Supplementary Information

Nanomolar fluorogenic detection of Al(III) by a series of Schiff bases in aqueous system and their application in cell imaging.

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Synthetic Procedures and Characterization.

Scheme S1. Synthesis of Sensors
**Fig. S1.** Showing the H-bonding interactions in DBIH1 resulting in the formation of undulating tapes of molecules (a) down a axis (b) down the b axis.

**Fig. S2.** The H-bonded 3D, double helical tapes in the crystal structure of DBIH1, shown down the b axis.
Fig. S3. $^1$H NMR of DBIH1.

Fig. S4. $^{13}$C NMR of DBIH1.
Fig. S5. IR of DBIH1.

Fig. S6. ESI-MS of DBIH1.
Fig. S7. $^1$H NMR of DBIH2.

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\[ \text{C}_{22}\text{H}_{18}\text{N}_4\text{O}_6+1(M+1)^+ \]

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Fig. S11. $^1$H NMR of DBIH3.

Fig. S12. $^{13}$C NMR of DBIH3.
Fig. S13. IR of DBIH3.

Fig. S14. ESI-MS of DBIH3.
Fig. S15. Changes in UV-vis spectrum of DBIH1 (10 μM) on the addition of different metal ions (100 μM) in HEPES buffer (pH 7.4, containing 30% DMSO as a co-solvent). Inset: Response of Al(III) towards DBIH1.

Fig. S16. Changes in UV-vis spectrum of DBIH2 (10 μM) on the addition of different metal ions (100 μM) in HEPES buffer (pH 7.4, containing 30% DMSO as a co-solvent). Inset: Response of Al(III) towards DBIH2.
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Fig. S18. Benesi-Hildebrand plot for stability constant of DBIH1 with Al(III) from absorbance data.
Fig. S19. Benesi-Hildebrand plot for stability constant of DBIH2 with Al(III) from absorbance data.

Fig. S20. Benesi-Hildebrand plot for stability constant of DBIH3 with Al(III) from absorbance data.
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Fig. S25. (a) Benesi-Hildebrand plot for stability constant of DBIH1 with Al(III). (b) Fluorescence intensity of DBIH1 for different concentrations of Al (III) normalized between the maximum emission and the minimum emission (0.0 µM Al (III)) intensity.

Fig. S26. Changes in fluorescence spectra of DBIH2 (2.5 µM) upon gradual addition of Al(III).
Fig. S27. (a) Benesi-Hildebrand plot for stability constant of DBIH2 with Al(III). (b) Fluorescence intensity of DBIH2 for different concentrations of Al(III), normalized between the maximum emission and the minimum emission (0.0 µM Al(III)) intensity.

Fig. S28. Changes in fluorescence spectra of DBIH3 (2.5 µM) upon gradual addition of Al(III).
**Fig. S29.** (a) Showing Benesi-Hildebrand plot for stability constant of DBIH3 with Al(III). (b) Fluorescence intensity of DBIH3 for different concentrations of Al(III), normalized between the maximum emission and the minimum emission (0.0 µM Al(III)) intensity.

**Calculation of change in Free energies of the Al(III) complexes of DBIH1-DBIH3**

The equation used for the calculation of free energy of the complexation process is:

\[
\Delta G = -2.303RT\log K_a
\]

Where \( R = 8.314 \text{ JK}^{-1}\text{mol}^{-1} \), \( T = 298 \text{ K} \) and

For **DBIH1**, \( \log K_a = 5.74, \Delta G = -32.75 \text{ KJmol}^{-1} \).

For **DBIH2**, \( \log K_a = 6.39, \Delta G = -36.50 \text{ KJmol}^{-1} \).

For **DBIH3**, \( \log K_a = 4.84, \Delta G = -27.64 \text{ KJmol}^{-1} \).
**Fig. S30.** The fluorescence responses of **DBIH1** (2.5 µM) towards different Al(III) salts (10 equiv.).

**Fig. S31.** Competitive Selectivity of **DBIH1** (2.5µM) towards Al(III) (10 equiv.) in the presence of other metal ions (50 equiv.) under study.
Fig. S32. The fluorescence responses of DBIH2 (2.5 µM) towards different Al(III) salts (10 equiv.).

Fig. S33. Competitive Selectivity of DBIH2 (2.5µM) towards Al(III) (10 equiv.) in the presence of other metal ions (50 equiv.) under study.
**Fig. S34.** The fluorescence responses of **DBIH3** (2.5 µM) towards different Al(III) salts (10 equiv.).

**Fig. S35.** Competitive Selectivity of **DBIH3** towards Al(III) (10 equiv.) in the presence of other metal ions (50 equiv.) under study.
Fig. S36. (a) $^1$H NMR (b) IR of DBIH1-Al(III).

Fig. S37. ESI-MS of DBIH1-Al(III).
Fig. S38. (a) $^1$H NMR (b) IR of DBIH2-Al(III).

Fig. S39. ESI-MS of DBIH2-Al(III).
Fig. S40. (a) $^1$H NMR (b) IR of DBIH3-Al(III).

Fig. S41. ESI-MS of DBIH3-Al(III).
**Fig. S42.** Cell viability values (%) estimated by an MTT proliferation test with HeLa and C6 glioma cells at 37°C. Blue bars represent the results with HeLa Cells and red bars represent the results with C6 cells.
Table S1. Crystal data and structure refinement for **DBIH1**.

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<th>Crystal data and structure refinement for DBIH1.</th>
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<td><strong>Identification code</strong></td>
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<tr>
<td><strong>Formula weight</strong></td>
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<tr>
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<td><strong>Density (calculated)</strong></td>
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<td><strong>R indices (all data)</strong></td>
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Table S2. Showing important hydrogen bonds in DBIH1 (Å, °)

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<th></th>
<th>X...Y</th>
<th>H...Y</th>
<th>X-H...Y</th>
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<td>2.678(4)</td>
<td>1.96(3)</td>
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<td>O5-H5A...N4</td>
<td>2.717(4)</td>
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<td>N1-H1B...O5</td>
<td>3.193(4)</td>
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<td>N1-H1B...O6</td>
<td>3.157(4)</td>
<td>2.67(3)</td>
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<td>N3-H3B...O3</td>
<td>2.876(4)</td>
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<td>3.398(4)</td>
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(i) \(x, y+1/2+1, z+1/2\)  (ii) \(-x+1, -y+1, -z+1\)  (iii) \(-x+1, +y-1/2, -z+1/2\)

(iv) \(-x+1, +y-1/2, -z+1/2+1\)  (v) \(-x+1, +y+1/2, -z+1/2+1\)  (vi) \(-x+1, +y+1/2, -z+1/2\)