Supporting Information

Triethylene glycol-modified iridium(III) complexes for fluorescence imaging of *Schistosoma japonicum*

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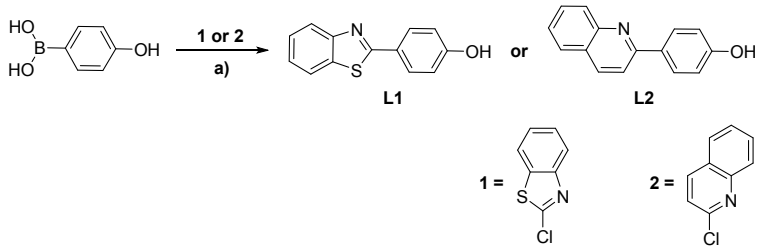
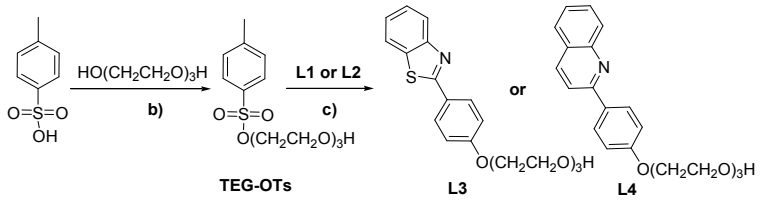
1. Synthesis of L1 and L2



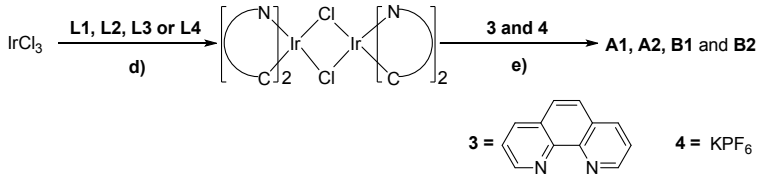
Scheme S1. Synthetic route of the ligands L1 and L2. Conditions: (a) $Pd[P(Ph)_3]_4$, K_2CO_3, THF/H_2O, reflux, 70 ^{0}C, N_2

2. Synthesis of L3 and L4



Scheme S2. Synthetic route of the ligands L3 and L4. Conditions: (b) pyridine, DCM, 0 ^{0}C; (c) Tetrabutyl ammonium bromide, K_2CO_3, CH_3CN, reflux 80 ^{0}C

3. Synthesis of complexes A1, A2, B1 and B2



Scheme S3. Synthetic route of complexes A1, A2, B1 and B2, Conditions: (d) 2-Ethoxyethanol/H_2O, reflux 110 ^{0}C; (e) methanol/DCM, reflux 50 ^{0}C

4. Summary of frontier MOs obtained the PBE/(DSPP/DNP) level

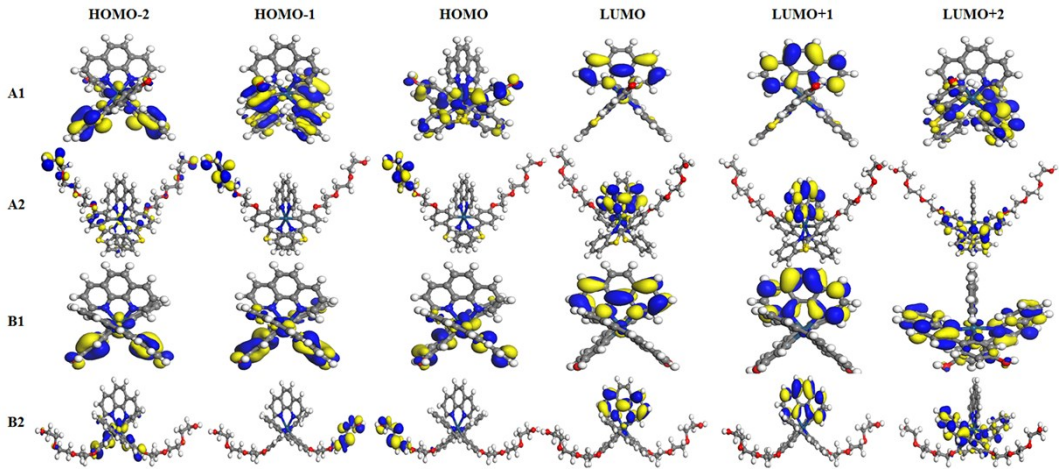


Figure S1. Representations of the frontier molecular orbitals (MOs) for ground state geometry of four iridium complexes as determined at the PBE/(DSPP/DNP) level of theory

Table S1. Energies for the frontier MOs obtained the PBE/(DSPP/DNP) level (in eV)

Complex	HOMO-2	HOMO-1	HOMO	LUMO	LUMO+1	LUMO+2	gap
A1	-8.18	-7.67	-7.61	-6.04	-5.96	-5.00	1.57
A2	-7.41	-7.19	-7.18	-5.82	-5.74	-4.85	1.36
B1	-7.88	-7.62	-7.39	-5.86	-5.78	-5.26	1.53
B2	-7.26	-7.21	-7.21	-5.74	-5.66	-5.12	1.47

5. Cytotoxicity of A1 and B1

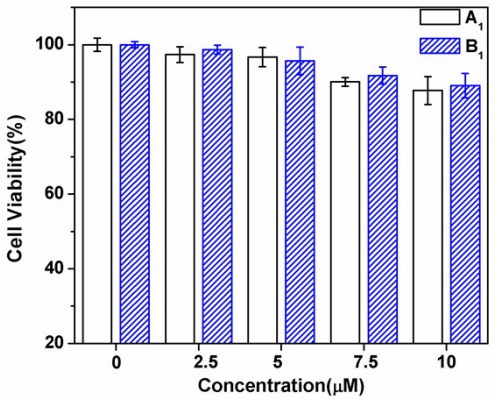


Figure S2. Cell viability values (%) estimated by MTT proliferation test versus incubation concentrations of A1 and B1, HeLa cells were cultured in the presence of 2.5 ~ 10 μM A1 and B1 at 37 °C for 24 h.

6. Photobleaching curves of A2 and B2

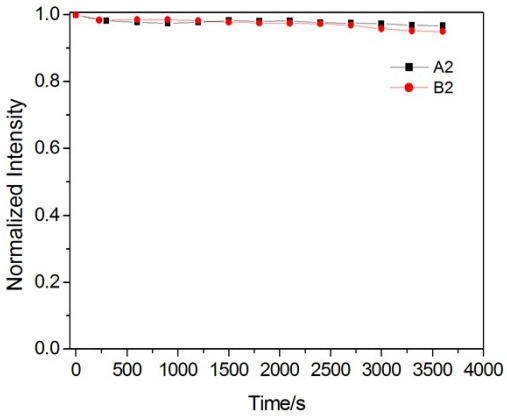


Figure S3. Photobleaching curves of A2 and B2 excitation at 365 nm, the emission signal at 560 nm was collected

7. Emission spectra of four Ir complexes at different pH values

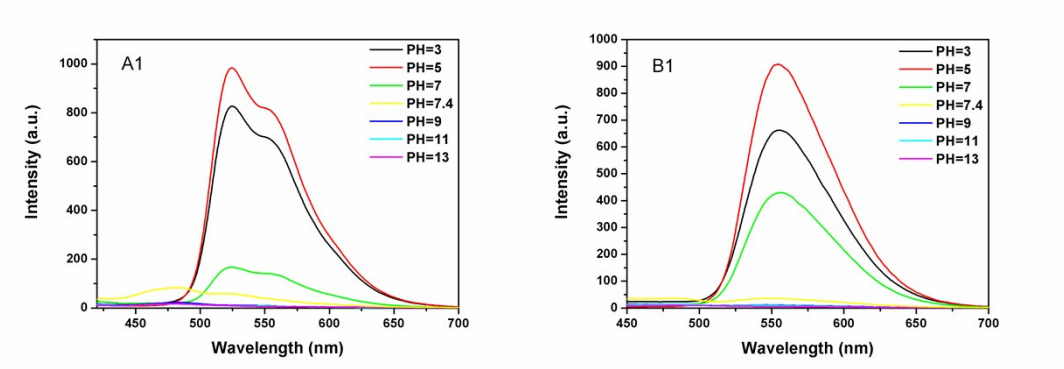


Figure S4. The luminescent spectra of A1 and B1 at different pH values

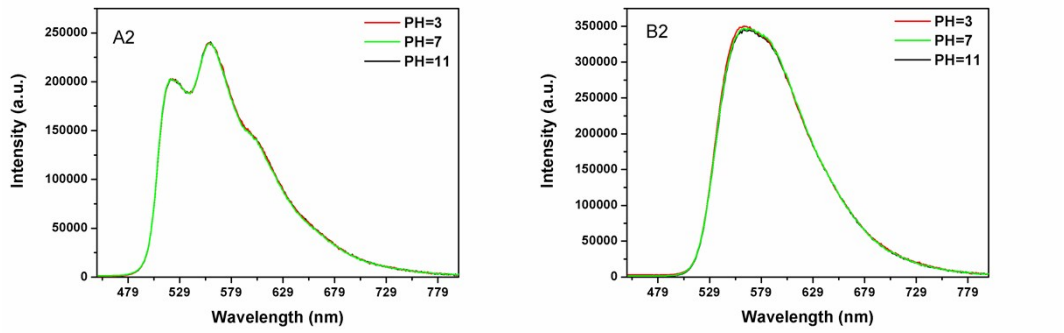


Figure S5. The luminescent spectra of A2 and B2 at different pH values