# Electronic Supplementary Information (ESI)

## AIE-active Ir(III) complexes as Type-I dominant photosensitizers for efficient photodynamic therapy

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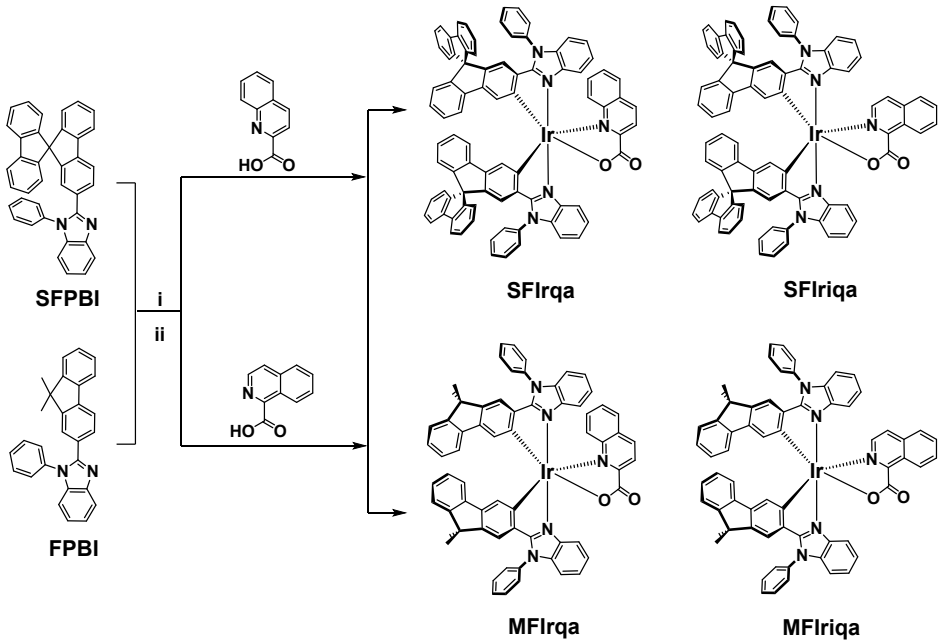
## 1. Synthesis and characterization




**Scheme S1**. Synthetic routes of the complexes. (i) $IrCl_3 \cdot 3H_2O$, ethoxyethanol, water (3:1, v/v), reflux, 24 h; (ii) μ-chloro-bridged dimer, $CH_2Cl_2$, ethanol, reflux, 12 h.

### Synthesis of SFIrqa

$IrCl_3 \cdot 3H_2O$ (0.35 g, 1.00 mmol) and ligand SFPBI[1] (1.12 g, 2.20 mmol) in a solution of 2-ethoxyethanol and water were refluxed for about 24 h under $Ar_2$ atmosphere. The mixture was filtered after cooling to room temperature, followed by washing with water and ethanol, obtaining about 0.68 g μ-chloro-bridged dimer. Then, the ancillary ligand (0.05 g, 0.28 mmol) and the corresponding dimer (0.30 g, 0.11 mmol) in a mixed solvent of $CH_2Cl_2$ and ethanol were allowed to reflux overnight. The residue was purified by silica gel column chromatography with ethyl acetate: $CH_2Cl_2$ in 1:10 (v:v) ratio as the eluent, giving a red powder. Yield 70%. $^1$H NMR (500 MHz, $d_6$-DMSO, $\delta$ [ppm]): 8.67 (d, $J$ = 9.0 Hz, 1H), 8.21 (d, $J$ = 8.4 Hz, 1H), 8.09 (d, $J$ = 7.8 Hz, 1H), 7.90-7.94 (m, 4H), 7.85 (d, $J$ = 9.0 Hz, 1H), 7.75-7.76 (m, 1H), 7.66 (t, $J$ = 7.8 Hz, 1H), 7.52 (t, $J$ = 7.8 Hz, 1H), 7.42-7.46 (m, 4H), 7.35-7.39 (m, 4H), 7.29-7.34 (m, 3H), 7.21-7.27 (m, 6H), 7.14-7.19 (m, 4H), 6.99-7.12 (m, 8H), 6.74-6.77 (m, 3H), 6.69 (d, $J$ = 7.8 Hz, 1H), 6.58-6.62 (m, 2H), 6.54 (t, $J$ = 8.4 Hz, 2H), 6.45 (d, $J$ = 7.8 Hz, 1H), 5.69 (d, $J$ = 8.4 Hz, 1H), 5.65 (s, 1H), 5.57 (s, 1H). $^{13}$C NMR (125 MHz,

$CDCl_3$, $\delta$ [ppm]): 175.27, 163.83, 163.75, 155.13, 150.55, 149.89, 149.38, 149.21, 149.02, 148.85, 148.42, 148.03, 146.25, 142,74, 142.26, 142.17, 142.04, 141.78, 141.71, 141.59, 141.36, 141.07, 141.04, 139.92, 139.75, 138.54, 136.31, 135.88, 134.87, 134.84, 133.60, 133.51, 130.33, 130.02, 129.92, 129.68, 129.61, 129.56, 129.44, 129.43, 128.19, 127.94, 127.79, 127.70, 127.53, 127.34, 127.27, 127.24, 127.15, 127.07, 125.49, 124.70, 124.47, 124.32, 124.25, 124.06, 124.02, 123.74, 123.26, 123.16, 122.89, 121.33, 120.67, 120.47, 119.96, 119.76, 119.43, 119.30, 119.15, 116.99, 114.43, 110.64, 110.08. MS [m/z]: Calcd for $C_{86}H_{52}IrN_5O_2$: 1379.4, Found 1379.4 $[M]^+$. Anal. calcd. For $C_{86}H_{52}IrN_5O_2$: C 74.87, H 3.80, N 5.08; Found: C 74.65, H 3.78, N 5.09.

**Synthesis of SFIriqa**

The synthesis method is the same as **SFIrqa**. Yield 73%. $^1$H NMR (500 MHz, $d_6$-DMSO, $\delta$ [ppm]): 9.95 (d, $J$ = 8.4 Hz, 1H), 8.15 (d, $J$ = 6.0 Hz, 1H), 8.06 (d, $J$ = 8.4 Hz, 1H), 7.87-7.92 (m, 7H), 7.81 (t, $J$ = 7.8 Hz, 1H), 7.49-7.53 (m, 2H), 7.45 (d, $J$ = 7.2 Hz, 1H), 7.29-7.39 (m, 10H), 7.22-7.26 (m, 3H), 7.11-7.19 (m, 9H), 6.98-7.09 (m, 5H), 6.79-6.84 (m, 2H), 6.68 (d, $J$ = 7.8 Hz, 1H), 6.54-6.59 (m, 3H), 6.44-6.48 (m, 2H), 5.69 (s, 2H), 5.56 (s, 1H). $^{13}$C NMR (125 MHz, $CDCl_3$, $\delta$ [ppm]): 174.41, 164.17, 163.33, 151.31, 150.48, 149.99, 149.45, 149.29, 149.19, 149.15, 148.96, 148.87, 142.79, 142.37, 142.15, 142.12, 141.75, 141.56, 141.39, 141.13, 141.05, 139.81, 139.77, 136.58, 136.45, 135.98, 134.91, 134.03, 133.47, 131.32, 130.01, 129.93, 129.72, 129.62, 129.54, 129.46, 129.17, 128.79, 128.23, 127.96, 127.92, 127.81, 127.67, 127.66, 127.45, 127.41, 127.35, 127.25, 127.20, 127.10, 127.05, 126.46, 126.12, 125.69, 124.78, 124.74, 124.50, 124.19, 124.07, 124.01, 123.76, 123.64, 123.41, 122.71, 121.02, 120.74, 120.34, 119.82, 119.61, 119.41, 119.29, 119.15, 117.44, 114.29, 110.63, 110.03. MS [m/z]: Calcd for $C_{86}H_{52}IrN_5O_2$: 1379.4, Found 1379.4 $[M]^+$. Anal. calcd. For $C_{86}H_{52}IrN_5O_2$: C 74.87, H 3.80, N 5.08; Found: C 74.72, H 3.92, N 4.90.

**Synthesis of MFIrqa**

The synthesis method is the same as **MFIriqa**. Yield 73%. $^1$H NMR (500 MHz, $d_6$-DMSO, $\delta$ [ppm]): 8.73 (d, $J$ = 8.4 Hz, 1H), 8.29 (d, $J$ = 8.4 Hz, 1H), 8.11 (d, $J$ = 7.8

Hz, 1H), 7.93-7.98 (m, 3H), 7.88-7.92 (m, 1H), 7.83-7.87 (m, 4H), 7.80 (d, *J* = 7.8 Hz, 1H), 7.72 (d, *J* = 7.8 Hz, 1H), 7.67 (d, *J* = 6.0 Hz, 1H), 7.59 (t, *J* = 7.8 Hz, 1H), 7.48 (d, *J* = 6.6 Hz, 1H), 7.42 (d, *J* = 7.2 Hz, 1H), 7.38 (d, *J* = 7.8 Hz, 1H), 7.28-7.32 (m, 2H), 7.24-7.28 (m, 2H), 7.14-7.23 (m, 6H), 7.11 (t, *J* = 7.8 Hz, 1H), 7.07 (d, *J* = 7.2 Hz, 1H), 6.93 (s, 1H), 6.80 (t, *J* = 7.8 Hz, 1H), 6.57 (d, *J* = 3.0 Hz, 2H), 6.52 (s, 1H), 5.68 (d, *J* = 8.4 Hz, 1H), 1.22 (s, 3H), 1.11 (s, 3H), 1.06 (s, 3H), 1.03 (s, 3H). $^{13}$C NMR (125 MHz, $CDCl_3$, $\delta$ [ppm]): 175.29, 164.23, 164.14, 155.22, 154.70, 154.59, 149.95, 148.12, 146.47, 145.96, 145.63, 140.79, 140.40, 140.04, 139.94, 139.10, 138.86, 138.47, 136.72, 136.29, 135.83, 135.80, 132.87, 132.83, 130.45, 130.40, 130.32, 130.18, 130.15, 130.11, 130.06, 129.72, 128.87, 128.65, 128.55, 128.14, 128.11, 128.06, 127.36, 126.97, 126.53, 126.41, 125.46, 124.77, 124.25, 123.81, 123.78, 123.20, 122.86, 122.41, 122.27, 120.27, 120.04, 119.87, 119.52, 116.98, 114.49, 110.65, 110.08. MS [m/z]: Calcd for $C_{66}H_{48}IrN_5O_2$: 1135.3, Found 1135.3 $[M]^+$. Anal. calcd. For $C_{66}H_{48}IrN_5O_2$: C 69.82, H 4.26, N 6.17; Found: C 69.70, H 4.18, N 6.19.

**Synthesis of MFIriqa**

The synthesis method is the same as **MFIriqa**. Yield 68%. $^1$H NMR (500 MHz, *d*$_6$-DMSO, $\delta$ [ppm]): 10.02 (d, *J* = 9.0 Hz, 1H), 8.15 (d, *J* = 6.0 Hz, 1H), 8.04-8.08 (m, 2H), 7.95-7.97 (m, 2H), 7.84-7.93 (m, 9H), 7.73 (d, *J* = 7.8 Hz, 1H), 7.68 (d, *J* = 7.2 Hz, 1H), 7.40 (d, *J* = 7.2 Hz, 1H), 7.36-7.38 (m, 1H), 7.32-7.34 (m, 2H), 7.23-7.26 (m, 3H), 7.14-7.20 (m, 4H), 7.11 (d, *J* = 7.8 Hz, 1H), 7.02 (d, *J* = 7.2 Hz, 1H), 6.92 (s, 1H), 6.84-6.88 (m, 1H), 6.63 (s, 1H), 6.57 (s, 1H), 6.52 (s, 1H), 5.71 (d, *J* = 7.8 Hz, 1H), 1.19 (s, 3H), 1.10 (s, 3H), 1.03 (d, *J* = 11.4 Hz, 6H). $^{13}$C NMR (125 MHz, $CDCl_3$, $\delta$ [ppm]): 173.44, 163.51, 162.73, 153.63, 153.58, 150.39, 149.10, 148.29, 145.21, 144.61, 141.38, 139.90, 139.82, 139.26, 138.93, 138.87, 138.17, 137.71, 135.82, 135.58, 135.38, 134.82, 132.35, 131.79, 130.22, 129.43, 129.34, 129.19, 129.11, 129.08, 129.05, 128.75, 128.10, 127.85, 127.76, 127.72, 127.55, 127.07, 126.38, 125.90, 125.54, 125.48, 125.38, 125.01, 124.58, 123.82, 123.59, 122.76, 122.34, 121.69, 121.40, 121.22, 119.12, 118.74, 118.62, 116.38, 113.31, 109.63, 109.01, 106.48. MS [m/z]: Calcd for $C_{66}H_{48}IrN_5O_2$: 1135.3, Found 1135.3 $[M]^+$. Anal. calcd. For $C_{66}H_{48}IrN_5O_2$: C 69.82, H 4.26, N 6.17; Found: C 69.75, H 4.18, N 6.19.

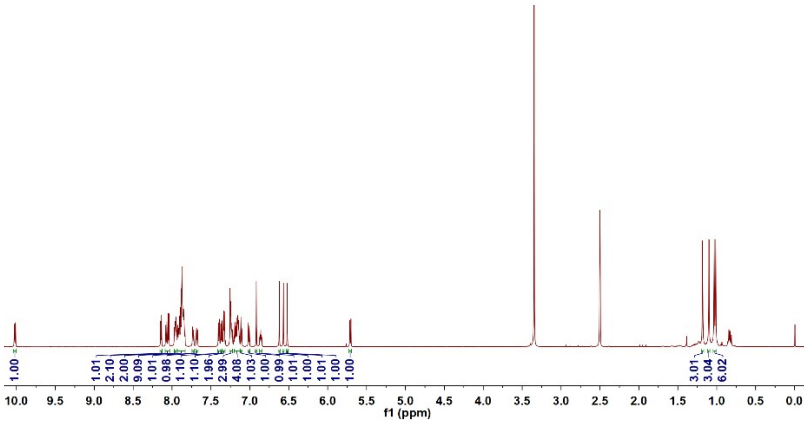



**Fig. S1** $^{1}$H NMR spectrum of **MFIriqa** in $d_6$-DMSO at room temperature.

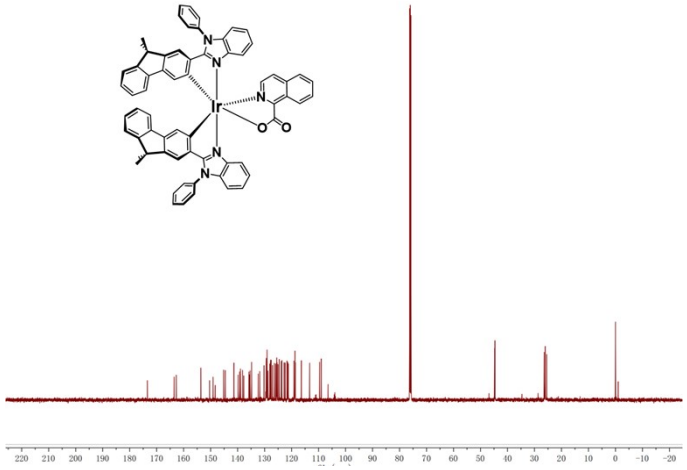



**Fig. S2** $^{13}$C NMR spectrum of **MFIriqa** in $CDCl_3$ at room temperature.

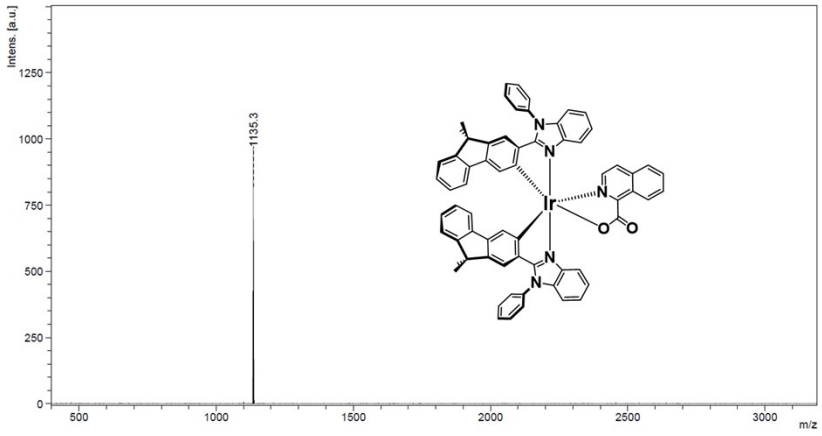



**Fig. S3** High-resolution MALDI-TOF mass spectrum of **MFIriqa**.

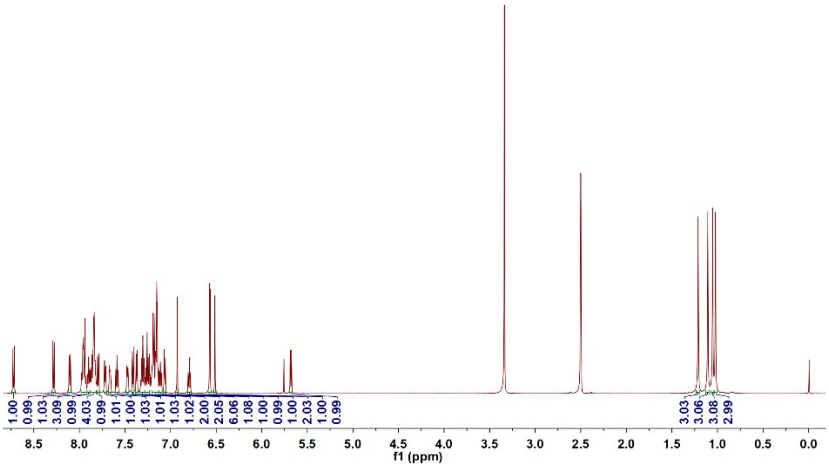



**Fig. S4** $^{1}$H NMR spectrum of **MFIrqa** in $d_6$-DMSO at room temperature.

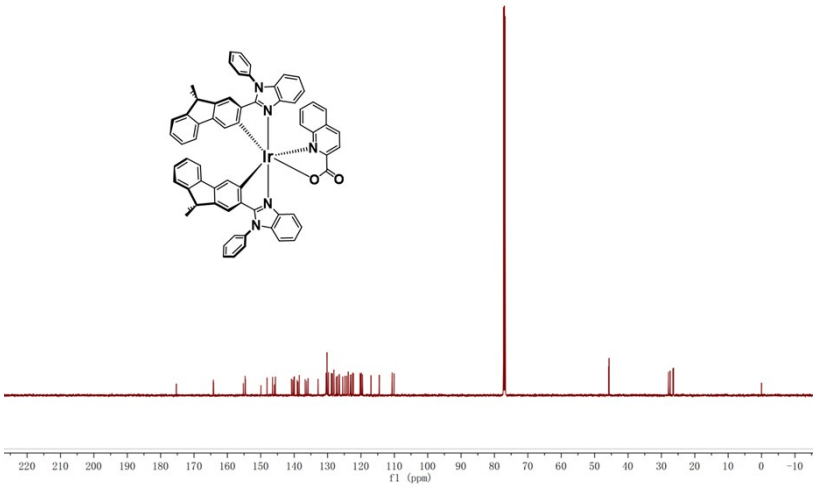



**Fig. S5** $^{13}$C NMR spectrum of **MFIrqa** in $CDCl_3$ at room temperature.

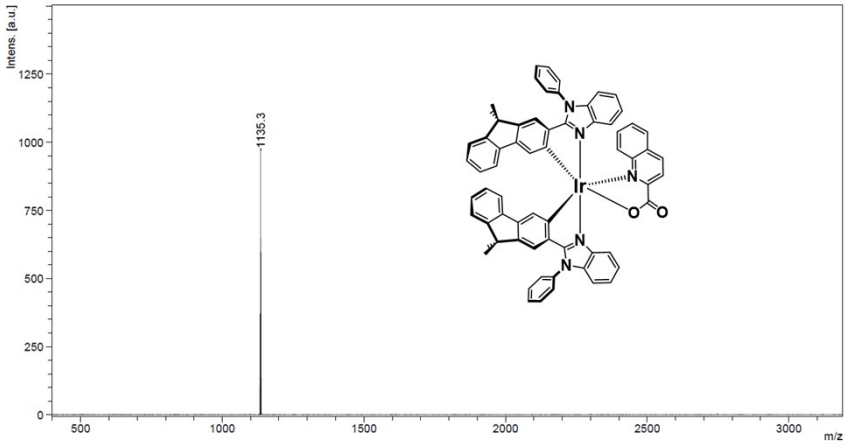



**Fig. S6** MALDI-TOF mass spectrum of **MFIrqa**.

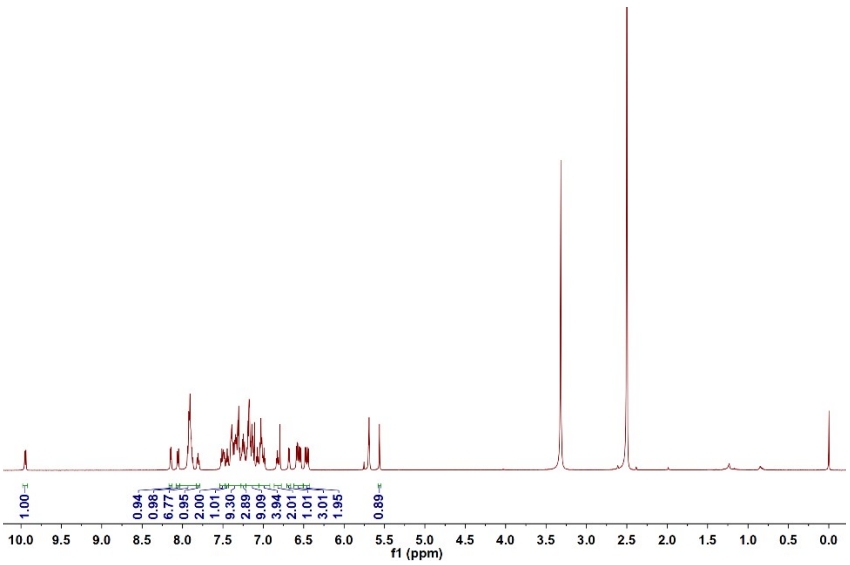



**Fig. S7** $^{1}$H NMR spectrum of **SFIriqa** in $d_6$-DMSO at room temperature.

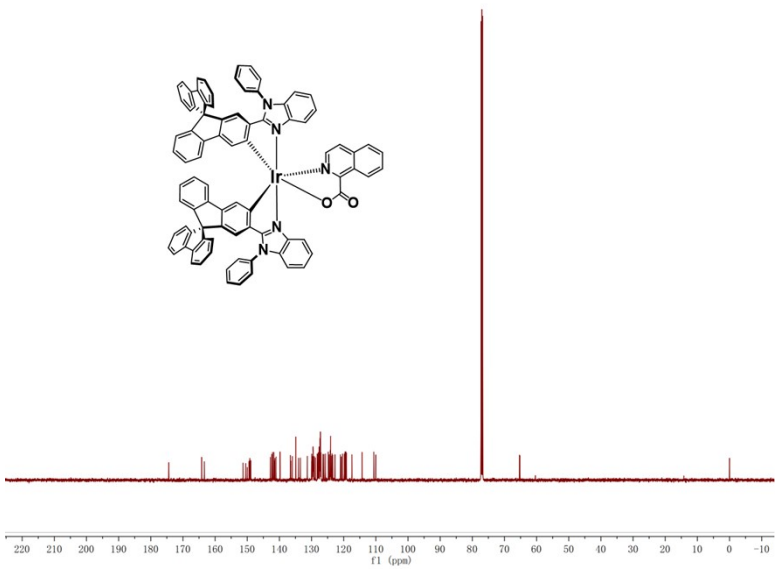



**Fig. S8** $^{13}$C NMR spectrum of **SFIriqa** in $CDCl_3$ at room temperature.

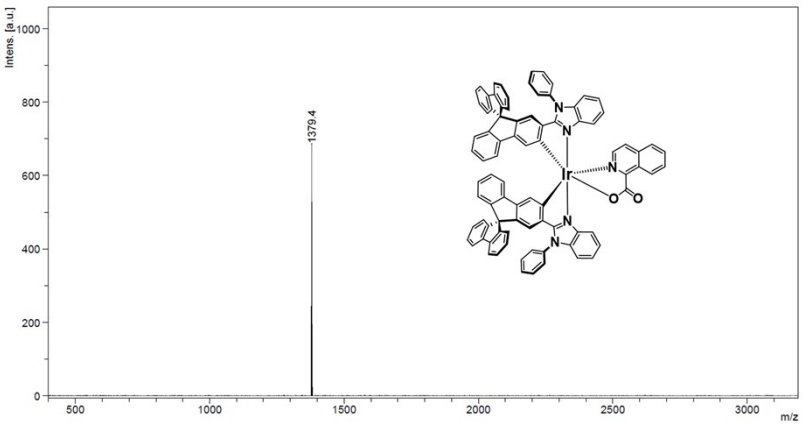



**Fig. S9** MALDI-TOF mass spectrum of SFIriqa.

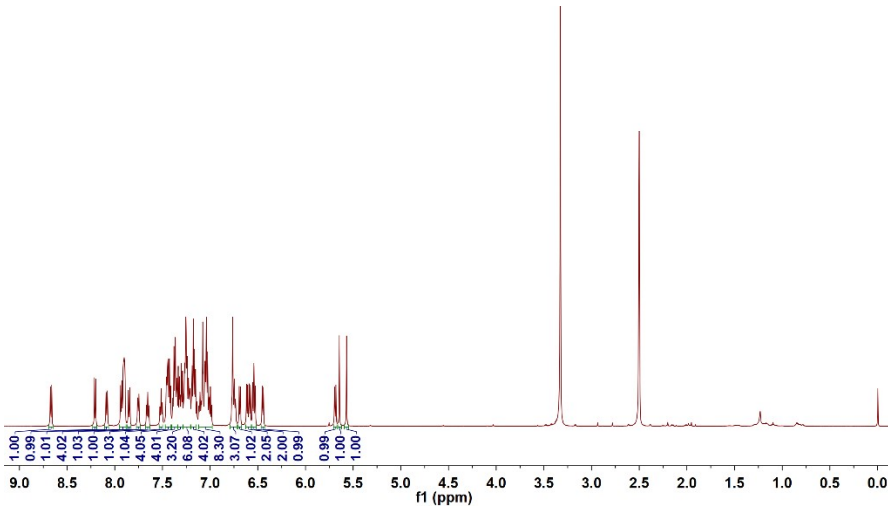



**Fig. S10** $^{1}$H NMR spectrum of **SFIrqa** in $d_6$-DMSO at room temperature.

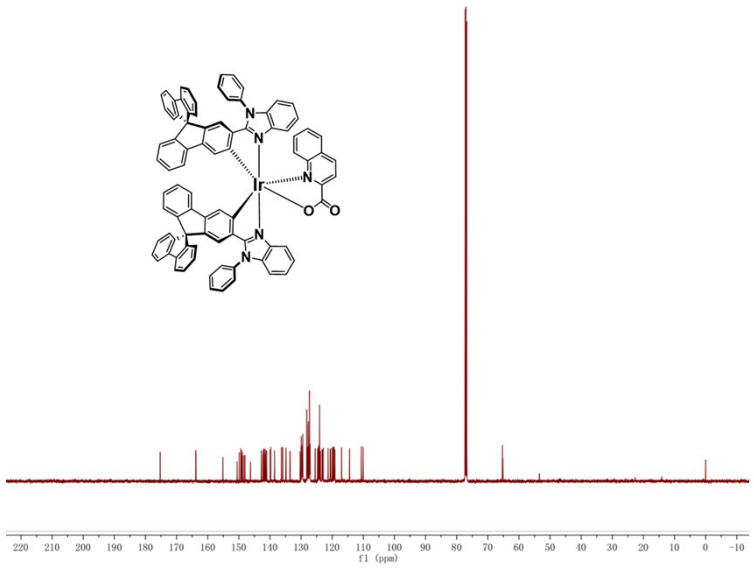



**Fig. S11** $^{13}$C NMR spectrum of **SFIrqa** in $CDCl_3$ at room temperature.

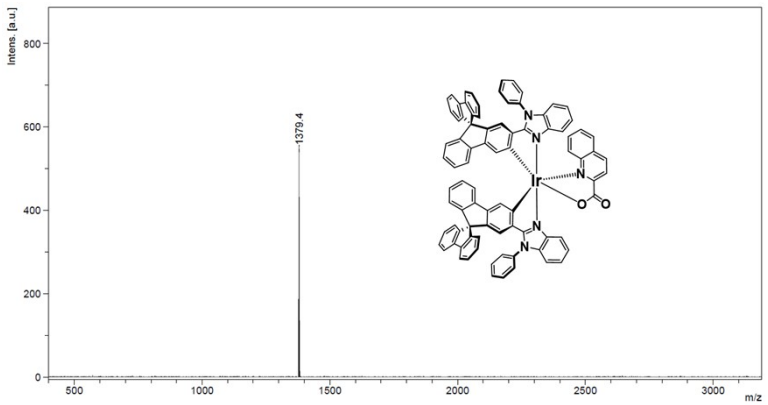



**Fig. S12** MALDI-TOF mass spectrum of **SFIrqa**.

**Table S1** Crystal data and structure refinement of **MFIriqa**, **MFIrqa** and **SFIriqa**.

| Name | **MFIriqa** | **MFIrqa** | **SFIriqa** |
|---|---|---|---|
| Identification code | CCDC 2212243 | CCDC 2212244 | CCDC 2212245 |
| Formula | $C_{66}H_{48}IrN_5O_2$ | $C_{66}H_{48}IrN_5O_2$ | $C_{86}H_{52}IrN_5O_2$ |
| Formula weight | 1135.29 | 1135.29 | 1379.52 |
| Crystal system | monoclinic | monoclinic | orthorhombic |
| Space group | $P2_1/n$ | $P2_1/n$ | $P2_12_12_1$ |
| Cell Lengths (Å) | a 17.0548(8) | a 19.1462(11) | a 16.8482(8) |
| | b 18.1638(8) | b 14.0770(8) | b 18.3470(9) |
| | c 19.8406(9) | c 22.2847(13) | c 22.5335(10) |
| Cell Angles (°) | α 90 | α 90 | α 90 |
| | β 97.298(3) | β 104.354(3) | β 90 |
| | γ 90 | γ 90 | γ 90 |
| Cell Volume (Å3) | 6096.4(5) | 5818.7(6) | 6965.4(6) |
| Z | 4 | 4 | 4 |
| Dcalcd.(g m-3) | 1.237 | 5.021 | 1.316 |
| F(000) | 2288.0 | 7540.0 | 2784.0 |
| Rint | 0.0685 | 0.0427 | 0.0534 |
| Goodness-of-fit on F2 | 1.034 | 0.824 | 1.020 |
| R1a, wR2b [I>=2σ (I)] | 0.0377, 0.0780 | 0.0285, 0.0961 | 0.0378, 0.0905 |
| R1, wR2 [all data] | 0.0533, 0.0834 | 0.0356, 0.1022 | 0.0446, 0.0949 |

[a] $R_1 = \Sigma||Fo|- |Fc||/\Sigma|Fo|$. [b] $wR_2 = |\Sigma w(|Fo|^2-|Fc|^2)|/\Sigma|w(Fo^2)^2|^{1/2}$.

**Table S2** Representative bond lengths and bond angles for **MFIriqa**, **MFIrqa**, and **SFIriqa**.

| Name | **SFIriqa** | **MFIrqa** | **MFIriqa** |
|---|---|---|---|
| bond lengths (Å) | Ir1-O1 [2.152(5)] | Ir1-O1 [2.138(3)] | Ir1-O2 [2.145(3)] |
| | Ir1-N1 [2.043(5)] | Ir1-N1 [2.040(3)] | Ir1-N1 [2.129(3)] |
| | Ir1-N4 [2.156(5)] | Ir1-N2 [2.219(2)] | Ir1-N2 [2.041(3)] |
| | Ir1-N5 [2.059(5)] | Ir1-N3 [2.042(2)] | Ir1-N3 [2.033(3)] |
| | Ir1-C1 [2.006(7)] | Ir1-C1 [2.012(3)] | Ir1-C1 [2.021(3)] |
| | Ir1-C8 [2.023(6)] | Ir1-C13 [1.995(4)] | Ir1-C2 [1.994(4)] |
| | **SFIriqa** | **MFIrqa** | **MFIriqa** |
| bond angles (°) | O1-Ir1-N4 | O1-Ir1-N2 | O2-Ir1-N1 |
| | [76.1(2)] | [75.95(9)] | [75.3(1)] |
| | N1-Ir1-C1 | N1-Ir1-C13 | N2-Ir1-C1 |
| | [80.1(2)] | [79.9(1)] | [80.0(1)] |
| | N5-Ir1-C8 | N3-Ir1-C1 | N3-Ir1-C2 |
| | [80.3(2)] | [80.2(1)] | [80.0(1)] |
| | O1-Ir1-C1 | O1-Ir1-C13 | O2-Ir1-C2 |
| | [173.9(2)] | [175.3(1)] | [170.6(1)] |
| | N1-Ir1-N5 | N1-Ir1-N3 | N2-Ir1-N3 |
| | [171.1(2)] | [171.9(1)] | [171.1(1)] |
| | N4-Ir1-C8 | N2-Ir1-C1 | N1-Ir1-C1 |
| | [170.7(2)] | [167.1(1)] | [173.9(1)] |

**Table S3.** The intermolecular interactions of **MFIriqa, MFIrqa,** and **SFIriqa** crystals.

| **MFIriqa** | | **MFIrqa** | | **SFIriqa** | |
|---|---|---|---|---|---|
| Types of bond | distance (Å) | Types of bond | distance (Å) | Types of bond | distance (Å) |
| C-H…C | 2.778, 2.780, 2.840, 2.841, 2.851, 2.855 | C-H…O | 2.561, 2.609 | C-H…π | 2.775, 2.791, 2.793, 2.801, 2.816 |
| C-H…O | 2.601, 2.680, 2.715 | C-H…π | 2.792, 2.824 | C-H…O | 2.541, 2.572 |
| C-H…π | 2.791, 2.851 | | | C-H…C | 2.835, 2.855 |
| π…π | 3.375 | | | C-H…H | 2.179 |

**Table S4** Calculated energy levels, oscillator strengths, and orbital transition analyses of lowest triplet state ($T_1$) states for complexes **MFIriqa**, **MFIrqa, SFIrqa,** and **SFIriqa**.

| **Complex** | **State** | **eV** | ***f*** | **Assignment** | **Character** |
|---|---|---|---|---|---|
| **MFIriqa** | $T_1$ | 1.83 | 0.00 | H→L(96%) | $^3$MLCT/ $^3$LLCT |
| **MFIrqa** | $T_1$ | 1.91 | 0.00 | H→L(36%) | $^3$MLCT$^3$LLCT /$^3$LC |
| | | | | H→L+1(44%) | $^3$MLCT$^3$LLCT /$^3$LC |
| **SFIriqa** | $T_1$ | 1.86 | 0.00 | H→L(95%) | $^3$MLCT/$^3$LLCT |
| **SFIrqa** | $T_1$ | 1.92 | 0.00 | H→L(37%) | $^3$MLCT$^3$LLCT /$^3$LC |
| | | | | H→L+1(42%) | $^3$MLCT$^3$LLCT /$^3$LC |

H stands for HOMO; L stands for LUMO.

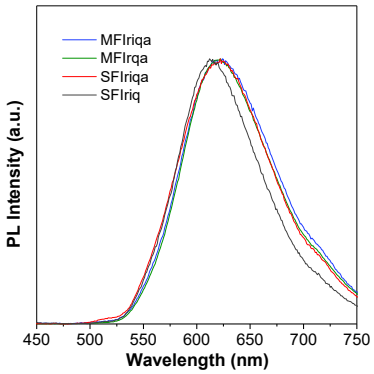



**Fig. S13** PL spectra of **MFIriqa**, **MFIrqa, SFIrqa,** and **SFIriqa** in the film.

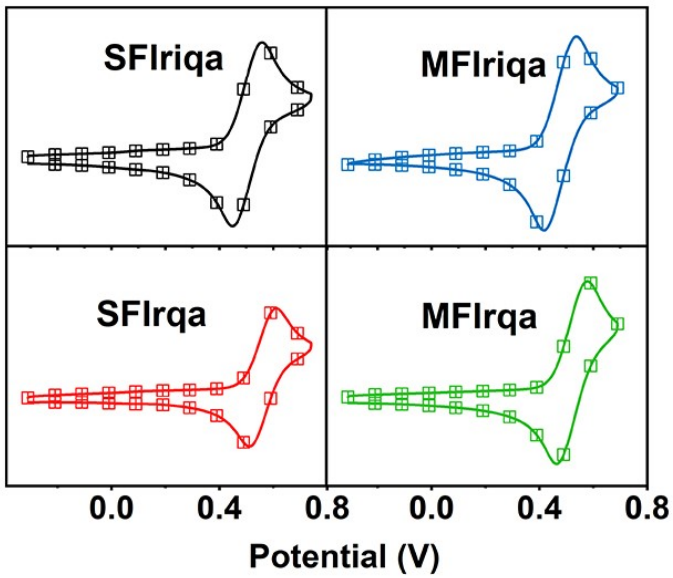



**Fig. S14** Cyclic voltammograms of complexes **MFIriqa**, **MFIrqa, SFIrqa,** and **SFIriqa** in degassed $CH_3CN$ solution with 0.1 M $TBAPF_6$ as electrolyte (scan rate = 100 mV/s)

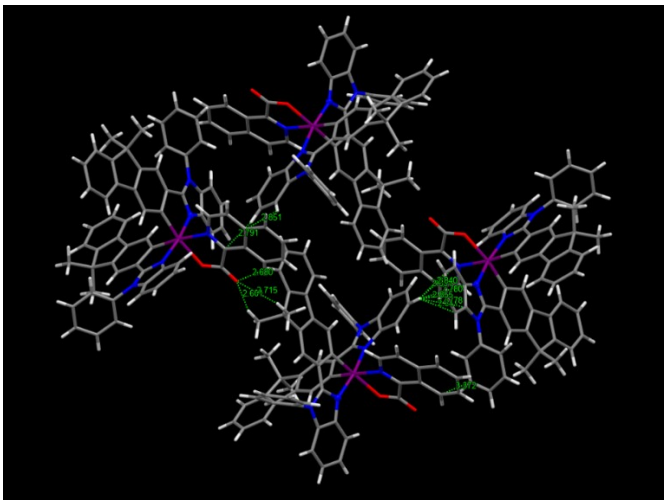


**Fig. S15** The intermolecular interactions of **MFIriqa.**

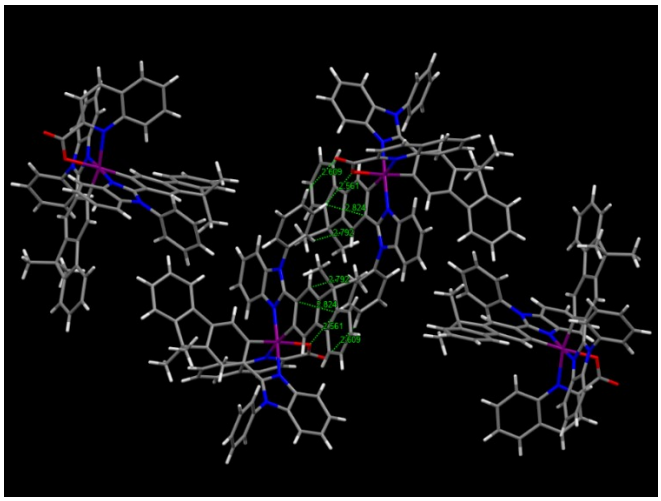


**Fig. S16** The intermolecular interactions of **MFIrqa.**

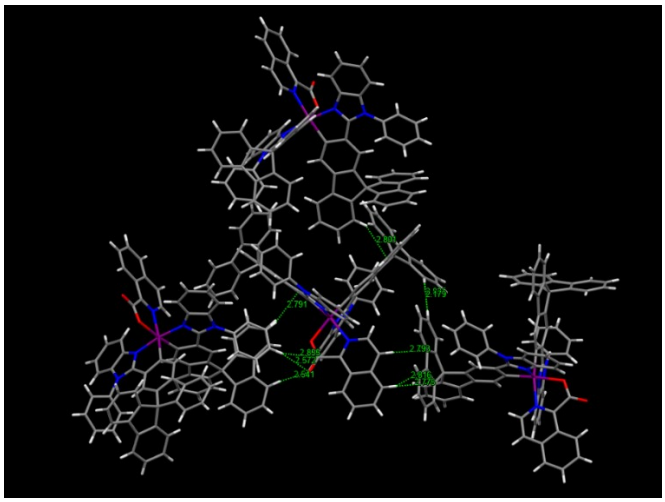


**Fig. S17** The intermolecular interactions of **SFIriqa.**

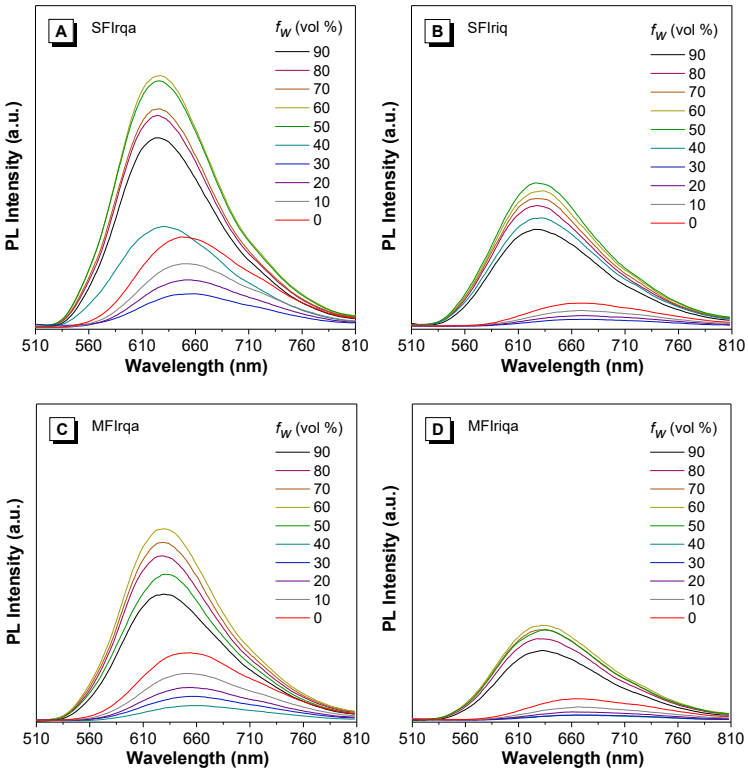



**Fig. S18** PL spectra of (A) **SFIrqa**, (B) **SFIriqa**, (C) **MFIrqa** and (D) **MFIriqa** in DMSO/$H_2O$ with different $H_2O$ fractions (*fw*). Concentration: 0.1 μM; Excitation wavelength: 460 nm.

## 2. ROS generation measurement

### General ROS detection by DCFH-DA

The general ROS generation assay used 2,7-dichlorodihydrofluorescein (DCFH) as an indicator, which was converted from 2,7- dichlorodihydrofluorescein diacetate (DCFH-DA), responded with an aqueous solution of NaOH for 30 min at 4°C. The hydrolysate was then neutralized with ultrapure water to get the stock solution with a concentration of 40 μM. Typically, DCFH-DA stock solution (working concentration: 5 μM) and PBS were mixed with NPs solution, the mixtures were exposed to white light irradiation (30 mW $cm^{-2}$), and the PL intensities at 525 nm (Excitation wavelength: 488 nm) were recorded at regular intervals in a PL spectrofluorometer.

### Detection of singlet oxygen($^1O_2$) by ABDA

The $^1O_2$ generation was studied by using ABDA as an indicator as the absorbance of

ABDA decreases upon reaction with $^1O_2$. ABDA solution (working concentration: 20 μM) was added to different AIE NPs (working concentration: 2 μM), and the mixtures were exposed to white light irradiation (30 mW $cm^{-2}$). After that, the absorbance of ABDA at 378 nm was recorded for different durations of white light irradiation to obtain the decay rate of the photosensitizing process.

**Detection of •OH by HPF**

The •OH generation measurements were conducted using hydroxyphenyl fluorescein (HPF) as the indicator. When •OH is generated in the solution, the HPF will be oxidized and fluoresce intensely green centered at 515 nm. HPF solution (working concentration: 5 μM) and PBS were added to different AIE NPs (working concentration: 2 μM), and the mixtures were exposed to white light irradiation (30 mW $cm^{-2}$). The PL intensities at 515 nm (Excitation wavelength: 490 nm) were recorded at regular intervals in a PL spectrofluorometer.

## 3. Cellular study

**Preparation of Nanoparticles**

5 mg of **MFIriqa**, **MFIrqa, SFIriqa,** and **SFIrqa**, and 10 mg of DSPE-mPEG-2000 were respectively dissolved in 10 mL THF solution, which was poured into 10 mL ultrapure water under sonication (200 W). The dissolution obtained was further kept in sonication (200 W) for 15 min. Subsequently, the AIE NPs were obtained by filtration through a polyethersulfone (PES) syringe-driven filter (0.45/0.22 μm). To purify AIE NPs, they were washed with a 10 K centrifuge filter units (Millipore) under centrifugation at 8000 r.p.m. for 8 min. Finally, the four AIE NPs solutions were concentrated into 5 mL ultrapure water and stored at 4°C for further investigation.

**Cell culture**

Hela cells were cultured DMEM (containing 10% FBS and 1% Penicillin-Streptomycin solution) at 37 °C in a humidified incubator with 5% $CO_2$.

**Cell cytotoxicity evaluations**

The cell viability of AIE NPs on Hela cancer cells was examined by CCK-8 assay. Briefly, Hela cells were seeded in 96-well microplates at a density of $5 \times 10^3$ cells/well in 100 μL of complete DMEM media and incubated at 37°C in a humidified incubator with 5% $CO_2$. Subsequently, the cells reached about 80% confluence, the culture medium was replaced with the fresh medium containing different concentrations (0, 50, 100, 150, and 200 μg/mL) of four NPs. After further incubation for 4 h, the cells were exposed to white light irradiation 30 mW $cm^{-2}$ for 30 min. Meanwhile, the **MFIriqa**, **MFIrqa, SFIriqa,** and **SFIrqa** NPs incubated cells without white light irradiation were also conducted for the dark cytotoxicity study. After an additional 24 h, each well was directly added 10 μL CCK-8 solution and incubated at 37 °C for 30 min. The absorbance of sample wells and control wells at 450 nm was also measured by a microplate reader.

**Cell imaging**

Before confocal microscopy imaging of cells with analytes, Hela cells in the exponential phase were plated on 35 nm glass bottom culture dishes for 24 h to reach around 80% confluency. After incubation with DMEM containing **MFIriqa**, **MFIrqa, SFIriqa,** and **SFIrqa** NPs solution (working concentration: 10 μg/mL) for 4 h, the cells were further washed by PBS three times and imaged by CLSM in the channel mode at excitation of 488 nm. The emission filter was 650 - 750 nm.

**Co-localization imaging**

Before confocal microscopy imaging of cells with analytes, Hela cells in the exponential phase were plated on 35 nm glass bottom culture dishes for 24 h to reach around 80% confluency. Cells were first incubated with 1 mL DMEM containing **MFIriqa**, **MFIrqa, SFIriqa,** and **SFIrqa** NPs (working concentration: 10 μg/mL), 37 °C for 4 h. The DMEM was then removed, and the cells were further washed by PBS three times. Subsequently, cells were incubated with 1 mL DMEM containing BODIPY (1 μM, stock solution: 1 mM in DMSO), 37 °C for 30 min. The cells were

further washed by PBS three times and imaged by CLSM. For NPs, the excitation was 488 nm and the emission filter was 650 - 750 nm. For BODIPY, the excitation was 488 nm and the emission filter was 500 - 540 nm.

**ROS generation measurement in vitro**

The Hela cells were seeded in 6-well microplates at a density of $5\times10^4$ cells/well in 1 mL of complete DMEM media and incubated at 37 °C in a humidified incubator with 5% $CO_2$. Cells were first incubated with 1 mL DMEM containing **MFIriqa**, **MFIrqa,** **SFIriqa,** and **SFIrqa** NPs (working concentration: 200 μg/mL), 37°C for 4 h. The DMEM was then removed, and the cells were further washed by PBS three times. Then, the cells were incubated with 1 mL DMEM containing DCFH-DA (10 μM, stock solution: 10 mM in DMSO), 37 °C for 20 min, the cells were further washed by PBS three times and imaged by CLSM in the channel mode at excitation of 488 nm. The emission filter was 500 - 600 nm.

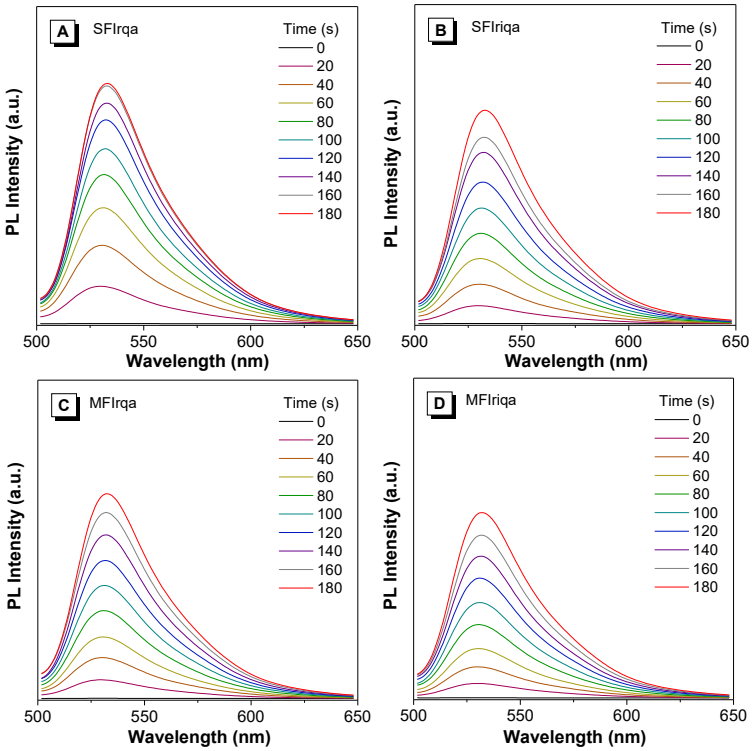



**Fig. S19** Fluorescence intensity changes of (A) **SFIrqa**, (B) **SFIriqa**, (C) **MFIrqa** and (D) **MFIriqa** (2 μM) in DCFH-DA with increasing irradiation time upon white light (30 mW $cm^{-2}$).

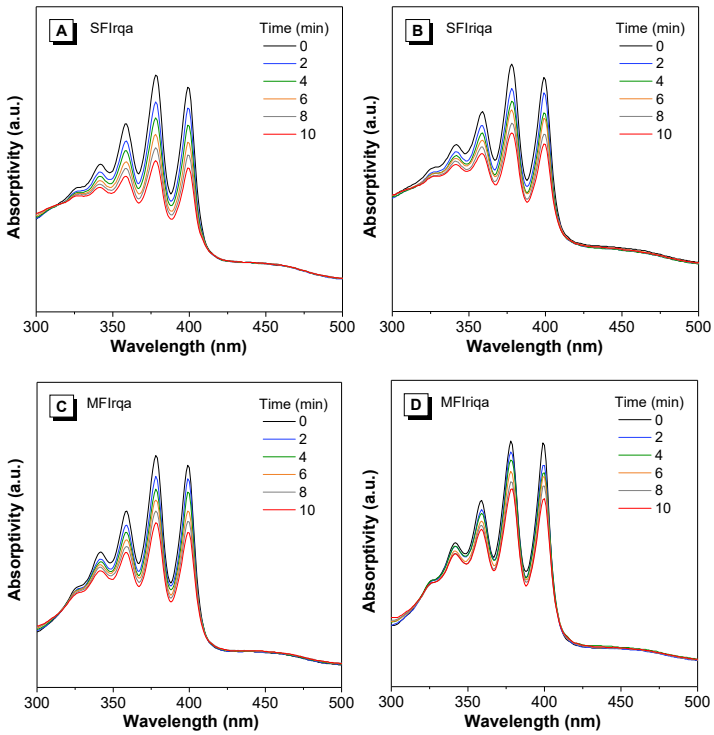



**Fig. S20** Absorption of ABDA in ultrapure water of (A) **SFIrqa**, (B) **SFIriqa**, (C) **MFIrqa** and (D) **MFIriqa** (2 μM) after exposure to white light irradiation of 30 mW $cm^{-2}$ with different time.

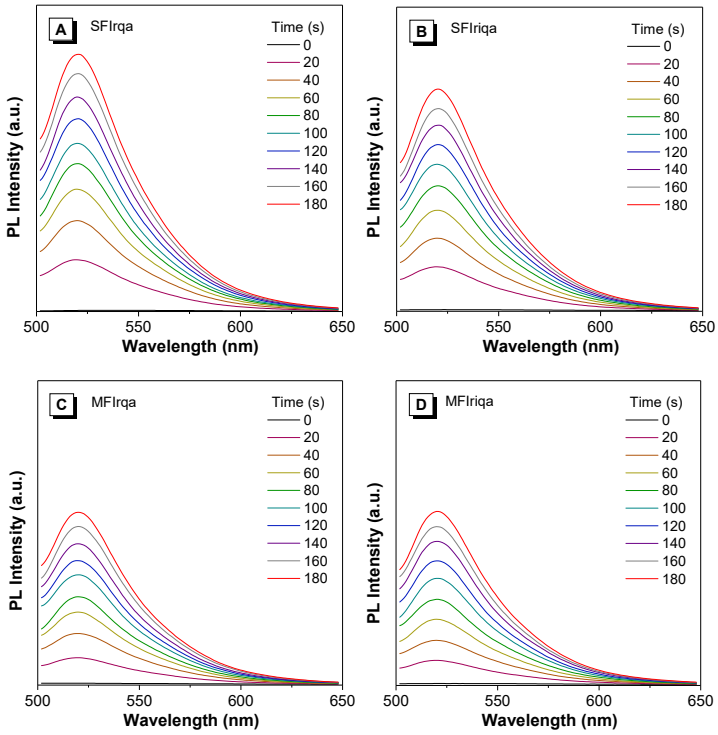



**Fig. S21** Fluorescence intensity changes of HPF for •OH detection. (A) **SFIrqa**, (B) **SFIriqa**, (C) **MFIrqa** and (D) **MFIriqa** (2 μM) after exposure to white light irradiation of 30 mW $cm^{-2}$ with different time.

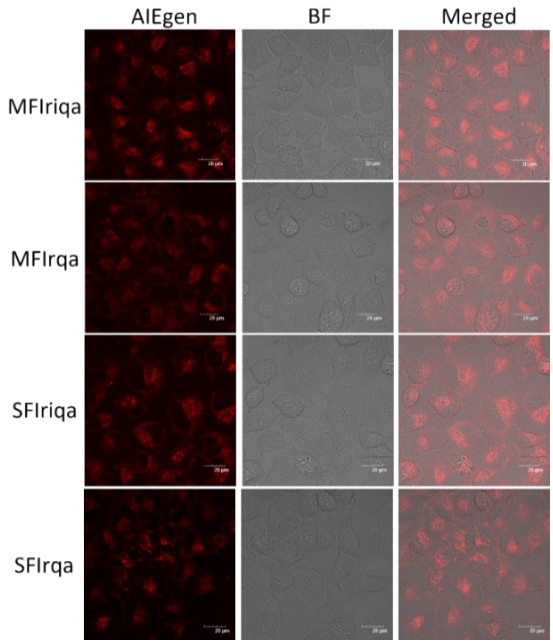



**Fig. S22** CLSM images of Hela with **MFIriqa**, **MFIrqa, SFIriqa,** and **SFIrqa** for 4 h. [AIE NPs 10μg/mL], Ex = 488 nm, Em = 650 - 750 nm.

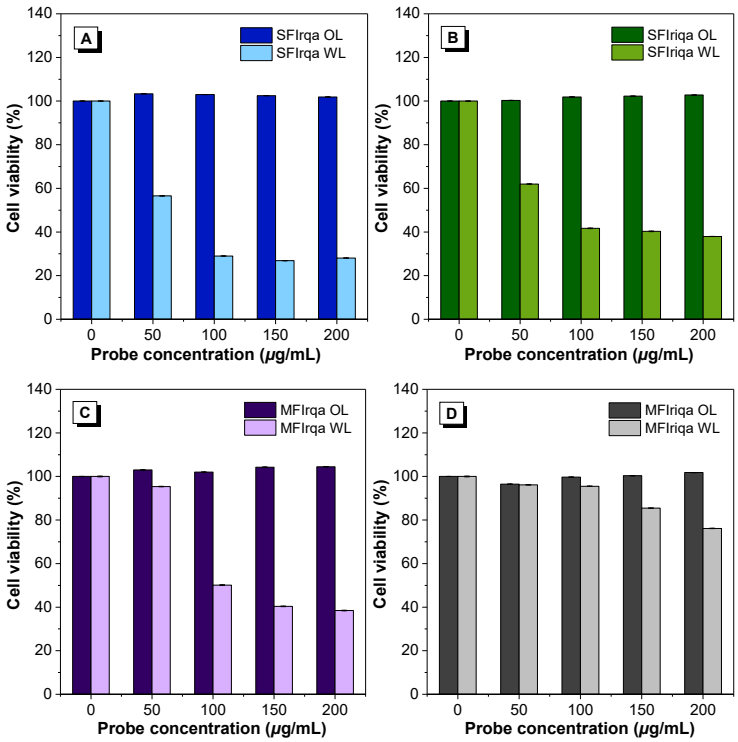



**Fig. S23** Viability of Hela cancer cells after treatment with a range of concentration with white light and without irradiation of 30 mW $cm^{-2}$ for 30 min for (A) **SFIrqa**, (B) **SFIriqa**, (C) **MFIrqa** and (D) **MFIriqa** for 4 h. The data were presented as mean ± SD (n = 3).

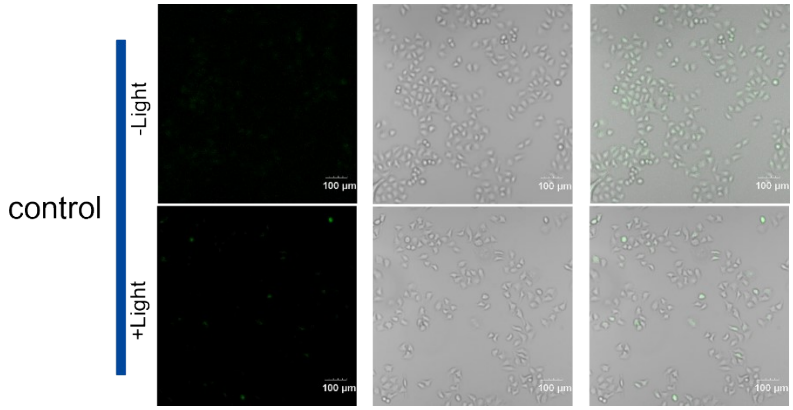



**Fig. S24** Intracellular ROS detection by CLSM after Hela cancer cells were incubated with DCFH-DA under white light irradiations (30 mW $cm^{-2}$, 10 min), Scale bar = 100 μm.

**List of acronyms**

CLSM = Confocal Laser Scanning Microscopy.

CCK-8 = Cell Counting Kit-8.

QY = Fluorescence quantum yield.

ROS = Reactive oxygen species.

PDT = Photodynamic therapy.

AIE = Aggregation-induced emission.

ACQ = Aggregation-caused quenching.

**Cartesian coordinates of optimized $T_1$ structures**

**MFIriqa** in $T_1$ state

| | | | |
|---|---|---|---|
| Ir | 0.14326000 | -0.58249500 | -0.73352000 |
| N | 1.75820200 | -2.04521600 | -1.03472100 |
| O | 0.49383400 | -2.63947800 | -4.33627400 |
| O | -0.22685300 | -1.40175100 | -2.62560100 |

| | | | |
|---|---|---|---|
| N | -1.28994100 | -1.90012400 | -0.01293400 |
| N | 1.49982800 | 0.84700000 | -1.34623800 |
| C | -1.48033600 | 0.61431600 | -0.75306300 |
| N | -3.41718300 | -2.34175800 | 0.48721100 |
| C | 0.85468800 | 0.00680900 | 1.05862400 |
| N | 3.12235700 | 2.29437900 | -0.87103000 |
| C | 1.74637700 | -2.65702600 | -2.28530300 |
| C | 2.75915000 | -3.62789000 | -2.63945200 |
| C | 3.78412600 | -3.92936800 | -1.67479900 |
| C | 3.74237400 | -3.24633600 | -0.41063800 |
| H | 4.49725800 | -3.44666900 | 0.34330800 |
| C | 2.73906900 | -2.34055200 | -0.15548100 |
| H | 2.69038500 | -1.82656800 | 0.79875000 |
| C | 4.78168500 | -4.87162200 | -1.98468100 |
| H | 5.54595800 | -5.08364800 | -1.24001200 |
| C | 4.80178600 | -5.52534900 | -3.21788100 |
| H | 5.58093800 | -6.24987600 | -3.44001800 |
| C | 3.80977100 | -5.23640100 | -4.16091500 |
| H | 3.81521800 | -5.73857800 | -5.12554100 |
| C | 2.80764300 | -4.30631800 | -3.88319900 |
| H | 2.04257600 | -4.07977600 | -4.61355100 |
| C | 0.64893400 | -2.24895200 | -3.16539300 |
| C | -2.71336000 | -0.01441500 | -0.36413800 |
| C | -3.93548500 | 0.67755700 | -0.38538000 |
| H | -4.85847500 | 0.18960100 | -0.09755900 |
| C | -3.94362400 | 2.00549600 | -0.78839300 |
| C | -5.13329300 | 2.95638800 | -0.88970600 |
| C | -4.44643900 | 4.23197900 | -1.37810700 |
| C | -5.01084200 | 5.47391100 | -1.65422600 |
| H | -6.07795700 | 5.64137000 | -1.53336100 |
| C | -4.18277200 | 6.51495900 | -2.09320700 |
| H | -4.61334900 | 7.48827000 | -2.31169700 |
| C | -2.80564700 | 6.31453900 | -2.25397700 |
| H | -2.17908400 | 7.13342800 | -2.59621800 |
| C | -2.23214300 | 5.07113800 | -1.97835700 |
| H | -1.16396100 | 4.91651700 | -2.10369500 |
| C | -3.05928600 | 4.03239900 | -1.53959600 |
| C | -2.74289200 | 2.64714500 | -1.17316000 |
| C | -1.53011700 | 1.95914900 | -1.16211100 |
| H | -0.62271600 | 2.46090100 | -1.48191000 |
| C | -6.17609800 | 2.44534800 | -1.90962400 |
| H | -5.72627400 | 2.28736400 | -2.89457600 |
| H | -6.99160500 | 3.16833500 | -2.01793400 |
| H | -6.60900200 | 1.49678500 | -1.57445300 |

| | | | |
|---|---|---|---|
| C | -5.80500300 | 3.16517300 | 0.48641500 |
| H | -6.23791400 | 2.22734100 | 0.85038100 |
| H | -6.61161100 | 3.90203600 | 0.41100200 |
| H | -5.08570300 | 3.52229100 | 1.22995400 |
| C | -2.53217000 | -1.39727500 | 0.03782600 |
| C | -1.34759000 | -3.21919000 | 0.40319000 |
| C | -0.35795000 | -4.20106000 | 0.55177300 |
| H | 0.67576400 | -3.99120700 | 0.30873200 |
| C | -0.75803300 | -5.44931100 | 1.01678100 |
| H | -0.01446700 | -6.23130400 | 1.13765200 |
| C | -2.10458900 | -5.72702500 | 1.33232200 |
| H | -2.37411500 | -6.71617100 | 1.68995900 |
| C | -3.09677400 | -4.76068500 | 1.19359800 |
| H | -4.13391400 | -4.96696900 | 1.43473900 |
| C | -2.69249400 | -3.50892700 | 0.72593400 |
| C | -4.83048100 | -2.20541300 | 0.72057100 |
| C | -5.27900000 | -1.74017800 | 1.95961100 |
| H | -4.55985700 | -1.47270100 | 2.72747000 |
| C | -6.65120600 | -1.61882500 | 2.18512700 |
| H | -7.00771900 | -1.25447000 | 3.14381800 |
| C | -7.56056000 | -1.96857900 | 1.18297500 |
| H | -8.62739500 | -1.87403400 | 1.36305100 |
| C | -7.10073600 | -2.44318800 | -0.04839300 |
| H | -7.80616700 | -2.71871800 | -0.82633600 |
| C | -5.73032700 | -2.56629100 | -0.28532800 |
| H | -5.35648800 | -2.92967800 | -1.23737300 |
| C | 1.88183400 | 1.01475300 | 1.00132800 |
| C | 2.46556400 | 1.53721900 | 2.16722000 |
| H | 3.22353200 | 2.30914200 | 2.11243200 |
| C | 2.05864100 | 1.04277400 | 3.39884400 |
| C | 2.55841200 | 1.43254300 | 4.78740400 |
| C | 1.71777600 | 0.50982800 | 5.67016300 |
| C | 0.86038200 | -0.29587700 | 4.89187100 |
| C | 0.00129700 | -1.21939300 | 5.49580400 |
| H | -0.65802700 | -1.84118200 | 4.89638100 |
| C | 0.00699200 | -1.32973100 | 6.88816200 |
| H | -0.65267300 | -2.04236400 | 7.37527000 |
| C | 0.85672100 | -0.52930600 | 7.66275200 |
| H | 0.84842200 | -0.62737500 | 8.74478200 |
| C | 1.71696200 | 0.39542900 | 7.05720400 |
| H | 2.37233000 | 1.01065500 | 7.66821700 |
| C | 1.07061900 | 0.03309800 | 3.47767900 |
| C | 0.47912800 | -0.47951400 | 2.32292200 |
| H | -0.27286500 | -1.25817400 | 2.39954300 |

| | | | |
|---|---|---|---|
| C | 2.27946100 | 2.92138000 | 5.09380300 |
| H | 2.84531000 | 3.56722600 | 4.41415100 |
| H | 2.58311900 | 3.16283900 | 6.11783400 |
| H | 1.21657900 | 3.15958900 | 4.98839000 |
| C | 4.06936300 | 1.14393200 | 4.93980300 |
| H | 4.29884700 | 0.09510400 | 4.72810300 |
| H | 4.39965100 | 1.36768000 | 5.95962500 |
| H | 4.65169900 | 1.76728700 | 4.25280100 |
| C | 2.20348600 | 1.41535300 | -0.35844300 |
| C | 2.98425000 | 2.27606300 | -2.26044300 |
| C | 3.65451400 | 2.97653300 | -3.26527500 |
| H | 4.44529600 | 3.68196400 | -3.03444400 |
| C | 3.25537600 | 2.72450100 | -4.57529800 |
| H | 3.75046900 | 3.24628700 | -5.38864800 |
| C | 2.22541100 | 1.80599300 | -4.87154200 |
| H | 1.94797700 | 1.63997800 | -5.90807500 |
| C | 1.55979900 | 1.10687000 | -3.87037700 |
| H | 0.77255300 | 0.39380600 | -4.08566200 |
| C | 1.95554900 | 1.35213500 | -2.54873000 |
| C | 4.09855000 | 3.07949200 | -0.16357600 |
| C | 3.81562000 | 4.41350500 | 0.14047200 |
| H | 2.85783800 | 4.83905800 | -0.14195300 |
| C | 4.77212100 | 5.17626700 | 0.81314800 |
| H | 4.55885400 | 6.21294400 | 1.05538900 |
| C | 5.99642700 | 4.60702000 | 1.17337100 |
| H | 6.73749500 | 5.20324700 | 1.69758200 |
| C | 6.27148600 | 3.27351600 | 0.85752200 |
| H | 7.22465400 | 2.83215300 | 1.13231100 |
| C | 5.32388300 | 2.50302500 | 0.18160500 |
| H | 5.52298600 | 1.46703000 | -0.07435100 |

**MFIrqa** in $T_1$ state

| | | | |
|---|---|---|---|
| Ir | 0.01823400 | -0.61167800 | -0.96354800 |
| O | -0.80994300 | -0.90312600 | -2.96400000 |
| O | -0.74484800 | -2.11008900 | -4.85462300 |
| N | 3.33364200 | 1.91191700 | -0.95991100 |
| N | -1.54835700 | -1.82913400 | -0.33206500 |
| N | 1.35999900 | -2.27101600 | -1.99291000 |
| N | 1.49121000 | 0.70685800 | -1.49746200 |
| N | -3.70873100 | -2.06718300 | 0.16732800 |
| C | 0.91742100 | -0.92070000 | 4.61144700 |
| C | 1.86989400 | -0.27532000 | 5.45019700 |
| C | -5.09665500 | -1.79194700 | 0.42496200 |
| C | 2.33288600 | 1.07079600 | -0.45895600 |

| | | | |
|---|---|---|---|
| C | 3.09145900 | 2.08401800 | -2.32031100 |
| C | 3.78289200 | 2.80166900 | -3.29317400 |
| C | 2.10051200 | 2.05539900 | -4.90994500 |
| C | 2.01920000 | 0.61597800 | 0.82065500 |
| C | 2.50127000 | -2.89838300 | -1.54315700 |
| C | 2.68432500 | 0.96636600 | 2.04990400 |
| C | -1.48589300 | -5.54299800 | 0.03542000 |
| C | 1.41306400 | 1.32491000 | -3.94482500 |
| C | -2.70433000 | -1.18108300 | -0.13375900 |
| C | -3.78615300 | 1.12051100 | -0.02364000 |
| C | -2.68525800 | 0.26695200 | -0.23695200 |
| C | -1.38946000 | 0.77762400 | -0.56568600 |
| C | -1.23485900 | 2.16709000 | -0.65298300 |
| C | -2.32760500 | 3.01086000 | -0.43385800 |
| C | -3.60263000 | 2.48958200 | -0.12687000 |
| C | 3.26897900 | 2.77560200 | -4.59450700 |
| C | 1.92424800 | 1.32817500 | -2.63390400 |
| C | -2.85370200 | -5.69705000 | 0.33841800 |
| C | 0.94660500 | -2.50466500 | -3.23729400 |
| C | 1.62905400 | -3.36653800 | -4.12687400 |
| C | -0.30818400 | -1.79936700 | -3.74112200 |
| C | 1.12654000 | -0.50958000 | 3.24969900 |
| C | 2.78232600 | -3.98460600 | -3.71689500 |
| C | 0.84459300 | -0.31240700 | 0.83532000 |
| C | -3.71048000 | -4.60013800 | 0.40948600 |
| C | 2.94201100 | -2.71054400 | -0.20858200 |
| C | -0.01157800 | -2.02503800 | 6.55035900 |
| C | 4.08663900 | -3.33244200 | 0.24471600 |
| C | 0.93083600 | -1.38824200 | 7.37220600 |
| C | 2.24324800 | 0.41319800 | 3.21833500 |
| C | -3.14955200 | -3.34646800 | 0.16308500 |
| C | -0.02988400 | -1.80162000 | 5.17486200 |
| C | -0.93105800 | -4.29045800 | -0.21281700 |
| C | 4.84508500 | -4.17041800 | -0.60735200 |
| C | -1.78291700 | -3.18087300 | -0.15273900 |
| C | 2.78490200 | 0.63825800 | 4.63097700 |
| C | -5.53269700 | -1.62928500 | 1.74274000 |
| C | -5.99227200 | -1.71840900 | -0.64531300 |
| C | 0.44419200 | -0.83491900 | 2.05710600 |
| C | 1.87696100 | -0.50749000 | 6.81671300 |
| C | -6.88325800 | -1.37469900 | 1.98780700 |
| C | 3.25579500 | -3.76631800 | -2.39970000 |
| C | 4.43346500 | -4.38472200 | -1.90370900 |
| C | -7.78519600 | -1.28827900 | 0.92384800 |

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|---|---|---|---|
| C | -7.34037600 | -1.46178600 | -0.38974400 |
| C | -4.12029000 | 6.18558000 | -0.15102700 |
| C | -3.75686000 | 4.84249600 | -0.18324000 |
| C | -2.42368400 | 4.47510900 | -0.46447700 |
| C | -1.45012200 | 5.44909000 | -0.70730200 |
| C | -1.82200600 | 6.79545200 | -0.67115100 |
| C | -3.14556500 | 7.16178700 | -0.39655600 |
| C | -4.62672400 | 3.60858100 | 0.05920900 |
| C | 6.86317200 | 3.18257300 | 0.97388400 |
| C | 5.94887500 | 4.12396800 | 0.49446400 |
| C | 4.77399600 | 3.70691600 | -0.13412300 |
| C | 4.52341000 | 2.33925800 | -0.29153500 |
| C | 5.44219800 | 1.39069400 | 0.17501100 |
| C | 6.60606700 | 1.81759800 | 0.81523200 |
| H | 0.12140400 | -4.17005500 | -0.43882700 |
| H | -0.85007400 | -6.42243300 | -0.00416000 |
| H | -3.24894000 | -6.69123600 | 0.52385000 |
| H | -4.76246800 | -4.71354500 | 0.64810200 |
| H | -5.63037100 | -1.85396000 | -1.65970800 |
| H | -8.04134400 | -1.39904000 | -1.21663200 |
| H | -8.83481200 | -1.08838100 | 1.11844900 |
| H | -7.22826100 | -1.24325000 | 3.00895300 |
| H | -4.81863300 | -1.69424100 | 2.55776900 |
| H | -4.76127000 | 0.71556200 | 0.21941600 |
| H | -0.26642300 | 2.59174700 | -0.89662300 |
| H | -1.07823100 | 7.56535900 | -0.85742300 |
| H | -0.42277700 | 5.16750900 | -0.92165300 |
| H | -3.41881900 | 8.21323800 | -0.37318100 |
| H | -5.14411800 | 6.48155600 | 0.06333400 |
| H | 0.51142900 | 0.77188500 | -4.17654900 |
| H | 1.72749300 | 2.07003100 | -5.92970900 |
| H | 3.78259500 | 3.32725900 | -5.37617500 |
| H | 4.67966600 | 3.36154100 | -3.05173600 |
| H | 4.04960800 | 4.43098300 | -0.49337600 |
| H | 5.24006300 | 0.33326700 | 0.03719100 |
| H | 7.31697800 | 1.08228500 | 1.18058300 |
| H | 7.77273800 | 3.51082200 | 1.46827600 |
| H | 6.14313400 | 5.18542900 | 0.61716500 |
| H | 0.92980000 | -1.57599000 | 8.44215300 |
| H | -0.76288400 | -2.30044700 | 4.54670600 |
| H | 2.60299900 | -0.01683000 | 7.46057500 |
| H | -0.73689200 | -2.70270200 | 6.99342600 |
| H | 3.50877000 | 1.66881800 | 2.04629900 |
| H | -0.40446400 | -1.51155600 | 2.09748000 |

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|---|---|---|---|
| H | 2.35330500 | -2.08226800 | 0.44644400 |
| H | 4.40700800 | -3.17953000 | 1.27119600 |
| H | 4.99724900 | -5.03348700 | -2.56819800 |
| H | 5.74572100 | -4.64740200 | -0.23242600 |
| H | 3.33615400 | -4.64251800 | -4.38125800 |
| H | 1.21138600 | -3.50072700 | -5.11667400 |
| C | 2.63222700 | 2.11586000 | 5.05592100 |
| H | 2.96121800 | 2.25456700 | 6.09170000 |
| H | 3.24118500 | 2.76618900 | 4.41855600 |
| H | 1.59069900 | 2.44388600 | 4.98230600 |
| C | 4.26529500 | 0.21248500 | 4.74070500 |
| H | 4.40138500 | -0.83391500 | 4.44965200 |
| H | 4.89523500 | 0.83151700 | 4.09253700 |
| H | 4.62397000 | 0.32791900 | 5.76942200 |
| C | -5.77085400 | 3.50867600 | -0.97403800 |
| H | -6.33428800 | 2.57987500 | -0.83355000 |
| H | -6.46890300 | 4.34538400 | -0.86097600 |
| H | -5.38507600 | 3.52202500 | -1.99822100 |
| C | -5.21296200 | 3.60532300 | 1.48883500 |
| H | -5.88698800 | 4.45668800 | 1.63263100 |
| H | -5.78664900 | 2.68925100 | 1.66677300 |
| H | -4.42196800 | 3.66389800 | 2.2429820 |

**SFIriqa** in $T_1$ state

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|---|---|---|---|
| Ir | 0.06676200 | 1.61385700 | 0.18357900 |
| O | -0.87611800 | 3.34985000 | 0.87259600 |
| O | -0.71169700 | 5.49723800 | 1.45393700 |
| N | 1.13523500 | 1.20569200 | 1.90207000 |
| N | 2.79085900 | 0.13407400 | 2.93389300 |
| N | -2.92199800 | 1.48170000 | -2.69768500 |
| N | 1.53484200 | 3.21784700 | -0.16410100 |
| N | -1.04650600 | 1.84974700 | -1.55005600 |
| C | 1.29639500 | 0.17384000 | -0.50966300 |
| C | 2.26502300 | -1.33515000 | -2.14632800 |
| C | 3.16896100 | -1.83023800 | -1.17904600 |
| C | 4.07086600 | -2.91036600 | -1.78207300 |
| C | -3.88682200 | -1.04305500 | 0.98151700 |
| C | 3.31843100 | 5.41765300 | -0.36775800 |
| C | -2.87682800 | -1.03920400 | 1.97094000 |
| C | -1.50289500 | 0.42167700 | 0.60160700 |
| C | 2.02622900 | 5.60021100 | 0.23971300 |
| C | 1.34555000 | -0.34020900 | -1.81668000 |
| H | 0.66814000 | 0.04121900 | -2.57351500 |
| C | 1.14055100 | 4.45927700 | 0.32825500 |

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|---|---|---|---|
| C | 3.91591500 | -0.71997800 | 3.21069100 |
| C | -2.13407900 | 2.33694100 | -3.46753600 |
| C | -1.69938400 | -0.31786500 | 1.78148900 |
| H | -0.93785300 | -0.31532100 | 2.55441100 |
| C | 2.22390600 | 1.00507600 | 3.86567000 |
| C | 5.56831900 | -2.58906100 | -1.69017300 |
| C | 4.00428700 | -4.25320400 | -1.04430900 |
| C | 5.28615100 | -4.64505500 | -0.60934800 |
| C | 5.46117700 | -5.84615500 | 0.08334500 |
| H | 6.44716000 | -6.15612900 | 0.41844300 |
| C | 4.34280600 | -6.64411200 | 0.34057100 |
| H | 4.46282000 | -7.58011300 | 0.87893300 |
| C | 3.06971600 | -6.25022500 | -0.08973400 |
| H | 2.21086100 | -6.88196100 | 0.11854800 |
| C | 2.89265100 | -5.04871900 | -0.78689300 |
| H | 1.90315600 | -4.74886500 | -1.12089900 |
| C | -0.95142000 | 2.56681000 | -2.72982800 |
| C | -3.73260200 | -0.32517400 | -0.19610200 |
| H | -4.51443600 | -0.33036600 | -0.94530300 |
| C | 2.23943300 | -0.33462800 | 0.45262300 |
| C | 2.10077900 | 0.28828200 | 1.75956100 |
| C | -6.40574600 | -1.15098400 | 1.45480900 |
| C | 3.16434000 | -1.33685500 | 0.11858500 |
| H | 3.86310100 | -1.72101200 | 0.85153000 |
| C | -2.54920500 | 0.40614900 | -0.38473800 |
| C | 1.17861800 | 1.68140600 | 3.19892800 |
| C | -5.07201900 | -1.90755900 | 1.41821800 |
| C | 1.69922800 | 6.89642400 | 0.71092100 |
| H | 0.72999000 | 7.03826100 | 1.16963800 |
| C | 2.50233900 | -2.04028100 | -3.41070400 |
| C | -2.22845600 | 1.21490300 | -1.54696100 |
| C | 3.54595600 | -2.96766400 | -3.22162500 |
| C | 6.25497200 | -3.61582600 | -1.01230300 |
| C | -0.19555900 | 4.49563600 | 0.92699500 |
| C | -4.23373200 | 1.03243900 | -3.08449100 |
| C | -4.36871800 | -0.14848900 | -3.81881300 |
| H | -3.48773900 | -0.73157700 | -4.06820100 |
| C | -5.64213600 | -0.56188300 | -4.21388700 |
| H | -5.75701400 | -1.48106200 | -4.78017600 |
| C | -6.76274200 | 0.20424700 | -3.88191200 |
| H | -7.75171400 | -0.12072100 | -4.19140500 |
| C | -6.61442200 | 1.38892400 | -3.15581900 |
| H | -7.48445300 | 1.98600700 | -2.90037100 |
| C | -5.34597900 | 1.81099400 | -2.75459800 |

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|---|---|---|---|
| H | -5.21212100 | 2.72773100 | -2.18911100 |
| C | 0.05570000 | 3.39430600 | -3.24516600 |
| H | 0.96489900 | 3.57711600 | -2.68693400 |
| C | -2.69405800 | -2.18412200 | 4.30370300 |
| H | -1.71228800 | -1.78401300 | 4.54044800 |
| C | -5.39753000 | -3.04638300 | 0.44332200 |
| C | -4.59696400 | -2.39177900 | 2.79310600 |
| C | -3.32128700 | -1.87371200 | 3.09308200 |
| C | -7.35563700 | -1.77858000 | 0.62444100 |
| C | -2.35759900 | 2.91392800 | -4.71913500 |
| H | -3.27274000 | 2.73105900 | -5.27171700 |
| C | 4.79478600 | -2.81623600 | 4.00752800 |
| H | 4.63400200 | -3.81721500 | 4.39609900 |
| C | 2.52939400 | 1.24895900 | 5.20618300 |
| H | 3.33550400 | 0.72595200 | 5.70883500 |
| C | 3.65977600 | 4.10556600 | -0.84553900 |
| H | 4.62491800 | 3.92772600 | -1.30955400 |
| C | 2.59795900 | 7.95688600 | 0.59310900 |
| H | 2.31283400 | 8.93791100 | 0.96598400 |
| C | -6.73124300 | -2.95271900 | -0.00185600 |
| C | 4.20337000 | 6.50643400 | -0.47119300 |
| H | 5.17556600 | 6.34412200 | -0.93167500 |
| C | 5.20948300 | -0.23294500 | 3.00638900 |
| H | 5.35146600 | 0.77139600 | 2.61993300 |
| C | -0.16436200 | 3.97042000 | -4.49164600 |
| H | 0.59521300 | 4.61999000 | -4.91596800 |
| C | 1.87645600 | -1.91674500 | -4.65496600 |
| H | 1.07224200 | -1.20173000 | -4.80381600 |
| C | 3.97105700 | -3.77766700 | -4.26971600 |
| H | 4.77514700 | -4.49446000 | -4.12916100 |
| C | 3.69746900 | -2.00411500 | 3.71614300 |
| H | 2.68277400 | -2.35679200 | 3.87168600 |
| C | 7.63722500 | -3.53627400 | -0.82251900 |
| H | 8.17273400 | -4.32499100 | -0.30136400 |
| C | -3.35518600 | -3.01917200 | 5.20683100 |
| H | -2.88319900 | -3.27017100 | 6.15242500 |
| C | 2.75827100 | 3.07459400 | -0.71643400 |
| H | 3.00282400 | 2.08047400 | -1.07635500 |
| C | 0.39579200 | 2.63095800 | 3.86950300 |
| H | -0.40253200 | 3.15163800 | 3.35384100 |
| C | -6.73406300 | -0.00478400 | 2.17111100 |
| H | -6.00249700 | 0.48164800 | 2.81031100 |
| C | 2.30576800 | -2.73097100 | -5.70509000 |
| H | 1.83130600 | -2.64868900 | -6.67879000 |

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|---|---|---|---|
| C | -4.57147200 | -4.07496000 | 0.00229700 |
| H | -3.54352600 | -4.15018900 | 0.34604700 |
| C | 6.09284900 | -2.34266100 | 3.79927600 |
| H | 6.94401600 | -2.97744600 | 4.02723900 |
| C | 6.25135900 | -1.47991300 | -2.17843400 |
| H | 5.72555500 | -0.68545200 | -2.70059300 |
| C | -8.02937100 | 0.51432500 | 2.05570000 |
| H | -8.30049800 | 1.40841300 | 2.60981400 |
| C | 3.34270200 | -3.65400000 | -5.51449100 |
| H | 3.66350600 | -4.28035700 | -6.34201800 |
| C | 7.63613800 | -1.40166000 | -1.98600100 |
| H | 8.18265600 | -0.54142600 | -2.36191800 |
| C | -5.25193100 | -3.22509900 | 3.69413700 |
| H | -6.23444300 | -3.62877300 | 3.46665800 |
| C | -8.64816500 | -1.25892700 | 0.51140700 |
| H | -9.38625500 | -1.73831800 | -0.12575600 |
| C | 3.85260800 | 7.77165600 | 0.00256100 |
| H | 4.54939200 | 8.60114000 | -0.08600700 |
| C | -8.97670800 | -0.10838500 | 1.23363900 |
| H | -9.97742800 | 0.30749900 | 1.15656700 |
| C | 6.29939800 | -1.05341100 | 3.30127000 |
| H | 7.30791900 | -0.68429600 | 3.14207500 |
| C | -7.24585500 | -3.89646900 | -0.89511800 |
| H | -8.27373200 | -3.83151000 | -1.24114400 |
| C | -1.35088200 | 3.73555200 | -5.21789700 |
| H | -1.48311200 | 4.20792300 | -6.18661000 |
| C | 8.32173800 | -2.42187600 | -1.31517300 |
| H | 9.39644800 | -2.34589900 | -1.17547300 |
| C | 1.74803500 | 2.19617000 | 5.86234300 |
| H | 1.95213800 | 2.41967900 | 6.90510300 |
| C | -4.62207400 | -3.53599300 | 4.90499600 |
| H | -5.12184200 | -4.18475600 | 5.61873600 |
| C | 0.69932500 | 2.87432700 | 5.20452700 |
| H | 0.11718200 | 3.60698900 | 5.75521300 |
| C | -5.08888400 | -5.01887600 | -0.89334900 |
| H | -4.45615000 | -5.82862600 | -1.24573600 |
| C | -6.41409600 | -4.92925000 | -1.33681700 |
| H | -6.79994600 | -5.67085500 | -2.03076100 |

**SFIrqa** in $T_1$ state

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|---|---|---|---|
| Ir | -0.08603400 | -1.91953600 | 0.33252800 |
| O | 1.05642200 | -3.50382400 | 1.30884400 |
| O | 1.16504000 | -5.69147800 | 1.79681900 |
| N | -2.89393600 | -0.20401400 | 2.88469000 |

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|---|---|---|---|
| N | 1.12862500 | -2.26796400 | -1.32422900 |
| N | -1.42466800 | -3.84815400 | 0.20120800 |
| N | -1.21816500 | -1.41160300 | 1.96336700 |
| N | 3.04232300 | -1.90995200 | -2.41339900 |
| C | -2.04779800 | 1.80390300 | -3.44714900 |
| C | -3.03441700 | 2.82585800 | -3.34735000 |
| C | -4.84641000 | 5.91337100 | -0.14806400 |
| C | 4.33873200 | -1.41359500 | -2.79173000 |
| C | -2.15434300 | -0.42151500 | 1.71965600 |
| C | -2.39875700 | -1.05636500 | 3.86317300 |
| C | -2.77591100 | -1.24495100 | 5.19063200 |
| C | -0.99325000 | -2.91670100 | 5.35928400 |
| C | -2.17244700 | 0.16035100 | 0.45283200 |
| C | -2.70203700 | -4.01255300 | -0.29106300 |
| C | -3.00663400 | 1.25180000 | 0.02090500 |
| C | 0.50845000 | -4.70496600 | -4.08601300 |
| C | -0.61746300 | -2.73705400 | 4.03090200 |
| C | 2.27067200 | -1.56563000 | -1.33177700 |
| C | 3.59704700 | 0.23279800 | -0.11226900 |
| C | 2.47558400 | -0.60715500 | -0.25981900 |
| C | 1.39280600 | -0.59004100 | 0.67529700 |
| C | 1.47971300 | 0.28724100 | 1.76356500 |
| C | 2.59456100 | 1.11568700 | 1.91156200 |
| C | 3.64802000 | 1.08983600 | 0.97467600 |
| C | -2.05691700 | -2.19028400 | 5.92983100 |
| C | -1.34022100 | -1.80191600 | 3.26757800 |
| C | 1.72120700 | -4.48478700 | -4.76921100 |
| C | -0.82535700 | -4.88372900 | 0.78740800 |
| C | -1.44038300 | -6.14789900 | 0.93753600 |
| C | 0.58375400 | -4.70132100 | 1.34008700 |
| C | -1.92989000 | 1.12299000 | -2.19001000 |
| C | -2.71915600 | -6.33509400 | 0.48016900 |
| C | -1.17886900 | -0.45345500 | -0.48645500 |
| C | 2.66038600 | -3.56736200 | -4.30286300 |
| C | -3.35447600 | -2.94802400 | -0.96310900 |
| C | -1.68510300 | 2.42417900 | -5.75528200 |
| C | -4.63436600 | -3.10784400 | -1.45105000 |
| C | -2.65890600 | 3.43080200 | -5.64610400 |
| C | -2.87657700 | 1.70719600 | -1.25807100 |
| C | 2.34316000 | -2.88280800 | -3.12909600 |
| C | -1.36980200 | 1.60969800 | -4.67093600 |
| C | 0.19678800 | -4.02058200 | -2.91442900 |
| C | 8.40526500 | 1.66043900 | 0.67580900 |
| C | 8.79101300 | 0.62010600 | 1.52574700 |

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|---|---|---|---|
| C | 7.85809700 | 0.00618200 | 2.37051000 |
| C | 6.52123100 | 0.42296200 | 2.37993800 |
| C | 6.13420000 | 1.45722600 | 1.53390600 |
| C | 7.07121200 | 2.07698000 | 0.68336900 |
| C | -5.32482500 | -4.33337600 | -1.29591800 |
| C | 1.13559600 | -3.10088900 | -2.42989000 |
| C | -3.64196700 | 2.85106400 | -1.93872900 |
| C | 4.42956800 | -0.37113800 | -3.71797800 |
| C | -3.49015100 | 4.19487400 | -1.21767100 |
| C | -4.74834600 | 4.69481100 | -0.82536000 |
| C | -3.67589900 | 6.62350800 | 0.13289500 |
| C | -2.42691100 | 6.12522100 | -0.25859700 |
| C | -2.32668800 | 4.90424100 | -0.93664000 |
| C | 5.48653300 | -2.00740400 | -2.25992800 |
| C | -1.09593000 | 0.06202400 | -1.77115800 |
| C | -3.33857700 | 3.63201200 | -4.43244200 |
| C | 5.68887200 | 0.09113600 | -4.10388600 |
| C | -3.39244300 | -5.26238300 | -0.15427100 |
| C | -4.71137800 | -5.39107400 | -0.66301500 |
| C | 6.84271400 | -0.48778200 | -3.56910700 |
| C | 6.74093800 | -1.53573700 | -2.65032300 |
| C | 4.72394400 | 3.63214400 | 3.50061300 |
| C | 4.17193200 | 2.67117300 | 2.65974100 |
| C | 2.92011900 | 2.09502900 | 2.95485200 |
| C | 2.21234200 | 2.48013700 | 4.09746200 |
| C | 2.76925300 | 3.44556300 | 4.93954800 |
| C | 4.01386700 | 4.01662100 | 4.64474000 |
| C | 6.38664300 | 3.12619000 | -0.08630800 |
| C | 5.02929000 | 3.14882800 | 0.29120900 |
| C | 4.14776800 | 4.05586300 | -0.28756700 |
| C | 4.63217400 | 4.94775600 | -1.25245000 |
| C | 5.98089500 | 4.92791900 | -1.62870900 |
| C | 6.86871000 | 4.01701700 | -1.04935200 |
| C | 4.74652300 | 2.08748900 | 1.36218800 |
| C | -6.21026200 | 2.34516800 | 3.43842900 |
| C | -4.95729900 | 2.71080800 | 3.93701500 |
| C | -3.85646300 | 1.87267900 | 3.75036900 |
| C | -4.01941700 | 0.66584200 | 3.06314300 |
| C | -5.27298000 | 0.28854900 | 2.57025900 |
| C | -6.36622400 | 1.13602100 | 2.75510400 |
| C | -7.93368900 | 2.73334700 | -1.63985900 |
| C | -7.17585000 | 3.78574200 | -1.11894200 |
| C | -5.78570400 | 3.74826000 | -1.25895000 |
| C | -5.16272400 | 2.66644200 | -1.91337000 |

| | | | |
|---|---|---|---|
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| H | -0.73905800 | -4.18681300 | -2.39544500 |
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| H | 7.82083700 | -0.12409500 | -3.86994100 |
| H | 5.76620800 | 0.90402300 | -4.81956800 |
| H | 3.52369400 | 0.07101100 | -4.12065400 |
| H | 4.40780800 | 0.20924300 | -0.83009300 |
| H | 0.68559300 | 0.31855700 | 2.50119800 |
| H | 2.23304700 | 3.75503900 | 5.83228800 |
| H | 1.24832700 | 2.03585300 | 4.32922600 |
| H | 4.43353500 | 4.76508400 | 5.31103400 |
| H | 5.68939700 | 4.07853000 | 3.27886200 |
| H | 3.10032900 | 4.07562400 | 0.00060900 |
| H | 3.95455000 | 5.66158500 | -1.71243300 |
| H | 6.34056200 | 5.62742900 | -2.37824800 |
| H | 7.91448200 | 4.00431900 | -1.34416800 |
| H | 9.13214400 | 2.13525700 | 0.02239000 |
| H | 9.82455400 | 0.28506000 | 1.53158100 |
| H | 8.17328900 | -0.80125000 | 3.02542100 |
| H | 5.80266600 | -0.05652800 | 3.03890300 |
| H | 0.20848000 | -3.28063300 | 3.59010800 |
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| H | -5.38125400 | -0.65453900 | 2.04365300 |
| H | -7.33929200 | 0.84914800 | 2.36773800 |
| H | -7.06385700 | 3.00121200 | 3.58178200 |
| H | -4.83283300 | 3.65025300 | 4.46726300 |
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| | | | |
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| H | -5.44383400 | 0.78803000 | -2.94210000 |
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| H | -6.33397000 | -4.43727300 | -1.68326400 |
| H | -3.22376000 | -7.29105000 | 0.59086100 |
| H | -0.86972500 | -6.92959900 | 1.42277700 |

## References

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