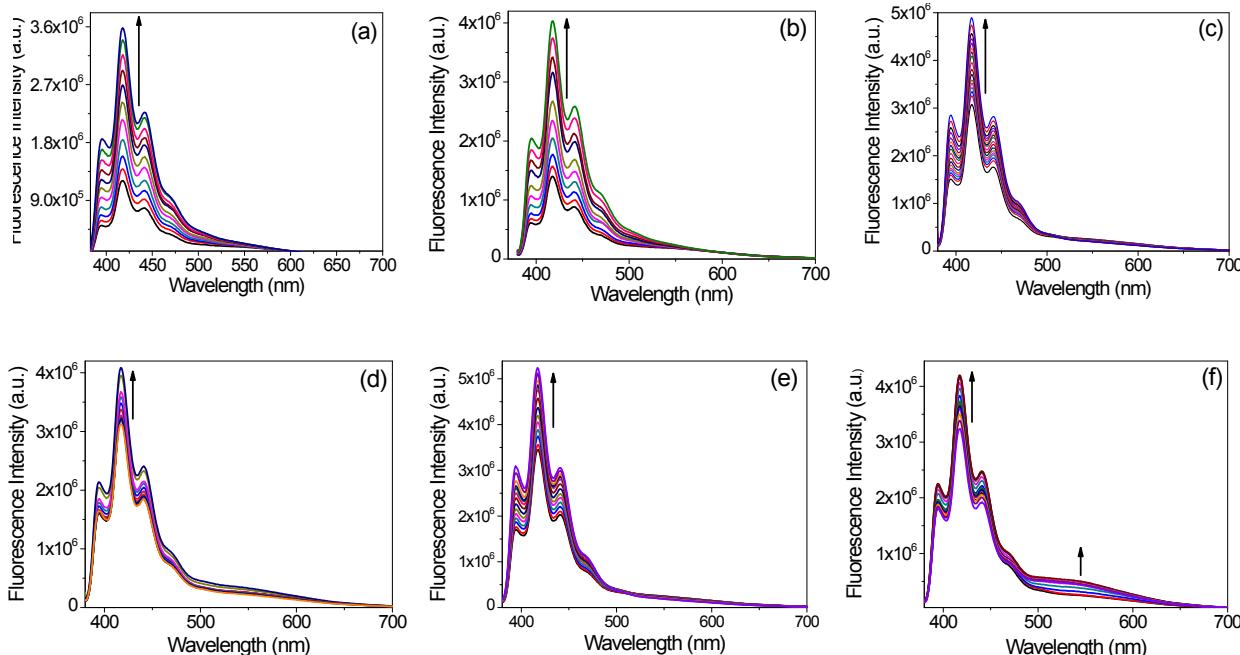


**Anthracene labeled poly(pyridine methacrylamide) as polymer-based chemosensors for detection of pyrophosphate ( $P_2O_7^{4-}$ ) in semi-aqueous media**

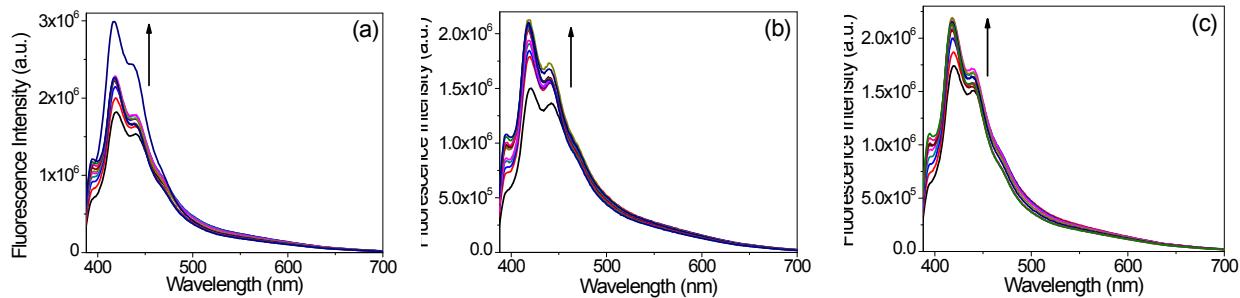
Saswati Ghosh Roy, Subhendu Mondal and Kumaresh Ghosh\*

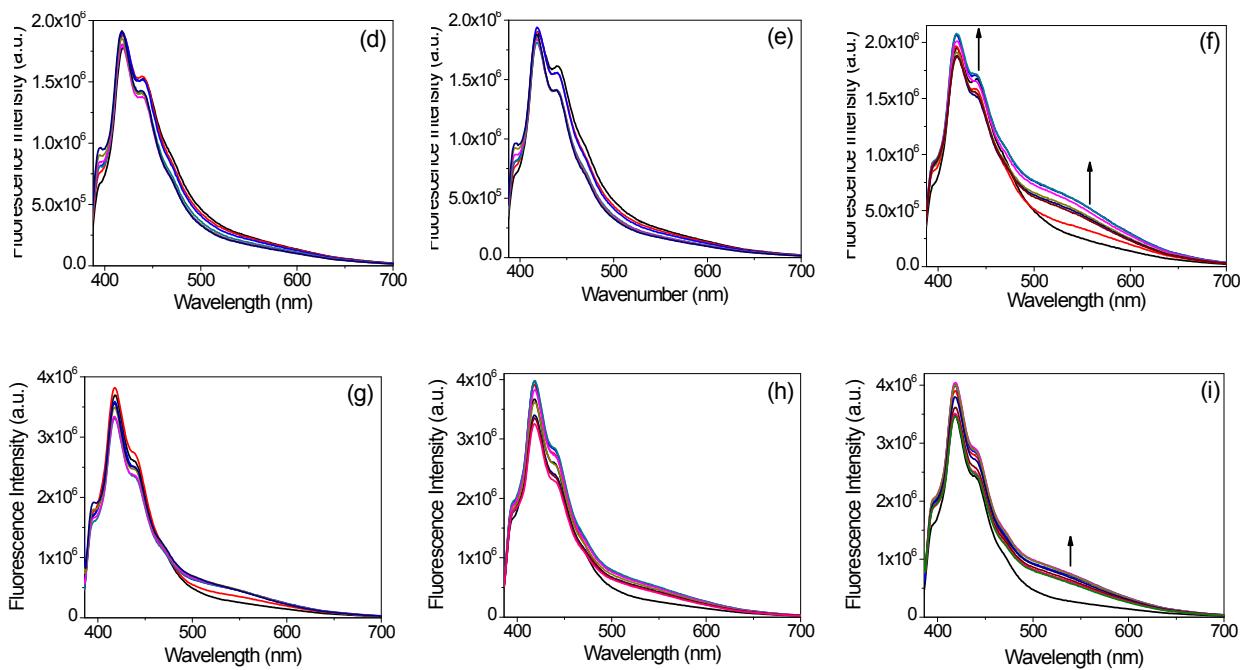
Department of Chemistry, University of Kalyani, Kalyani-741235, Nadia, West Bengal, India.

E-mail: ghosh\_k2003@yahoo.co.in; kumareshchem18@klyuniv.ac.in

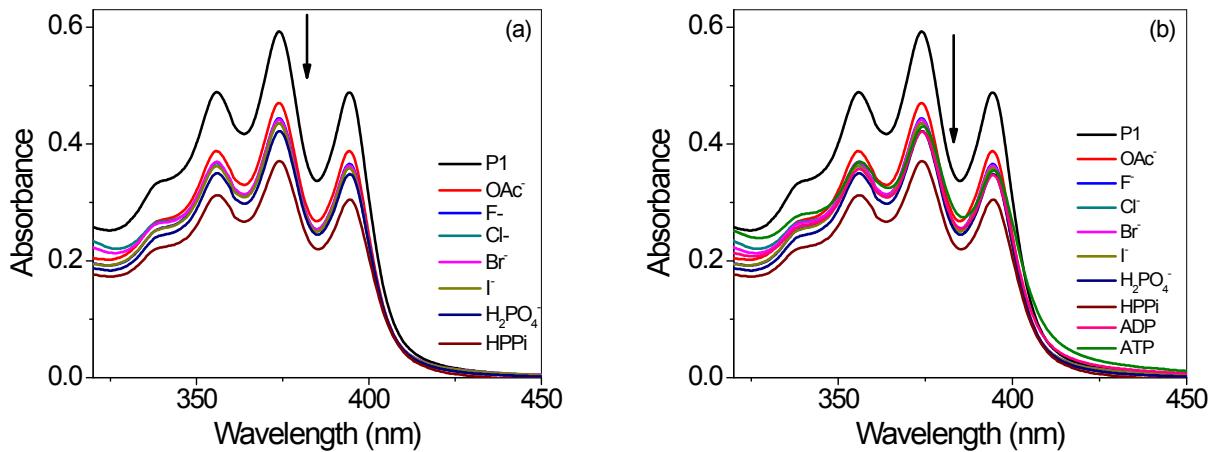


**Fig. S1.** Change in emission of **P1** ( $c = 0.06 \text{ mg/mL}$ ) upon successive addition of (a) acetate ( $\text{OAc}^-$ ) (b)  $\text{F}^-$  (c)  $\text{Cl}^-$  (d)  $\text{Br}^-$  (e)  $\text{I}^-$  and (f)  $\text{HSO}_4^-$  (taken as tetrabutyl ammonium salt) ( $c = 1.0 \times 10^{-3} \text{ M}$ ) from 0 to 0.4 mL in DMSO.

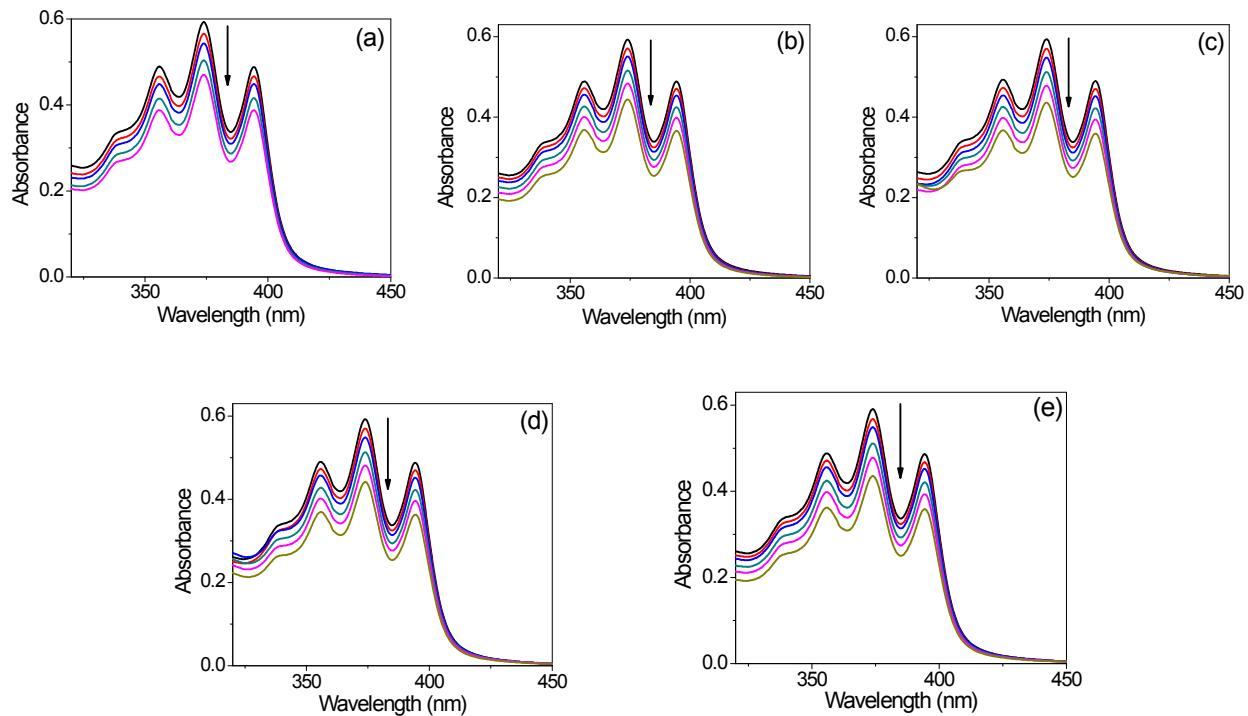




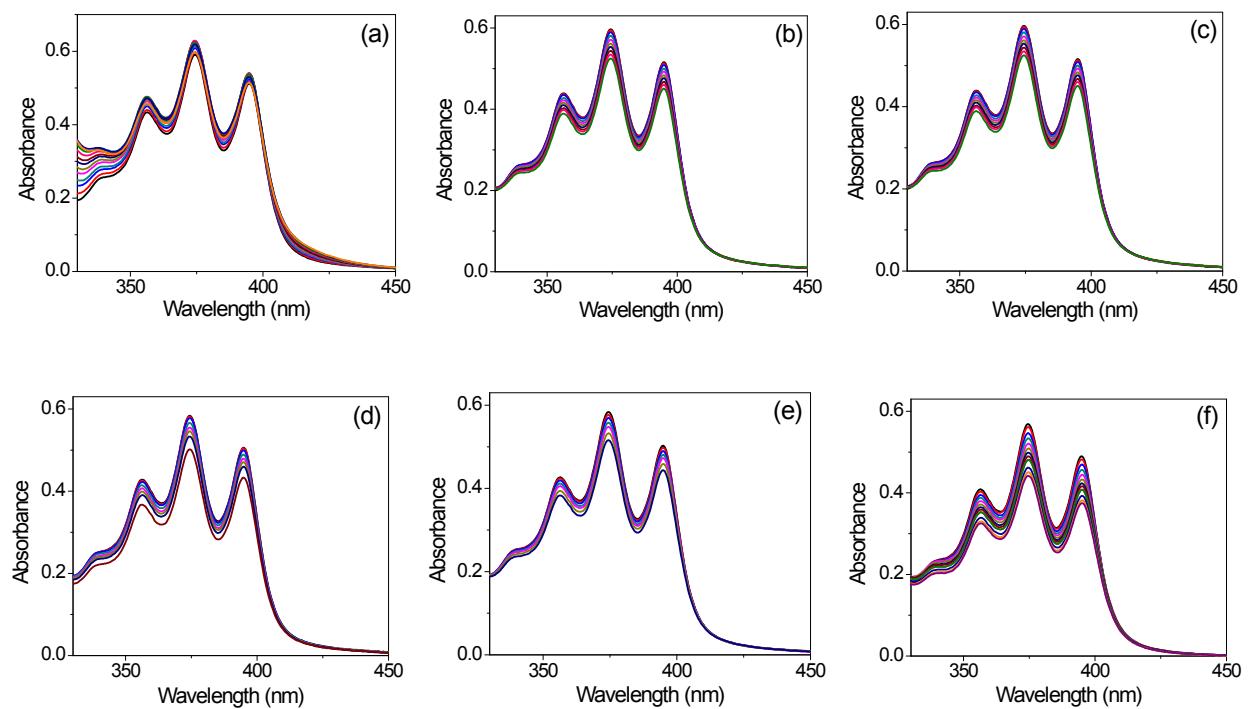
**Fig. S2.** Change in emission of **P1** ( $c = 0.06$  mg/mL,  $\lambda_{\text{ex}} = 370$  nm) upon successive addition of (a) acetate ( $\text{OAc}^-$ ) (b)  $\text{F}^-$  (c)  $\text{Cl}^-$  (d)  $\text{Br}^-$  (e)  $\text{I}^-$ , (f)  $\text{HSO}_4^-$  (g) AMP, (h) ADP and (i) ATP (taken as tetrabutyl ammonium salt) ( $c = 1.0 \times 10^{-3}$  M) from 0 to 0.4 mL in DMSO- $\text{H}_2\text{O}$  (3:1, v/v).

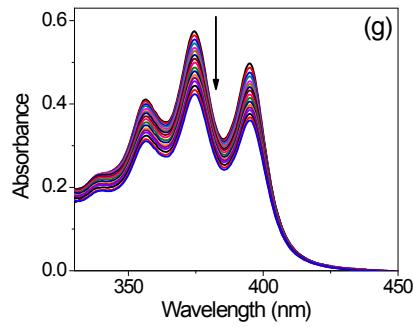


**Fig. S3.** Changes in absorption of **P1** ( $c = 0.06$  mg/mL) upon addition of 0.4 mL solution of various anions (a) ( $\text{OAc}^-$ ,  $\text{F}^-$ ,  $\text{Cl}^-$ ,  $\text{Br}^-$ ,  $\text{I}^-$ ,  $\text{H}_2\text{PO}_4^-$ , HPPi as  $\text{Bu}_4\text{N}$  salt) in DMSO and (b) ( $\text{OAc}^-$ ,  $\text{F}^-$ ,  $\text{Cl}^-$ ,  $\text{Br}^-$ ,  $\text{I}^-$ ,  $\text{H}_2\text{PO}_4^-$ , HPPi, ADP and ATP in DMSO- $\text{H}_2\text{O}$  ( $c = 1 \times 10^{-3}$  M).

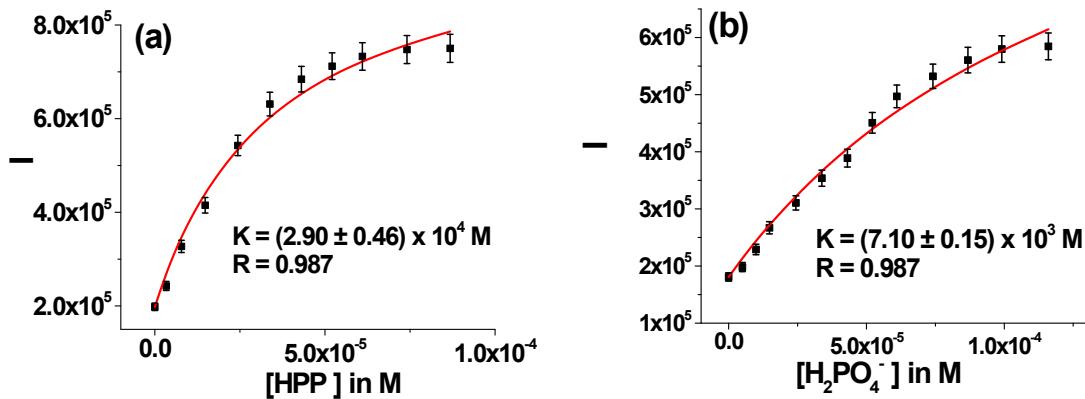


**Fig. S4.** Changes in absorption of **P1** ( $c = 0.06 \text{ mg/mL}$ ) upon the successive addition of solution of various anions ( $\text{OAc}^-$ ,  $\text{F}^-$ ,  $\text{Cl}^-$ ,  $\text{Br}^-$  and  $\text{I}^-$  from 0 mL to 0.4 mL in DMSO ( $c = 1 \times 10^{-3} \text{ M}$ ).

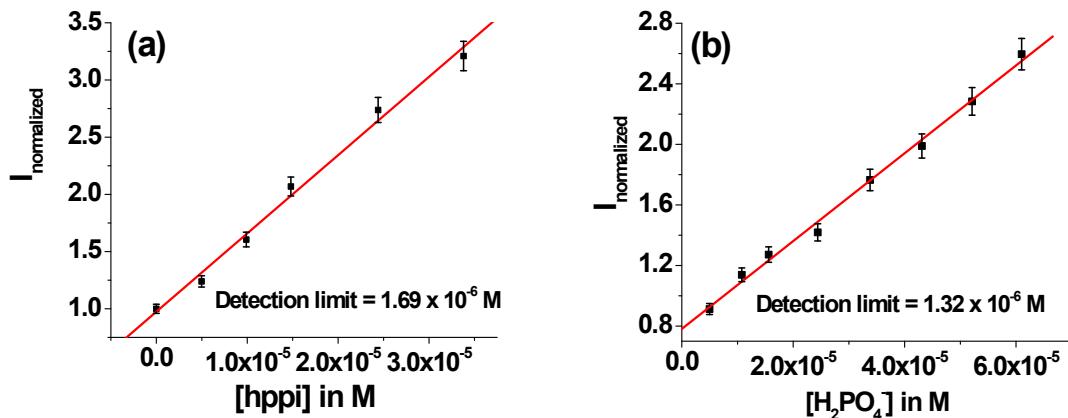




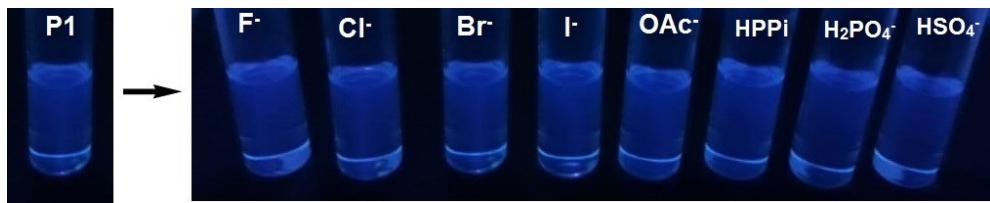
**Fig. S5.** Changes in absorption of **P1** ( $c = 0.06 \text{ mg/mL}$ ) upon the successive addition of solution of various anions ( $\text{OAc}^-$ ,  $\text{F}^-$ ,  $\text{Cl}^-$ ,  $\text{Br}^-$ ,  $\text{I}^-$ , ADP and ATP from 0 mL to 0.4 mL in DMSO-H<sub>2</sub>O ( $c = 1 \times 10^{-3} \text{ M}$ ).



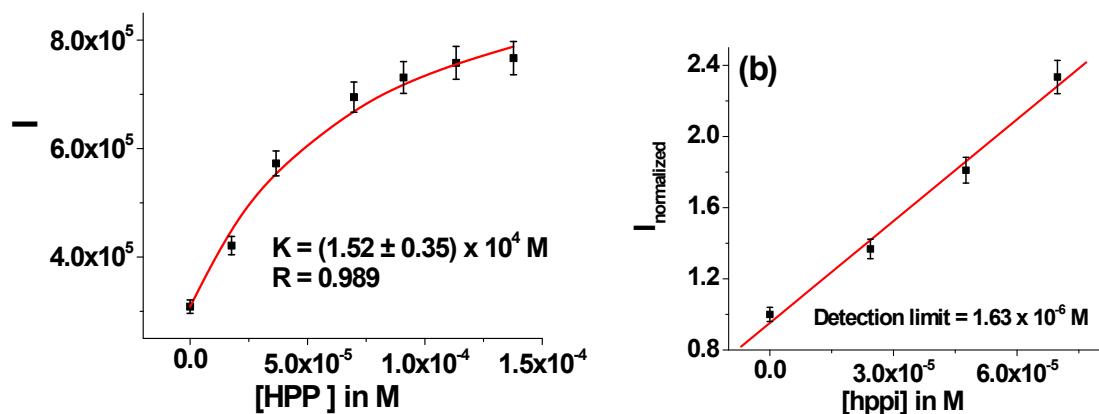
**Fig. S6.** Binding constant curves for **P1** with (a) hydrogen pyrophosphate and (b) dihydrogen phosphate from non-linear fitting of fluorescence titration data in DMSO at 520 nm.



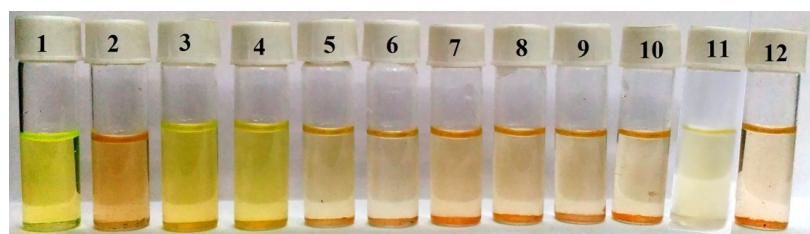
**Fig. S7.** Detection limits for polymer **P1** ( $c = 0.06 \text{ mg/mL}$ ) with (a) HPPi and (b)  $\text{H}_2\text{PO}_4^-$  ( $c = 1.0 \times 10^{-3} \text{ M}$ ) ions in DMSO.



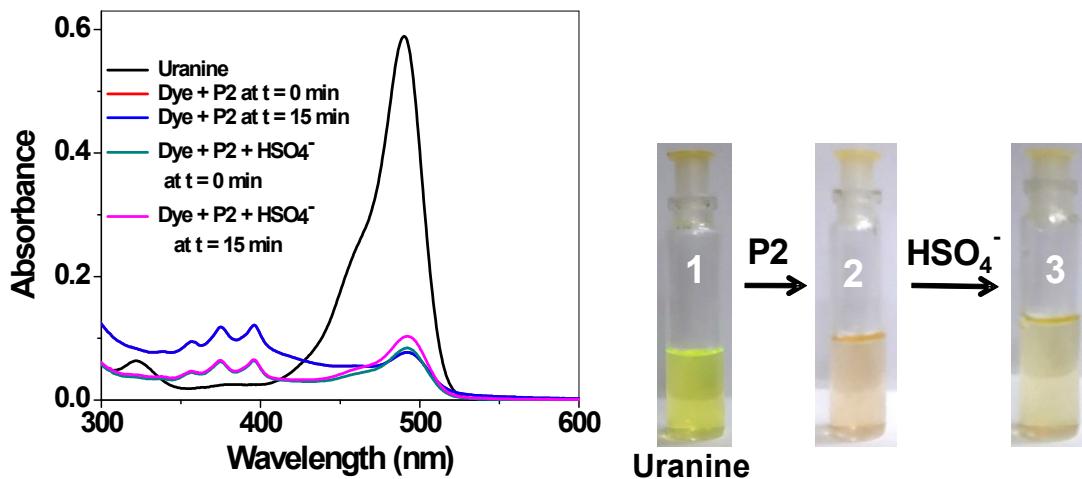
**Fig. S8.** Photograph showing solution of **P1** in absence and presence of 0.4 mL solution of various anions ( $c = 1.0 \times 10^{-3}$  M) as tetrabutylammonium salts in DMSO-H<sub>2</sub>O (3:1, v/v), ([**P1**] = 0.06 mg/mL) under hand held UV light.



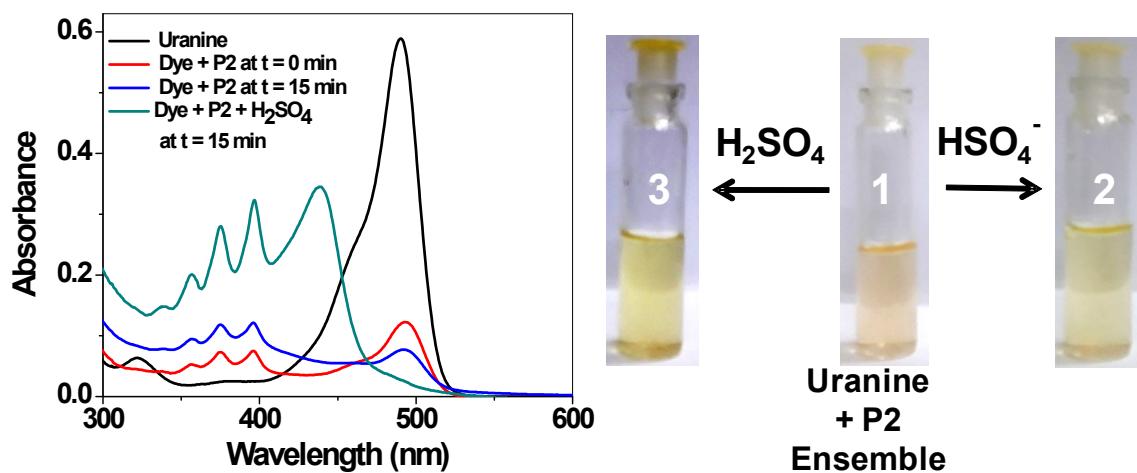
**Fig. S9.** (a) Binding constant curve for **P1** with hydrogen pyrophosphate from non-linear fitting of fluorescence titration data in DMSO-H<sub>2</sub>O (3:1, v/v) at 530 nm and (b) detection limit for **P1** ( $c = 0.06$  mg/mL) with HPPi ( $c = 1.0 \times 10^{-3}$  M) in DMSO-H<sub>2</sub>O (3:1, v/v).



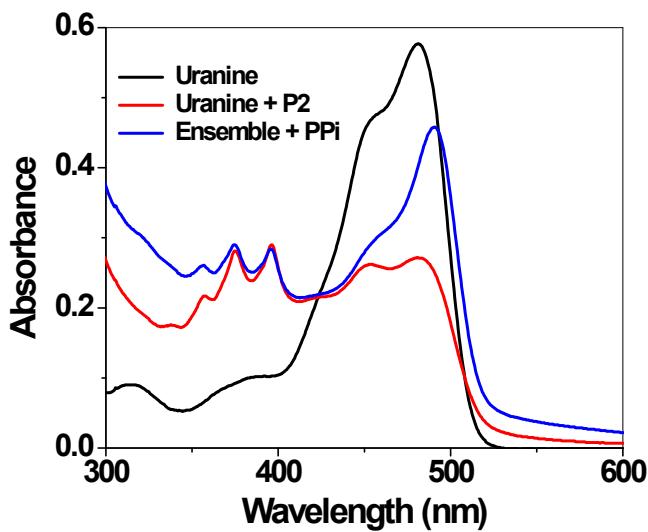
**Fig. S10.** Photograph showing (1) Uranine dye, (2) dye + 0.3 mL polymer solution (1 mg/mL), ensemble with (3) PPi, (4) HPPi, (5) H<sub>2</sub>PO<sub>4</sub><sup>-</sup>, (6) OAc<sup>-</sup>, (7) F<sup>-</sup>, (8) Cl<sup>-</sup>, (9) Br<sup>-</sup>, (10) I<sup>-</sup>, (11) HSO<sub>4</sub><sup>-</sup> and (12) NO<sub>3</sub><sup>-</sup> in DMSO/H<sub>2</sub>O (1:1 v/v, pH = 6.8, 10 mM Tris HCl buffer) [anions were taken as tetrabutylammonium salt and pyrophosphate as sodium salt].



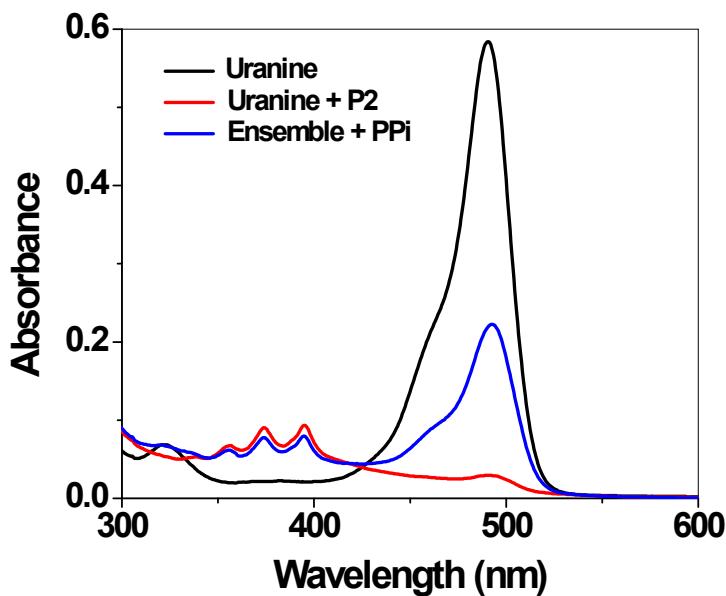
**Fig. S11.** Change in absorbance of uranine dye upon addition of 0.3 mL of **P2** solution and absorbance of **P2**-dye ensemble after addition 0.6 ml amounts of HSO<sub>4</sub><sup>-</sup> ( $c = 5 \times 10^{-3}$  M) to the ensemble in DMSO-H<sub>2</sub>O (1:1 v/v, pH = 6.8, 10 mM TrisHCl buffer) ([dye] =  $2.5 \times 10^{-5}$  M, [polymer **P2**] = 0.06 mg/mL) (left); Photograph showing color of (1) Uranine dye, (2) dye + 0.3 mL of **P2** polymer ensemble and (3) ensemble treated with HSO<sub>4</sub><sup>-</sup> [HSO<sub>4</sub><sup>-</sup> taken as tetrabutylammonium salt] (right).



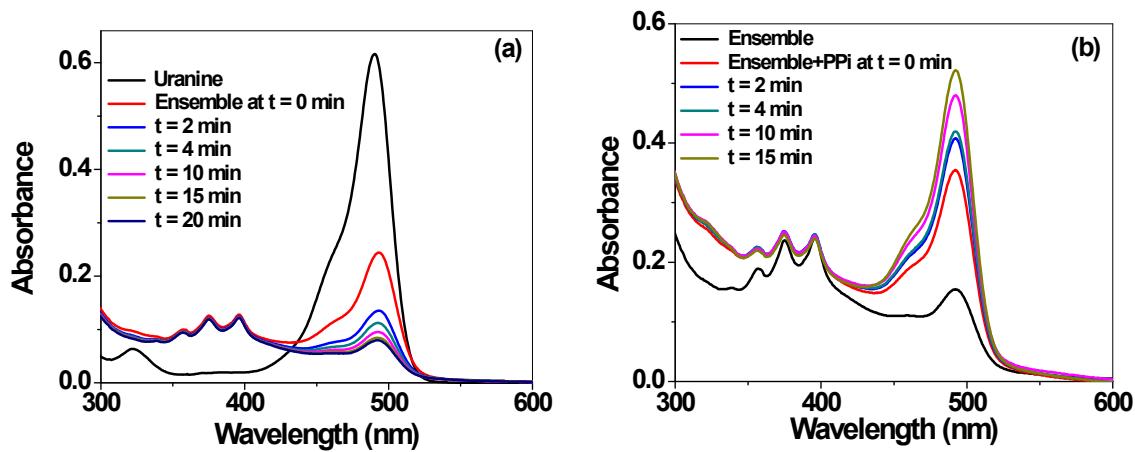
**Fig. S12.** Change in absorbance of uranine dye upon addition of 0.3 mL of **P2** solution and absorbance of **P2**-dye ensemble after addition 0.6 ml amounts of H<sub>2</sub>SO<sub>4</sub> ( $c = 5 \times 10^{-3}$  M) to the ensemble in DMSO-H<sub>2</sub>O (1:1 v/v, pH = 6.8, 10 mM TrisHCl buffer) ([dye] =  $2.5 \times 10^{-5}$  M, [polymer **P2**] = 0.06 mg/mL) (left); Photograph showing color change (right).



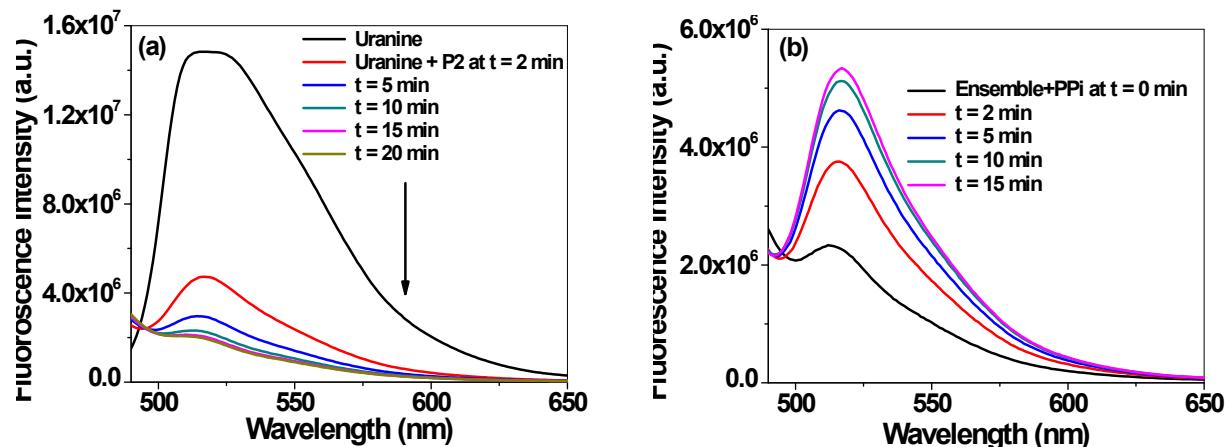
**Fig. S13.** Change in absorption intensity of Uranine dye upon addition of **P2** (0.3 mL) and dye-ensemble upon the addition of 0.6 mL of PPi ( $c = 5 \times 10^{-3}$  M) in DMSO-H<sub>2</sub>O (1:1 v/v, pH = 4.0, 10 mM TrisHCl buffer) ([dye] =  $2.5 \times 10^{-5}$  M, [polymer **P2**] = 0.06 mg/mL).



**Fig. S14.** Change in absorption intensity of Uranine dye upon addition of **P2** (0.3 mL) and dye-ensemble upon addition of 0.6 mL of PPi ( $c = 5 \times 10^{-3}$  M) in DMSO-H<sub>2</sub>O (1:1 v/v, pH = 10.0, 10 mM TrisHCl buffer) ([dye] =  $2.5 \times 10^{-5}$  M, [polymer **P2**] = 0.06 mg/mL).

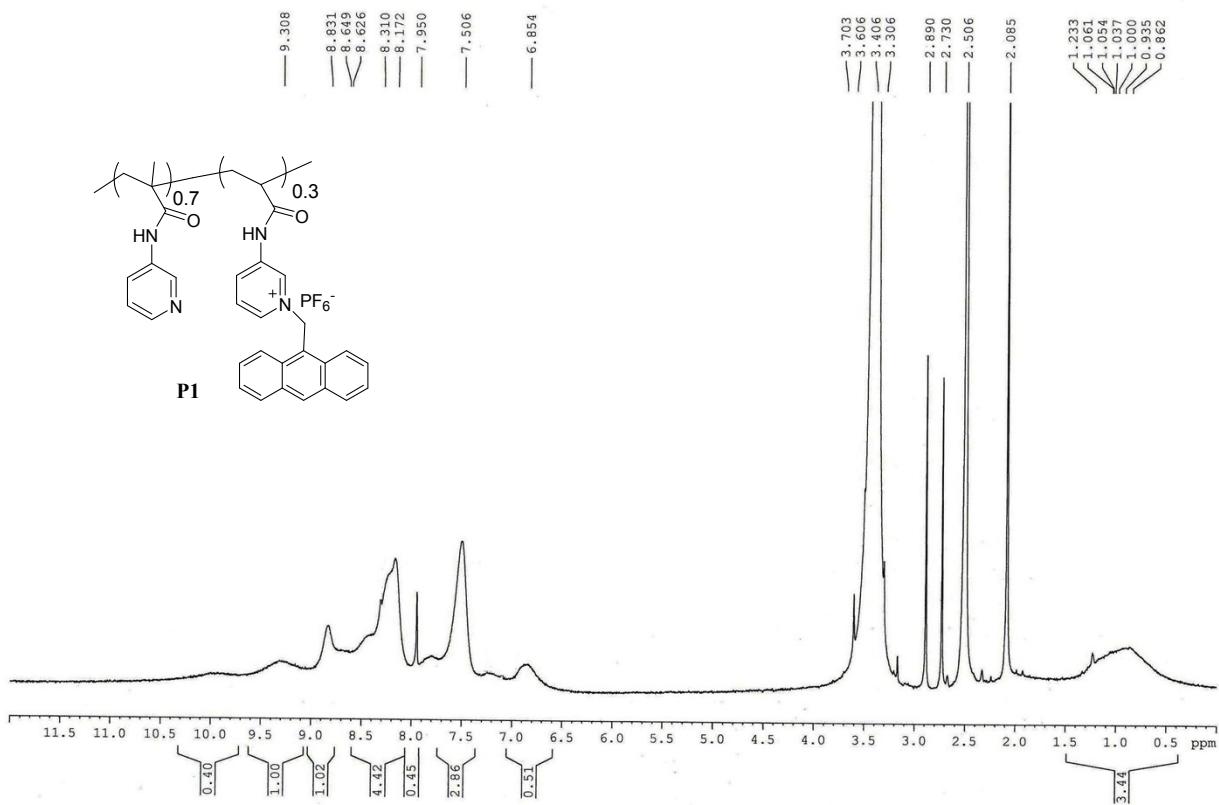


**Fig. S15.** Change in absorption intensity with time of (a) uranine dye upon addition of 0.3 mL of **P2** solution and (b) **P2**-dye ensemble after addition 0.6 ml amounts of PPi ( $c = 5 \times 10^{-3}$  M) to the ensemble in DMSO-H<sub>2</sub>O (1:1 v/v, pH = 6.8, 10 mM TrisHCl buffer) ([dye] =  $2.5 \times 10^{-5}$  M, [polymer **P2**] = 0.06 mg/mL).

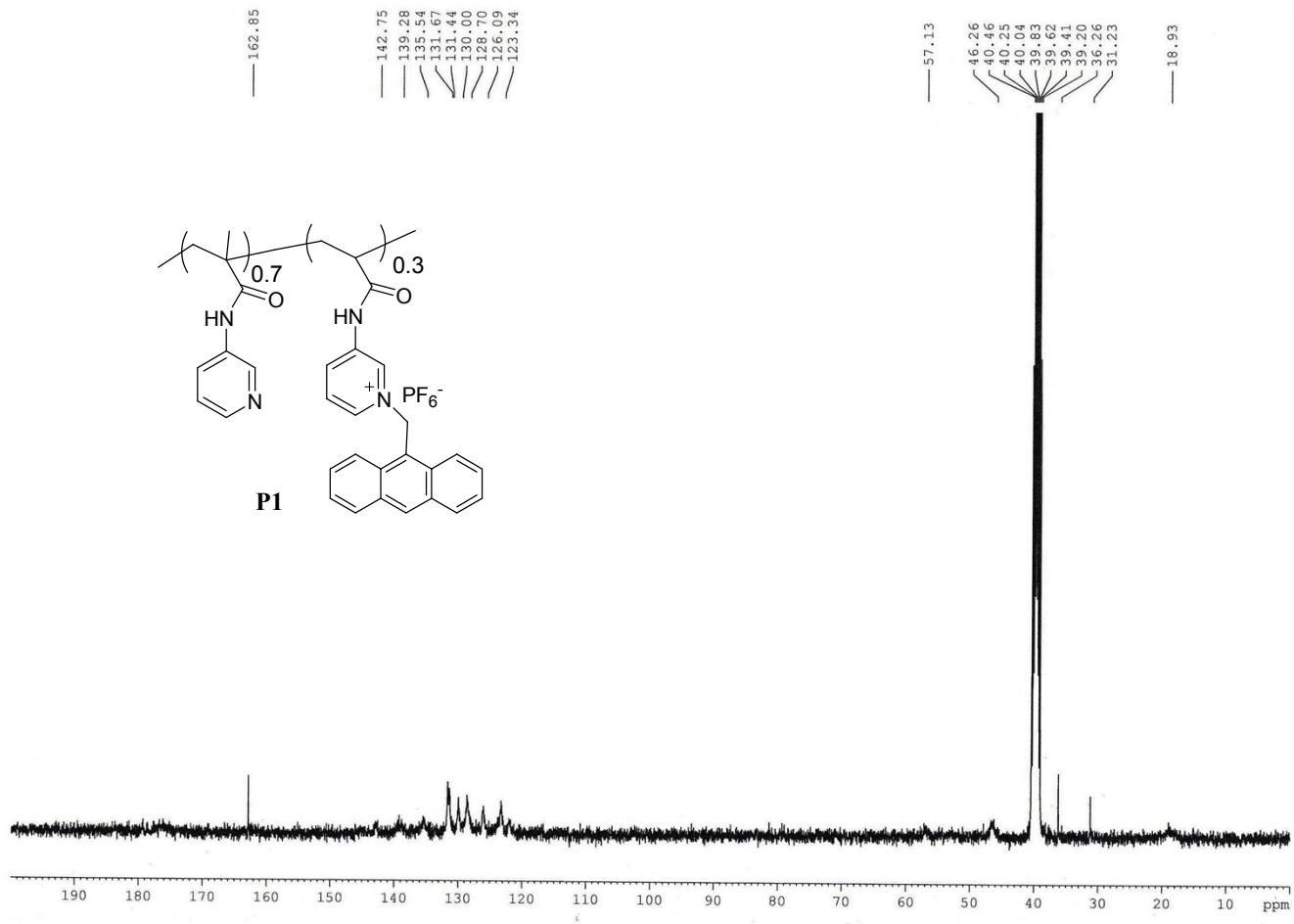


**Fig. S16.** (a) Decrease in fluorescence intensity of uranine dye upon addition of 0.3 mL of **P2** with time and (b) retrieval of fluorescence intensity of uranine dye with time upon addition of 0.6 mL of PPi ( $c = 5 \times 10^{-3}$  M) to the **P2**-dye ensemble in DMSO-H<sub>2</sub>O (1:1 v/v, pH = 6.8, 10 mM Tris HCl buffer).

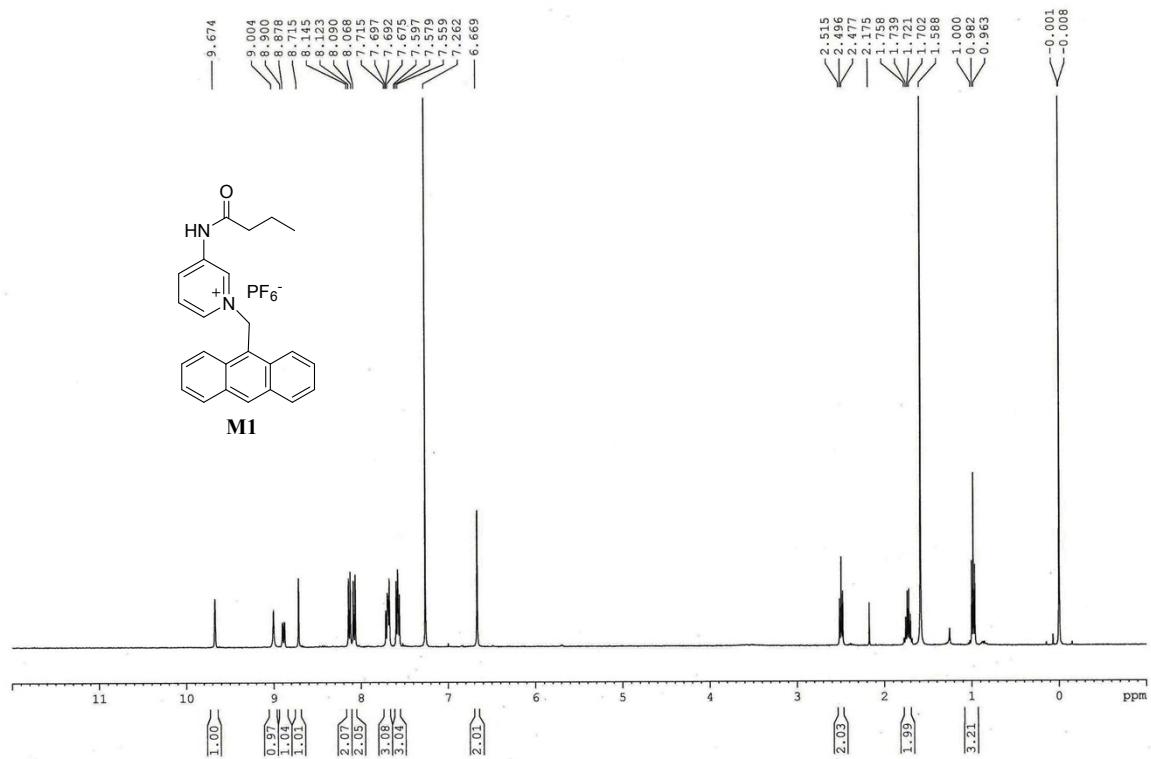
**<sup>1</sup>H NMR of P1 in d<sub>6</sub>-DMSO (400 MHz)**



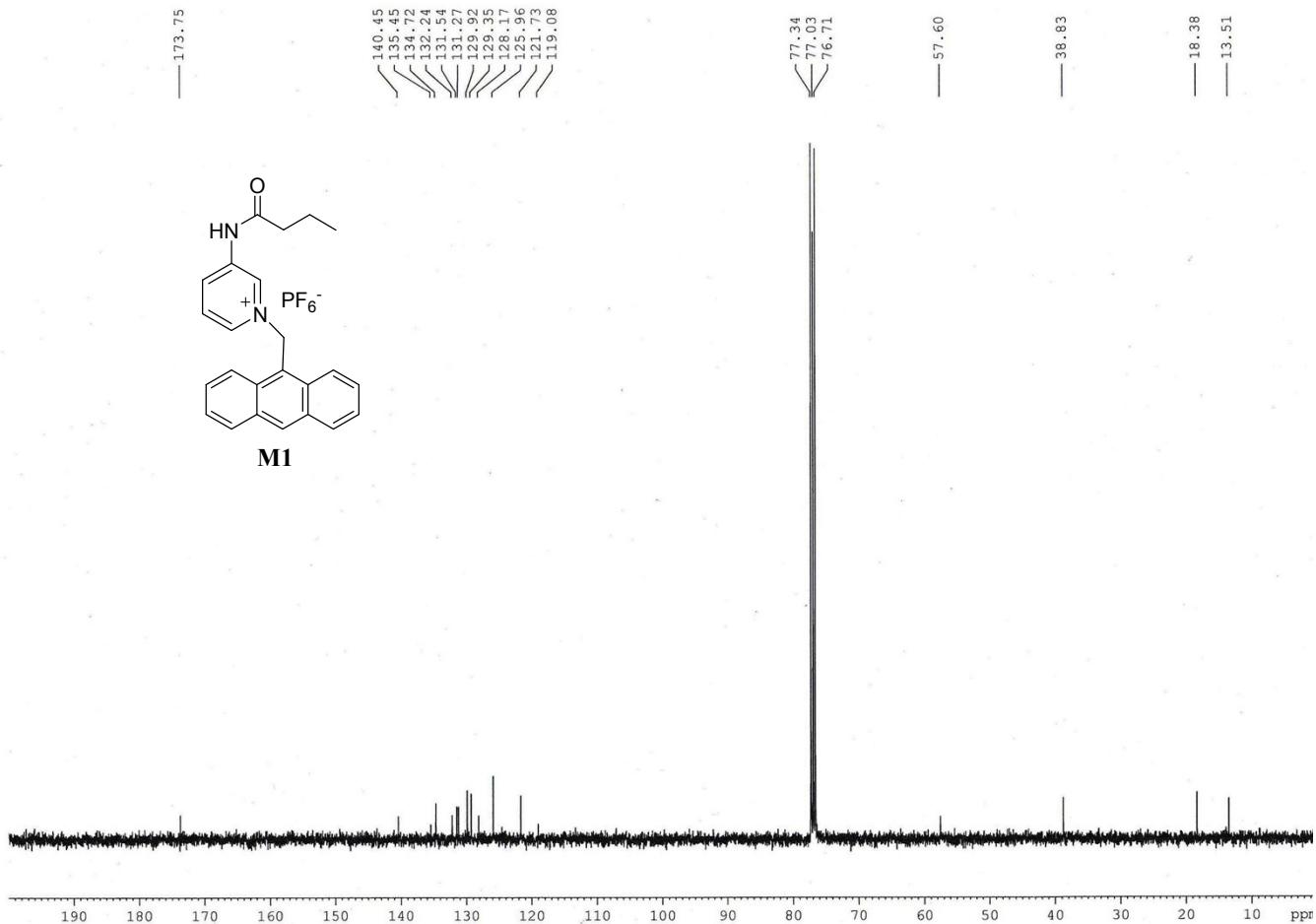
**$^{13}\text{C}$  NMR of P1 in  $\text{d}_6\text{-DMSO}$  (100 MHz)**



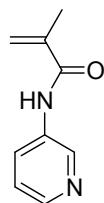
**$^1\text{H}$  NMR of M1 in  $\text{CDCl}_3$  (400 MHz)**



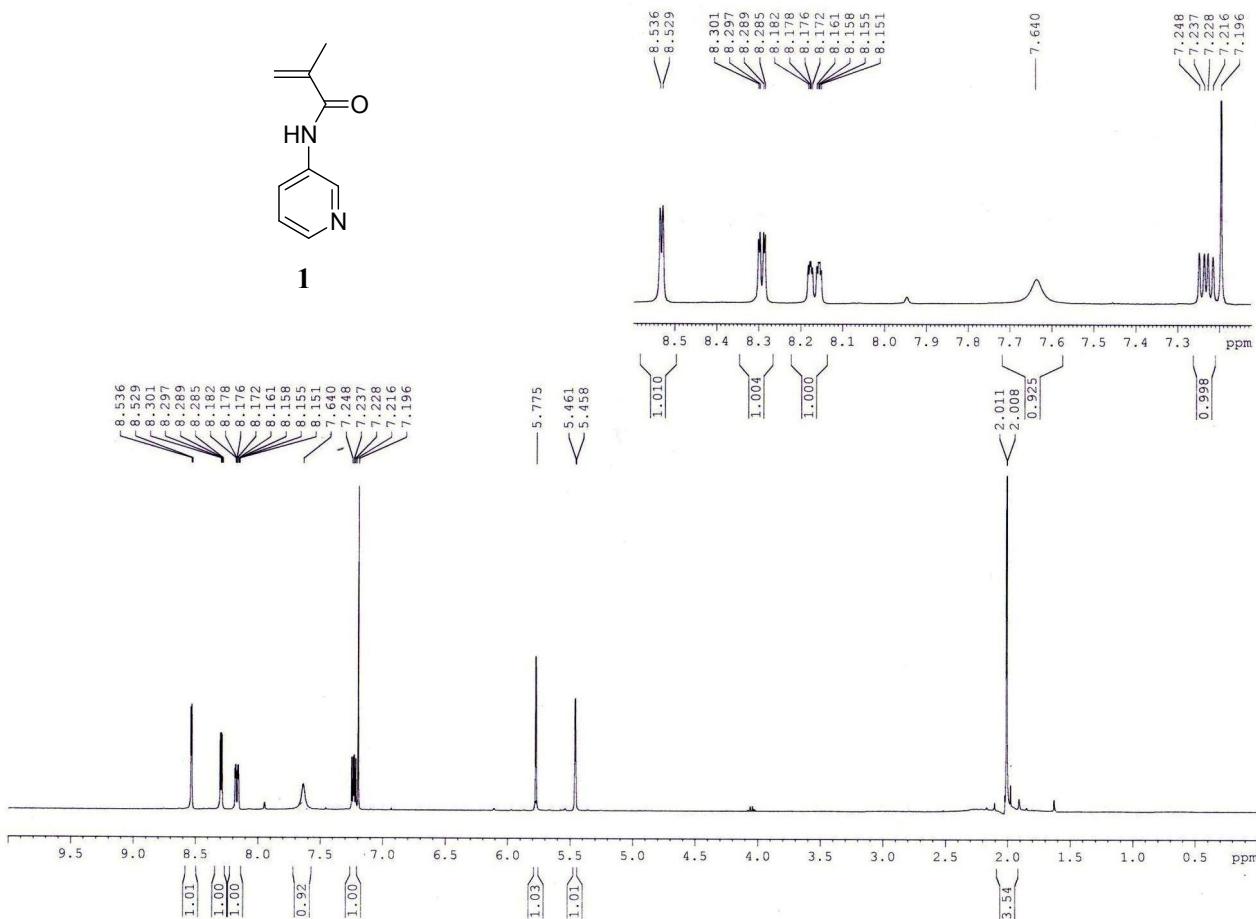
**$^{13}\text{C}$  NMR of M1 in  $\text{CDCl}_3$  (100 MHz)**



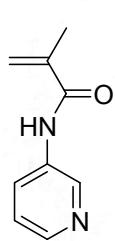
**<sup>1</sup>H NMR of 1 in CDCl<sub>3</sub> (400 MHz)**



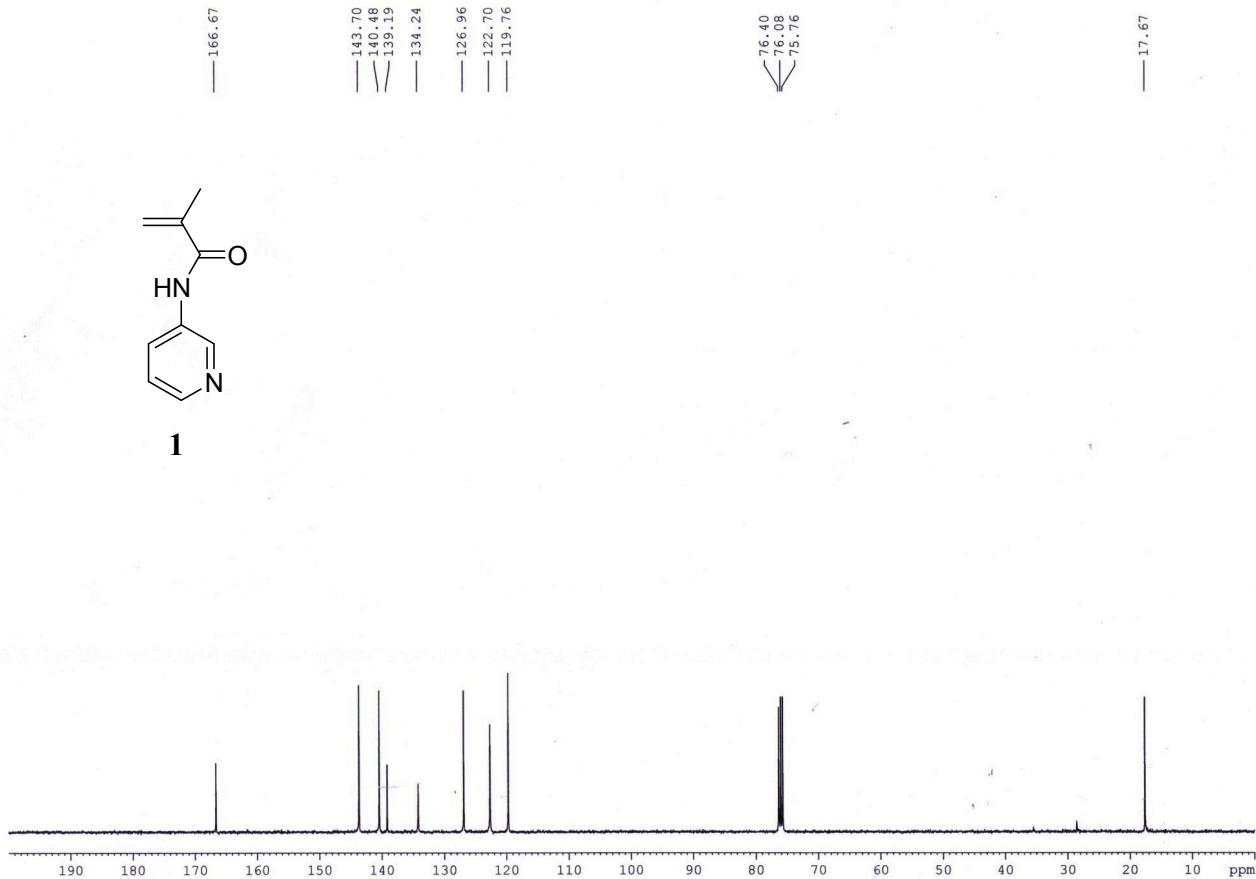
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**$^{13}\text{C}$  NMR of 1 in  $\text{CDCl}_3$  (100 MHz)**



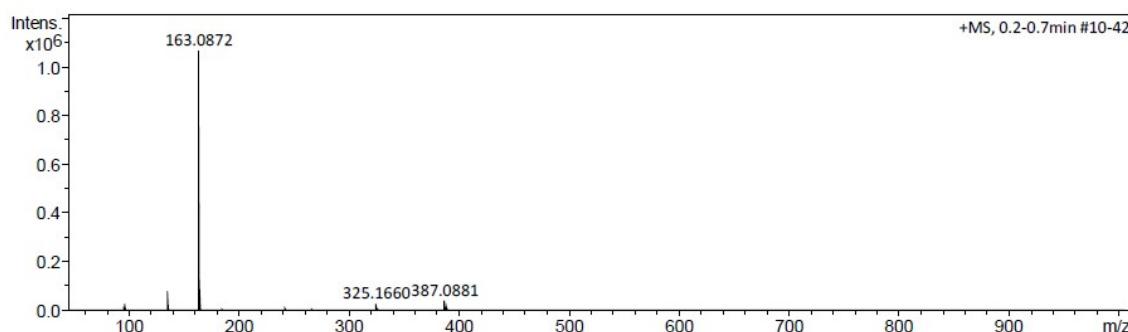
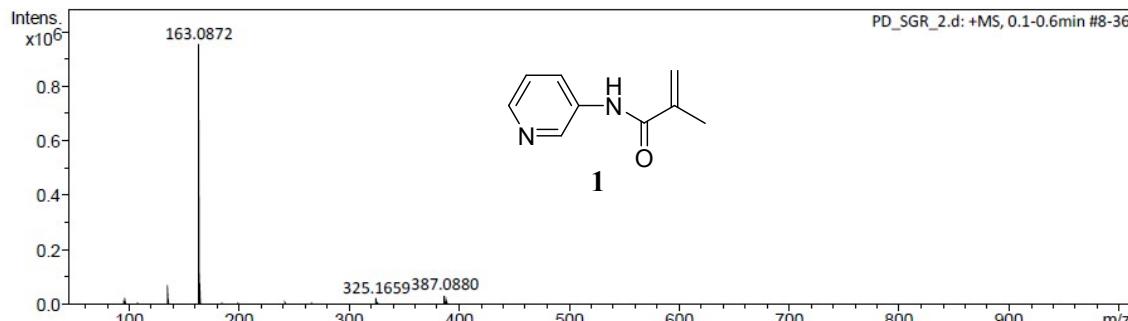
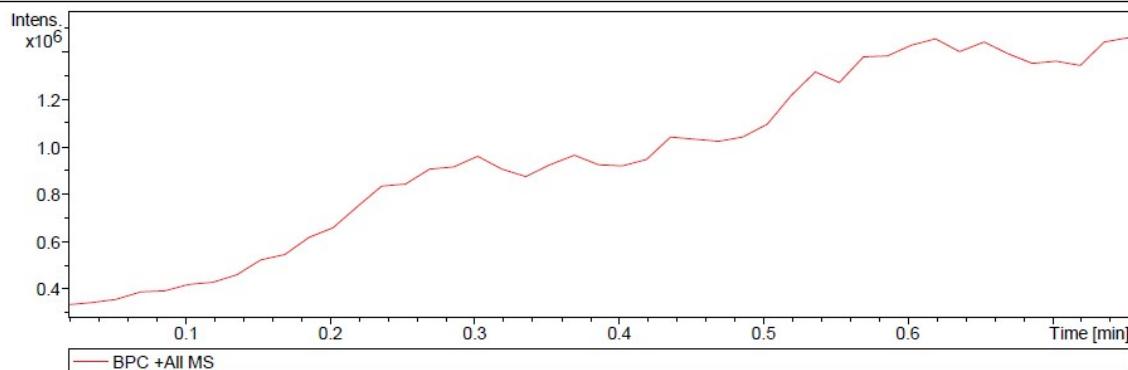
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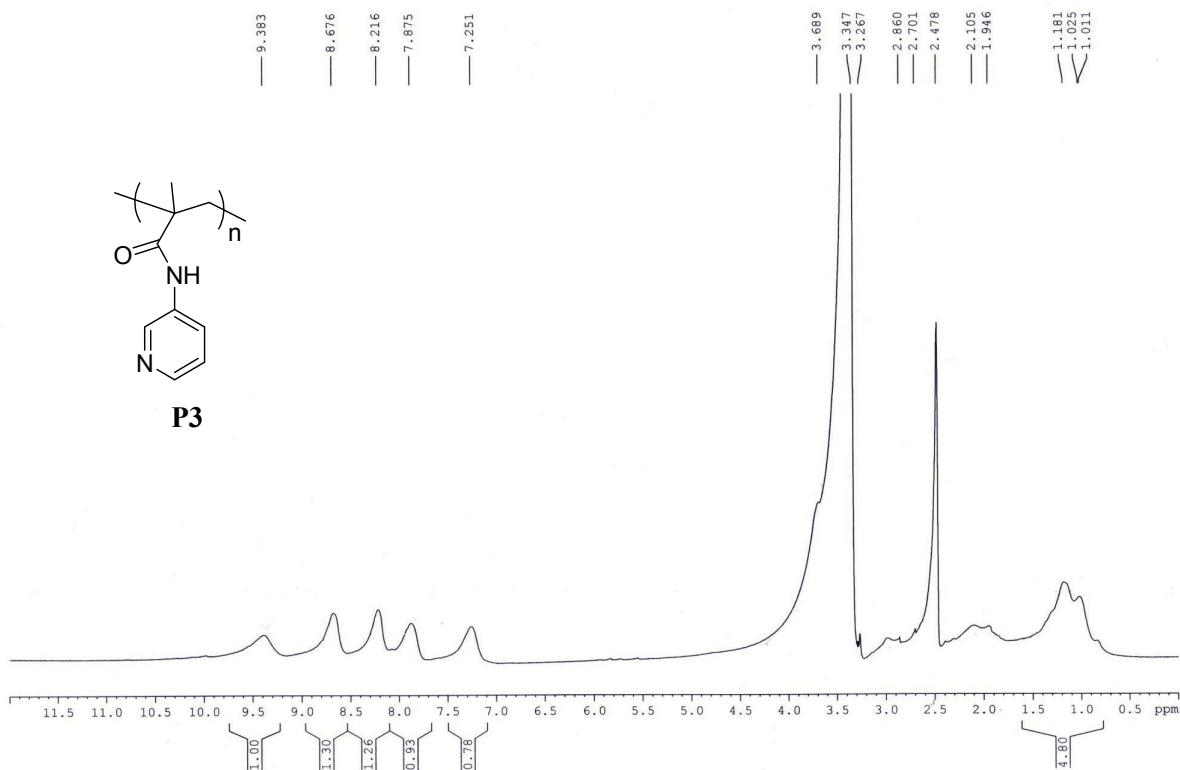
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Scan End	1000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



**$^1\text{H}$  NMR of P3 in  $\text{d}_6\text{-DMSO}$  (400 MHz)**



**$^{13}\text{C}$  NMR of P3 in  $\text{d}_6\text{-DMSO}$  (100 MHz)**

