

Supporting Information for

**Prominent Bathochromic Shift Effect of Indole-Containing
Diarylethene Derivatives**

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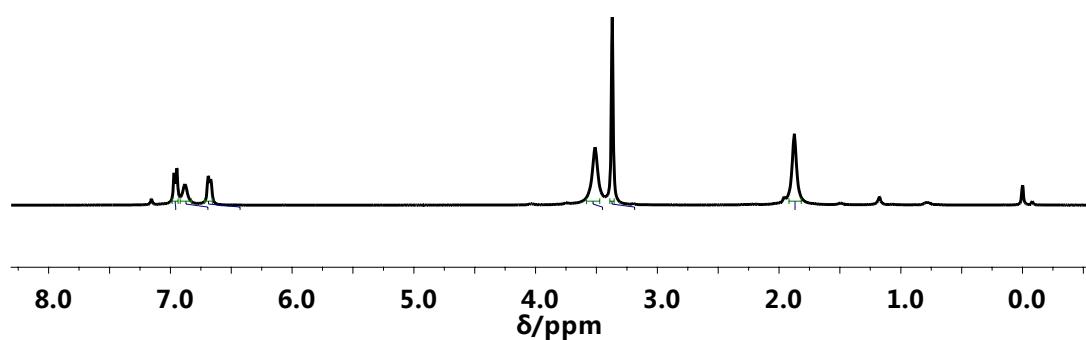


Figure S1. ¹H NMR spectrum of **1o** (CDCl₃, 400 MHz, 298 K).

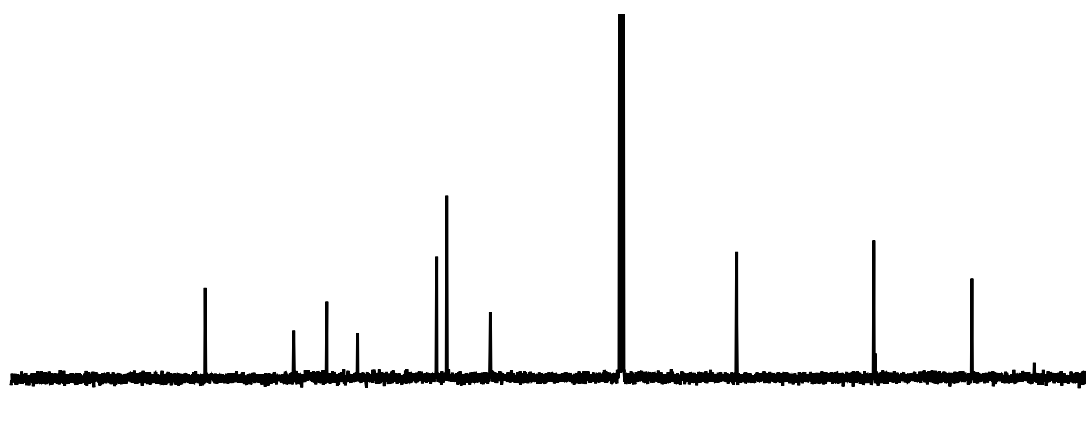


Figure S2. ¹³C NMR spectrum of **1o** (CDCl₃, 100 MHz, 298 K).

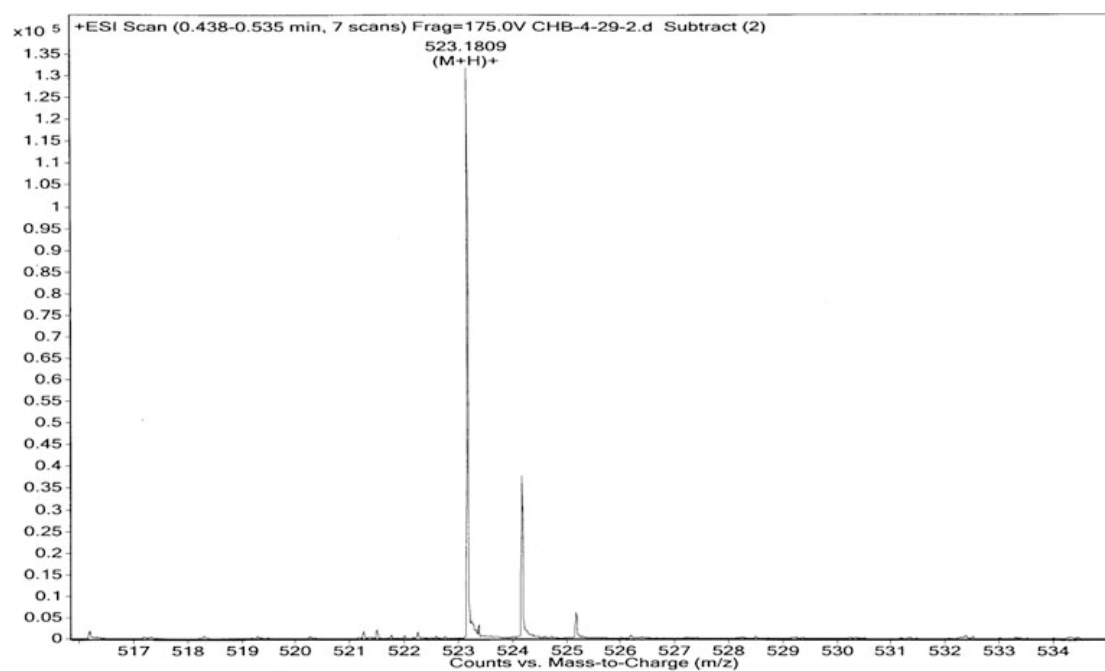


Figure S3. HRMS (ESI) spectrum of **1o**

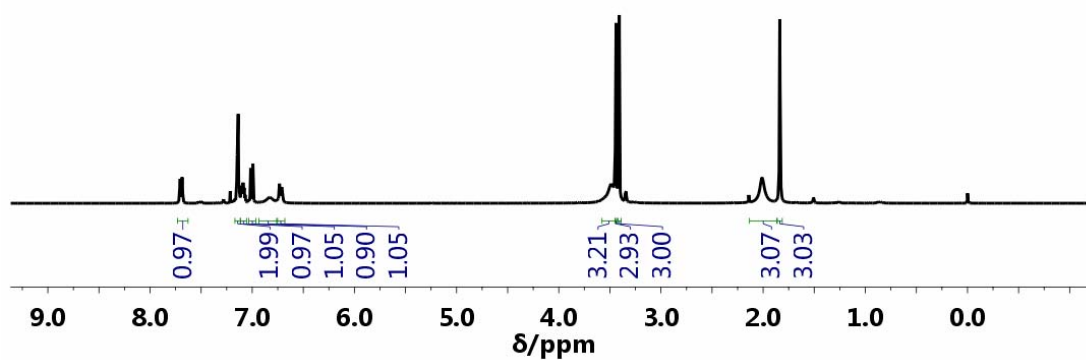


Figure S4. ^1H NMR spectrum of **2o** (CDCl_3 , 400 MHz, 298 K).

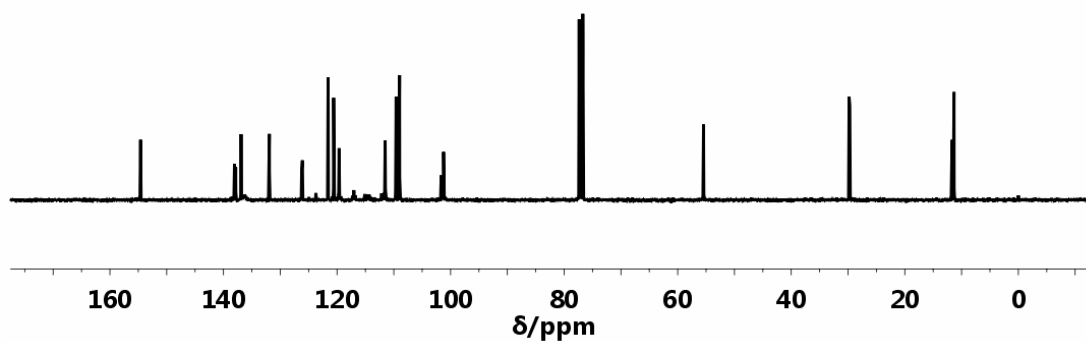


Figure S5. ^{13}C NMR spectrum of **2o** (CDCl_3 , 100 MHz, 298 K).

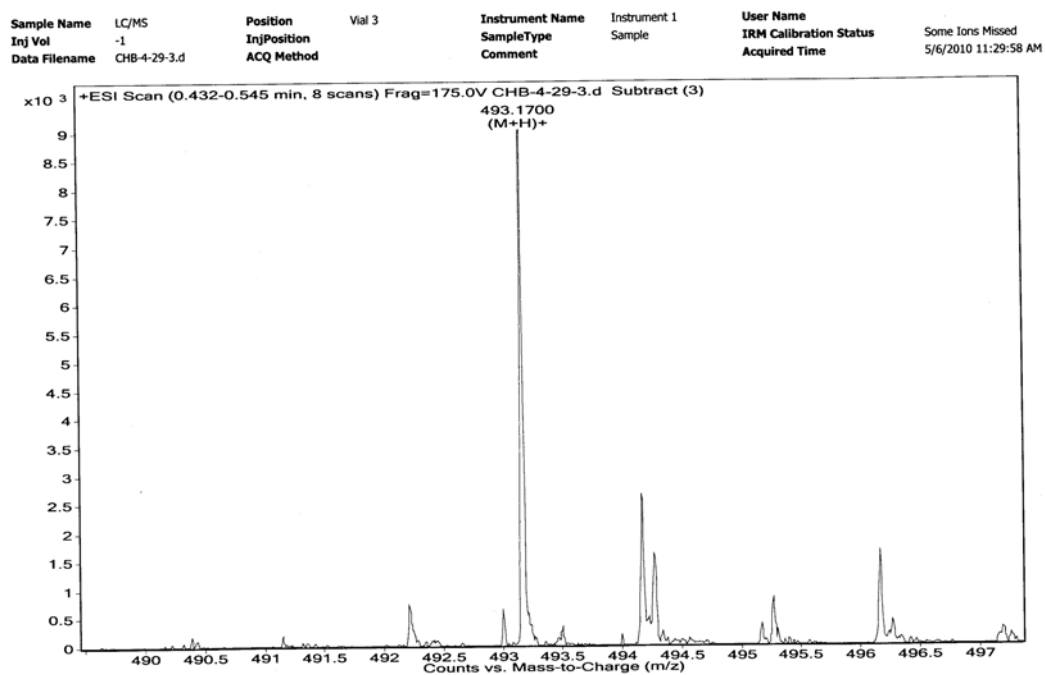


Figure S6. HRMS (ESI) spectrum of **2o**

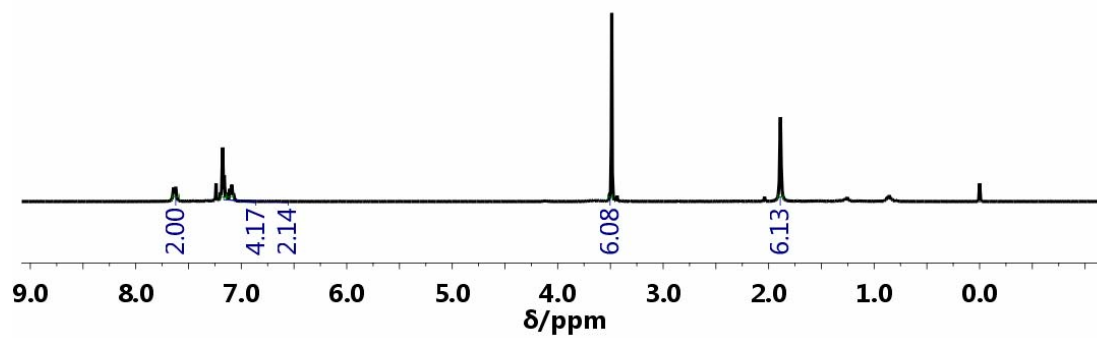


Figure S7. ^1H NMR spectrum of **3o** (CDCl_3 , 400 MHz, 298 K).

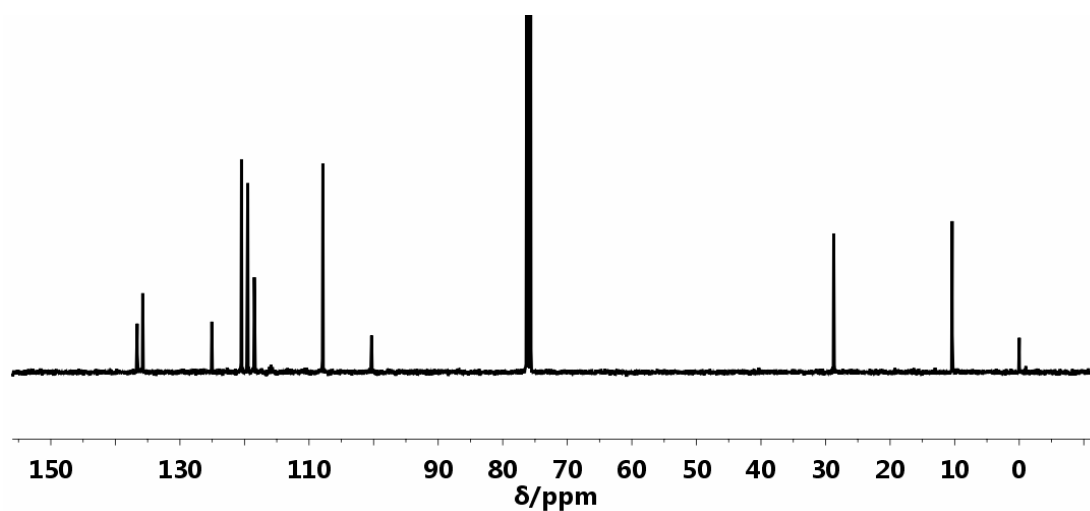


Figure S8. ^{13}C NMR spectrum of **3o** (CDCl_3 , 100 MHz, 298 K).

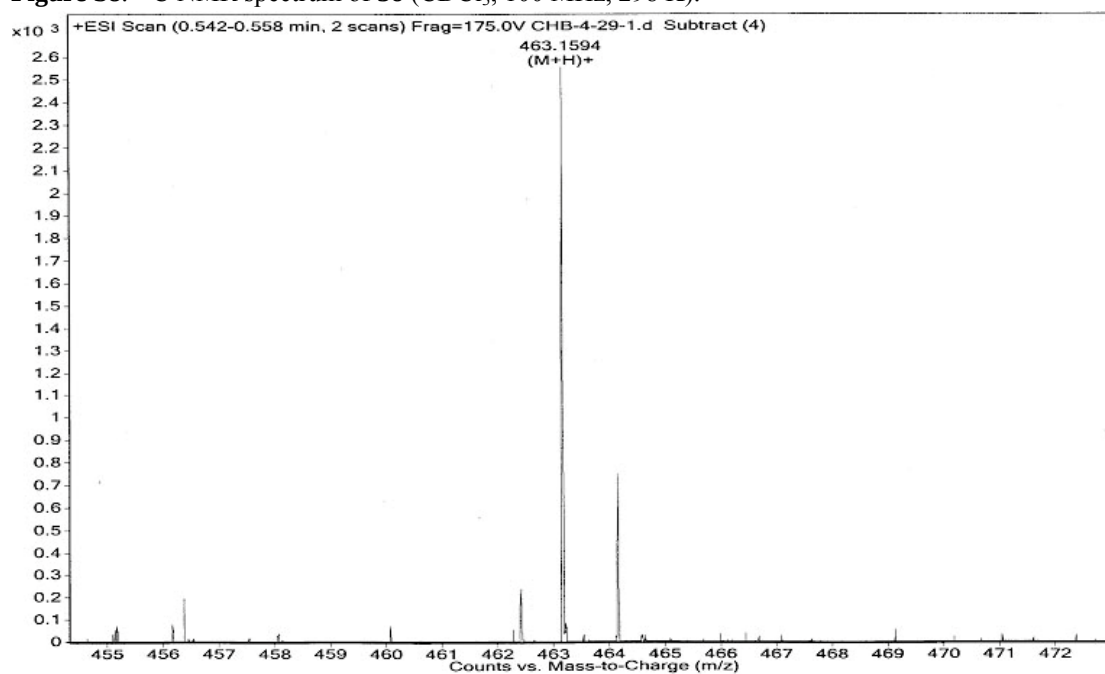


Figure S9. HRMS (ESI) spectrum of **3o**

Table S1. Crystallographic data for **1o**

Empirical formula	$\text{C}_{27}\text{H}_{24}\text{F}_6\text{N}_2\text{O}_2$
Formula weight	522.48
Crystal size (mm^3)	0.10 x 0.10 x 0.08
Temperature (K)	113(2)
Wavelength ($\text{\AA}$)	0.71073
Crystal system	Monoclinic
Space group	$\text{P2}(1)/n$
a / $\text{\AA}$	12.040(4)
b / $\text{\AA}$	11.834(3)
c / $\text{\AA}$	17.361(5)
α / $^\circ$	90

$\beta/^\circ$	105.585(5)
$\gamma/^\circ$	90
$V/\text{\AA}^3$	2382.5(12)
Z	4
Calculated density ($\text{Mg}\cdot\text{m}^{-3}$)	1.457
Absorption coefficient(mm^{-1})	0.124
$F(000)$	1080
θ range($^\circ$)	1.85-25.02
Limiting indices	-10 $\leq h \leq$ 14 -14 $\leq k \leq$ 14 -20 $\leq l \leq$ 19
Reflections collected / unique	16979 / 4187 [$R(\text{int}) = 0.0303$]
Data / restraints / parameters	4187 / 0 / 340
Goodness-of-fit on F^2	1.062
Final R indices [$I > 2\sigma(I)$]	$R_1 = 0.0384$, $wR_2 = 0.0960$
R indices (all data)	$R_1 = 0.0468$, $wR_2 = 0.1008$

$$R_1 = \sum \|F_0\| - |F_c| / \sum \|F_0\|, \quad \omega R_2 = \{ \sum \omega (F_0^2 - F_c^2)^2 / \sum \omega (F_0^2)^2 \}^{1/2}$$

Table S2. Hydrogen bond lengths ($\text{\AA}$) and bond angles ($^\circ$) for complexes 1o.

D–H $\cdots$ A	d(D–H)	d(H $\cdots$ A)	d(D $\cdots$ A)	$\angle(\text{D–H}\cdots\text{A})$
C(2)–H(2) $\cdots$ F(3)#i	0.95	2.52	3.467(2)	173
C(3)–H(3) $\cdots$ O(1)#ii	0.95	2.52	3.403(2)	154
C(5)–H(5) $\cdots$ F(2)	0.95	2.36	3.083(2)	132

#i -1/2+x, 1/2-y, -1/2+z; #ii -x, -y, -z.

Table S3. Photochromic parameters of compounds 1, 2 and 3 in toluene at 5.0×10^{-5} M

compounds	$\lambda_{\text{max}}/\text{nm}^{\text{a}}$ ($\epsilon/\text{L mol}^{-1}\text{cm}^{-1}$)	$\lambda_{\text{max}}/\text{nm}^{\text{b}}$ ($\epsilon/\text{L mol}^{-1}\text{cm}^{-1}$)	$\Phi^{\text{a-b}}$	Φ^{c}	$\Phi^{\text{b-a}}$
1	282 (1.76×10^4)	638 (4.8×10^3)	0.28		0.26
2	289 (3.35×10^4)	620 (8.9×10^3)	0.20		0.17
3	286 (1.62×10^4)	593 (4.2×10^3)	0.25		0.15

^aAbsorption maxima of open-ring forms. ^bAbsorption maxima of closedring forms. ^cQuantum yields of cyclization ($\Phi^{\text{a-b}}$) and cycloreversion ($\Phi^{\text{b-a}}$), respectively.

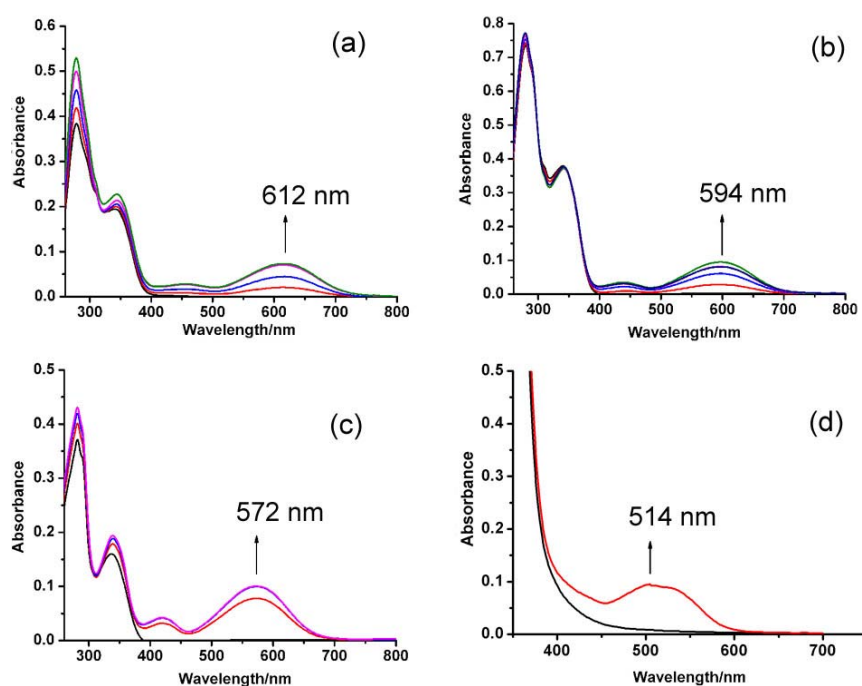


Figure S10. UV-vis spectral changes of (a) **1o**, (b) **2o**, (c) **3o** and (d) **4o** upon 365 nm light irradiation in hexane at 25 °C (0–2 min).

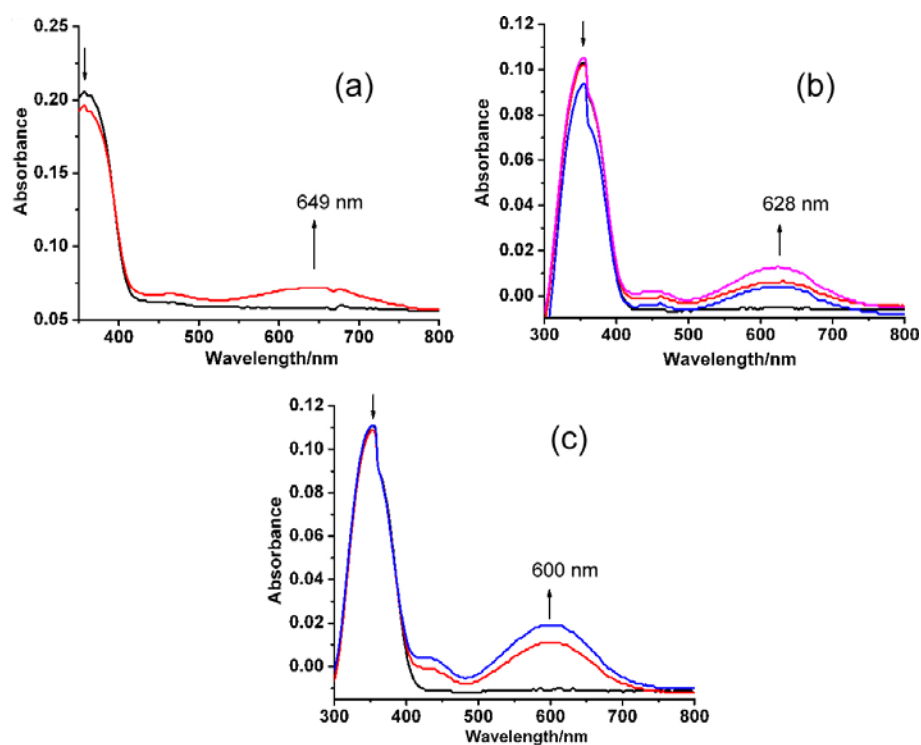


Figure S11. UV/Vis spectral changes of a 2 wt% (a) **1o**, (b) **2o** and (c) **3o** loaded poly(methyl methacrylate) (PMMA) film at 25 °C (0–2 min) after irradiation with 365 nm light.

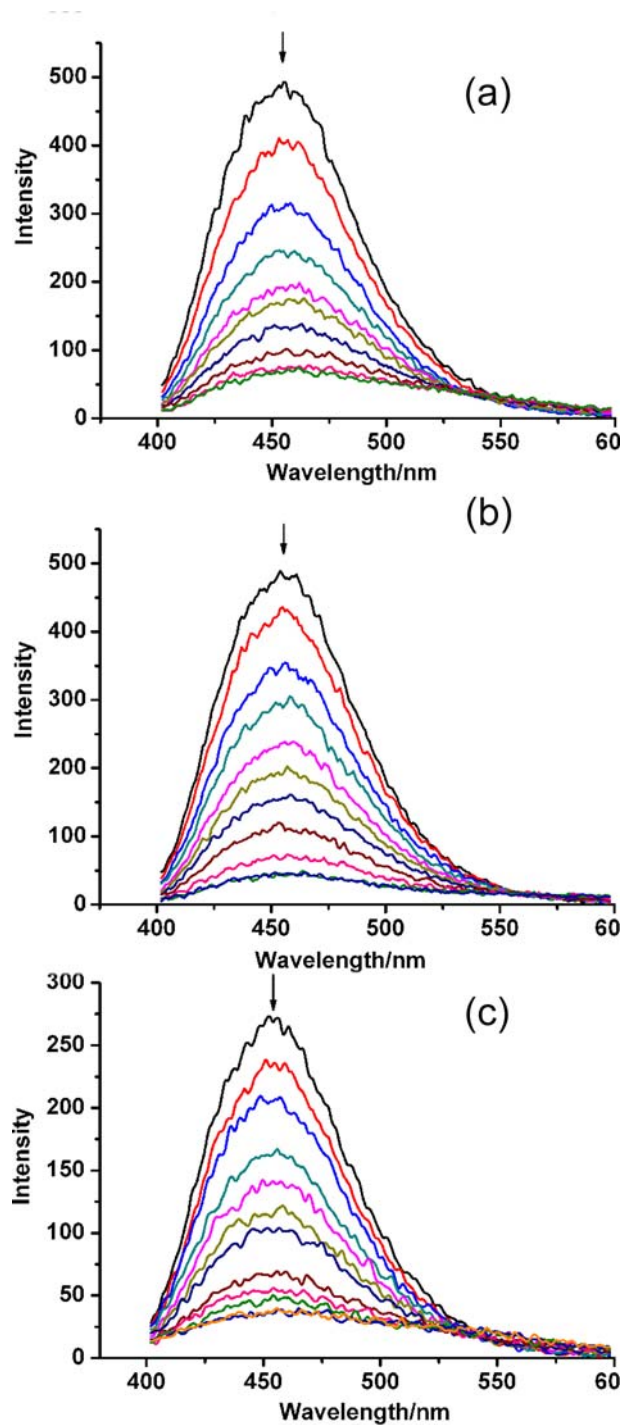


Figure S12. Fluorescence spectral changes of **1o**, **2o** and **3o** upon 365 nm light irradiation in toluene at 25 °C (0–2 min).

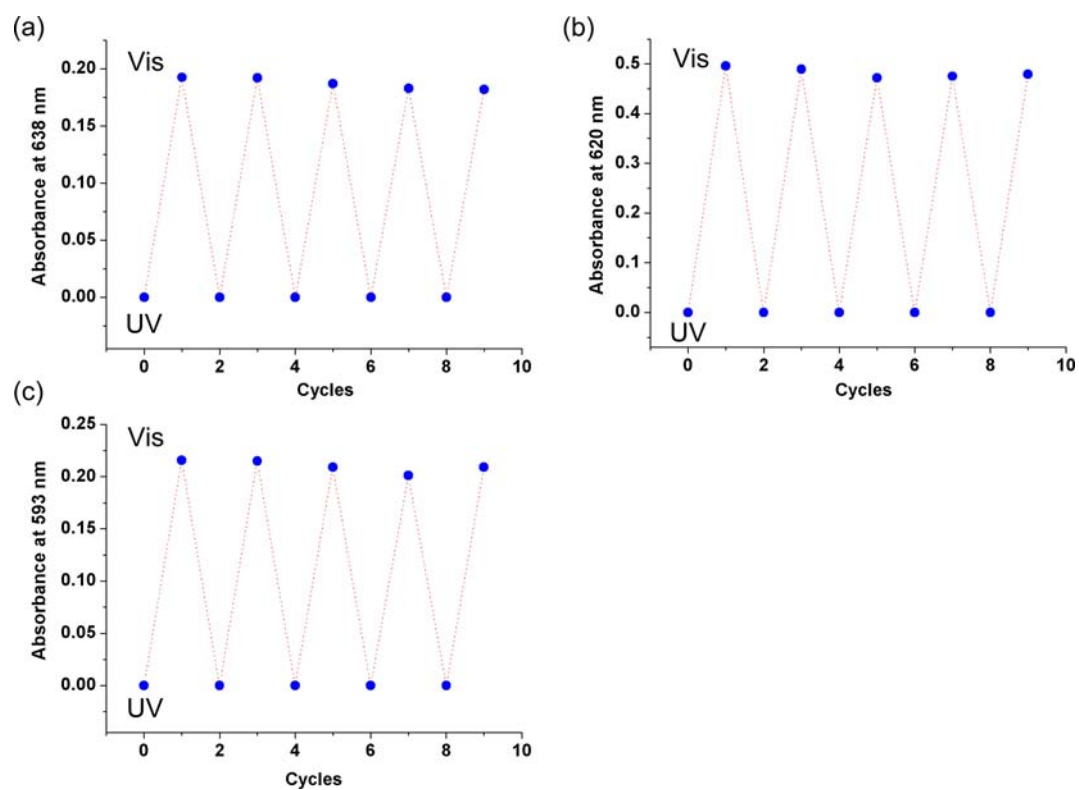


Figure S13. The absorption maxima changes of (a) **1o**, (b) **2o**, (c) **3o** (in toluene at 25 °C) observed upon alternating UV (365 nm) and Vis-light (> 400 nm) irradiation.