Electronic Supplementary Information (ESI)

Phosphorescent biscyclometallated iridium(III) ethylenediamine complexes functionalised with polar ester or carboxylate groups as bioimaging and visualisation reagents

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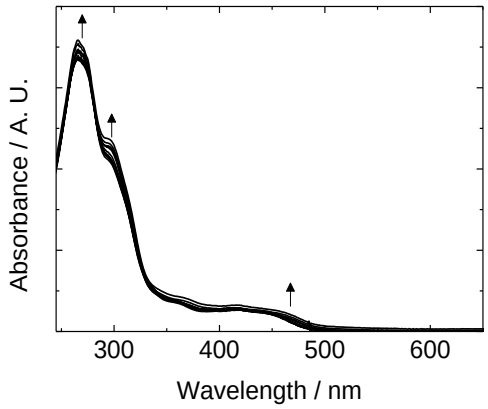
Table S1 Electronic absorption data of the iridium(III) complexes in MeOH at 298 K

Complex	λ_{abs}/nm (ε/dm^3 mol^{-1} cm^{-1})
1a	267 (38840), 277 sh (36000), 300 sh (23490), 367 sh (3610), 420 (3080), 458 sh (2855)
2a	271 (36670), 294 (30740), 359 (22180), 436 sh (5080), 493 (3870)
1b	267 (44325), 279 sh (41220), 300 sh (26585), 360 sh (4900), 418 (4010), 440 sh (3935)
2b	271 (38870), 290 sh (31400), 346 (20220), 408 sh (4820), 462 (4250)

(a)



(b)

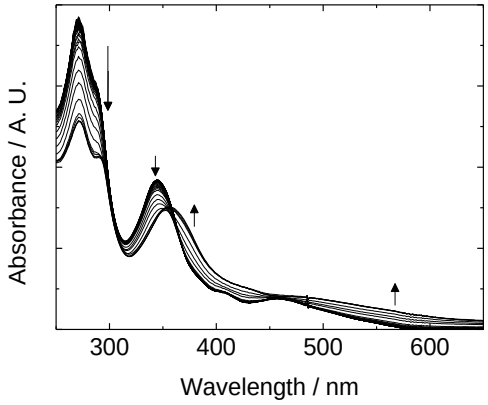
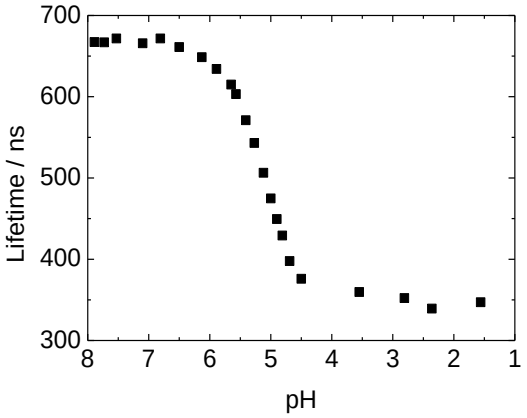


Figure S1 Electronic absorption spectral traces of (a) complex **1b** (50 μM) and (b) complex **2b** (50 μM) in aerated 10 mM KOH(aq) and 100 mM KCl(aq)/DMSO (9:1, v/v) at 298 K upon decreasing the pH.

(a)



(b)

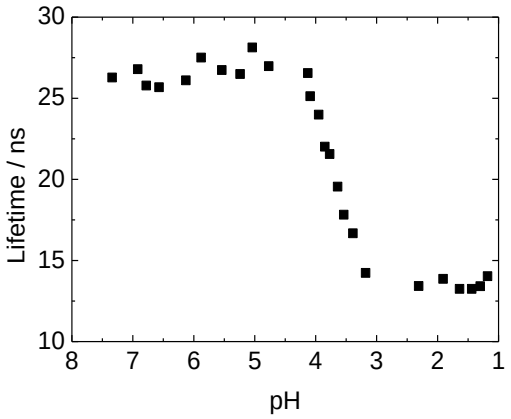


Figure S2 Lifetime-based pH titration curves of (a) complex **1b** (50 μM) and (b) complex **2b** (50 μM) in aerated 10 mM KOH(aq) and 100 mM KCl(aq)/DMSO (9:1, v/v) at 298 K upon decreasing the pH.

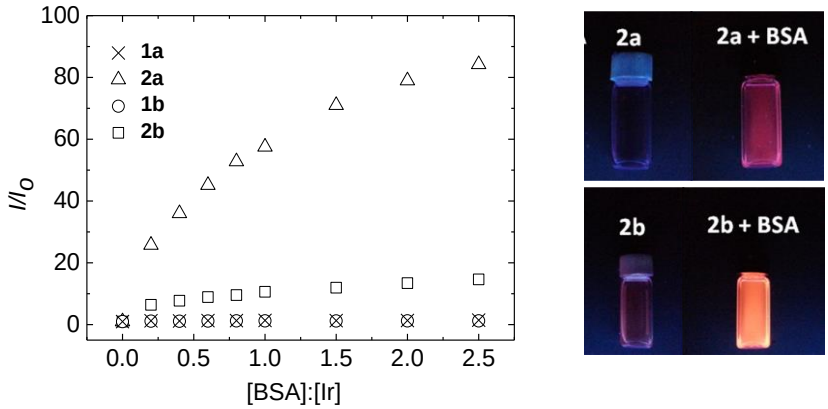


Figure S3 Change of emission intensity of a solution of complexes **1a** (crosses), **2a** (triangles), **1b** (circles) and **2b** (squares) and BSA upon incubation in the dark at 298 K for 24 h. I and I_o are the emission intensities of the solutions in the presence and absence of BSA, respectively.

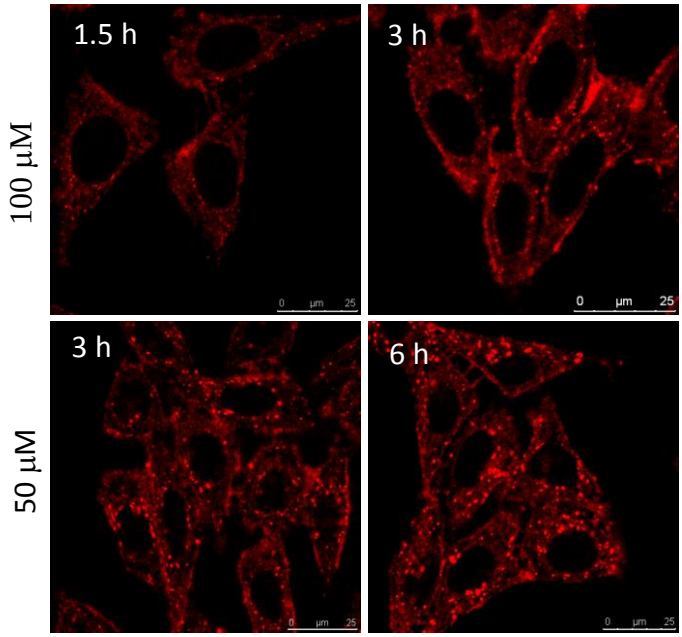
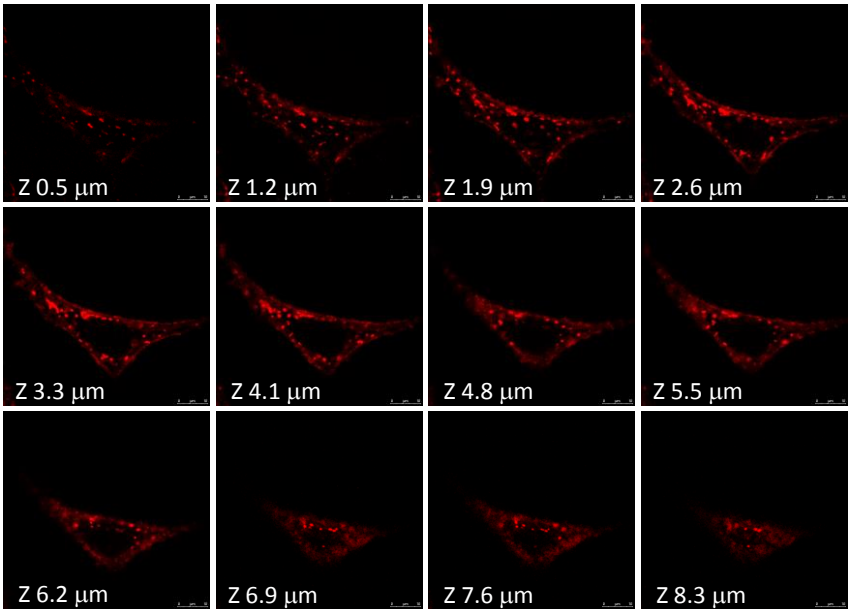


Figure S4 LSCM images of HeLa cells incubated with complex **1a** for different time at 37 °C (λ_{ex} = 405 nm).

(a)



(b)

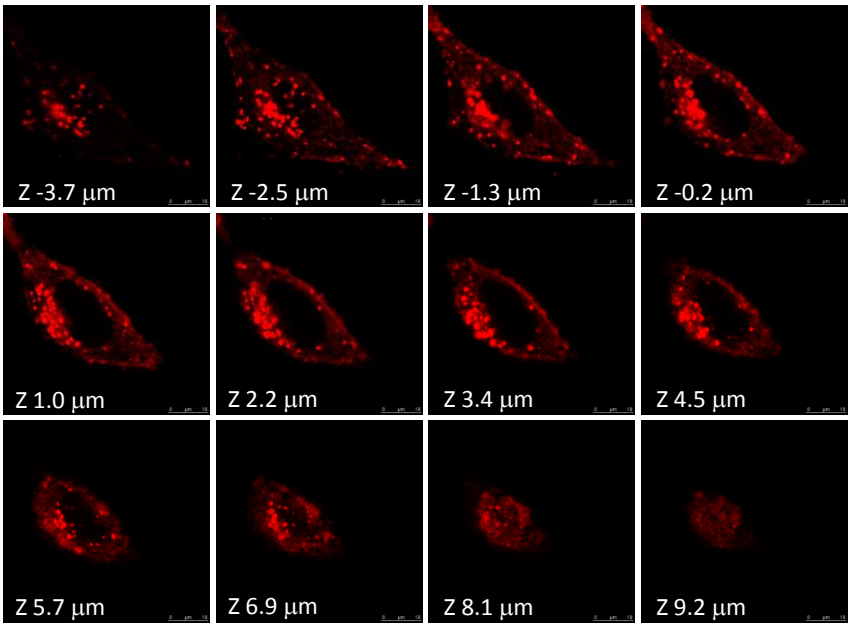


Figure S5 *Z*-scan images of HeLa cells incubated with complex **1a** (50 μM) for (a) 6 h and (b) 12 h at 37 °C (λ_{ex} = 405 nm).

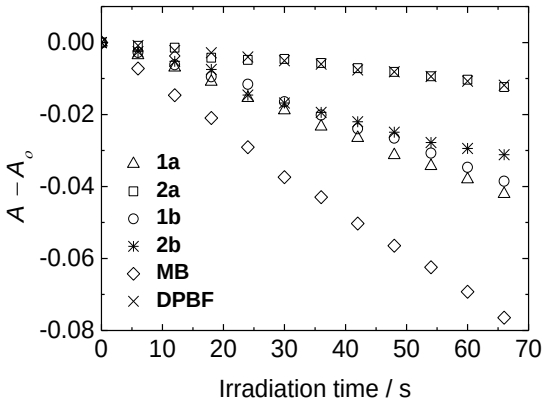


Figure S6 Plot of rates of decay in absorbance of DPBF (10 μM) at 417 nm in aerated DMSO in the presence of complexes **1a** (triangles), **2a** (squares), **1b** (circles), **2b** (asterisks) and methylene blue (diamonds), respectively, upon irradiation at 365 nm. A solution of DPBF without any sensitisers (crosses) was used as the negative control.

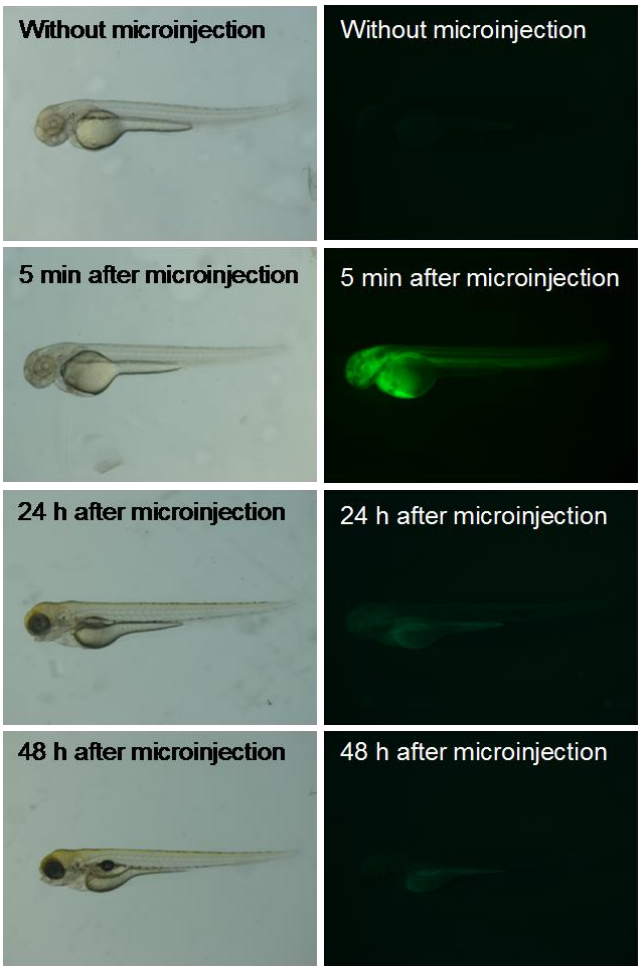


Figure S7 Brightfield (left) and fluorescence (right) microscopy images of a 48 hpf zebrafish larva that was microinjected with complex **1b** (2 mM, 40 nL); the images were taken at 5 min, 24 h and 48 h after microinjection. A 48 hpf zebrafish larva without microinjection was shown for reference.