

ANION-BINDING AND SENSING PROPERTIES OF NOVEL RECEPTORS BASED ON N-(INDOL-3-YLGLYOXYLYL)BENZYLAMINE

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The detailed characterization data for receptor 1–5 were as follows:

Receptor 1 (C₂₆H₁₈N₄O₄): Yield: 78%; Light yellow crystal; M.p. > 300 °C; ε: 27107 M⁻¹·cm⁻¹ (λ_{DMSO} = 332 nm); IR (KBr, cm⁻¹): 3300, 3225, 1680, 1620, 1527, 1486, 1310, 1239, 1129, 1011, 895, 756, 741; ¹H NMR (400 MHz, DMSO-*d*₆): δ 12.44 (s, 2H, N-H), 10.60 (s, 2H, N-H), 8.95 (d, 2H, Ar-H), 8.33 (m, 2H, Ar-H), 7.79 (m, 2H, Ar-H), 7.59 (m, 2H, Ar-H), 7.36 (m, 2H, Ar-H), 7.32 (m, 2H, Ar-H); ¹³C NMR (100 MHz, DMSO-*d*₆): δ 180.94, 161.87, 139.15, 136.37, 130.10, 126.28, 126.02, 125.32, 123.71, 122.88, 121.40, 112.74, 111.96; MS (ESI): 451.1 ([M+H]⁺).

Receptor 2 (C₂₆H₁₈N₄O₄): Yield: 74%; Light yellow crystal; M.p. > 300 °C; ε: 28309 M⁻¹·cm⁻¹ (λ_{DMSO} = 326 nm); IR (KBr, cm⁻¹): 3340, 3261, 2930, 1673, 1638, 1597, 1505, 1313, 1245, 1169, 1141, 1125, 860, 821, 802, 784, 743, 685; ¹H NMR (400 MHz, DMSO-*d*₆): δ 12.39 (s, 2H, N-H), 10.77 (s, 2H, N-H), 8.78 (s, 1H, Ar-H), 8.53 (s, 2H, Ar-H), 8.32 (m, 4H, Ar-H), 7.60 (t, 2H, J = 16 Hz, Ar-H), 7.39 (t, 2H, J = 16 Hz, Ar-H), 7.32 (m, 3H, Ar-H); ¹³C NMR (100 MHz, DMSO-*d*₆): δ 182.05, 162.50, 138.53, 138.34, 136.43, 128.91, 126.16, 123.61, 122.74, 121.25, 116.57, 112.70, 112.61, 112.00; MS (ESI): 451.1 ([M+H]⁺).

Receptor 3 (C₂₆H₁₈N₄O₄): Yield: 80%; Yellow powder; M.p. > 300 °C; ε: 30174 M⁻¹·cm⁻¹ (λ_{DMSO} = 339 nm); IR (KBr, cm⁻¹): 3447, 3309, 3258, 2930, 1668, 1600, 1503, 1308, 1240, 1204,

1125, 1009, 949, 878, 856, 823, 775, 732, 688, 658; ¹H NMR (400 MHz, DMSO-*d*₆): δ 12.38 (s, 2H, N-H), 10.75 (s, 2H, N-H), 8.83 (s, 4H, Ar-H), 8.32 (m, 2H, Ar-H), 7.91 (d, 2H, J = 8 Hz, Ar-H), 7.59 (m, 2H, Ar-H), 7.32 (m, 4H, Ar-H); ¹³C NMR (100 MHz, DMSO-*d*₆): δ 181.94, 162.12, 138.69, 136.41, 134.36, 126.24, 123.61, 122.76, 121.28, 120.59, 112.71, 112.01; MS (ESI): 451.1 ([M+H]⁺).

Receptor 4 (C₂₂H₁₈N₄O₄): Yield: 82%; White powder; M.p. > 300 °C; ε: 20237 M⁻¹·cm⁻¹ (λ_{DMSO} = 324 nm); IR (KBr, cm⁻¹): 3298, 3190, 3057, 2935, 1651, 1600, 1582, 1538, 1510, 1492, 1234, 1165, 1131, 745, 717; ¹H NMR (400 MHz, DMSO-*d*₆): δ 12.26 (s, 2H, N-H), 8.92 (s, 2H, N-H), 8.82 (s, 2H, Ar-H), 8.27 (t, 2H, J = 8 Hz, Ar-H), 7.55 (t, 2H, J = 8 Hz, Ar-H), 7.28 (t, 4H, J = 8 Hz, Ar-H), 2.89 (s, 4H, CH₂-H); ¹³C NMR (100 MHz, DMSO-*d*₆): δ 181.96, 163.83, 138.58, 136.25, 126.22, 123.42, 122.55, 121.28, 112.55, 112.16, 38.28; MS (ESI): 403.1 ([M+H]⁺).

Receptor 5 (C₂₀H₁₄N₄O₄): Yield: 68%; Yellow powder; M.p. > 300 °C; ε: 16230 M⁻¹·cm⁻¹ (λ_{DMSO} = 318 nm); IR (KBr, cm⁻¹): 3224, 3126, 2929, 1595, 1513, 1431, 1235, 1143, 927, 784, 742; ¹H NMR (400 MHz, DMSO-*d*₆): δ 12.38 (s, 2H, N-H), 10.82 (s, 2H, N-H), 8.74 (d, 2H, J = 4 Hz, Ar-H), 8.27 (t, 2H, J = 8 Hz, Ar-H), 7.60 (t, 2H, J = 8 Hz, Ar-H), 7.30 (m, 4H, Ar-H); ¹³C NMR (100 MHz, DMSO-*d*₆): δ 181.86, 163.12, 138.56, 136.53, 125.80, 123.73, 122.82, 121.28, 112.75, 112.52; MS (ESI): 375.1 ([M+H]⁺).

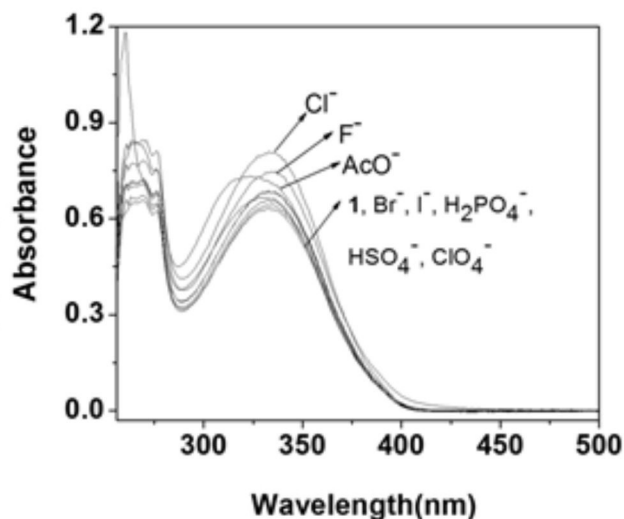


Figure 1S. Changes in the UV-Vis absorption spectra of receptor 1 (2.5×10^{-5} mol·L⁻¹) in DMSO–H₂O (9:1, v/v) solution upon the addition of various anions

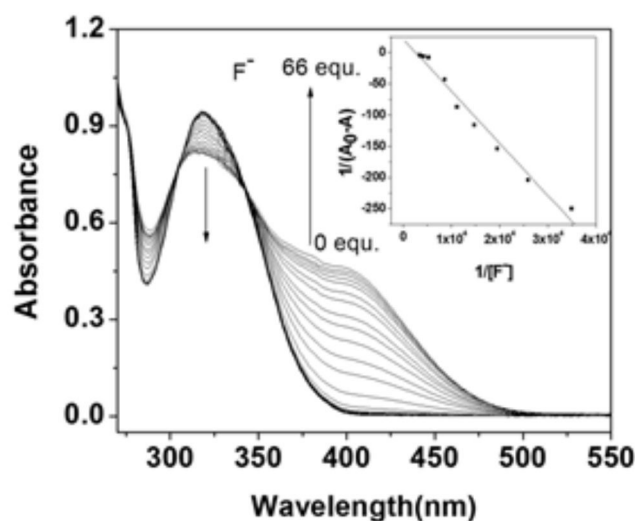


Figure 2S. Changes in the UV-Vis absorption spectra of receptor 5 (5.0×10^{-5} mol·L⁻¹) in DMSO–H₂O (9:1, v/v) solution upon the addition of F⁻

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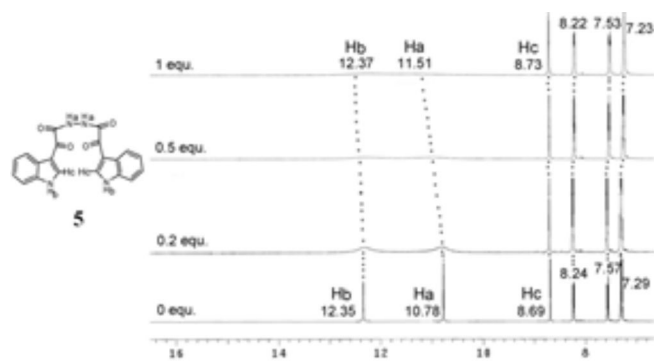
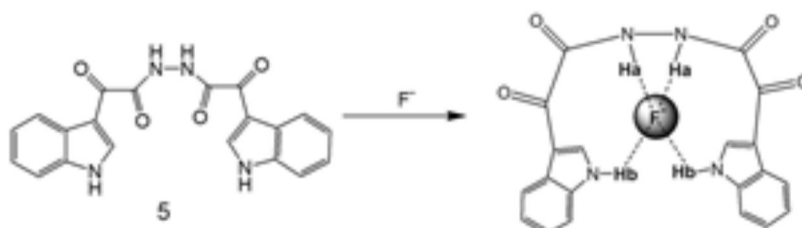


Figure 3S. Changes in ^1H NMR spectra of receptor **5** in the presence of F^- in DMSO-d_6



Scheme 1S. Possible binding modes of receptor **5** with fluoride ions