Electronic Supplementary Information

Fluorescent Aggregates of Hetero-oligophenylene Derivative as "No Quenching" Probe for Detection of Picric Acid at Femtogram Level

Sharanjeet Kaur, Vandana Bhalla, Varun Vij, Manoj Kumar**

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

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S12 Selectivity bar graph of derivative **3** towards picric acid and Fluorescence lifetime decay profile of derivative **3** with the addition of picric acid.

S13 detection limit plot of derivative **3** and effect of PA on derivative 3 at different pH.

S14 Fluorescence emission spectra of derivative **5** with the addition of TFA and scanning electronic microscopic images of derivative **5**.

S15 – S17 ^{1}H NMR, ^{13}C NMR and mass spectrum of derivative **3**.

S18 – S20 ^{1}H NMR, ^{13}C NMR and mass spectrum of derivative **4**.

S21 Comparison of selectivity, K_{sv} and detection limit of derivative **3** towards picric acid with literature Reports.

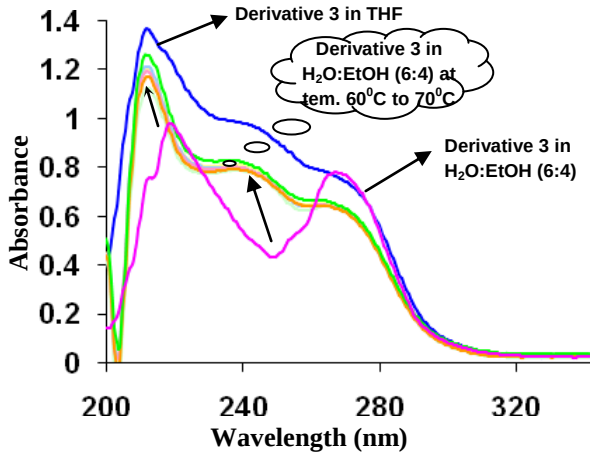

Figure S1: UV-vis absorption spectra of derivative **3** upon increasing temperature up to 70^0C in H_2O:EtOH (6:4).

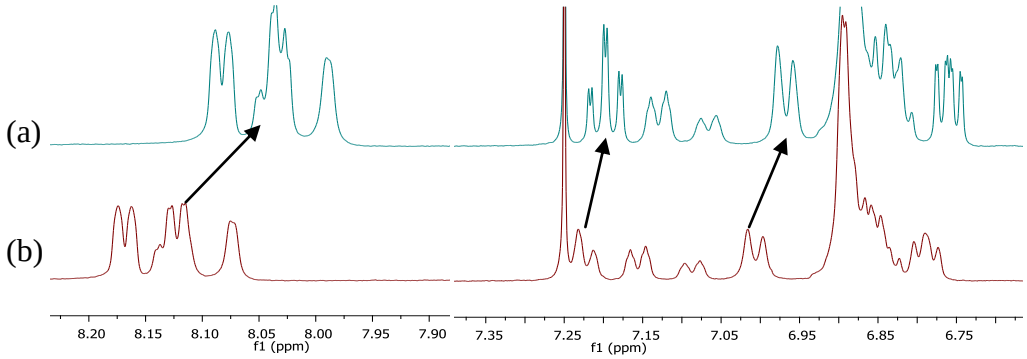

Figure S2: Concentration dependent ^{1}H NMR spectrum of derivative **3,** (a) 15 mg (b) 5 mg, each in 0.6 ml $CDCl_3$. NMR frequency is 300 MHz.

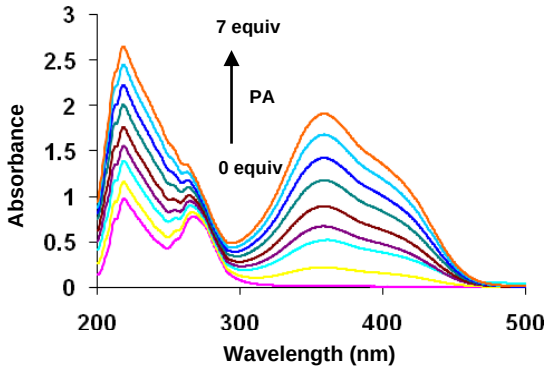

Figure S3. UV-vis absorption spectra of derivative **3** (50 μM) with the addition of picric acid in H_2O:EtOH (6:4) buffered with HEPES, pH = 7.

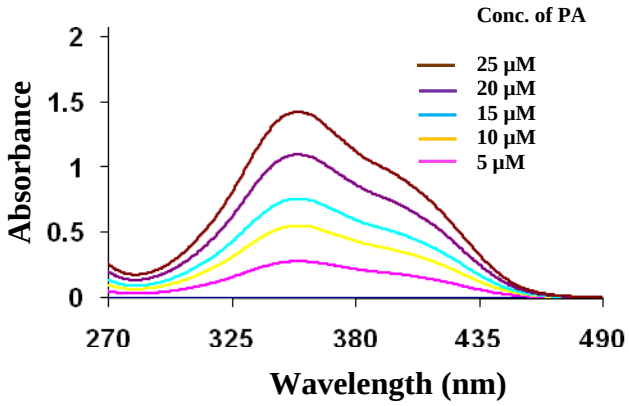

Figure S4. UV-vis absorption spectra of picric acid at different concentrations in H_2O:EtOH (6:4).

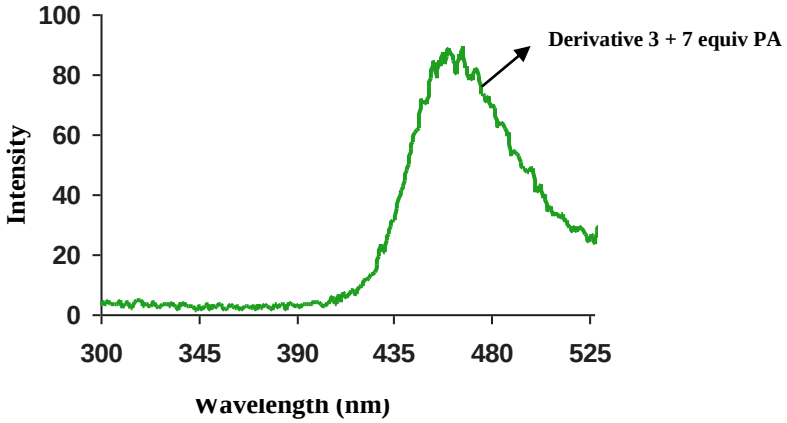

Figure S5. Fluorescence emission spectrum of derivative **3** (50 µM) after the addition of 350 µM of picric acid in H_2O:EtOH (6:4) buffered with HEPES, pH = 7.0; λ_{exc} = 273 nm.

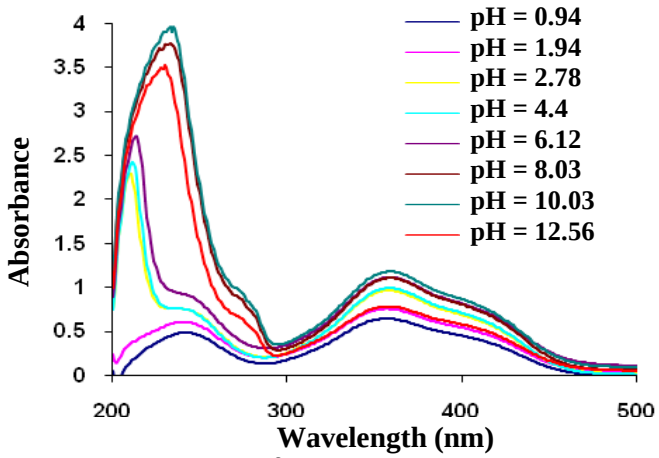

Figure S6. UV-VIS absorption spectra of picric acid at variable pH in H_2O:EtOH (6:4) buffered with HEPES.

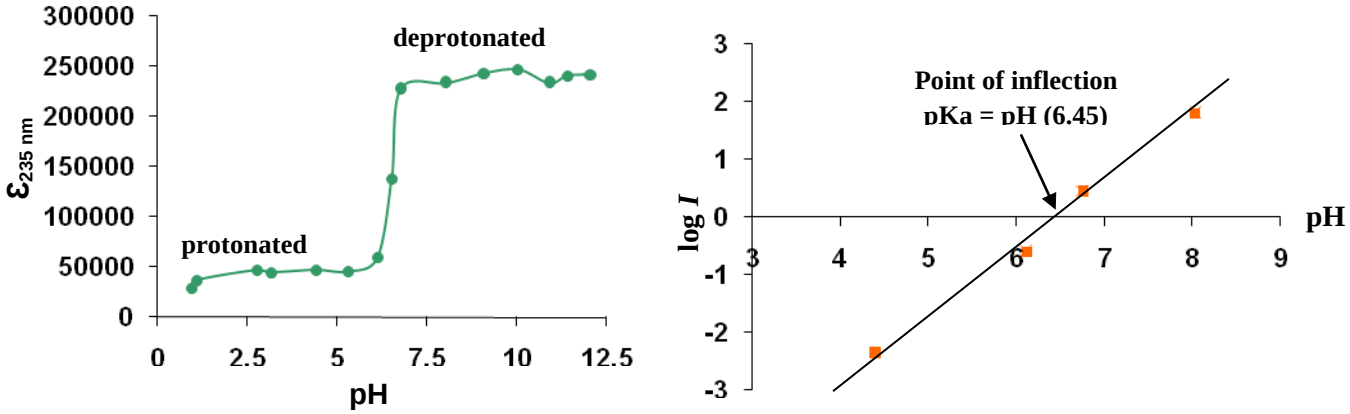

Figure S7. (A) The sigmoid curve **pH-ε$_{235}$** nm plot. **b)** The log *I*−pH plot for the protonation of PA.

Calculations:

Using equation: $pK_a = m.H_{1/2} + \log I$, where $I = (\varepsilon_{obs}-\varepsilon_{fb})/(\varepsilon_{ca}-\varepsilon_{obs})$

(at half protonation point log *I* will be equal to zero)

from graph, pKa = $H_{1/2}$ = 6.45

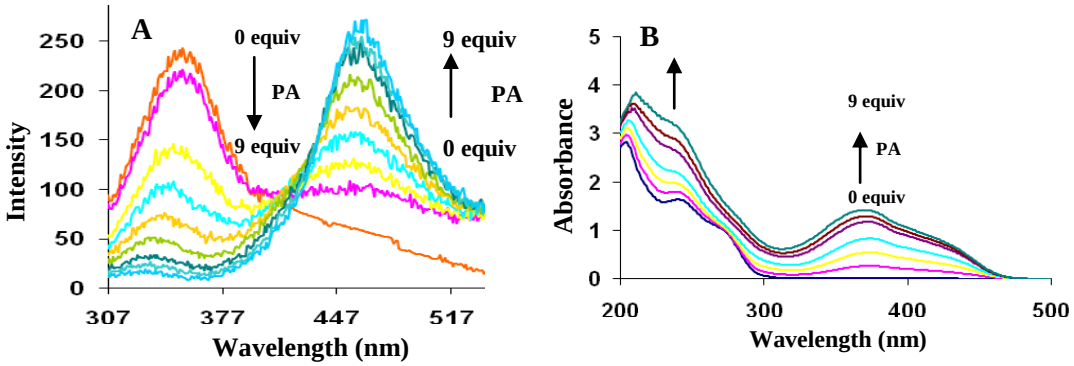

Figure S8. (A & B) Fluorescence and absorption spectra of derivative **3** (50 µM) with the addition of PA in pure acetonitrile.

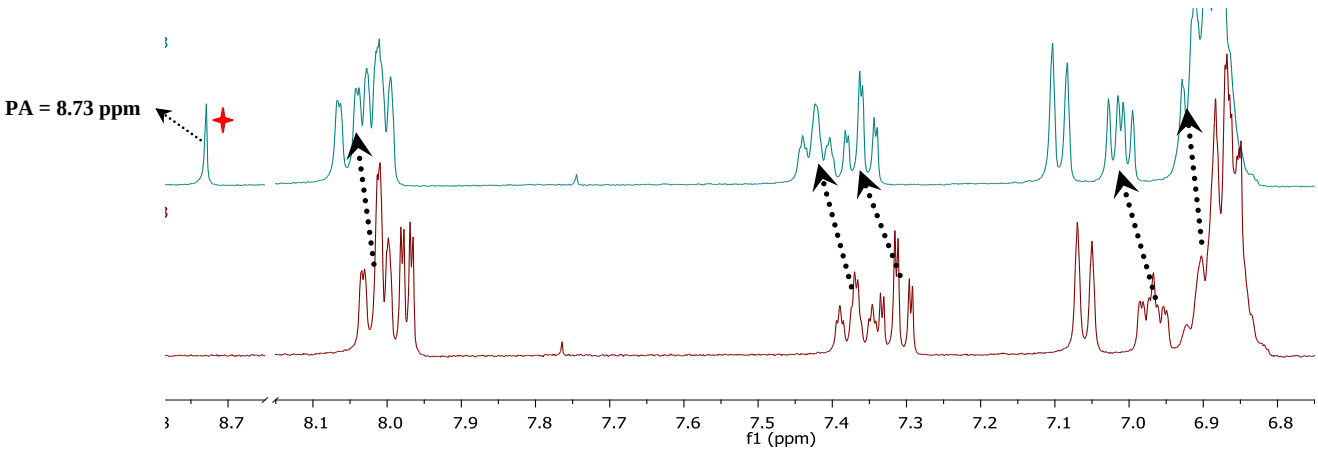

Figure S9: Overlay ^{1}H NMR spectra of derivative **3** and titration with PA respectively in D_2O:CD_3OD (6:4) showing downfield shift in the signals of aromatic protons with the average shift of 0.05 ppm.

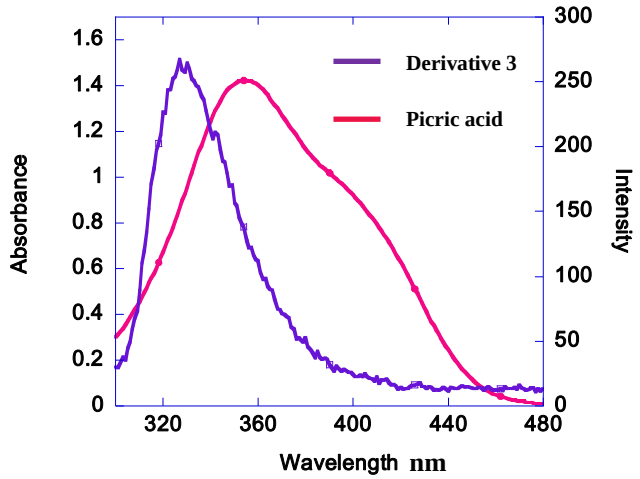

Figure S10. The spectral overlay of emission spectrum of derivative **3** with the absorption spectrum of picric acid in H_2O:EtOH (6:4).

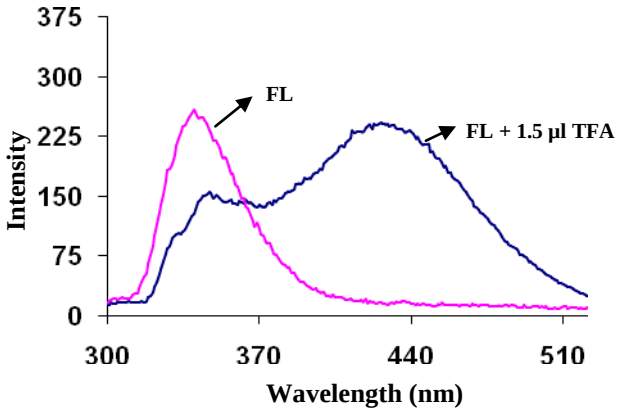

Figure S11. Fluorescence emission spectra of derivative **3** (50 µM) with the addition of 1.5 µl of 10^{-1}M TFA in H_2O:EtOH (6:4) buffered with HEPES, pH = 7.0; λ_{exc} = 273 nm.

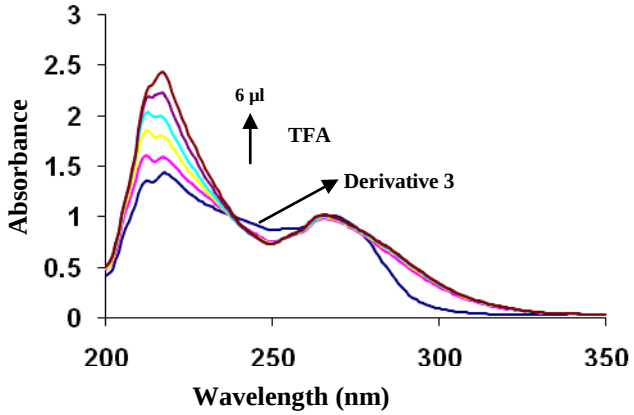

Figure S12. UV-vis absorption spectra of derivative **3** (50 µM) with the addition of 6 µl of 10^{-1}M TFA in H_2O:EtOH (6:4) buffered with HEPES, pH = 7.

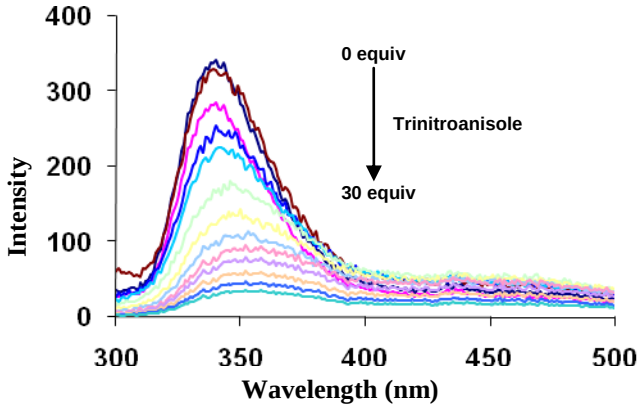

Figure S13. Fluorescence emission spectra of derivative **3** (50 µM) with the addition 1.5 mM of 2,4,6-trinitroanisole (protecting –OH of PA by $–OCH_3$) in H_2O:EtOH (6:4) buffered with HEPES, pH = 7.

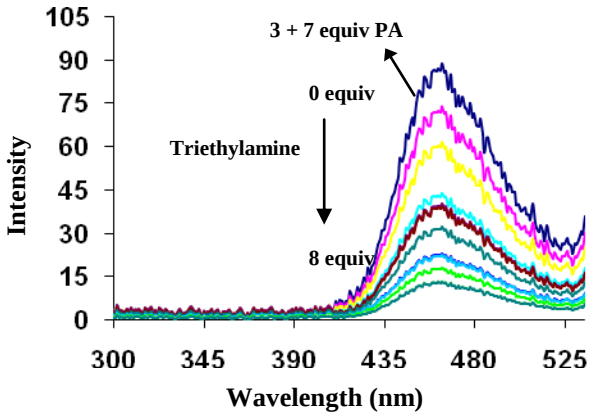

Figure S14. Fluorescence emission spectra of derivative **3 + 7equiv PA** upon the addition of 8 equiv of base triethylamine (10^{-2} M) in H_2O:EtOH (6:4) buffered with HEPES, pH = 7.0; λex = 273 nm.

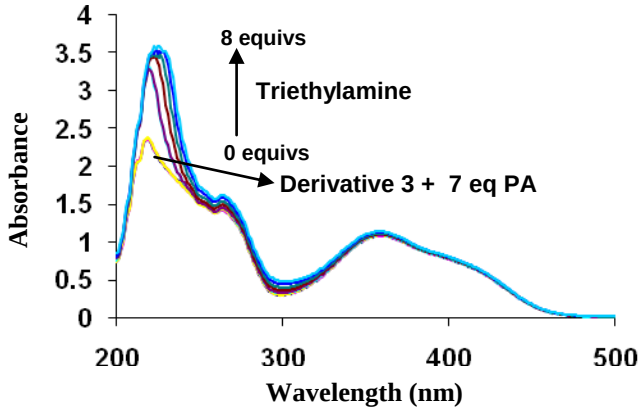

Figure S15. UV-vis absorption spectra of derivative **3 + PA** with the addition of 8 equivs of triethylamine (10^{-2} M) in H_2O:EtOH (6:4) buffered with HEPES, pH = 7.

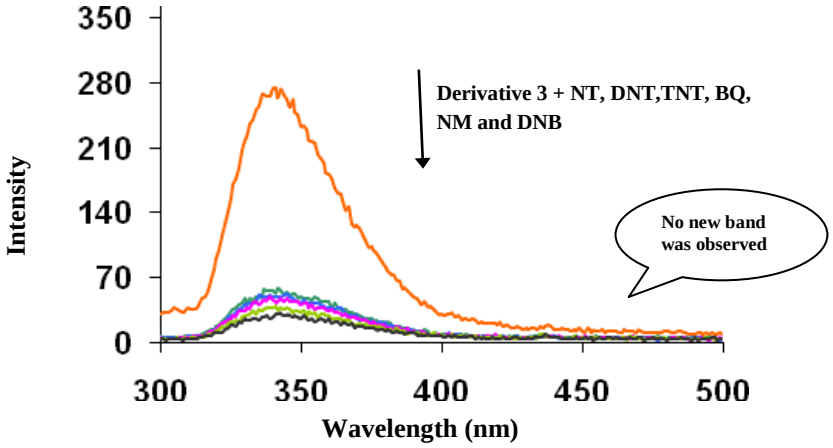

Figure S16. Fluorescence emission spectra of **3** with the addition of nitro derivatives such as NT(40 equiv),DNT(62 equiv), TNT (65 equiv), BQ (120 equiv), NM (135 equiv) and DNB (82 equiv) in H_2O:EtOH (6:4) buffered with HEPES, pH = 7.0; λ_{ex} = 273 nm.

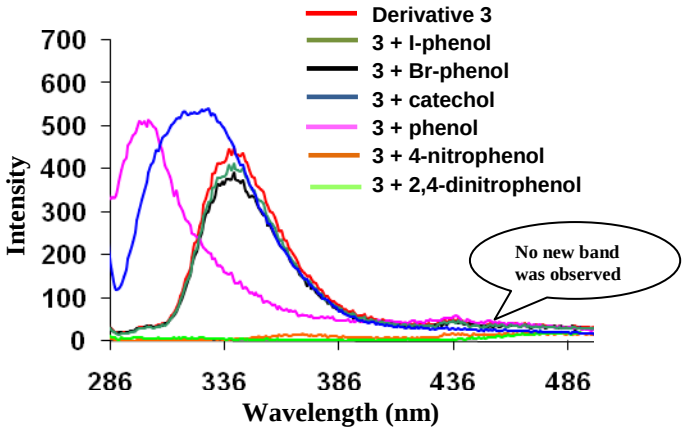

Figure S17. Fluorescence emission spectra of derivative **3** (50 μM) with the addition of 20 equiv. of phenol derivatives in H_2O:EtOH (6:4) buffered with HEPES, pH = 7.0; λ_{exc} = 273 nm.

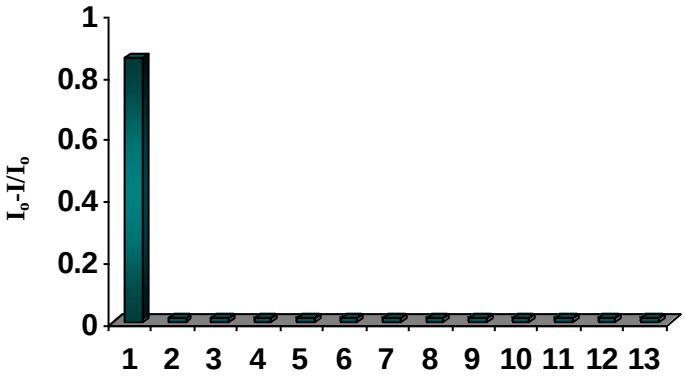

Figure S18. Selectivity graph of derivative **3** (50 µM) towards PA amongst nitro derivatives and phenol derivatives with respect to emission band at 460 nm, (1) PA, (2) TNT, (3) DNT, (4) DNB, (5) BQ, (6) NM, (7) NT, (8) phenol (9) catechol (10) I-phenol, (11) Br-phenol (12) DNP and (13) p-NP.

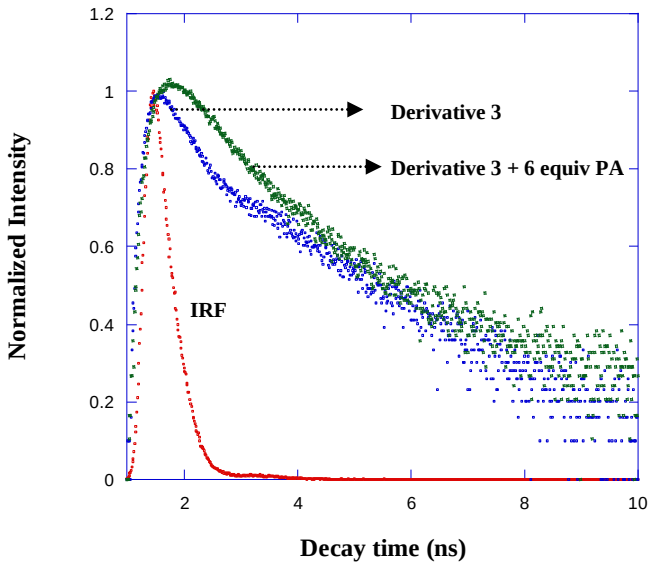

Figure S19. Fluorescence lifetime decay profile of derivative **3** (50 µM) with the addition of 300 µM of picric acid in H_2O:EtOH (6:4) buffered with HEPES, pH = 7.0. λex = 273 nm.

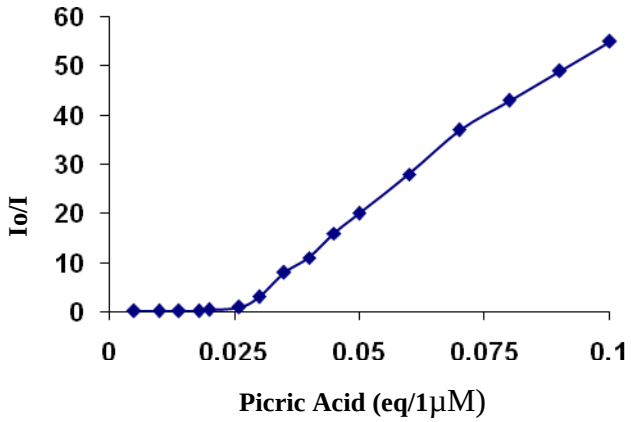

Figure S20. The detection limit plot of derivative **3** (1 μM) in H_2O:EtOH (6:4) with Picric Acid.

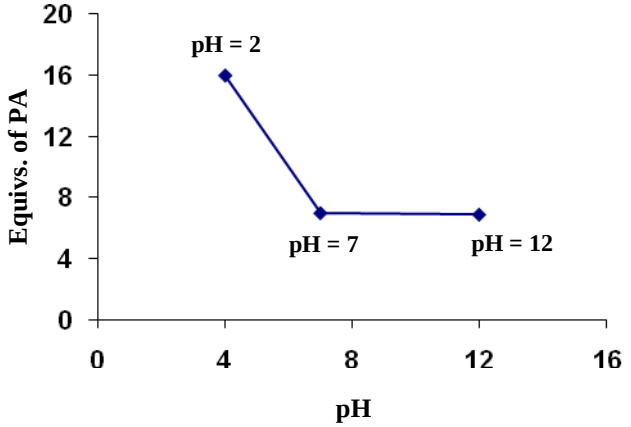

Figure S21. Effect of picric acid on derivative **3** (50 μM) at different pH scale.

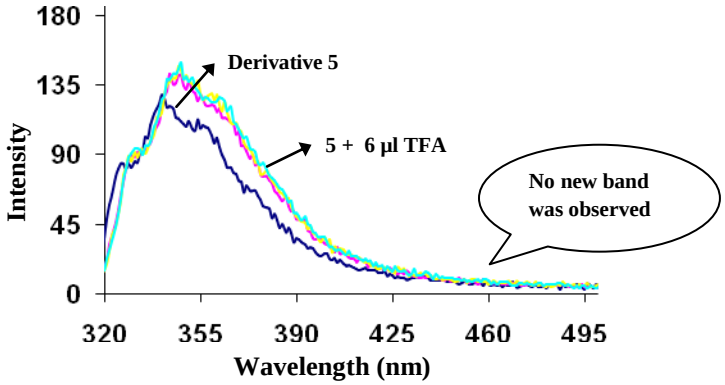

Figure S22. Fluorescence emission spectra of derivative **5** (5 µM) with the addition of 6 µl of 10^{-1}M TFA in H_2O:EtOH (6:4) buffered with HEPES pH = 7; λ_{ex} = 290 nm.

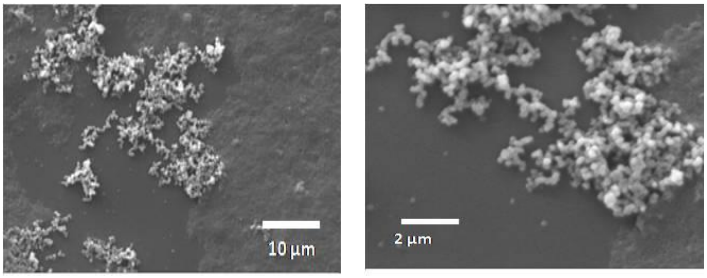

Figure S23. Scanning electron microscopic (SEM) images of aggregates of derivative **5** in H_2O:THF (8:2).

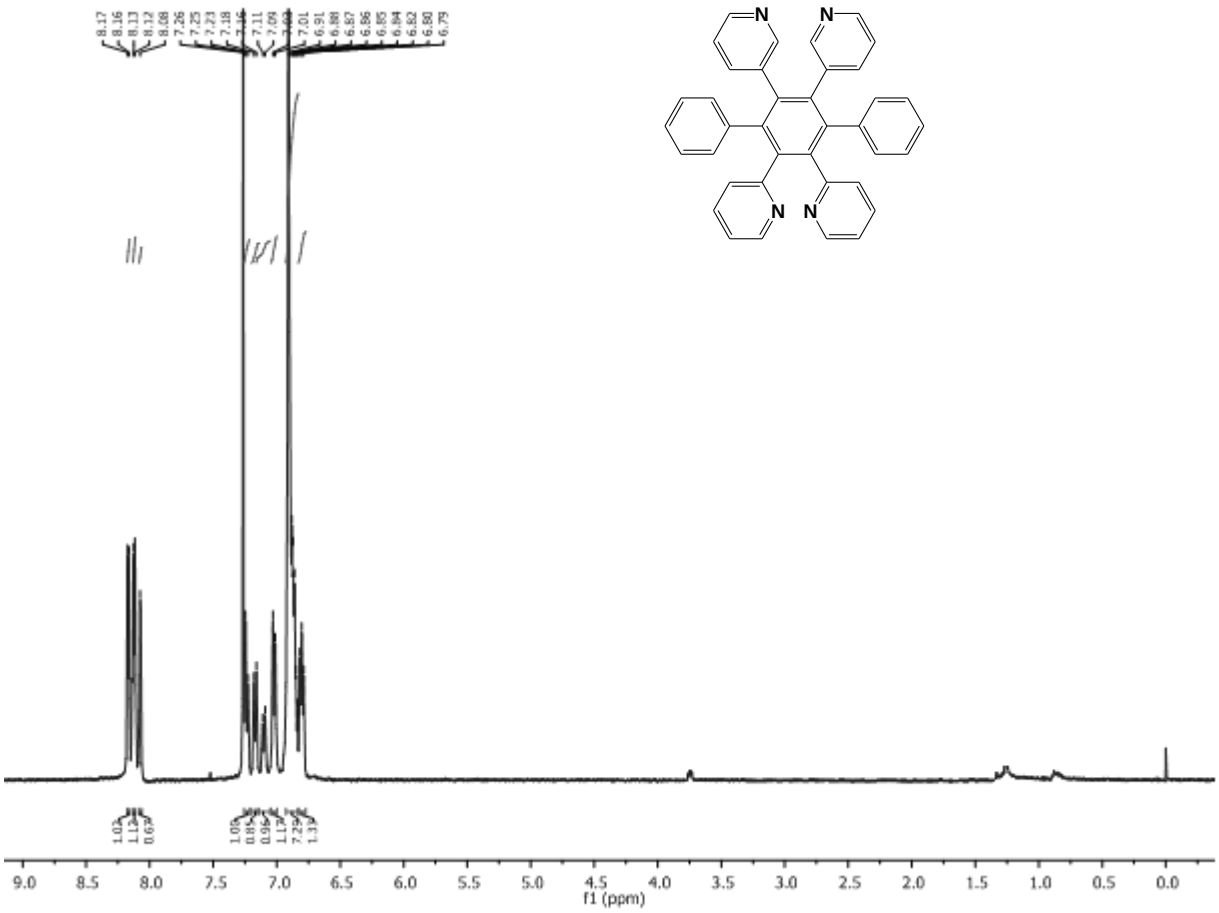

Figure S24. ^{1}H NMR spectrum of derivative **3** (400 MHz, $CDCl_3$).

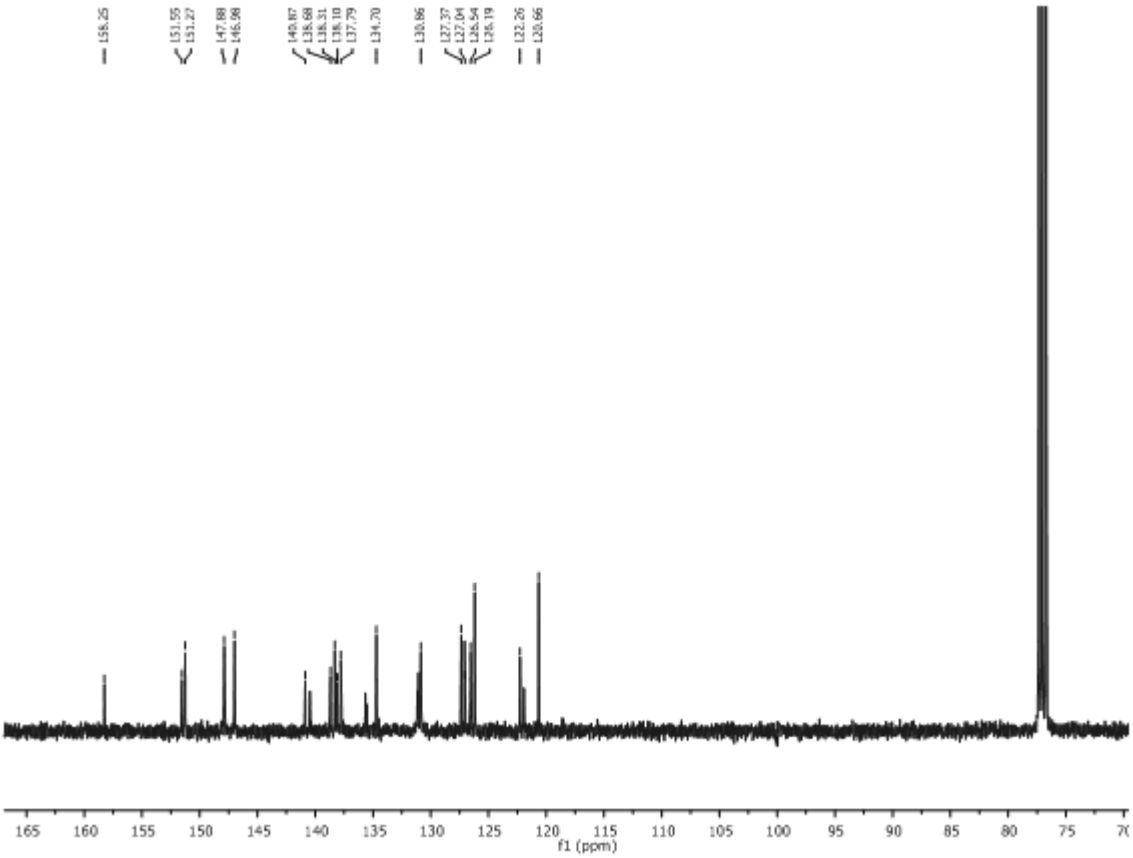

Figure S25 ^{13}C NMR spectrum of derivative **3** (100 MHz, $CDCl_3$).

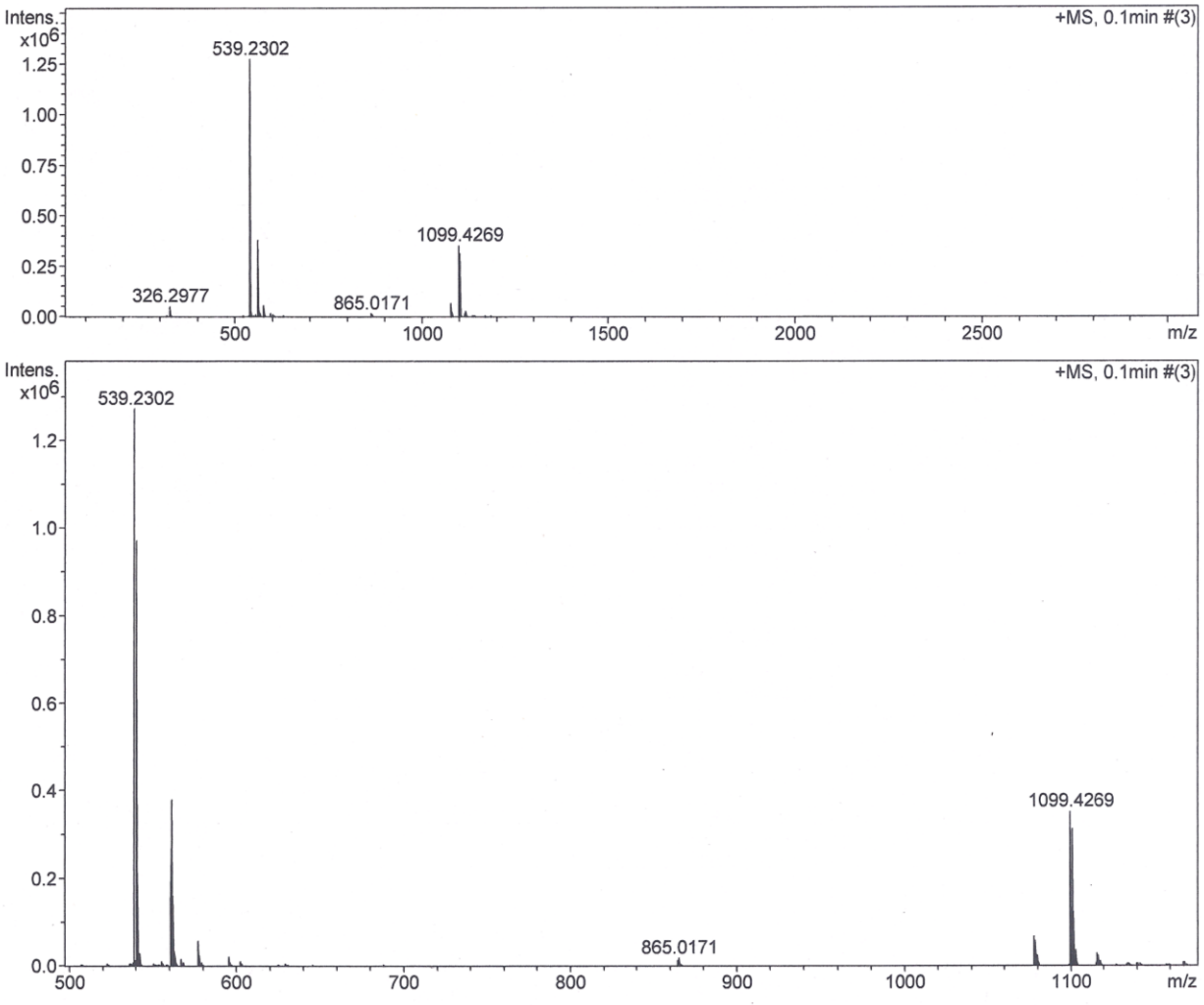

Figure S26 Mass spectrum of derivative **3.**

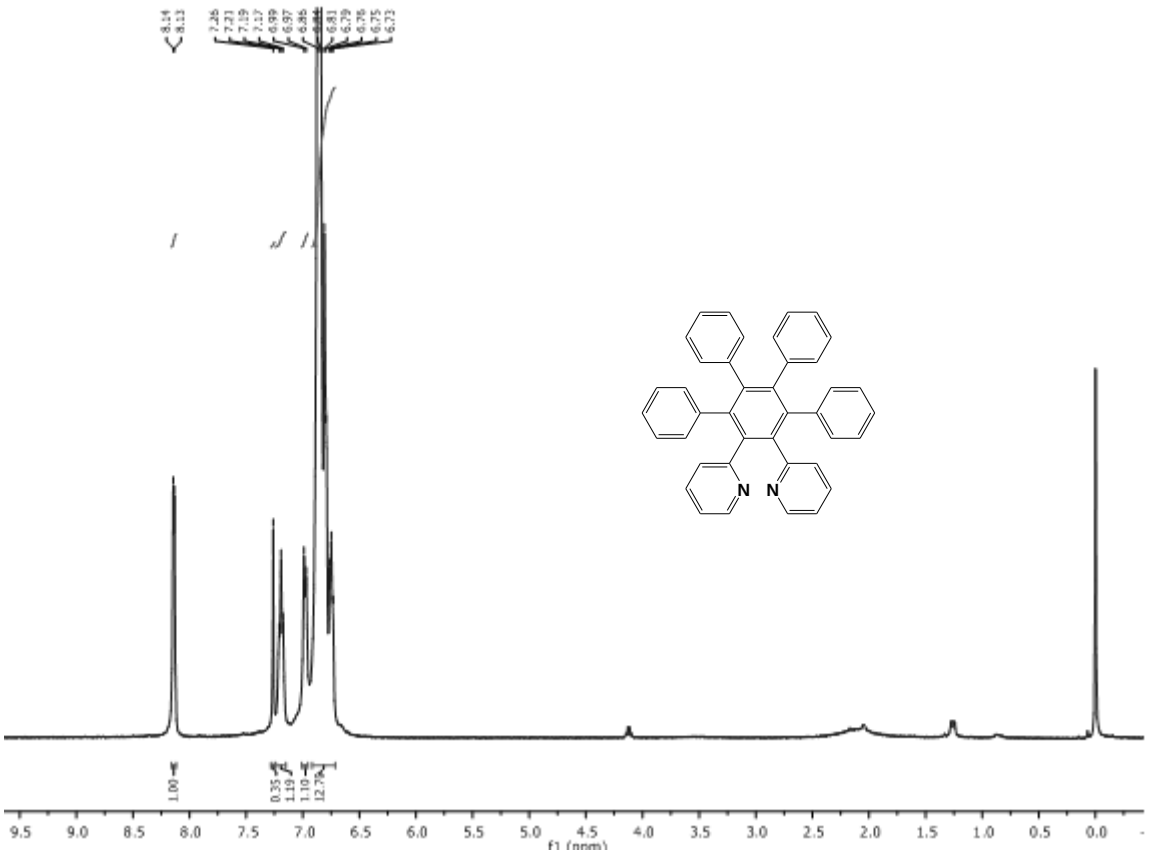

Figure S27 ^{1}H NMR spectrum of derivative **4** (400 MHz, $CDCl_3$).

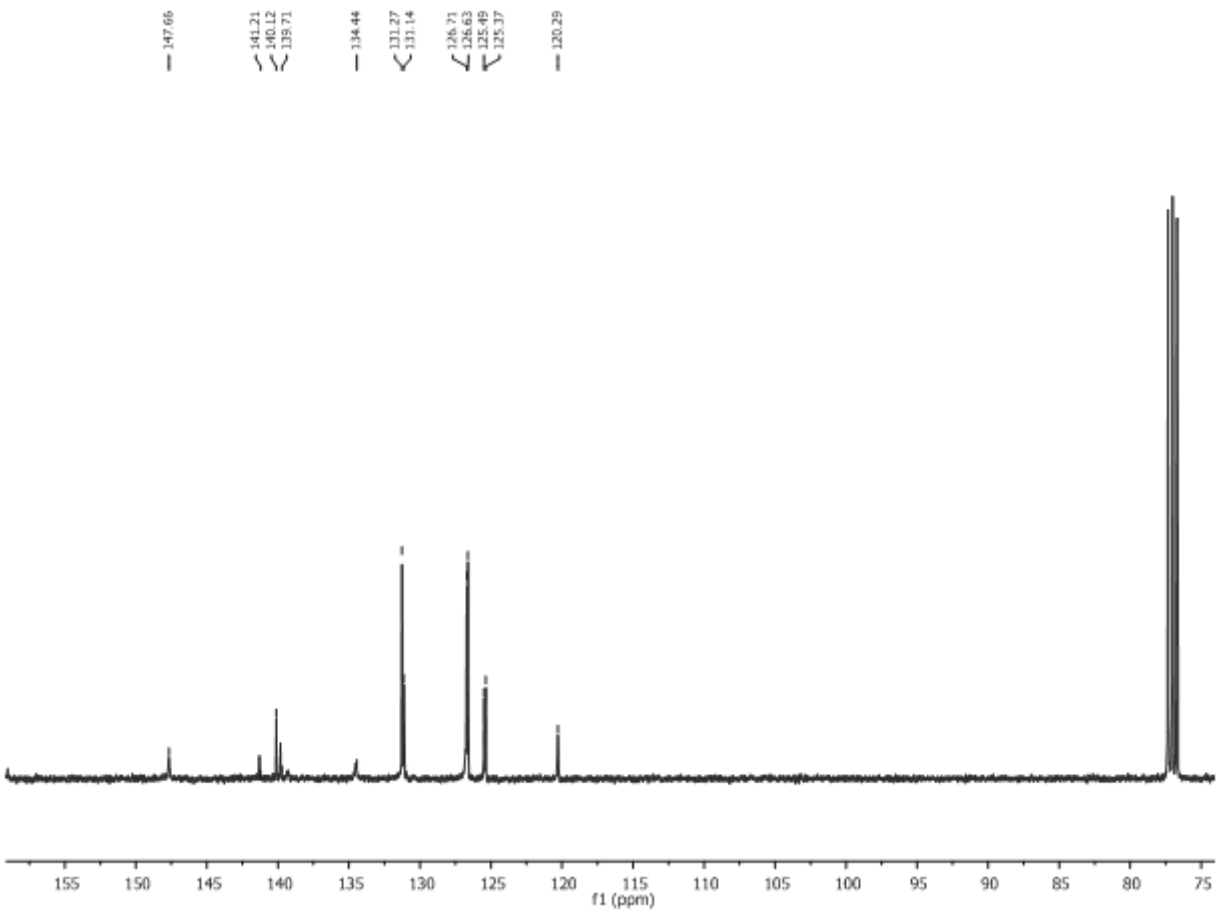

Figure S28[13]C NMR spectrum of compound **4** (100 MHz, $CDCl_3$).

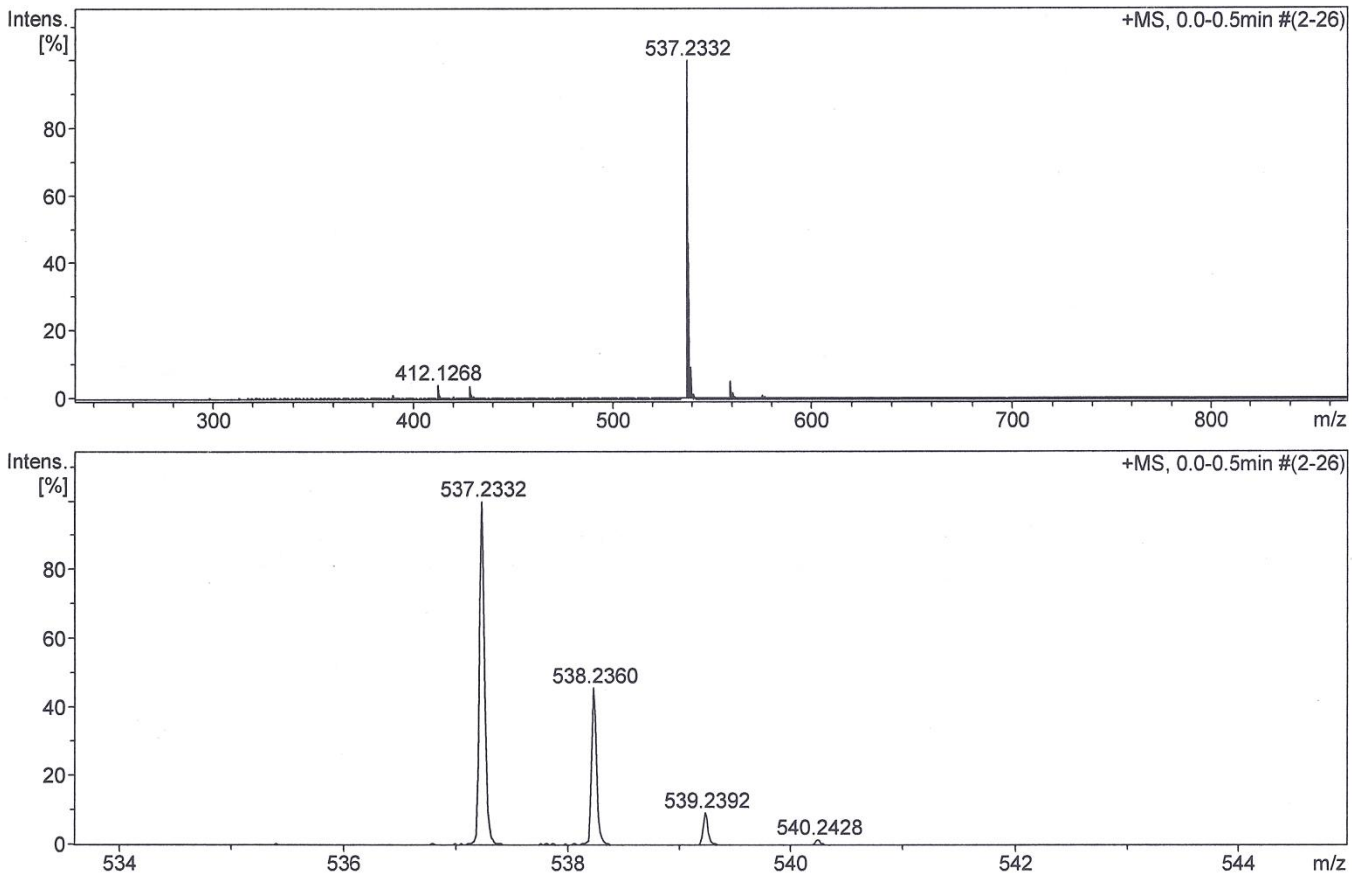

Figure S29. Mass spectrum of compound **4.**

Publication	Selectivity Towards PA	K_{SV} (M^{-1})	Detection limit	Response with PA
Present Manuscript	High	1.27 X 10^6	2.29 fg	Turn on
Angew. Chem. Int. Ed. **2013**, *52*, 2881	high	3.5 x 10^4	---------	Turn-off
Chem.Commun. **2012,** *48*, 5007	moderate	9.9 x 10^4	1.37 ng -13.7 ng	Turn-off
J. Mater. Chem. **2012**, *22*, 11574	moderate	3.04 x 10^4	0.15 ng	Turn-off
J. Org. Chem. **2013**, *78*, 1306	moderate	3.8 × 10^4 and 3.3 × 10^4	0.32 µg – 0.23 µg	Turn-off
J. Phys. Chem. C **2013**, *117*, 7236	low	2.405 × 10^5	1.15 fg/cm^2	Turn-off
J. Mater. Chem. A, **2013**, *1*, 8745	high	3.14 x 10^4	55.64 ng	Turn-off
J. Mater.Chem. **2008**, *18*, 3143	Low	-	1pg	Turn on
Chem. Commun. **2013**, *49*, 4764	high	-	47.49 ng	Turn on

Table S1. Comparison of selectivity, K_{sv} and detection limit of derivative **3** towards PA with literature reports.