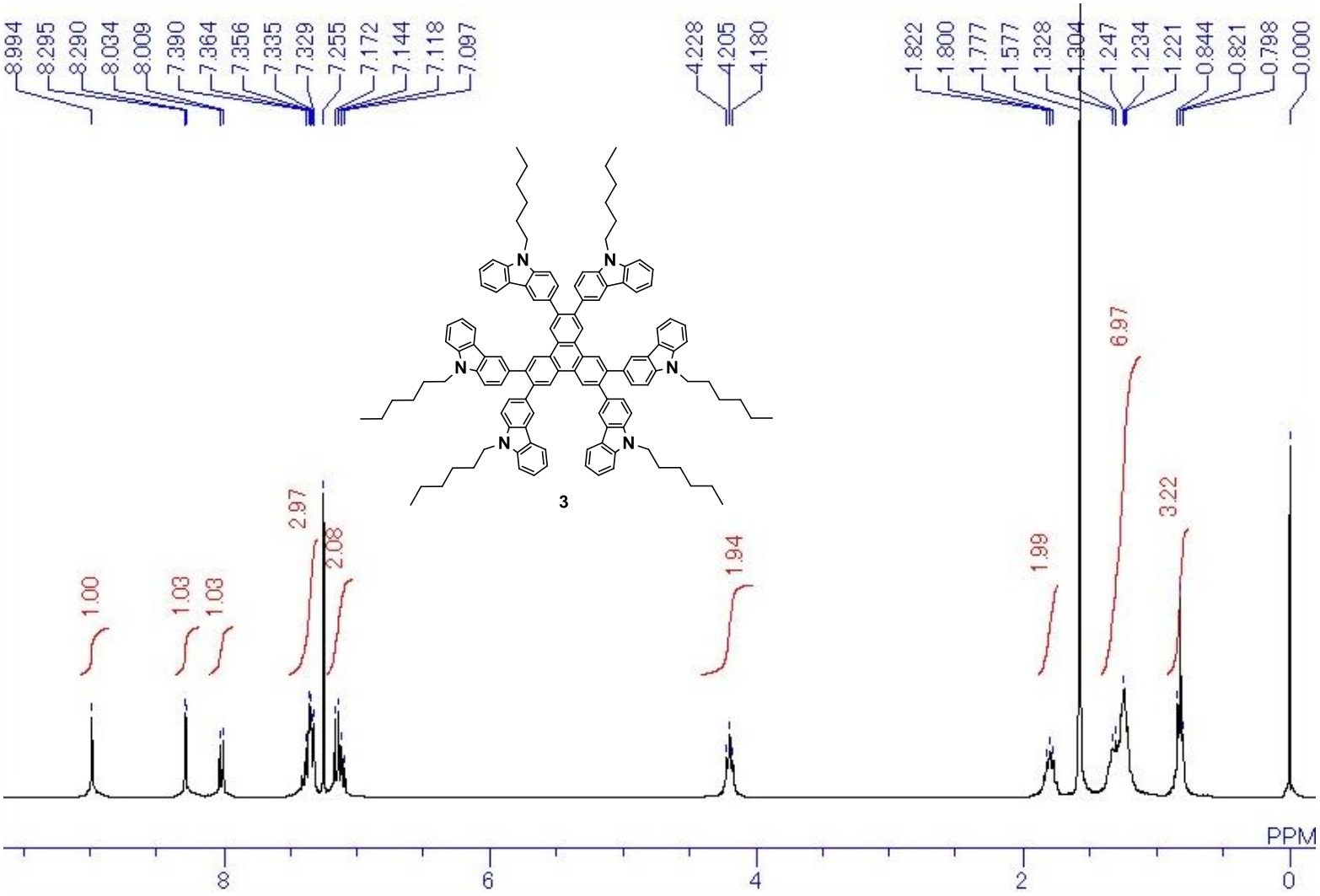
This journal is © The Royal Society of Chemistry 2012

Calculated Stern-Volmer constant for compounds 3 and 5 with various nitroaromatic derivatives

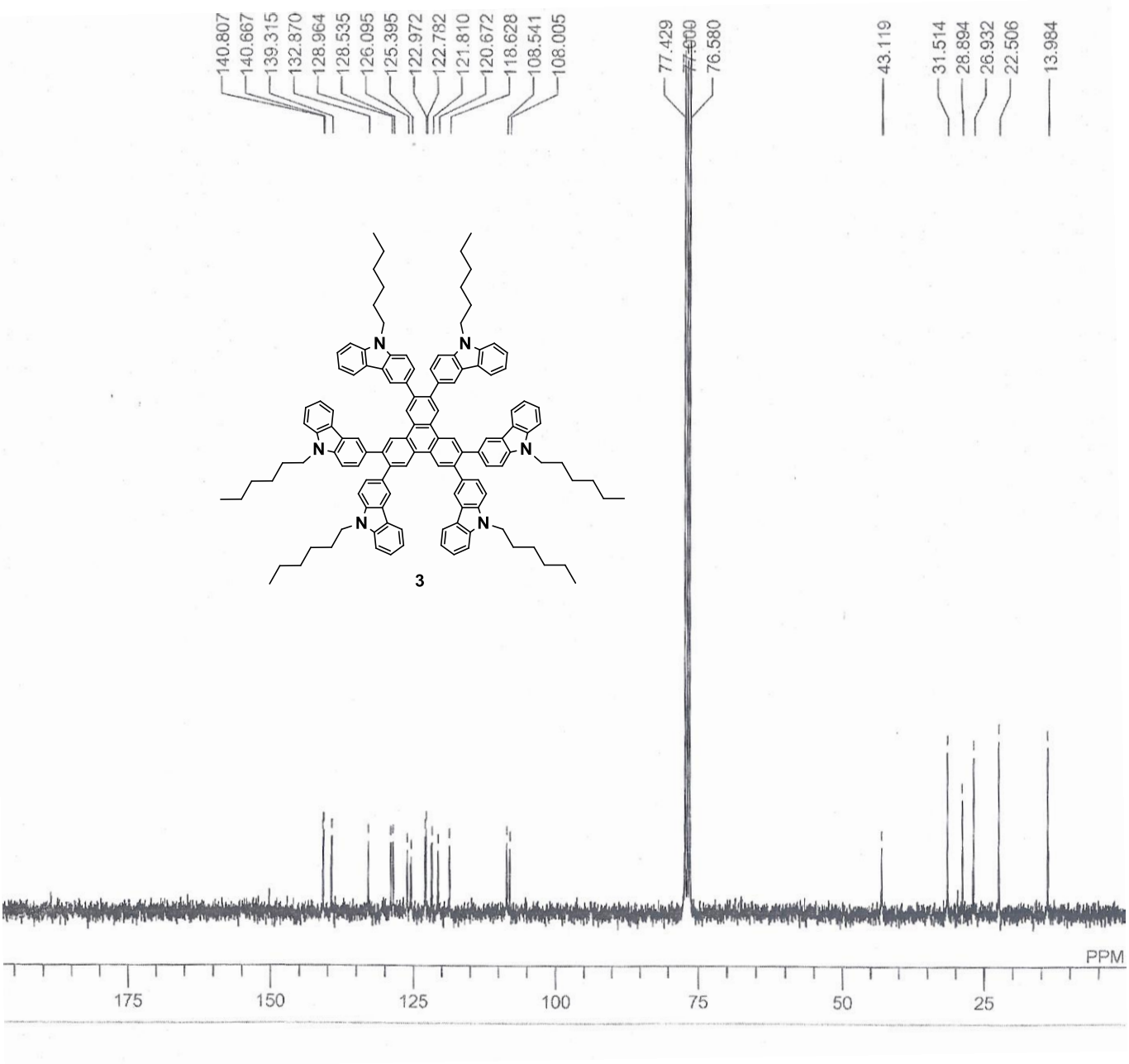
Calculated Ksv for Compound	PA	4-NT	DNT	TNT	DNB	NB
3	2.91×10^5 M^{-1}	1.85×10^4 M^{-1}	3.41×10^3 M^{-1}	2.4×10^3 M^{-1}	4.02×10^3 M^{-1}	1.81×10^3 M^{-1}
5	2.93×10^5 M^{-1}	1.95×10^4 M^{-1}	2.20×10^4 M^{-1}	8.29×10^3 M^{-1}	1.92×10^4 M^{-1}	1.32×10^4 M^{-1}

Table 2: Calculated Stern-Volmer constants for compounds **3** and **5** with various nitroaromatics

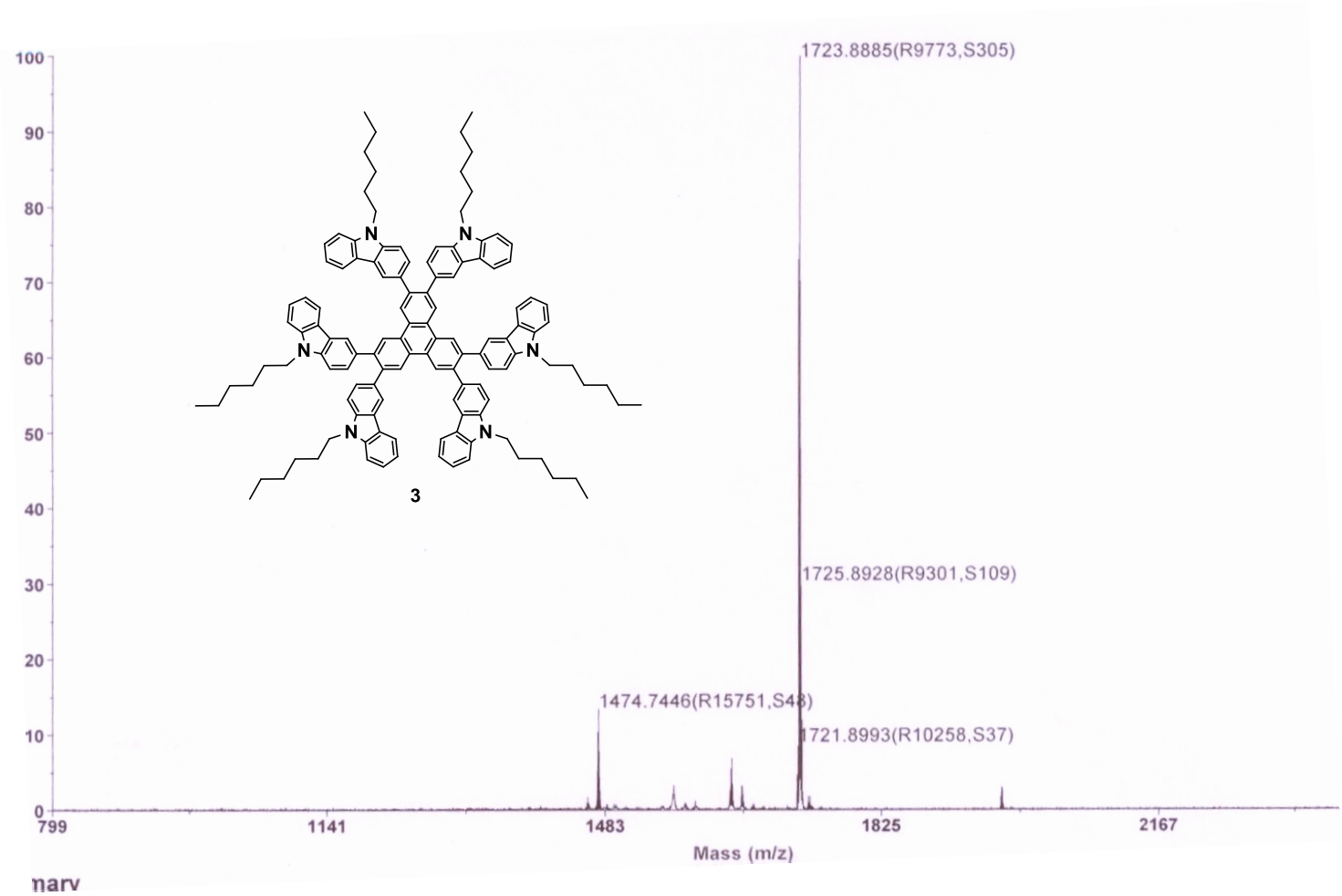
^{1}H NMR of compound 3



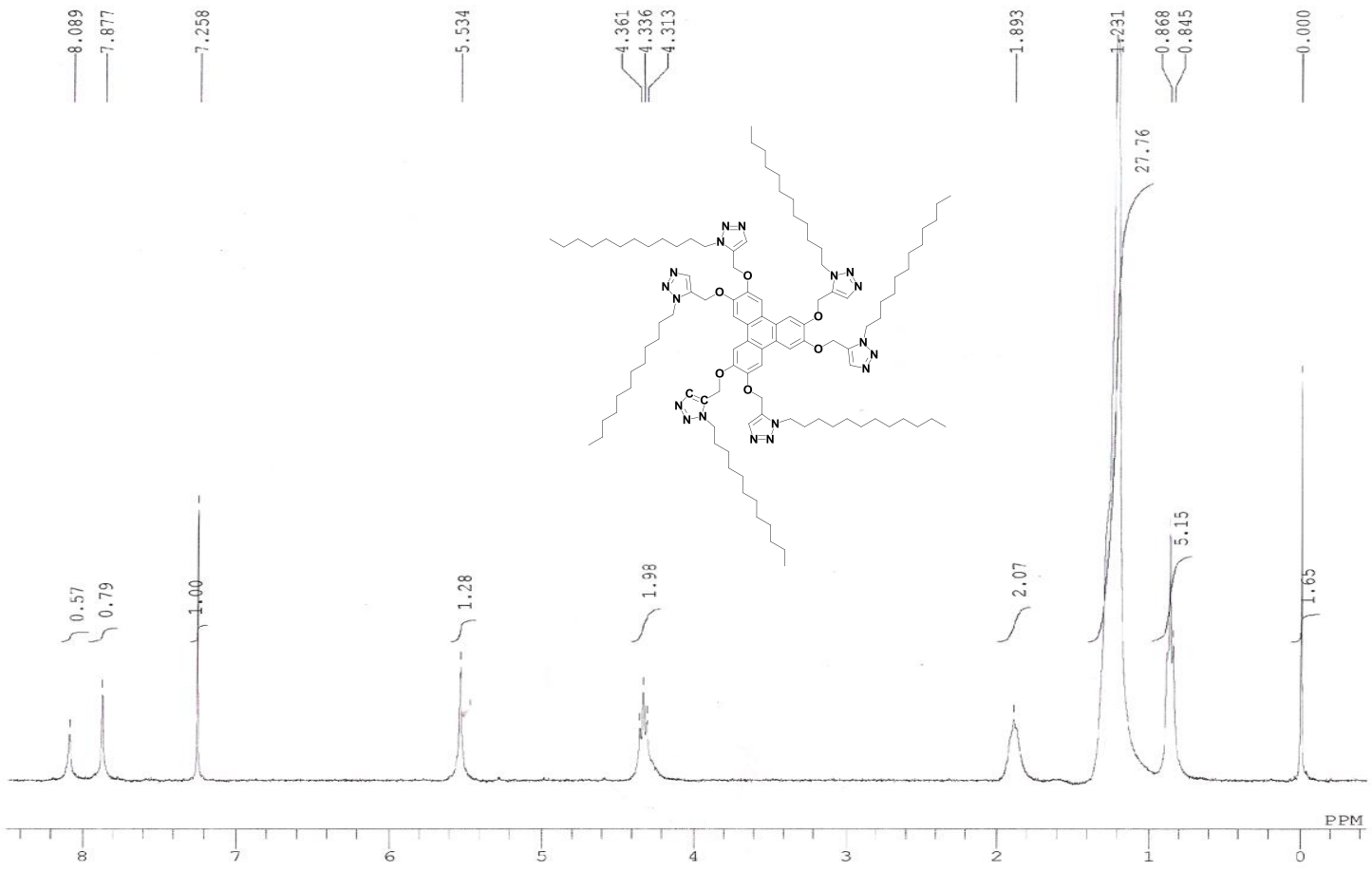
^{13}C NMR of compound 3



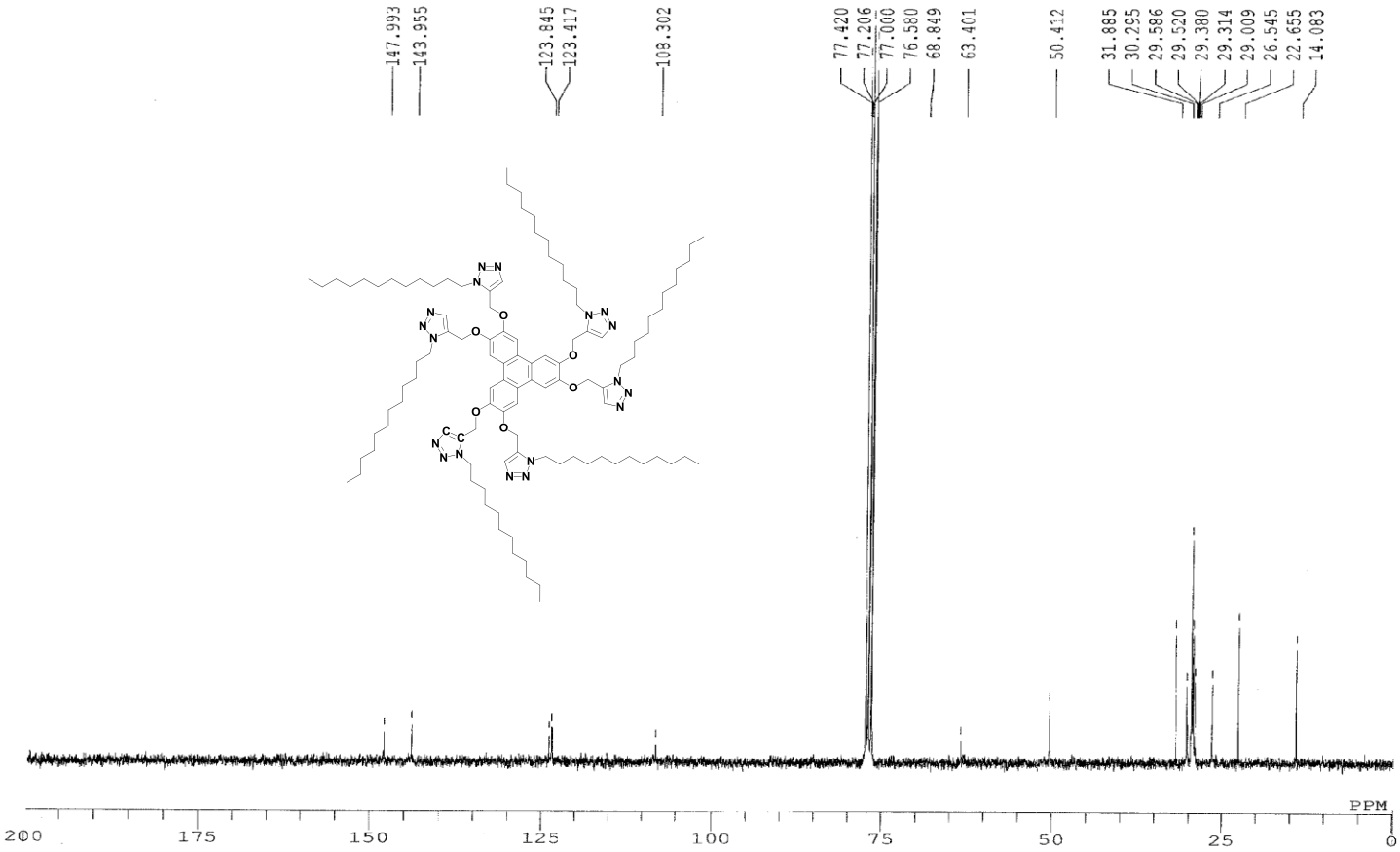
MALDI-TOF Mass Spectrum of compound 3.



^{1}H NMR spectrum of Compound 5



^{13}C NMR spectrum of compound 5



Mass Spectrum of compound 5

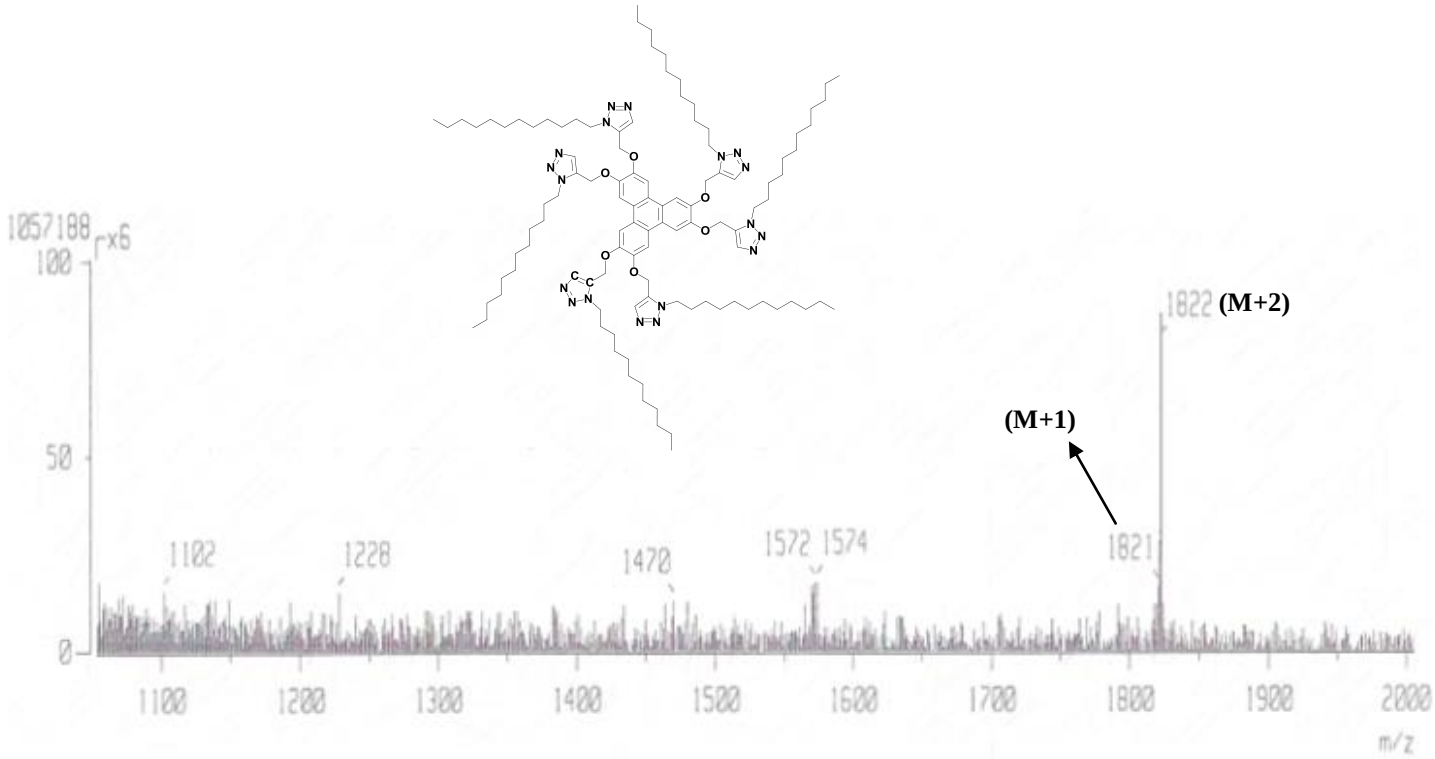


Table: 1 Comparison of derivative 5 with previous reports

S.No.	Reference	Detection limit	Calculated Stern-Volmer constant with PA	Contact mode detection of explosives with test strips.
1.	Derivative 5	50 nM	2.93×10^{5} M^{-1} for 5	YES
2	*Dalton Trans.*, 2011, 40, 12333	*	2.0×10^{4} M^{-1} and 5.0×10^{4} M^{-1}	No
3	*Dalton Trans.*, 2011, 40, 2257	*	3.1×10^{4} M^{-1} $1.9 \times 10^{4}M^{-1}$	No
4	*Chem. Commun.*, 2012, 48, 5007.	0.87 µM	9.9×10^{4} M^{-1}	No
5	*Polym. Chem.*, 2010, 1, 426	4.3 µM	1.5×10^{5} M^{-1}	No
6	*Sensors and Actuators B* 2012,161 251.	*	6.21×10^{3} M^{-1}	No

* No data available