Electronic Supplementary Information for:

Analytically useful blue chemiluminescence from a water-soluble iridium(III) complex containing a tetraethylene glycol functionalised triazolylpyridine ligand

Zoe M. Smith, Emily Kerr, Egan H. Doeven, Timothy U. Connell, Neil W. Barnett, Paul S. Donnelly, Stephen J. Haswell and Paul S. Francis^{*}

Figure S1. Photoluminescence emission spectrum of $[Ir(df-ppy)_2(STP)]$ (blue line) and $[Ir(df-ppy)_2(BPS)]^-$ (green line), in aqueous solution at a concentration of 10 μ M.



Figure S2. Chemical structure and selected properties of [Ir(ppy-SO₃)₂(pt-TEG)]⁻.



green emitter (λ_{max} = 482, 512 nm) soluble in water E_{ox} = 1.09 V vs Ag/AgCl

Figure S3. Photoluminescence of $[Ir(df-ppy)_2(pt-TEG)]^+$ (left), $[Ir(ppy-SO_3)_2(pt-TEG)]^-$ (middle), and $[Ru(bpy)_3]^{2+}$ (right) at 1 mM in aqueous solution under ultraviolet light (LED: $\lambda_{max} = 370$ nm).



Figure S4. Compounds selected for the comparison of the chemiluminescence intensities.



Figure S5. Relative chemiluminescence (signal-to-blank) response for $[Ru(bpy)_3]^{2+}$ and $[Ir(df-ppy)_2(pt-TEG)]^+$ at 1 mM reagent concentration, with cerium(IV) sulfate (1 mM) and various pharmaceuticals and related compounds (10 μ M), using flow injection analysis methodology.



Figure S6. Chemiluminescence responses (signal/blank ratios) of various loop diuretics and related compounds: (1) furosemide, (2) 4-chloro-3-sulfamoyl-benzoic acid, (3) *N*-benzyl-4-chloro-sulfamoylanthranillic acid, (4) piretanide, (5) bumetanide, at 1 μ M, with [Ru(bpy)₃]²⁺ (red columns) and [Ir(df-ppy)₂(pt-TEG)]⁺ (blue columns), using flow injection analysis methodology. Reagent concentration: 0.1 mM. Oxidant: 1 mM cerium(IV) sulfate in 0.05 M H₂SO₄.



Figure S7. Calibrations for furosemide prepared using flow injection analysis methodology with 0.1 mM $[Ir(df-ppy)_2(pt-TEG)]^+$ (blue plot) or $[Ru(bpy)_3]^{2+}$ (red plot) and 1 mM cerium(IV) sulfate in 0.05 mM H₂SO₄. Each point is an average of three replicate injections. The precision was evaluated using a 3×10^{-7} M furosemide solution (n = 5), which showed a relative standard deviation of less than 2% with both reagents. The limits of detection (1 × 10⁻⁸ M and 7 × 10⁻⁸ M, respectively) were established using a smaller range calibration at low concentrations.

