Electronic Supporting Information

New triangular steroid-based A(\text{LS})_3 type gelators for selective fluoride sensing application

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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 ^1\text{H} 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:H₂O (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.
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.

<table>
<thead>
<tr>
<th>Compounds</th>
<th>Minimized Energy</th>
<th>Gradient</th>
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<tbody>
<tr>
<td>Compound 2</td>
<td>196.712 Kcal/mol</td>
<td>0.0924</td>
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<tr>
<td>Compound 3</td>
<td>171.807 Kcal/mol</td>
<td>0.0715</td>
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<tr>
<td>Compound 4</td>
<td>180.694 Kcal/mol</td>
<td>0.0909</td>
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</table>

### References
1. HyperChem(TM), Hypercube, Inc., 1115 NW 4th Street, Gainesville, Florida 32601, USA.
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.

<table>
<thead>
<tr>
<th>Compound</th>
<th>$\nu_{\text{max}}$/cm$^{-1}$</th>
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<tbody>
<tr>
<td></td>
<td>N-H strech</td>
<td>C=O ester</td>
<td>C=O amide</td>
<td>N-H bend</td>
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<td>Solid 2</td>
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<td>1727</td>
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<td>2/TEA</td>
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<tr>
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<tr>
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<td>4/DIPEA</td>
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