Supporting Information

Exploration of selective recognition of iodide with dipodal sensor: 2,2’- [ethane-1,2-diylbis(iminoethane-1,1-diyl)]diphenol

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Figure S1. IR spectra of receptor 2

Figure S2. $^1$H-NMR spectra of receptor 2
Figure S3. $^{13}$C-NMR spectra of receptor 2

Figure S4. LC-MS spectra of receptor 2 (M+H$^+$)
**Fig. S5.** Fluorescent titrations of receptor 2 (0.1 mM) with tetrabutylammonium iodide in CH$_3$CN.

**Figure S6.** A sensing of I$^-$ by receptor 2 (0.1 mM) in the presence of other competing anions.
To determination of binding constant

Linear fitting of the titration profiles using Benesi-Hildebrand methodology (Eq.1), Scatchard methodology (Eq.2) and Connor’s fitting method (Eq.3) based on a 1:1 binding mode results in a good linearity. The binding constant was calculated to be $8.6 \pm 0.01 \times 10^4 \text{M}^{-1}$. We calculated the association constant ($K_a$) by using the following equation.

$$
\frac{1}{(F-F_0)} = \frac{1}{(F_\infty-F_0)K_a[G]} + \frac{1}{(F_\infty-F_0)} \tag{Eq.1}
$$

$$
\frac{(F-F_0)}{[G]} = (F_\infty-F_0)K_a - (F - F_0)K_a \tag{Eq.2}
$$

Connor’s fitting method was carried out by the following equation as,

$$
K_a [H] + [G] \xrightarrow{\text{[HG]}} [HG] \\
F = k_s[H] + k_p[HG] \\
F_0 = k_s [H]_t \\
[H]_t = [H] + [HG] \\
K_a = \frac{[HG]}{[H][G]} \\
F = \frac{(1 + \frac{k_p}{k_s})}{(1 + K_a[G])} \implies \frac{(1 - \frac{F}{F_0})}{[F]} = K_a(\frac{F}{F_0}) - aK \quad (as \frac{k_p}{k_s} = a) \tag{Eq.3}
$$

Where, $F_0$ represents the fluorescence intensity in the absence of guest ion ($\Gamma$ ion), $F$ represents the fluorescence intensity in presence of guest ion, $F_\infty$ represents fluorescence intensity after titration and $[G]$ represents the concentration of guest.
Figure S7. A Benesi-Hildebrand methodology for receptor 2, \((1/\Delta F)\) vs \(1/[G]\), \(K_a = 8.57 \times 10^4 \text{M}^{-1}\).

Figure S8. A Scatchard methodology for receptor 2, \(\Delta F/[G]\) vs \(\Delta F\), \(K_a = 8.62 \times 10^4 \text{M}^{-1}\).
**Figure S9.** Connor’s fitting method for receptor 2, \((1-F/F_0)/[G] vs F/F_0\), \(K_a = 8.62 \times 10^4\) M\(^{-1}\).

**Figure S10.** 1:1 Stoichiometry of the host guest relationship realized from the Job’s plot for receptor 2.
Figure S11. LC-MS spectrum of receptor 2.l ion complex \([\text{M+H}^+.\text{(H}_2\text{O})_{0.5}]\)
Figure S12. A change in fluorescence intensity of receptor 2 with time (sec.) upon addition of 3 equiv. of $\Gamma$. 
Table S1. A comparison of literature reported synthesis with present methodology

<table>
<thead>
<tr>
<th>Group</th>
<th>Synthetic strategy</th>
<th>Detection limit</th>
<th>Fluorescence response</th>
<th>Ref.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Singh et al.</td>
<td>Multistep tripodial</td>
<td>2.1 µM</td>
<td>quenching</td>
<td>1a</td>
</tr>
<tr>
<td>Wang et al.</td>
<td>Multistep Ag-complex</td>
<td>7.16 µM</td>
<td>quenching</td>
<td>21</td>
</tr>
<tr>
<td>Shang et al.</td>
<td>Capped CdSe nanoparticles</td>
<td>0.28 µM</td>
<td>quenching</td>
<td>22</td>
</tr>
<tr>
<td>Yang et al.</td>
<td>Multistep PVC membrane</td>
<td>0.5 µM</td>
<td>quenching</td>
<td>23</td>
</tr>
<tr>
<td>Wang et al.</td>
<td>Capped Au nanoclusters</td>
<td>118 nM</td>
<td>quenching</td>
<td>24</td>
</tr>
<tr>
<td>Lin et al.</td>
<td>Multistep Hg-complex</td>
<td>0.45 µM</td>
<td>enhancement</td>
<td>25</td>
</tr>
<tr>
<td><strong>Present work</strong></td>
<td><strong>Simple condensation</strong> &amp; reduction</td>
<td><strong>1.38 µM</strong></td>
<td><strong>enhancement</strong></td>
<td><strong>-</strong></td>
</tr>
</tbody>
</table>

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Table S2  Crystallographic details for receptor 2

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Receptor 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Formula</td>
<td>C_{18}H_{24}N_{2}O_{2}</td>
</tr>
<tr>
<td>Formula weight</td>
<td>300.39</td>
</tr>
<tr>
<td>Temperature</td>
<td>150(2) K</td>
</tr>
<tr>
<td>Wavelength</td>
<td>0.71073 Å</td>
</tr>
<tr>
<td>Crystal system</td>
<td>Tetragonal</td>
</tr>
<tr>
<td>Space group</td>
<td>P 41212</td>
</tr>
<tr>
<td>Unit cell dimensions</td>
<td>a = 7.5161(6) Å</td>
</tr>
<tr>
<td></td>
<td>c = 29.023(2) Å</td>
</tr>
<tr>
<td>Volume</td>
<td>1639.6(3) Å</td>
</tr>
<tr>
<td>Z</td>
<td>4</td>
</tr>
<tr>
<td>Density (calculated)</td>
<td>1.217 Mg/m³</td>
</tr>
<tr>
<td>Absorption coefficient</td>
<td>0.080 mm⁻¹</td>
</tr>
<tr>
<td>F(000)</td>
<td>648</td>
</tr>
<tr>
<td>Crystal size</td>
<td>0.23 x 0.23 x 0.27 mm³</td>
</tr>
<tr>
<td>Theta range for data collection</td>
<td>2.799 to 24.988°</td>
</tr>
<tr>
<td>Index ranges</td>
<td>-8&lt;=h&lt;=8, -5&lt;=k&lt;=6, -33&lt;=l&lt;=34</td>
</tr>
<tr>
<td>Reflections collected</td>
<td>10916</td>
</tr>
<tr>
<td>Independent reflections</td>
<td>1434 [R(int) = 0.050]</td>
</tr>
<tr>
<td>Completeness to theta = 25.00°</td>
<td>99.7 %</td>
</tr>
<tr>
<td>Refinement method</td>
<td>Full-matrix least-squares on F²</td>
</tr>
<tr>
<td>Data / restraints / parameters</td>
<td>1434 / 0 / 109</td>
</tr>
<tr>
<td>Goodness-of-fit on F²</td>
<td>1.041</td>
</tr>
<tr>
<td>Final R indices [I&gt;2sigma(I)]</td>
<td>R1 = 0.0590, wR2 = 0.1365</td>
</tr>
<tr>
<td>R indices (all data)</td>
<td>R1 = 0.0807, wR2 = 0.1539</td>
</tr>
<tr>
<td>Largest diff. peak and hole</td>
<td>0.500 and -0.222 e/Å³</td>
</tr>
</tbody>
</table>

Table S3. Hydrogen bonds for receptor 2 [Å and °].

<table>
<thead>
<tr>
<th>D-H...A</th>
<th>d(D-H)</th>
<th>d(H...A)</th>
<th>d(D...A)</th>
<th>&lt;(DHA)</th>
</tr>
</thead>
<tbody>
<tr>
<td>C(8)-H(8A)...O</td>
<td>0.98</td>
<td>2.57</td>
<td>3.156(6)</td>
<td>118.6</td>
</tr>
<tr>
<td>N-H(1N)...O</td>
<td>1.10(5)</td>
<td>2.20(5)</td>
<td>2.993(5)</td>
<td>127(3)</td>
</tr>
<tr>
<td>O-H(1O)...N#2</td>
<td>0.95(7)</td>
<td>1.81(7)</td>
<td>2.760(5)</td>
<td>171(7)</td>
</tr>
</tbody>
</table>

Symmetry transformations used to generate equivalent atoms:
#1 y,x,-z  #2 y,x+1,-z
Table S4: An optimized bond angles, dihedral angles, bond length and energy calculated at B3LYP/ LANL2DZ level.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Ligand 2</th>
<th>2.I</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Dihedral angles (°)</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>N25-C29-C30-N26</td>
<td>61.09</td>
<td>91.88</td>
</tr>
<tr>
<td>C29-C30-N26-C24</td>
<td>-135.57</td>
<td>-169.19</td>
</tr>
<tr>
<td>C5-C4-C23-N25</td>
<td>33.34</td>
<td>69.46</td>
</tr>
<tr>
<td>O21-C3-C4-C23</td>
<td>-0.50</td>
<td>-2.44</td>
</tr>
<tr>
<td>C3-C4-C23-N25</td>
<td>-147.43</td>
<td>-108.38</td>
</tr>
<tr>
<td>O22-C12-C11-C24</td>
<td>-2.34</td>
<td>0.35</td>
</tr>
<tr>
<td>C11-C24-N26-C30</td>
<td>157.50</td>
<td>-179.05</td>
</tr>
<tr>
<td><strong>Bond angles (°)</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C23-N25-C29</td>
<td>116.22</td>
<td>112.14</td>
</tr>
<tr>
<td>C5-C4-C23</td>
<td>121.38</td>
<td>121.06</td>
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<tr>
<td>C30-N26-C24</td>
<td>120.29</td>
<td>114.74</td>
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<tr>
<td>N26-C24-C28</td>
<td>113.49</td>
<td>110.27</td>
</tr>
<tr>
<td>N25-C29-C30</td>
<td>109.24</td>
<td>112.12</td>
</tr>
<tr>
<td><strong>Bond Length (Å)</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>N25-C29</td>
<td>1.46</td>
<td>1.52</td>
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<tr>
<td>C30-N26</td>
<td>1.46</td>
<td>1.54</td>
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<tr>
<td>C24-N26</td>
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<tr>
<td>C23-N25</td>
<td>1.47</td>
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<tr>
<td>C12-O22</td>
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<tr>
<td>C3-O21</td>
<td>1.40</td>
<td>1.43</td>
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<tr>
<td>O22-H45</td>
<td>0.97</td>
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<tr>
<td>O21-H44</td>
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<tr>
<td>N25-H42</td>
<td>1.01</td>
<td>1.05</td>
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<tr>
<td>N26-H43</td>
<td>1.01</td>
<td>1.06</td>
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<tr>
<td>C23-C27</td>
<td>1.54</td>
<td>1.56</td>
</tr>
<tr>
<td><strong>Energy (a.u.)</strong></td>
<td>-960.28</td>
<td>-959.48</td>
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</table>