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<td>Author(s)</td>
<td>Wang, Yue; Harada, Takunori; Shiota, Yoshihito; Yoshizawa, Kazunari; Wang, Heng; Wang, Sheng; Ye, Xichong; Ogasawara, Masamichi; Nakano, Tamaki</td>
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Electronic Supplementary Information to:

**Isolation and Photo Transformation of Enantiomerically Pure Iridium(III) Bis[(4,6-difuorophenyl)pyridinato-N,C\textsubscript{2}]picolinate**

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**Experimental**

**Materials.** Iridium(III) Bis[(4,6-difuorophenyl)pyridinato-N,C2]picolinate (FIrpic) was purchased from Sigma-Aldrich and used as obtained. Chromatographic eluents were used as obtained.

**Instrumentation and measurements.** Analytical HPLC resolution was performed using a JASCO’s chromatographic setup consisting of a DG-980-50 degasser, a PU-980 pump, a UV-2070 detector, and a CD-2095plus detector equipped with a Daicel ChiralPak IA column or IC column (25 cm x 0.42 cm (i.d.)). Preparative HPLC resolution was conducted using JASCO PU-2086/UV-2075/R1-2031 equipped with a Daicel ChiralPak IC column (25 cm x 2 cm (i.d.)). Circular dichroism (CD) spectra were taken with a JASCO-820 spectrometer. UV-vis absorption spectra were measured on a JASCO V-570 spectrophotometer. Emission spectra were taken using a JASCO FP-8500 fluorescence spectrophotometer. FT-IR spectra were measured with a JASCO FT/IR6100 spectrometer. Photo irradiation was performed using an Ushio Optical Modulux SX-UlDS00MAMQQ 500-W Hg-Xe lamp equipped with a quartz-made collimating lens with a Gran-Taylor prism to obtain linearly polarized light (LPL) (ca. 40 mW/cm²) or without any prism to obtain non-polarized light (NPL) (ca. 200 mW/cm²). The distance between the source light and the sample was 35 cm. The light power was measured using a Coherent PM10 thermal sensor with a Coherent FieldmaxII-TO power meter.

**CPL emission measurements.** Circularly polarized luminescence (CPL) and nonpolarized fluorescence spectra were measured by using a dual-purpose CD and CPL spectrophotometer (J-700CPL) equipped with Stokes-Mueller matrix analysis system.¹ The excitation wavelength was set to 286 nm and the emission wavelengths were recorded over a wavelength range of 600–420 nm with 3 mm slit width and 10 nm spectral bandwidth for the excitation and emission monochromators, respectively. For the solid-state CPL measurements, artifact-free CPL spectra were measured carefully for both enantiomeric films (FIrpic 1 and 2 films), employing the set of procedures based on Stokes–Mueller matrix equations to remove parasitic artifacts.

**Computational method.** Geometrical optimization of iridium complexes without any symmetry constraint was carried out with the B3LYP functional in the Gaussian 09 program package.² The SDD basis³ for Ir atom and the 6-311+G* basis⁴ for C, N, O, F, and H atoms were used. The electronic excitation energies, rotational strengths of the iridium complexes have been calculated using time-dependent density functional theory (TDDFT).² Rotational strengths were calculated using the velocity representation.⁵ In comparison of calculated ECD spectra with experimental spectra, Gaussian bandshapes with a bandwidth of 0.25 eV were used to simulate the UV–Vis and ECD spectra.
Chromatographic resolution of Flrpic using a Daicel ChiralPak IA column hexane/2-propanol or hexane/2-propanol/CH₂Cl₂ as eluent

Figure S1. HPLC resolution profiles of Flrpic obtained using a Daicel ChiralPak IA column (25 cm x 0.46 cm (i.d.)) with binary (hexane/2-propanol (A-C)) and ternary (hexane/2-propanol/CH₂Cl₂ (D-F)) eluent systems where α denotes separation factor. HPLC conditions: flow rate = 0.5 ml/min, detection = UV at 250 nm.
Chromatographic resolution of Flrpic using a Daicel ChiralPak IA column
hexane/2-propanol/CHCl₃ as eluent

A. hexane/2-propanol/CHCl₃ = 75/15/10 (v/v/v); \( \alpha = 1.21 \)

B. hexane/2-propanol/CHCl₃ = 70/15/15 (v/v/v); \( \alpha = 1.28 \)

C. hexane/2-propanol/CHCl₃ = 65/15/20 (v/v/v); \( \alpha = 1.29 \)

Figure S2. HPLC resolution profiles of Flrpic obtained using a Daicel ChiralPak IA column (25 cm x 0.46 cm (i.d.)) with ternary (hexane/2-propanol/chloroform) eluent systems \( \alpha \) denotes separation factor. HPLC conditions: flow rate = 0.5 ml/min, detection = UV at 254 nm.
Chromatographic resolution of FIrpic using a Daicel ChiralPak IC column under various eluent conditions

**Figure S3.** HPLC resolution profiles of FIrpic obtained using a Daicel ChiralPak IC column (25 cm x 0.46 cm (i.d.)) with ternary hexane/2-propanol/dichloromethane eluent systems at various ratios where \( \alpha \) denotes separation factor. HPLC conditions: flow rate = 0.5 ml/min, detection = UV at 254 nm.
Chromatographic resolution of FIrpic using a Daicel ChiralPak OD column under various eluent conditions

Figure S4. HPLC resolution profiles detected with CD and UV (top and bottom of each, respectively) of FIrpic obtained using a Daicel ChiralPak OD column (25 cm x 0.46 cm (i.d.)) with binary hexane/2-propanol eluent systems (A, B) and with pure 2-ProOH as eluent (C) where \( \alpha \) denotes separation factor. HPLC conditions: flow rate = 0.5 ml/min, detection = UV at 250 nm.

*The CD signs of the first- and second-eluted isomer were opposite to those reported in ref. 9 under the same separation condition.
Comparison of theoretical and experimental CD spectra

Figure S5. Theoretical and experimental CD spectra of the Δ- and Λ-isomers. The experimental spectra were taken in MeOH at room temperature at 5.0 x 10^{-5} M in a 1-mm cell.
Figure S6. ESI mass spectra of rac-FIrpic (A) and the optically active, photo-transformation product isolated by HPLC (B).
Effects of light power and air on photo-induced transformation

Figure S7. $g_{CD}$-vs.-irradiation (A) and HPLC peak area of L-isomer-vs.-irradiation time (B) plots for the experiments using NPL (ca. 200 mW/cm$^2$) under N$_2$ (blue circle), LPL (ca. 40 mW/cm$^2$) under N$_2$ (red circle), and NPL (ca. 200 mW/cm$^2$) under air (green circle).
Reference
4  Gaussian 09, Revision E01: Gaussian, Inc., Wallingford CT, 2009.