Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information

Pyridine/pyridinium Symmetrical Bisamides as Functional Materials: Aggregation, Selective Sensing and Drug release

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Table 1S. Results of gelation test for **1** and **2**.

Solvent	1	2
$CHCl_3$	PS	I
DCM	I	I
$CHCl_3$: MeOH (10:1,v/v)	S	PS
$CHCl_3$: MeOH (1:1,v/v)	S	S
MeOH	S	S
Acetonitrile	PS	I
n-Hexane	I	I
Diethyl ether	I	I
1,4-Dioxane	S	PS
THF	S	I
DMF	S	S
DMSO	S	S
THF : H_2O (1:1, v/v)	P	P
DMF : H_2O (1:1, v/v)	S	S
MeOH : H_2O (1:1, v/v)	S	P
Acetonitrile : H_2O (1:1, v/v)	I	I
1,4-Dioxane : H_2O (1:1, v/v)	S	I
DMSO: H_2O (1:1, v/v)	S	S
MeOH : H_2O (1:1, v/v) + Ag^+	G	P
MeOH : H_2O (1:1, v/v) + Cu^{2+}	G	P
THF : H_2O (1:1, v/v) + Ag^+	G	P
THF : H_2O (1:1, v/v) + Cu^{2+}	G	P
1,4-Dioxane : H_2O (1:1, v/v) + Ag^+	G	P
1,4-Dioxane : H_2O (1:1, v/v) + Cu^{2+}	G	P
DMF : H_2O (1:1, v/v) + Ag^+	G	G
DMF : H_2O (1:1, v/v) + Cu^{2+}	G	P
DMSO : H_2O (1:1, v/v) + Ag^+	G (2 mg/mL)	G (2.2 mg/mL)
DMSO : H_2O (1:1, v/v) + Cu^{2+}	G (1.8 mg/mL)	P

S = solution; G = gel (minimum gelatination concentration); I = insoluble; P = precipitation; PS = partially soluble.

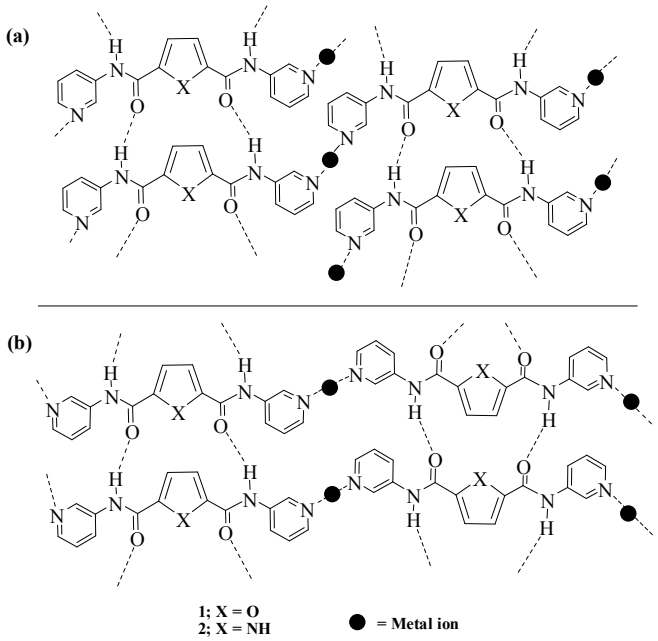


Fig. 1S. Suggested modes of interactions of **1** and **2** in gel states.

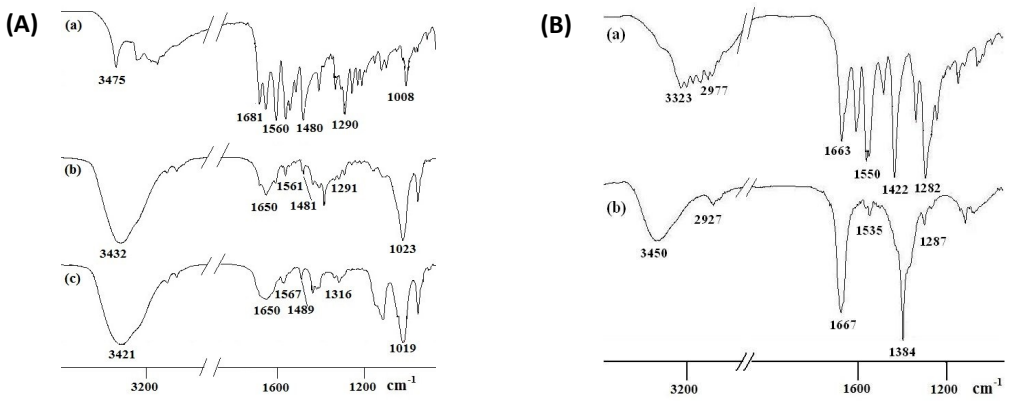


Fig. 2S. (A) Partial FTIR spectra of **1** in its amorphous (a) and gel states with Ag^{+} (b) and Cu^{2+} (c); (B) Partial FTIR spectra of **2** in its (a) amorphous and (b) gel state with Ag^{+}.

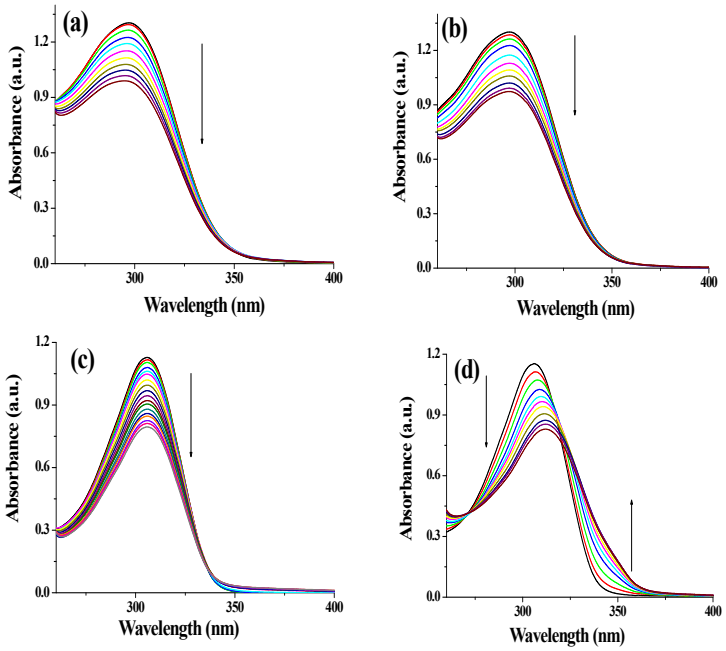


Fig. 3S. Change in UV-vis spectra of (a) **1**-Ag^{+}, (b) **1**-Cu^{2+}, (c) **2**-Ag^{+} and (d) **2**-Cu^{2+} ([ligand]= 2.50 x 10^{-5} M and [metal]= 1.0 x 10^{-3} M) in presence of 15 equiv. amounts of metal ions in DMSO: H_2O (1:1, v/v).

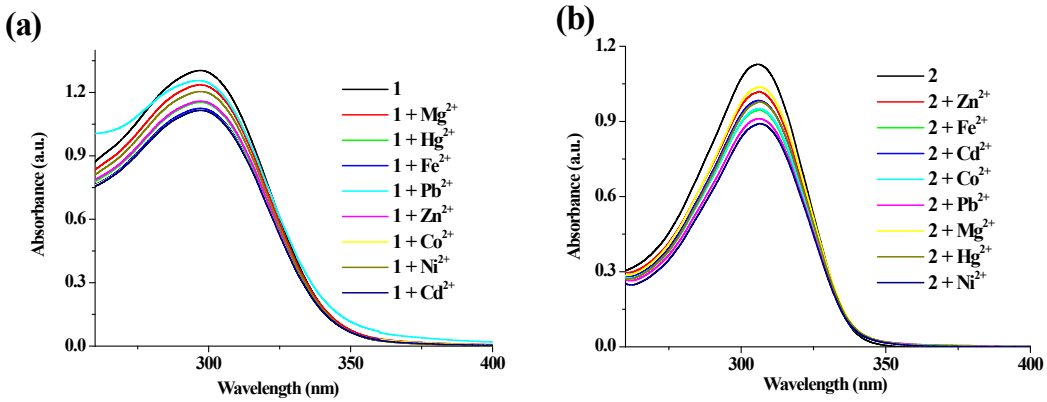


Fig. 4S. UV-vis spectra of (a) **1** and (b) **2** (*c* = 2.50 x 10^{-3} M) in presence of 15 equiv. amounts of different metal ions (*c* = 1.0 x 10^{-3} M) in DMSO: H_2O (1:1, v/v).

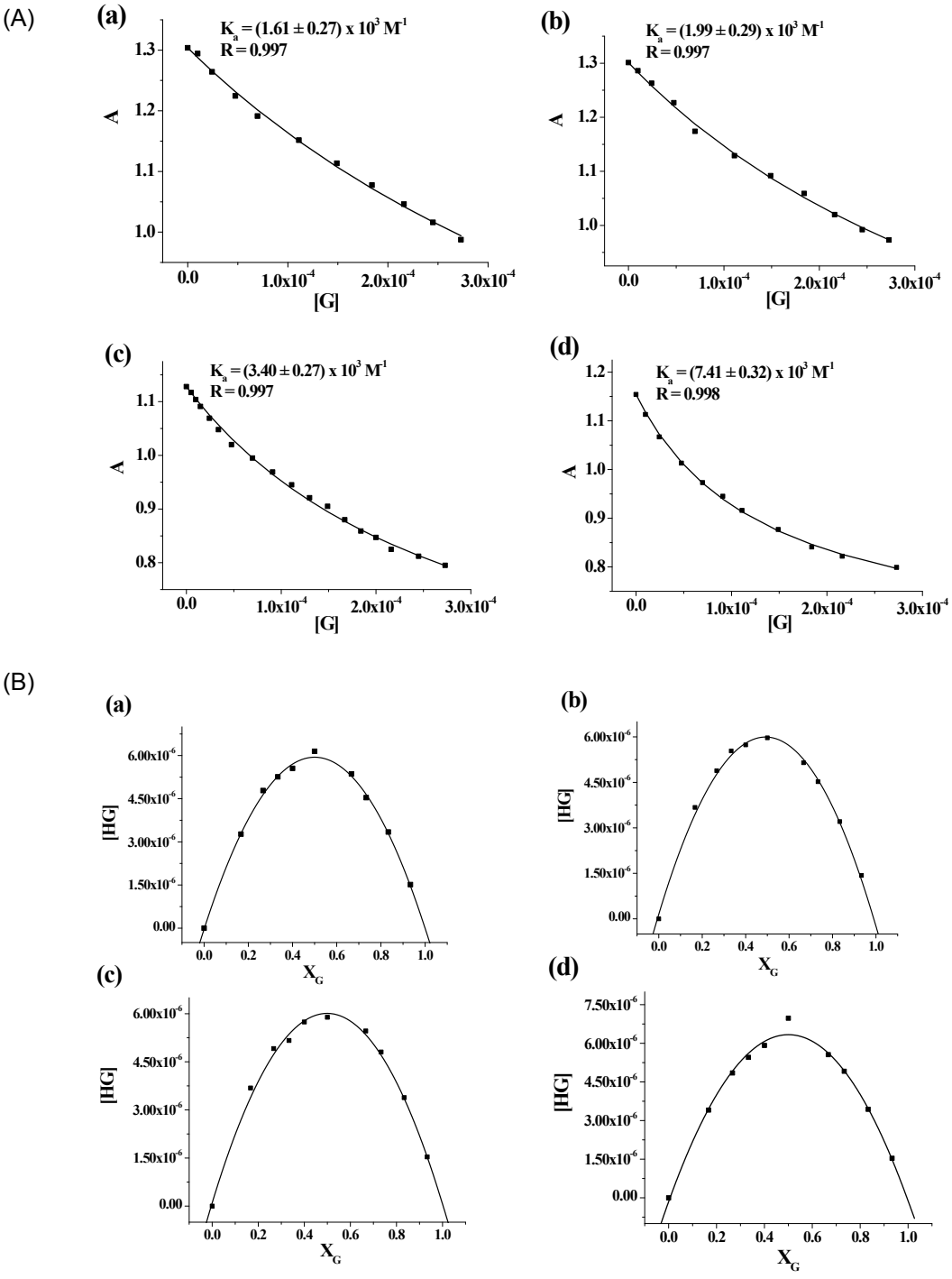


Fig. 5S. (A) Non linear binding constant curves for (a) **1**-Ag^+, (b) **1**-Cu^{2+}, (c) **2**-Ag^+ and (d) **2**-Cu^{2+} in DMSO: H_2O (1:1, v/v) and (B) Job plots for (a) **1**-Ag^+, (b) **1**-Cu^{2+}, (c) **2**-Ag^+ and (d) **2**-Cu^{2+} using UV titration data ([H] = [G] = 2.5 x 10^{-5} M).

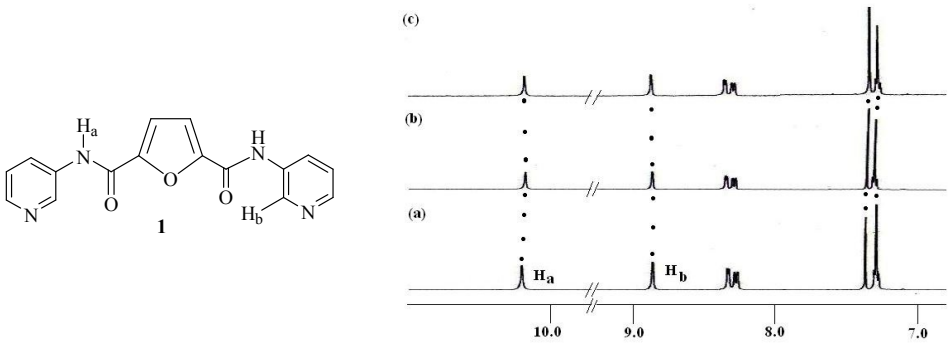


Fig. 6S. Partial ^{1}H-NMR spectra of (a) **1** (c = 1.38 x 10^{-2} M), (b) **1** with Cu^{2+} (1:1) and (c) **1** with Ag^{+} (1:1) in $CDCl_3$ containing few drops of d_6-DMSO.

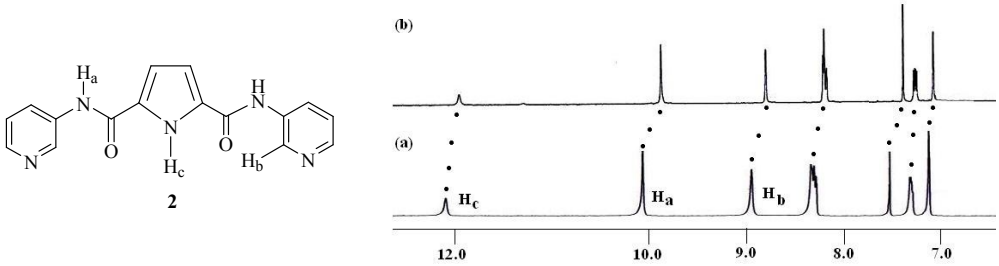


Fig. 7S. ^{1}H-NMR spectra of (a) **2** (c = 1.38 x 10^{-2} M) and (b) **2** with Ag^{+} (1:1) in $CDCl_3$ containing few drops of d_6-DMSO.

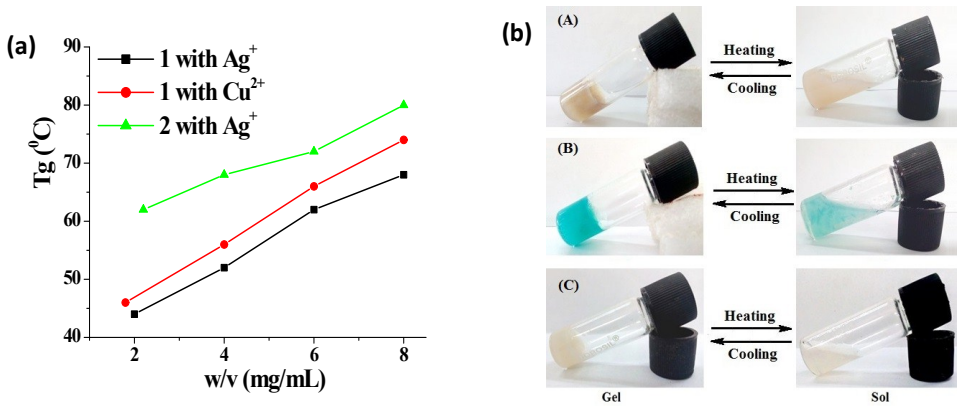


Fig. 8S. (a) Variation of gel melting temperature (Tg) with increasing concentration of gelators in DMSO: H_2O (1:1, v/v) in presence of 2 equiv. amounts of respective metal ions and (b) Pictorial representation of the thermo reversibility of the DMSO: H_2O (1:1, v/v) gels of (A) **1**-Ag^{+} (B) **1**-Cu^{2+} and (C) **2**-Ag^{+} ([gelator] = 5 mg/mL with 2 equiv. of metal ions).

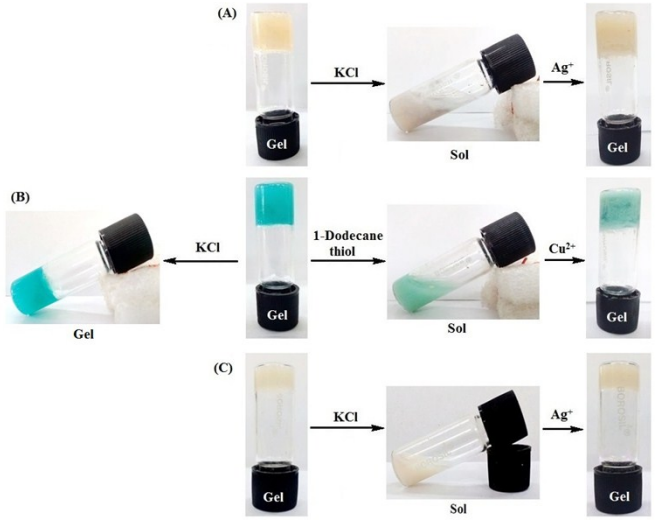


Fig. 9S. Chemical responsiveness of the gel of (A) **1**-Ag^{+} (B) **1**-Cu^{2+} and (C) **2**-Ag^{+} ([gelator] = 5 mg/mL with 2 equiv. of metal ions) in presence of external chemical stimulus (*c* = 0.05 M).

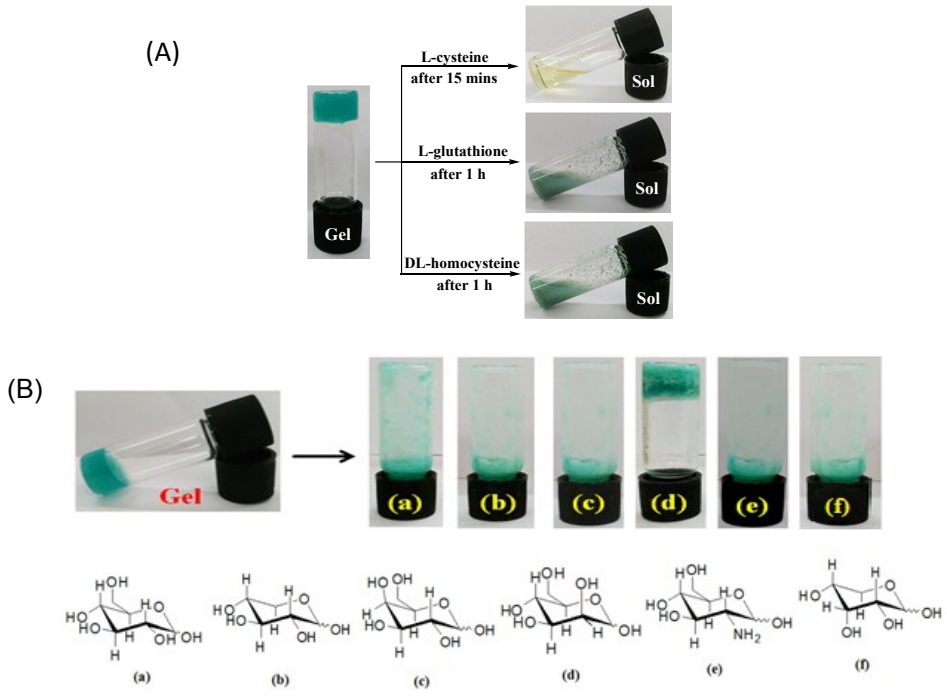


Fig. 10S. Photograph showing the phase change of the Cu^{2+} gel of **1** ([gelator] = 5 mg/mL with 2 equiv. of Cu^{2+} in 1:1 DMSO: H_2O) in the presence of 2 equiv. amounts of various (A) thiol containing amino acids (*c* = 0.03 M) and carbohydrates such as (B) (a) D-glucose, (b) D-xylose, (c) D-galactose, (d) D-mannose, (e) glucoseamine and (f) D-ribose (*c* = 0.03 M).

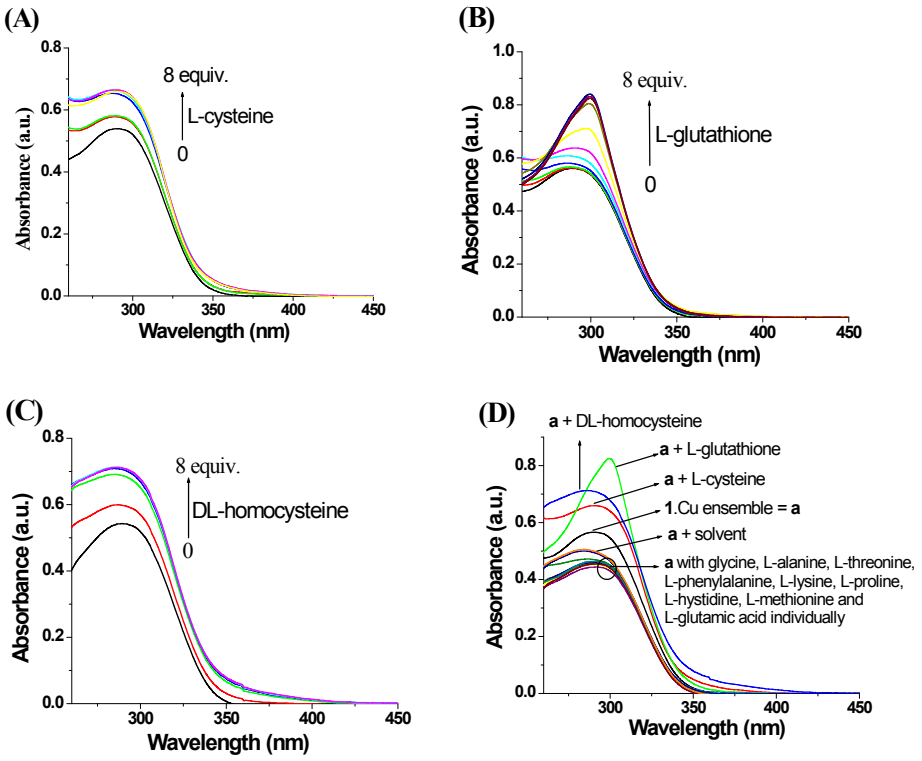


Fig. 11S. Change in absorbance of **1**.Cu ensemble (prepared by mixing **1** with 2 equiv. of $Cu(ClO_4)_2$; c = 2.5 x 10^{-5} M) upon gradual addition of 8 equiv. of (A) L-cysteine, (B) L-glutathione, (C) DL-homocysteine and (D) comparative views on absorption change of the same ensemble in presence of 8 equiv. amounts of all the amino acids examined [conc. of amino acids: c = 1.0 x 10^{-3} M] in DMSO:H_2O (1:1, v/v).

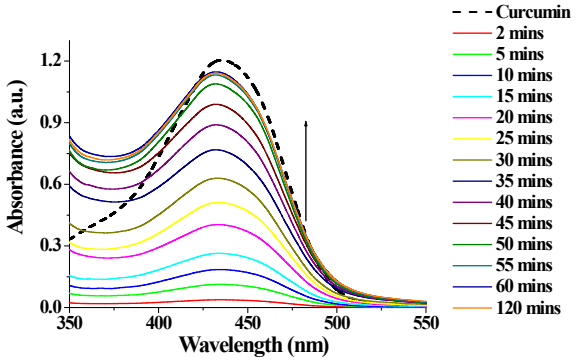


Fig. 12S. UV-vis spectra of the resulting supernatant solution obtained from L- cysteine responsive release of curcumin from the composite gel at different time intervals (the dotted line indicates the absorbance of curcumin before loading).

Table 2S. Results of gelation test for **3** and **4**.

Solvent	3	4
DMSO	S	S
DMF	S	S
$CHCl_3$: MeOH (1:1, v/v)	S	S
$CHCl_3$	PS	I
CH_3CN	I	I
n-Hexane	I	I
DMSO : $CHCl_3$ (1:1, v/v)	S	S
Diethyl ether	I	I
DCM	I	I
MeOH : H_2O (1:1 , v/v)	I	I
CH_3CN: H_2O (1:1 , v/v)	I	I
DMF : H_2O (1:1 , v/v)	S	G (48 mg/ml)
DMSO: H_2O (1:1 , v/v)	S	G (48 mg/ml)
Cyclohexane	I	I
S = solution; G = gel (minimum gelatination concentration); I = insoluble; PS = partially soluble.		

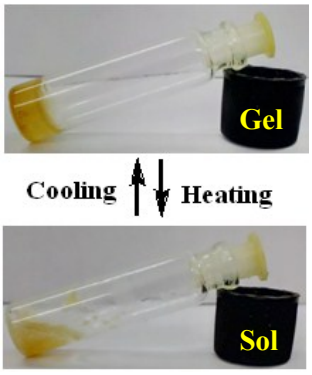


Fig. 13S. Pictorial representation of the thermo reversibility of the DMSO: H_2O (1:1, v/v) gel of **4** (48 mg/mL).

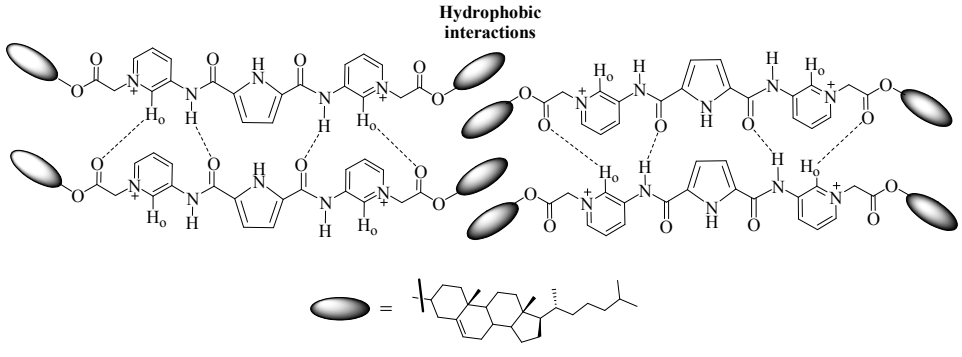


Fig. 14S. Schematic representation of the possible arrangement of molecules during gelation of **4**.

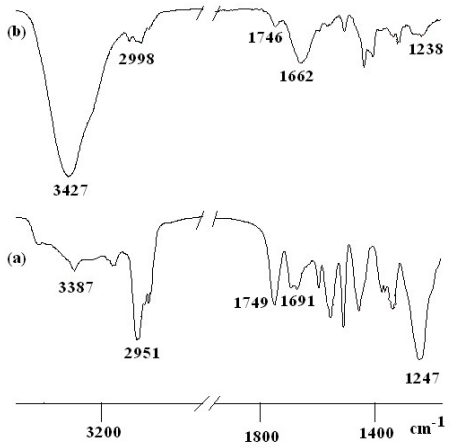


Fig. 15S. Partial FTIR spectra of **4** in its (a) amorphous and (b) gel states.

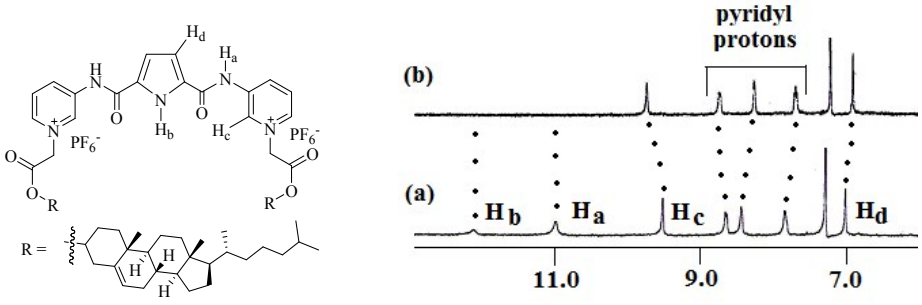


Fig. 16S. Partial ^{1}H-NMR spectra of (a) **4** (c = 5.34 x 10^{-3} M) and (b) **4** with AcO^{-} (1:1) in $CDCl_3$ containing few drops of d_6-DMSO.

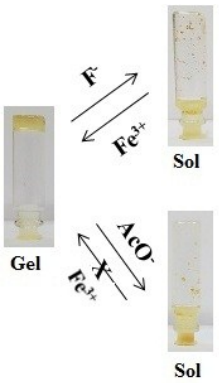


Fig. 17S. Photograph showing the chemical reversibility of F^{-} and AcO^{-} induced broken gels of **4** (48 mg/mL) in the presence of Fe^{3+}.

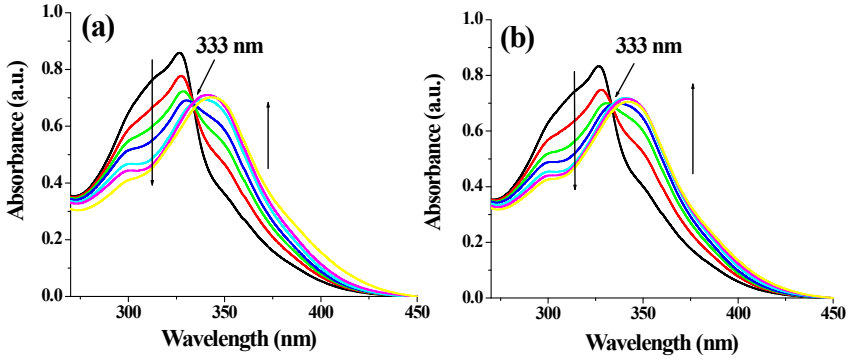


Fig. 18S. Change in UV-vis spectra of **4** (c = 2.50 x 10^{-5} M) in presence of 5 equiv. amounts of (a) F^- and (b) AcO^- (c = 1.0 x 10^{-3} M) in DMSO.

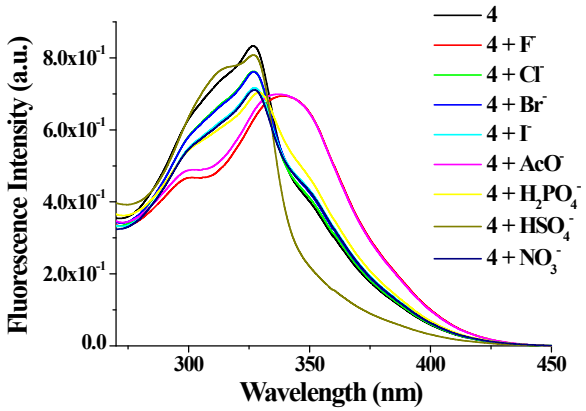


Fig. 19S. UV-vis spectra of **4** (c = 2.50 x 10^{-3} M) in presence of 5 equiv. amounts of different anions (c = 1.0 x 10^{-3} M) in DMSO.

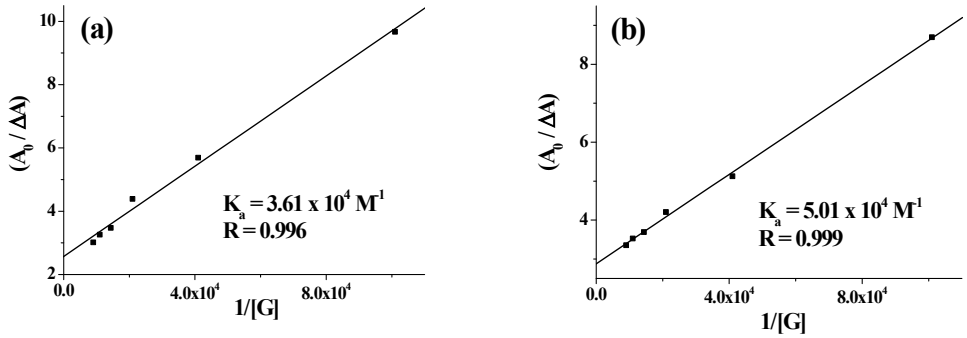
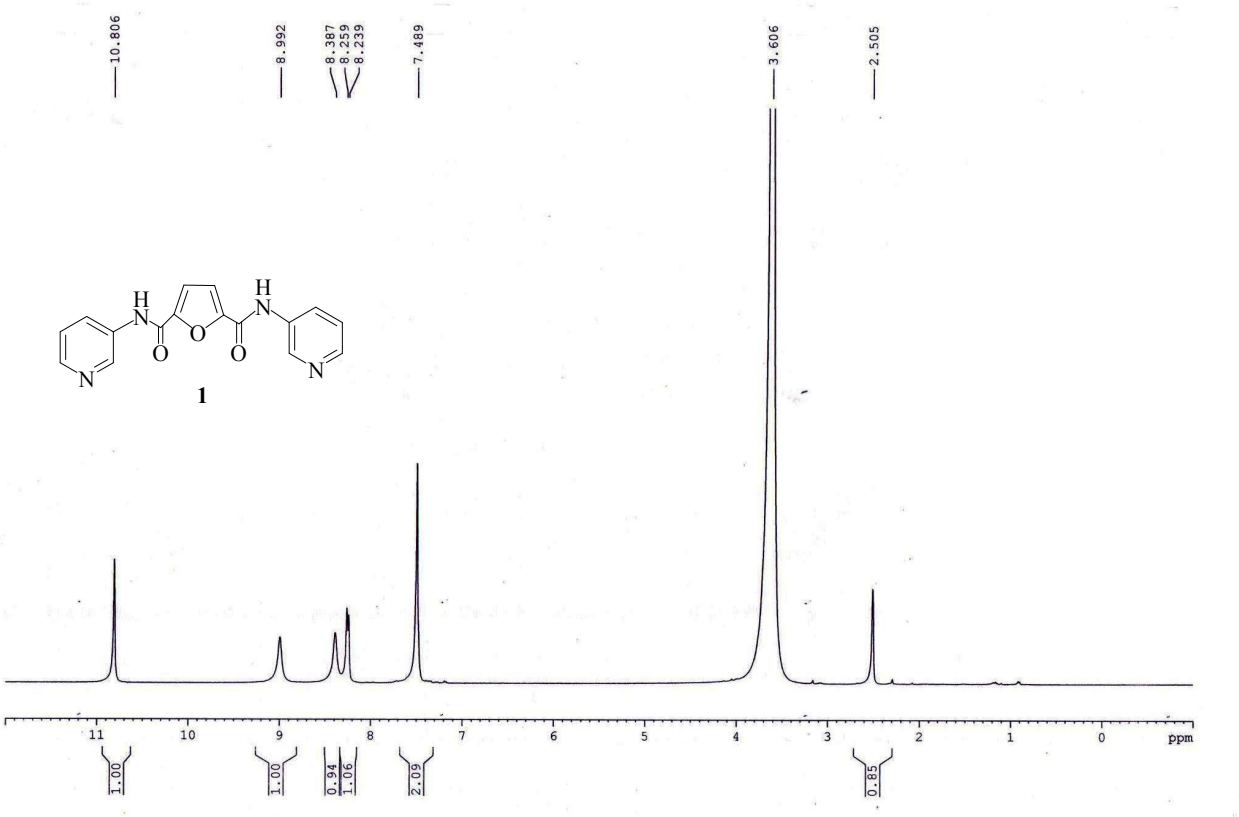


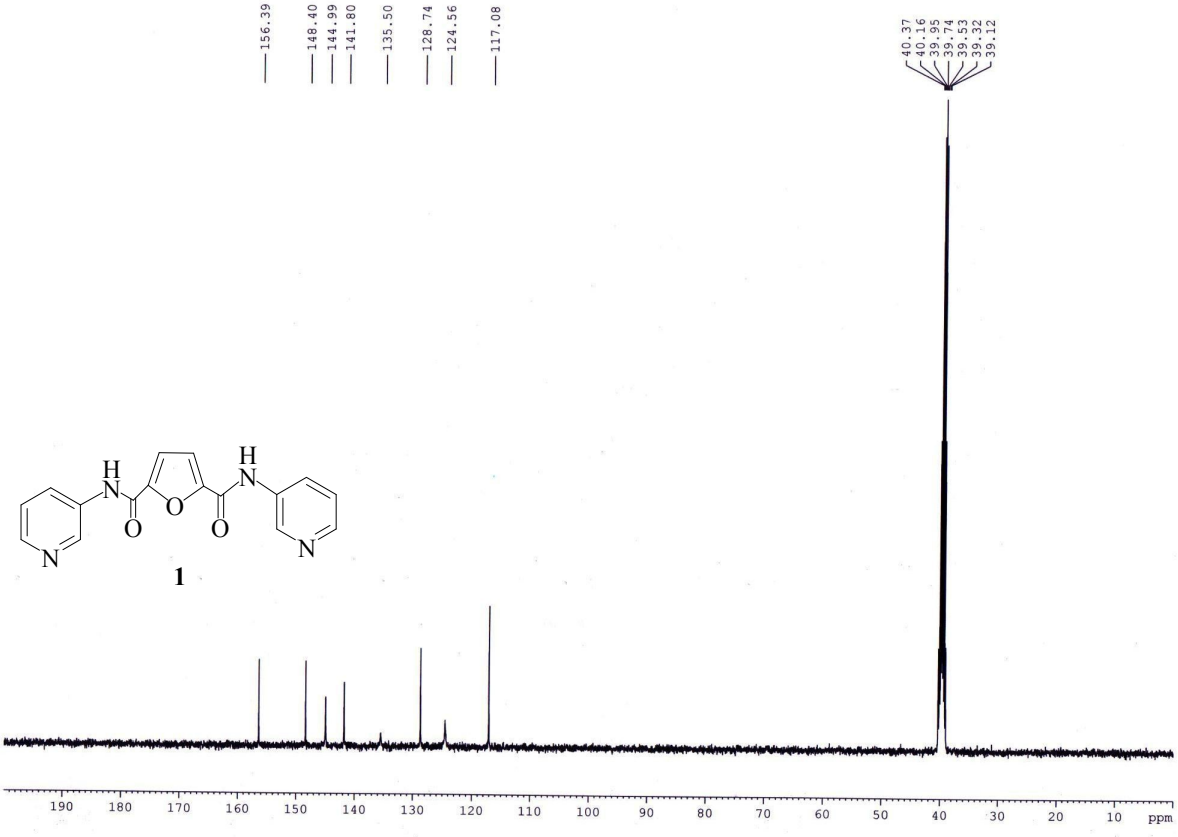
Fig. 20S. Benesi-Hildebrand plots using UV titration data for **4** with (a) F^- and (b) AcO^- ions in DMSO.

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

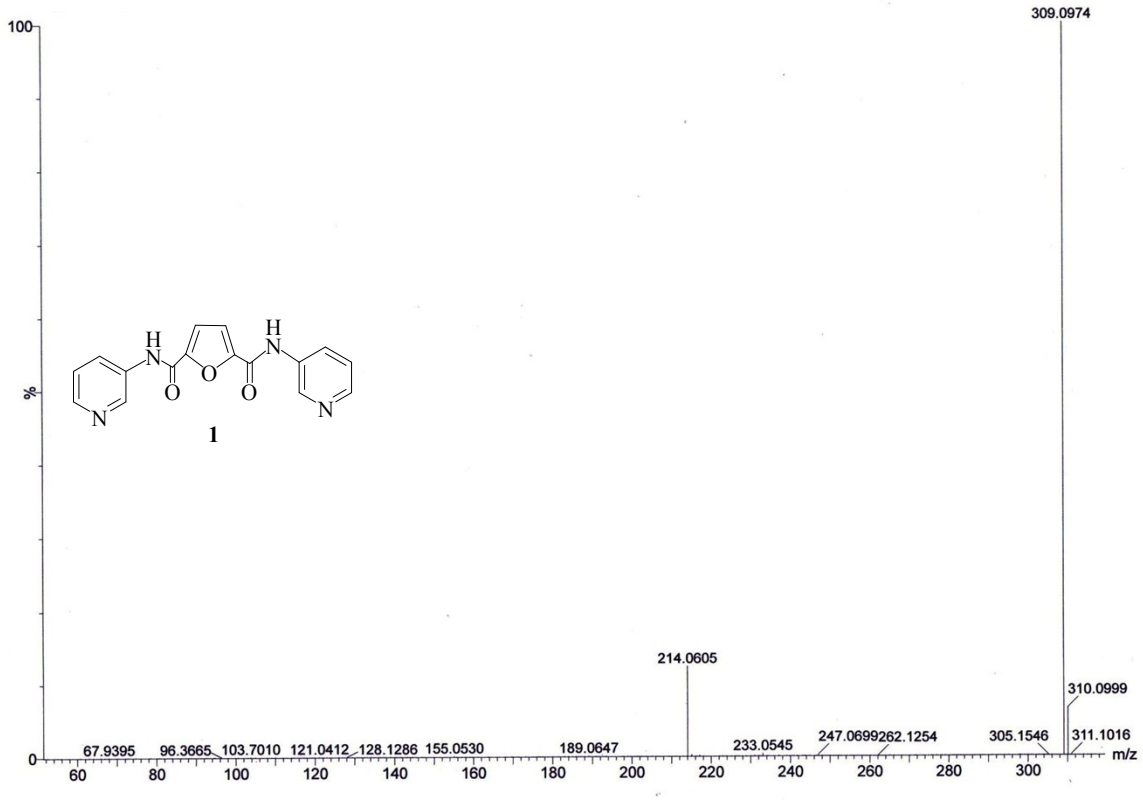


1

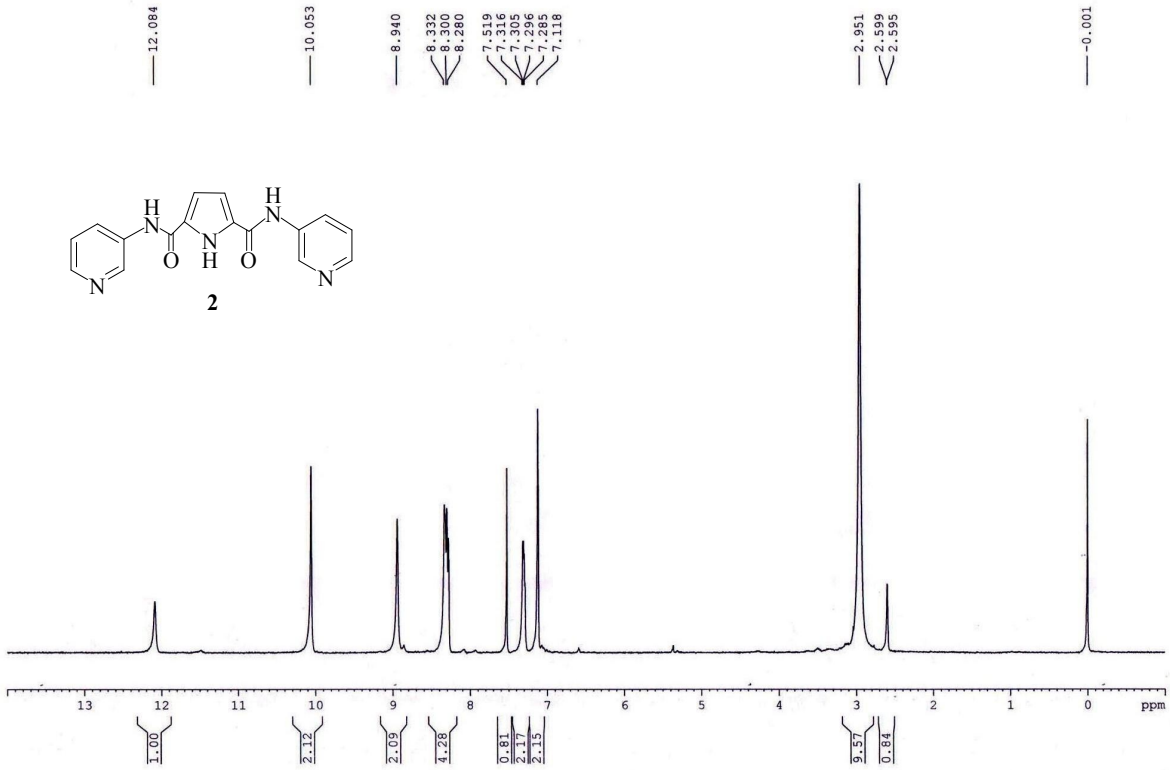
^{13}C NMR (d_6-DMSO, 100 MHz)



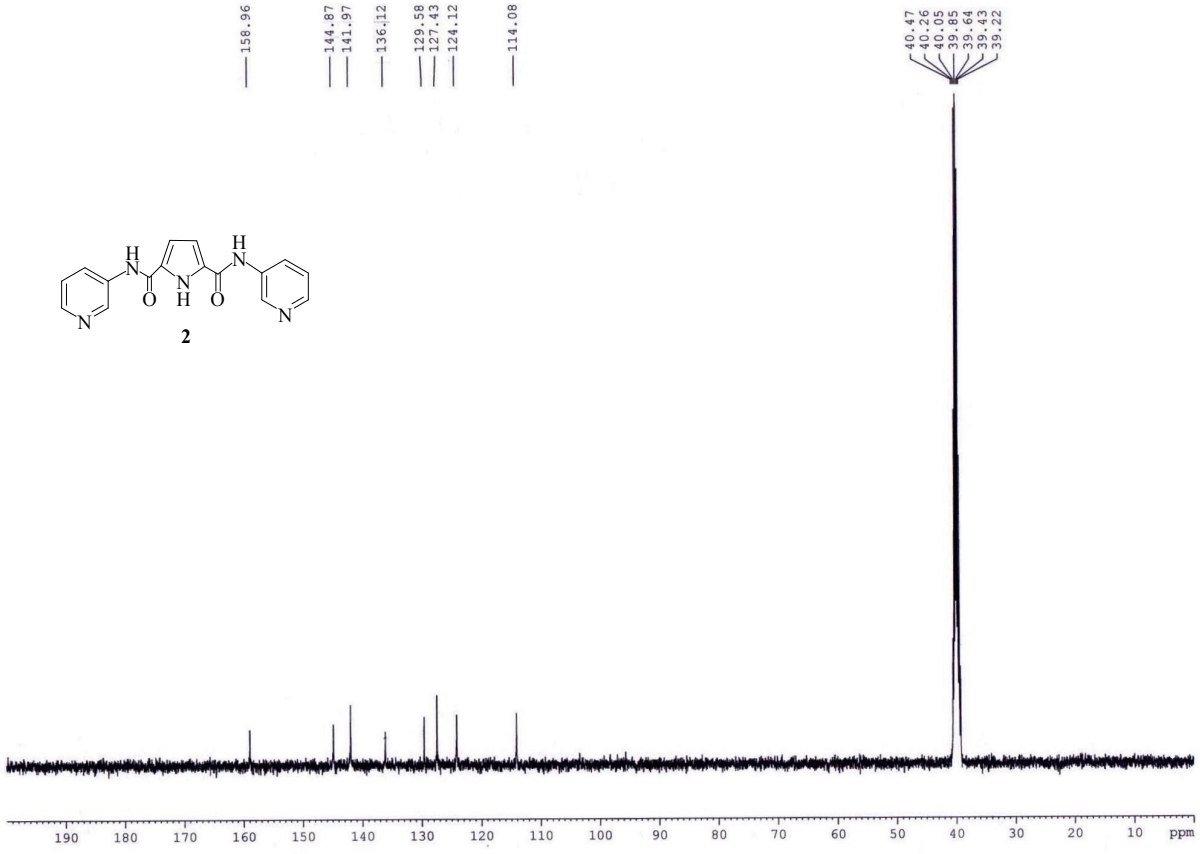
Mass spectrum of 1.



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

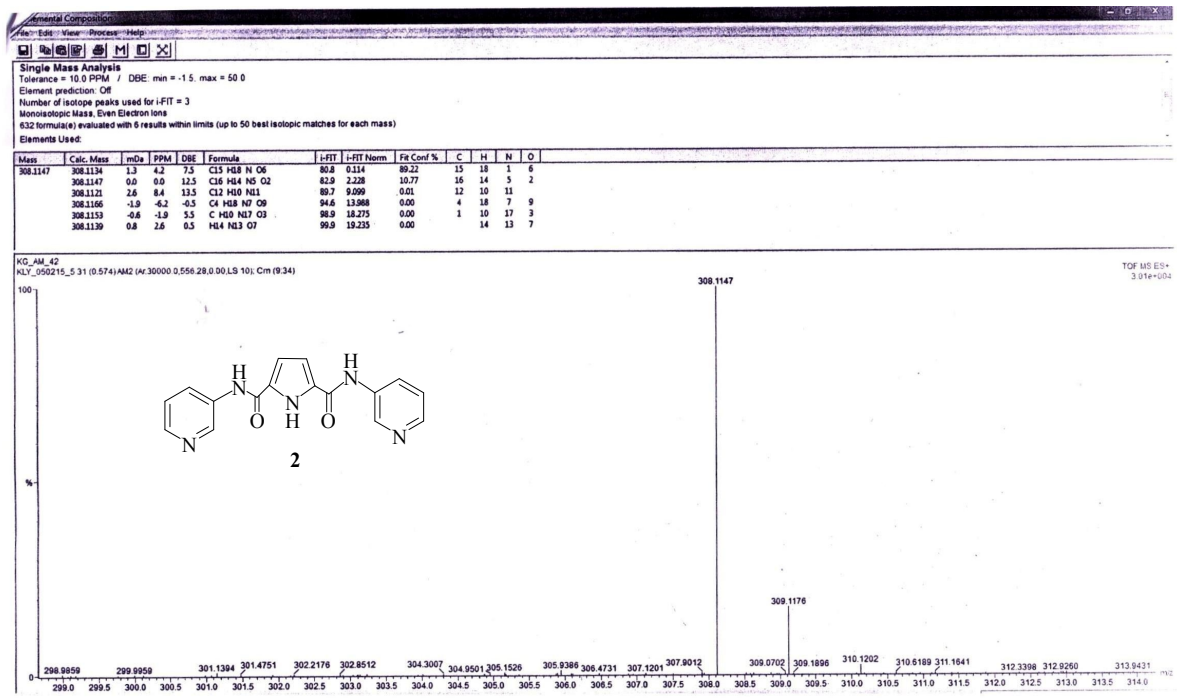


^{13}C NMR (d_6-DMSO, 100 MHz)

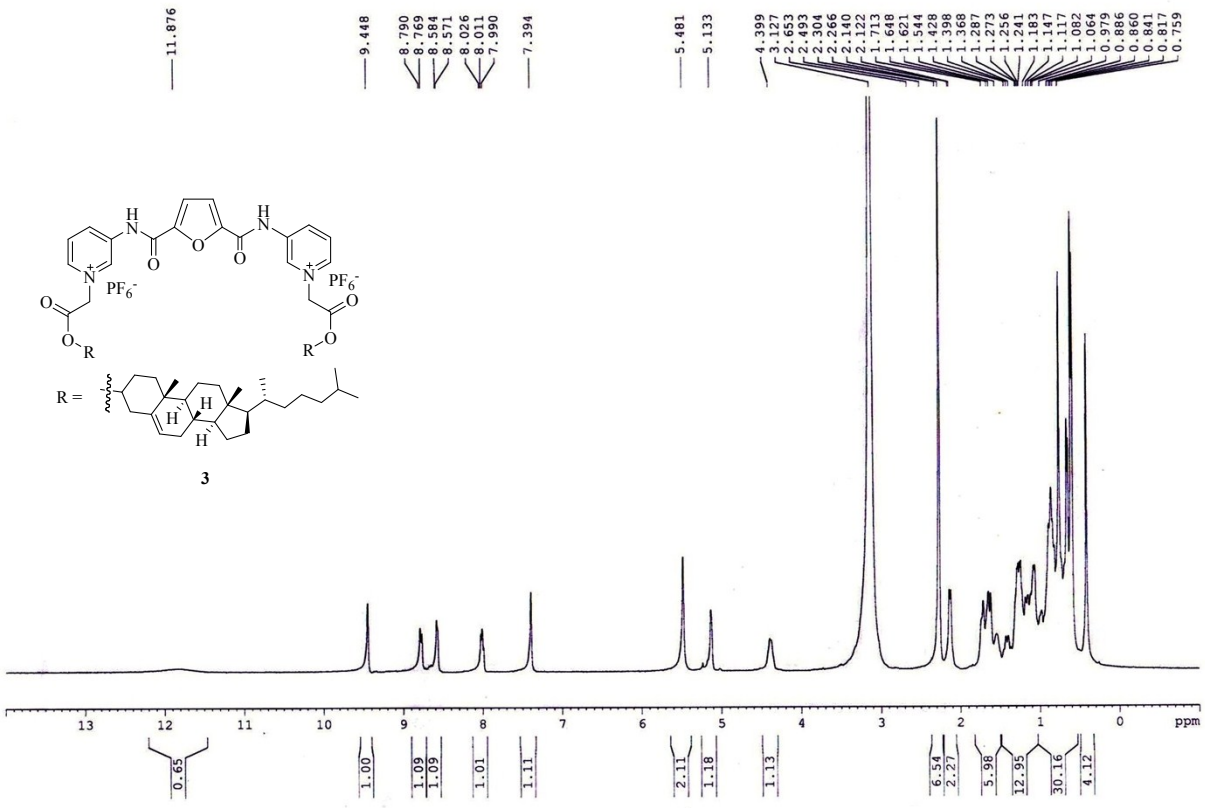


2

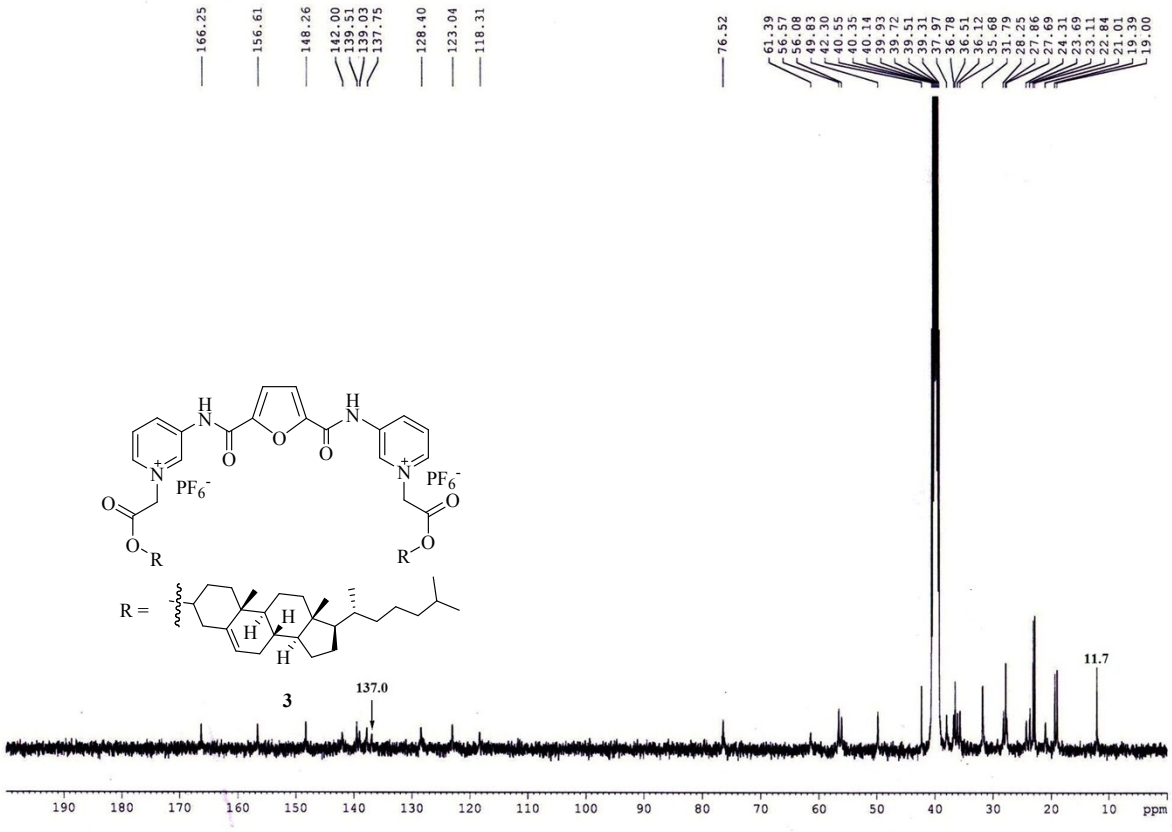
Mass spectrum of 2.



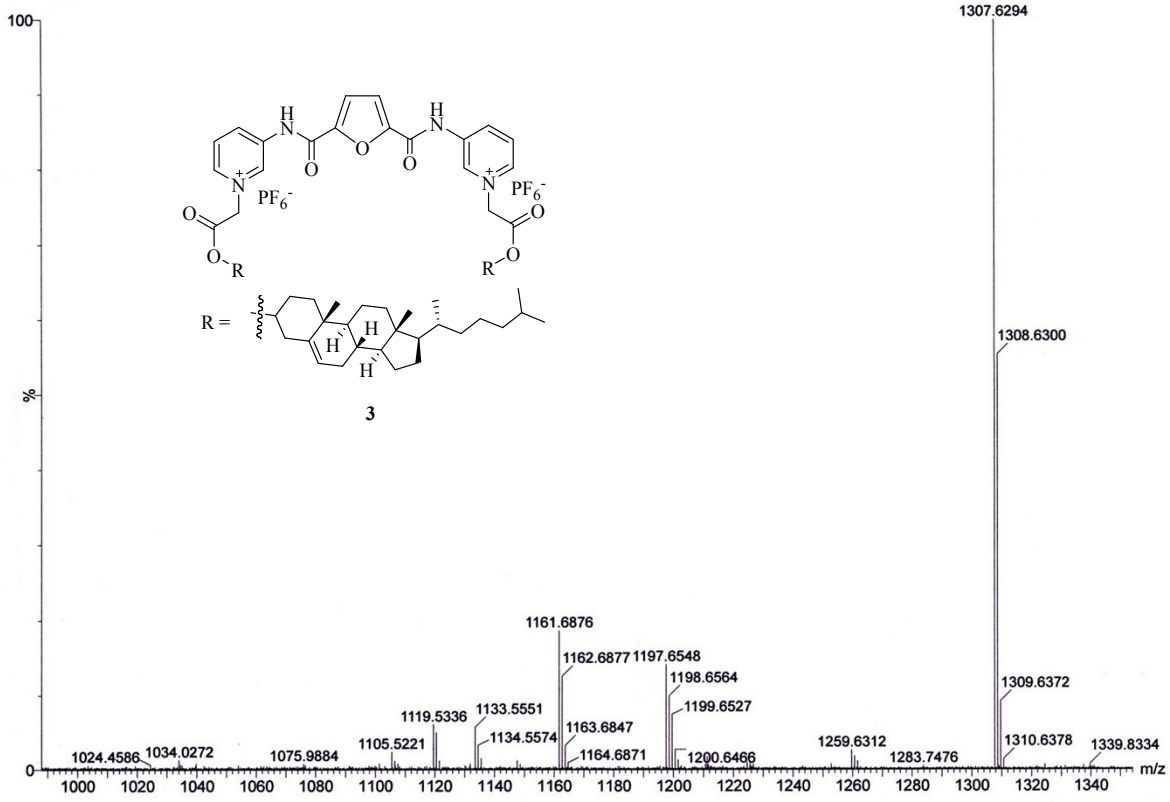
^{1}H NMR (d_6-DMSO, 400 MHz)



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

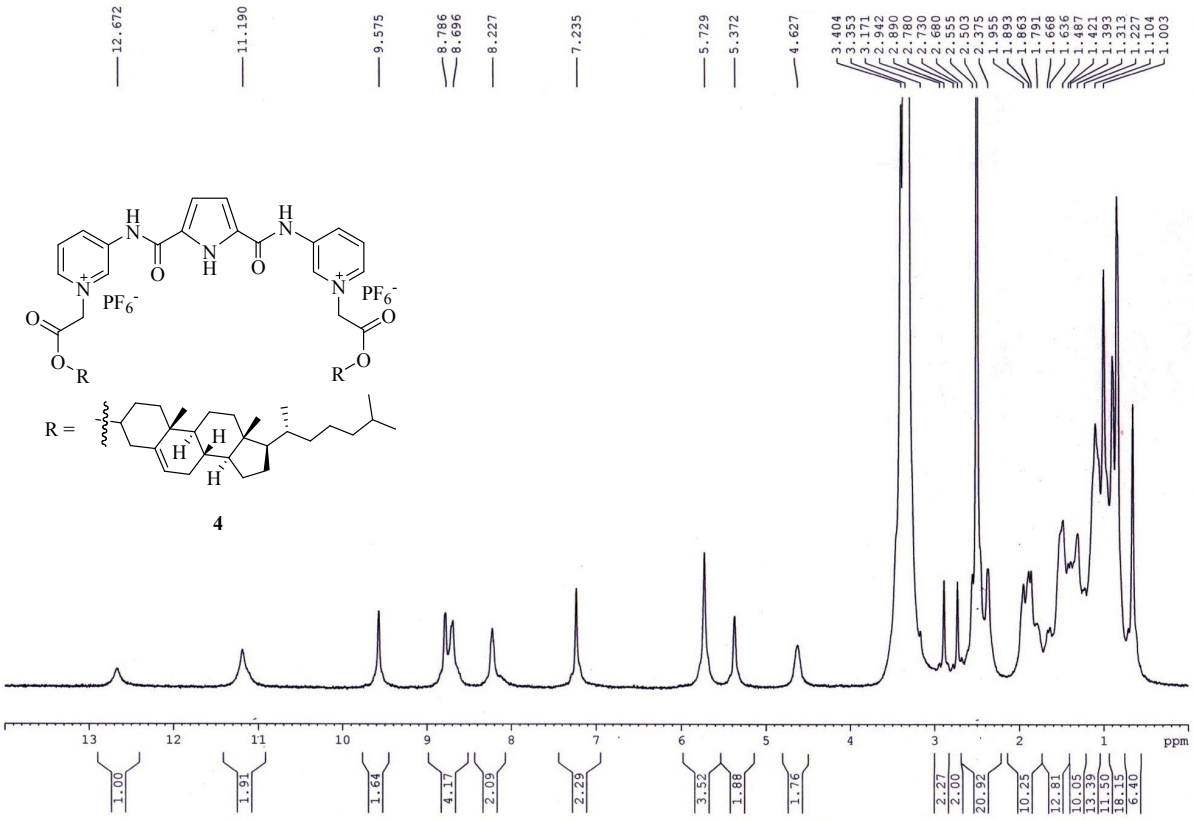


Mass spectrum of 3



3

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



4

Mass spectrum of 4