Supporting Information

Tuning of H-bonding ability of imidazole N-H towards colorimetric sensing of fluoride and cyanide ions as their sodium salt in aqueous medium

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Figure S1. Change in UV-Vis spectra for \{(A)-2a, (B)-2b, (C)-2c, (D)-2d, (E)-2e, (F)-2f, (G)-2g, (H)-2h\}(6.25x10^{-4} \text{ M}) in DMSO with the addition of (1.25x10^{-6} - 0.625x10^{-5}\text{ M}) of fluoride ion.
Figure S2. Change in UV-Vis spectra for ((A)- 2a, (B)-2b, (C)-2c, (D)-2d, (E) 2e, (F)-2f, (G)-2g, (H)-2h)(6.25x10^{-4} M) in DMSO with the addition of (1.25x10^{-6} - 0.625x10^{-5}M) of Cyanide ion.
Figure S3. UV-Vis spectra of mixture of 2f (1.25 x 10^{-4} M) and fluoride and cyanide (1.25 x 10^{-4} M) ions in DMSO-water mixtures of varying composition.
Figure S4. Change in fluorescence emission spectra for {(A) - 2a, (B) - 2b, (C) - 2c, (D) - 2d, (E) - 2e, (F) - 2f, (G) - 2g, (H) - 2h} (6.25x10^{-4} M) in DMSO with the addition of (1.25x10^{-6} - 6.25x10^{-4} M) of Cyanide ion.
Optimized structure for 2a, 2a-F and 2a-CN
Optimized structure for 2b, 2b-F and 2b-CN
Optimized structure for 2c, 2c-F and 2c-CN
Optimized structure for 2d, 2d-F and 2d-CN
Optimized structure for 2e, 2e-F and 2e-CN
Optimized structure for 2f, 2f-F and 2f-CN
Optimized structure for 2g, 2g-F and 2g-CN
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Figure S6. HOMO- LUMO for (2a-h)-F complexes.
Figure S7. HOMO- LUMO for (2a-h)-CN⁻ complexes.
$^1$H NMR for 1
$^1$H NMR for 2a, 2a-F$^-$ and 2a-CN$^-$
LCMS for 2a
H NMR for 2b, 2b-F⁻ and 2b-CN⁻
$^{13}$C NMR for 2b
LCMS for 2b
$^1$H NMR for 2c, 2c-$\text{F}^-$ and 2c-$\text{CN}^-$
LCMS for 2c
$^1$H NMR for 2d, 2d-F$^-$ and 2d-CN$^-$
LCMS for 2d
$^1$H NMR for 2e, 2e-F$^-$ and 2e -CN$^-$
LCMS for 2e
$^1$H NMR for 2f, 2f-F and 2f -CN
LCMS for 2f
$^1$H NMR for 2g, 2g-F$^-$ and 2g -CN$^-$
$^{13}$C NMR for 2g
LCMS for 2g
$^1$H NMR for 2h, 2h-F$^-$ and 2h-CN$^-$
LCMS for 2h

A mixture of compound 1 (0.5 g, 2.65 mmol) and benzaldehyde (0.280 g, 2.65 mmol) in DMSO (5 mL) was heated at 90º C with stirring for 6 h. After cooling to room temperature, the precipitate obtained from the reaction mixture was filtered through a filter paper and washed with cold ethanol to get the pure product as a yellow solid (0.626 g, yield = 85%).

Synthesis of 2-(naphthalen-1-yl)-1H-naphtho[2,3-d]imidazole-4,9-dione (2b).

A mixture of compound 1 (0.5 g, 2.65 mmol) and 1-naphthaldehyde (0.4134 g, 2.65 mmol) in DMSO (5 mL) was heated at 90º C with stirring for 6 h. After cooling to room temperature, the precipitate obtained from the reaction mixture was filtered through a filter paper and washed with cold ethanol to get the pure product as a yellow solid (0.7916 g, yield = 91%).

Synthesis of 2-(4-nitrophenyl)-1H-naphtho[2,3-d]imidazole-4,9-dione (2c).

A mixture of compound 1 (0.5 g, 2.65 mmol) and 4-nitrobenzaldehyde (0.4015 g, 2.65 mmol) in DMSO (5 mL) was heated at 90º C with stirring for 8 h. After cooling to room temperature, the precipitate obtained from the reaction mixture was filtered through a filter paper and washed with cold ethanol to get the pure product as a greenish yellow solid (0.6926 g, yield = 81%).


A mixture of compound 1 (0.5 g, 2.65 mmol) and 3-phenoxybenzaldehyde (0.5247 g, 2.65 mmol) in DMSO (5 mL) was heated at 90º C with stirring for 12 h. After cooling to room temperature, the precipitate obtained from the reaction mixture was filtered through
a filter paper and washed with cold ethanol to get the pure product as a brown solid (0.8012 g, yield =82%).

**Synthesis of 2-(pyridin-2-yl)-1H-naphtho[2,3-d]imidazole-4,9-dione (2e).**

A mixture of compound 1 (0.5 g, 2.65 mmol) and pyridine 2-carbaldehyde (0.2836 g, 2.65 mmol) in DMSO (5 mL) was heated at 90º C with stirring for 4 h. After cooling to room temperature, the precipitate obtained from the reaction mixture was filtered through a filter paper and washed with cold ethanol to get the pure product as a yellow solid (0.6210 g, yield =85%).

**Synthesis of 2-(thiophen-2-yl)-1H-naphtho[2,3-d]imidazole-4,9-dione (2f).**

A mixture of compound 1 (0.5 g, 2.65 mmol) and thiophene-2-carbaldehyde (0.2968 g, 2.65 mmol) in DMSO (5 mL) was heated at 90º C with stirring for 5 h. After cooling to room temperature, the precipitate obtained from the reaction mixture was filtered through a filter paper and washed with cold ethanol to get the pure product as a dark redish brown solid (0.6175 g, yield =83%).

**Synthesis of 2-isopropyl-1H-naphtho[2,3-d]imidazole-4,9-dione (2g).**

A mixture of compound 1 (0.5 g, 2.65 mmol) and isobutyraldehyde (0.1909 g, 2.65 mmol) in DMSO (5 mL) was heated at 70º C with stirring for 12 h. After cooling to room temperature, the precipitate obtained from the reaction mixture was filtered through a filter paper and washed with cold ethanol to get the pure product as a dark redish brown solid (0.410 g, yield =64%).

**Synthesis of 2-(trifluoromethyl)-1H-naphtho[2,3-d]imidazole-4,9-dione (2h).**

A mixture of compound 1 (0.5 g, 2.65 mmol) in trifluoro acetic acid (2 mL) was heated at
100°C with stirring for 12 h. After cooling to room temperature, the precipitate obtained from the reaction mixture was filtered through a filter paper and washed with cold ethanol to get the pure product as a dark brown solid (0.5039 g, yield =71%).