Electronic Supplementary Information for

1,8-Naphthyridinic fluorescent ‘turn-on’ and ‘turn-off’
chemosensors for detecting of F\(^{-}\) and Hg\(^{2+}\) mimicking INHIBIT
molecular logic behaviour

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Figure S20. HOMO-LUMO energy gap for 1b and 1b+F⁻ complex in gas phase and CH₃CN.

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Scheme S1. Schematic representation of binding events while adding 4 equivalents of F⁻ ions to 1a and its regeneration upon addition of protic solvents such as methanol.

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Figure S4. $^1$H-NMR spectrum of 1b in CDCl$_3$. 
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Figure S6. UV-Visible spectral changes of receptor 1a (40 μM) upon addition of different anions (4 eq.) in CH₃CN at 298 K.
Figure S7. Colorimetric naked eye detection upon addition of fluoride ions in CH$_3$CN.

Figure S8. UV-Vis spectra of 1a (40 µM), after the addition of F$^-$ ion (120 µM) and strong base TBAOH (80 µM).
**Figure S9.** The fluorescence spectra of 1a (40 µM), and after the addition of F⁻ (120 µM) and TBAOH (80 µM) supporting the deprotonation of amide NH-proton.

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Figure S13. Absorption spectra of 1b (4.0 × 10⁻⁵ M) in presence of varying concentration of F⁻ (0 to 1.60 × 10⁻⁴ M) in CH₃CN medium. Inset: Benesi-Hildebrand plot of 1b with F⁻ ion when monitoring absorbance changes at 378 nm show the 1:1 stoichiometry.

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Gas Phase

CH3CN
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**Table S1.** Computed vertical excitation wavelength and their orbital contribution using B3LYP/6-311+G(2df,2p).

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<th>λ_{abs}, nm</th>
<th>f^a</th>
<th>assignment</th>
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<tr>
<td>1a</td>
<td>306.7</td>
<td>0.2089</td>
<td>HOMO → LUMO (90%)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>HOMO-2→ LUMO+1 (5%)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>HOMO-4→ LUMO+1 (3%)</td>
</tr>
<tr>
<td></td>
<td>269.5</td>
<td>0.0143</td>
<td>HOMO-2→ LUMO (68%)</td>
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<td></td>
<td></td>
<td></td>
<td>HOMO → LUMO+1 (15%)</td>
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<tr>
<td></td>
<td></td>
<td></td>
<td>HOMO-4→ LUMO (14%)</td>
</tr>
<tr>
<td>1a.F−</td>
<td>369.3</td>
<td>0.1926</td>
<td>HOMO→ LUMO (94%)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>HOMO → LUMO+2 (3%)</td>
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<tr>
<td></td>
<td></td>
<td></td>
<td>HOMO-3 → LUMO+2 (2%)</td>
</tr>
<tr>
<td></td>
<td>297.1</td>
<td>0.2588</td>
<td>HOMO→ LUMO+2 (85%)</td>
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<td></td>
<td></td>
<td></td>
<td>HOMO-3 → LUMO (9%)</td>
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<td></td>
<td></td>
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<td>HOMO→ LUMO (2%)</td>
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^aoscillator strength

**Note:**

Δλ = 63 nm (Theoretically) for 1a to 1a+F−

Δλ = 69 nm (Experimentally) for 1a to 1a+F−

The electronic spectral data obtained through computational studies are in close agreement with experimental data.
**Figure S24.** HRMS (ESI+) mass spectra of (1:1) complex of 1a and Hg$^{2+}$ ion.

**Figure S25.** Absorbance of 1a in CH$_3$CN, normalized between the minimum absorbance was found at zero equiv of F$^-$ and the maximum absorbance was found at 4.0 eq. of F$^-$. 

\[ y = 1.1261x + 5.2226 \]
\[ R^2 = 0.9614 \]
**Figure S26.** Normalized response of fluorescence signal to changing $F^-$ concentrations for 1a.

\[
y = 1.4763x + 6.698 \\
R^2 = 0.9359
\]

**Figure S27.** Normalized response of fluorescence signal to changing $\text{Hg}^{2+}$ concentrations for 1a.

\[
y = 0.3856x + 2.4981 \\
R^2 = 0.9584
\]
**Scheme S1.** Schematic representation of binding events while adding 4 equivalents of F⁻ ions to 1a and its regeneration upon addition of protic solvents such as methanol.

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