

# A Newly Developed Highly Selective Ratiometric Fluoride Ion Sensor: Spectroscopic, NMR and Density Functional Studies

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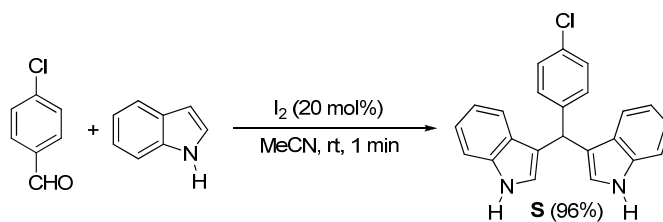
## SUPPLEMENTARY INFORMATION

**Synthesis of Sensor:** The synthesis of sensor **S** is shown in Scheme 1. This is synthesized simply by condensation of 4-chlorobenzaldehyde and indole. A mixture of 4-chlorobenzaldehyde (1 mmol), indole (2 mmol) and I<sub>2</sub> (0.2 mmol) in acetonitrile (10 ml) was stirred at room temperature for one minute. After completion of the reaction (TLC, <1 min), the mixture treated with aq. Na<sub>2</sub>S<sub>2</sub>O<sub>3</sub> solution (5%, 10 ml) and the product was extracted with ethyl acetate (3×5 ml). The combined organic layer was dried with anhydrous sodium sulphate, concentrated in vacuo and purified by column chromatography (ethyl acetate:petroleum ether=1:9) to afford the pure product. Product was characterized by NMR and elemental analysis data.

NMR: <sup>1</sup>H(CDCl<sub>3</sub>) 5.87 (1H, s), 6.59 (2H, d, *J* = 1.4 Hz), 7.04 (2H, t, *J* = 7.4 Hz), 7.10-7.41 (10H, m), 7.82 (2H, s, br).

<sup>13</sup>C(CDCl<sub>3</sub>) 39.6, 111.2, 119.2, 119.4, 119.8, 122.1, 123.6, 126.9, 128.4, 130.1, 131.8, 136.7, 142.6.

**CHN:** Anal. (C<sub>23</sub>H<sub>17</sub>ClN<sub>2</sub>) calcd, C: 77.41, H: 4.80, N: 7.85; found, C: 77.09, H: 4.94, N: 7.61.



**Scheme 1.** Synthesis of chemosensor **S**

Ref: Bandgar, B. P.; Shaikh, K. A. *Tetrahedron Lett.* **2003**, 44, 1959–1961.