Supporting Information

Diiridium(III) Complexes: Luminescent Probes and Sensors for G-Quadruplex DNA and Endoplasmic Reticulum Imaging

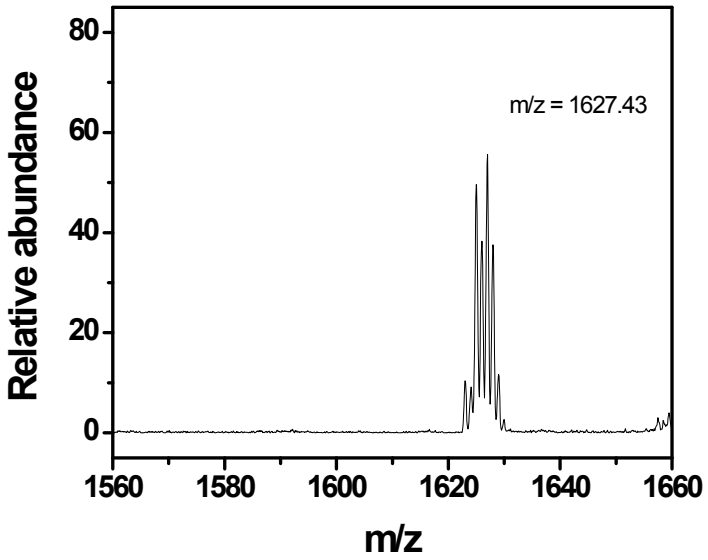
Tikum Florence Anjong, Gyungmi Kim, Ha Yoon Jang, Juyoung Yoon,* Jinheung Kim*

Department of Chemistry and Nano Science, Global Top 5 Research Program,

Ewha Womans University, Seoul 120-750, Korea

[**] This work is supported by the National Research Foundation of Korea's (NRF) grant funded by the Korean government (MEST) (NRF-2013R1A2A2A03015101). This work was also supported by a grant from the National Creative Research Initiative programs of the National Research Foundation of Korea (NRF) funded by the Korean government (MSIP) (No. 2012R1A3A2048814).

(a)



(b)

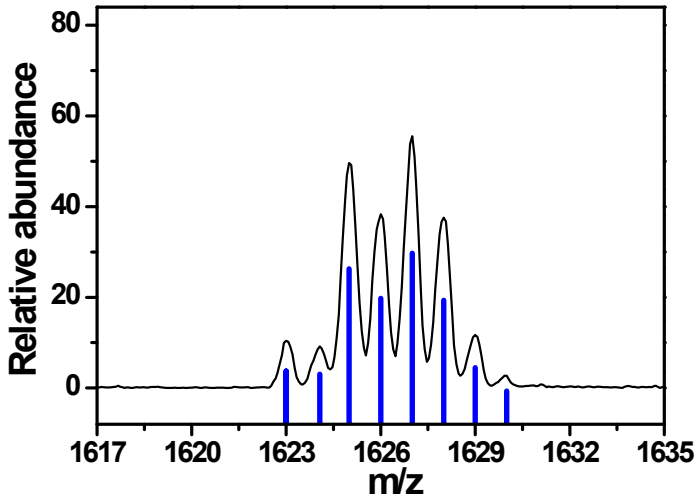


Figure S1. (a) Positive ESI-MS of **1** in acetonitrile and (b) peaks of an ion cluster of $[2Ir^{3+} + tppz + 4bhq^{-} + PF_6^{-}]^{+}$ and the calculated isotope distribution patterns.

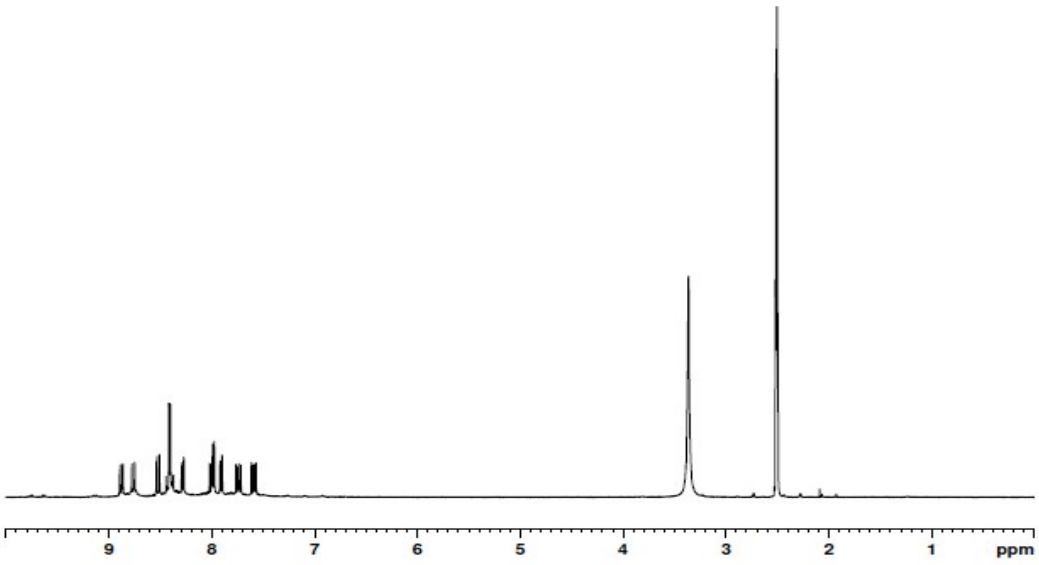
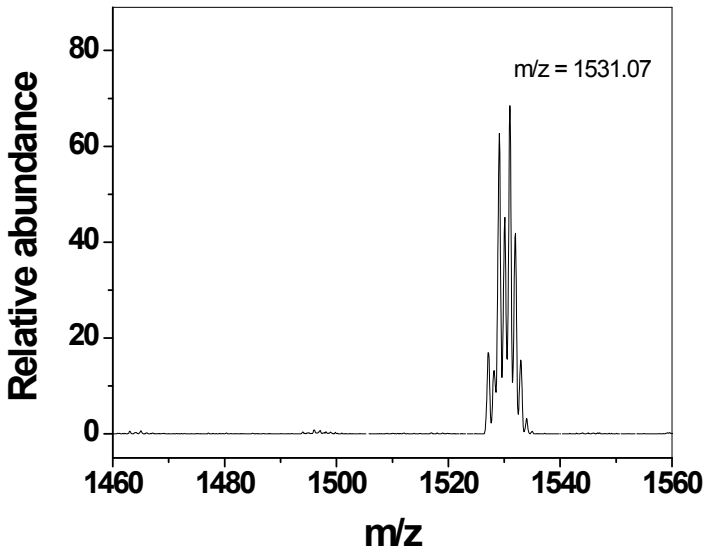


Figure S2. ^{1}H-NMR spectrum of **1** in acetonitrile-d_3.

(a)



(b)

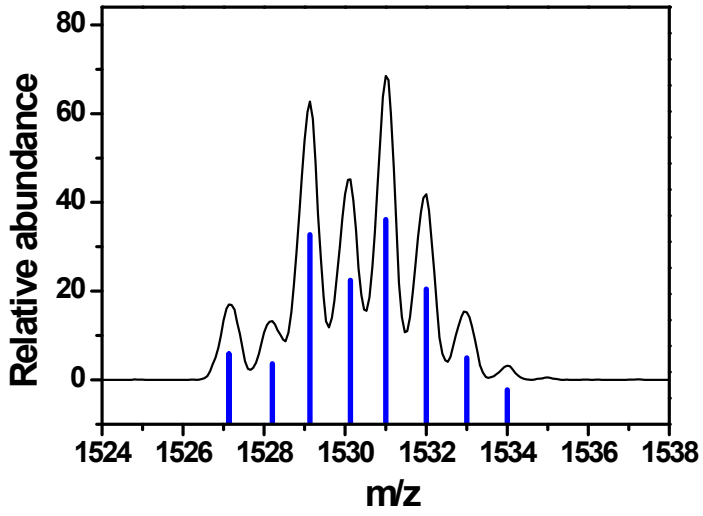


Figure S3. (a) Positive ESI-MS of **2** in acetonitrile and (b) peaks of an ion cluster of $[2Ir^{3+} + tppz + 4pph^{-} + PF_6^{-}]^{+}$ and the calculated isotope distribution patterns.

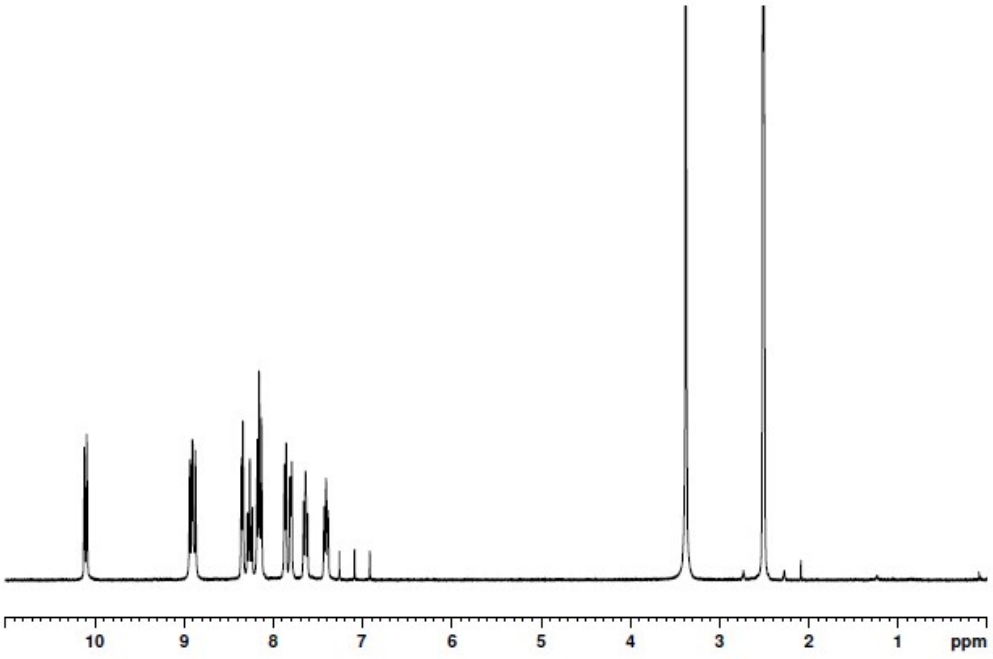
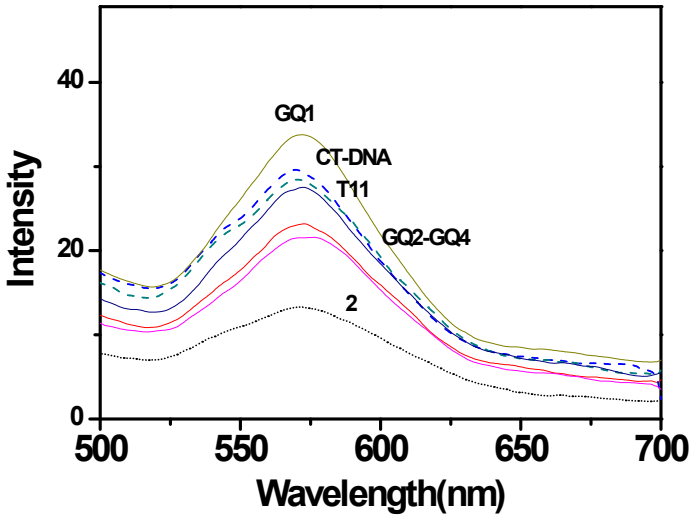


Figure S4. ^{1}H-NMR spectrum of **2** in acetonitrile-d_3.



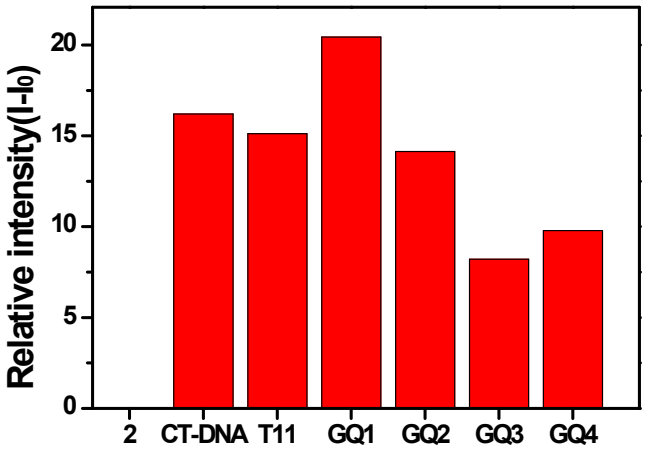
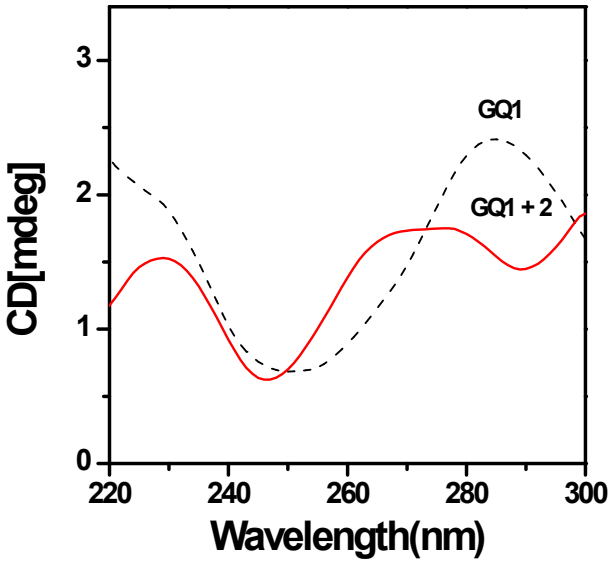
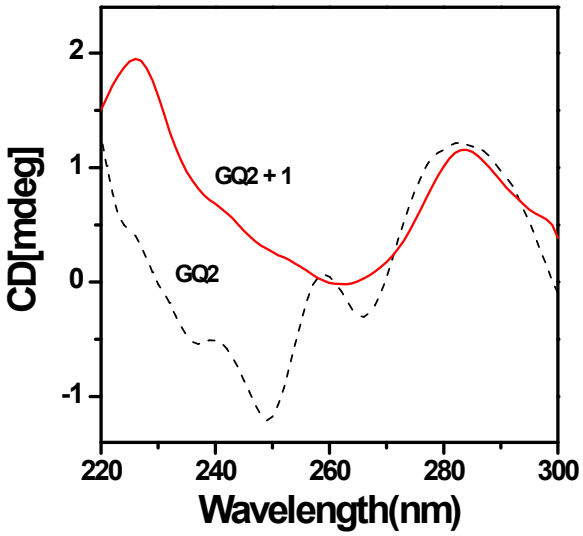
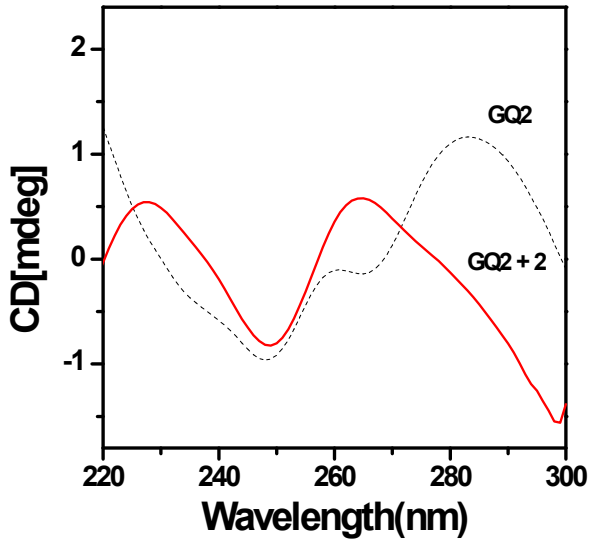
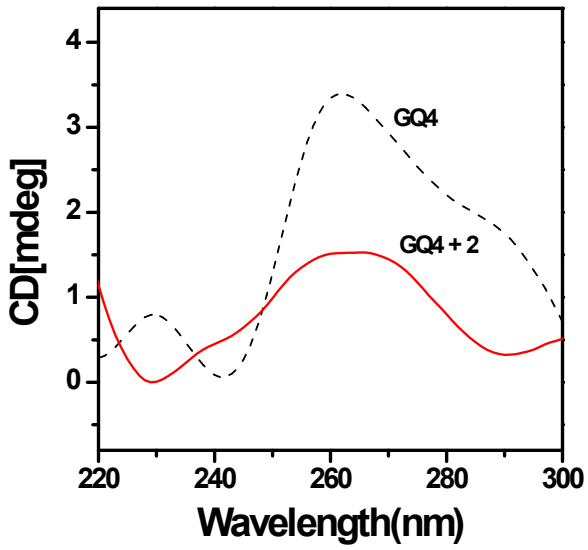


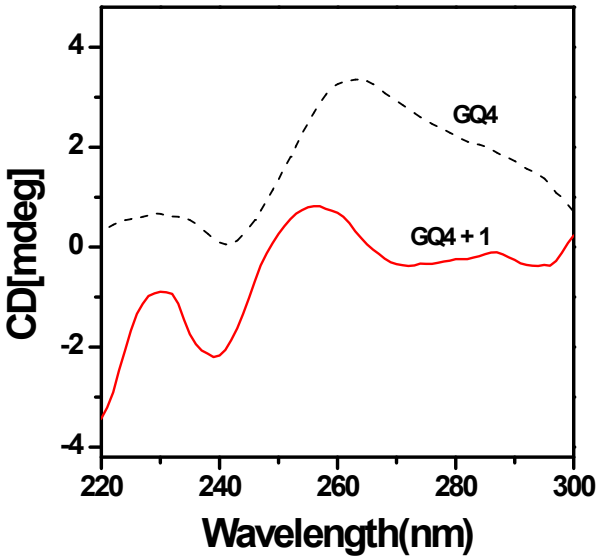
Figure S5. (a) Luminescence spectra of **2** in the presence of G1-G4, CT-DNA, and single-stranded T11 in 50 mM Na-phosphate buffer (pH = 7.4). (b) Relative intensity ($I - I_o$) plots for **2**. The concentration of each complex is 2.0 μM.


CD[mdeg]
3
2
1
0
220
240
260
280
300
Wavelength(nm)
GQ1
GQ1 + 2


CD[mdeg]
2
1
0
-1
GQ2 + 1
GQ2
220
240
260
280
300
Wavelength(nm)


CD[mdeg]
2
1
0
-1
GQ2
GQ2 + 2
220
240
260
280
300
Wavelength(nm)


CD[mdeg]
Wavelength(nm)
GQ4
GQ4 + 2
4
3
2
1
0
220
240
260
280
300


CD[mdeg]
Wavelength(nm)
GQ4
GQ4 + 1
4
2
0
-2
-4
220
240
260
280
300

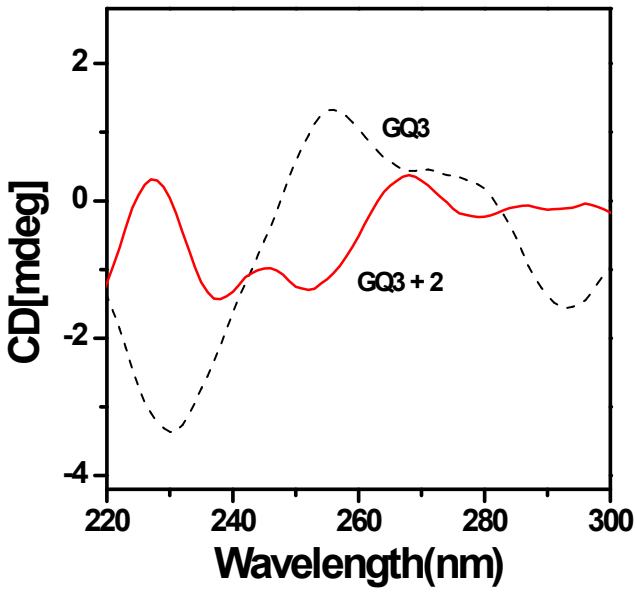


Figure S6. CD spectra of GQ1 and GQ1 + **2**, GQ2 and GQ2 + **1**, GQ2 and GQ2 + **2**, GQ3 and GQ3 + **2**, GQ4 and GQ4 + **1**, GQ4 and GQ4 + **2** at 5 μM concentration.

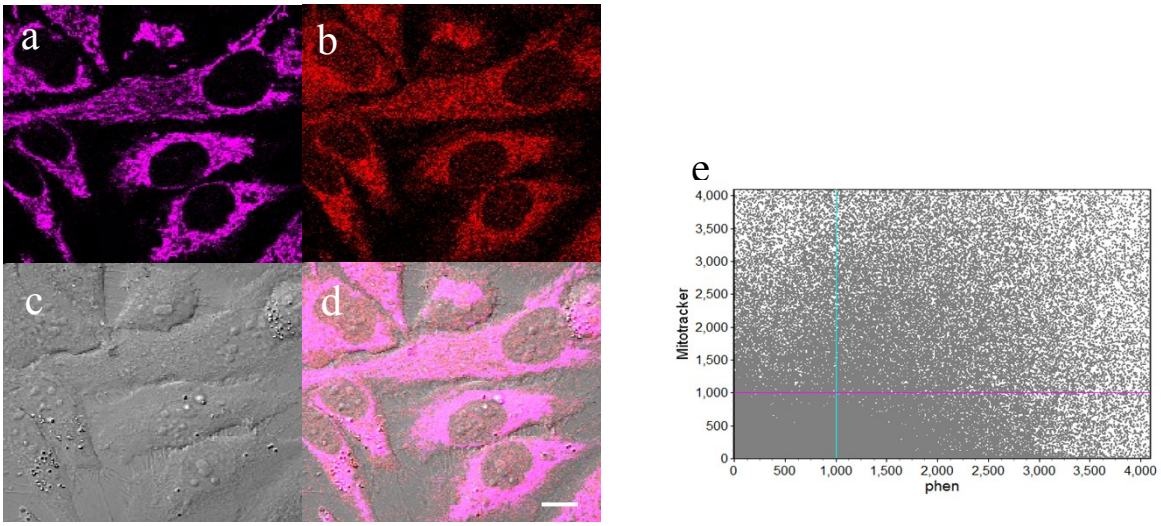


Figure S7. HeLa cells were incubated with 10 μM **1** for 1 hr at 37 ℃. After washing with the DPBS, the cells were incubated with 50 nM Mitotracker Deep Red (for mitochondria staining) in HBSS (Hank's Balanced Salt Solution with calcium and magnesium) media for 30 min at 37 ℃. After washing with DPBS, fluorescence images were acquired by confocal microscopy. (a) Mitotracker: ex. 635 nm/em. 655-755 nm, (b) **1**: ex. 405 nm/em. 490-590 nm, (c) DIC, (d) merge, (e) Co-localization analysis of Mitotracker and **1**. Scale bar: 10 μm.

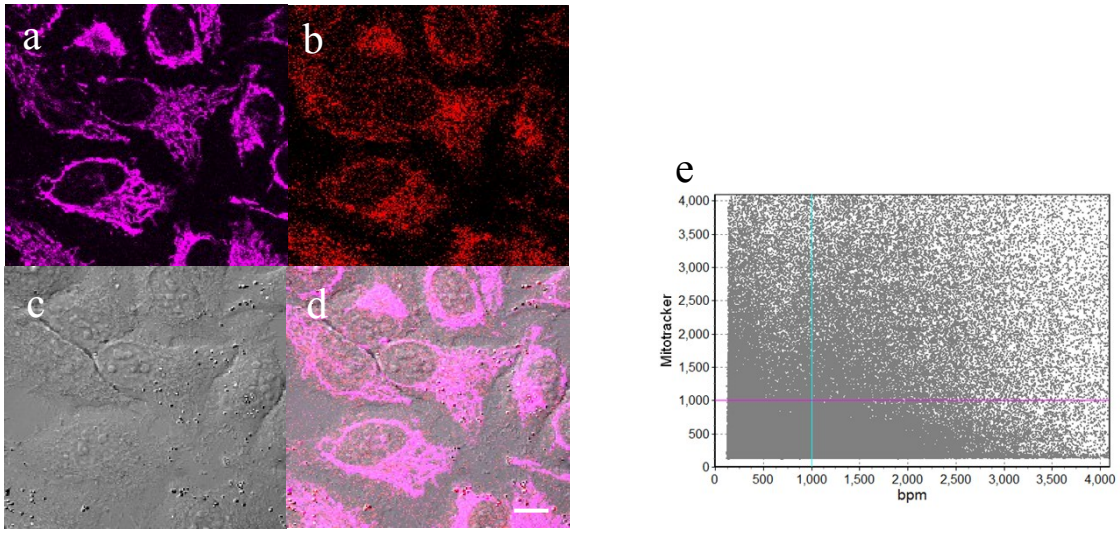


Figure S8. HeLa cells were incubated with 10 μM **2** for 1 hr at 37 ℃. After washing with the DPBS, the cells were incubated with 50 nM Mitotracker Deep Red (for mitochondria staining) in HBSS (Hank's Balanced Salt Solution with calcium and magnesium) media for 30 min at 37 ℃. After washing with DPBS, fluorescence images were acquired by confocal microscopy. (a) Mitotracker: ex. 635 nm/ em. 655-755 nm, (b) **2**: ex. 405 nm/ em. 490-590 nm, (c) DIC, (d) merge, (e) Co-localization analysis of Mitotracker and **2**. Scale bar: 10 μm.

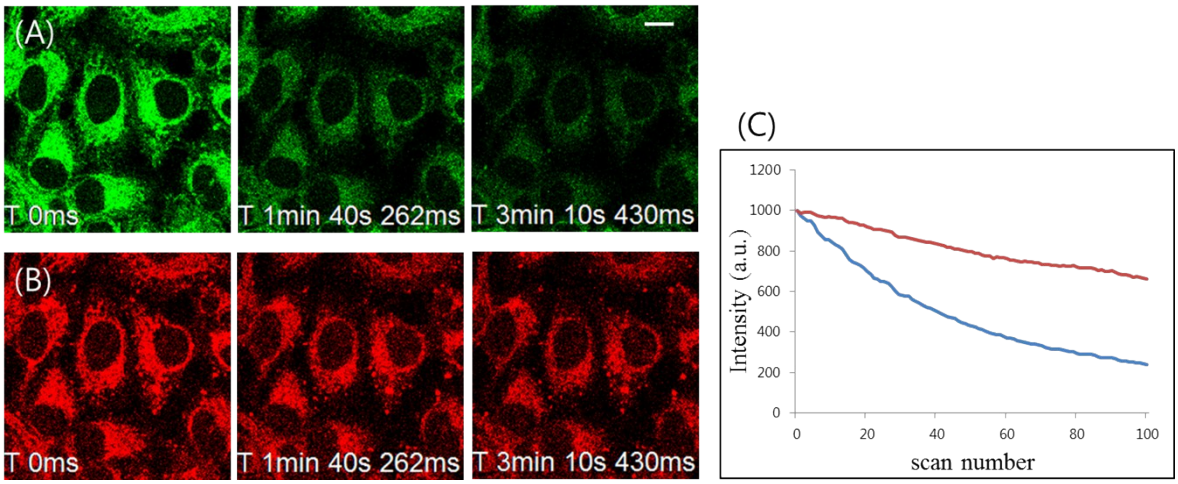


Figure S9. Analysis of the photostability of **2** and ER Tracker by continuous illumination in the live cell. HeLa cells were stained with 10 μM **2** for 1hr and 1 μM ER Tracker for 30 min and the fluorescence images were captured by 100 scans (2'04"/scan). Fluorescence intensity were analyzed by Olympus Fluoview Ver.4.0b software. (A) ER Tracker, (B) **2**. (C) Fluorescence intensities at different scan numbers (blue line: ER Tracker, red line: **2**). Scale bar: 10 μm.