Electronic Supporting Information

Naphthalene linked pyridyl urea as supramolecular gelator: A new insight in naked eye detection of I^- in the gel state with semiconducting behaviour

Kumaresh Ghosh[*a], Santanu Panja[a] and Subratanu Bhattacharya[b]

[a]Department of Chemistry, University of Kalyani, Kalyani-741235, India. Email: ghosh_k2003@yahoo.co.in, Fax: +913325828282; Tel: +913325828750; [b]Department of Physics, University of Kalyani, Kalyani-741235, India

Table 1S. Result of gelation test for **1-5**.

Solvents	**1**	**2**	**3**	**4**	**5**
$CHCl_3$	I	I	I	S	I
2% Methanol in $CHCl_3$	S	S	I	S	I
CH_3COCH_3	S	I	I	S	I
CH_3COCH_3:H_2O (1:1, v/v)	P	I	I	S	I
DMF	S	S	S	S	I
DMF :H_2O (1:1, v/v)	S	G (8 mg/mL)	P	S	I
CH_3CN	S	I	I	S	I
CH_3CN :H_2O (1:1, v/v)	P	I	I	S	I
CH_3OH	S	I	I	S	S
CH_3OH : :H_2O (1:3, v/v)	G (10 mg/mL)	I	I	S	P
DMSO	S	S	S	S	P
DMSO : H_2O (1:1, v/v)	S	G (8 mg/mL)	P	S	I
DMSO : H_2O (1:2, v/v)	G (6 mg/mL)	G (5 mg/mL)	P	P	I
S = solution, G = gel (minimum gelation concentration), I= insoluble, P = precipitation.					

Fig. 1S. Hydrogels of **2** prepared from (a) DMSO: H_2O (1:2, v/v) and (b) DMF:H_2O (1:1, v/v).

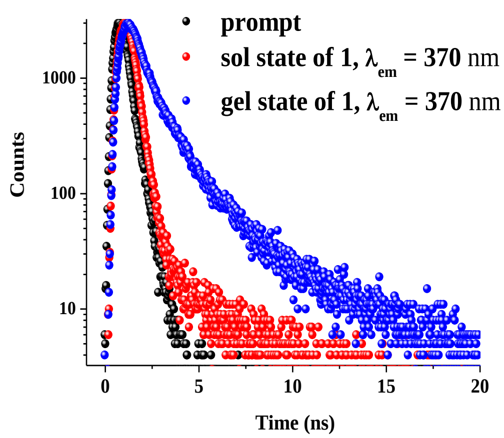


Fig. 2S. Comparison of fluorescence decays of **1** (λ_{ex} = 295 nm, λ_{em} = 370 nm) in solution and gel states in DMSO: H_2O (1:2, v/v).

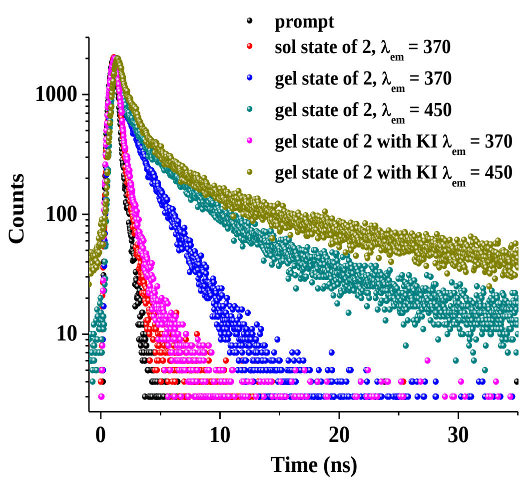


Fig. 3S. Comparison of fluorescence decays of **2** (λ_{ex} = 295 nm) in solution and gel states in DMSO: H_2O (1:2, v/v).

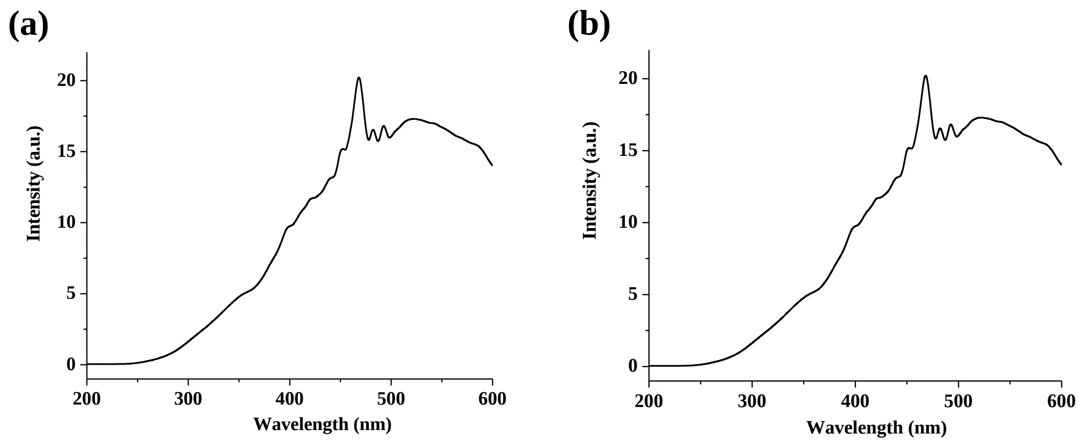


Fig 4S. Excitation spectra of **1** in gel state at emissions (a) 365 nm and (b) 416 nm.

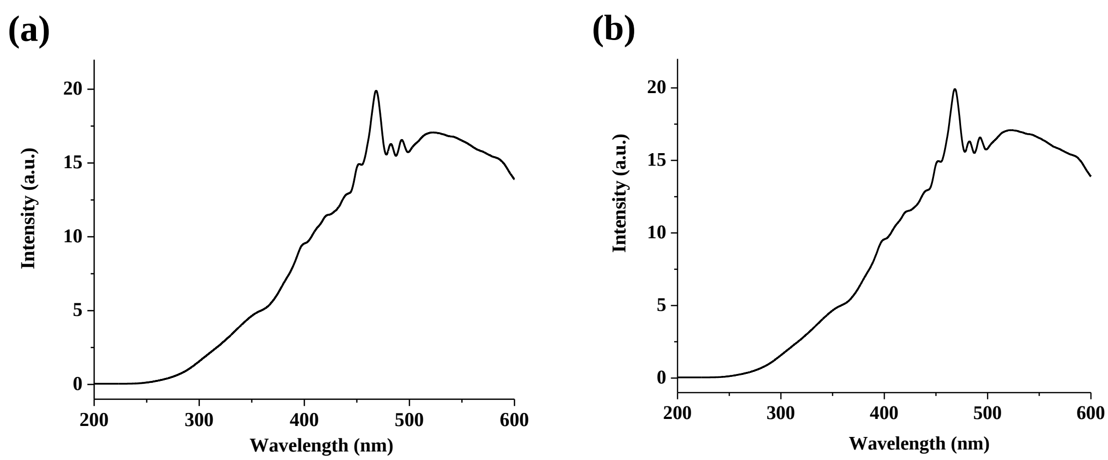


Fig. 5S. Excitation spectra of gel state of **2** at emissions (a) 367 nm and (b) 435 nm.

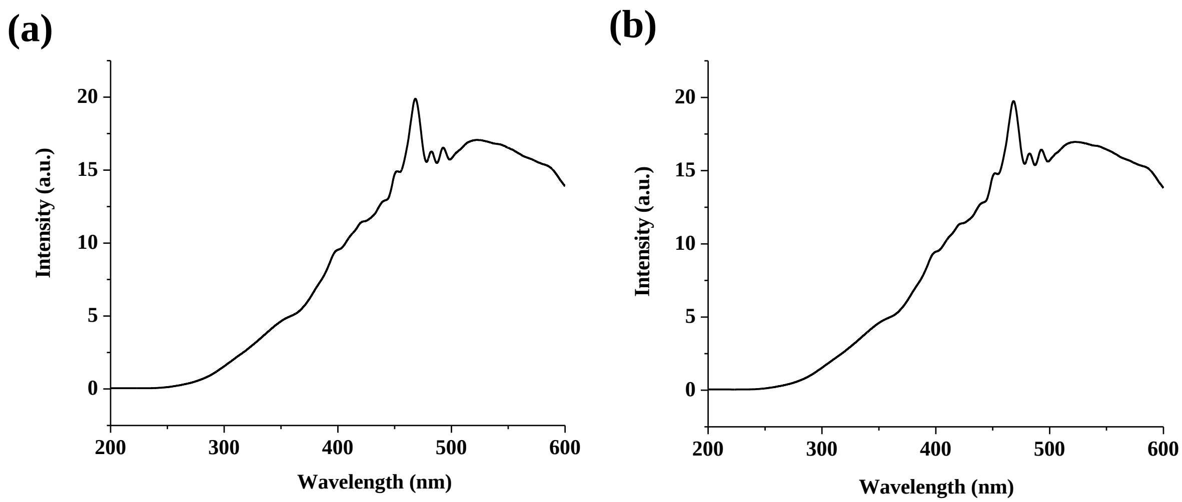


Fig. 6S. Excitation spectra of sol state of **1** (a) and **2** (b) at emissions 374 nm and 380 nm.

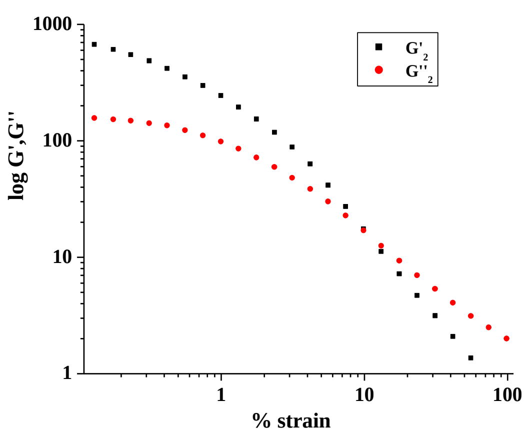
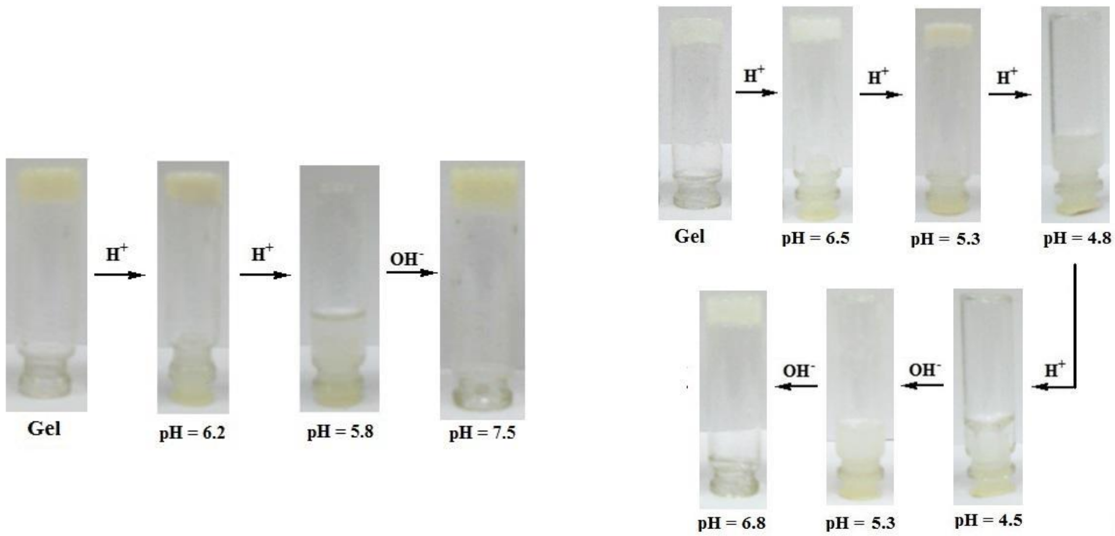


Fig. 7S. Rheological data for DMSO : H_2O (1:2, v/v) gel of **2**.



(a) (b)

Fig. 8S. Photograph showing the pH dependency of the hydrogels of **1** (a) and **2** (b) **(**in DMSO: H_2O, 1:2 v/v, 10 mg/ mL).

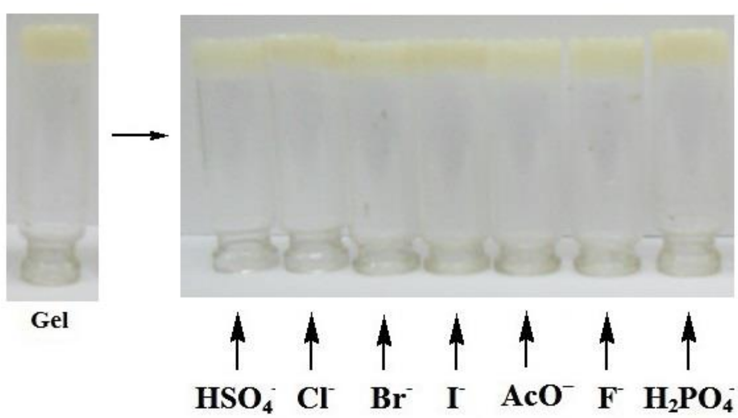


Fig. 9S. Photograph showing the changes in the DMSO: H_2O (1:2, v/v) gel of **1** (10 mg/ mL) after keeping contact with 1 mL aqueous solution of different anions (c = 9.5 x 10^{-2} M as K^+ salt) for 2h.

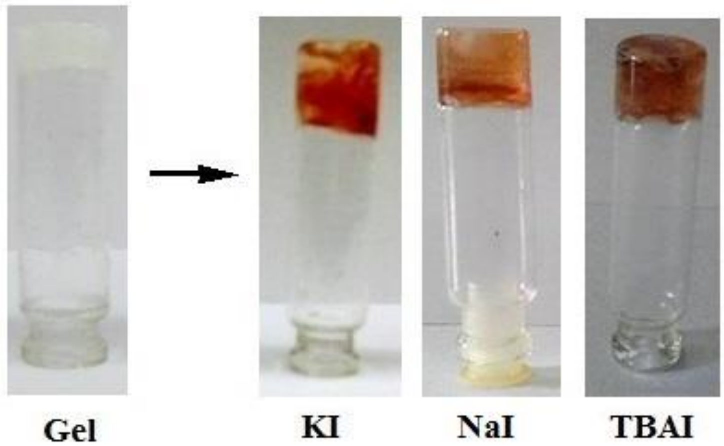


Fig. 10S. Photograph showing the colour change of the hydrogel of **2 (**in DMSO: H_2O, 1:2 v/v, 10 mg/mL) in presence of KI, NaI and TBAI after 2h, respectively.

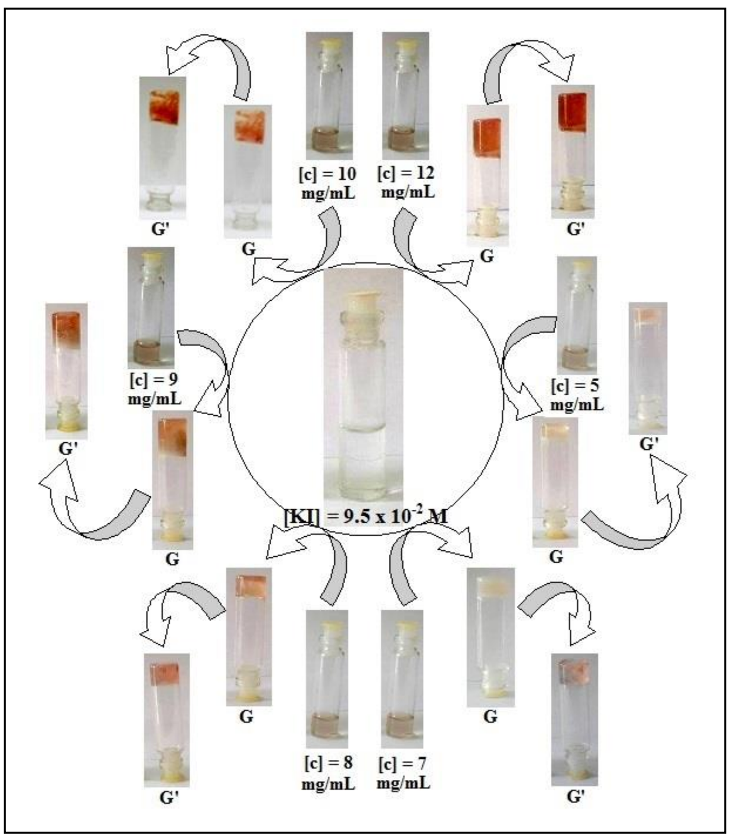


Fig. 11S. Photograph showing the color changes in the gel state of **2** (where [c] represent the amount of gelators taken) in presence of 4 equiv amounts of aqueous KI (c = 9.5 x 10^{-2} M) with time (where G and G' represent states of the gels after 1h and 2h, respectively).

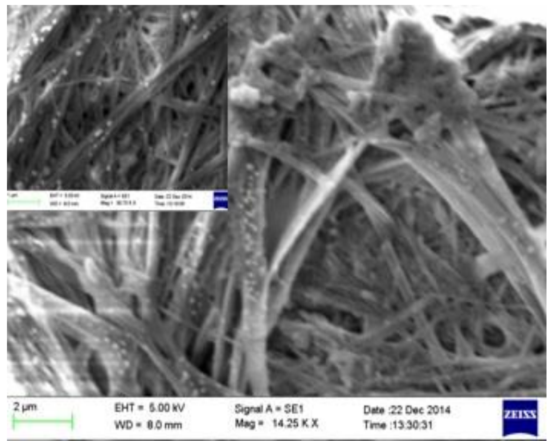


Fig. 12S. (a) SEM image of hydrogel of **2** with KI from DMSO : H_2O (1:2, v/v); (b) Photograph showing the color change of iodide treated gel of **2** in the presence of $AgNO_3$ (c = 0.5 M).

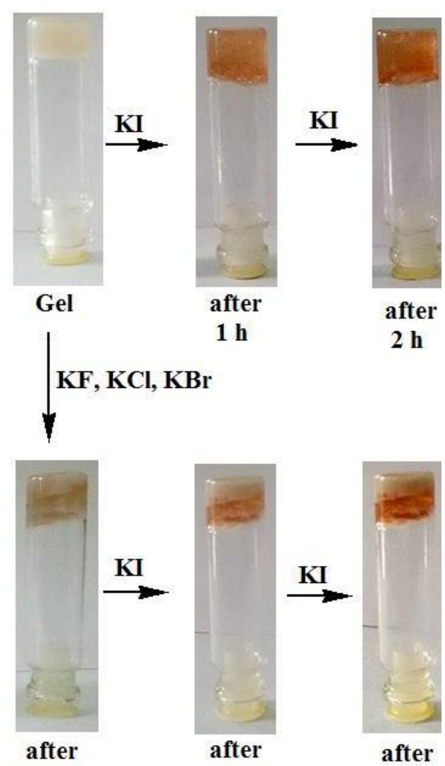


Fig. 13S. Photograph showing the colour change and selectivity of the hydrogel of **2 (**in DMF: H_2O, 1:1 v/v, 10 mg/ mL) towards KI (c = 0.2 M; added in 500 μL amount) in absence and presence of 100 μL of each solution of KF, KCl and KBr (c = 0.2 M).

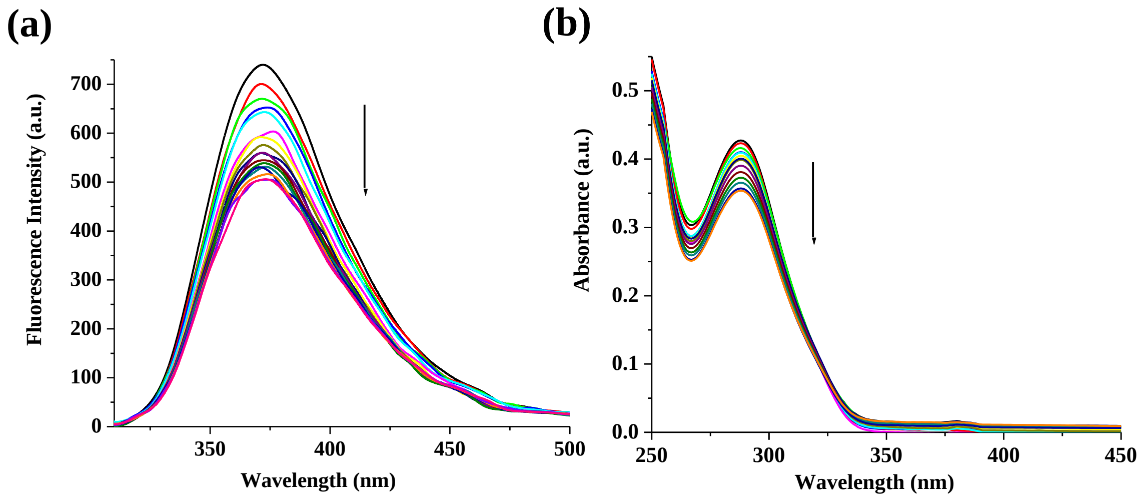


Fig. 14S. Change in (a) emission and (b) absorbance of **1** (c = 3.85 x 10^{-5} M) upon addition of 30 equiv. of TBAI (c = 1.54 x 10^{-3} M) in DMSO: H_2O (1:2, v/v).

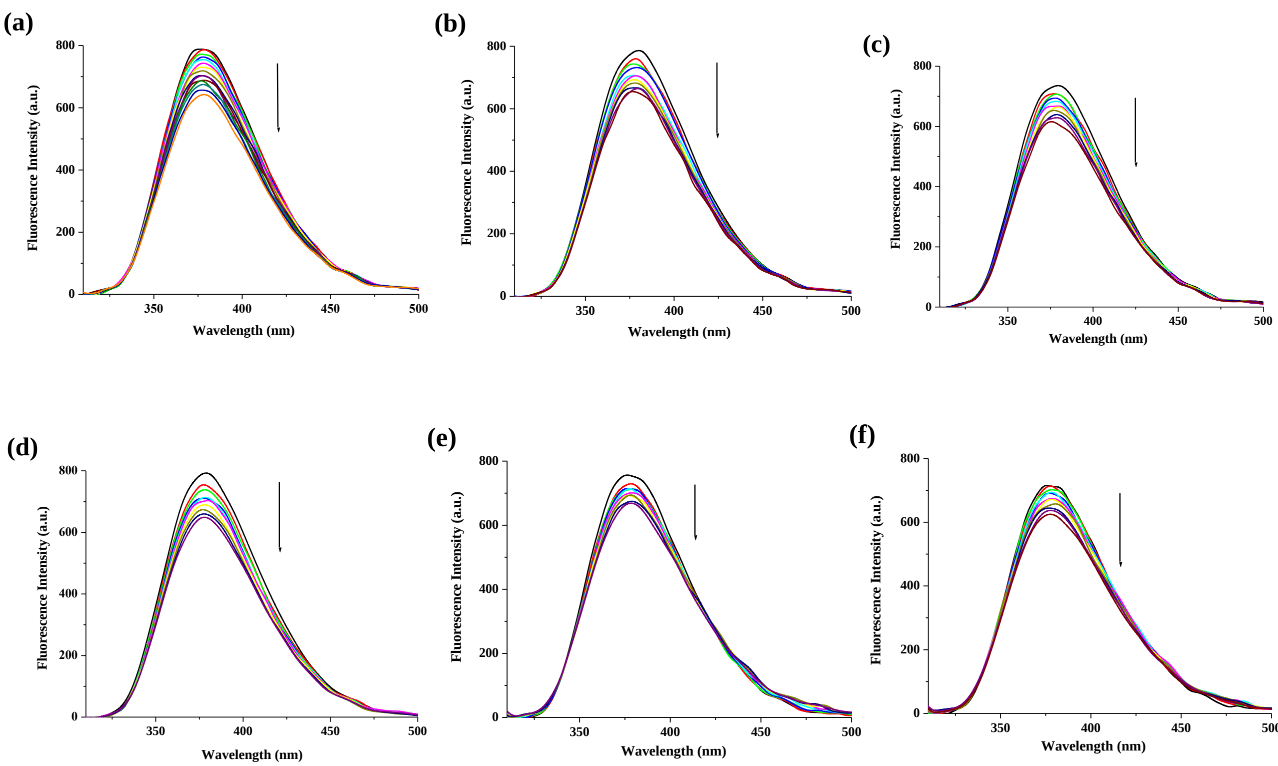


Fig. 15S. Change in emission of **2** (c = 3.85 x 10^{-5} M) upon addition of 30 equiv. of (a) F^-, (b) Cl^-, (c) Br^-, (d) AcO $^-$, (e) $H_2PO_4^-$, (f) HSO_4^- (c = 1.54 x 10^{-3} M) in DMSO: H_2O (1:2, v/v) (counter cation: tetrabutylammonium ion).

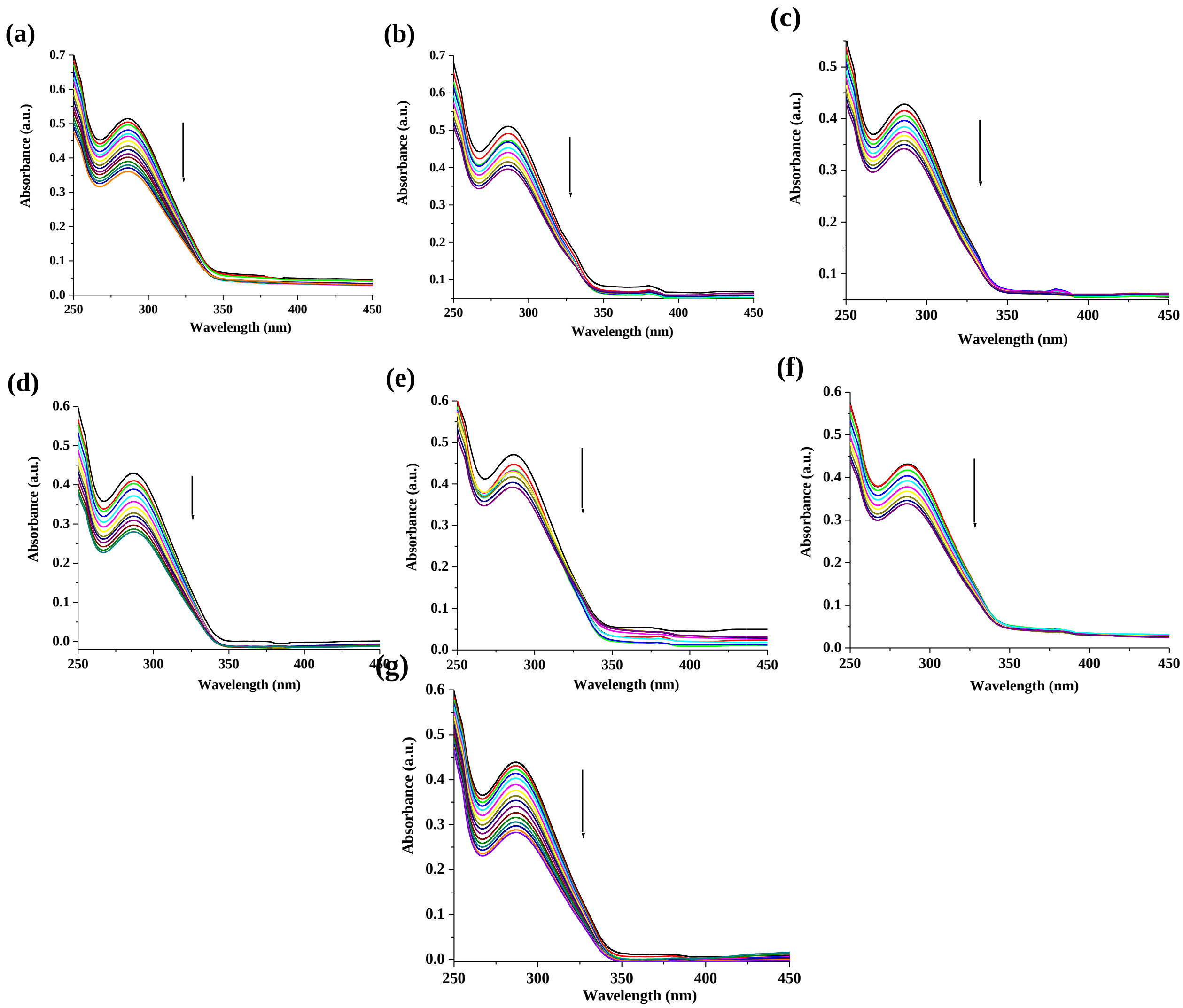


Fig. 16S. Change in absorbance of **2** (c = 3.85 x 10^{-5} M) upon addition of 30 equiv. of (a) F^-, (b) Cl^-, (c) Br^-, (d) AcO $^-$, (e) $H_2PO_4^-$, (f) HSO_4^-, (g) I^- (c = 1.54 x 10^{-3} M) in DMSO: H_2O (1:2, v/v) (counter cation: tetrabutylammonium ion).

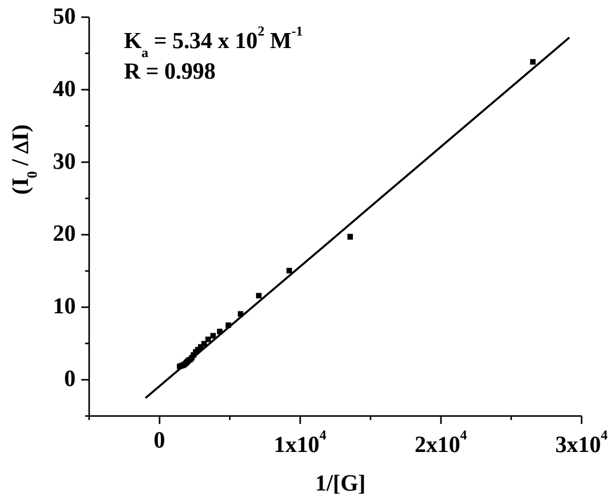
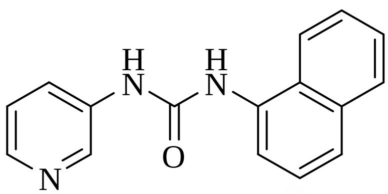
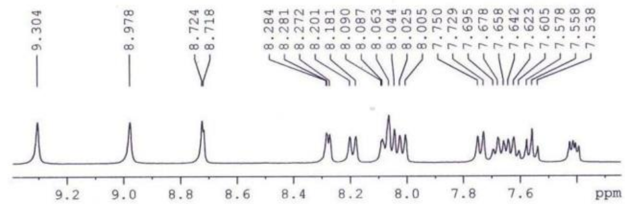


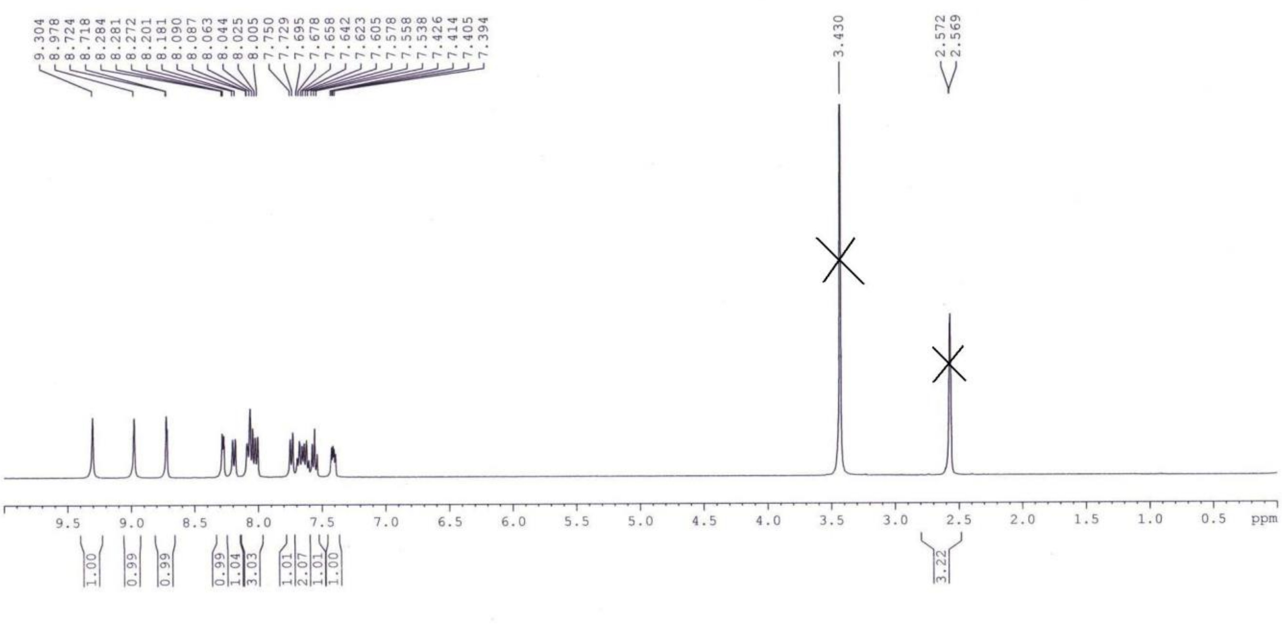
Fig. 17S. Benesi–Hilderband plot for **2** (c = 3.85 x 10^{-5} M) with I^- (c = 1.54 x 10^{-3} M) at 378 nm.

^{1}H NMR (d_6-DMSO, 400 MHz)

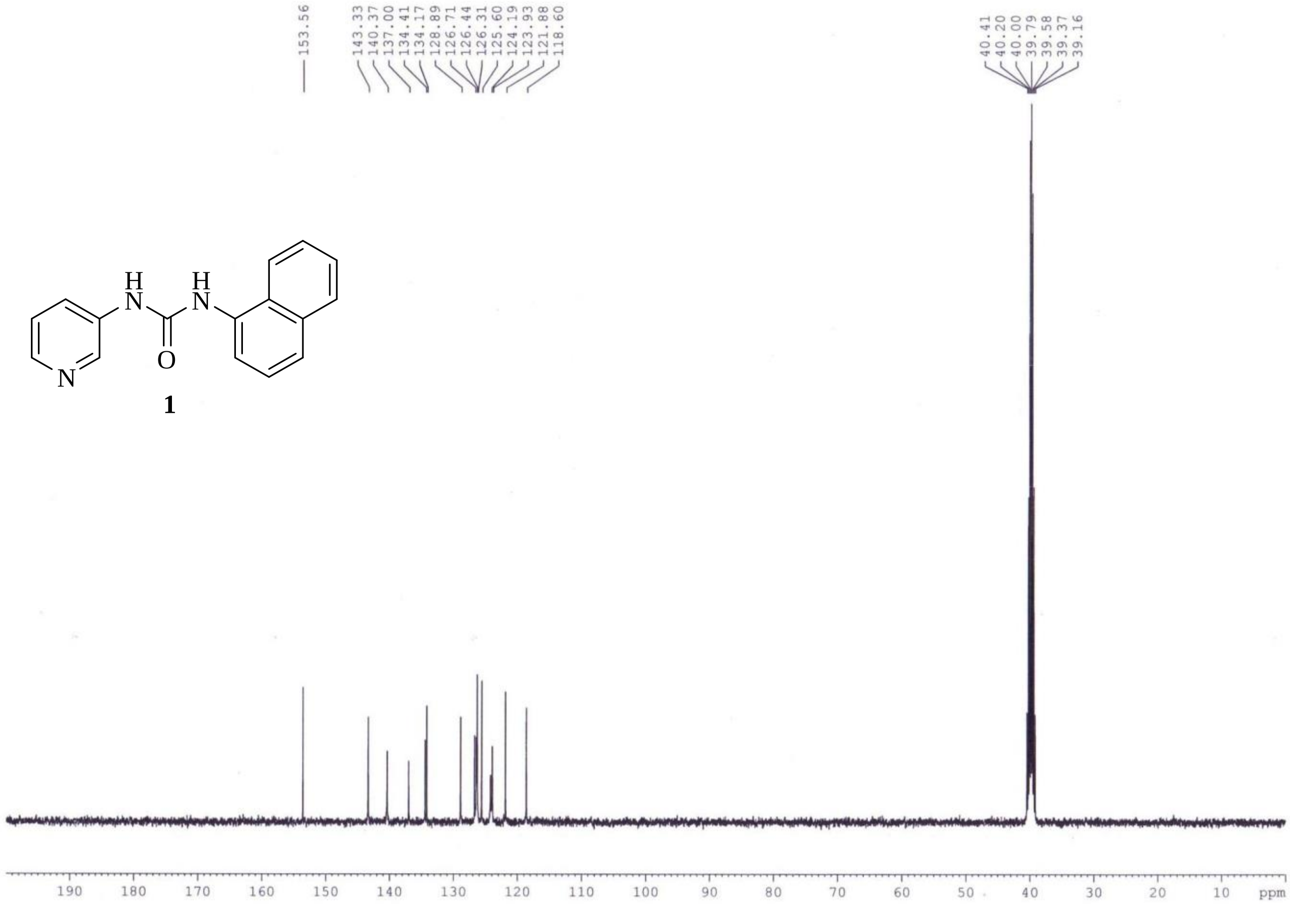


1



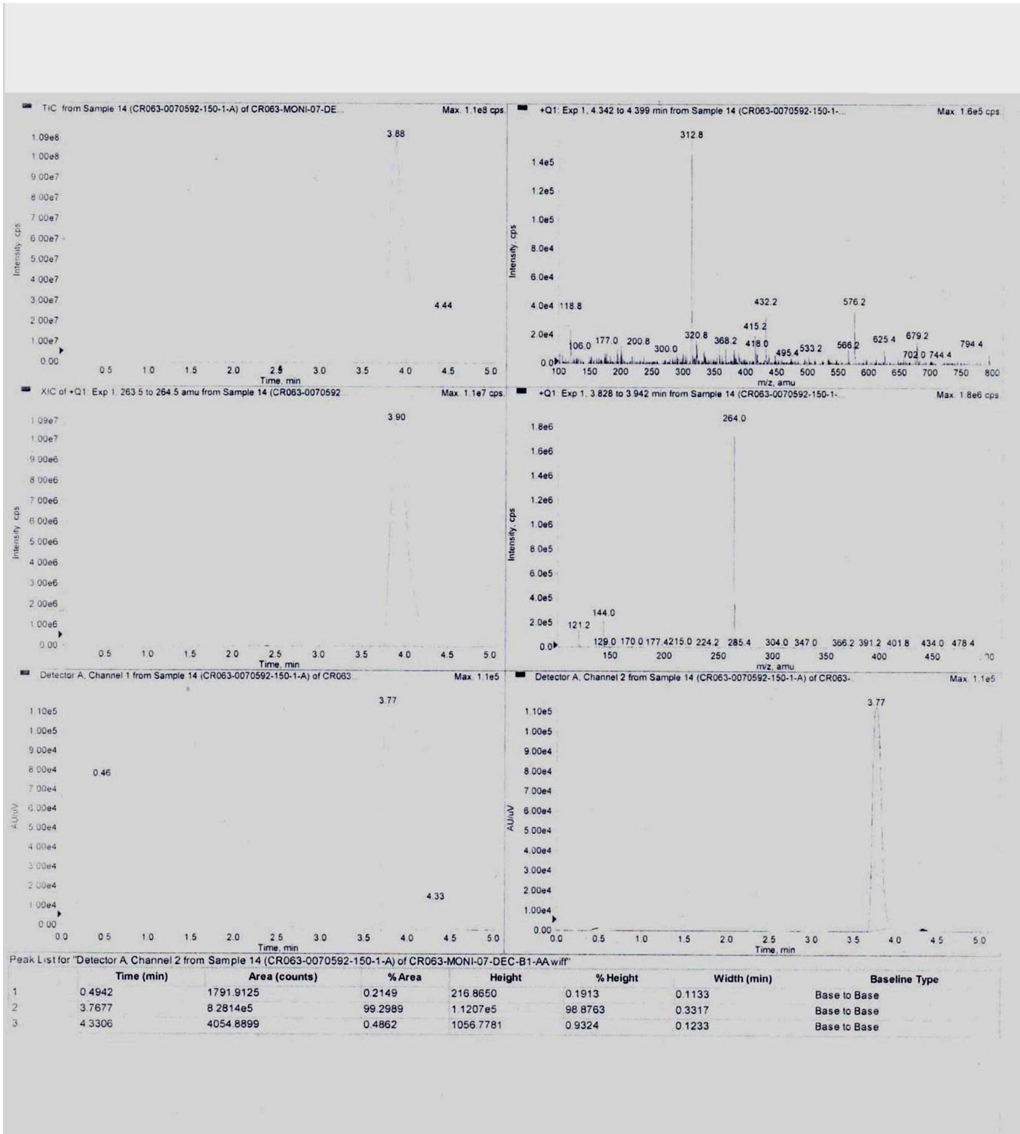


^{13}C NMR (d_6-DMSO, 100 MHz)

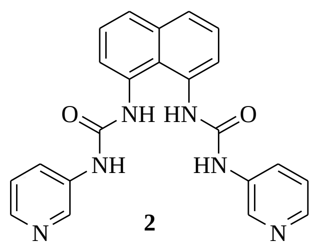


1

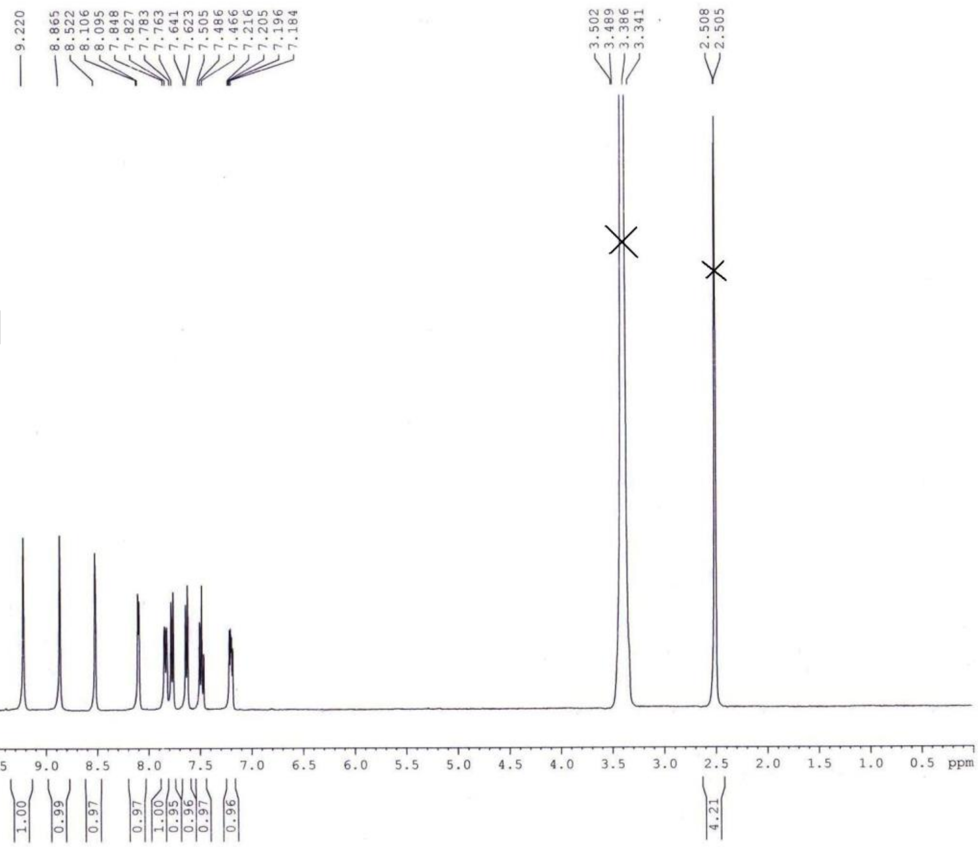
Mass spectrum of 1.



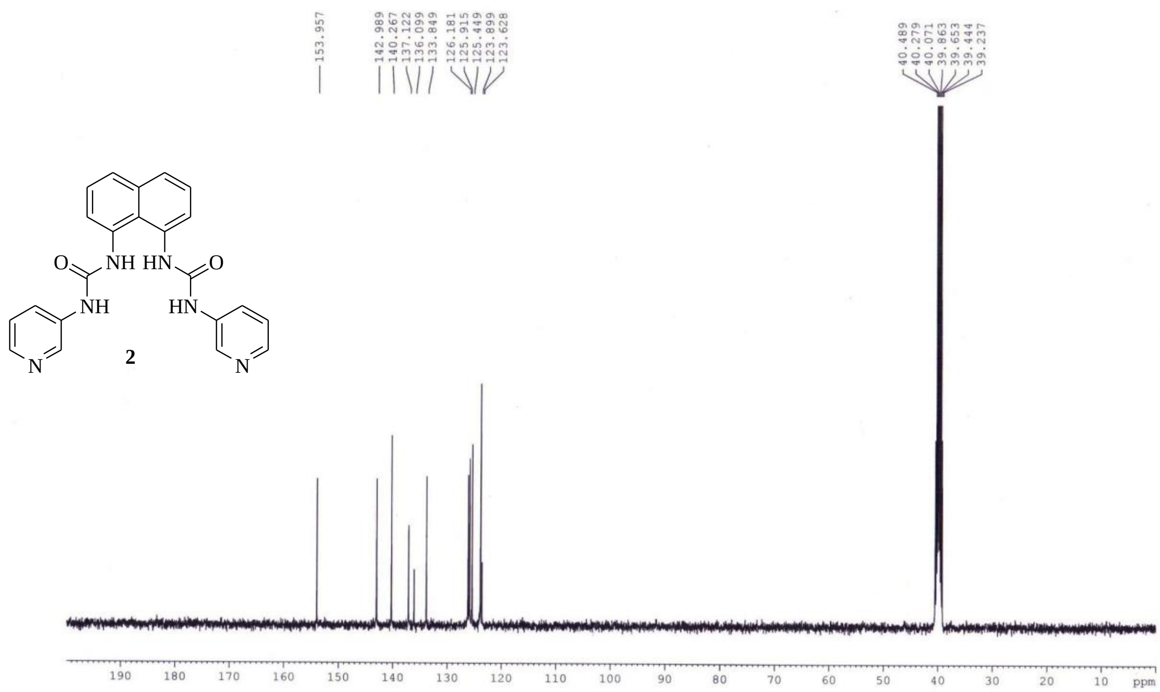
^{1}H NMR (d_6-DMSO, 400 MHz)



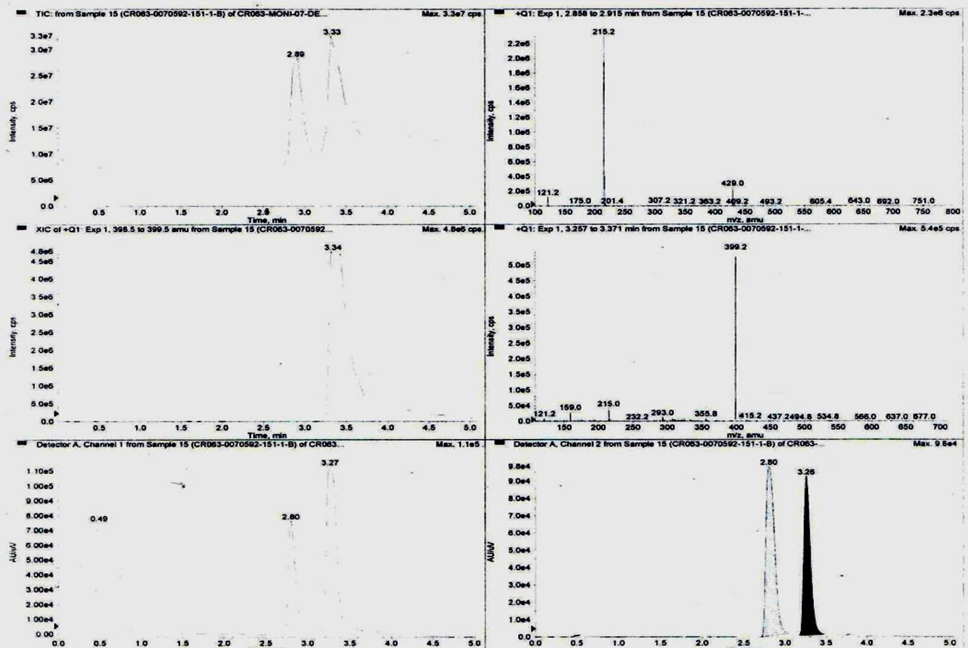
2



^{13}C NMR (d_6-DMSO, 100 MHz)



Mass spectrum of 2.



Peak List for "Detector A, Channel 2 from Sample 15 (CR063-0070592-151-1-B) of CR063-MONI-07-DEC-81-AA.wiff"

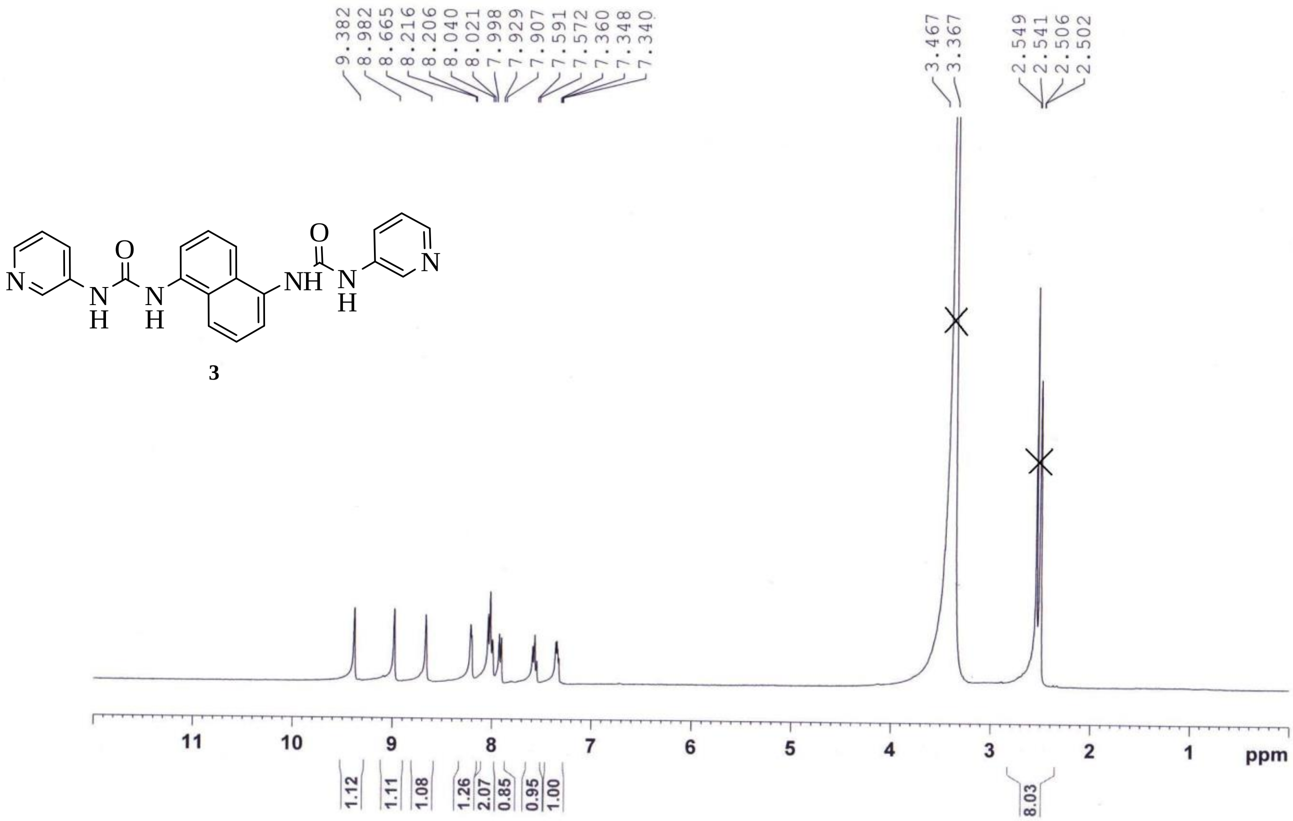
	Time (min)	Area (counts)	% Area	Height	% Height	Width (min)	Baseline Type
1	0.5342	1690.9735	0.1374	189.3480	0.0997	0.1200	Base to Base
2	2.8044	7.1894e5	58.4023	9.7888e4	51.5308	0.3350	Base to Base
3	3.2600	5.0993e5	41.4231	9.1707e4	48.2767	0.3083	Base to Base
4	3.7869	457.7405	0.0372	176.3530	0.0928	0.0600	Base to Base

LCMS REACTION MONITORING SAMPLE — COLUMN: Zorbax

Channel 1 at wavelength 220 nm,
Channel 2 at wavelength 260 nm

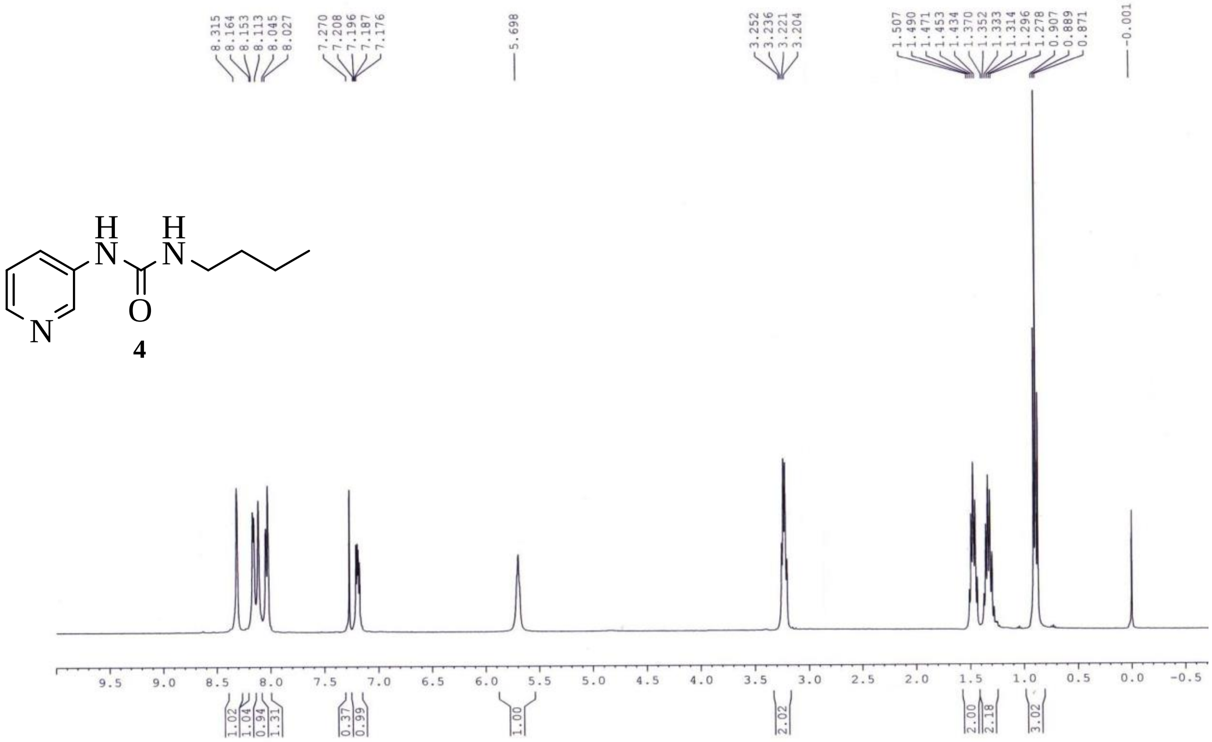
NH4OAc:ACN

^{1}H NMR (d_6-DMSO, 400 MHz)



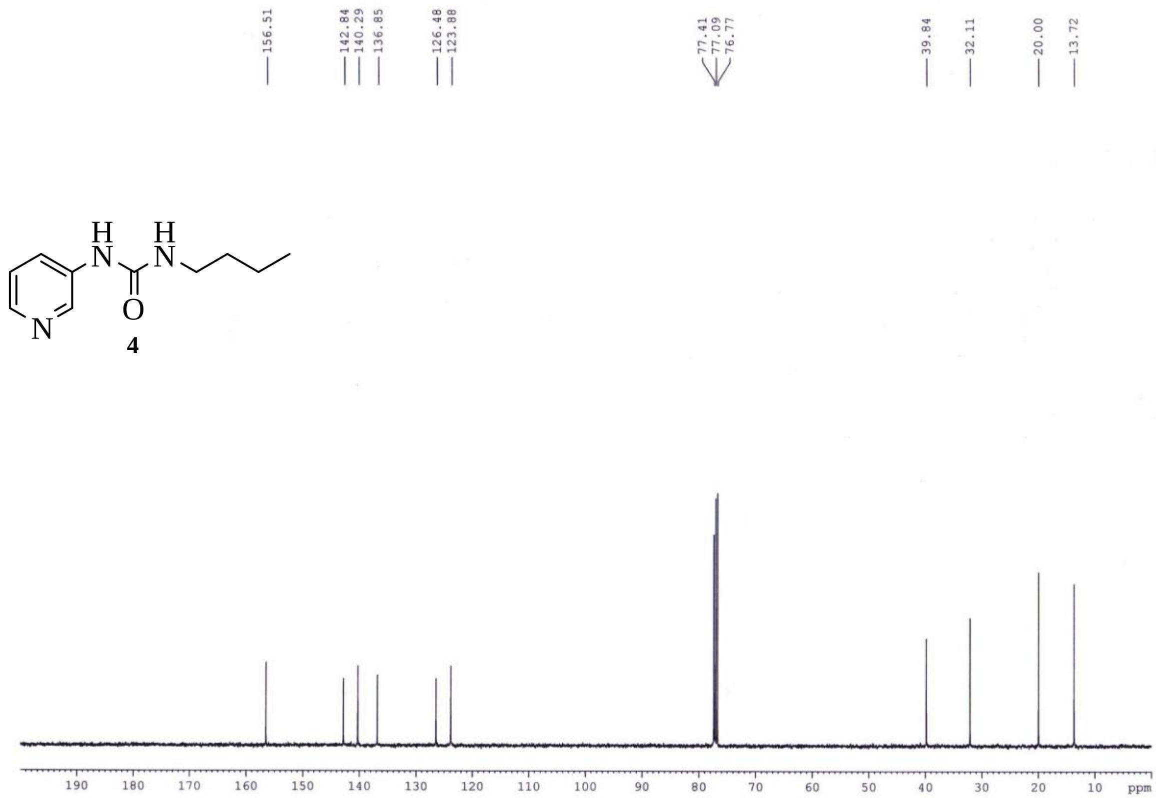
3

^{1}H NMR ($CDCl_3$, 400 MHz)



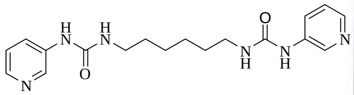
4

[13]C NMR ($CDCl_3$, 100 MHz)

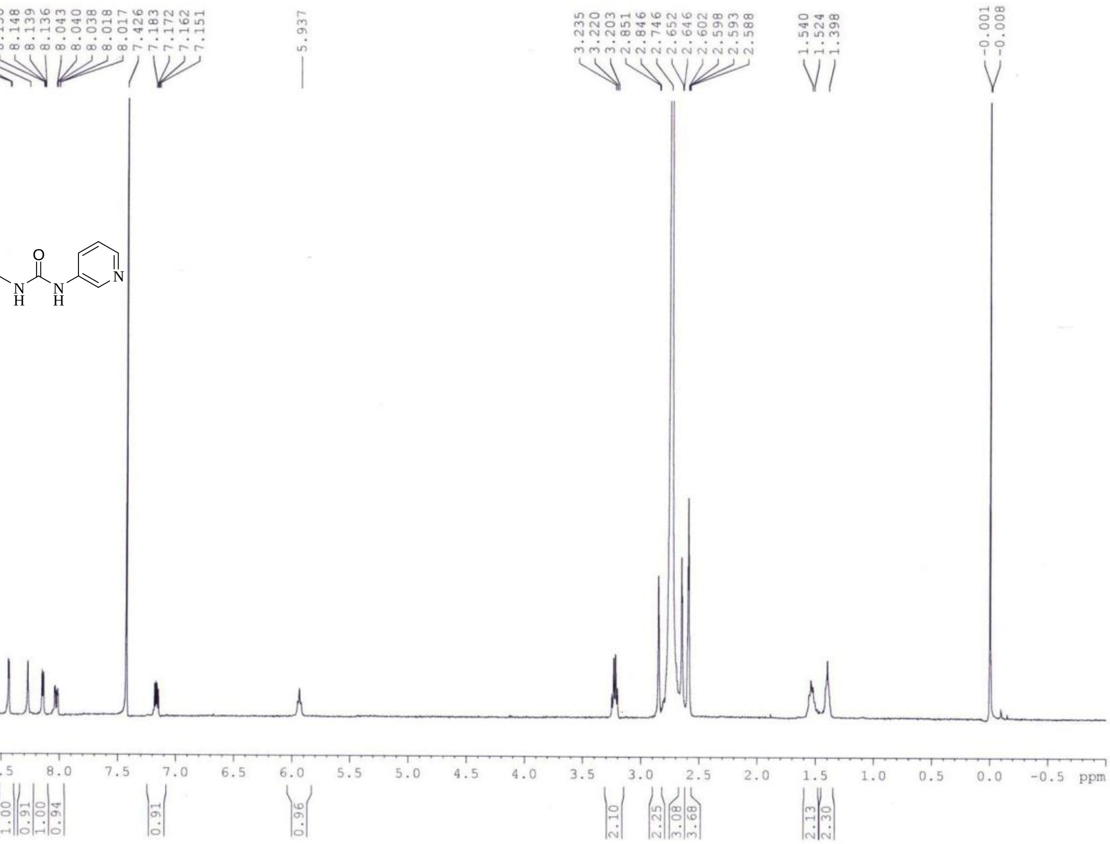


4

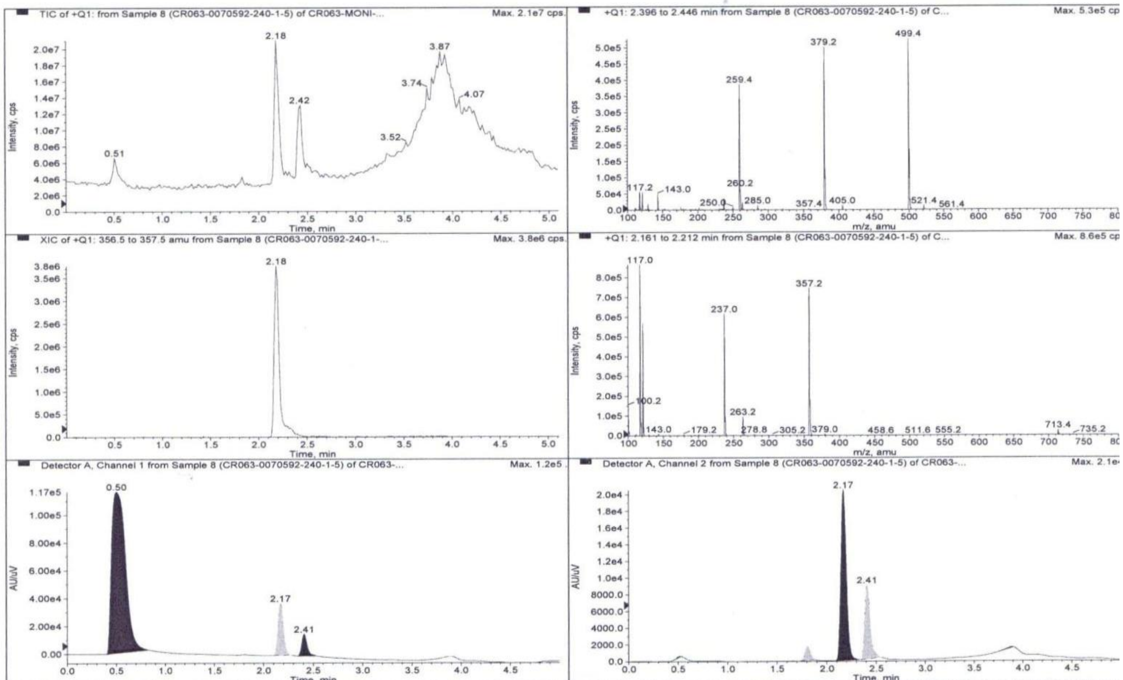
^{1}H NMR ($CDCl_3$ containing one drop of d_6-DMSO, 400 MHz)



5



Mass spectrum of 5.



Peak List for "Detector A, Channel 1 from Sample 8 (CR063-0070592-240-1-5) of CR063-MONI-22-MA

	Time (min)	Area (counts)	% Area	Height	% Height	Width (min)
1	0.5017	1.1611e6	85.1930	1.1602e5	68.5214	0.4283
2	2.1707	1.4061e5	10.3170	3.7395e4	22.0859	0.1867
3	2.4091	6.0095e4	4.4092	1.5657e4	9.2469	0.1967
4	3.8913	1100.8090	0.0808	246.9217	0.1458	0.0950

Peak List for "Detector A, Channel 2 from Sample 8 (CR063-0070592-240-1-5) of CR063-MONI-22-M

	Time (min)	Area (counts)	% Area	Height	% Height	Width (min)
1	0.5192	297.8191	0.2486	93.6618	0.3005	0.0733
2	1.8053	6145.8421	5.1303	1684.0760	5.4028	0.1517
3	2.1687	7.8826e4	65.8012	2.0435e4	65.5589	0.2517
4	2.4069	3.4086e4	28.4535	8883.7564	28.5006	0.2150
5	3.8908	438.9685	0.3664	73.9284	0.2372	0.1433

LCMS MONITORING SAMPLE

COLUMN: Zorbax Extend C18(4.6X50mm)

Channel 1 at wavelength 220 nm,
Channel 2 at wavelength 260 nm

NH4OAc:ACN