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

Supporting Information

Cholesterol linked benzothiazole: A versatile gelator for detection of picric acid and metal ions such as Ag^+, Hg^{2+}, Fe^{3+} and Al^{3+} under different conditions

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Table S1: Results of gelation test for **1**

Solvent	**1**
$CHCl_3$	S
DCM	S
Nitrobenzene	G (mgc = 18 mg/mL, T_{gel} = 44 °C)
Benzene	G (mgc = 56 mg/mL, T_{gel} = 40 °C)
1,4-Dioxane	G (mgc = 25 mg/mL, T_{gel} = 52 °C)
Toluene	G (mgc = 45 mg/mL, T_{gel} = 42 °C)
MeOH	I
CH_3CN	I
$CHCl_3$ – MeOH (1:1, v/v)	I
DMSO	I
$CHCl_3$-PET ether (1:1,v/v)	I
Cyclohexane	PS
n-Hexane	I
Diethyl ether	I
Acetone	PS
THF	S
DMF	G (mgc = 10 mg/mL, T_{gel} = 50 °C)
DMF : H_2O (1:1, v/v)	P
MeOH : H_2O (1:1, v/v)	I
CH_3CN : H_2O (1:1, v/v)	I
S = solution; G = gel; I = insoluble; PS = partially soluble; PG = partial gelation. Gelation studies were carried out by taking 60 mg of compound **1** in 1 mL of each solvent. Gels were primarily characterized by inversion of vial method after ~5 min of sample preparation.	

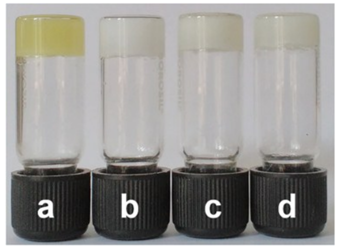


Fig S1. Pictorial representation of gel of **1** in (a) nitrobenzene, (b) DMF, (c) toluene and (d) benzene.

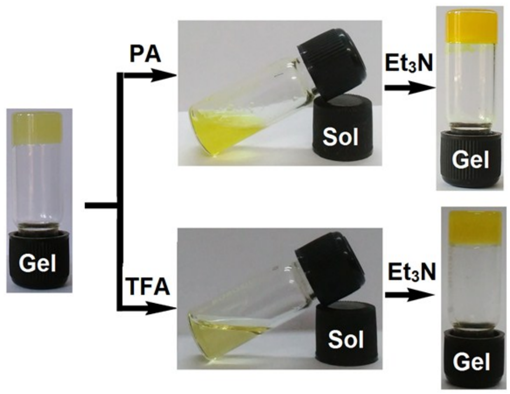


Fig S2. Photograph representing the phase change of the nitrobenzene gel of **1** (20 mg/mL) upon successive addition of 1 equiv. amount of picric (PA), trifluoroacetic acid (TFA) and Et_3N.

(a) (b)

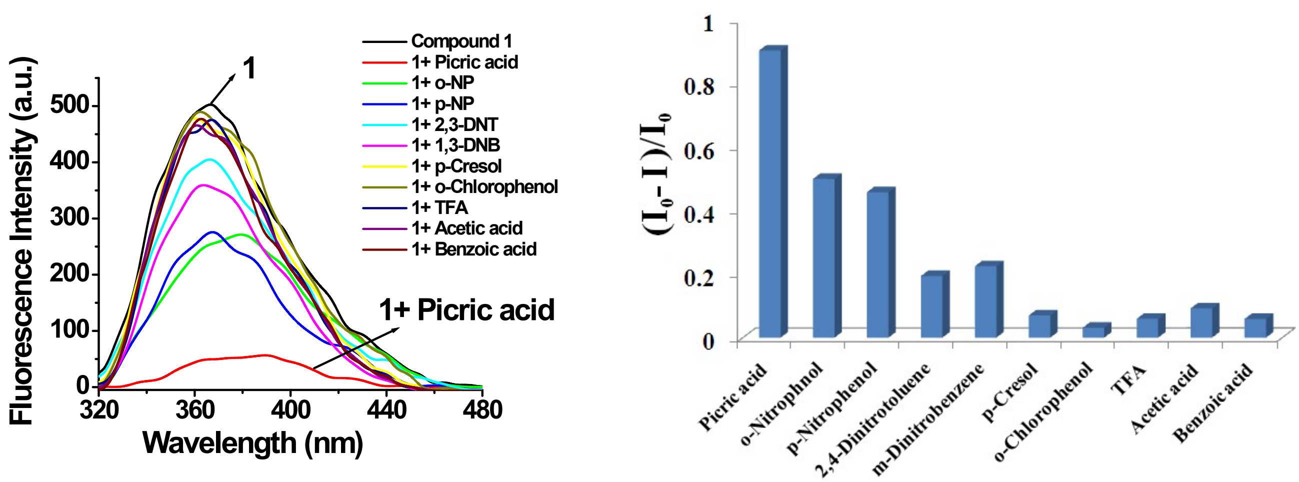


Fig S3. Change in (a) emission and (b) fluorescence ratio $[I\text{-}I_0/I_0]$ of **1** (c = 2.50 x 10^{-5} M) upon addition of 12 equiv. amounts of different guests (c = 1.0 x 10^{-3} M) in CH_3CN containing 1% $CHCl_3$.

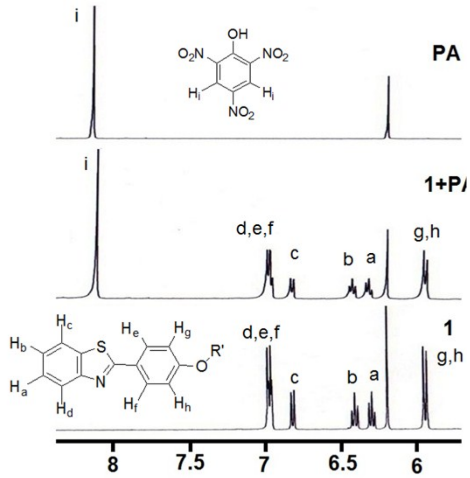


Fig S4. Partial ^{1}H NMR (400 MHz) of **1** (c = 3.07 x 10^{-3} M) in absence and presence of 1 equiv. amount of PA.

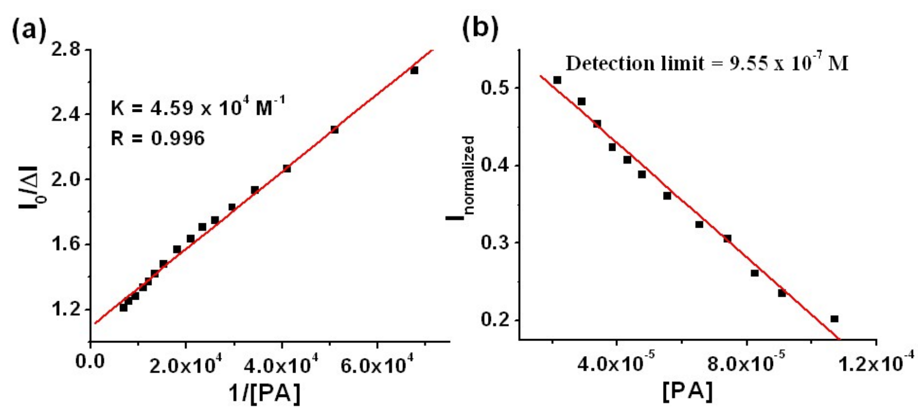


Fig S5. (a) Benesai-Hildebrand plot and (b) detection limit of **1** for with picric acid (*c* = 1 x 10^{-3} M) in CH_3CN containing 1% $CHCl_3$.

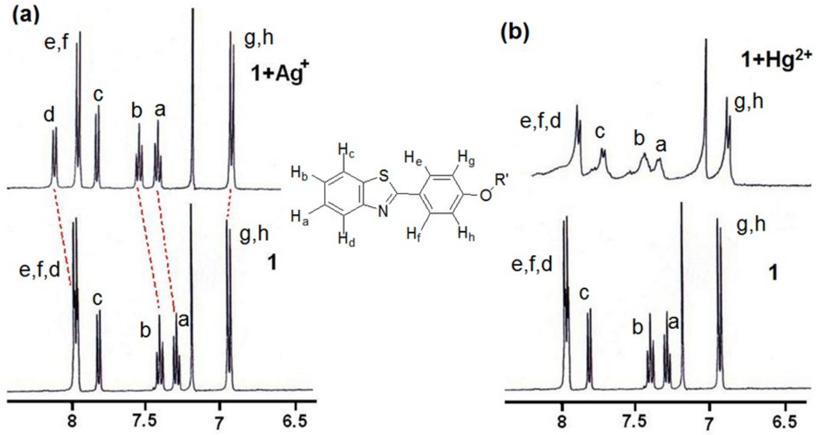


Fig S6. Partial [1]H NMR (400 MHz) of **1** (c = 3.07 x 10^{-3} M) in absence and presence of 1 equiv. amount of (a) Ag^+ and (b) Hg^{2+} in $CDCl_3$.

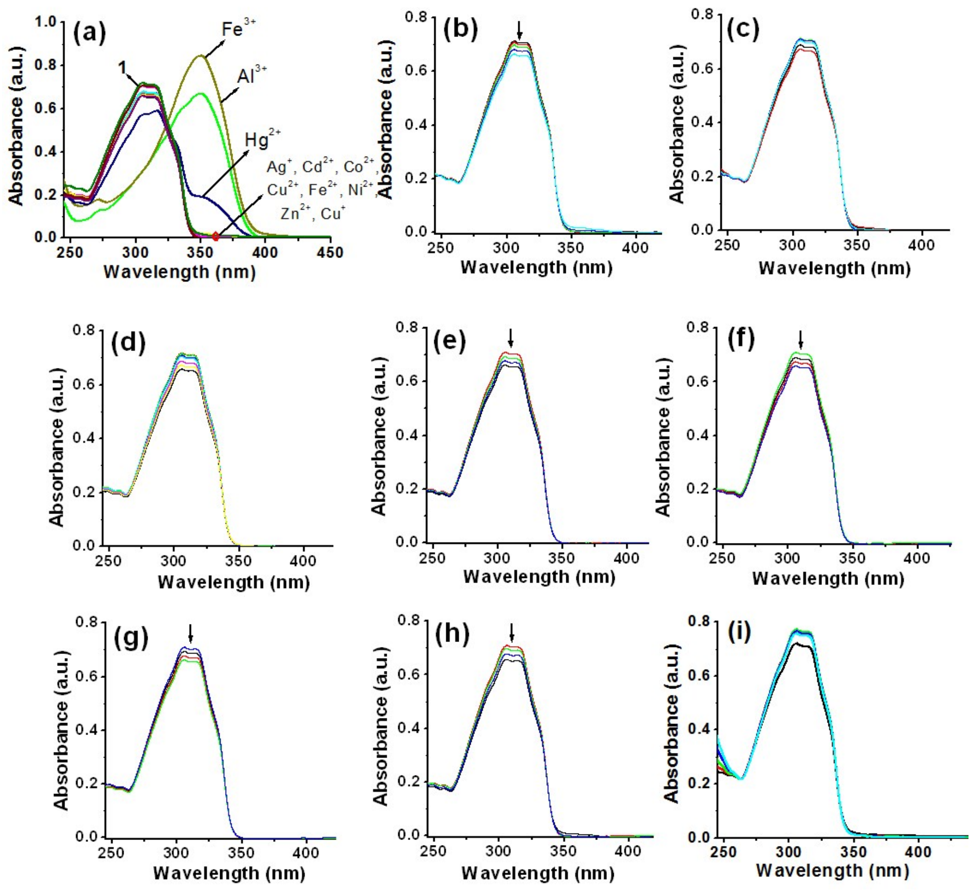


Fig S7. Change in UV-vis spectra of **1** with addition of 3 equiv. amounts of (a) all the metal ions, (b) Fe^{2+}, (c) Cu^{2+}, (d) Ag^+ (e) Co^{2+}, (f) Ni^{2+} , (g) Zn^{2+}, (h) Cd^{2+} and (i) Cu^+ (c = 1 x 10^{-3} M) in CH_3CN containing 1% $CHCl_3$.

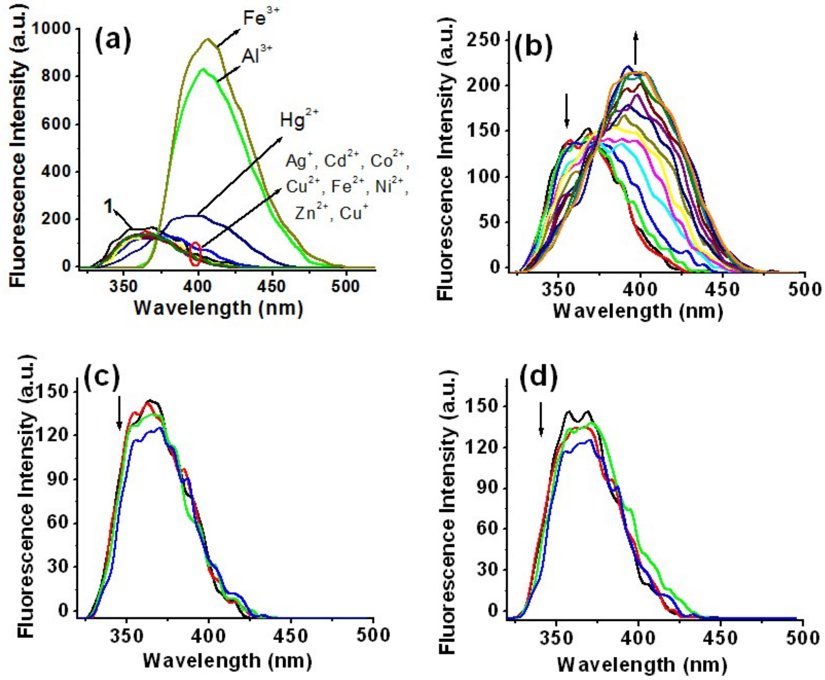


Fig S8. Change in emission of **1** with addition of 3 equiv. amounts of (a) all the metal ions, (b) Hg^{2+}, (c) Cu^{2+} and (d) Fe^{2+} (c = 1 x 10^{-3} M) in CH_3CN containing 1% $CHCl_3$.

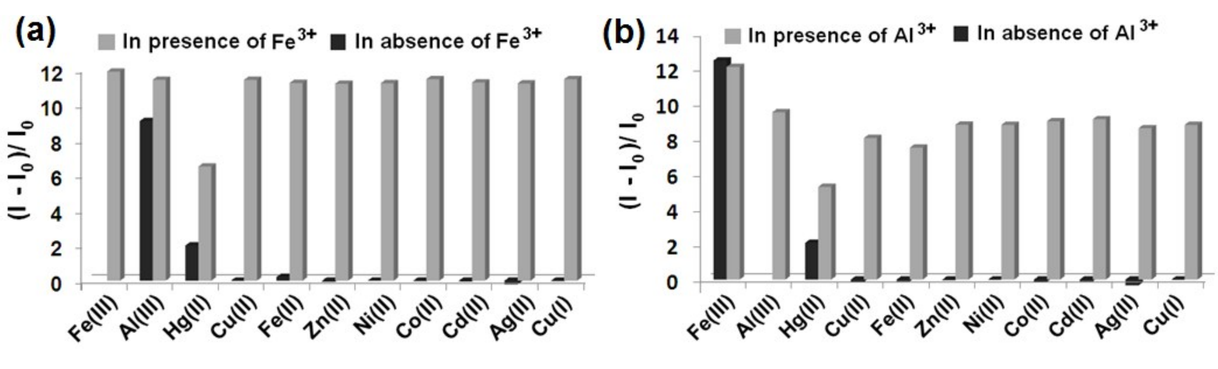


Fig S9. Change in fluorescence ratios of **1** (c = 2.5 x 10^{-5} M) with (a) Fe^{3+} and (b) Al^{3+} (c = 1 x 10^{-3} M) in the absence and presence of 3 equiv. amounts of different metal ions in CH_3CN containing 1% $CHCl_3$.

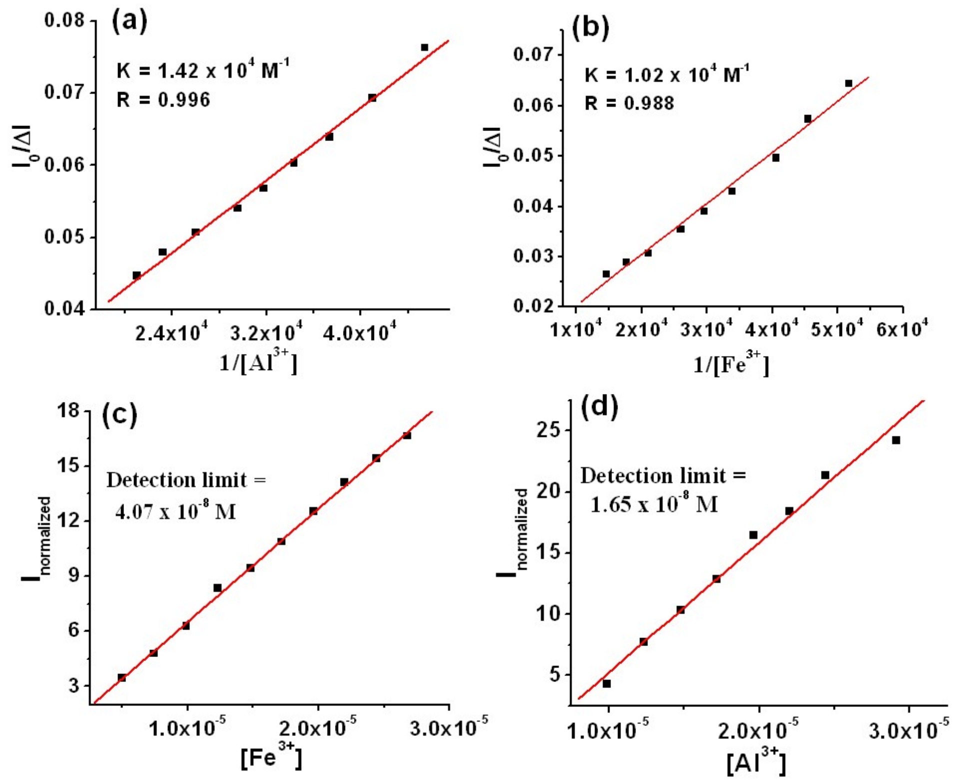


Fig S10. Benesai-Hildebrand plots of **1** with (a) Fe^{3+} and (b) Al^{3+}; Detection limit plots of **1** for (c) Fe^{3+} and (d) Al^{3+} ($c = 1 \times 10^{-3}$ M) in CH_3CN containing 1% $CHCl_3$.

Table S2: Reported PA sensors in gel phase

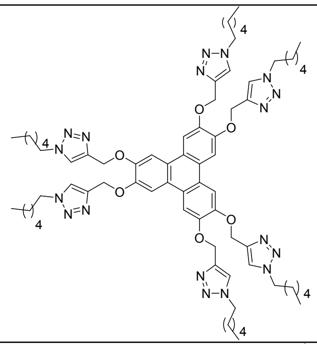
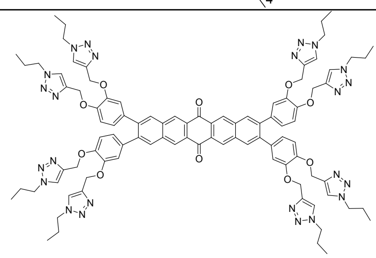
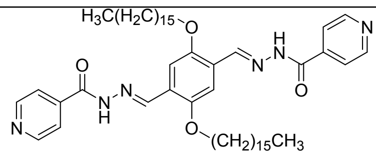
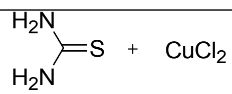
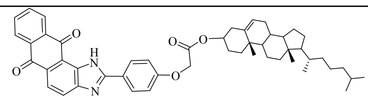
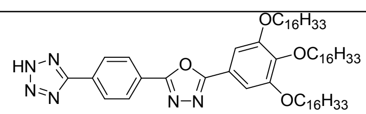
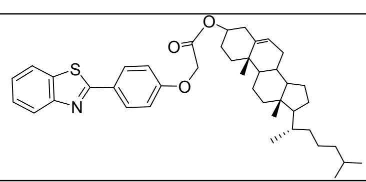
Entry	Structure of compounds	Medium of Gelation	Sensing	Ref.
1		Cyclohaxane and DCM/Haxane (1:4)	Detection of picric acid vapor through gel to sol transition	*Langmuir* 2011, **27**, 15275.
2		Toluene/DCM (8:2), Benzene/DCM (8:2) and o-Xylene/DCM (8:2)	Detection of picric acid through gel to sol transition	*ACS Appl. Mater. Interfaces* 2013, **5**, 672−679
3		THF	Detection of picric acid through gel to sol transition	*Appl. Mater. Interfaces* 2013, **5**, 8394
4		Water	Detection of picric acid through gel to sol transition	*ACS Appl. Mater. Interfaces* 2014, **6**, 6308
5		Nitrobenzene, Toluene, benzene and 1,2-dichlorobenzene	Detection of picric acid through gel to sol transition	*ChemistrySelect* 2017, **2**, 4800.
6		DMSO	Detection of picric acid through gel to sol transition	*New J. Chem.* 2018,**42**, 5382-5394
Our Work		Nitrobenzene	Detection of picric acid through gel to sol transition	

Table S3: List of different Hg^{2+} ion responsive supramolecular gelators

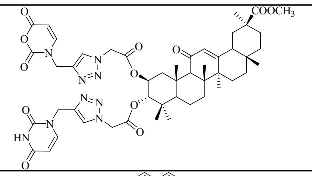
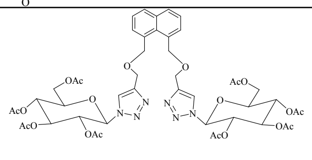
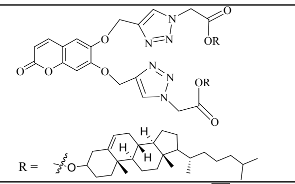
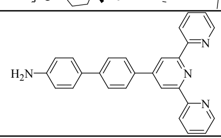
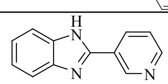
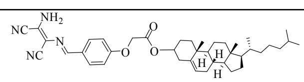
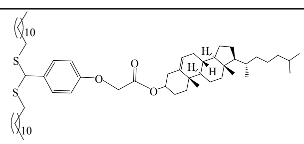
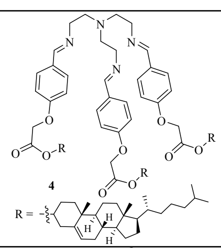
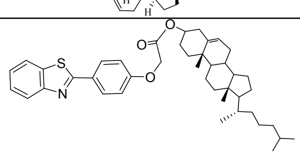
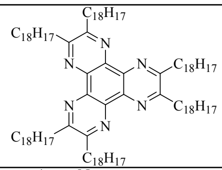
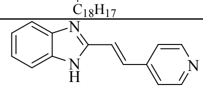
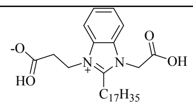
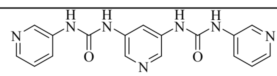
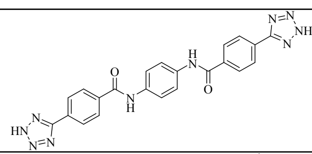
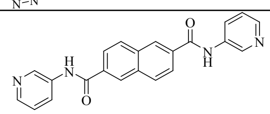
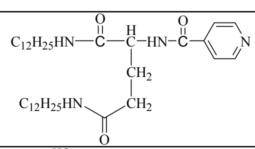
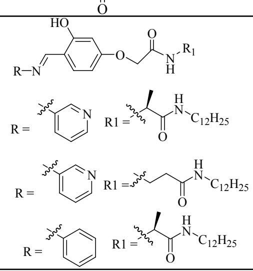
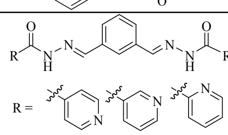
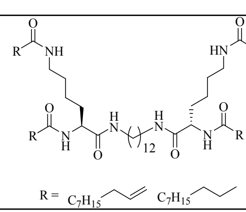
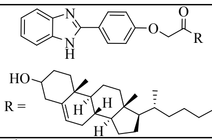
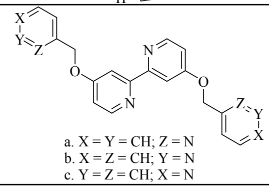
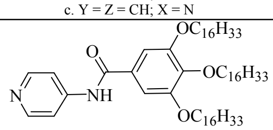
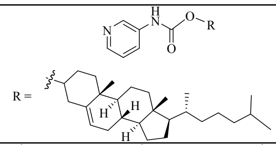
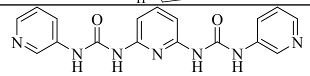
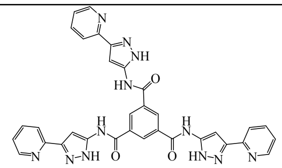
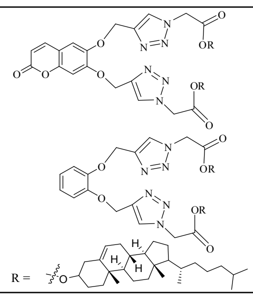
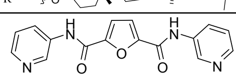
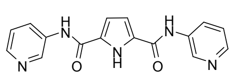
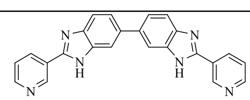
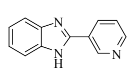
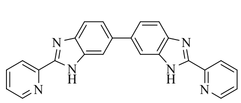
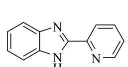
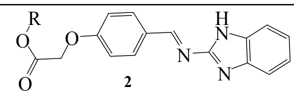
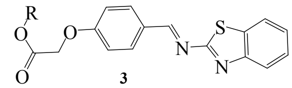
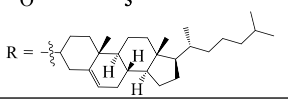
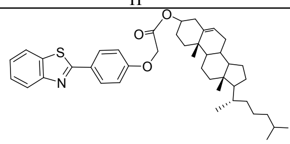
Entry	Structure	Solvent	Phase transformation in presence of Hg^{2+} ions	Interfering metal ions	Detection limit for Hg^{2+} (M)	Ref.
1		1,2-dichloroethane	Gel to Sol	-	-	*Org. Lett.,* 2011, **13**, 3372.
2		1,2-dichloroethane	Gel to Sol	-	-	*New J. Chem*., 2013*,* **37**, 2419.
3		$CHCl_3$:CH_3OH (2:1, v/v)	Gel to Sol	Cu^{2+}, Ag^{+}	-	*New. J. Chem*., 2016, **40**, 3476.
4		0.2 N HCl	Sol to gel	-	-	*Chem. Commun*., 2014, **50**, 734.
5		DMSO : H_2O = (1 : 6, v/v)	Gel to Sol	Cu^{2+}, Ag^{+}	2.02 x 10^{-6}	*Mater. Chem. Front.*, 2018, **2**, 385.
6		DMF : H_2O = (1 : 1, v/v)	Gel to Sol	Cu^{2+}	2.61 x 10^{-6}	*New. J. Chem*., 2018, **42**, 13718-13725
7		DMF : H_2O = (1 : 1, v/v)	Sol to gel Chemodosimetric approach	-	5.71 x 10^{-6}	*Supramol. Chem.,* 2018, **30**, 722.
8		DMF : H_2O = (1 : 1, v/v)	Sol to gel Chemodosimetric approach	-	5.51 x 10^{-6}	*New J. Chem.*, 2019, DOI: 10.1039/c8nj05056b
		Nitrobenzene	Gel to Sol	-	-	*Present work*

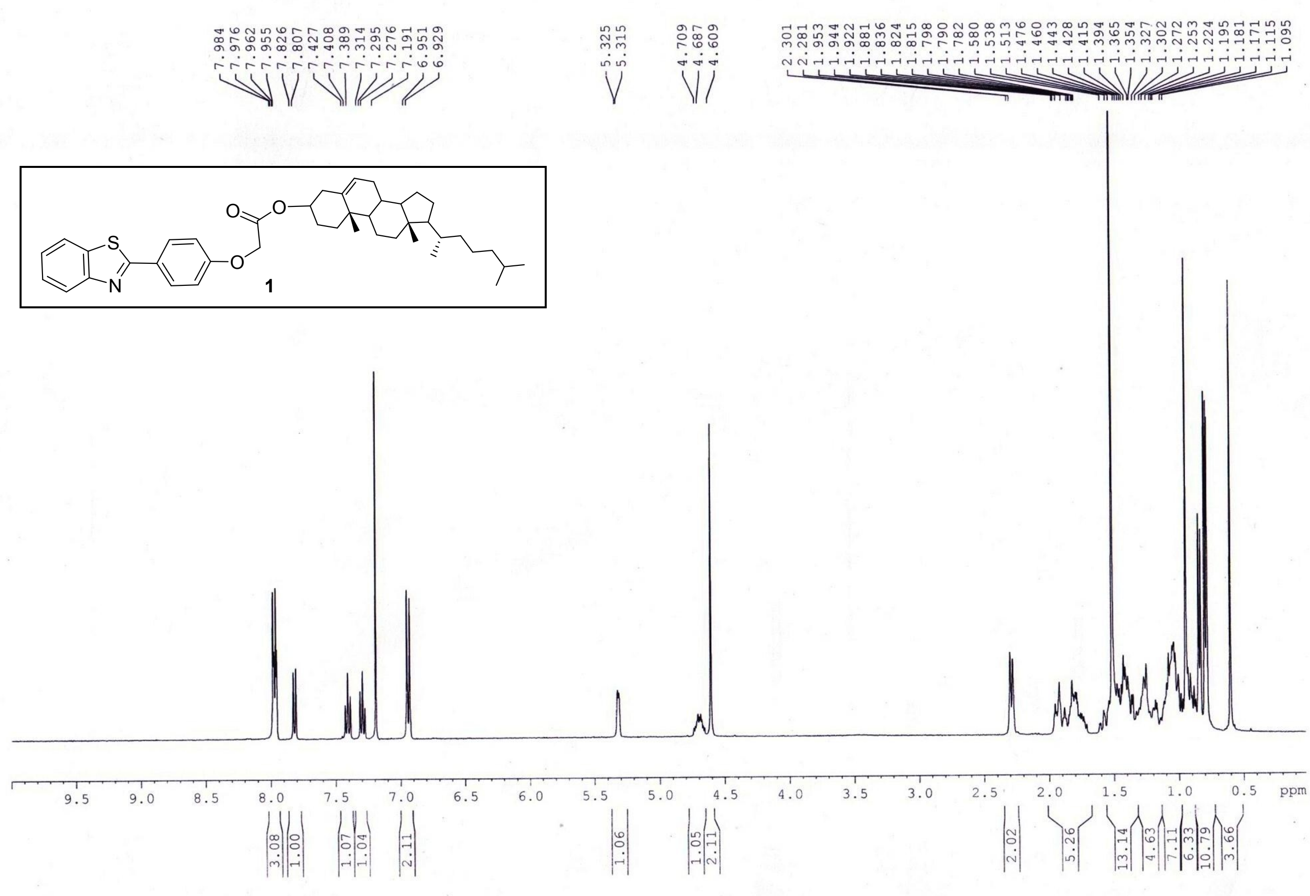
Table S4: List of different Ag^{+} ion responsive supramolecular gelators

Entry	Structure	Solvent	Phase transformation in presence of Ag^{+} ions	Interfering metal ions	Detection limit for Ag^{+} (M)	Ref.
1		EtOH	Gel to sol	-	-	*Tetrahedron Lett*. 2012, **53**, 1840.
2		MeOH	Sol to gel	-	-	*Chem. Commun*. 2013, **49**, 4181.
3		$MeOH:H_2O$ (1:1, v/v)	Sol to gel	-	-	*Supramol. Chem*. 2014, **26**, 39.
4		THF/ H_2O	Sol to gel	-	-	*Soft Matter*, 2011, **7**, 2412.
5		H_2O	Sol to gel	-	-	*Soft Matter*, 2012, **8**, 6557.
6		DMF: H_2O (2:3, v/v)	Sol to gel	-	-	*Cryst. Growth Des*. 2015, **15**, 4635.
7		CH_2Cl_2, $CHCl_3$, THF	Sol to gel	-	-	*Langmuir*, 2012, **28**, 27.
8		Toluene: EtOH (99:1, v/v)	Sol to gel	-	-	*Chem. Commun*. 2015, **51**, 13929.
9		DMF, DMF/ H_2O, DMSO/ H_2O	Sol to gel	-	-	*Cryst. Growth Des*. 2015, **15**, 5360.
10		EtOAc	Gel to sol	Li^{+}	-	*Chem. Commun*. 2012, **48**, 2767.

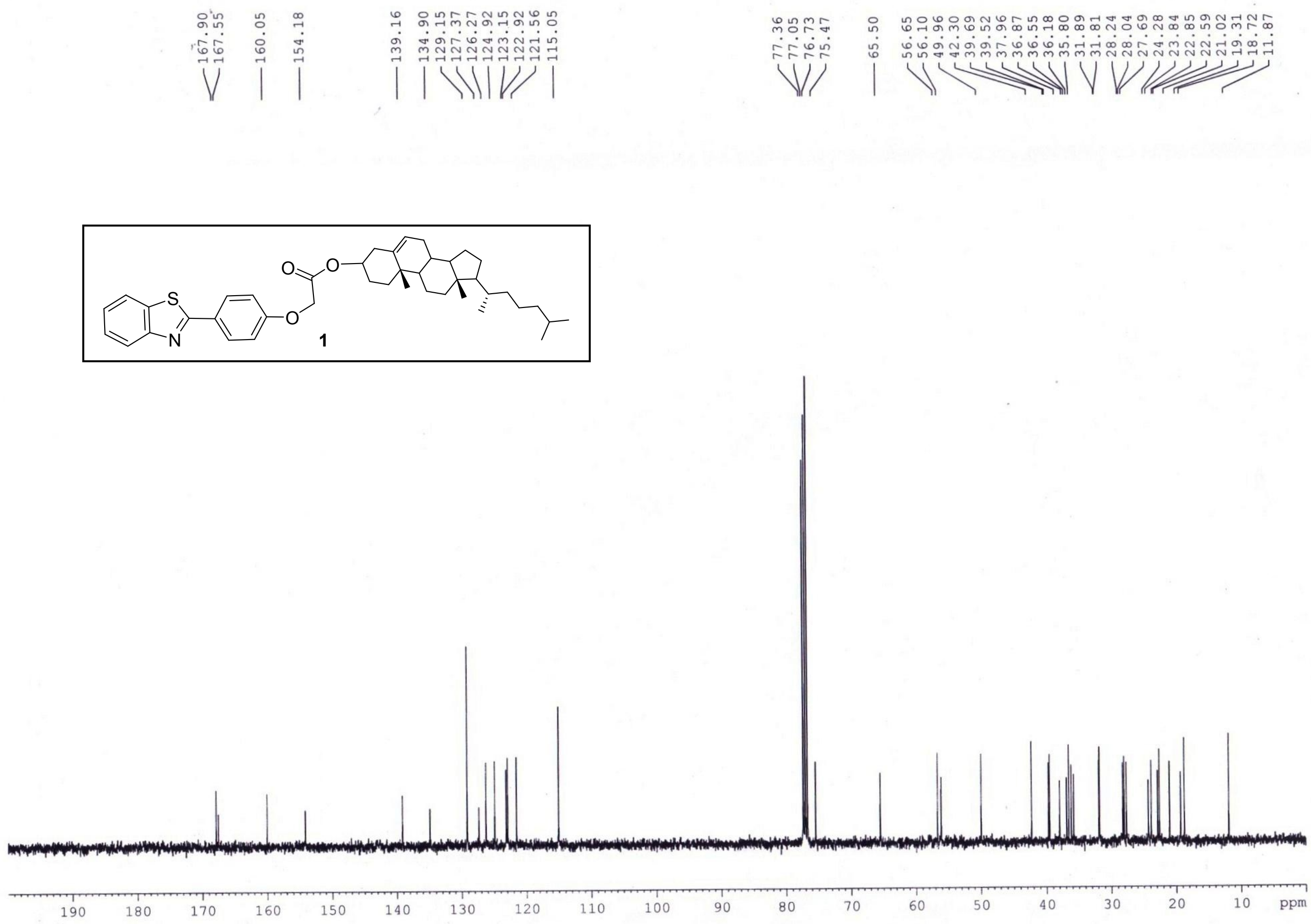
11		DMF : H_2O (1:1, v/v)	Sol to gel	-	4.31 x 10^{-5}	*ChemistrySelect*, 2017, **2**, 959.
12		DMSO: H_2O	Sol to gel	-	-	*Dalton Trans.*, 2017, **46**, 2793.
13		Toluene/ethanol (10:1, v/v)	Sol to gel	-	-	*Langmuir,* 2007, **23**, 8217.
14		Diphenyl ether	Sol to gel	-	-	*Chem. Lett.*, 2003, **32**, 12.
15		THF-H_2O (3 : 2)	Sol to gel	-	-	*New J. Chem.*, 2010, **34**, 2261.
16		H_2O	Sol to gel	-	-	*New J. Chem.*, 2014, **38**, 2470.
17		$CHCl_3$:CH_3OH (2:1, v/v)	Gel to Sol	Cu^{2+}, Hg^{2+}	-	*New. J. Chem.*, 2016, **40**, 3476.
18	 	DMSO: H_2O (1:1, v/v)	Sol to gel	Cu^{2+} -	- -	*New. J. Chem.*, 2018, **42**, 6488.
19	   	DMSO: H_2O DMSO: H_2O DMSO: H_2O DMSO: H_2O	Gel to sol Gel to sol Sol to gel Sol to gel	Cu^{2+} Cu^{2+}, Hg^{2+} - -	3.69 x 10^{-6} 3.34 x 10^{-6} 1.93 x 10^{-7} 1.28 x 10^{-6}	*Mater. Chem. Front.*, 2018, **2**, 385.

20	 2  3 	1,4-dioxane-MeOH (1:1, v/v) 1,4-dioxane-H_2O (1:1, v/v)	Gel to sol Sol to gel	- -	3.27×10^{-5} 9.27×10^{-5}	*New J. Chem.*, 2019, DOI: 10.1039/c8nj05056b
		Nitrobenzene	Gel to Sol	-		*Present work*

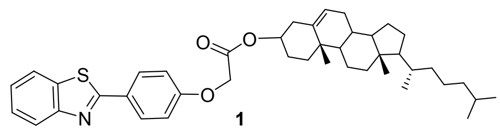
[1]H NMR ($CDCl_3$, 400 MHz) of 1

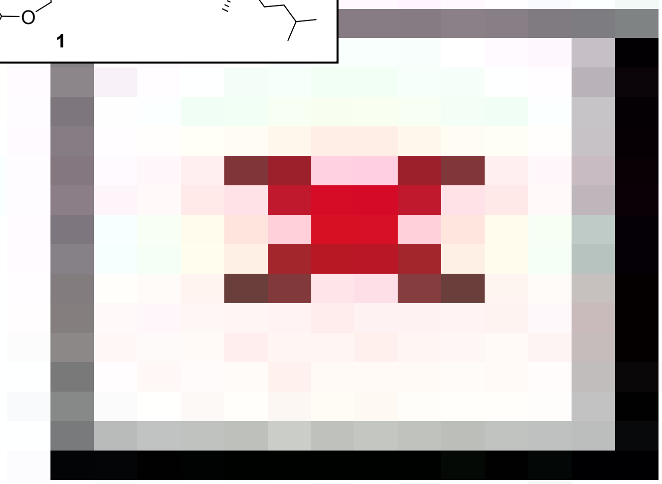


^{13}C NMR ($CDCl_3$, 100 MHz) of 1

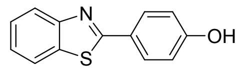


Mass spectrum of 1.


1



^{1}H NMR ($CDCl_3$ containing 8% d_6-DMSO, 400 MHz) of 3



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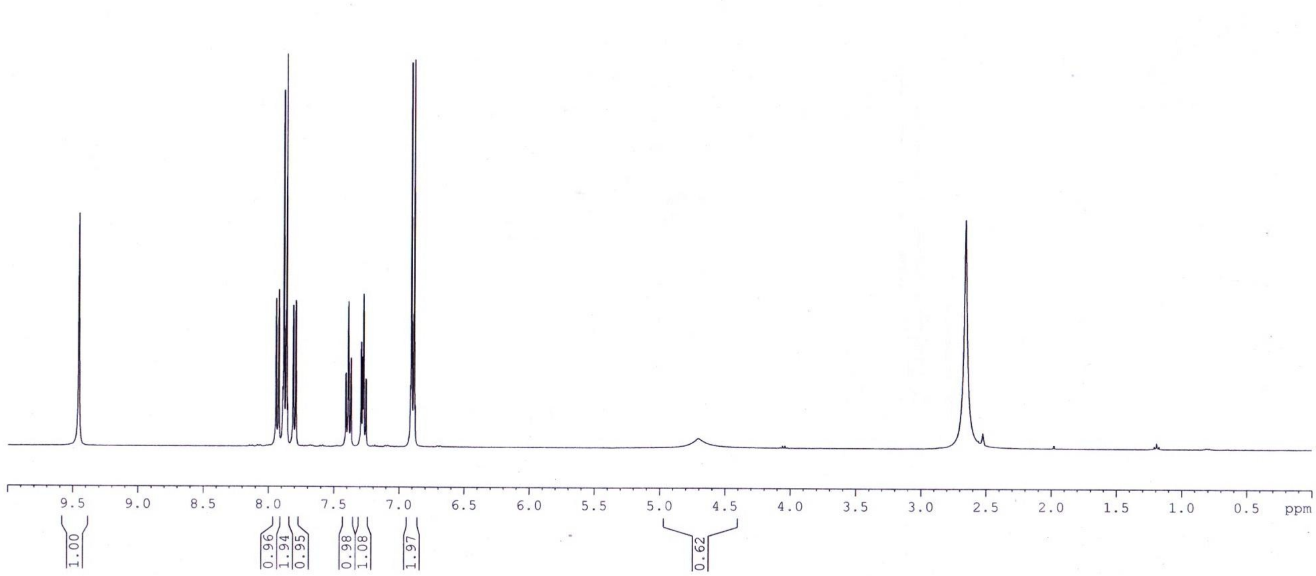
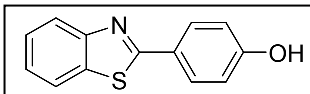


^{13}C NMR ($CDCl_3$ containing 8% d_6-DMSO, 100 MHz) of 3



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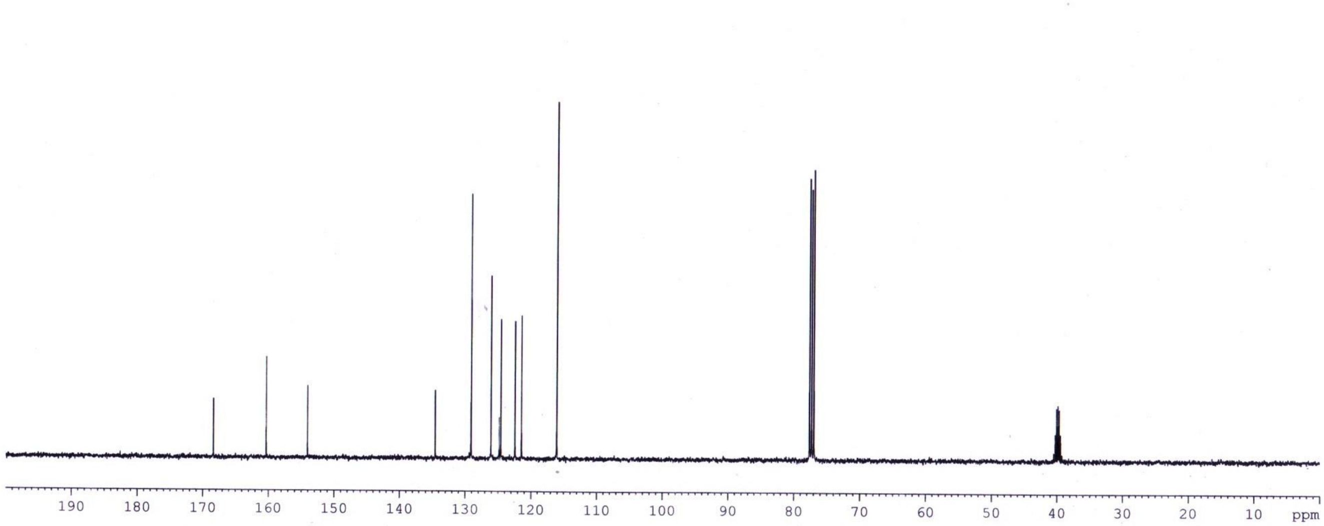
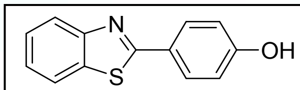


Mass spectrum of 3



3