Supporting Information

Naphthalimide-linked new pyridylazo phenol derivative for selective sensing of cyanide ion (CN^-) in sol-gel medium

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

Solvent	1	2
DMSO	S	S
DMF	S	S
THF	I	I
CH_3CN	I	I
CH_3OH	I	I
$CHCl_3$	S	S
Diethyl ether	I	I
Hexane	I	I
Petroleum ether	I	I
DCM	S	S
Toluene	I	I
DMSO: H_2O (1:1, v/v)	P	P
DMF: H_2O (1:1, v/v)	**G** (6 mg/mL)	P

S = Solution; G = Gel (mgc); I = Insoluble; P = Precipitation. Gelation was primarily investigated by inversion of vial method after 10-15 mins of sample preparation ([Gelator] = 20 mg/mL).

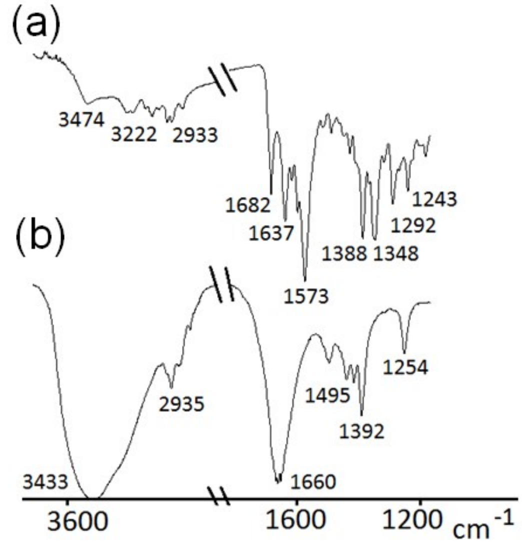


Fig. 1S. Partial FTIR spectra of **1** in (a) amorphous and (b) gel state.

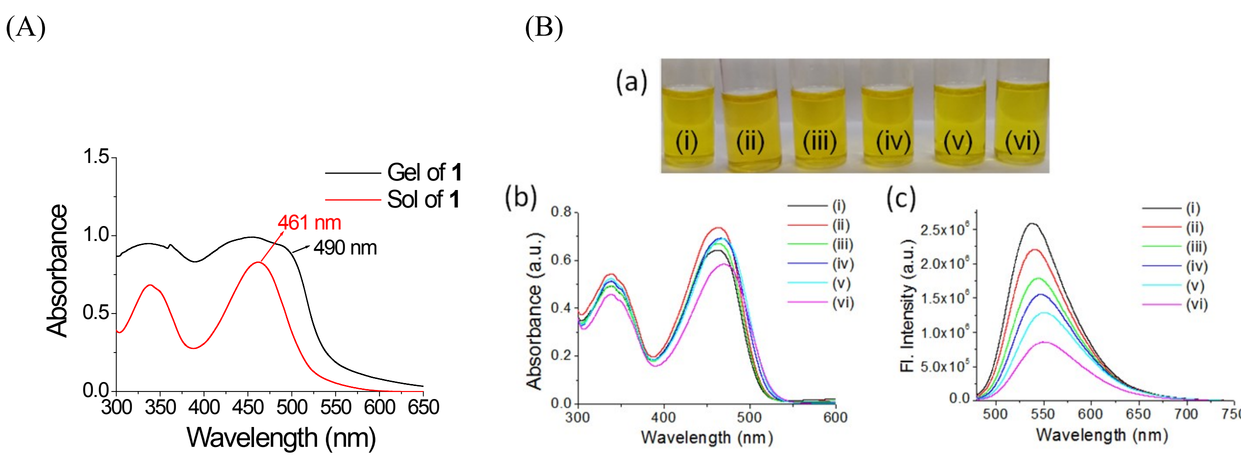


Fig. 2S. (A) Comparison of UV–Vis spectra of **1** in the sol and xerogel states; (B) Change in (a) color, (b) absorbance and (c) emission of **2** (c = 2.5 x 10^{-5} M) in (i) DMF, (ii) DMF-H_2O (19:1, v/v), (iii) DMF-H_2O (17:3, v/v), (iv) DMF-H_2O (3:1, v/v), (v) DMF-H_2O (3:2, v/v) and (vi) DMF-H_2O (1:1, v/v).

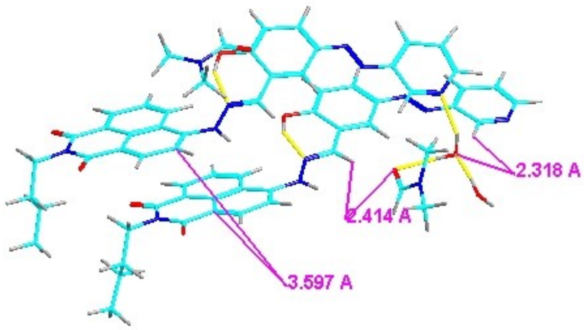


Fig. 3S. MMX optimized docked structure of **1** in presence of DMF and water.

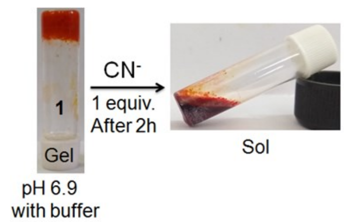


Fig. 4S. Phase change of DMF-H_2O (1:1, v/v) gel of **1** (pH = 6.9 using 10 mM HEPES buffer) after the addition of 1 equiv. amount of TBACN.

(a)

(b)

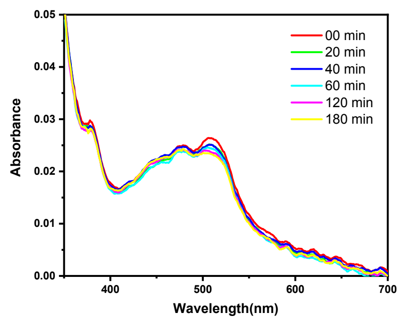
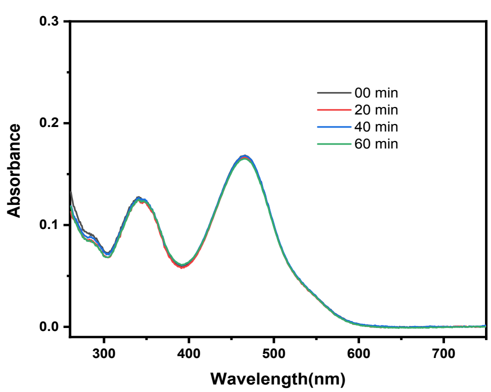


Fig. 5S. (a) Irradiation of DMF:H_2O (1:1, v/v) gel of **1** with 366 nm UV light at 273K for 5h; (b) UV-vis spectral changes in isomerization study of the gel under 366 nm light irradiation on a thin film for 3h.

(a)



(b)

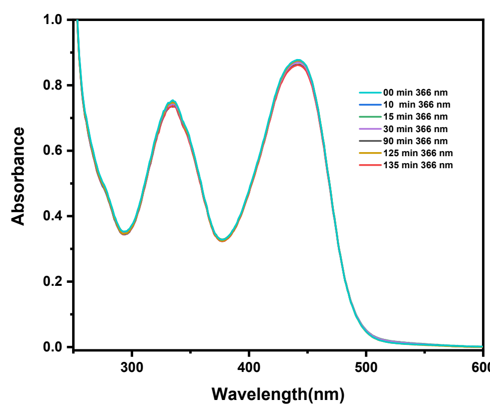


Fig. 6S. Change in UV-vis spectra of **1** in (a) DMF:H_2O (1:1, v/v; c = 1.67 x 10^{-5} M) and (b) CH_3CN (c = 2.5 x 10^{-5} M) upon irradiation of 366 nm light at 273K.

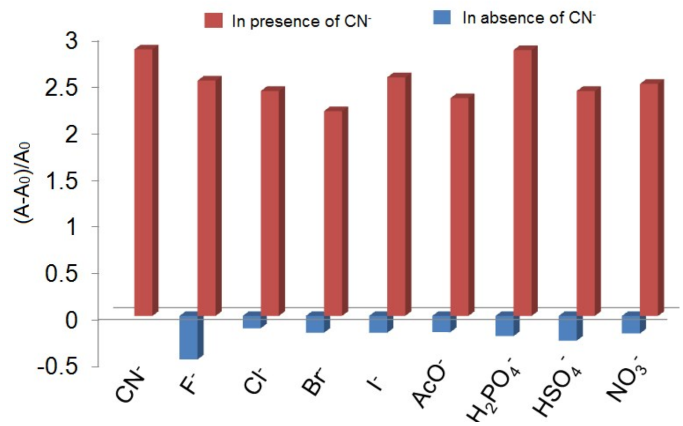


Fig. 7S. Selectivity plot of **1** (c = 2.5 x 10^{-5} M) for CN^- ion at 522 nm (c = 1.0 x 10^{-3} M) in DMF-H_2O (1:1, v/v) from UV-vis titration.

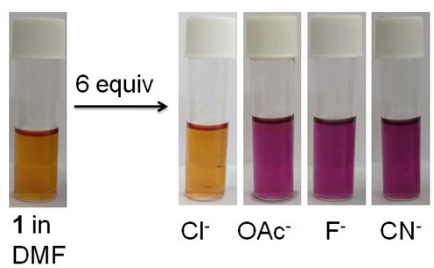


Fig. 8S. Change in colour of DMF solution of **1** (c = 2.5 × 10^{-5} M) in presence of different anions.

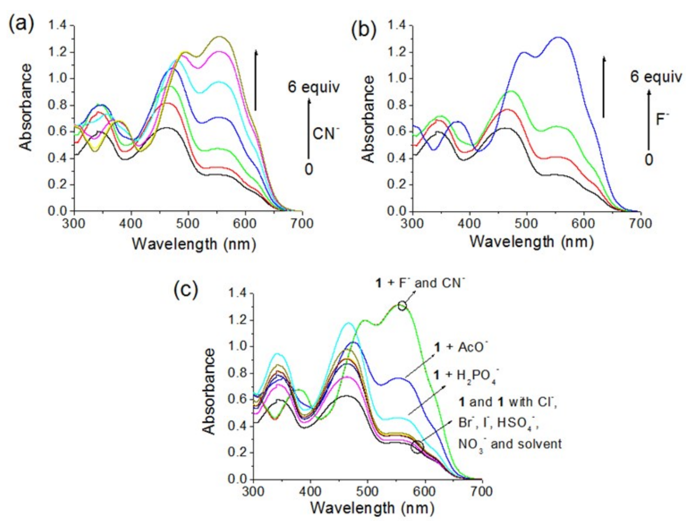


Fig. 9S. Change in absorbance of DMF solution of **1** (c= 2.5×10^{-5} M) upon addition of (a) CN^-, (b) F^- and (c) all anions (c = 1×10^{-3} M) (anions were taken as tetrabutylammonium salts).

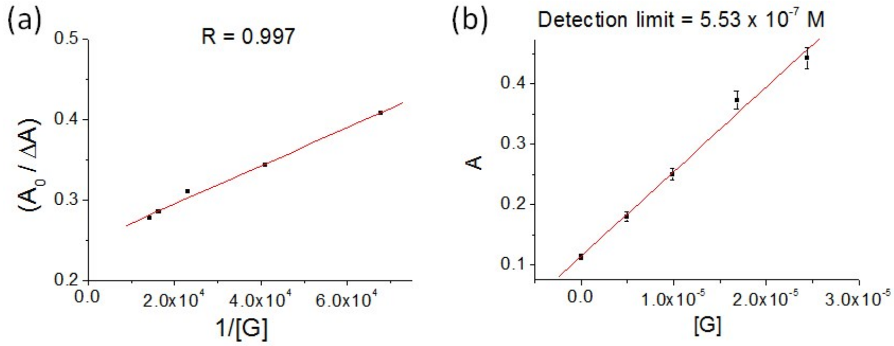


Fig. 10S. (a) Benesi–Hildebrand plot and (b) detection limit of **1** (c = 2.5 x 10^{-5} M) for TBACN at 522 nm (c = 1.0 x 10^{-3} M) in DMF-H_2O (1:1, v/v) from UV-vis titration.

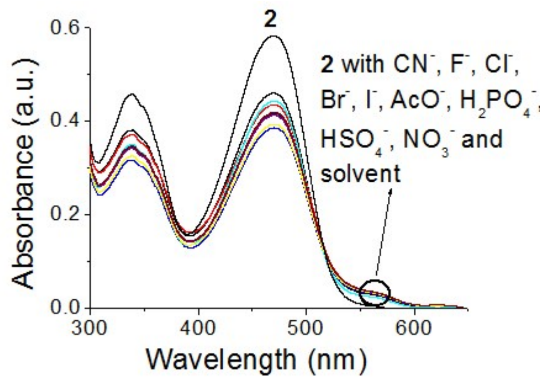


Fig. 11S. UV-vis titration spectra of **2** (c = 2.50 × 10^{-5} M) upon addition of 6 equiv. amounts of different anions (c = 1.0 ×10^{-3} M) in DMF-H_2O (1:1, v/v).

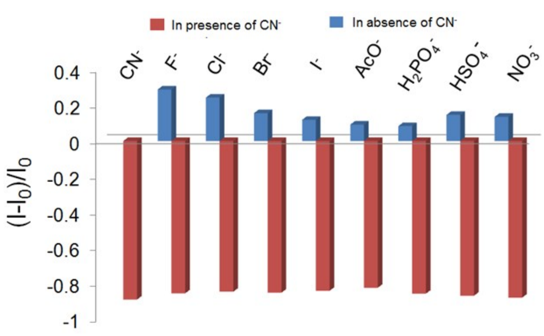


Fig. 12S. Selectivity plot of **1** (c = 2.5 x 10^{-5} M) for CN^- ion at 552 nm (c = 1.0 x 10^{-3} M) in DMF-H_2O (1:1, v/v) from fluorescence titration.

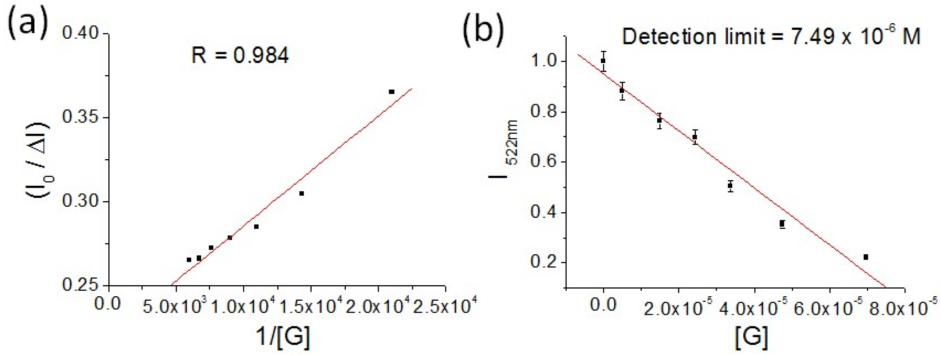


Fig. 13S. (a) Benesi–Hildebrand plot and (b) detection limit of **1** (c = 2.5 x 10^{-5} M) for TBACN at 552 nm (c = 1.0 x 10^{-3} M) in DMF-H_2O (1:1, v/v) from fluorescence titration.

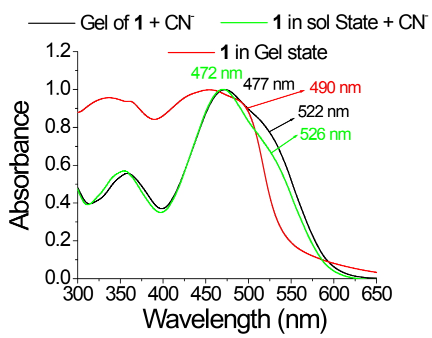
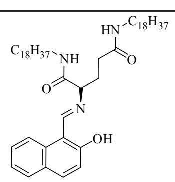
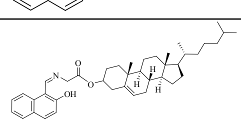
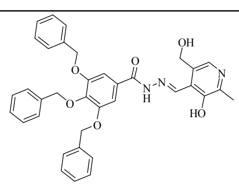
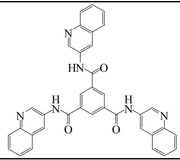
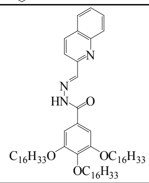
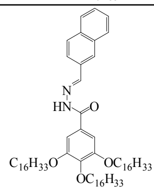
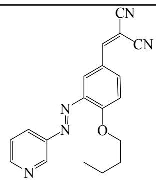
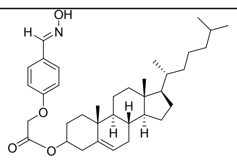
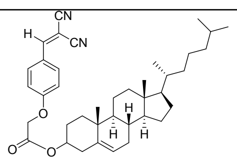
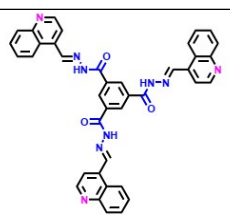
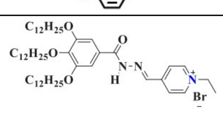
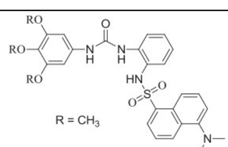
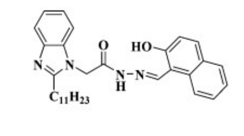
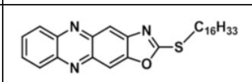
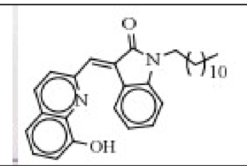
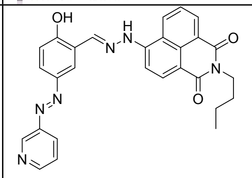


Fig. 14S. Comparison of normalized UV-vis spectra of CN$^-$ broken gel of **1** with the gel of **1** and solution of **1** containing CN$^-$.

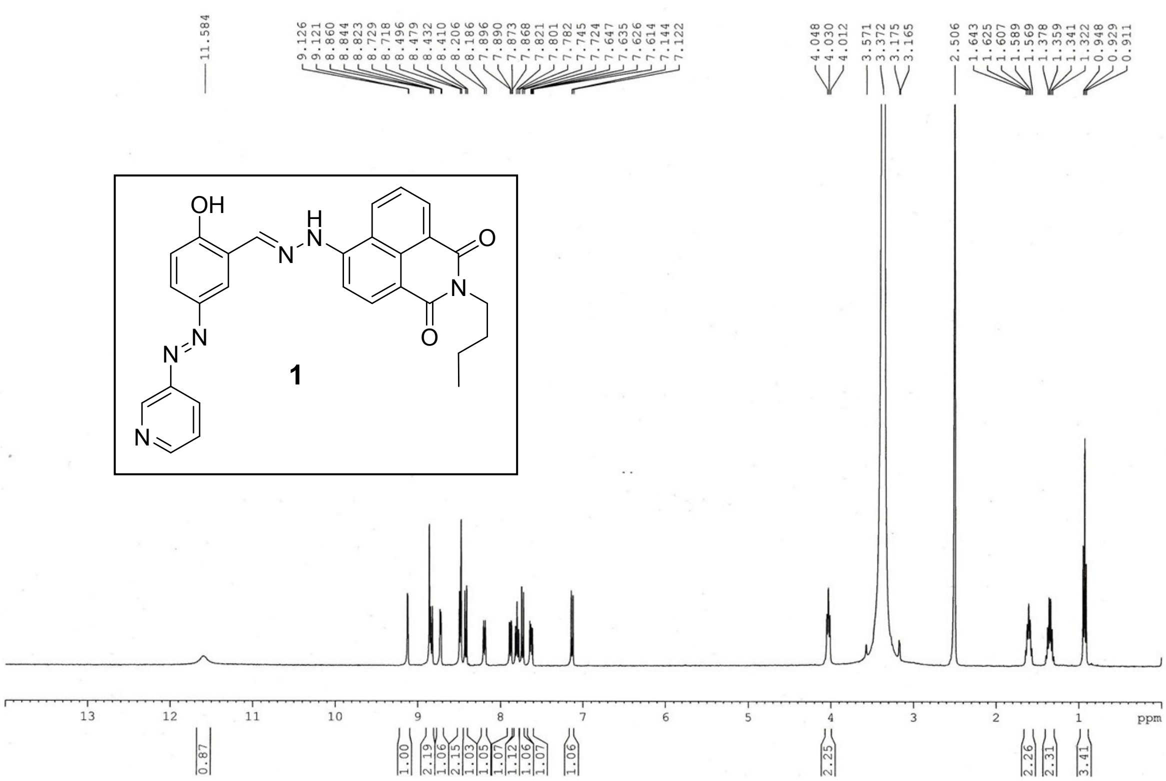
Table 2S : Reported structures for CN$^-$ sensing in gel phase.

Entry	Gelator structure	Detection media	Sensing mechanism	solvent	Detection limit (M)	Interference from other anions	Ref.
1		Gel-to-gel state	Metal Displacement	DMSO	1.6 x 10^{-6}	-	1
2		Gel-to-sol state	Reaction-based	DMF:H_2O (2:1, v/v)	1.36 x 10^{-5}	-	2
3		Gel-to-sol state	Deprotonation	DMSO	-	F$^-$ and AcO$^-$	3

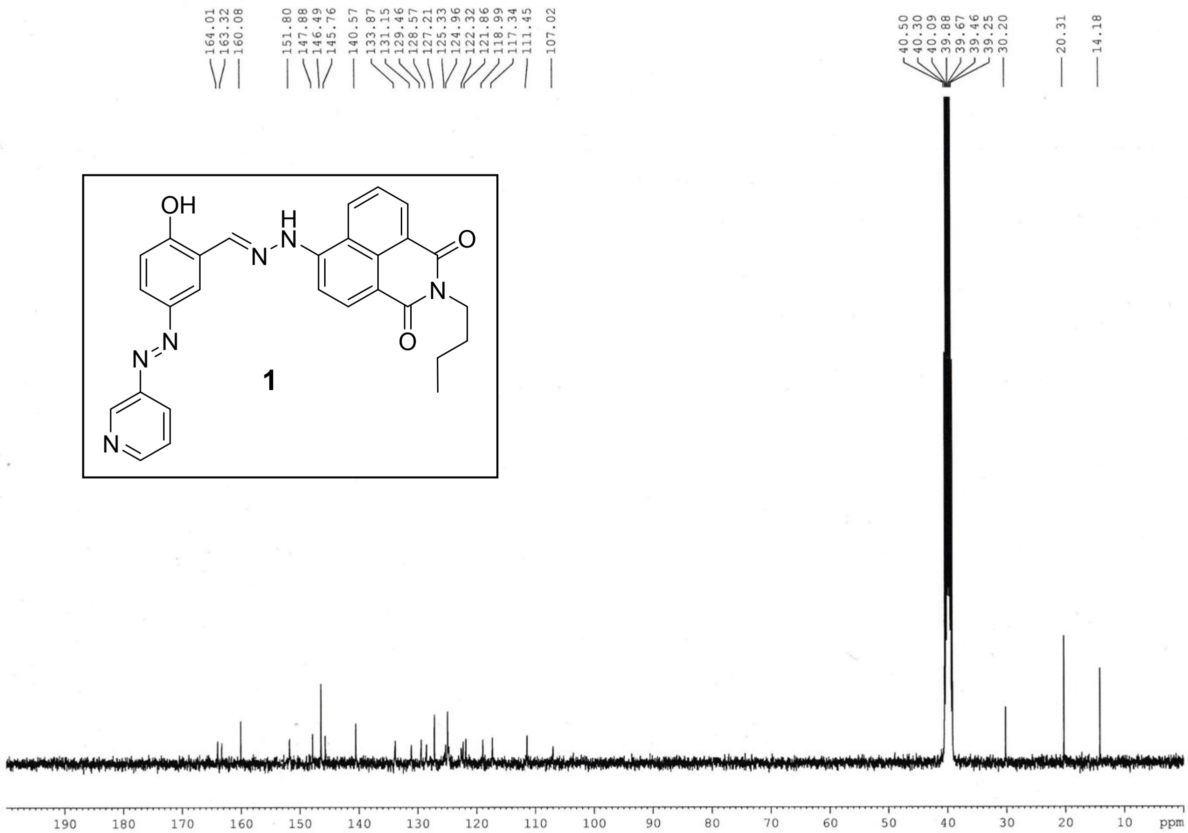
4		Gel-to-gel state	Deprotonation	DMSO:H_2O (8:2, v/v)	-	F^-, AcO^- and $H_2PO_4^-$	4
5		Gel-to-gel state	Metal Displacement	DMF	1.0×10^{-5} 1.0×10^{-7}	-	5
6		Gel-to-gel state	Metal Displacement	EtOH	1.0×10^{-6}	-	6
7	Two component gel from citrazinic acid and melamine	Gel-to-sol state	Deprotonation	Air dried gel	-	S^{2-}	7
8		Gel-to-sol state	Reaction-based	CH_3CN	9.36×10^{-6}	-	8
9		Gel-to-sol state	Deprotonation	Toluene		F^- and AcO^-	9
10		Gel-to-sol state	Reaction-based	Toluene-MeOH (1:2)	4.17×10^{-6}	-	9
11		Gel-to-sol state	H-bonding based	DMSO-H_2O (1:1, v/v)	1.5 mM	No other anions tested	10
12		Gel-to-sol state	Deprotonation	DMF:H_2O (1:1, v/v)	0.368 mM	-	11
13		Gel-to-sol state	Deprotonation	DMSO	0.4×10^{-8}	No other anions tested	12

14		Gel-to-sol state	Deprotonation	glycerol	In gel: 3.02×10^{-6}	-	13
15		Gel-to-sol state	Reaction-based	DMSO-H_2O (1:1, v/v)	4.18 $\times 10^{-10}$ (gel)	-	14
16		Gel-to-sol state	Reaction-based	DMSO	1.36×10^{-4}	-	15
This work		Gel-to-sol state	Deprotonation	DMF-H_2O (1:1, v/v)	5.53×10^{-7} (in DMF-H_2O (1:1, v/v))	-	-

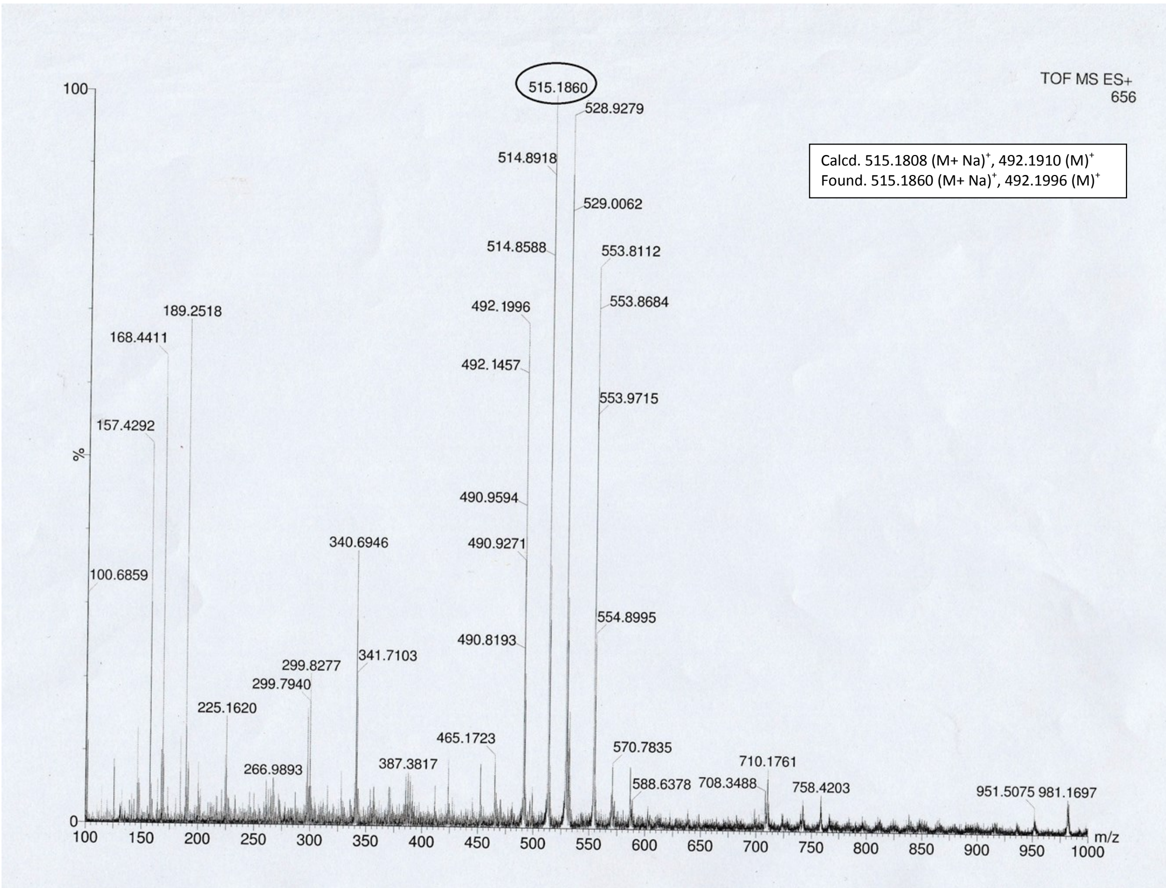
^{1}H NMR (d$_6$- DMSO, 400 MHz) of 1



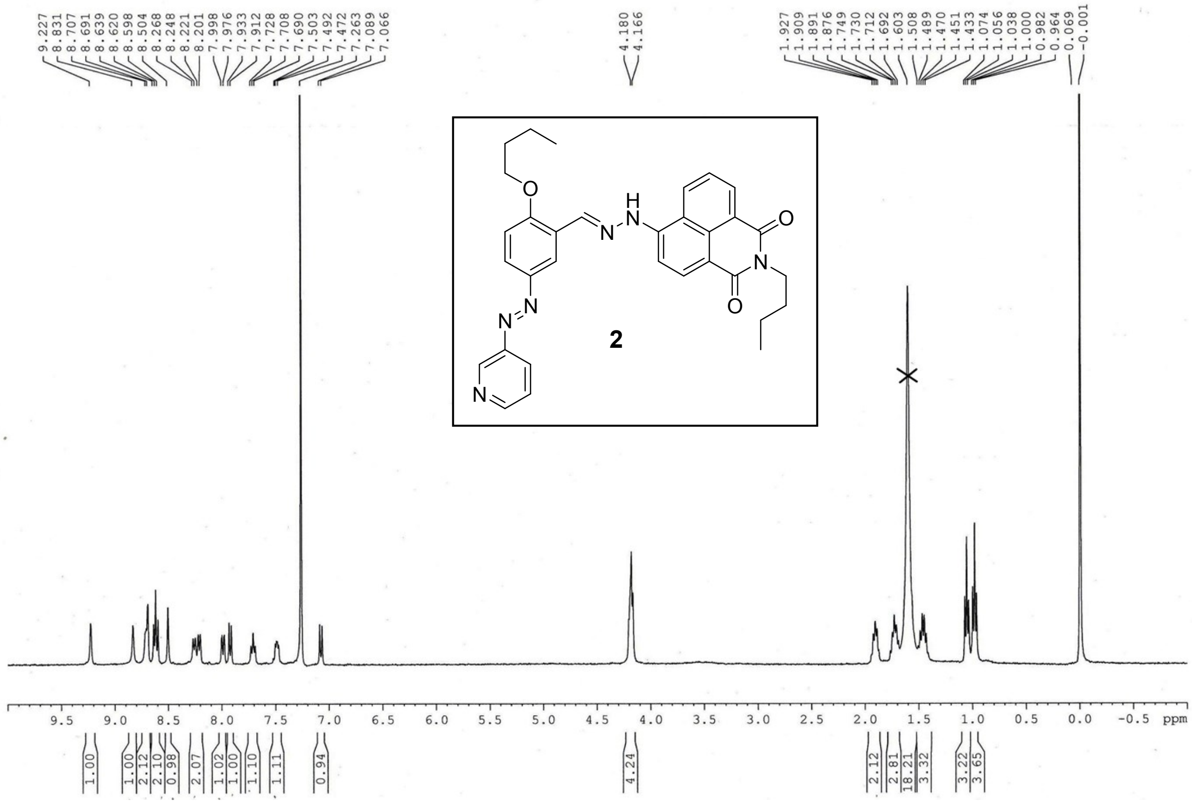
^{13}C NMR (d$_6$- DMSO, 100 MHz) of 1



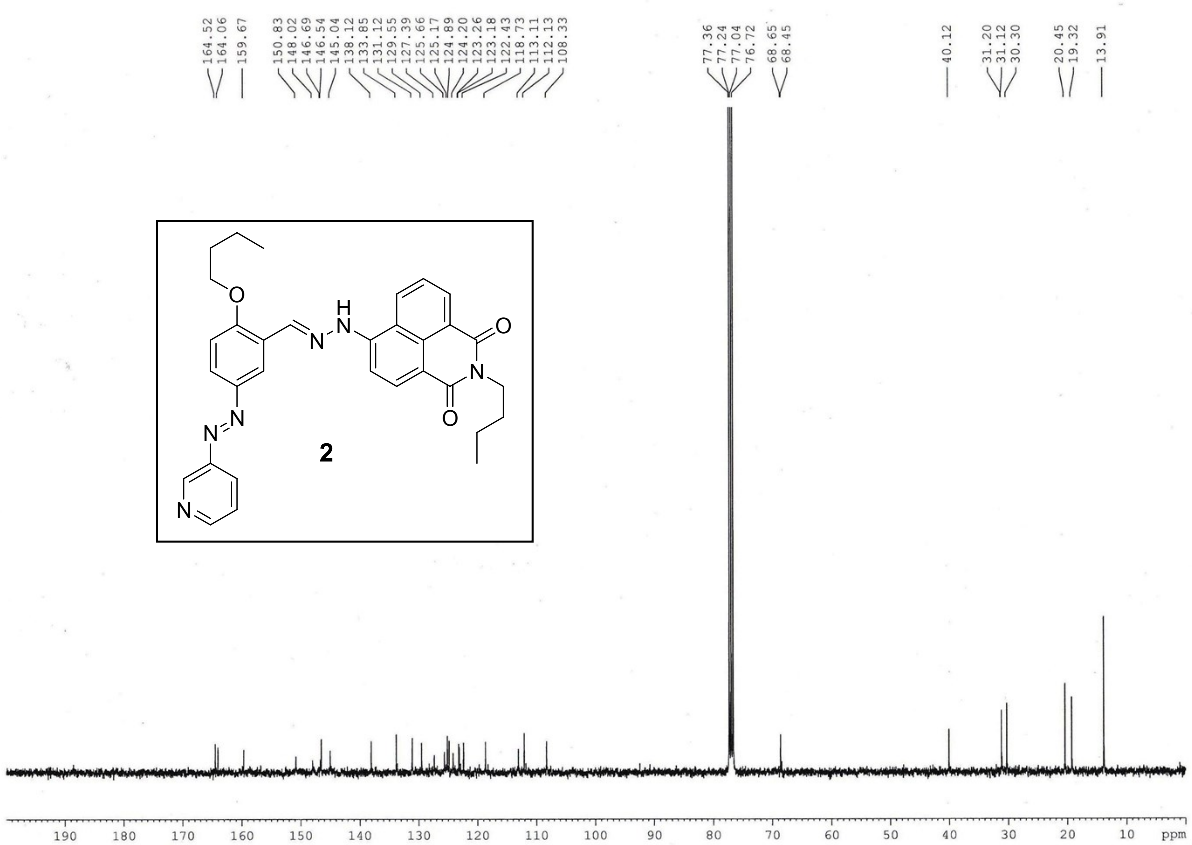
Mass spectrum of 1.



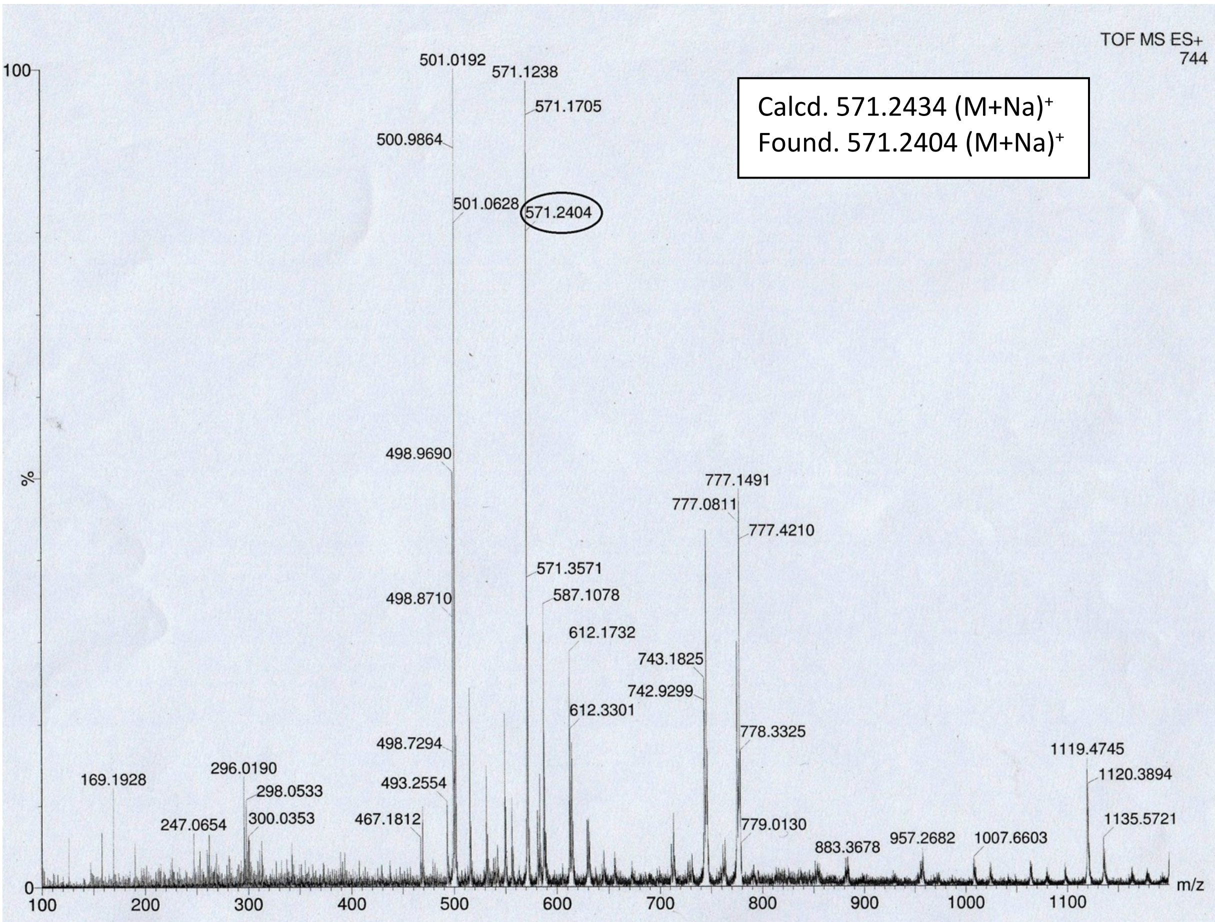
^{1}H NMR ($CDCl_3$, 400 MHz) of 2



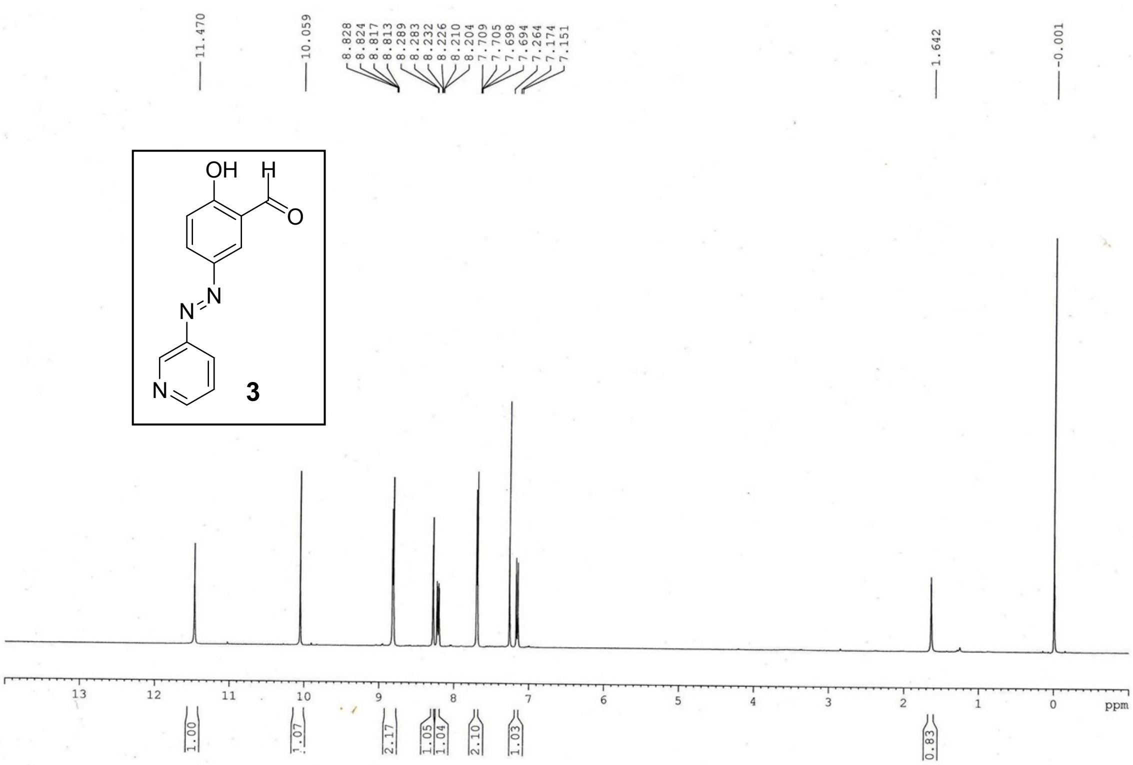
^{13}C NMR ($CDCl_3$, 100 MHz) of 2



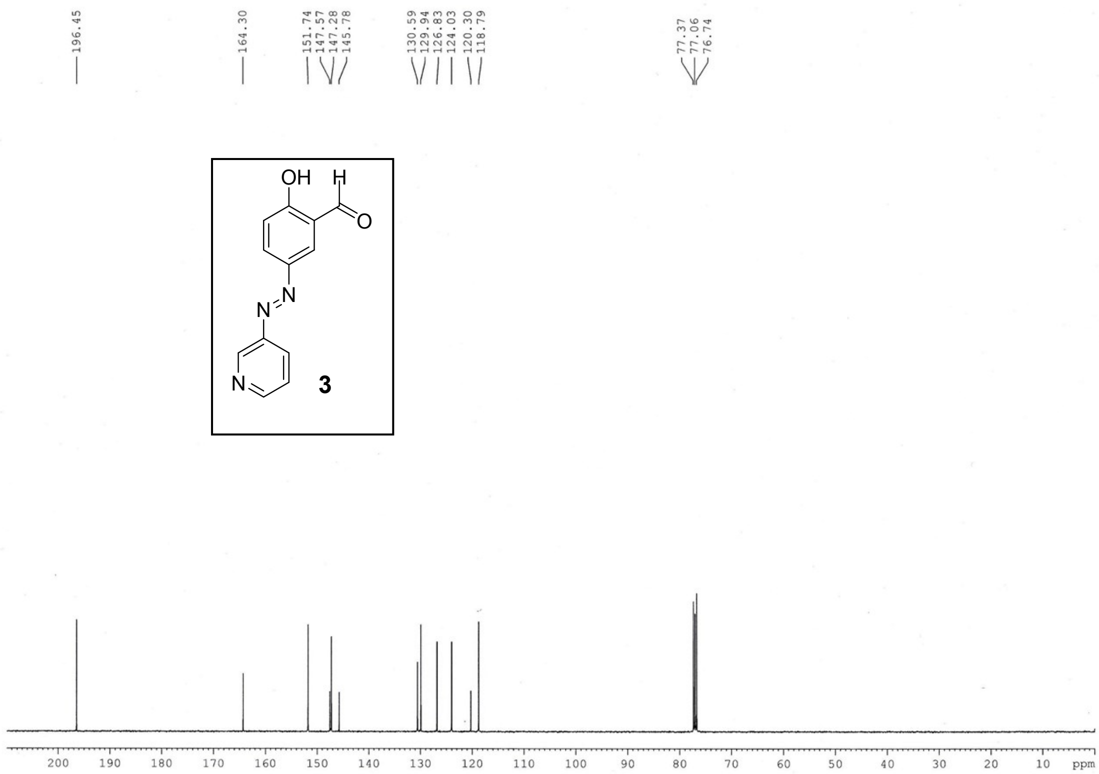
Mass spectrum of 2.



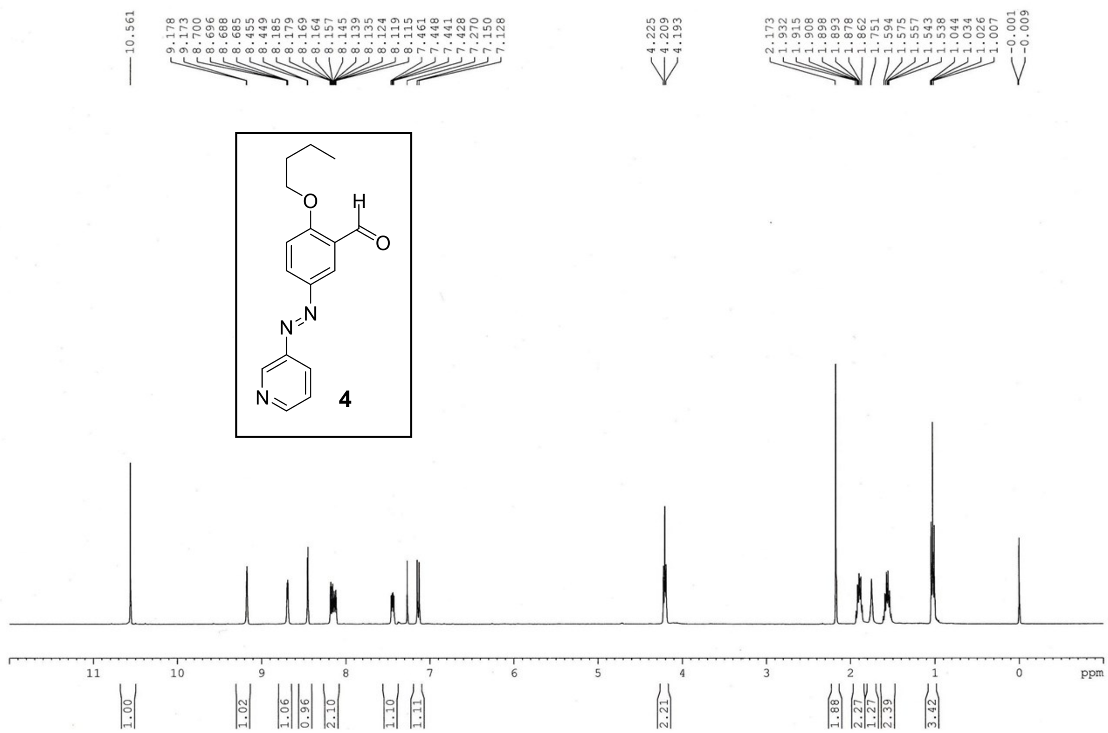
^1H NMR ($CDCl_3$, 400 MHz) of 3



^{13}C NMR ($CDCl_3$, 100 MHz) of 3



^{1}H NMR ($CDCl_3$, 400 MHz) of 4



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