

Electronic Supplementary Information for

## Phenothiazine and semi-cyanine based colorimetric and fluorescent probes for detection of sulfites in solutions and in living cells

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## I. Photophysical and sensing properties of four probes

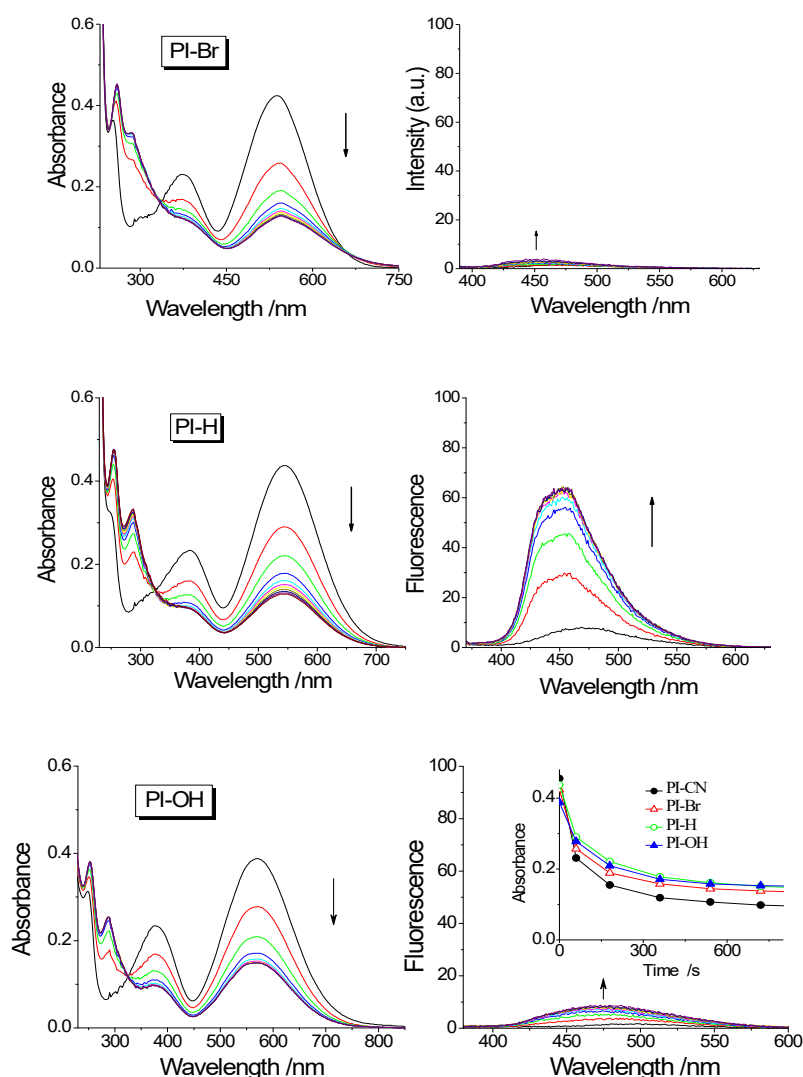
Table S1. Photophysical and sensing properties of four probes

probe	$\lambda_{\text{abs}}(\epsilon)^a$ /nm	$(\epsilon)/(\text{L}\cdot\text{mol}^{-1}\cdot\text{cm}^{-1})^a$	$\lambda_{\text{em}}^b$ /nm	LOD
PI-CN	518	30320	499	22 nM
PI-Br	537	28320	452	28 nM
PI-H	545	29180	455	27 nM
PI-OH	568	25846	470	37 nM

<sup>a</sup> absorption maxima (nm) and molar absorption coefficients

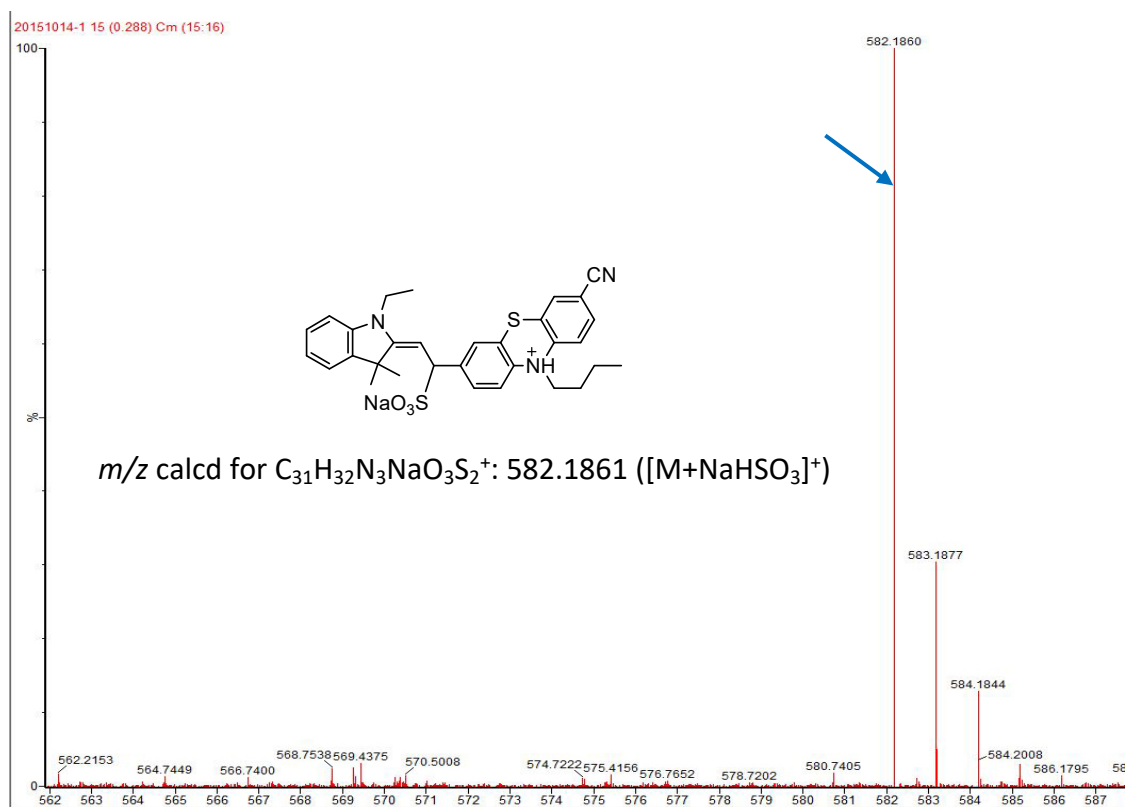
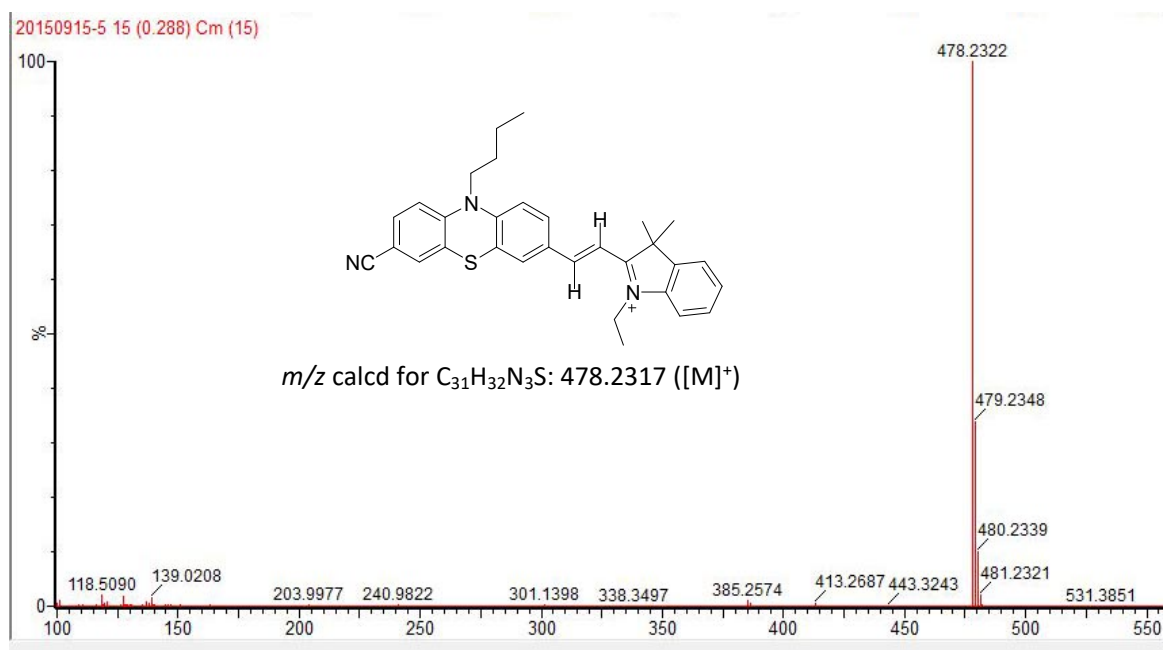
<sup>b</sup> emission maxima (nm)

## II. Spectral response of probes to $\text{HSO}_3^-/\text{SO}_3^{2-}$



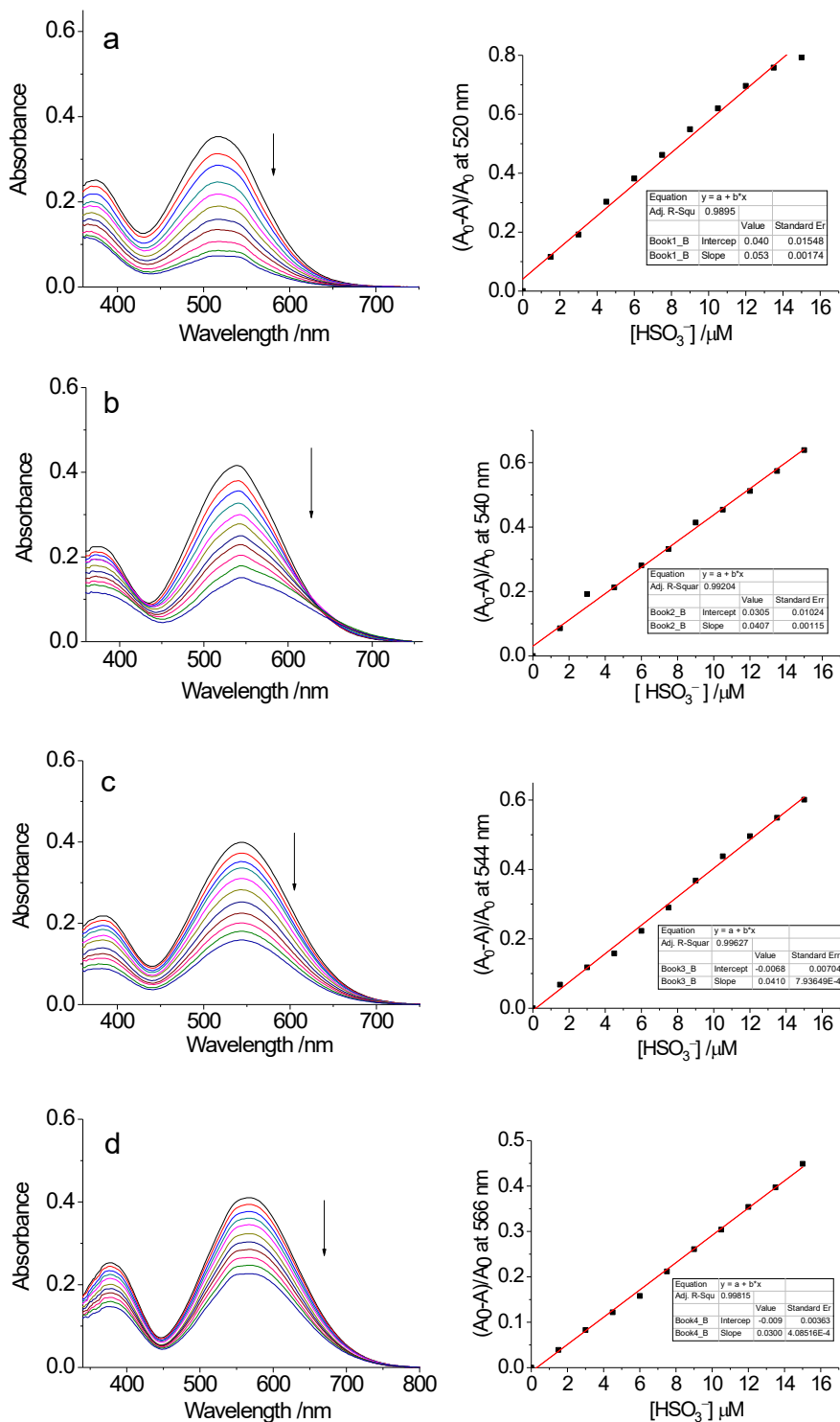
**Fig. S1** Time-dependent UV/vis absorption (left) and fluorescence spectra (right) of probes (15  $\mu\text{M}$ ) in EtOH/PBS (v/v1:3, pH 7.4) in the presence of  $\text{HSO}_3^-$  (1.0 equiv.) recorded at 0-30 min, excitation at 320 nm. Inset of PI-OH: plots of absorption maxima of probes vs time in the presence of  $\text{HSO}_3^-$  incubation for 15 min

### III. Mass spectra of PI-CN without and with NaHSO<sub>3</sub>



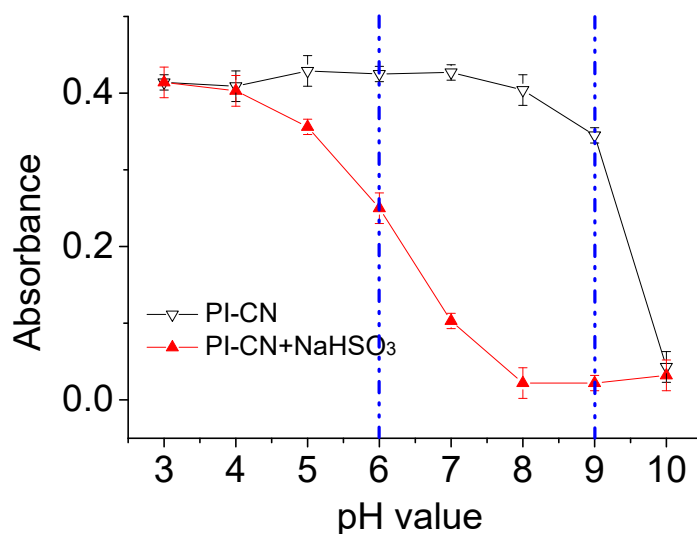
**Fig. S2** High-resolution MS of probe PI-CN (upper) and the mixture of PI-CN+NaHSO<sub>3</sub> (bottom).

## IV. Measurements of detection limits

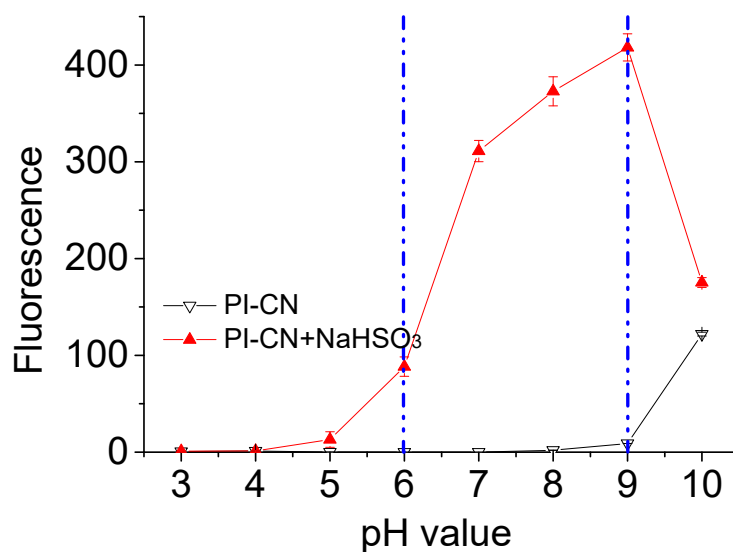


**Figure S3.** UV/vis absorption PI-CN (a), PI-Br (b), PI-H (c) and PI-OH (d) in EtOH/PBS (v/v1:3, pH 7.4) with titration of various amounts of  $\text{HSO}_3^-$  (0–15  $\mu\text{M}$ ), and the corresponding linear correlation between the absorbance toward concentrations of  $\text{HSO}_3^-$ .

V. pH effects on optical response of PI-CN to  $\text{HSO}_3^-/\text{SO}_3^{2-}$



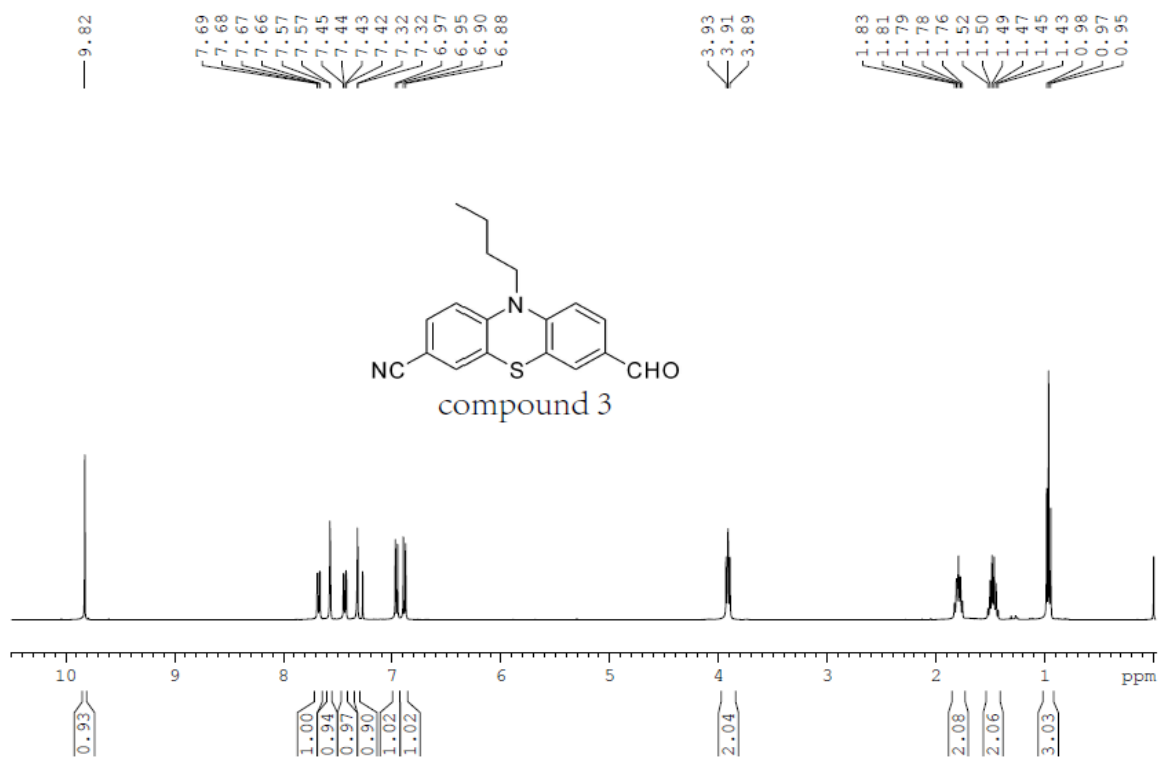
**Figure S4a.** Plots of absorbance at 520 nm to pH values for 15 $\mu\text{M}$  PI-CN solutions (EtOH/PBS v/v 1:3) before (black) and after (red) the addition of 15  $\mu\text{M}$   $\text{HSO}_3^-$ .



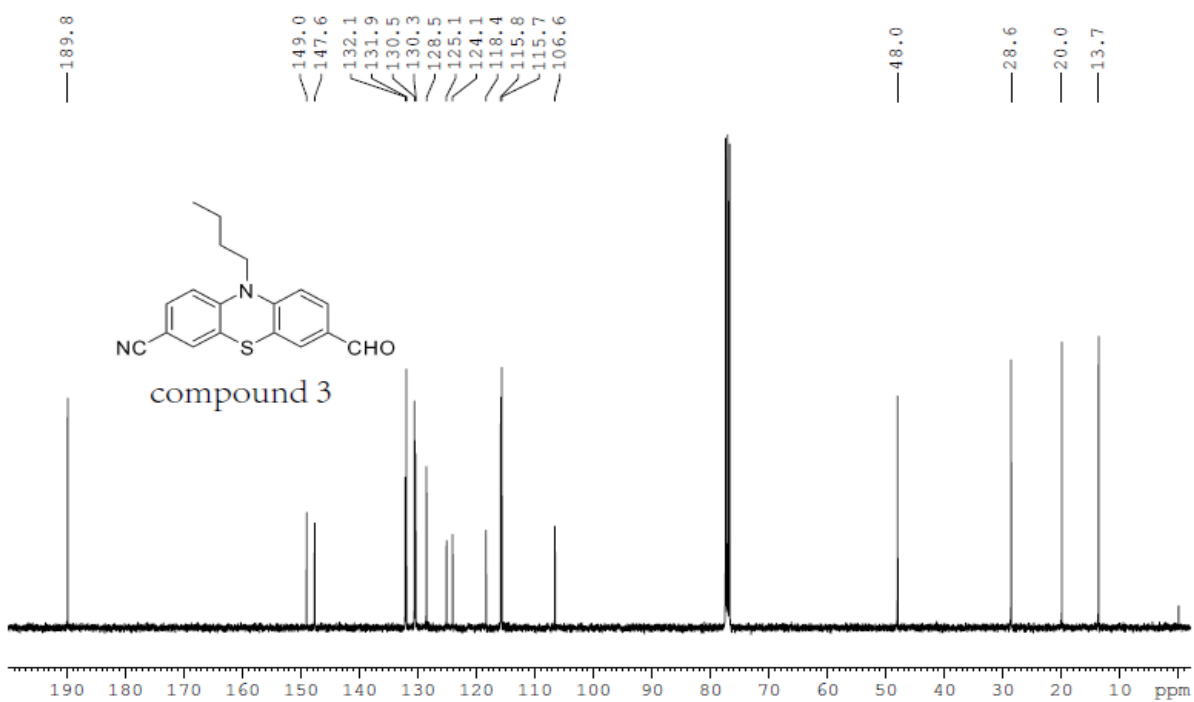
**Figure S4b.** Plots of fluorescence intensity at 499 nm to pH values for 15 $\mu\text{M}$  PI-CN solutions (EtOH/PBS v/v 1:3) before and after the addition of 15  $\mu\text{M}$   $\text{HSO}_3^-$ .

## IV. NMR spectra of related compounds

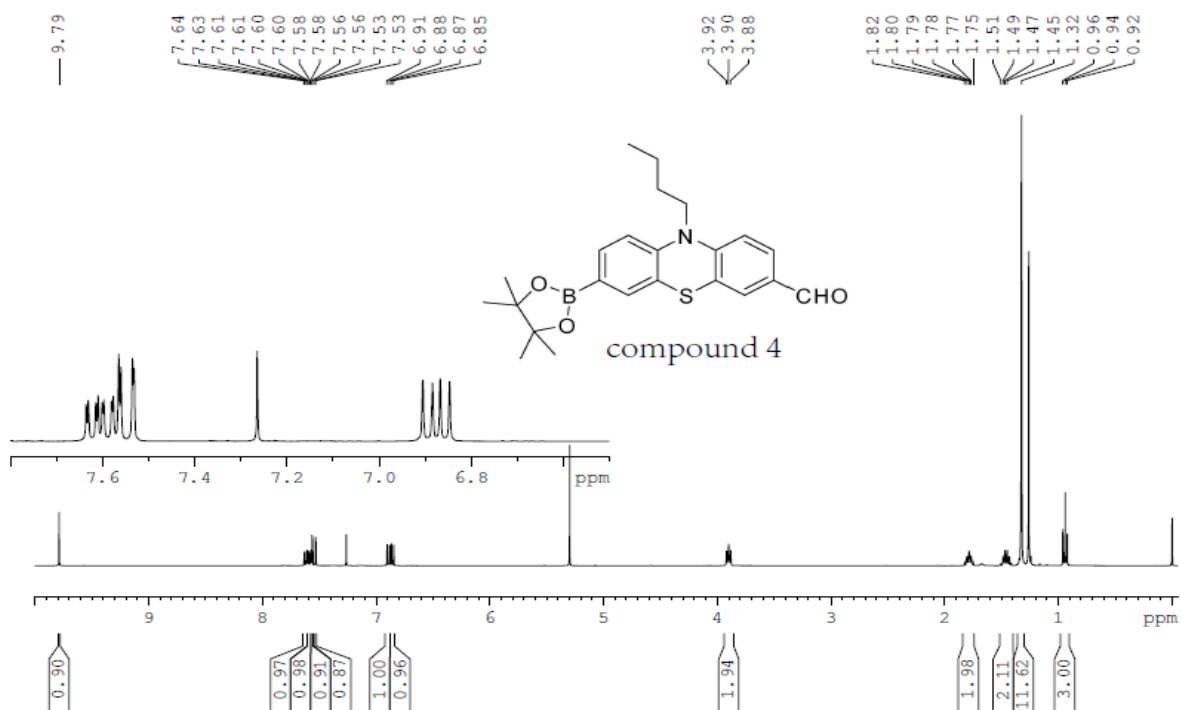
### $^1\text{H}$ NMR of compound **3**.



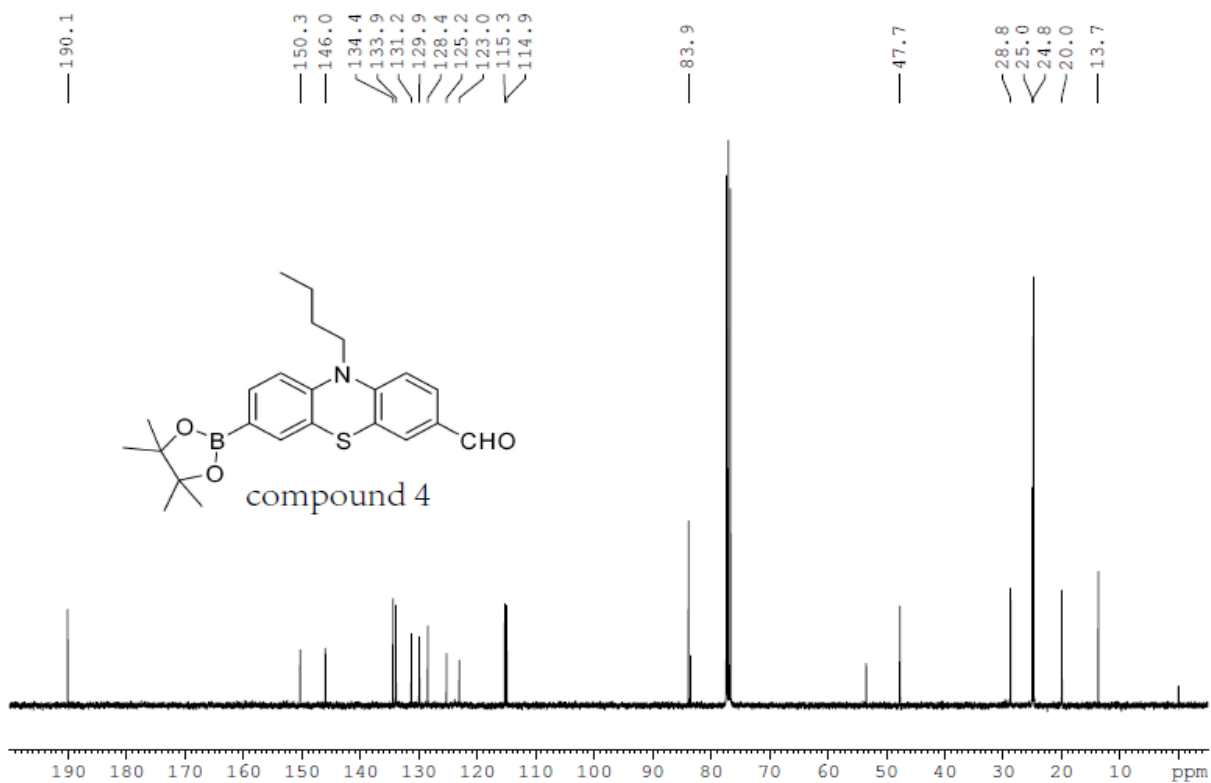
### $^{13}\text{C}$ NMR of compound **3**.



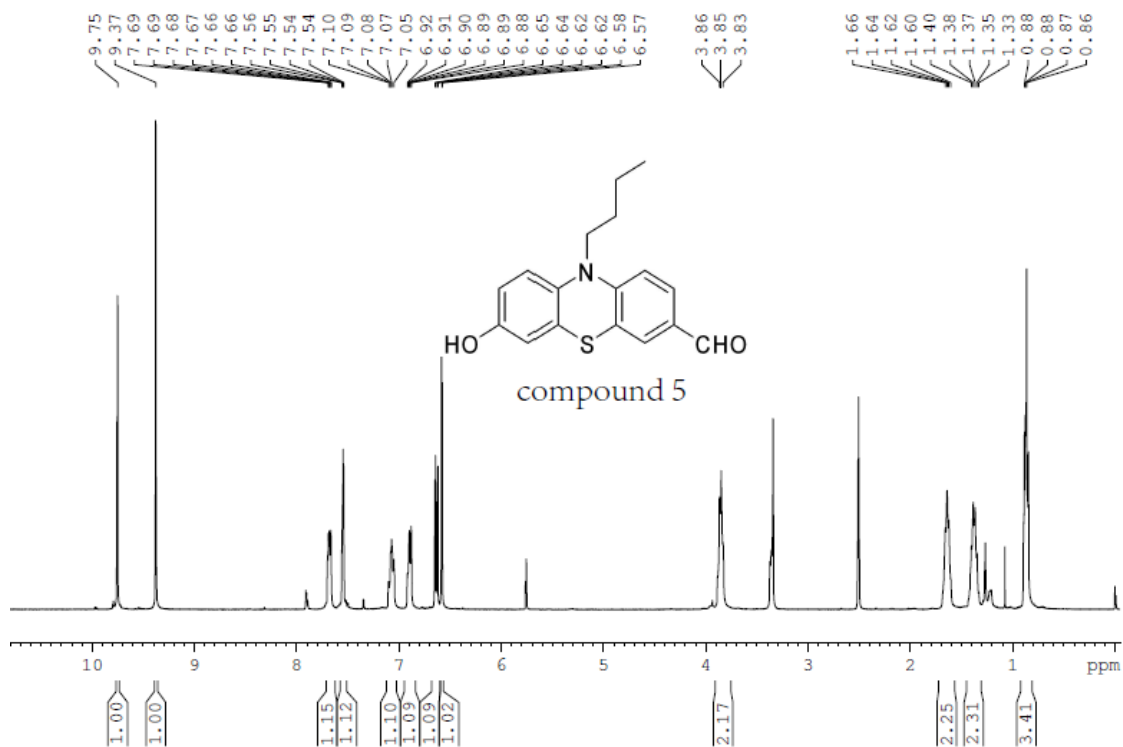
<sup>1</sup>H NMR of compound 4.



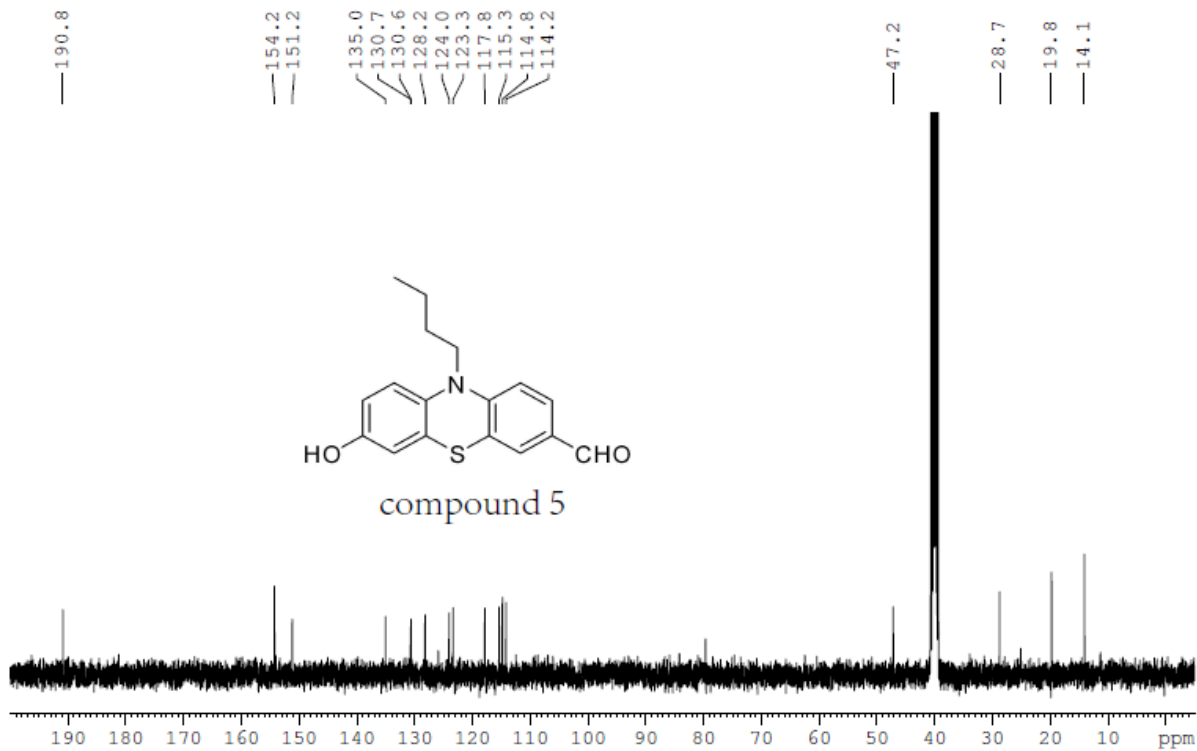
<sup>13</sup>C NMR of compound 4.



$^1\text{H}$  NMR of compound **5**.

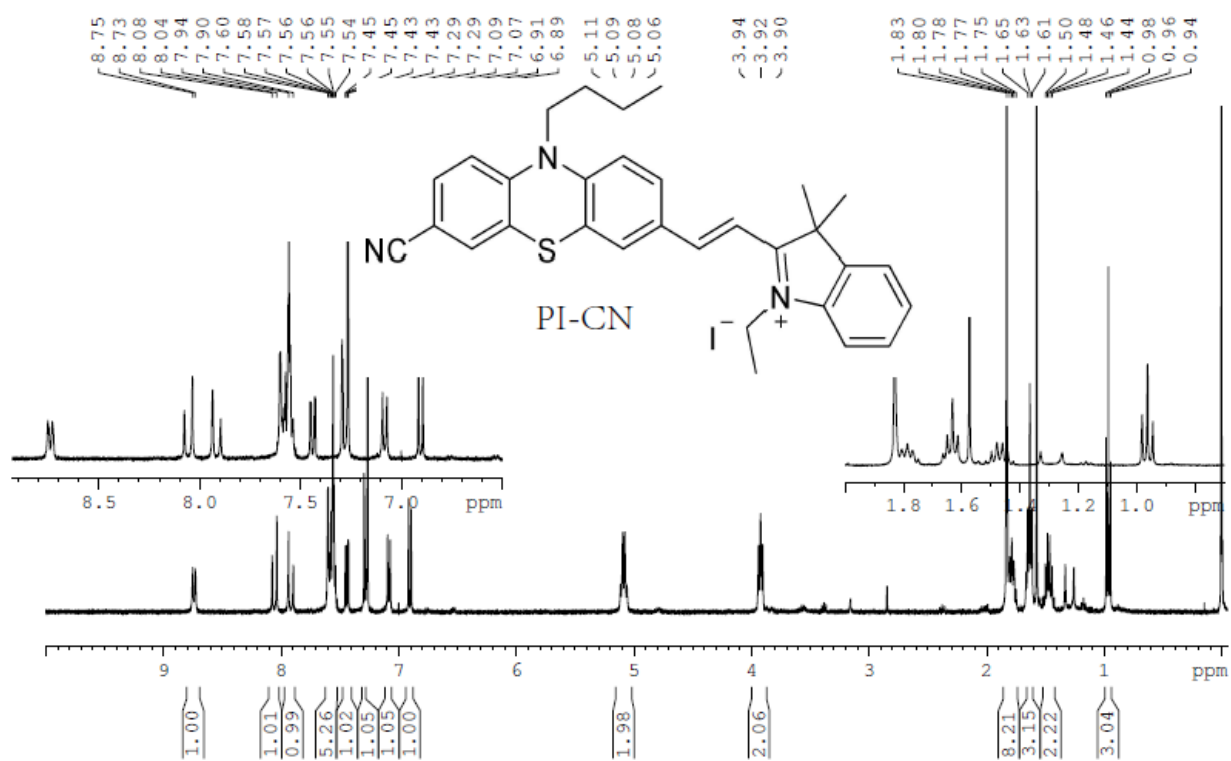


$^{13}\text{C}$  NMR of compound **5**.

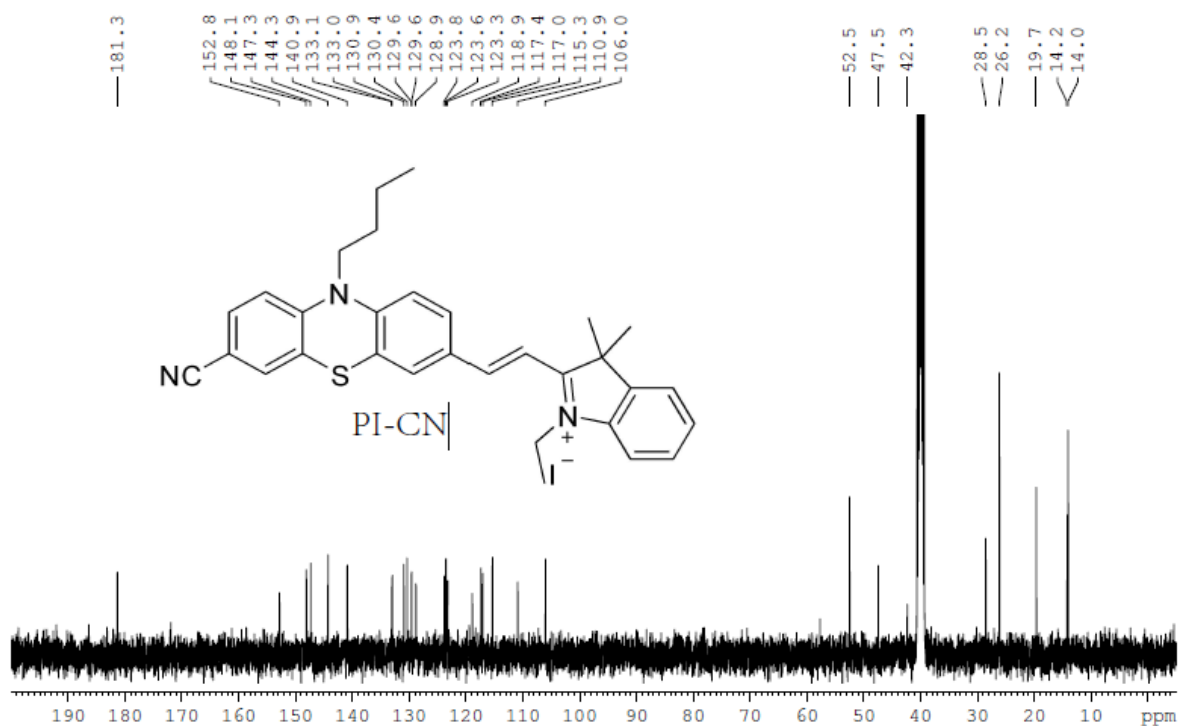




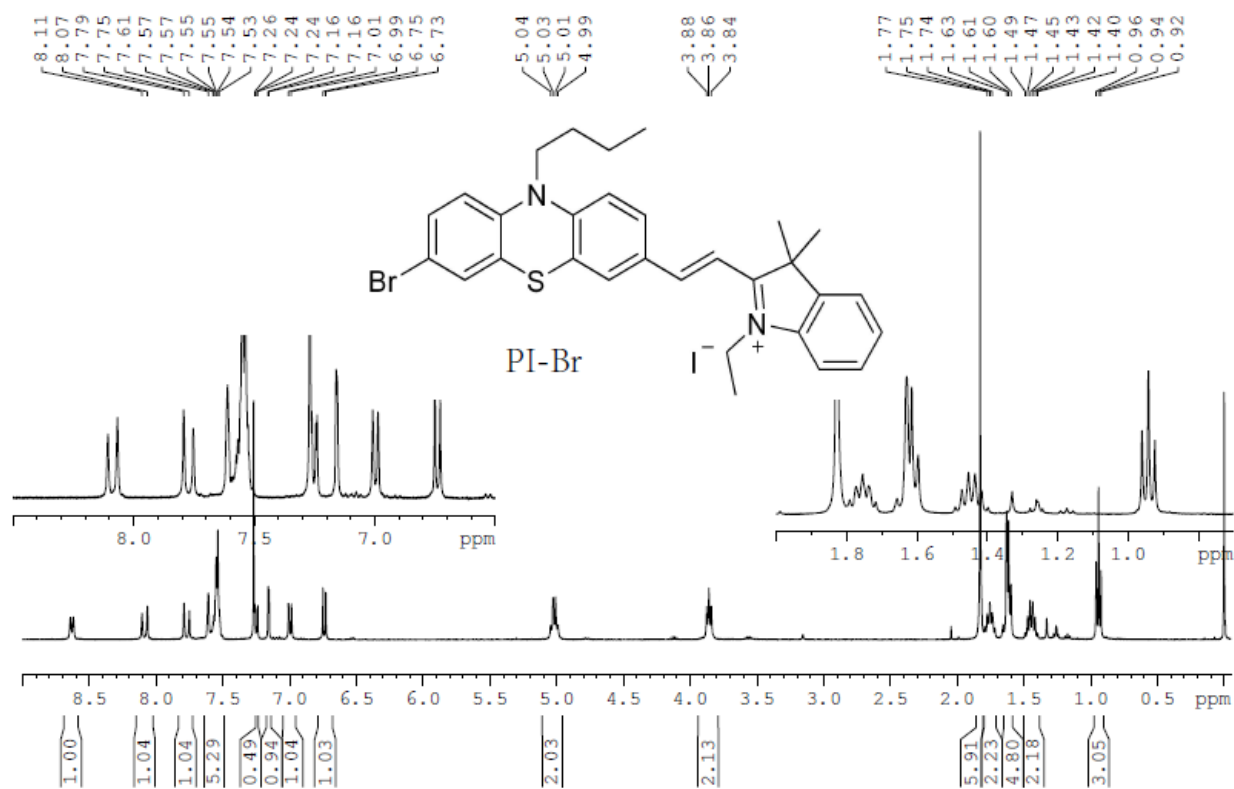
<sup>1</sup>H NMR of PI-CN.



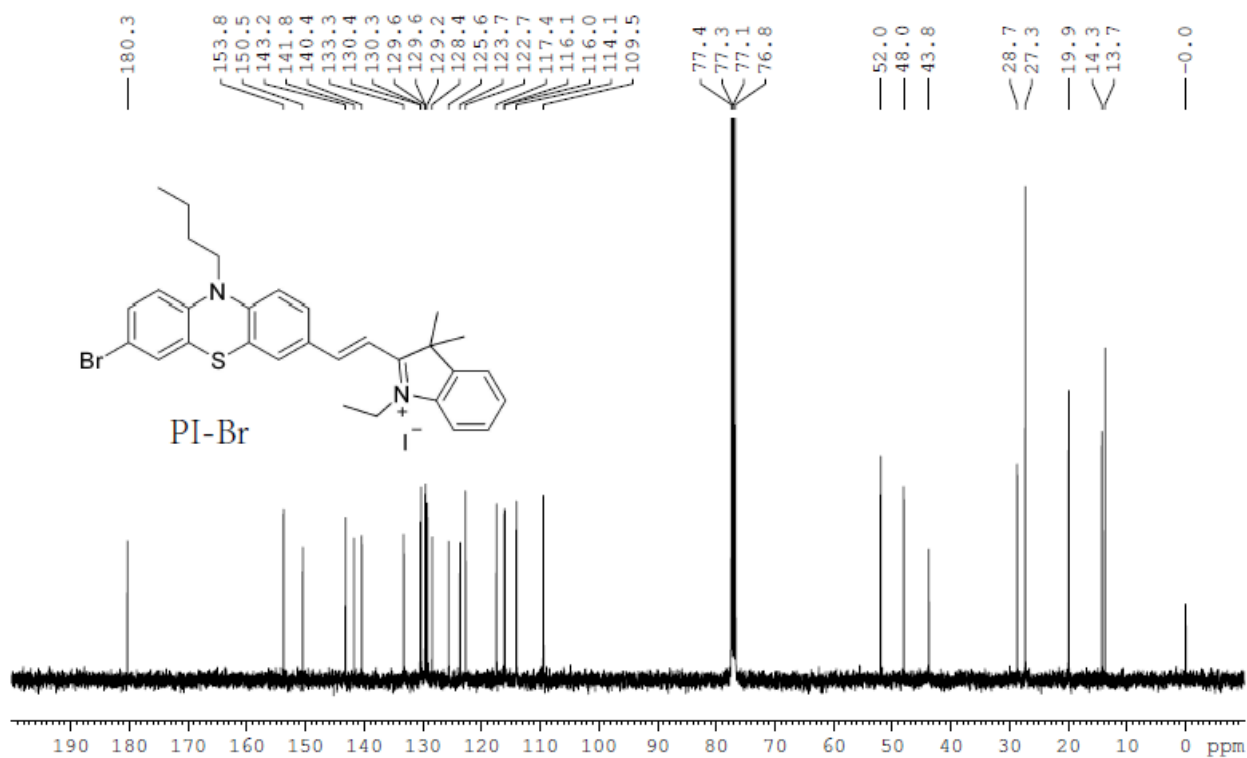
<sup>13</sup>C NMR of PI-CN.



<sup>1</sup>H NMR of PI-Br.

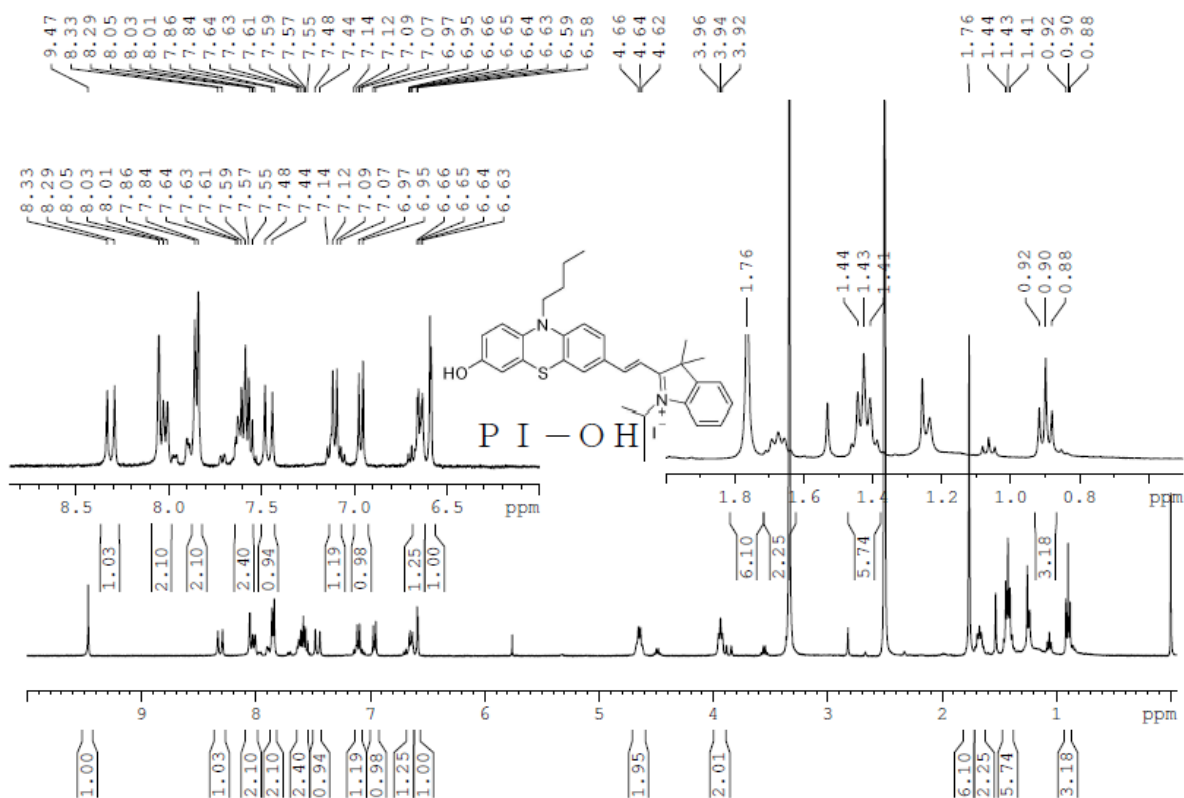


<sup>13</sup>C NMR of PI-Br.





$^1\text{H}$  NMR of PI-OH.



$^{13}\text{C}$  NMR of PI-OH

