Supporting Information for

An investigation into the phosphorescence of a series of regioisomeric Ir(III) complexes

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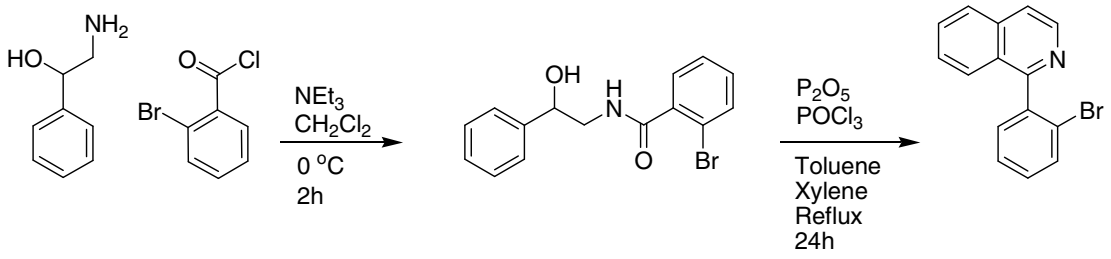

Fig. S1: Synthesis of 1-(2-bromophenyl)-isoquinoline. An adaptation of this route is used for all the regioisomers.

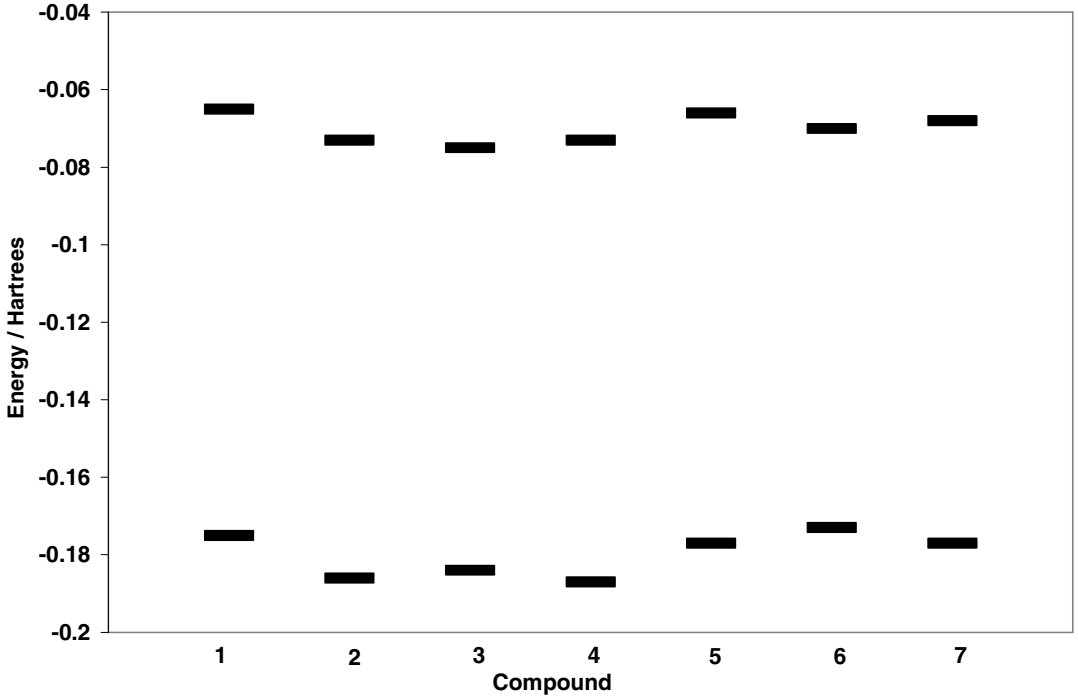

Fig. S2: The HOMO and LUMO energies for compounds **1**-**7** calculated by DFT using the B3LYP hybrid functional.

Experimental Section

2-Bromo-N-(2-hydroxy-2-phenylethyl)-benzamide

To a stirred solution of (±)-2-amino-1-phenylethanol (3.14 g, 22.8 mmol) and Et_3N (3.14 mL, 22.9 mmol) in CH_2Cl_2 (50 mL) at 0 °C was added 2-bromobenzoyl chloride (5.00 g, 22.8 mmol) dropwise. Stirring was continued for 2 h, after which time a white precipitate was observed. Filtration afforded the desired product in quantitative yield (7.28 g, 100%).

1-(2-Bromophenyl)-isoquinoline

2-Bromo-*N*-(2-hydroxy-2-phenylethyl)-benzamide (7.28 g , 22.75 mmol) was heated to reflux overnight in a 1:1 mixture of toluene and xylene (200 mL) with P_2O_5 (18 g, 64 mmol) and $POCl_3$ (25 mL, 273 mmol). The reaction mixture was cooled to room temperature and quenched by addition of MeOH. Addition of NaOH pellets until pH = 11, followed by extraction with EtOAc, gave the crude title compound. Column chromatography (silica, petroleum ether: EtOAc 6:1) afforded the pure title compound as a colourless oil (4.51 g, 70%).

^{1}H NMR (270 MHz, $CDCl_3$, ppm) δ: 8.62 (d, J = 5.7 Hz, 1H, Ar*H*), 7.89 (d, *J* = 8.2 Hz, 1H, Ar*H*), 7.75 - 7.35 (m, 8H, Ar*H*); *m/z* (CI) 285 ($[M+H]^+$ 100%).

1-(3-Bromophenyl)-isoquinoline

Synthesised using the same procedure as for 1-(2-bromophenyl)-isoquinoline. The compound was isolated as a white solid (4.88 g, 75%).

Anal. Calcd. for $C_{15}H_{10}BrN$: C 64.40%, H 3.55%, N 4.93%; Found C 64.40%, H 3.57%, N 4.91%; m.p. 52-53 °C; ^{1}H NMR (270 MHz, $CDCl_3$, ppm) δ: 8.58 (d, *J* = 5.6 Hz, 1H, Ar*H*), 8.02 (d, *J* = 8.5 Hz, 1H, Ar*H*), 7.83 (m, 2H, Ar*H*), 7.68 — 7.57 (m, 4H, Ar*H*), 7.48 (t, *J* = 7.3 Hz, 1H, Ar*H*), 7.37 (t, J = 7.7 Hz, 1H, Ar*H*); $^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$, ppm) δ: 159.0, 142.2, 141.6, 136.9, 132.9, 131.7, 130.2, 129.9, 128.7, 127.6, 127.1, 126.6, 122.5, 120.4; *m/z* (CI) 285 ($[M+H]^+$, 100%).

1-(4-Bromophenyl)-isoquinoline

Synthesised using the same procedure as for 1-(2-bromophenyl)-isoquinoline. The compound was isolated as a white solid (3.97 g, 61%).

Anal. Calcd. for $C_{15}H_{10}BrN$: C 64.40%, H 3.55%, N 4.93%; Found C 64.39%, H 3.63%, N 4.90%; m.p. 67 – 69 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ: 8.62 (d, *J* = 5.7 Hz, 1H, Ar*H*), 8.08 (d, *J* = 8.5 Hz, 1H, Ar*H*), 7.01 (d, *J* = 8.0 Hz, 1H, Ar*H*), 7.80 (m, 4H, *ArH*), 7.58 (m, 3H, ArH); $^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$, ppm) δ: 142.3, 142.2, 132.0, 131.6, 130.6, 130.2, 128.8, 127.5, 127.1, 126.9, 120.2, 120.0; *m/z* (CI): 284 $[M+H]^+$.