Electronic Supplementary Material (ESI) for RSC Advances.

Electronic Supporting Information

New triangular steroid-based $A(LS)_3$ type gelators for selective fluoride sensing application

Manisha Devi, Abhimanew Dhir, Pooja and Chullikkattil P. Pradeep*

*School of Basic Sciences, Indian Institute of Technology Mandi, Kamand-175005, Himachal Pradesh, India.
Fax: +91 1905 300009; Tel: +91 1905 300045; E-mail: pradeep@iitmandi.ac.in

S2 Synthetic scheme of compound **1**

S3 Fluorescence spectrum of compound **1**

S4 Synthetic scheme of compound **2**

S5 Fluorescence spectrum of compound **2**

S6 Photographs of sol-gel of compound **2**

S7 Synthetic scheme of compound **3**

S8 Fluorescence spectrum of compound **3**

S9 Photographs of sol-gel of compound **3**

S10 Synthetic scheme of compound **4**

S11 Fluorescence spectrum of compound **4**

S12 Photographs of sol-gel of compound **4**

S13 UV spectra of compounds **2**, **3** and **4** with fluoride and hydroxide anions

S14 Mass spectrum of compound **4** + F^-

S15 ^1H NMR titration data of compound **4**

S16 Optimized structures of compounds **2**, **3** and **4**

S17 Additional TEM images of compounds **1**, **2**, **3** and **4**

S18 IR table of compounds **2**, **3**, and **4** and their xerogels

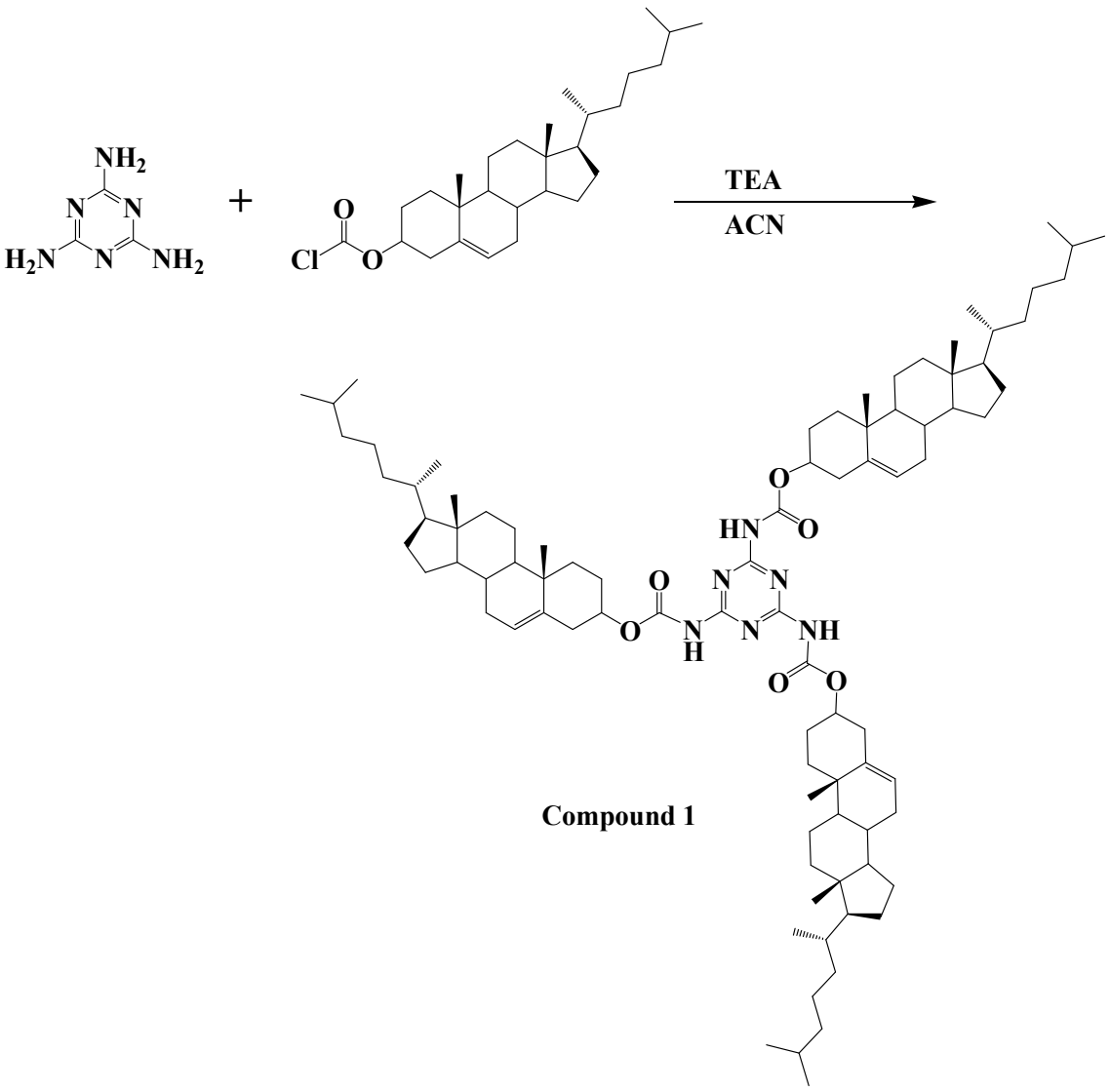

Fig. S2 Synthetic scheme of compound **1.**

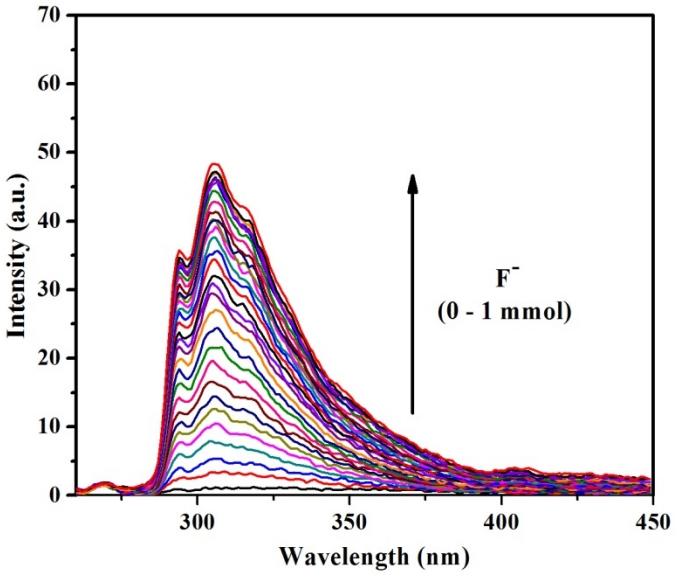

Fig. S3(a) Fluorescence of compound **1** (1×10^{-6} M) in response to fluoride anion.

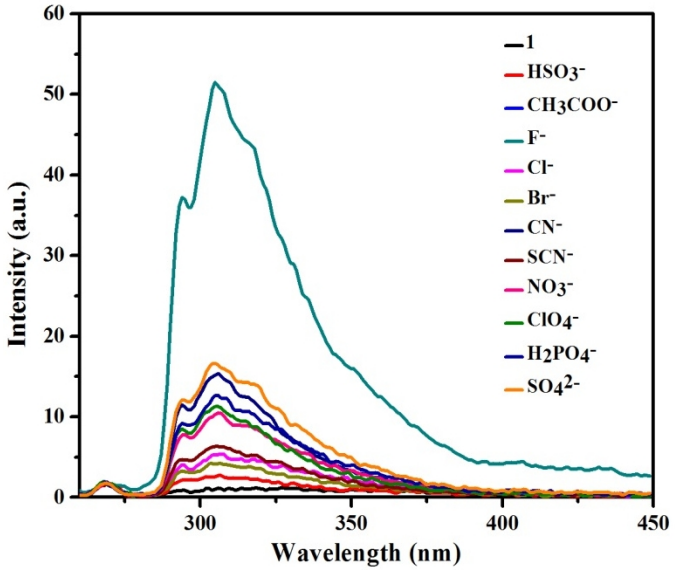

Fig. S3(b) Comparative graph of fluorescence spectra of compound **1** (1×10^{-6} M) in response to 11 different anions.

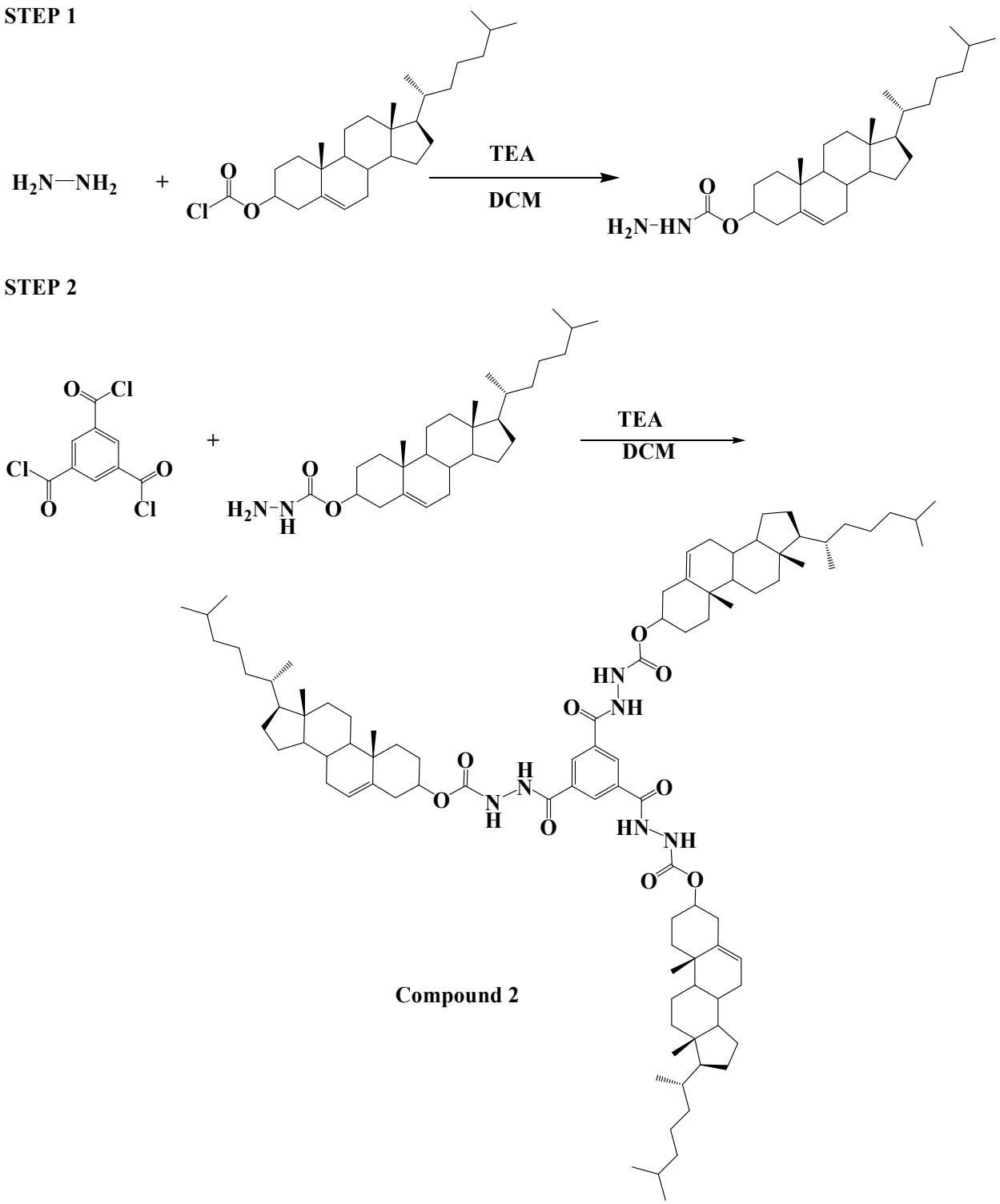

Fig. S4 Synthetic scheme of compound **2.**

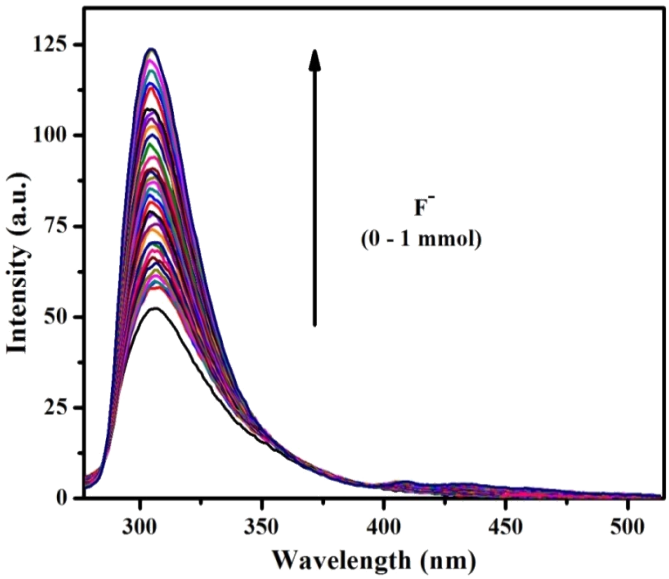

Fig. S5(a) Fluorescence of compound **2** (1×10^{-6} M) in response to fluoride anion.

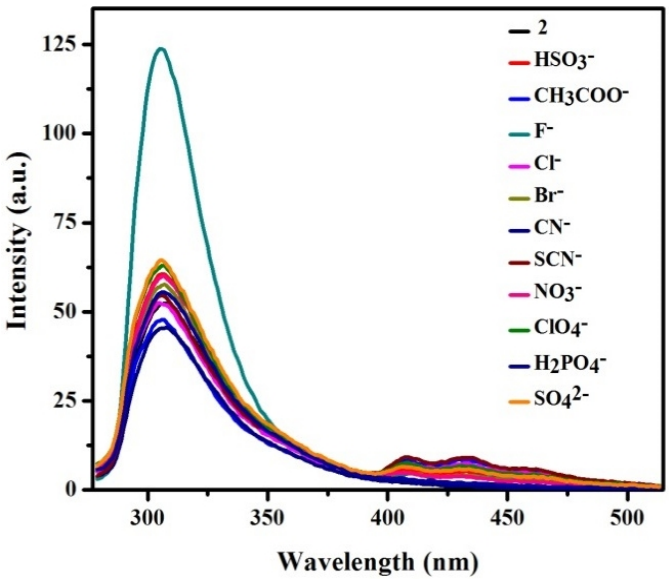

Fig. S5(b) Comparative graph of fluorescence spectra of compound **2** (1×10^{-6} M) in response to 11 different anions.

Fig. S6(a) Gel obtained from **2** with N,N-diisopropylethylamine (DIPEA) and degradation of gel after addition of TBAF.

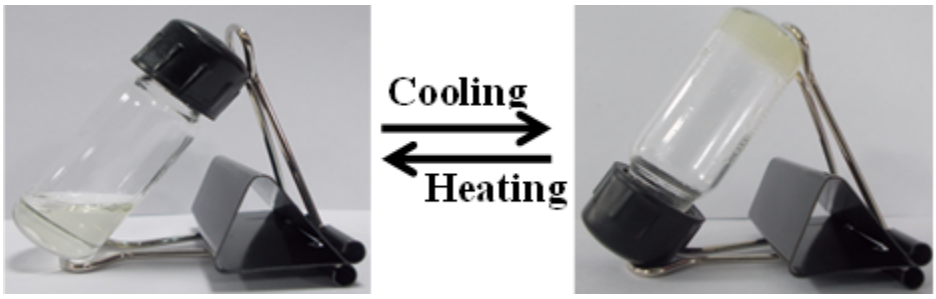

Fig. S6(b) Gel obtained from **2** with triethylamine (TEA).

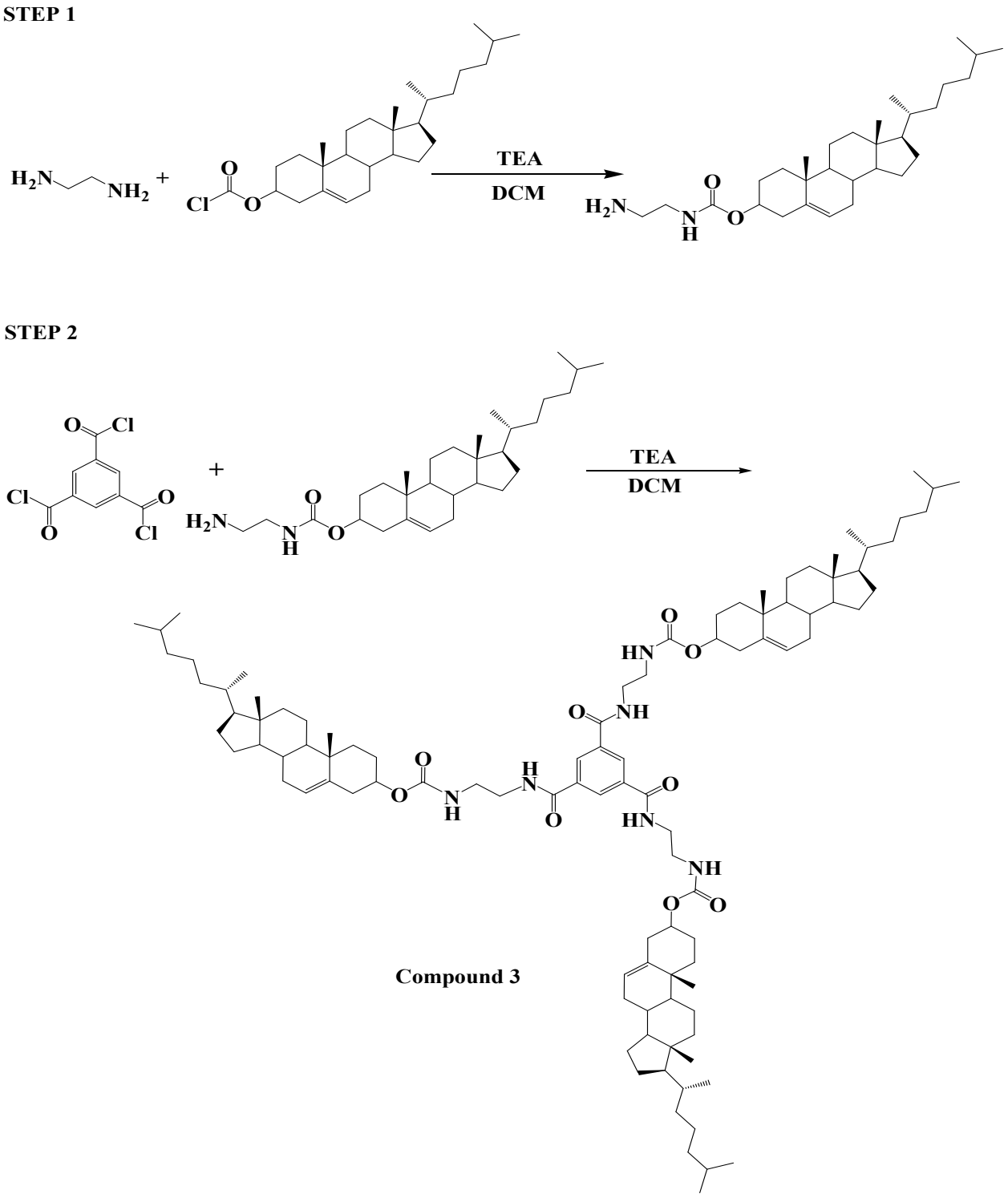

Fig. S7 Synthetic scheme of compound **3.**

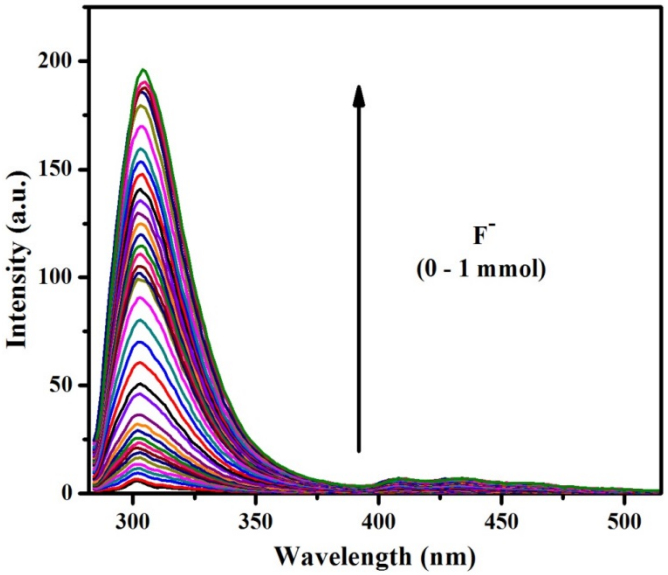

Fig. S8(a) Fluorescence of **3** (1×10^{-6} M) in response to fluoride anion.

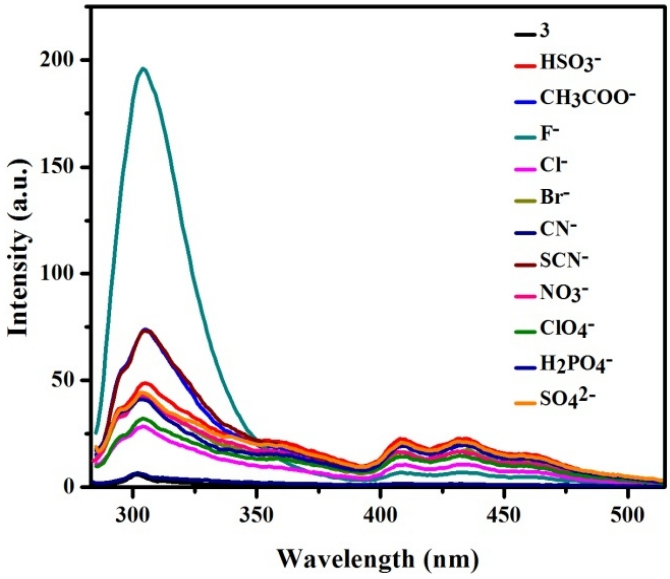

Fig. S8(b) Comparative graph of fluorescence spectra of compound **3** (1×10^{-6} M) in response to 11 different anions.

Fig. S9(a) Gel obtained from **3** with N,N-diisopropylethylamine (DIPEA) and degradation of gel after addition of TBAF.

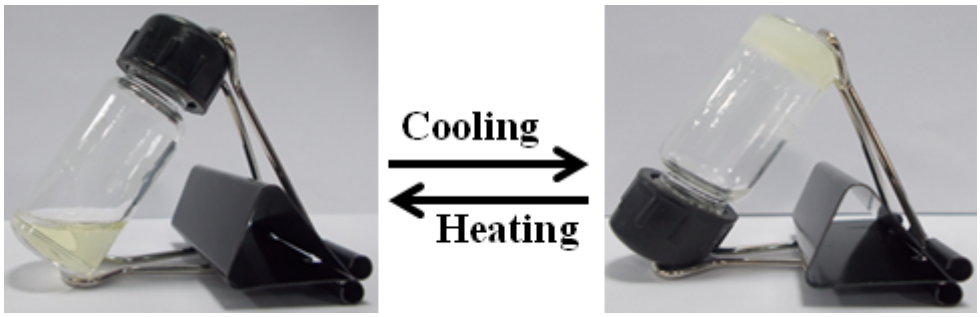

Fig. S9(b) Gel obtained from **3** with triethylamine (TEA).

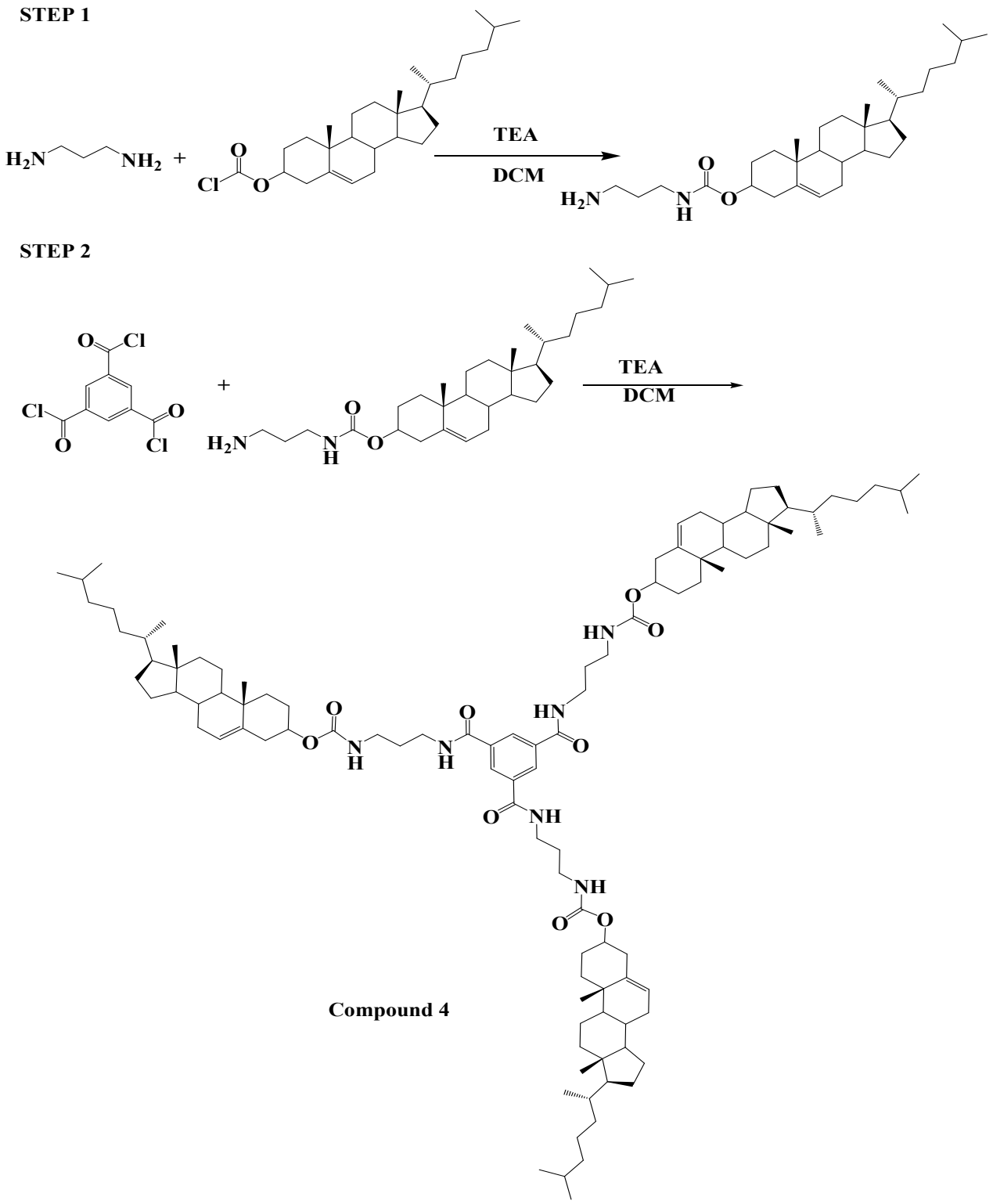

Fig. S10 Synthetic scheme of compound **4.**

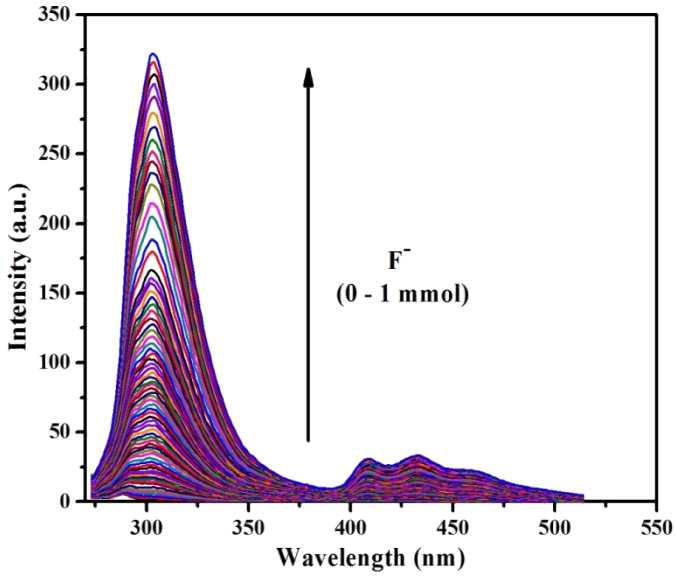

Fig. S11(a) Fluorescence of **4** (1×10^{-6} M) in response to fluoride anion.

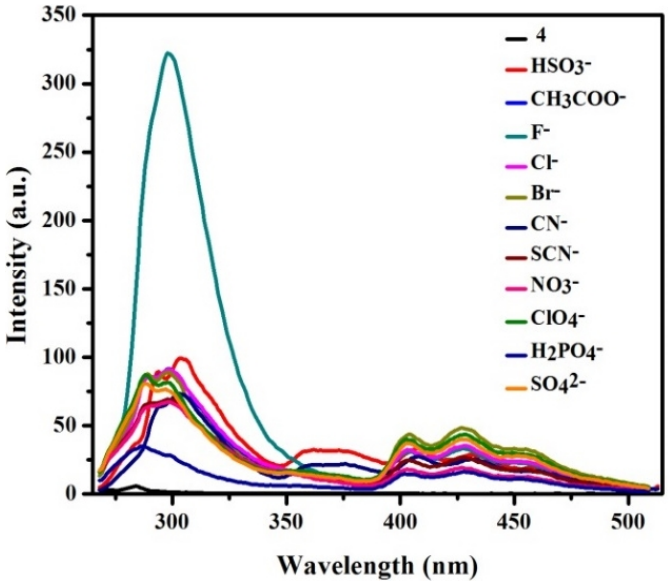

Fig. S11(b) Comparative graph of fluorescence spectra of compound **4** (1×10^{-6} M) in response to 11 different anions.

Fig. S12(a) Gel obtained from **4** with N,N-diisopropylethylamine (DIPEA) and degradation of gel after addition of TBAF.

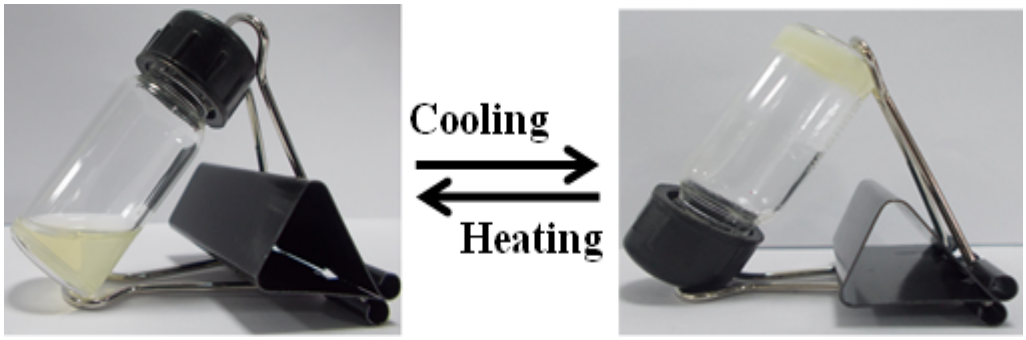

Fig. S12 (b) Gel obtained from **4** with triethylamine (TEA).

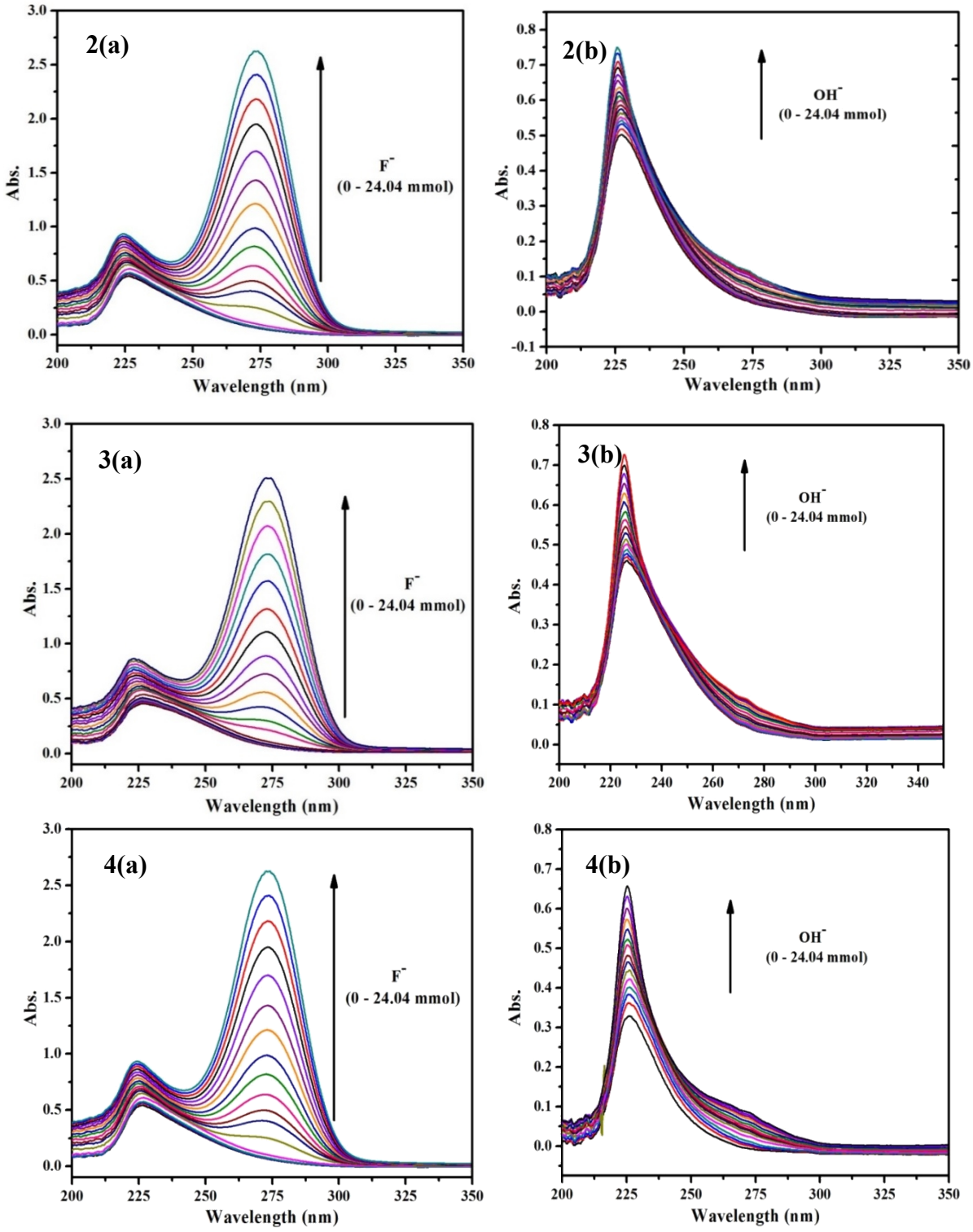

Fig. S13 UV spectra of **2**, **3** and **4** in THF:H_2O (9.5:0.5 *v/v*) solution with TBAF and TBAOH. 2(a,b) compound **2**; 3(a,b) compound **3**; 4(a,b) compound **4.**

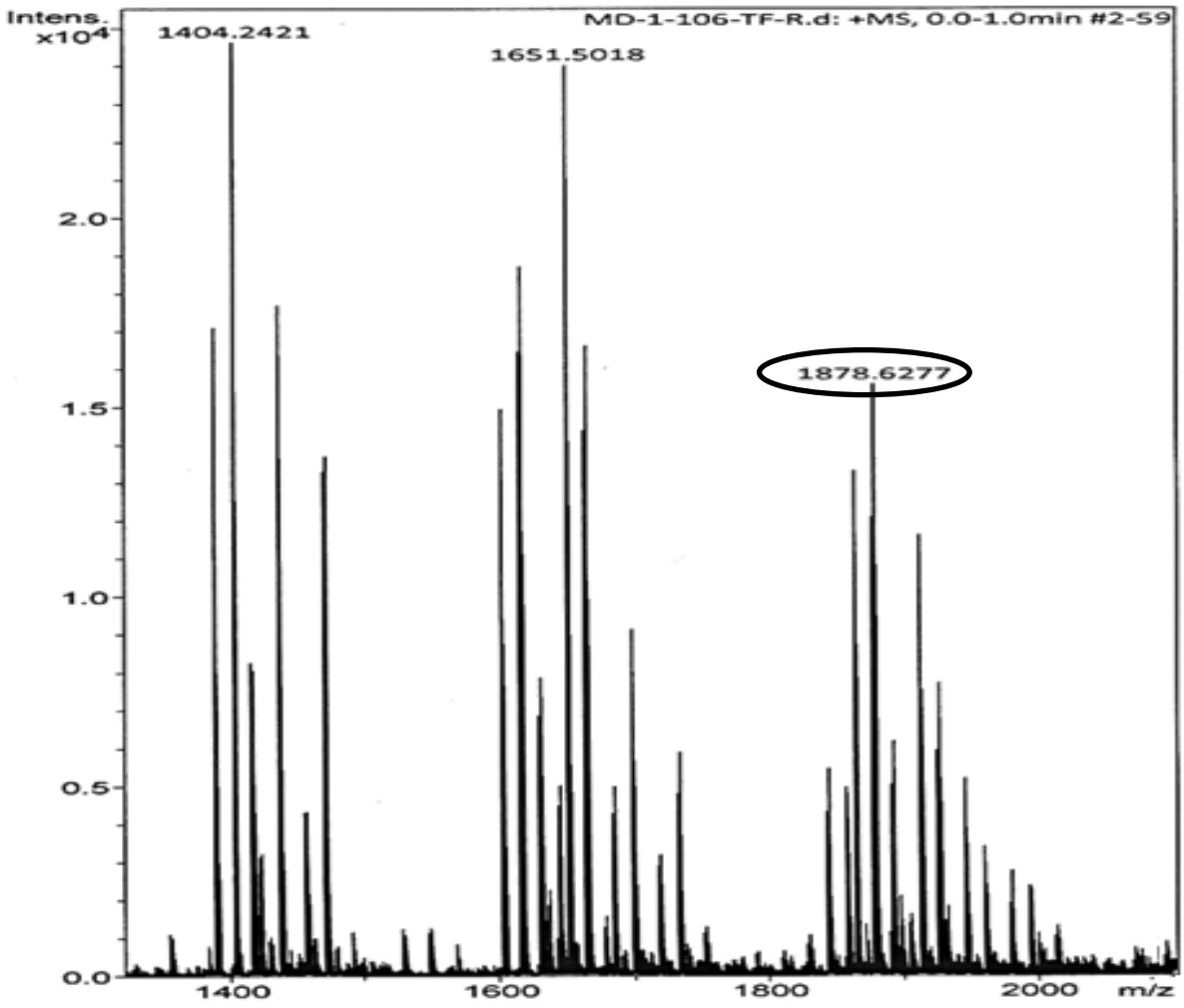

Fig. S14 Mass spectrum of compound **4** with fluoride anion.

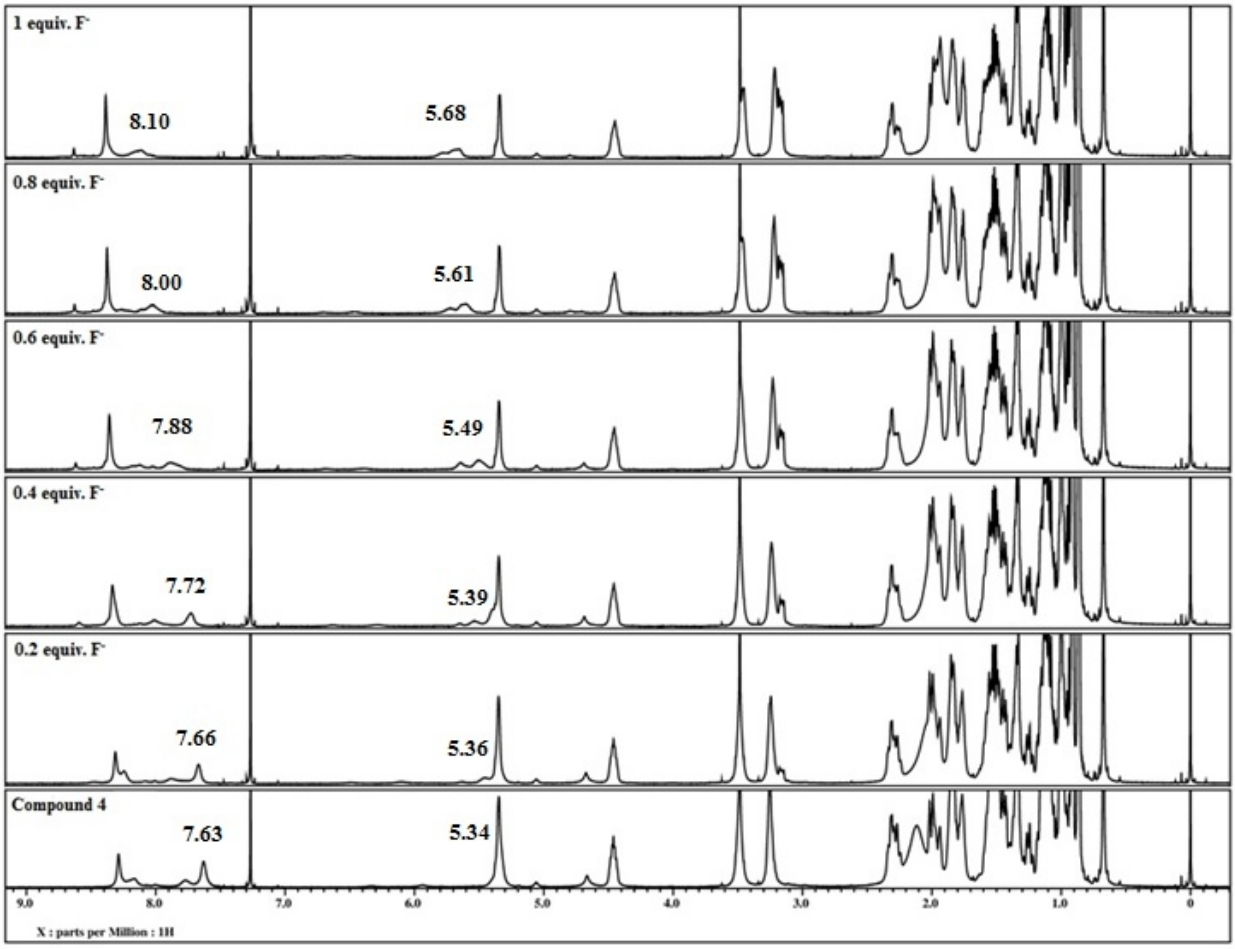

Fig. S15 ^{1}H NMR titration studies on compound **4** by addition of various equivalents of fluoride ions.

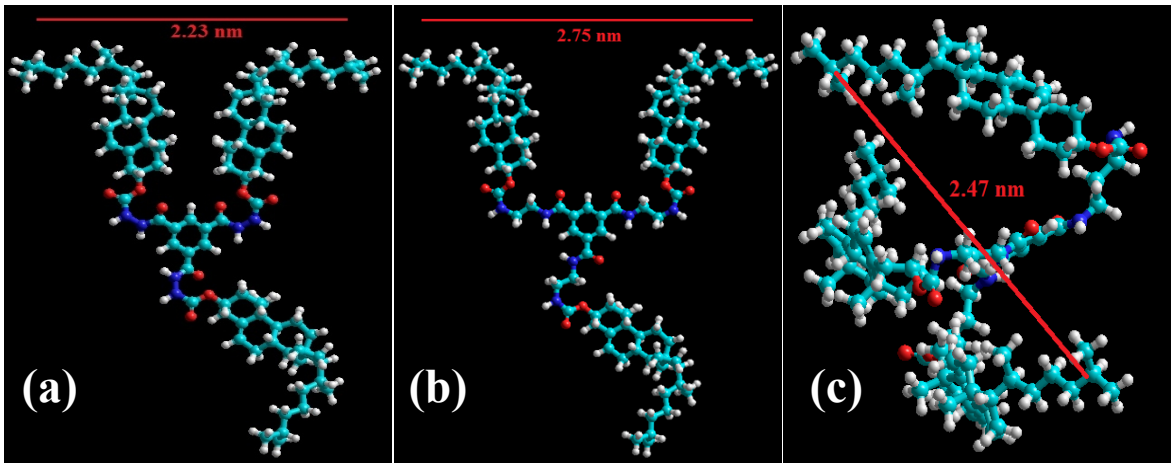

Fig. S16 Optimized structures of (a) compound **2**; (b) compound **3**; (c) compound **4** using Hyperchem professional; Red = Oxygen, Dark blue = Nitrogen, Light blue = carbon, White = hydrogen.

The ground state geometry of the compounds **2-4** has been optimized for minimum energy as mentioned in Table S1 using molecular mechanics method and Polak-Riviere (conjugate gradient) algorithm as implemented in quantum chemistry package Hyperchem Professional version 8.[1,2] RMS gradient of 0.1 Kcal/mole is used.

Table S1 Minimum energy and gradient of optimized structures of compound **2-4**.

Compounds	**Minimized Energy**	**Gradient**
Compound **2**	196.712 Kcal/mol	0.0924
Compound **3**	171.807 Kcal/mol	0.0715
Compound **4**	180.694 Kcal/mol	0.0909

References

1. HyperChem(TM), Hypercube, Inc., 1115 NW 4th Street, Gainesville, Florida 32601, USA.
2. (a) V. C. Edelsztein, A. S. Mac Cormack, M. Ciarlantini and P. H. Di Chenna, *J. Org. Chem.* 2013**, 9**, 1826; (b) F. W¨urthner, C. Thalacker, S. Diele and C. Tschierske, *Chem.–Eur. J.*, 2001, **7**, 2245; (c) L. E. Sinks, B. Rybtchinski, M. Limura, B. A. Jones, A. J. Goshe, X. Zuo, D. M. Tiede, X. Li and M. R.Wasielewski, *Chem. Mater.*, 2005, **17**, 6295.

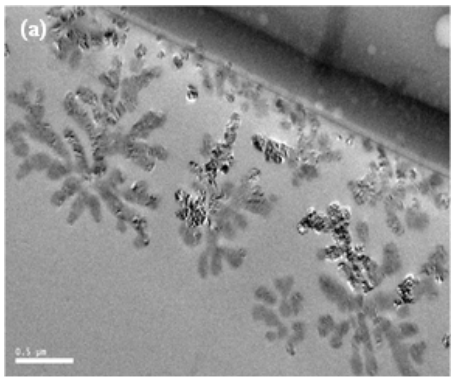

Fig. S17 (a) TEM image of compound **1** at 500 nm.

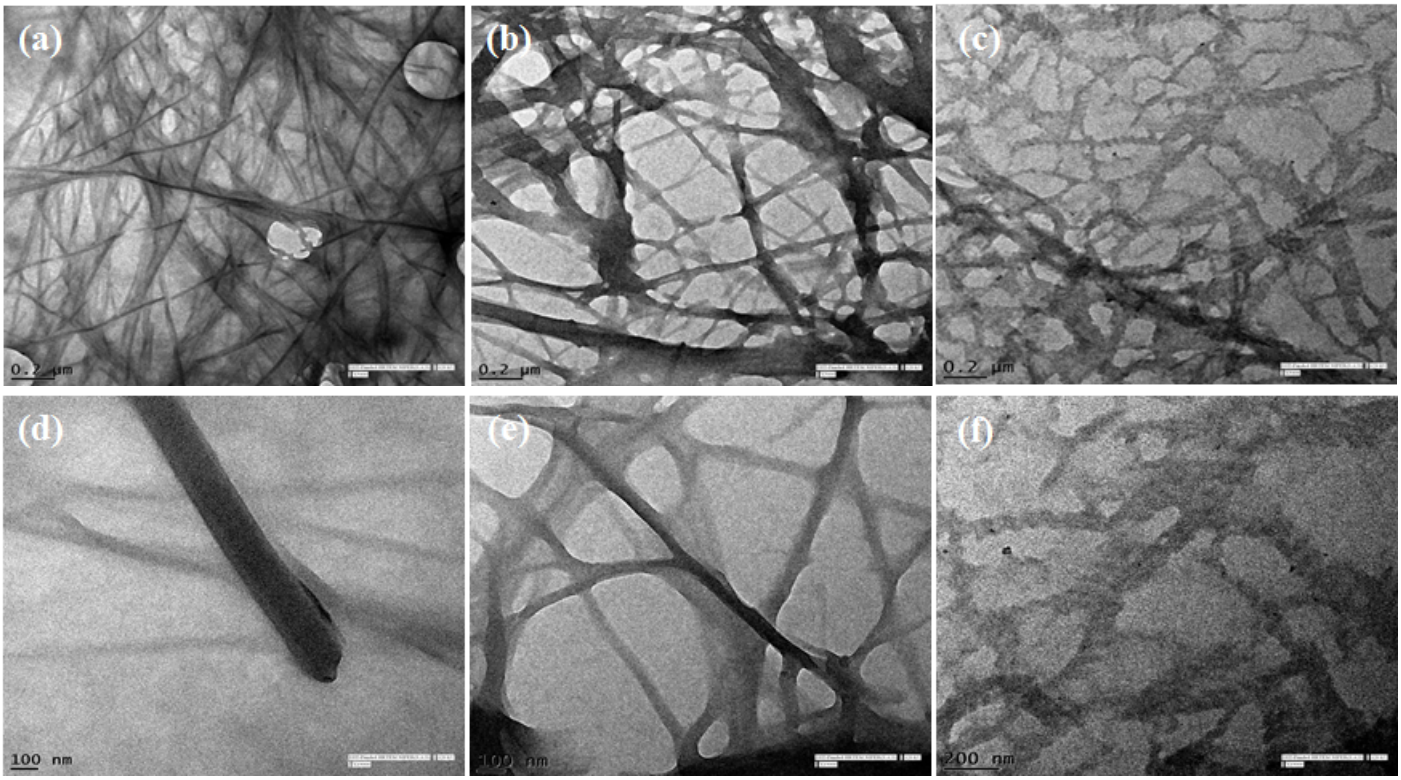

Fig. S17 (b) TEM images of gels obtained from triethylamine: (a, d) compound **2**; (b, e) compound **3**, (c, f) compound **4.**

Table S2 FT-IR data for gelators as solid and xerogels from TEA and DIPEA.

Compound	υ_{max}/cm^{-1}			
	N-H strech	**C=O ester**	**C=O amide**	**N-H bend**
Solid **2**	3291	1727	1690	1525
2/TEA	3268	1732	1680	1531
2/DIPEA	3274	1732	1680	1531
Solid **3**	3340	1708	1653	1531
3/TEA	3332	1713	1655	1538
3/DIPEA	3313	1726	1655	1538
Solid **4**	3346	1708	1659	1537
4/TEA	3366	1713	1642	1551
4/DIPEA	3352	1713	1655	1538