Supporting Information

Pyridoxal-derived a new gelator for selective recognition of CN^- and F^- under different conditions

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Table 1S: Summary of gel property of compound **1** in different solvents

Solvents	Results
DMF	S
DMF:H_2O(10:1, v/v)	**G(7 mg/mL)**
DMSO	S
DMSO:H_2O(10:1, v/v)	**G(7 mg/mL)**
$CHCl_3$:CH_3OH	S
$CHCl_3$	I
Benzene	I
Toluene	I
Nitrobenzene	I
CH_3CN	I
THF	I
1,4-Dioxane	S
1,4-Dioxane:H_2O	I

S = Soluble, G = Gel, I = Insoluble

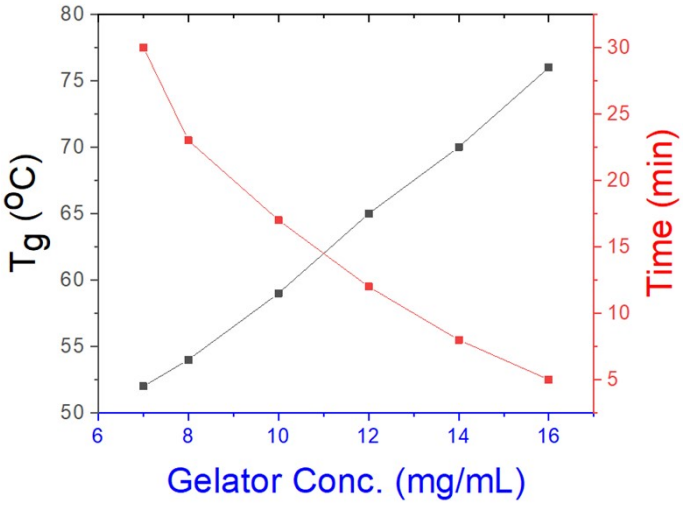


Figure 1S. Plots showing variation of conc. (mg/mL) of **1** *vs* T_{gel} (°C) *vs* Time (min) taken for gel formation.

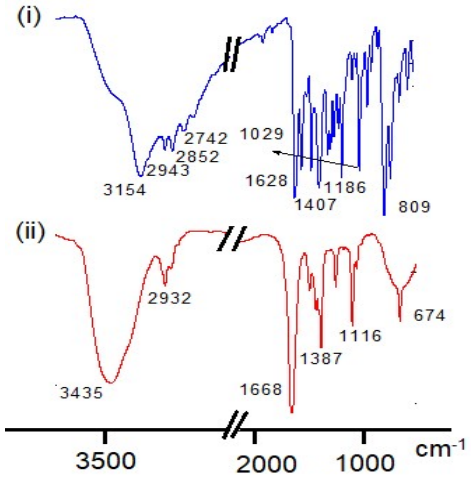


Figure 2S. Partial FTIR spectra of compound **1** (i) in amorphous and (ii) gel states.

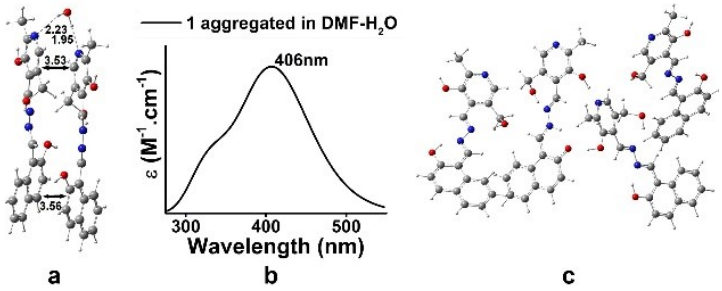


Figure 3S: (a) Optimized geometry of **1**-dimer in DMF-H_2O, (b) UV-Vis spectra of **1**-dimer in DMF-H_2O, and (c) Optimized geometry **1**-tetramer in DMF without H_2O molecules.

Table 2S. Simulated absorption wavelengths (λ_{max}), oscillator strengths (*f*), and the composition of the corresponding electronic transitions (H = HOMO; L = LUMO) calculated using B3LYP/6-31g(d) level of theory.

Compound	λ_{max} (nm)	*f*	ε (10^4)	Main compositions (contribution)
1- in DMF-H_2O	421 (397)[a]	0.80	2.37	H→L (99%)
1-aggregated in DMF-H_2O	427 (406)[a]	0.46	2.34	H-1→L+2 (76%)
1-dianionic in DMF-H_2O	490 (500)[a]	0.98	2.04	H→L (99%)
1- monoanionic in DMF-water	498 (500)[a]	0.89	2.01	H→L (100%)

*a indicates the experimental values

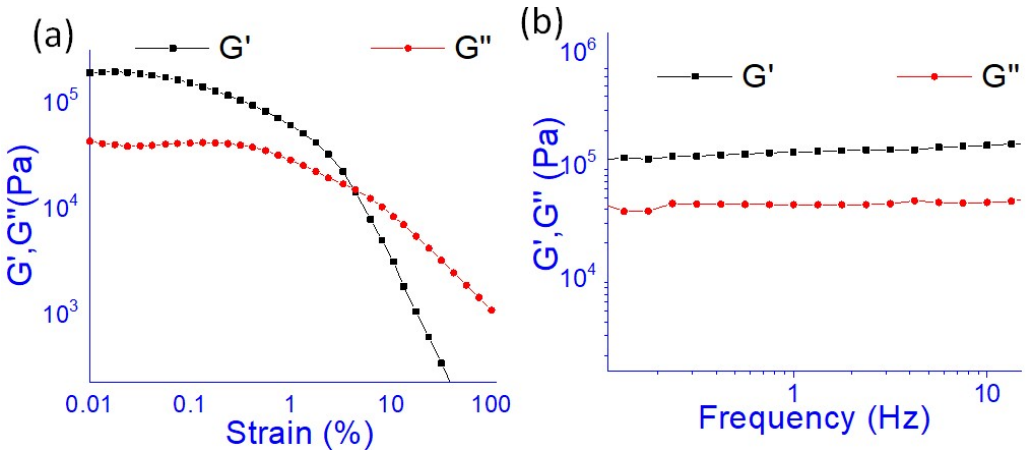


Figure 4S. Rheological studies of the gel of **1** with 1 equivalent amounty of F^- ion: (a) amplitude sweep (at constant frequency of 1Hz) and (b) frequency sweep (at constant 0.1% strain) experiments [gel was prepared at its cgc in DMF/H_2O (10:1, v/v)].

Table 3S. Summary of rheological properties of the F^- treated gel of **1**.

Gel	Critical strain (%)	Cross-over (% strain)	G'_{av} (Pa)	G''_{av} (Pa)	G'_{av}/G''_{av}	tan δ (G''_{av}/G'_{av})
1.F^-	0.01	4.2	127294	43941	2.89	0.346

Figure 5S. Photograph showing the minimum amount of CN^- needed to break the gel of **1** [7 mg dissolved in 1 mL of DMF: H_2O (10:1, v/v); c = 2.08 x 10^{-2} M].

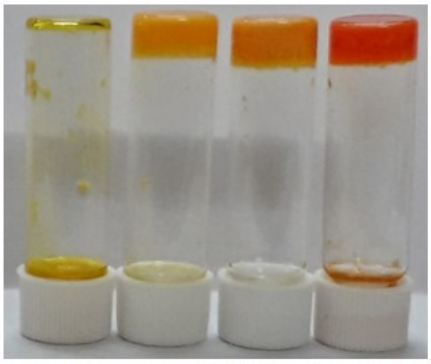


Figure 6S. Photograph showing the phase change with pH.

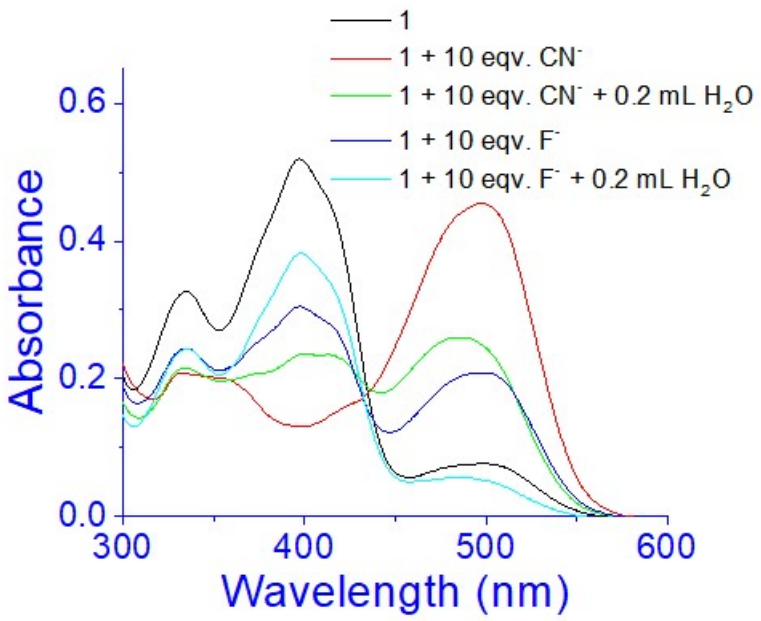


Figure 7S: UV-vis spectra of **1** (c = 2.5 x 10^{-5} M) to distinguish CN^- from F^- through addition of H_2O.

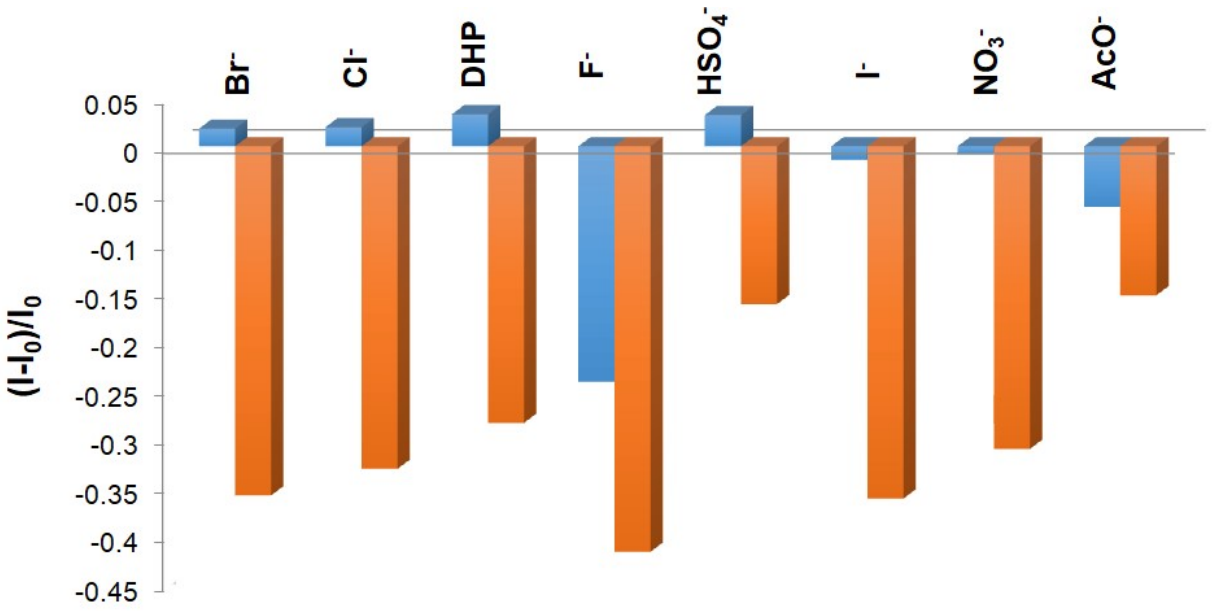


Figure 8S. Photograph showing Selectivity of **1** (c = 2.5 x 10^{-5} M) for CN^- ion in DMF: H_2O (10:1, v/v).

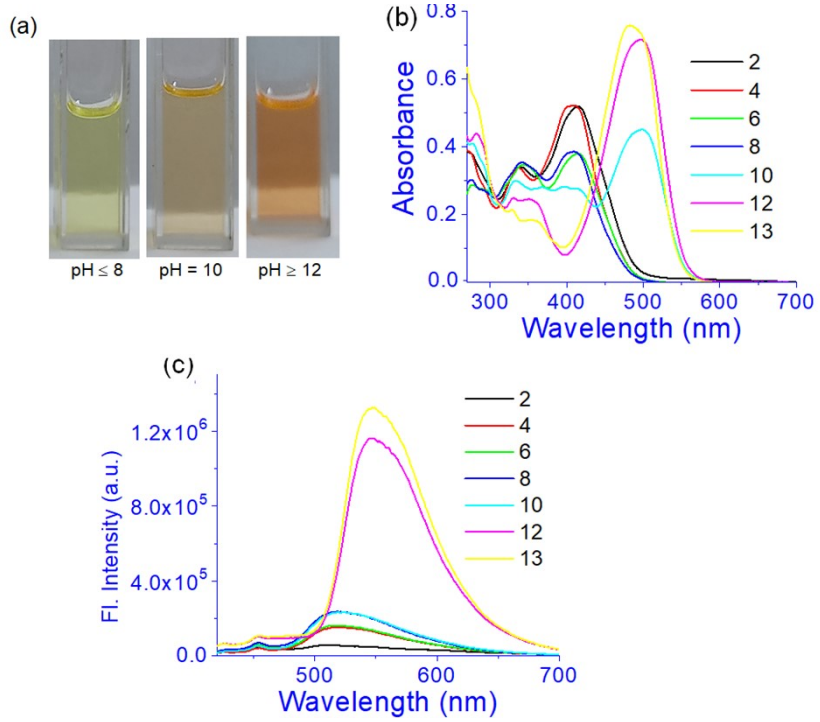


Figure 9S. The change in (a) color, (b) absorbance and (c) emission of compound **1**(c = 2.5 x 10^{-5} M) with variation of pH.

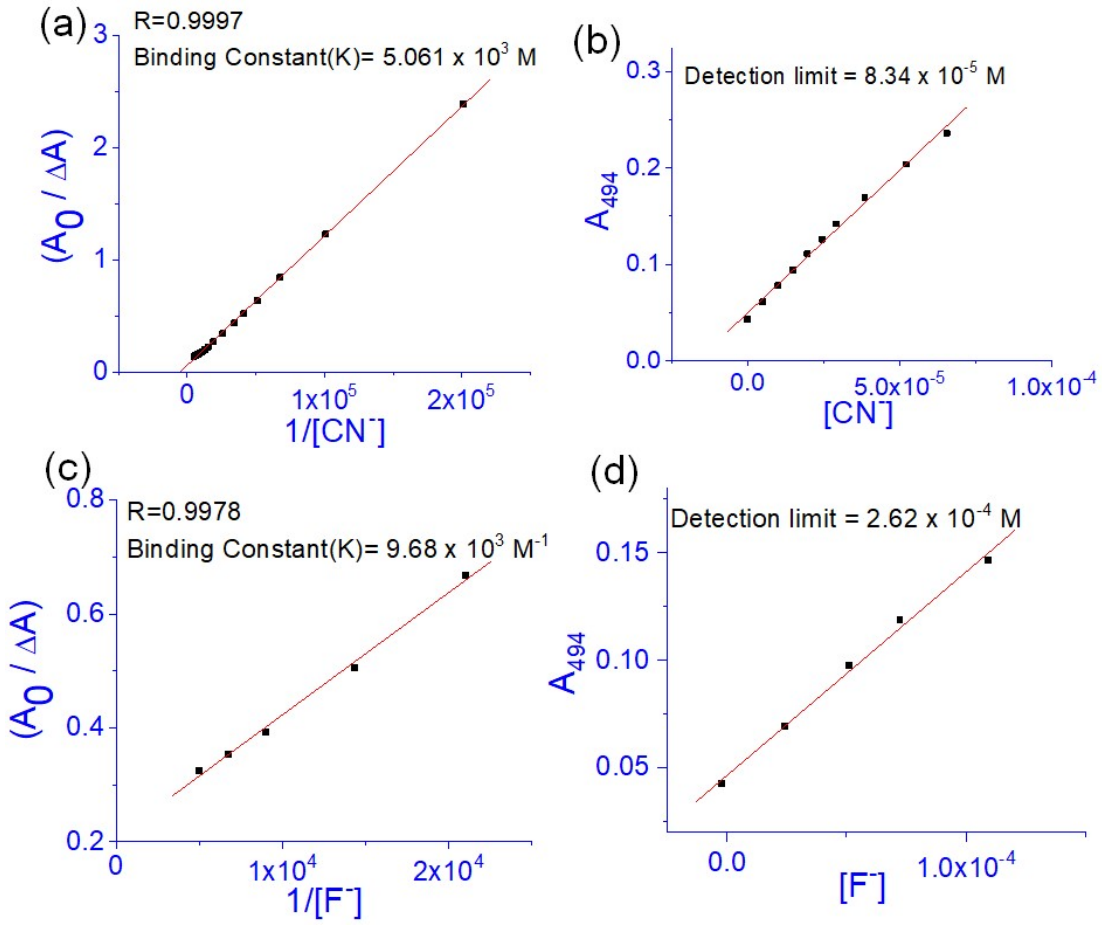


Figure 10S. Benesi–Hildebrand plots for **1** with (a) CN^- and (c) F^- and detection limits of **1** (c = 2.5 x 10^{-5} M) with (b) CN^- and (d) F^- (c = 1.0 x 10^{-3} M) in DMF: H_2O (10:1, v/v) by considering absorbance change at 494 nm.

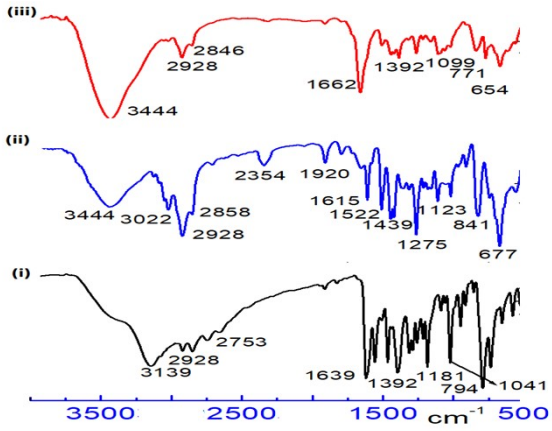
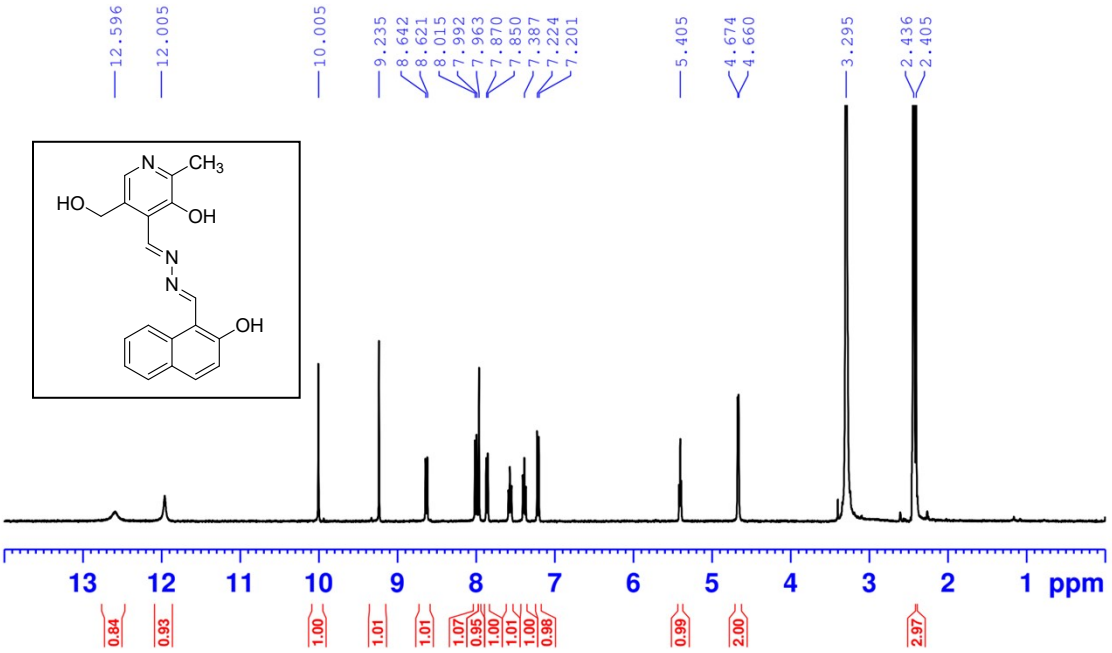
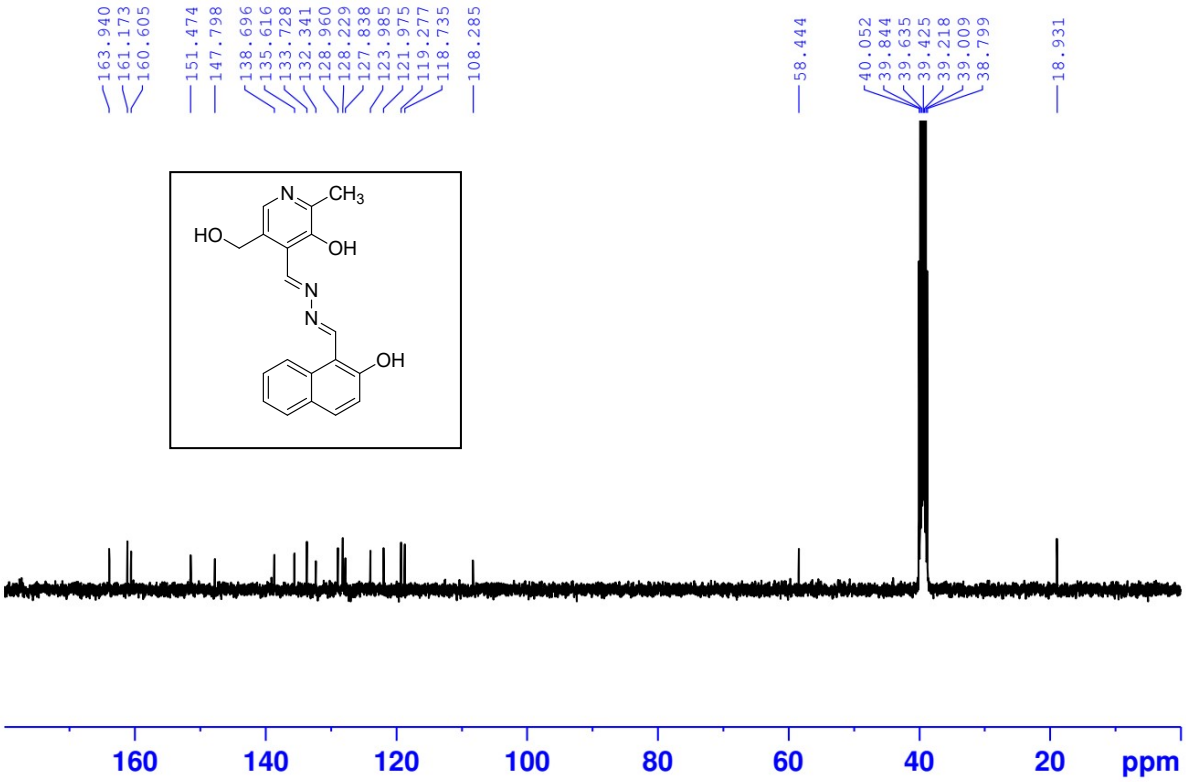


Figure 11S: FTIR spectra of: (i) **1**, (ii) Merrifield resin and (iii) **1** hooked to Merrifield resin (**1a**).

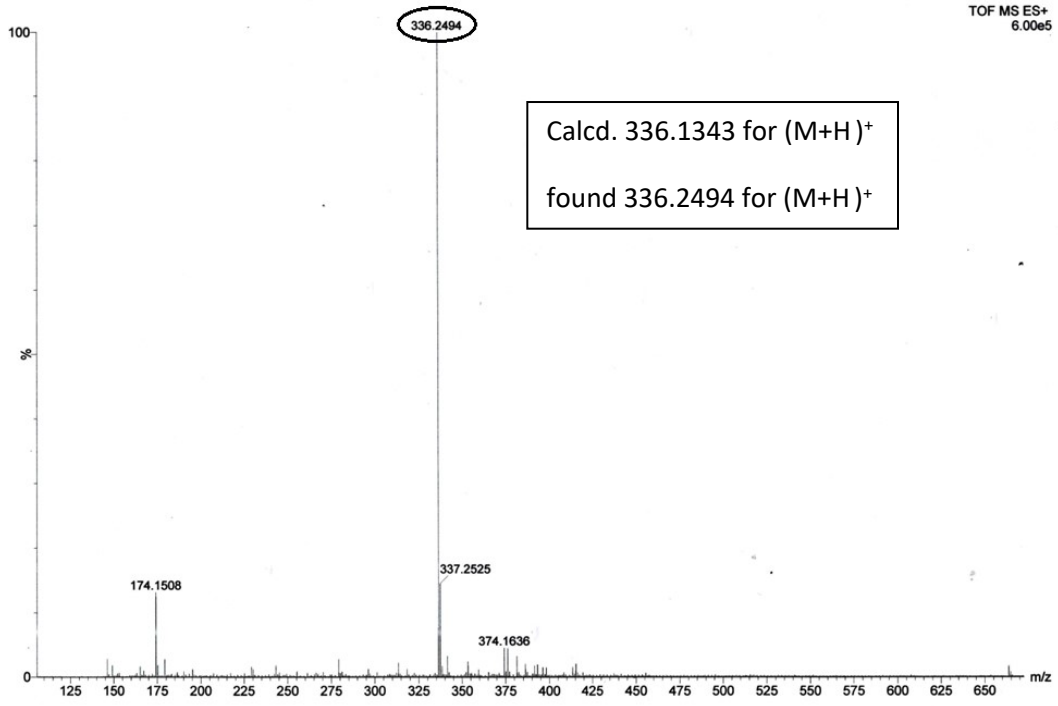
^{1}H NMR of compound **1** in d_6-DMSO (400 MHz)



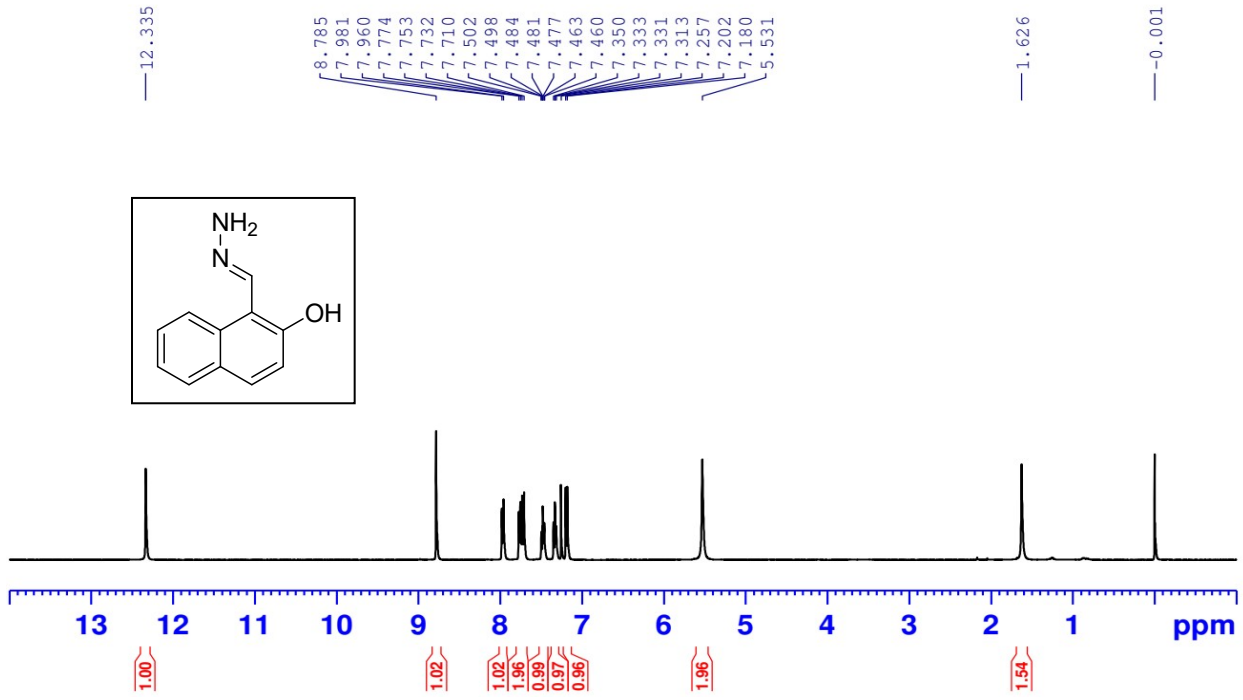
^{13}C of compound **1** in d_6-DMSO (100 MHz)



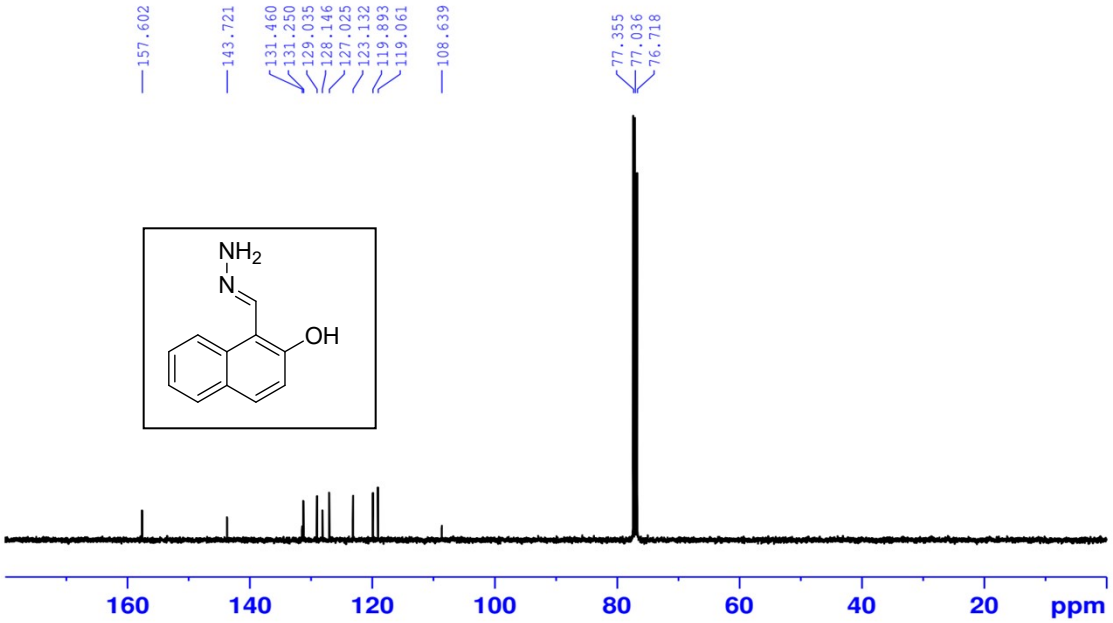
Mass spectra of Compound **1**



^{1}H NMR of compound **4** in $CDCl_3$ (400 MHz)



^{13}C NMR of compound **4** in $CDCl_3$ (100 MHz)



^{1}H NMR of compound **3** in $CDCl_3$ (400 MHz)