Supporting Information

CN\textsuperscript{−} Scavenger: A Leap Towards Development of CN\textsuperscript{−} antidote

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Equation for calculation of binding constants

Binding constants of compound-anion complex were calculated using Benesi-Hildebrand Equation.

\[
\frac{1}{(A_f - A_{obs})} = \frac{1}{(A_f - A_{fc})} + \frac{1}{K (A_f - A_{fc})} \quad \text{[Ligand]}
\]

Where \(A_f\) is absorbance of free host, \(A_{obs}\) is absorbance observed, \(A_{fc}\) is absorbance at saturation, \(K\) is the binding constant.

EXPERIMENTAL SECTION

Melting points were determined in capillaries and are uncorrected. \(^1\)H and \(^{13}\)C NMR spectra were recorded on JEOL 300 MHz and 75 MHz NMR spectrometer, respectively using CDCl\(_3\) and/or DMSO-d\(_6\) as solvent. Chemical shifts are given in ppm with TMS as an internal reference. \(J\) values are given in Hertz. Signals are abbreviated as singlet, s; doublet, d; double-doublet, dd; triplet, t; multiplet, m. In \(^{13}\)C NMR spectral data, +ve, -ve terms correspond to CH\(_3\), CH, CH\(_2\) signals in DEPT-135 NMR spectra. Chromatography was performed with silica 100-200 mesh and reactions were monitored by thin layer chromatography (TLC) with silica plates coated with silica gel HF-254. Elemental analysis was performed on Thermoelectron FLASH EA1112 CHN analyzer. Reactions under microwaves were performed using microwave oven (INALSA model 1MW17EG) with microwave power 700 W and operating frequency 2450 MHz. IR and UV spectral data were recorded on Varian 660-IR FT-IR Spectrometer and BioTek PowerWave XS instruments respectively.

5-(4-Hydroxy-3,5-dimethoxybenzylidene) pyrimidine-2,4,6 (1\(H\),3\(H\),5\(H\))-trione (3a). A finely ground mixture of syringaldehyde (100 mg, 1 mmol) and barbituric acid (84.34 mg, 1.2 mmol) was irradiated in microwave oven for 1 min. The completion of the reaction was checked by TLC. The solid mass was washed with diethyl ether to get pure 155 mg 3a (97%). mp >250 °C. \(\nu_{\text{max}}\) (KBr)/cm\(^{-1}\) 3475 (NH), 3202 (OH), 1743 (C=O); \(\delta_H\) (300 MHz, CDCl\(_3\)+DMSO-d\(_6\)) 3.06 (s, 6H, 2×OCH\(_3\)), 7.14 (s, 2H, ArH), 7.47 (s, 1H, CH), 10.31 (br, 1H, NH), 10.44 (br, 1H, NH); \(\delta_C\) (normal/DEPT-135, CDCl\(_3\)+DMSO-d\(_6\)) 54.69 (OCH\(_3\)), 112.33 (CH), 112.57 (CH), 121.58 (C), 141.38 (C), 145.71 (C), 148.85 (CH), 155.92 (C), 160.99 (C), 162.88 (C); MS (FAB) 293 (M+1); Anal. Calcd. for C\(_{13}\)H\(_{12}\)N\(_2\)O\(_6\): C, 53.43; H, 4.14; N, 9.59%. Found: C, 53.40; H, 4.16; N, 9.57%.
5-(4-Hydroxy-3,5-dimethoxybenzylidene)-1,3-dimethyl pyrimidine-2,4,6 \((1H,3H,5H)\)-trione (3b). A finely ground mixture of syringaldehyde (100 mg, 1 mmol) and 1,3 dimethyl barbituric acid (103 mg, 1.2 mmol) was irradiated in microwave oven for 1 min. The completion of the reaction was checked by TLC. The solid mass was washed with diethyl ether to get pure 165 mg 3b (95%). mp 237 ºC.

\(\nu_{\text{max}}\) (KBr)/cm\(^{-1}\) 3425 (OH), 1656 (C=O); \(\delta_H\) (300 MHz, CDCl\(_3\)) 3.30 (s, 3H, CH\(_3\)), 3.31 (s, 3H, CH\(_3\)), 3.99 (s, 6H, 2×OCH\(_3\)), 6.27 (br, 1H, OH), 7.86 (s, 2H, ArH), 8.44 (s,1H, CH); \(\delta_C\) (normal/DEPT-135, CDCl\(_3\)+DMSO-d\(_6\)) 24.52 (CH\(_3\)), 32.46 (CH\(_3\)), 54.41 (OCH\(_3\)), 111.87 (CH), 112.33 (CH), 121.20 (C), 141.26 (C), 145.44 (CH), 149.28 (C), 156.20 (C); MS (FAB) 321 (M+1); Anal. Calcd for C\(_{15}\)H\(_{16}\)N\(_2\)O\(_6\): C, 56.25; H, 5.04; N, 8.75%. Found: C, 56.28; H, 5.01; N, 8.76%.

\((4Z)-4-(4-Hydroxy-3,5-dimethoxybenzylidene)-1-(3-chlorophenyl)-3-methyl-1H-pyrazol-5(4H)-one (4). A finely ground mixture of syringaldehyde (100 mg, 1 mmol) and 1-(3-chlorophenyl)-3-methyl-2-pyrazolin-5-one (137 mg, 1.2 mmol) was irradiated in microwave oven for 1 min. The completion of the reaction was checked by TLC. The solid mass was washed with diethyl ether to get pure 158 mg 4 (81%). mp 184 ºC.

\(\nu_{\text{max}}\) (KBr)/cm\(^{-1}\) 3205 (OH), 1598 (C=O); \(\delta_H\) (300 MHz, CDCl\(_3\)) 2.33 (s, 3H, CH\(_3\)), 4.01 (s, 6H, 2×OCH\(_3\)), 6.20 (br, 1H, OH), 7.11-7.33 (m, 4H, ArH), 7.89 (d, 1H, ArH, \(J = 6\) Hz), 8.07 (d, 3H, \(J = 9.3\) Hz CH); \(\delta_C\) (normal/DEPT-135) 13.32 (CH\(_3\)), 56.58 (OCH\(_3\)), 111.76 (CH), 116.76 (CH), 118.85 (CH), 124.43 (CH), 124.58 (C), 129.69 (CH), 134.41 (C), 140.47 (C), 146.79 (CH), 147.89 (CH), 151.30 (C), 162.31 (C); MS (FAB) 373 (M+1); Anal. Calcd for C\(_{19}\)H\(_{17}\)N\(_2\)O\(_4\): C, 61.21; H, 4.60; N, 7.51%. Found: C, 61.19; H, 4.61; N, 7.49%.

4-[2-(3-Chlorophenyl)-5-methyl-3-oxo-2,3-dihydro-1H-pyrazol-4-ylmethyl]-2,6-dimethoxybenzonitrile (7): A mixture of 4 (50 mg, 1 mmol) and NaCN (1 equiv) in ethanol-water (1:1, v/v) was kept for 2-3 h. Extraction of aqueous solution with ethyl acetate and concentration under vacuum, after column chromatography provided compound 7 (59%). mp 165 ºC.

\(\nu_{\text{max}}\) (KBr)/cm\(^{-1}\) 2213 (C≡N), 1593 (C=O); \(\delta_H\) (300 MHz, CDCl\(_3\)+TFA) 2.18 (s, 3H, CH\(_3\)), 2.65 (s, 2H, CH\(_2\)), 3.97 (s, 6H, 2×OCH\(_3\)), 6.76 (s, 1H, ArH), 7.25-8.02 (m, 5H, ArCH); \(\delta_C\) (normal/DEPT-135, CDCl\(_3\)+DMSO-d\(_6\)) 15.13 (CH\(_3\)), 28.60 (CH\(_2\)), 54.73 (OCH\(_3\)), 108.94 (CH), 115.53 (CH), 116.25 (C), 117.21 (CH), 117.70 (C), 121.53 (CH), 122.83 (C), 128.61 (CH), 140.47 (C), 146.79 (CH), 147.89 (CH), 151.30 (C), 162.31 (C); MS (FAB) 373 (M+1); Anal. Calcd for C\(_{19}\)H\(_{17}\)N\(_2\)O\(_4\): C, 61.21; H, 4.60; N, 7.51%. Found: C, 61.19; H, 4.61; N, 7.49%.
132.78 (C), 140.55 (C), 147.35 (C), 149.83 (C), 171.44 (C); MS (FAB) 384 (M+1); Anal. Calcd for C_{20}H_{18}ClN_{3}O_{3}: C, 62.58; H, 4.73; N, 10.95%. Found: C, 62.59; H, 4.74; N, 10.94%.

4-[[2-(3-Chlorophenyl)-5-methyl-3-oxo-2,3-dihydro-1H-pyrazol-4-ylmethyl]-2,6-dimethoxybenzoic acid (10): Mixture of compound 7 (25 mg, 1mmol) and NaOH (1.2 mmol) in HEPES buffer-ethanol (1:1, v/v) was refluxed for 3 hours. Extraction of reaction mixture with ethyl acetate provided compound 10 (15 mg, 58%), mp 210 °C. \( \nu_{\text{max}} \) (KBr)/cm\(^{-1}\) 3412 (OH), 1619 (C=O), 1590 (C=O); \( \delta_{\text{H}} \) (300 MHz, CDCl\(_3\)+DMSO-d\(_6\)) 1.60 (s, 3H, CH\(_3\)), 2.36 (s, 2H, CH\(_2\)), 3.58 (s, 6H, 2×OCH\(_3\)), 6.48 (s, 2H, ArH), 6.77 (d, \( J = 7.8 \text{ Hz}, 1\text{H}, \text{ArH}\)), 6.97 (t, \( J = 7.7 \text{ Hz}, 1\text{H}, \text{ArH}\)), 7.70 (d, \( J = 8.1 \text{ Hz}, 1\text{H}, \text{ArH}\)), 8.01 (s, 1H, ArH); \( \delta_{\text{C}} \) (normal/DEPT-135, CDCl\(_3\)+DMSO-d\(_6\)) 16.44 (CH\(_3\)), 29.212 (CH\(_2\)), 55.97 (OCH\(_3\)), 105.56 (CH), 116.97 (CH), 118.76 (CH), 123.03 (CH), 123.64 (CH), 128.1 (CH), 132.06 (C), 145.80 (C), 188.08 (C), 199.22 (C). MS (FAB) 403 (M+1). Anal. Calcd for C_{20}H_{19}ClN_{2}O_{5}: C, 59.63; H, 4.75; N, 6.95%. Found: C, 59.62; H, 4.76; N, 6.94%.

**SI Scheme 1.** Synthesis of compounds.
Spectroscopic Data

**SI Figure 1**: $^1$H NMR spectrum of compound 3a.

**SI Figure 2**: $^{13}$C NMR spectrum of compound 3a.
SI Figure 3: FTIR spectrum of compound 3a.

SI Figure 4: $^1$H NMR spectrum of compound 3b.
SI Figure 5: $^{13}$C NMR spectrum of compound 3b.

SI Figure 6: FTIR spectrum of compound 3b.
**SI Figure 7:** $^1$H NMR spectrum of compound 4.

**SI Figure 8:** $^{13}$C NMR spectrum of compound 4.
**SI Figure 9:** DEPT-135 NMR spectrum of compound 4.

**SI Figure 10:** FTIR spectrum of compound 4.
SI Figure 11: (a) $^1$H NMR spectrum of compound 7 in (CDCl$_3$+ TFA). (b) $^1$H NMR spectrum of compound 7 in (CDCl$_3$+ CD$_3$OD).

SI Figure 12: $^{13}$C NMR spectrum of compound 7 in (CDCl$_3$+DMSO-d$_6$).
**SI Figure 13**: (a) DEPT-135 NMR spectrum of compound 7 in (CDCl₃+DMSO-d₆).

**SI Figure 14**: FTIR spectrum of compound 7.
SI Figure 15: $^1$H NMR spectrum of compound 10.

SI Figure 16: $^{13}$C NMR spectrum of compound 10.
SI Figure 17: DEPT-135 NMR spectrum of compound 10.

SI Figure 18: FTIR spectrum of compound 10.
UV-Vis titrations

**SI Figure 19**: UV-vis spectra of compound 4 (1 x 10^{-5} M) in presence of tetrabutyl ammonium salt of various anionic analytes (1 equiv) in EtOH-water (1:1, v/v) solution.

**SI Figure 20**: Job’s plot for compound 4 with CN⁻ in EtOH-water (1:1, v/v), monitored at 520 nm.
**SI Figure 21:** UV-vis spectra of compound 4 ($1 \times 10^{-5}$ M) (purple line) in EtOH-water (1:1, v/v). Addition of sodium cyanide (1 equiv) (red line) and recording of spectra as a function of time. Overlapping of lines (over red line) indicate no change in spectra with time.

**SI Figure 22:** Graph between change in absorbance at 520 nm for compound 4 on addition of cyanide indicating a first order reaction between 4 and CN⁻.
SI Figure 23: UV-Vis spectrum of compound 7 isolated from the solution of 4 and CN⁻ showing absorption band at 590 nm.

NMR titrations:

SI Figure 24: (a) ¹H NMR spectrum (CDCl₃) of compound 3a, OH signal at δ 6.24, (b) ¹H NMR spectrum of compound 3a in presence of 0.2 equiv. of tetrabutylammonium cyanide, signal due to OH disappeared.
SI Figure 25. (a) $^1$H NMR spectrum (CDCl$_3$) of compound 4, (b) in the presence of 0.2 equiv. of tetrabutylammonium cyanide, OH signal disappeared.
**SI Figure 26:** UV-Vis spectrum of compound 8 (1x10^{-5} M, EtOH-water (1:1, v/v), green line) changed to maroon line in presence of sodium cyanide (50 equiv).

**SI Figure 27:** UV-Vis titration of compound 9 (1x10^{-5} M, EtOH-water (1:1, v/v), red line) with sodium cyanide (10 equiv).
**SI Figure 28:** UV-Vis titration of compound 4 (1x10^{-5} M, CH$_3$CN, purple line) with tetrabutylammonium cyanide.

**SI Figure 29:** UV-Vis titration of compound 4 (1x10^{-5} M, CHCl$_3$, purple line) with tetrabutylammonium cyanide.
SI Figure 30: Absorbance of compound 4 (purple line) at 520 nm increases on addition of CN⁻ in acidic medium (pH 3.8).

SI Figure 31: Absorbance of compound 4 (blue line) at 520 nm (pH 8.8) increases on addition of CN⁻.
**SI Figure 32:** Absorbance of compound 4 (blue line) at 520 nm (pH 12.05) increases on addition of CN⁻.

**SI Figure 33.** Bar graph shows absorbance of compound 4 at 520 nm in presence of 1 equiv of various anions.
**SI Figure 34**: Color change of compound 4 (10 µM, EtOH-water, 1:1, v/v) in presence of anions: CN⁻, F⁻, Br⁻, Cl⁻, I⁻, HSO₄⁻, H₂PO₄⁻, NO₃⁻, AcO⁻.

**SI Figure 35.** UV-vis spectrum of compound 4 (ethanol-water, 1:1, v/v) in presence of sodium carbonate (upto 10 equiv); further addition of sodium cyanide intensified the absorption band at 520 nm.
SI Figure 36. UV-vis titration of compound 4 (ethanol-water, 1:1, v/v) with sodium bicarbonate (upto 10 equiv). Further addition of sodium cyanide intensified the absorption band at 520 nm.

SI Figure 37: UV-Vis titration of compound 4 (purple line, $1 \times 10^{-5}$ M) with sodium carbonate in EtOH-water (1:1, v/v).
**SI Figure 38:** UV-Vis spectra of compound 4 (purple line, 1×10⁻⁵ M) with sodium bicarbonate in EtOH-water (1:1, v/v).

**SI Figure 39:** (a) UV-vis spectra of compound 4 (ethanol-tap water, 1:1, v/v, purple line) with sodium cyanide (1 and 10 equiv). (b) Absorption spectrum of receptor 4 (purple), 4+CN⁻ (1:1) (green) and 4+CN⁻+Fe³⁺ (1:1:20) (red).
**SFigure 40.** Absorption intensity of compound 4 (5x10^-8 M) at 520 nm in presence of 5x10^-6 M of anions: 4+CN^- (green bar), 4+AcO^-+CN^- (light blue bar), 4+F^-+CN^- (red bar), 4+Cl^-+CN^- (dark green bar), 4+Br^-+CN^- (dark red bar), 4+I^-+CN^- (blue bar), 4+NO_3^-+CN^- (yellow bar), 4+H_2PO_4^-+CN^- (purple bar), 4+HSO_4^-+CN^- (maroon bar), 4+CO_3^{2-}+CN^- (brown bar), 4+HCO_3^-+CN^- (orange bar).

**SI Figure 41:** UV-Vis titration of receptor 3a (1x10^-5 M, EtOH-water (1:1, v/v), pink line) with sodium cyanide. Binding constant is 10^6 M^-1.
**SI Figure 42.** Job’s plot for compound 3a with CN⁻ in EtOH-water (1:1, v/v) monitored at 413 nm.

**SI Figure 43:** Bar graph showing absorbance of compound 3a (10 μM, EtOH-water (1:1, v/v)) at 501 nm in the presence of 1 equiv of various anions.
**SI Figure 44:** 3a (5 x 10^{-8} M) at 500 nm in presence 5 x 10^{-6} M of anion: 3a+CN^- (green bar), 3a+AcO^-+CN^- (light blue), 3a+F^-+CN^- (red bar), 3a+Cl^-+CN^- (dark green bar), 3a+Br^-+CN^- (pink bar), 3a+I^-+CN^- (royal blue bar), 3a+NO_3^-+CN^- (yellow bar), 3a+H_2PO_4^-+CN^- (purple bar), 3a+HSO_4^-+CN^- (maroon bar), 3a+CO_3^{2-}+CN^- (brown bar), 3a+HCO_3^-+CN^- (orange bar).

**SI Figure 45:** Absorption spectrum of compound 3a (pink), 3a +CN^- (1:1) (green), 3a +CN^- + Fe^{3+} (1:1:10) (red).
**SI Figure 46:** UV-Vis titration of receptor 3b (purple line, 1x10^{-5} M) with sodium cyanide in EtOH-water (1:1, v/v). Binding constant is 10^6 M^{-1}.

**SI Figure 47:** Job’s plot for compound 3b with CN^- in EtOH-water (1:1, v/v) monitored at 402 nm.
**SI Figure 48:** Bar graph showing absorbance of compound 3b (10 µM) in EtOH-water (1:1, v/v) at 501 nm in the presence of 1 equiv of various anions.

**SI Figure 49:** Competitive binding of 3b with CN⁻ in presence of other anions. Absorption intensity of compound 3b (5 x 10⁻⁸ M) at 500 nm in presence 5 x 10⁻⁶ M of anion: 3b+CN⁻ (green bar), 3b+AcO⁻+CN⁻ (light blue), 3b+F⁻+CN⁻ (red bar), 3b+Cl⁻+CN⁻ (dark green bar), 3b+Br⁻+CN⁻ (pink bar), 3b+I⁻+CN⁻ (royal blue bar), 3b+NO₃⁻+CN⁻ (yellow bar), 3b+H₂PO₄⁻+CN⁻ (purple bar), 3b+HSO₄⁻+CN⁻ (maroon bar), 3b+CO₃²⁻+CN⁻ (orange bar), 3b+HCO₃⁻+CN⁻ (brown bar),
SI Figure 50: Color changes of receptor 3b (10 µM, EtOH-water (1:1, v/v)) in presence of anions: CN⁻, F⁻, AcO⁻, Br⁻, Cl⁻, I⁻, HSO₄⁻, H₂PO₄⁻, NO₃⁻.
**SI Figure 51:** Experiments showing removal of CN\(^{-}\) from water by compound 4.
**SI Figure 52.** UV-vis spectra of compound 10 (ethanol-water, 1:1, v/v).