

*Electronic Supplementary Information*

**A novel family of AIE-active *meso*-2-ketopyrrolylBODIPYs:  
Bright solid-state red fluorescence, morphological properties and  
application as viscosimeters in live cells**

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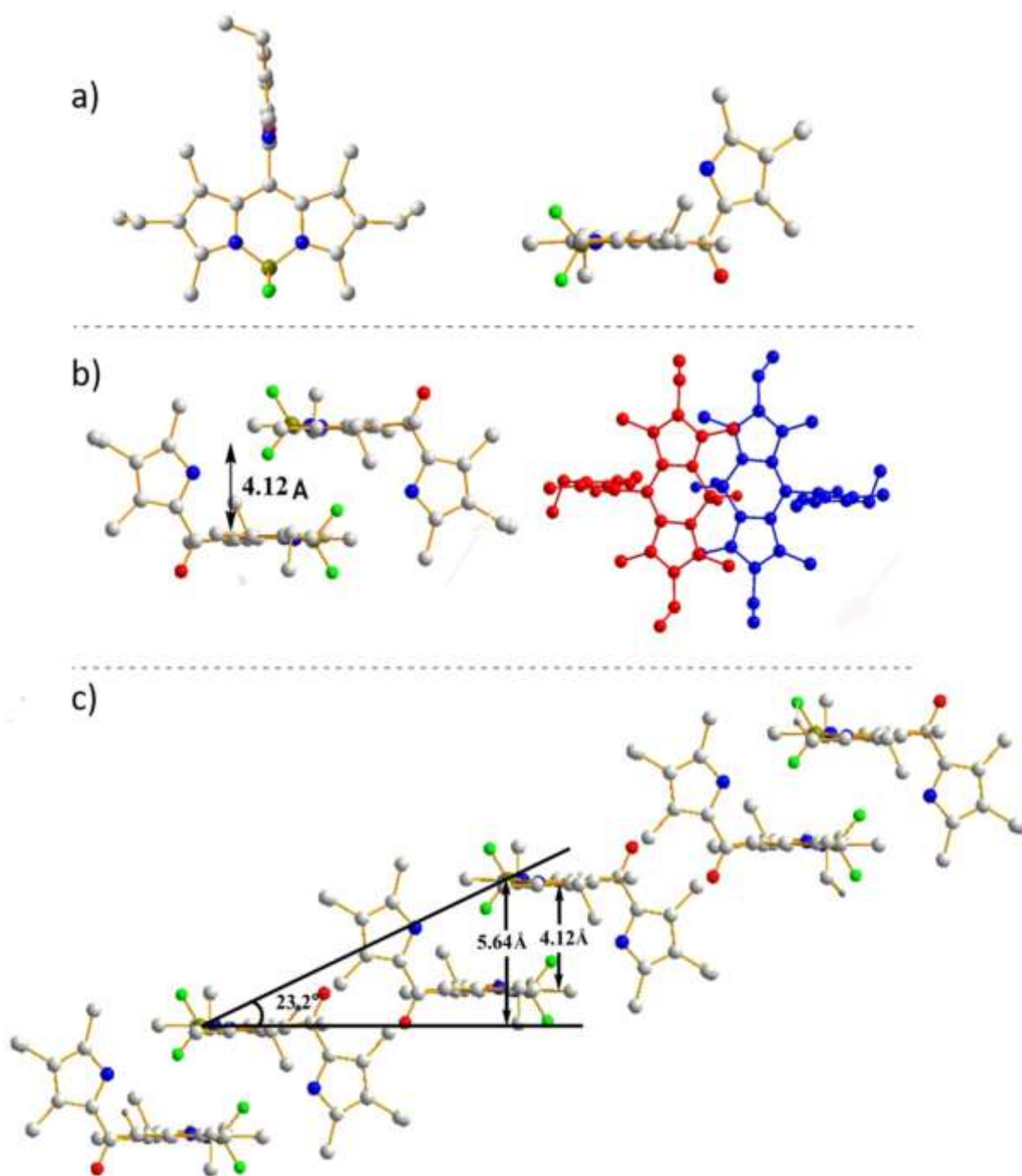
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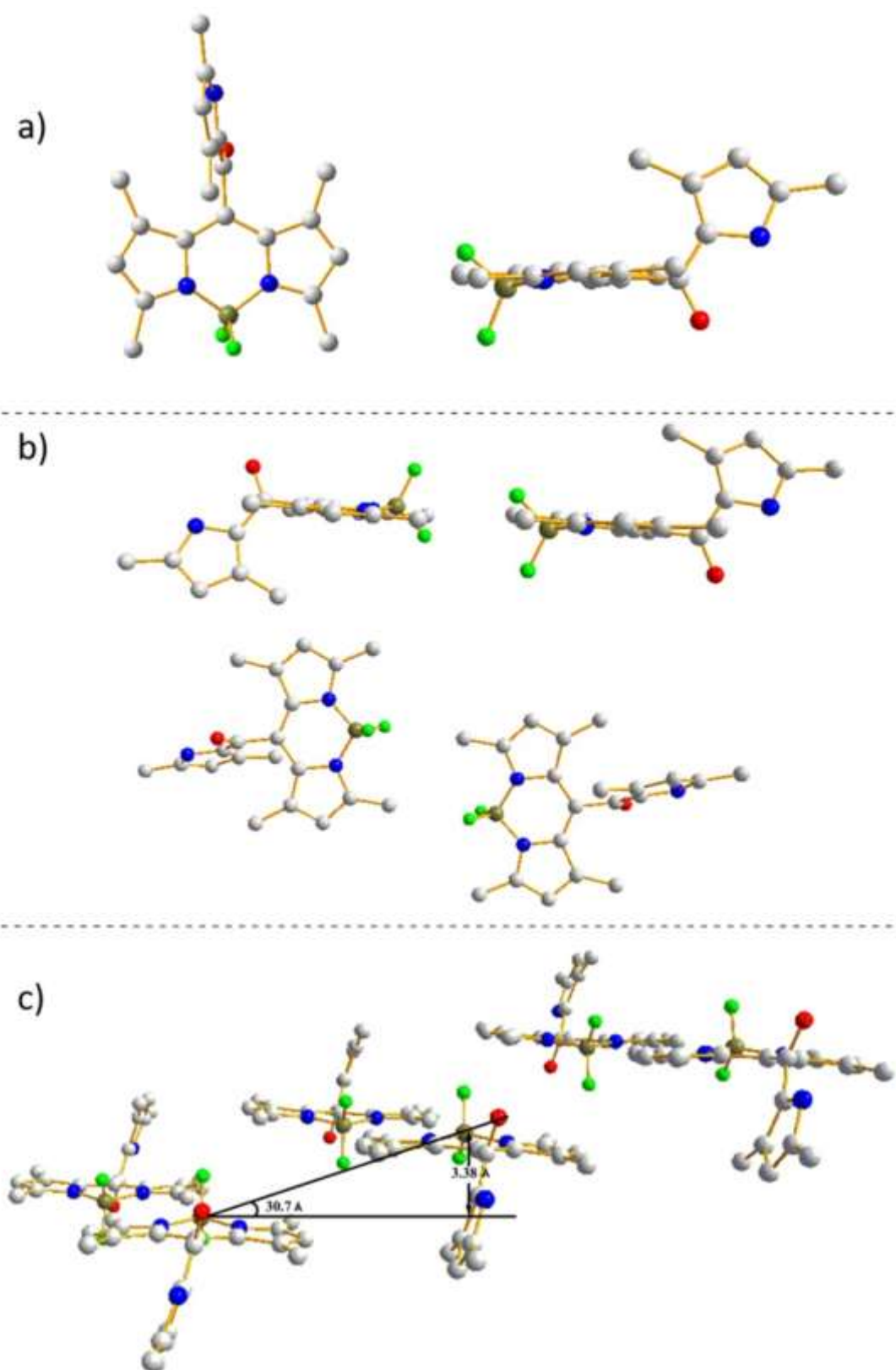
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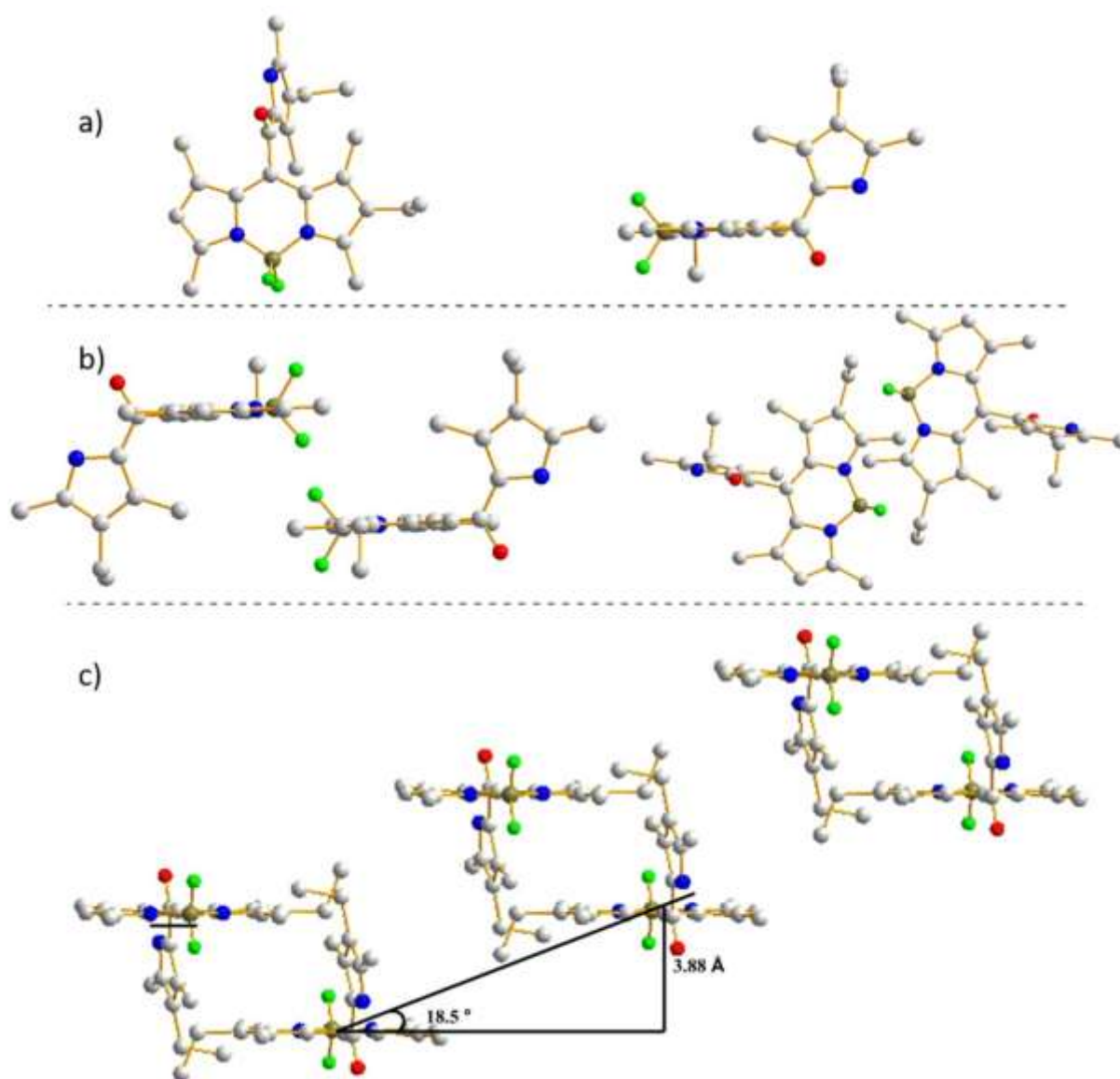
## 1. Crystal diagrams and selected data



**Figure S1.** Crystal-packing pattern of **1a** between the adjacent interlayered crystals from side view. Interlayer distance is  $4.12 \text{ \AA}$  and tilt angle is  $23.2^\circ$  for coplanar inclined arrangements of its transition dipole. C, light gray; N, blue; B, dark yellow; F, green; O, red; H atoms are omitted for clarity.

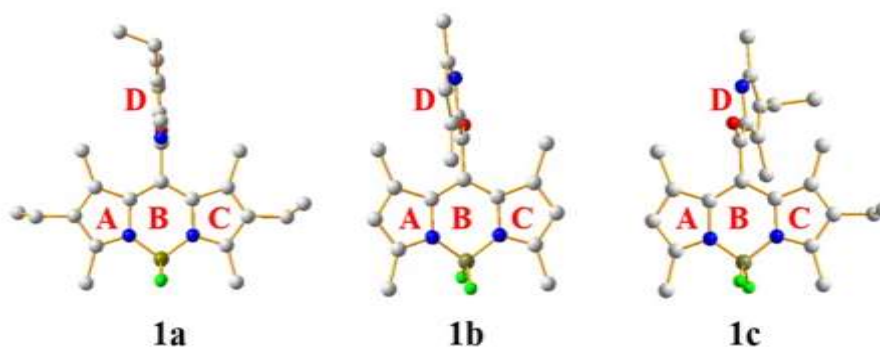


**Figure S2.** Crystal-packing pattern of **1b** between the adjacent interlayered crystals from side view. Interlayer distance is 3.38 Å and tilt angle is 30.7° for coplanar inclined arrangements of its transition dipole. C, light gray; N, blue; B, dark yellow; F, green; O, red; H atoms are omitted for clarity.



**Figure S3.** Crystal-packing pattern of **1c** between the adjacent interlayered crystals from side view. Interlayer distance is 3.88 Å and tilt angle is 18.5° for coplanar inclined arrangements of its transition dipole. C, light gray; N, blue; B, dark yellow; F, green; O, red; H atoms are omitted for clarity.

**Table S1.** Selected bond lengths [ $\text{\AA}$ ] and dihedral angles [deg] of *meso*-2-ketopyrrolyl-BODIPYs **1a-c** obtained from X-ray crystallography.



	<b>1a</b>	<b>1b</b>	<b>1c</b>
the B-F bond distances ( $\text{\AA}$ )	1.390 1.392	1.377 1.383	1.381 1.389
the B-N bond distances ( $\text{\AA}$ )	1.536 1.536	1.549 1.550	1.533 1.547
dihedral angles of two coordinated pyrrolic rings <b>A</b> and <b>C</b> (deg)	5.0(2)	8.78(2)	1.51(1)
dihedral angles between the six-membered ring <b>B</b> composed of NBN and the BODIPY core (deg)	0.53(1)	0.61(2)	0.40(2)
dihedral angles between the <i>meso</i> -uncoordinated pyrrolic ring <b>D</b> and the BODIPY core (deg)	88.8(2)	72.9(1)	81.4(1)
intramolecular C-H $\cdots$ F hydrogen bond distances ( $\text{\AA}$ )	2.602, 2.611, 2.680, 2.759	2.542, 2.728, 2.726, 2.878	2.571, 2.600, 2.707, 2.772
intermolecular C-H $\cdots$ F hydrogen bond distances ( $\text{\AA}$ )		2.695, 2.695, 2.827, 2.827	2.578, 2.612
intermolecular N-H $\cdots$ F hydrogen bond distances ( $\text{\AA}$ )	2.075, 2.075		

**Table S2.** Crystal data collection parameters for *meso*-2-ketopyrrolyl BODIPYs **1a**, **1b** and **1c** obtained from X-ray crystallography.

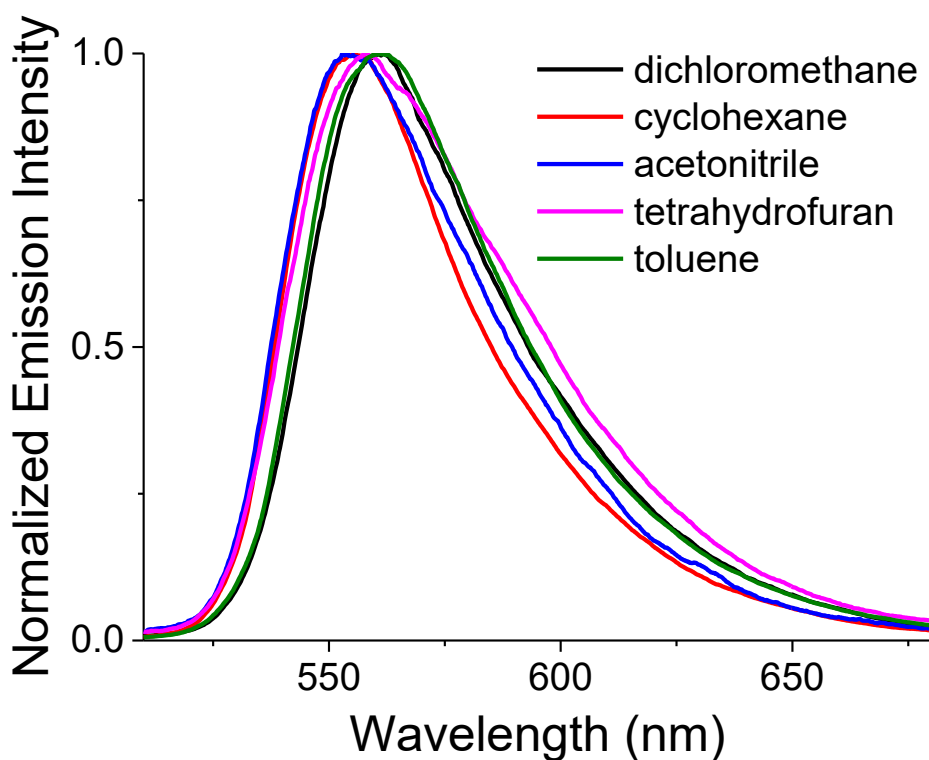
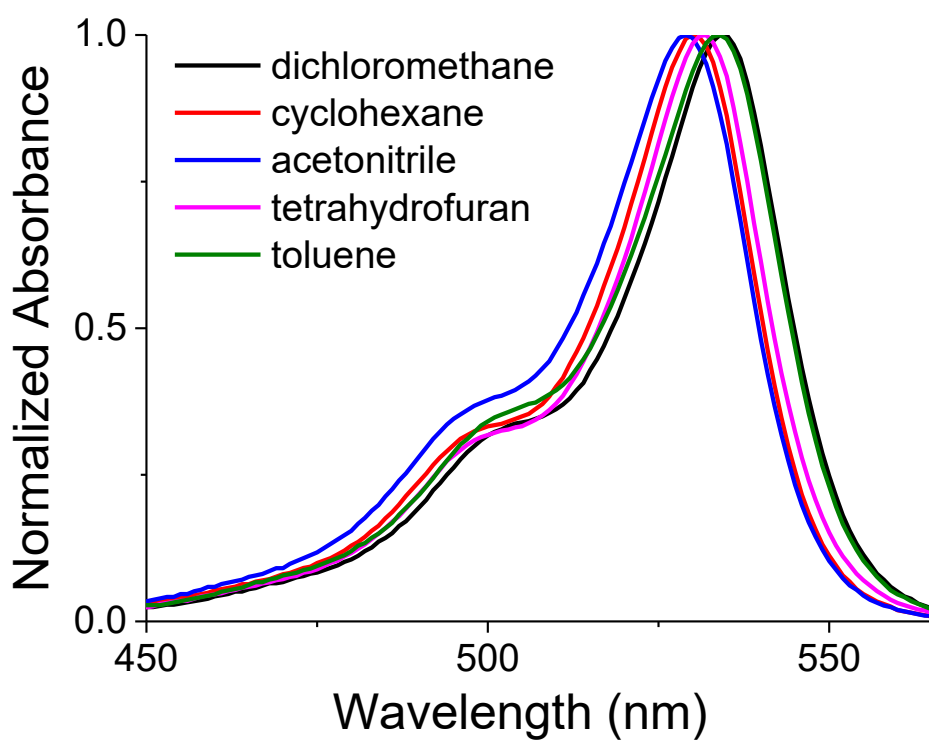
	<b>1a</b>	<b>1b</b>	<b>1c</b>
CCDC no.	1541729	1541728	1901461
formula	C <sub>26</sub> H <sub>34</sub> BF <sub>2</sub> N <sub>3</sub> O	C <sub>20</sub> H <sub>22</sub> BF <sub>2</sub> N <sub>3</sub> O	C <sub>24</sub> H <sub>30</sub> BF <sub>2</sub> N <sub>3</sub> O
M	453.37	369.22	425.32
T (K)	293(2)	293(2)	293(2)
$\lambda$ (Å)	0.71073	0.71073	0.71073
crystal system	Monoclinic	Monoclinic	Monoclinic
space group	C2/c	C2/c	C2/c
a (Å)	26.649(3)	12.8894(18)	23.744(3)
b (Å)	9.8463(10)	9.0135(12)	12.2488(12)
c (Å)	19.4482(19)	31.806(4)	19.0154(18)
$\alpha$ (deg)	90	90	90
$\beta$ (deg)	101.3930(10)	93.146(2)	101.276(2)
$\gamma$ (deg)	90	90	90
V (Å <sup>3</sup> )	5002.5(9)	3689.6(9)	5423.7(10)
Z	8	8	8
D <sub>calcd</sub> (mg m <sup>-3</sup> )	1.204	1.329	1.042
$\mu$ mm <sup>-1</sup>	0.083	0.096	0.073
F(000)	1936	1552	1808.0
$\theta$ range (deg)	1.56 - 27.63	2.76 - 27.62	1.249 to 24.996
reflections collected/unique	21129 / 5791	15525 / 4277	18895 / 4776
R (int)	0.0294	0.0222	0.0339
goodness-of-fit on F <sup>2</sup>	1.058	1.047	1.094
R1, wR2 [I > 2 $\sigma$ (I)]	0.0637, 0.2012	0.0458, 0.1300	0.0544, 0.1846
R1, wR2 (all data)	0.1044, 0.2386	0.0618, 0.1441	0.0718, 0.1948
Largest diff. peak and hole, e. Å <sup>-3</sup>	0.306, -0.240	0.277, -0.210	0.21, -0.17

## 2. Photophysical properties

**Table S3.** Photophysical properties of *meso*-2-ketopyrrolyl BODIPYs **1a** and **1b** in several organic solvents and powder state.

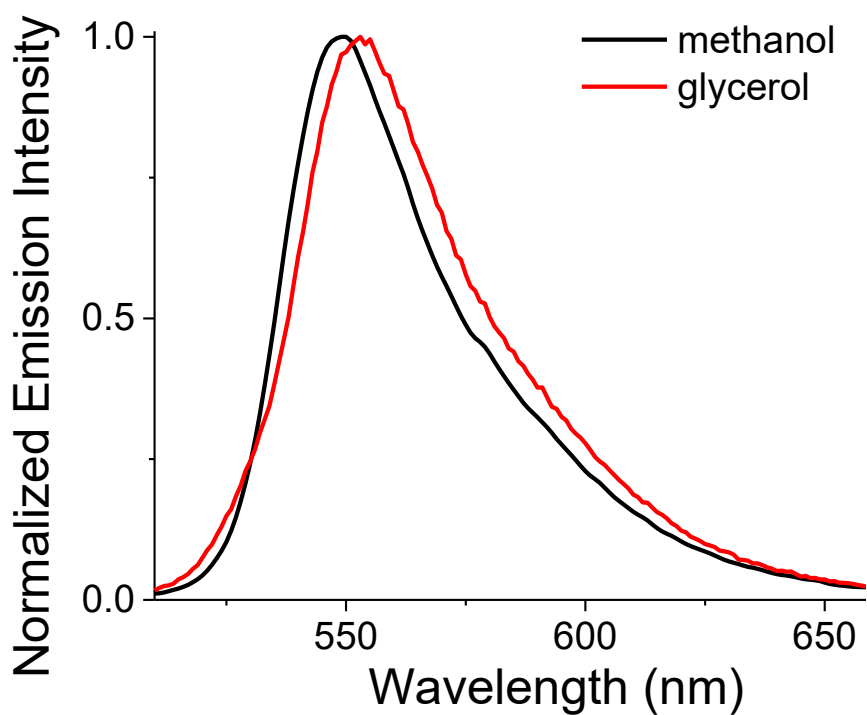
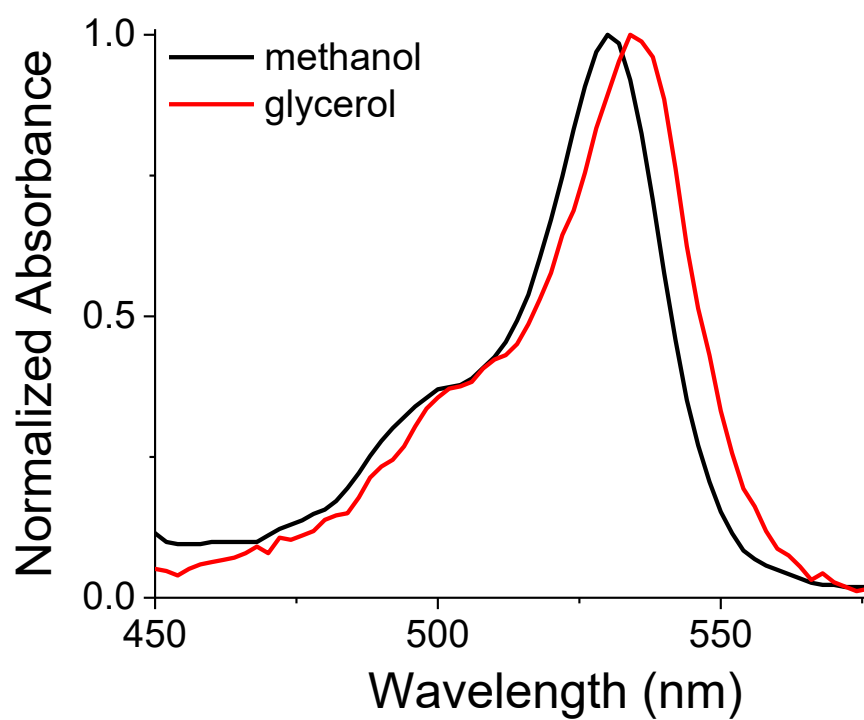
dyes	solvents	$\lambda_{\text{abs}}^{\text{max}}$ (nm)	$\lambda_{\text{em}}^{\text{max}}$ (nm)	$\log \epsilon_{\text{max}}^{\text{a}}$	$\phi^{\text{b}}$	Stokes shift ( $\text{cm}^{-1}$ )
<b>1a</b>	cyclohexane	532	557	4.89	0.12	844
	toluene	534	561	4.84	0.19	901
	dichloromethane	534	560	4.81	0.21	869
	tetrahydrofuran	530	554	4.84	0.18	817
	acetonitrile	529	555	4.79	0.10	886
	methanol	530	549	4.80	0.13	653
	glycerol	534	554	4.82	0.43	676
	solid state	-	661	-	0.13	-
<b>1b</b>	cyclohexane	508	534	4.91	0.12	958
	toluene	510	537	4.91	0.07	986
	dichloromethane	509	533	4.90	0.08	885
	tetrahydrofuran	507	530	4.93	0.05	856
	acetonitrile	504	526	4.88	0.03	830
	methanol	506	522	4.86	0.06	606
	glycerol	510	526	4.89	0.15	596
	solid state	-	620	-	0.21	-
<b>1c</b>	cyclohexane	520	548	4.88	0.03	983
	toluene	522	549	4.86	0.08	942
	dichloromethane	521	548	4.83	0.10	946
	tetrahydrofuran	518	544	4.80	0.03	923
	acetonitrile	517	543	4.78	0.01	926
	solid state	-	653	-	0.25	-
<b>1d</b>	cyclohexane	519	547	4.87	0.03	986
	toluene	522	549	4.84	0.08	942
	dichloromethane	521	548	4.80	0.10	946
	tetrahydrofuran	518	543	4.81	0.03	889
	acetonitrile	517	541	4.79	0.01	858
	solid state	-	644	-	0.22	-

<sup>a</sup>Molar absorption coefficients of **1a-d** are calculated at the maximum of the highest peak in their absorption spectra. <sup>b</sup>Fluorescence quantum yields ( $\phi$ ) of **1a-d** were evaluated by using integrating sphere in the above solvents (excited at 480 nm for **1b-d** in the above solvents, excited at 500 nm for **1a**) and powder state (excited at 550 nm for **1a** and 500 nm for **1b-d**). The standard errors are less than 5%.

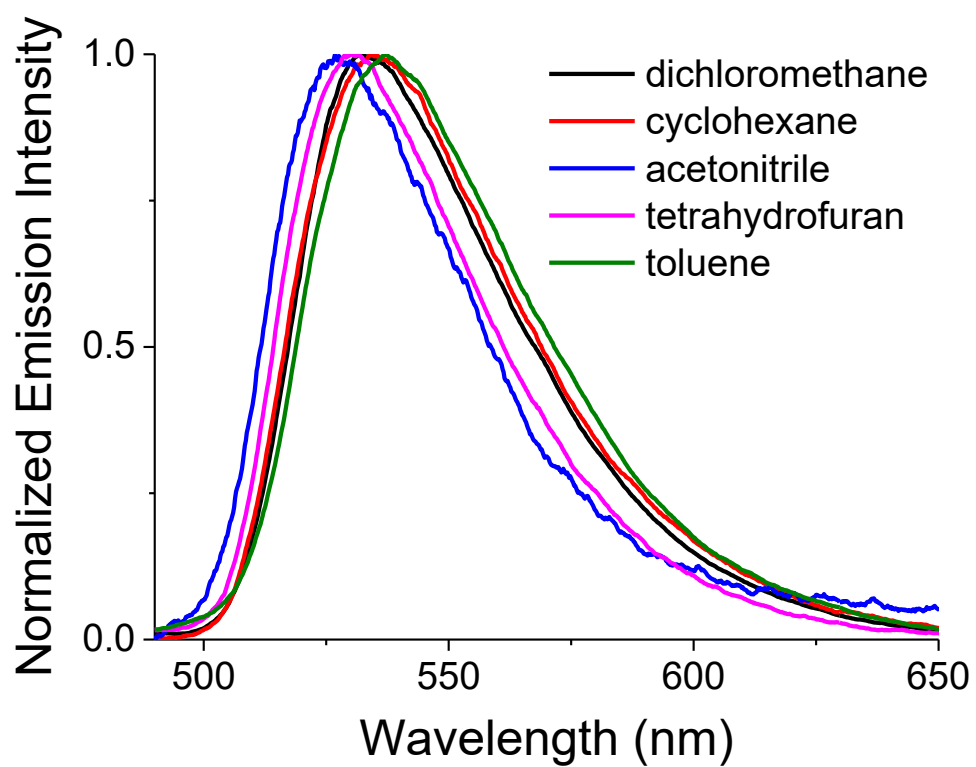
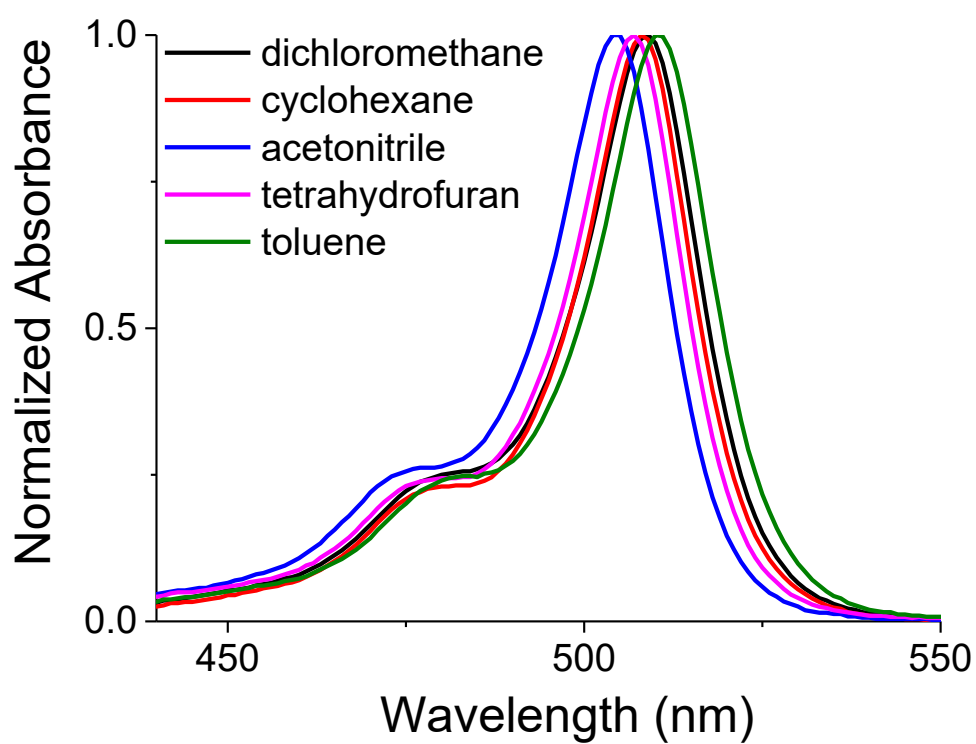


**Figure S4.** Normalized UV-vis (top) and fluorescence spectra (bottom) of **1a** (5 μM) in different solvents, excited at 500 nm.

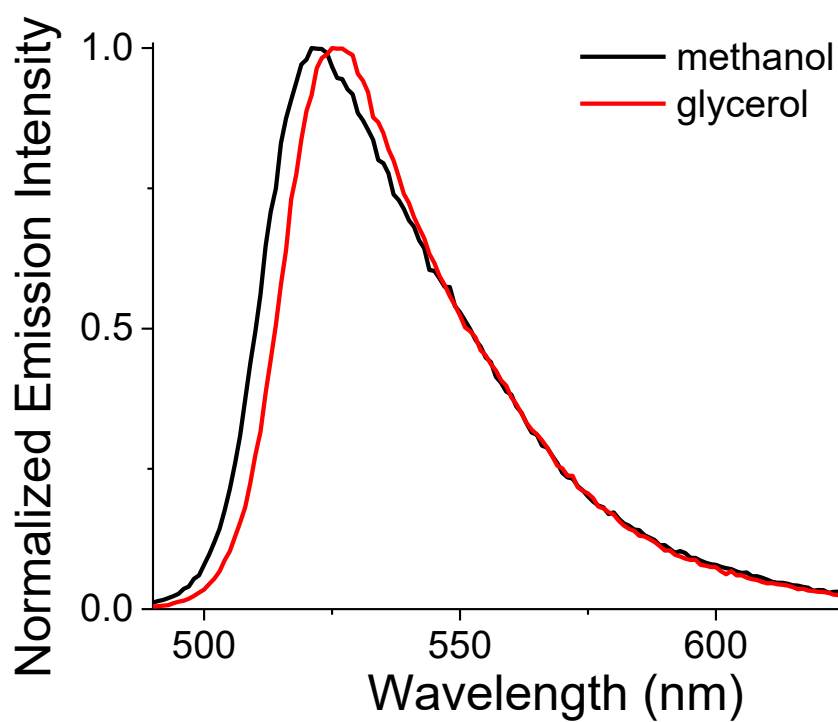
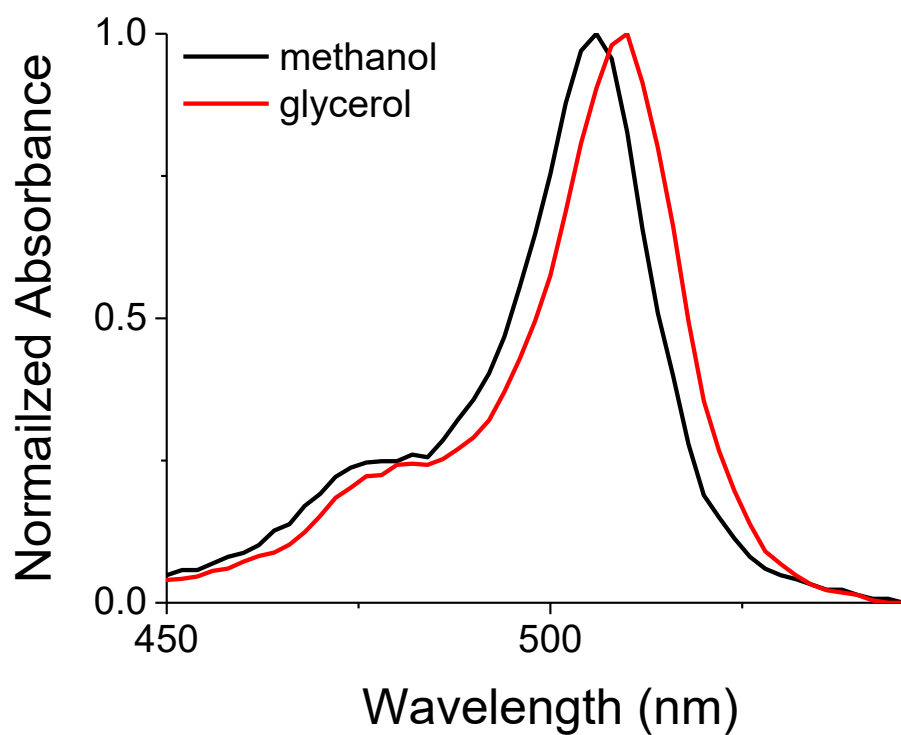




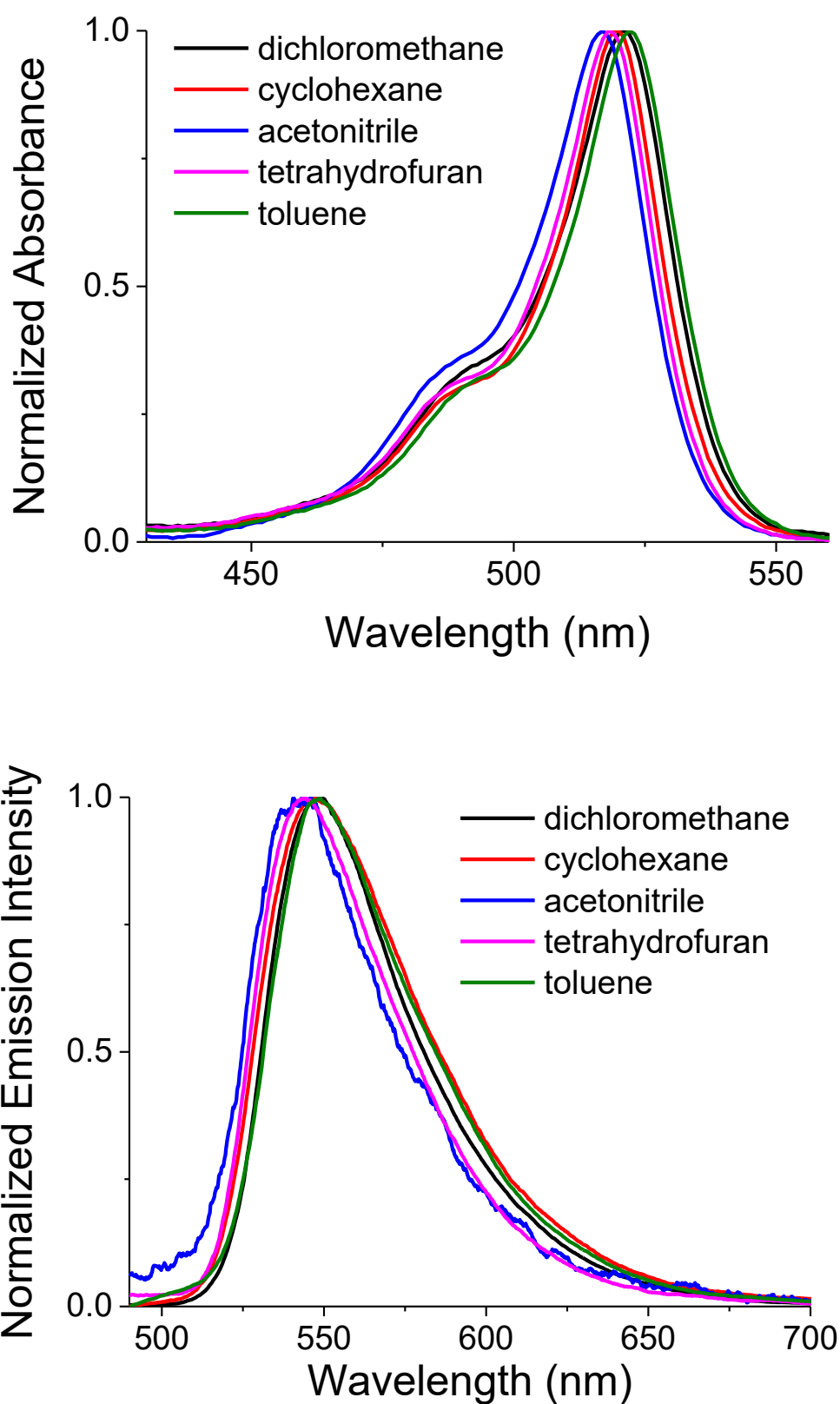
**Figure S5.** Normalized UV-vis (top) and fluorescence spectra (bottom) of **1a** (5  $\mu\text{M}$ ) in methanol and glycerol, excited at 500 nm.



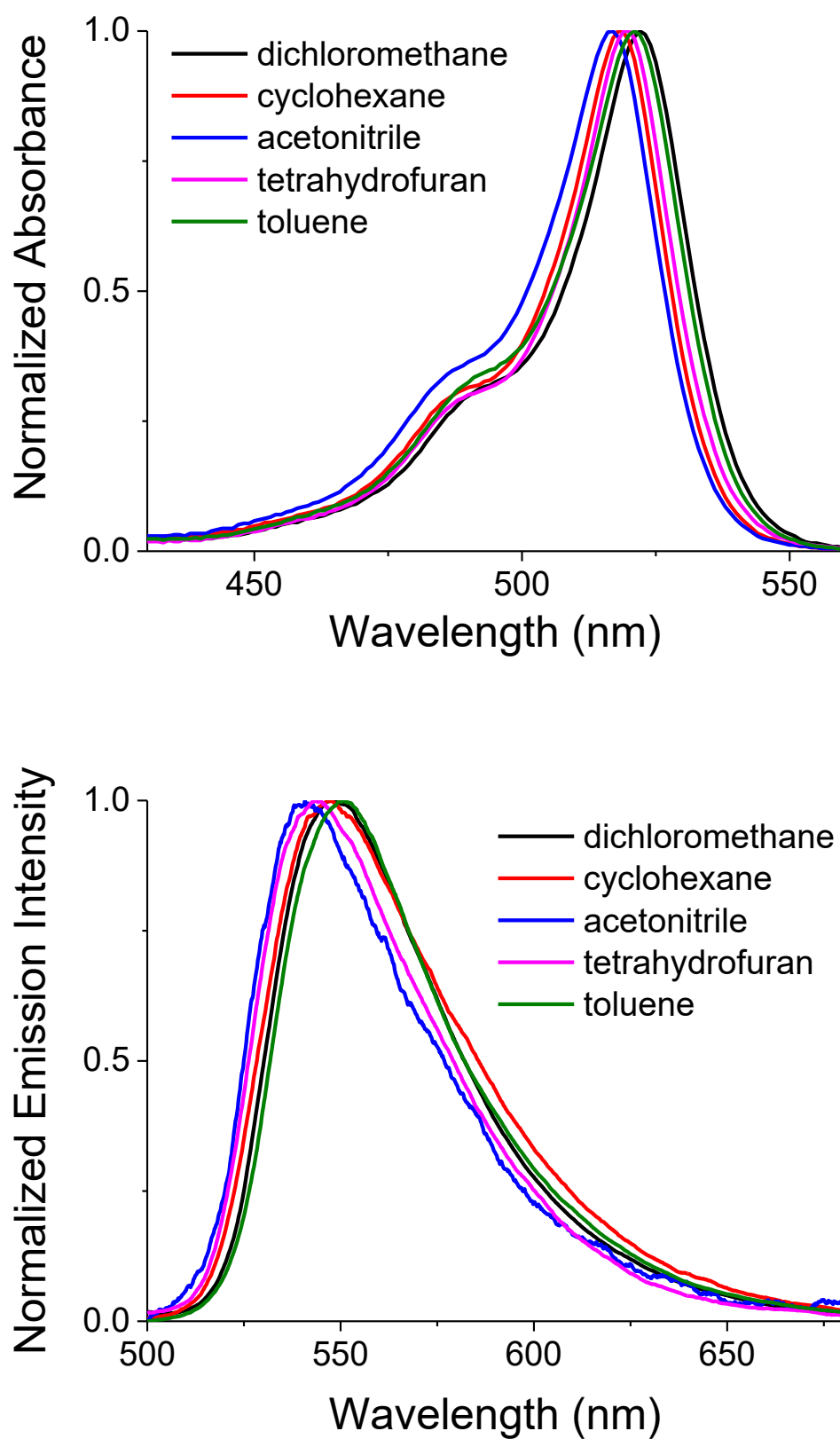
**Figure S6.** Normalized UV-vis (top) and fluorescence spectra (bottom) of **1b** (5  $\mu\text{M}$ ) in different solvents, excited at 480 nm.



**Figure S7.** Normalized UV-vis (top) and fluorescence spectra (bottom) of **1b** (5  $\mu\text{M}$ ) in methanol and glycerol, excited at 480 nm.

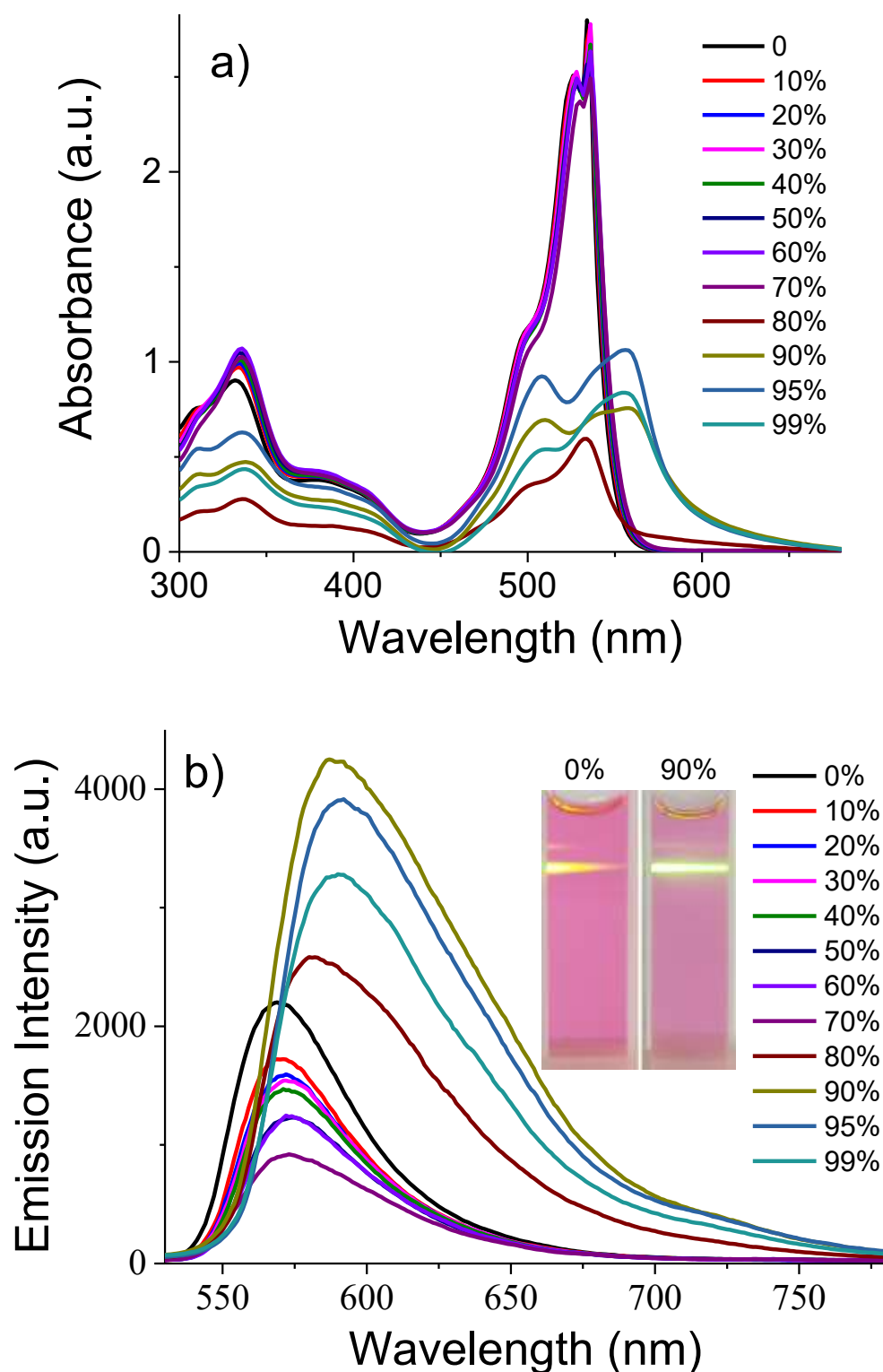


**Figure S8.** Normalized UV-vis (top) and fluorescence spectra (bottom) of **1c** in different solvents, excited at 480 nm.

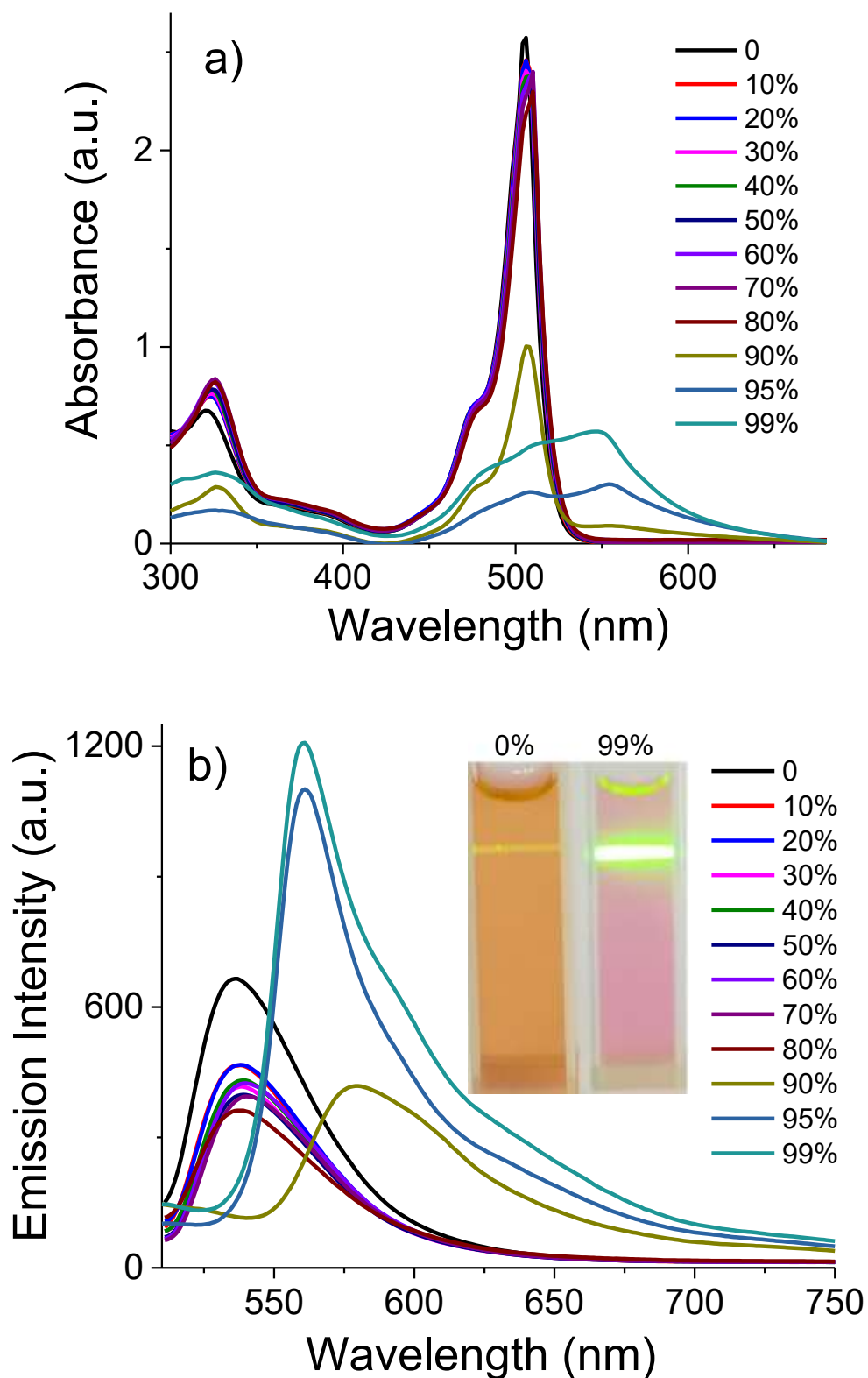


**Figure S9.** Normalized UV-vis (top) and fluorescence spectra (bottom) of **1d** in different solvents, excited at 480 nm.

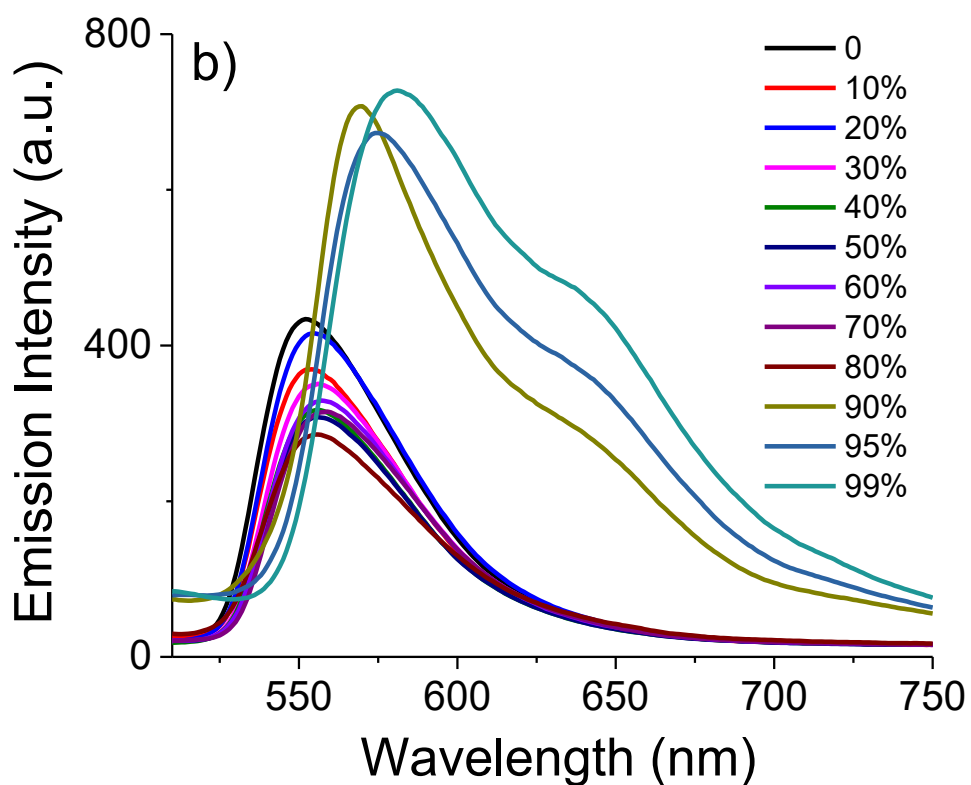
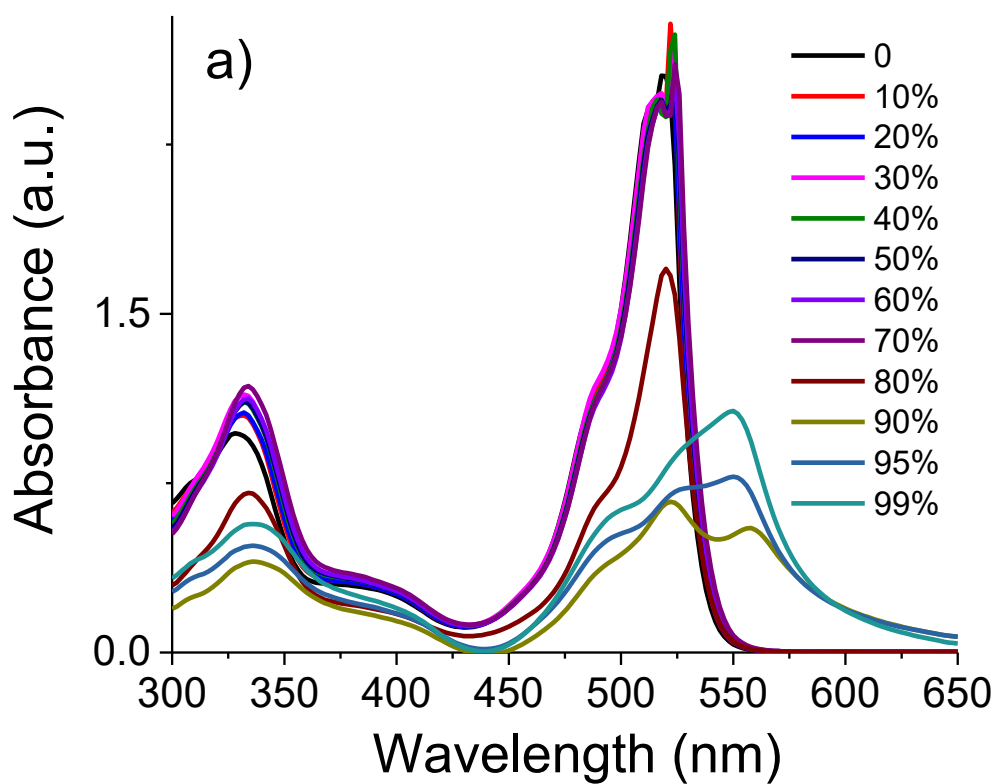
### 3. Aggregation-induced emission properties



**Figure S10.** Absorbance (a) and fluorescence (b) spectra of **1a** (50  $\mu\text{M}$ ) in acetonitrile/water with different water fractions ( $f_w$ ), excited at 500 nm. Photographs of acetonitrile and the mixed acetonitrile-water system containing 90% water of **1a** under 365 nm handheld UV lamp irradiation condition.

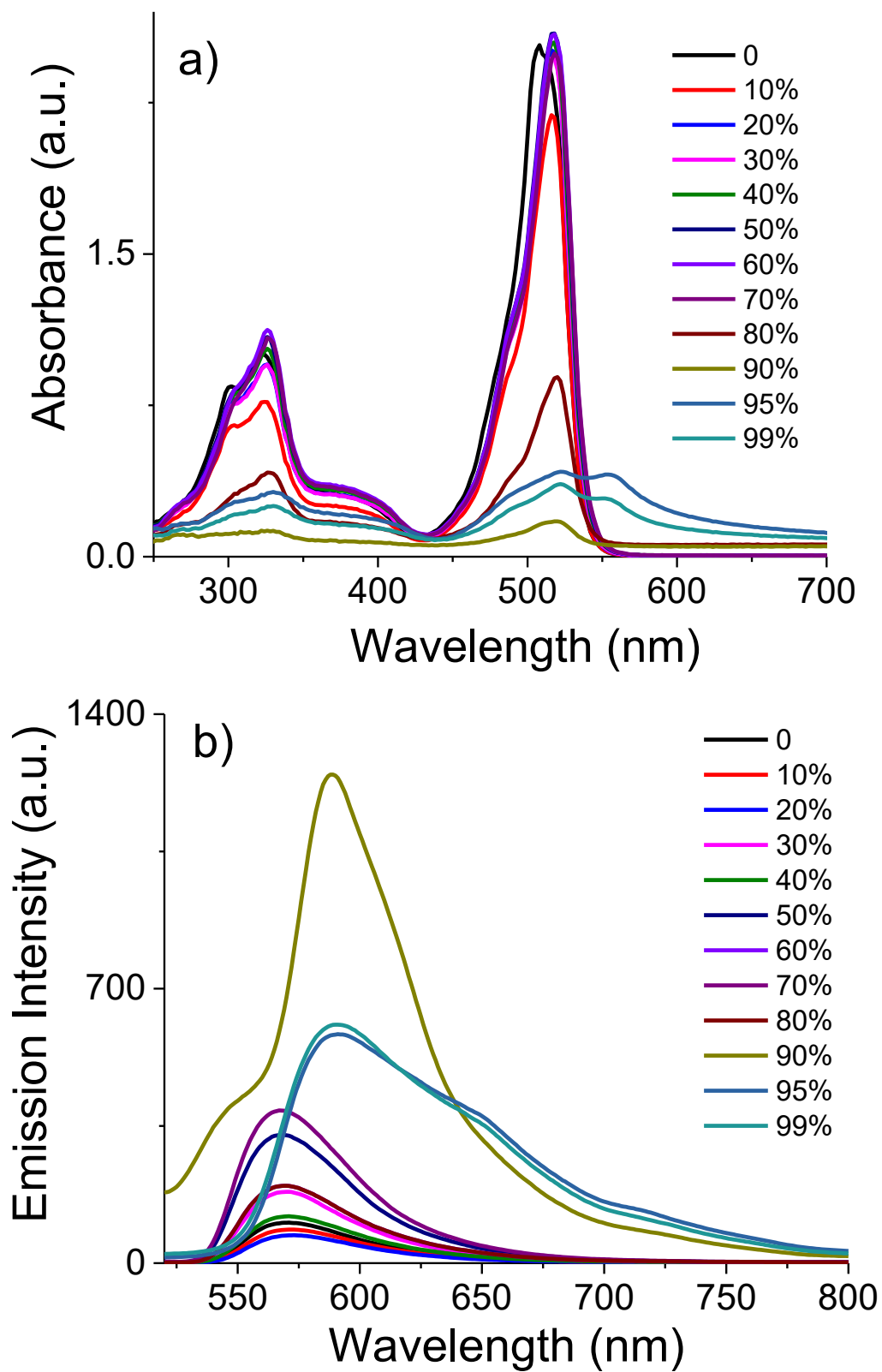


**Figure S11.** Absorbance (a) and fluorescence (b) spectra of **1b** (30  $\mu\text{M}$ ) in acetonitrile/water with different water fractions ( $f_w$ ), excited at 480 nm. Photographs of acetonitrile and the mixed acetonitrile-water system containing 99% water of **1b** under 365 nm handheld UV lamp irradiation condition.



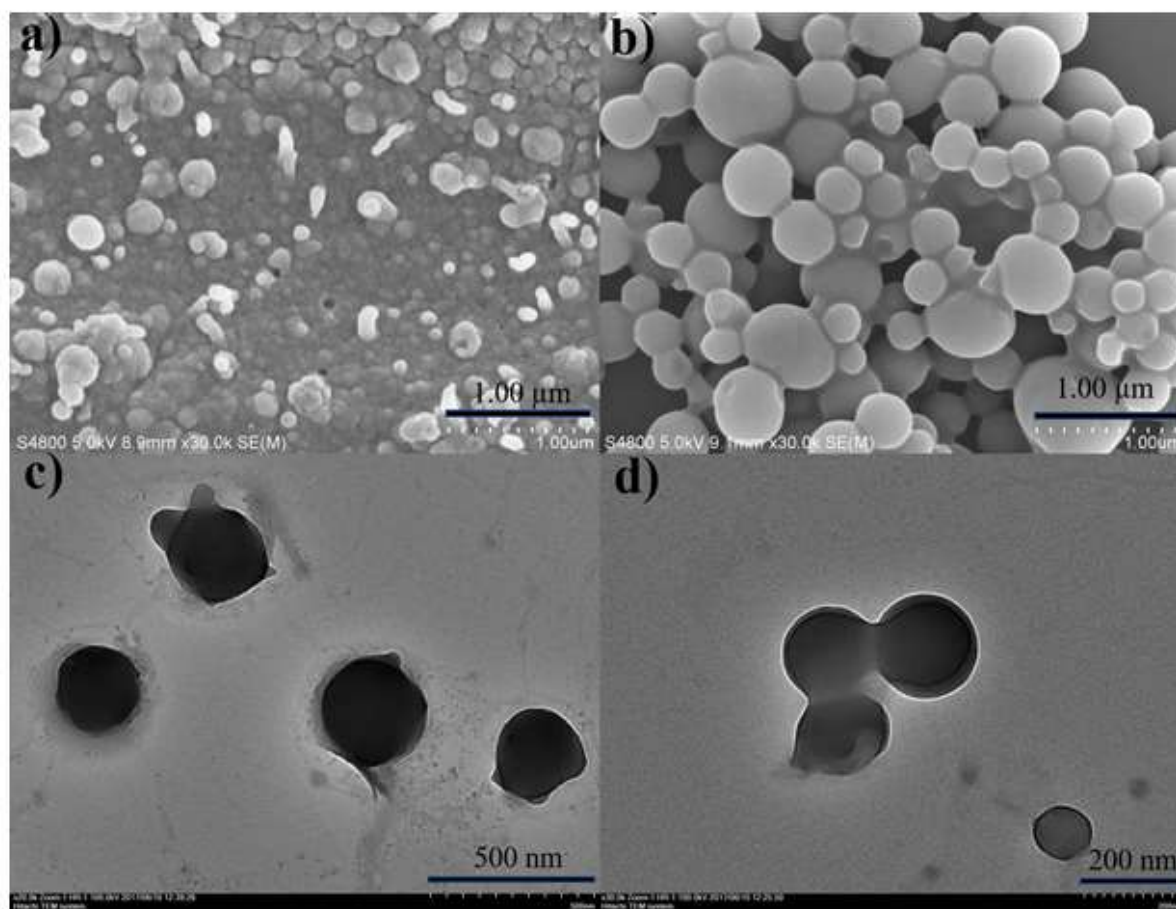
**Figure S12.** Absorbance (a) and fluorescence (b) spectra of **1c** (30  $\mu\text{M}$ ) in acetonitrile/water with different water fractions ( $f_w$ ), excited at 480 nm.





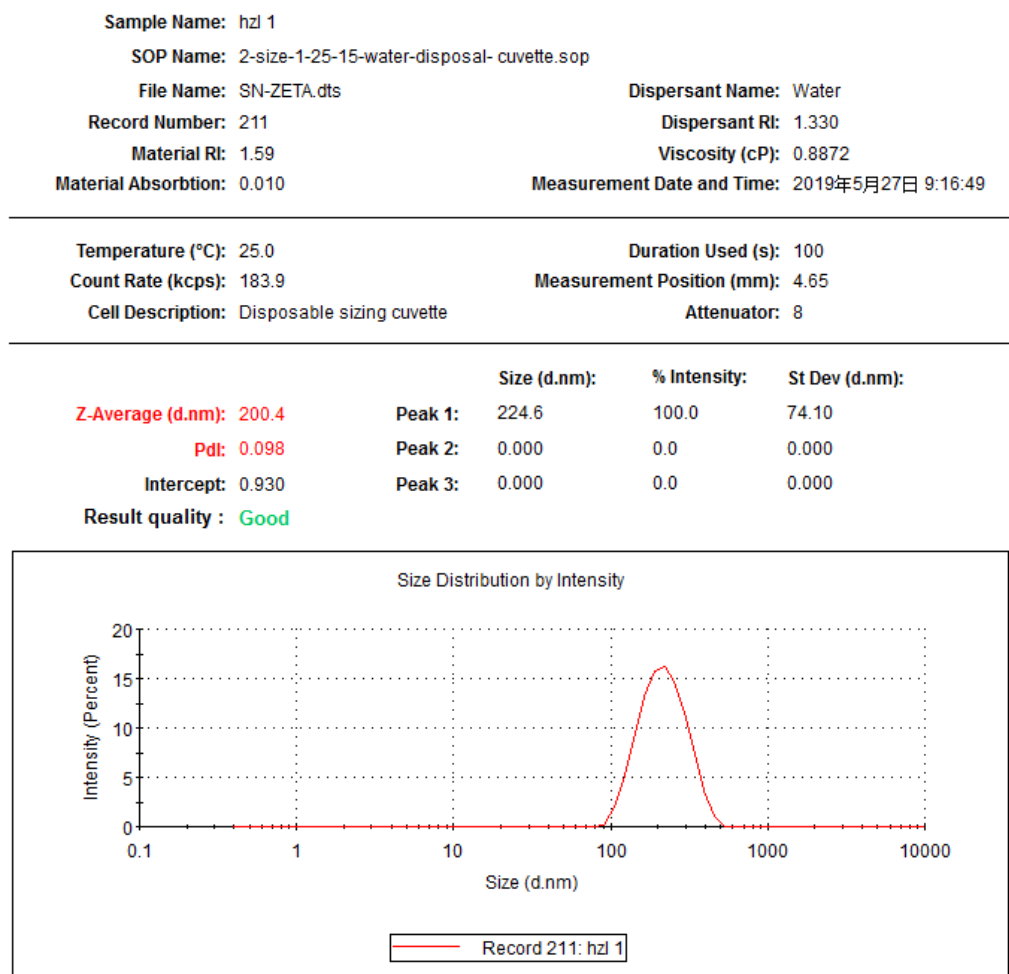
**Figure S13.** Absorbance (a) and fluorescence (b) spectra of **1d** (30  $\mu\text{M}$ ) in acetonitrile/water with different water fractions ( $f_w$ ), excited at 480 nm.

#### 4. SEM and TEM images



**Figure S14.** SEM (a, b) and TEM (c, d) images of nanoballs for **1c** (30 μM) and nanocuboid for **1d** (30 μM) in acetonitrile-water system with  $f_w = 90\%$ .

## 5. Dynamic light scattering



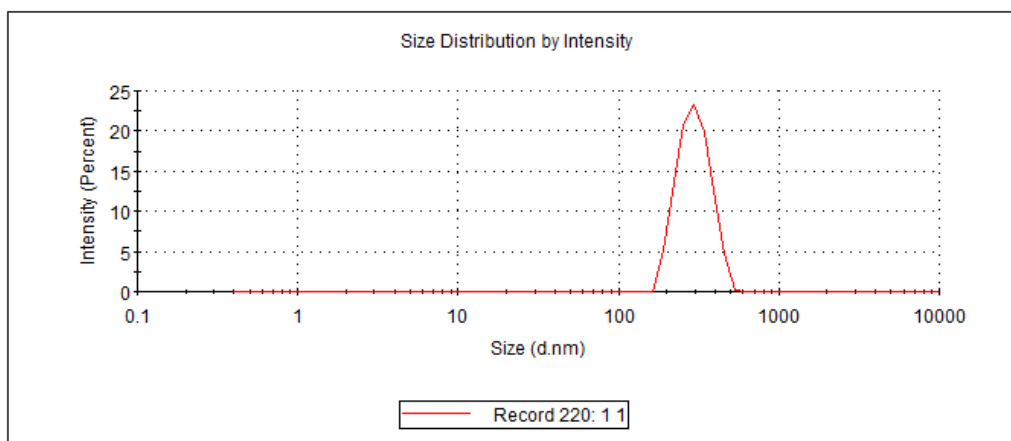
**Figure S15.** Dynamic light scattering (DLS) of the nanoparticles **1a** (50  $\mu\text{M}$ ) in acetonitrile-water system with water fraction equal to 99%.

**Sample Name:** 1 1  
**SOP Name:** 2-size-1-25-15-water-disposal- cuvette.sop  
**File Name:** dspe-1-zeta.dts **Dispersant Name:** Water  
**Record Number:** 220 **Dispersant RI:** 1.330  
**Material RI:** 1.59 **Viscosity (cP):** 0.8872  
**Material Absorbion:** 0.010 **Measurement Date and Time:** 2019年5月23日 10:16:19

**Temperature (°C):** 25.0 **Duration Used (s):** 100  
**Count Rate (kcps):** 355.3 **Measurement Position (mm):** 4.65  
**Cell Description:** Disposable sizing cuvette **Attenuator:** 9

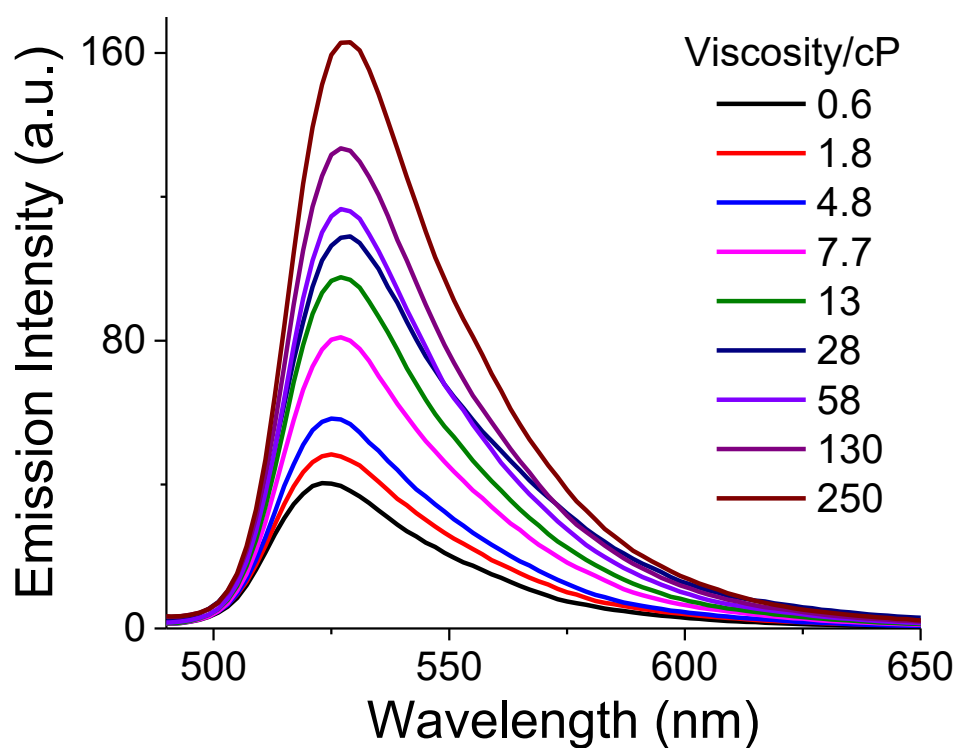
	Size (d.nm):	% Intensity:	St Dev (d.nm):
<b>Z-Average (d.nm):</b> 347.1	<b>Peak 1:</b> 301.3	100.0	68.36
<b>PdI:</b> 0.283	<b>Peak 2:</b> 0.000	0.0	0.000
<b>Intercept:</b> 0.825	<b>Peak 3:</b> 0.000	0.0	0.000

**Result quality :** Good

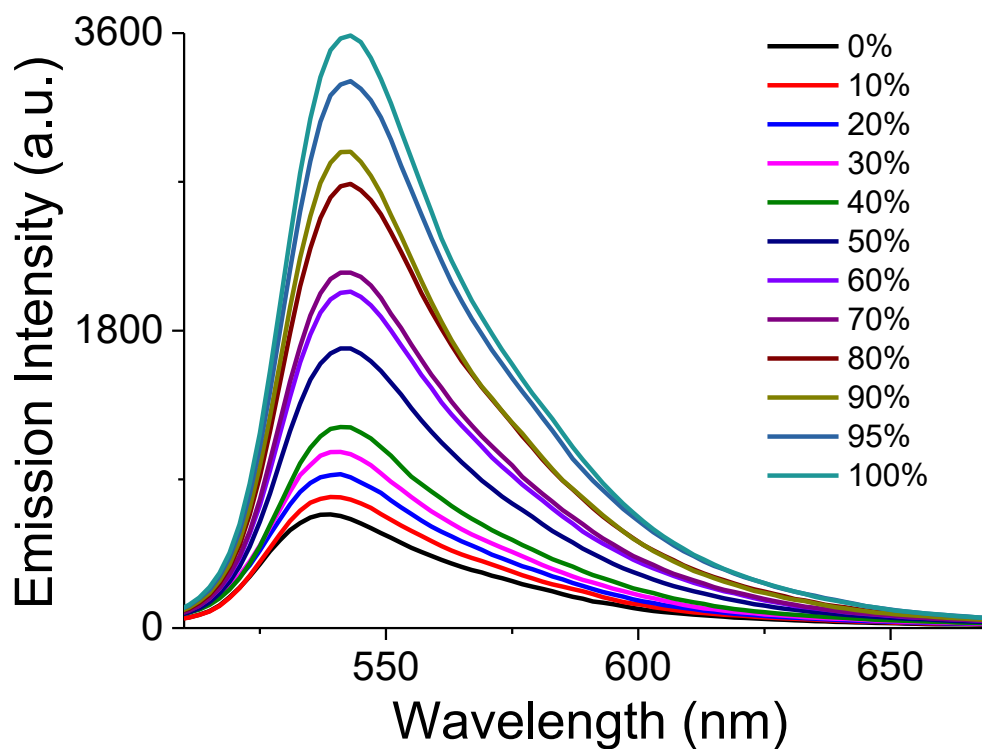


**Figure S16.** Dynamic light scattering (DLS) of the nanoparticles **1b** (30  $\mu$ M) in acetonitrile-water system with water fraction equal to 99%.

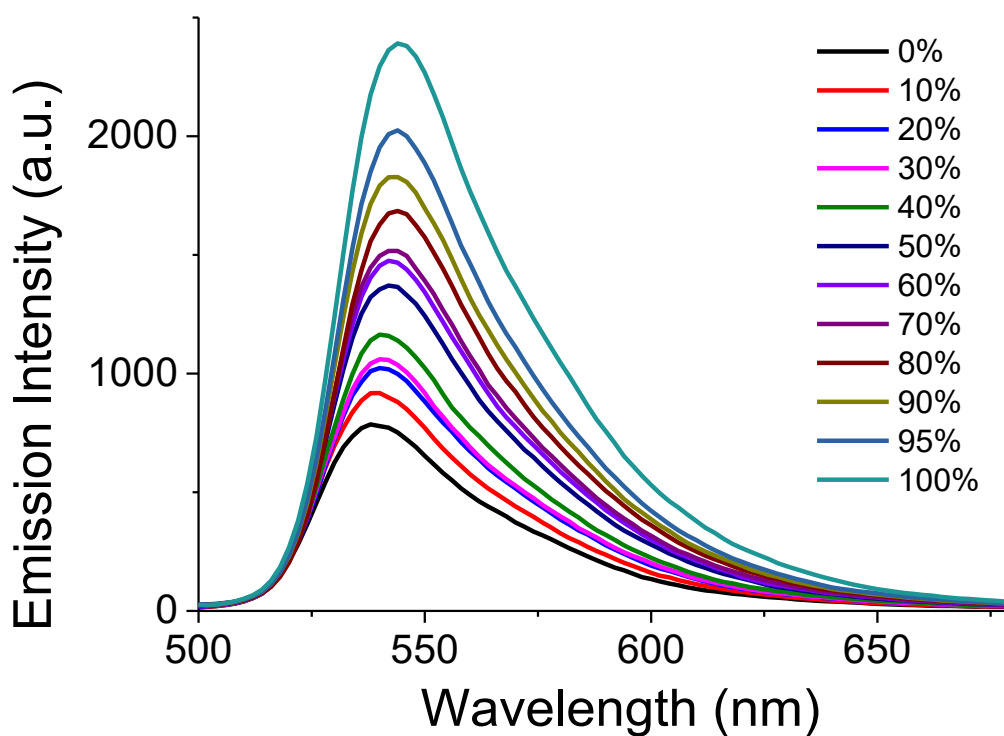
## 6. Viscosity sensitivity studies



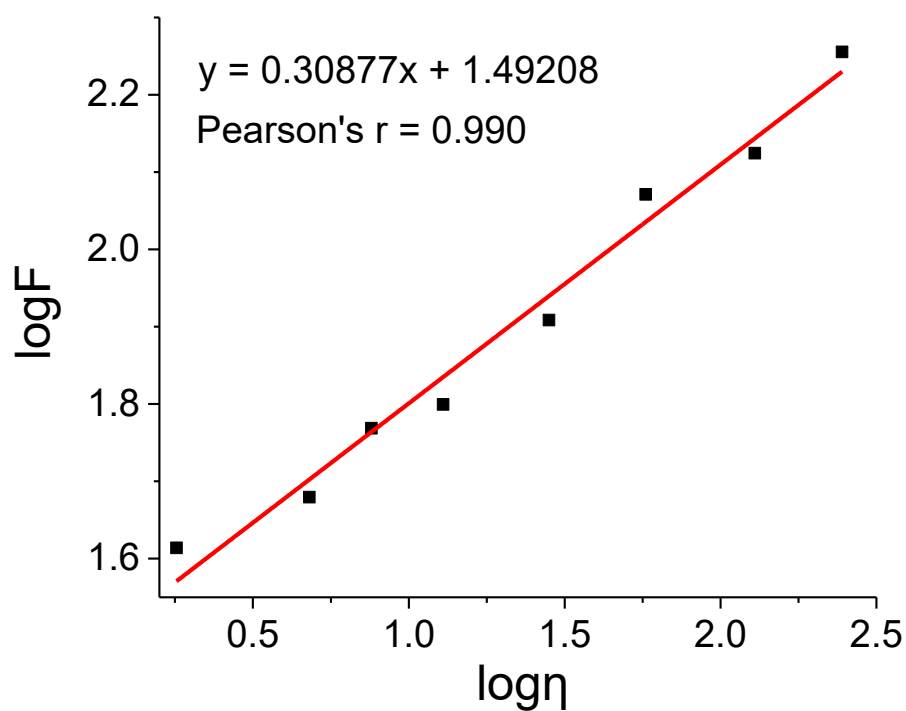
**Figure S17.** Changes of fluorescence intensity of **1b** (5  $\mu\text{M}$ , excited at 480 nm) in methanol-glycerol system with the variation of solution viscosity.



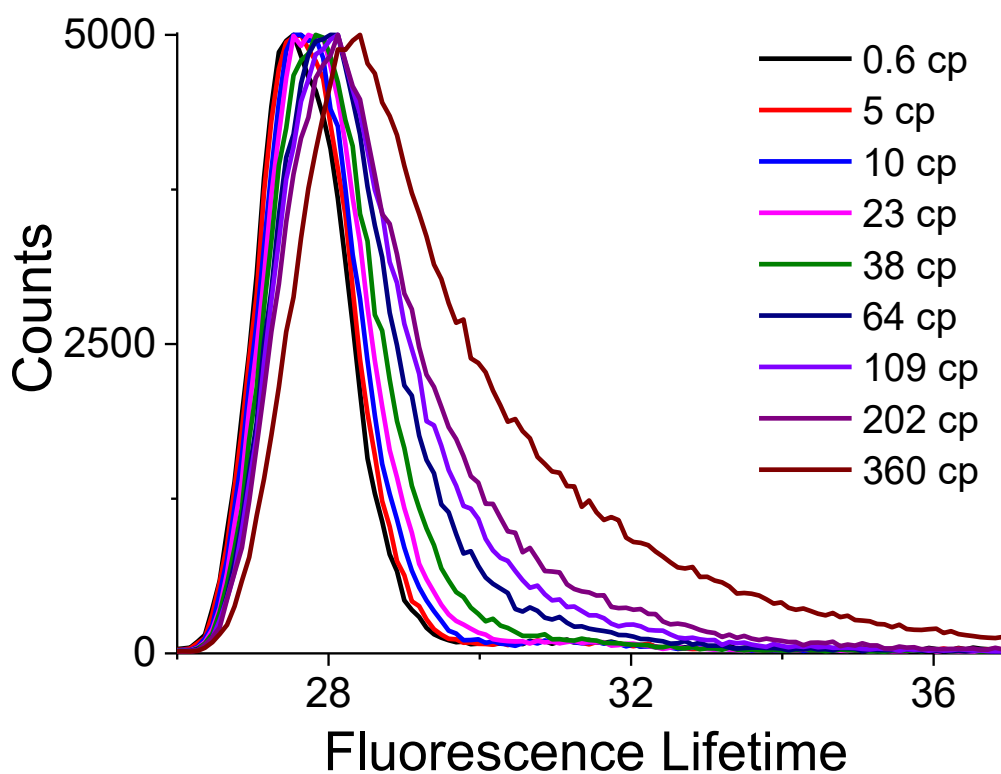
**Figure S18.** Viscosity change of the absorbance and fluorescence emission spectra of **1c** (5  $\mu\text{M}$ ) in methanol-glycerol mixtures, excited at 500 nm.



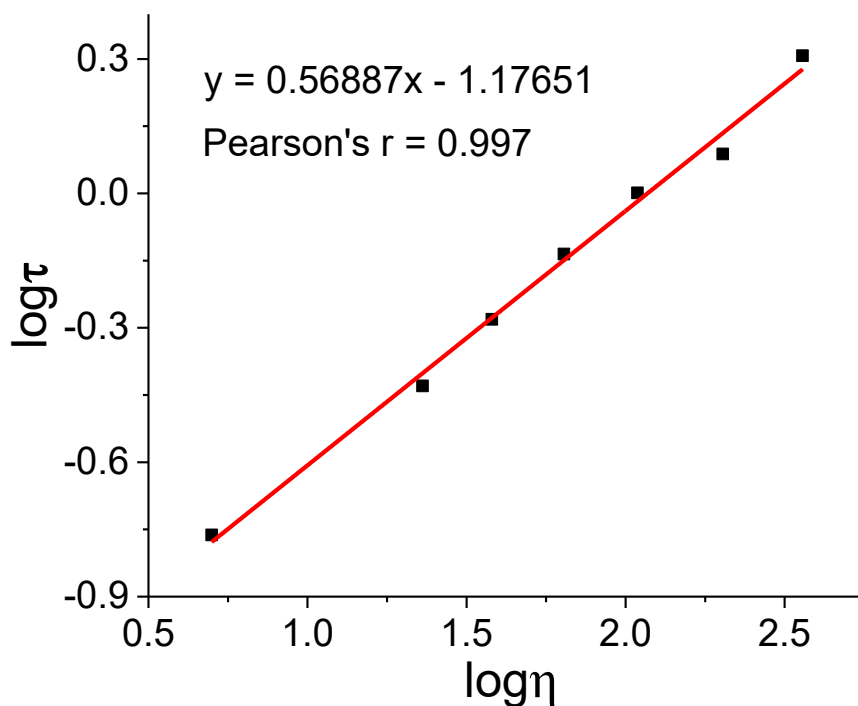
**Figure S19.** Viscosity change of the absorbance and fluorescence emission spectra of **1d** (5  $\mu\text{M}$ ) in methanol-glycerol mixtures, excited at 480 nm.



**Figure S20.** The linear relationship of **1b** between the fluorescent intensity and the viscosity  $\eta$ .

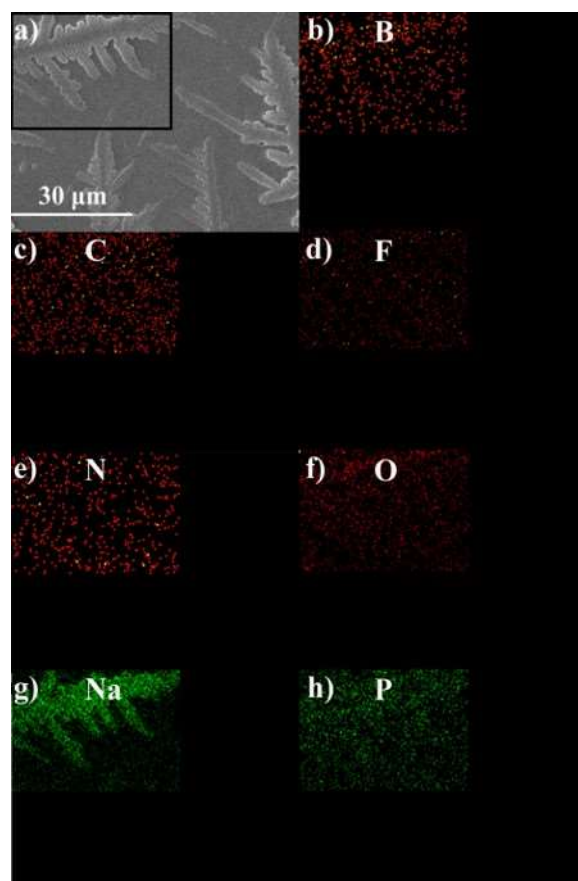


**Figure S21.** The fluorescence lifetime spectra of **1b** with different viscosity collected at 560 nm.

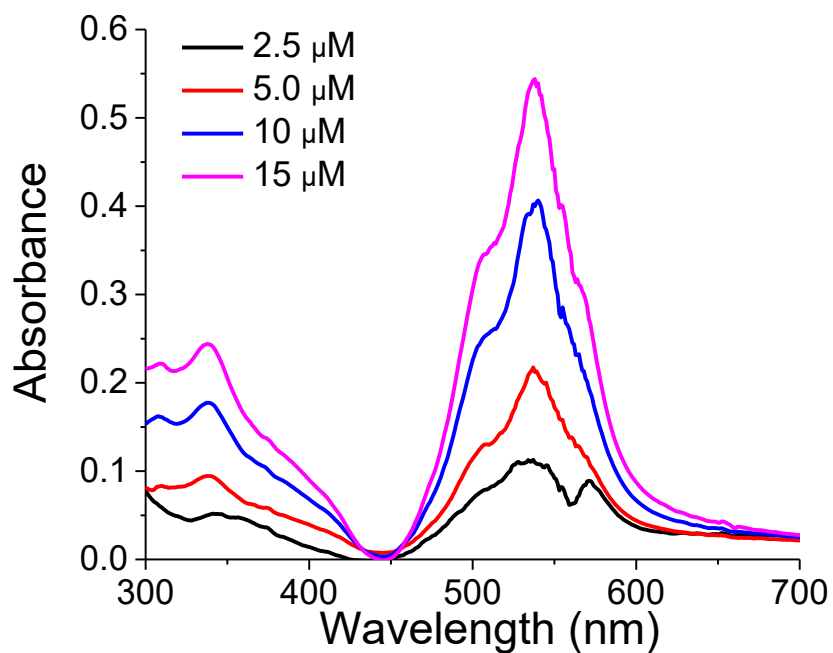


**Figure S22.** The linear relationship of **1b** between the fluorescence lifetime and the viscosity  $\eta$ .

## 7. Cell culture

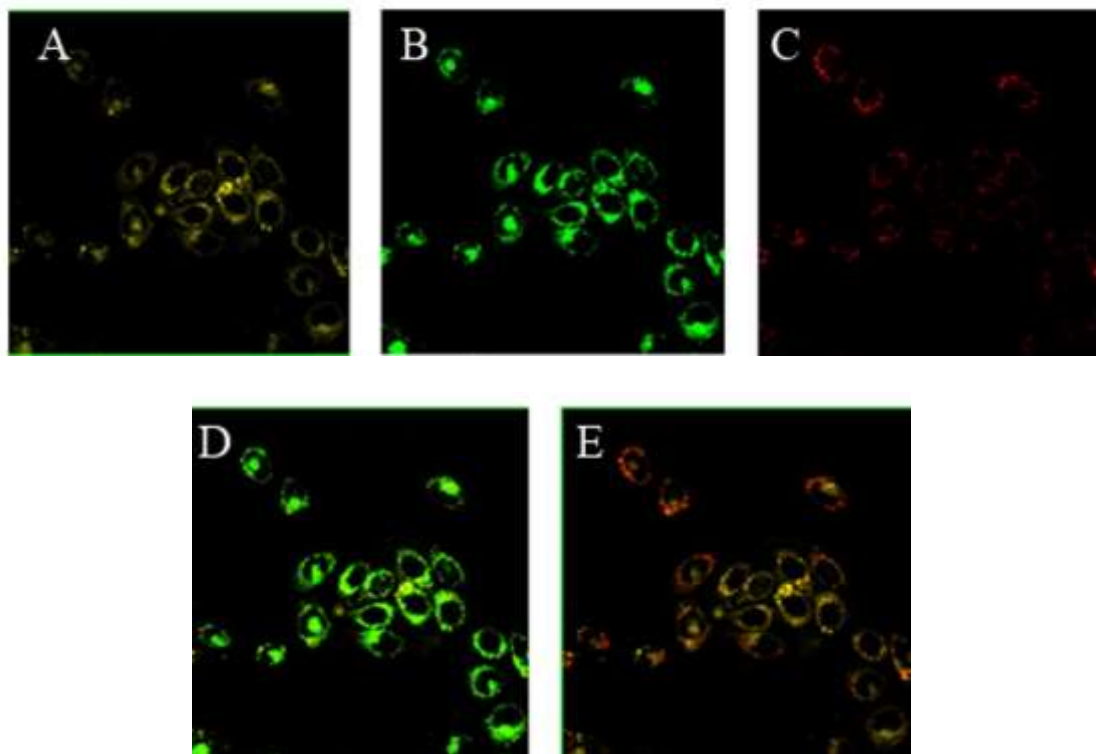


**Figure S23.** a) SEM image of BODIPY 1a (5  $\mu\text{M}$ ) in phosphate-buffered saline (PBS) and EDS mapping in the rectangle frame for B (b), C (c), F (d), N (e), O (f), Na (g) and P (h).

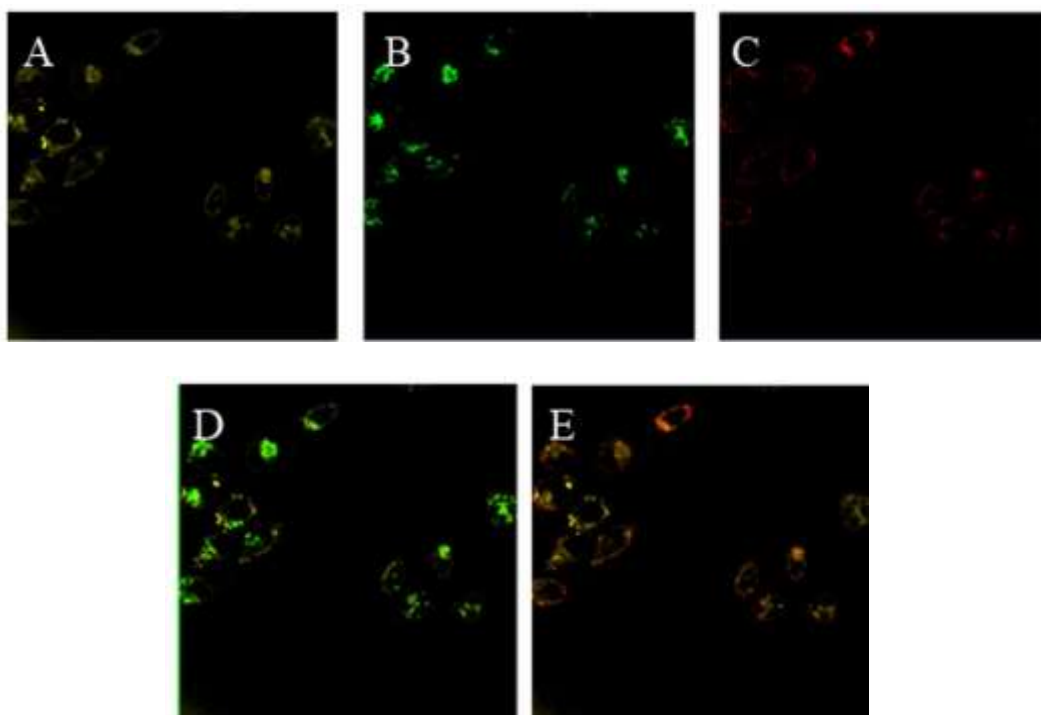


**Figure S24.** Absorbance of BODIPY 1a with different concentrations of 2.5  $\mu\text{M}$ , 5  $\mu\text{M}$ , 10  $\mu\text{M}$  and 15  $\mu\text{M}$  in dulbecco's modified eagle medium (DMEM).

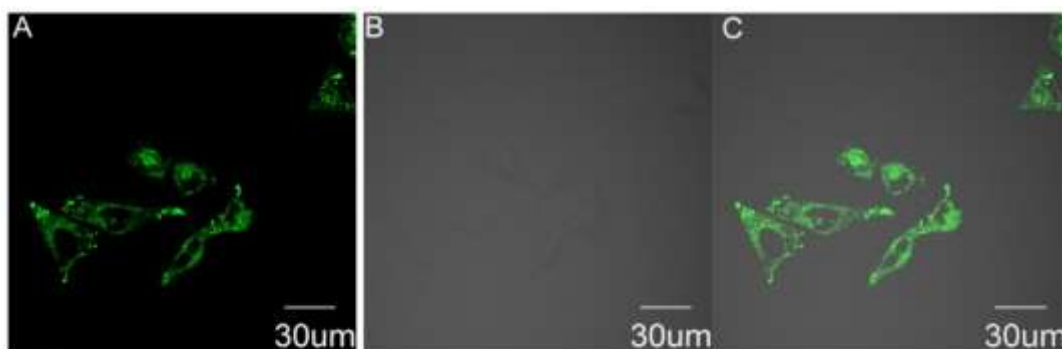




**Figure 25.** Co-location imaging studies in MCF-7 cells: (A) Stained with **1a** (5  $\mu$ M,  $\lambda_{\text{ex}}$  = 515 nm,  $\lambda_{\text{em}}$  = 520-600 nm); (B) Stained with DND-99 (1  $\mu$ M,  $\lambda_{\text{ex}}$  = 559 nm,  $\lambda_{\text{em}}$  = 575-620 nm); (C) Stained with Mito Deep Red (1  $\mu$ M  $\lambda_{\text{ex}}$  = 635 nm,  $\lambda_{\text{em}}$  = 655-755 nm); (D) Merge of A and B; (E) Merge of A and C.



**Figure 26.** Co-location imaging studies in MCF-7 cells: (A) Stained with **1b** (5  $\mu$ M,  $\lambda_{ex}$  = 515 nm,  $\lambda_{em}$  = 520-600 nm); (B) Stained with DND-99 (1  $\mu$ M,  $\lambda_{ex}$  = 559 nm,  $\lambda_{em}$  = 575-620 nm); (C) Stained with Mito Deep Red (1  $\mu$ M,  $\lambda_{ex}$  = 635 nm,  $\lambda_{em}$  = 655-755 nm); (D) Merge of A and B; (E) Merge of A and C.



**Figure S27.** Imaging of **1b** in MCF-7 cells. (A) MCF-7 cells were stained with **1b** (5  $\mu$ M,  $\lambda_{ex}$  = 488 nm,  $\lambda_{em}$  = 510-600 nm); (B) DIC image; (C) Merge of A and B.

## 8. MTT Assay

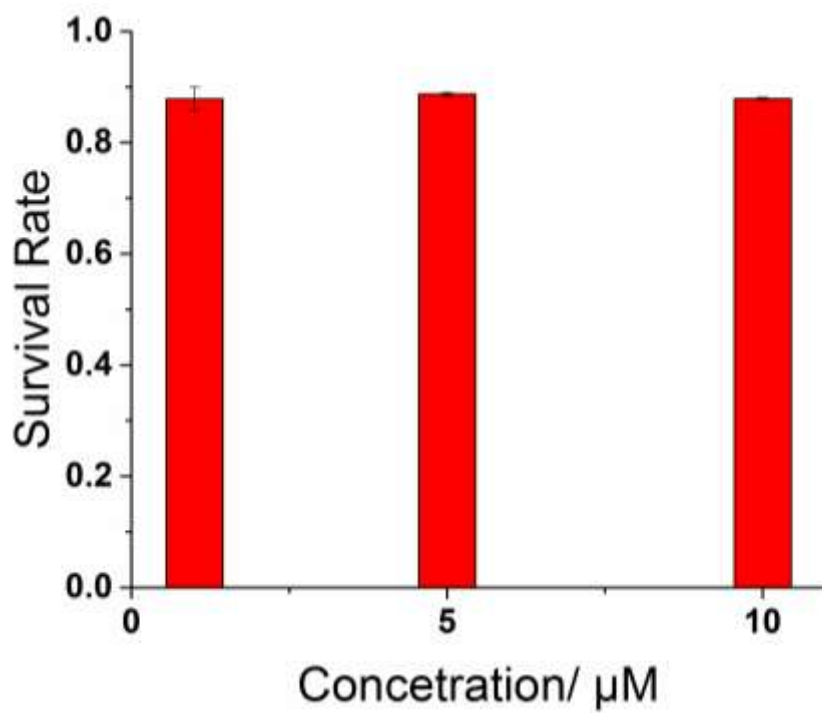


Figure S28. Cell viability of **1a** at different concentrations.

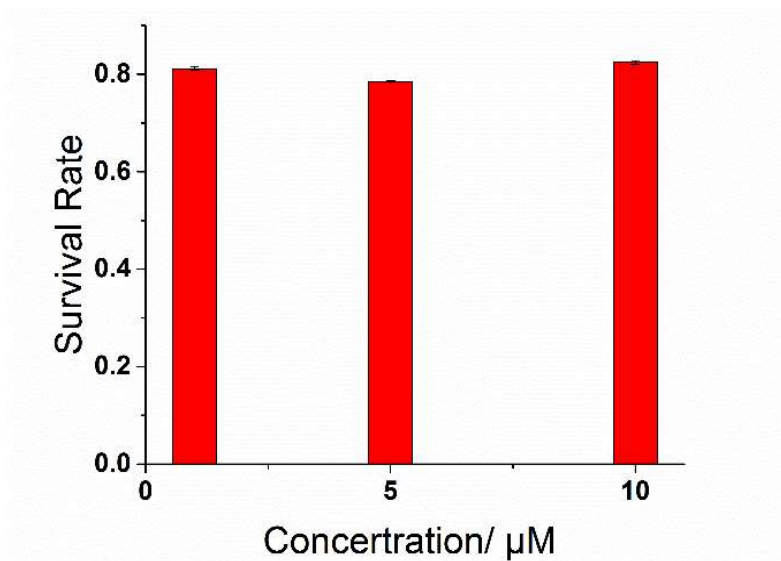
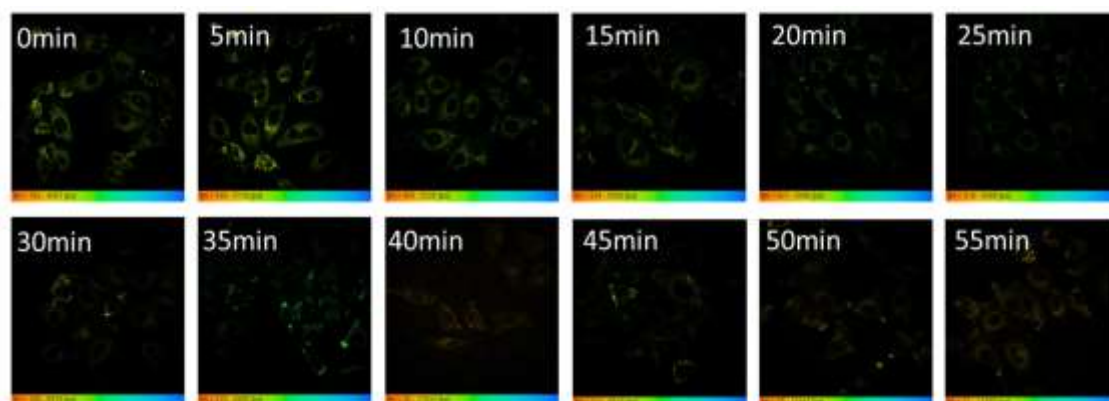
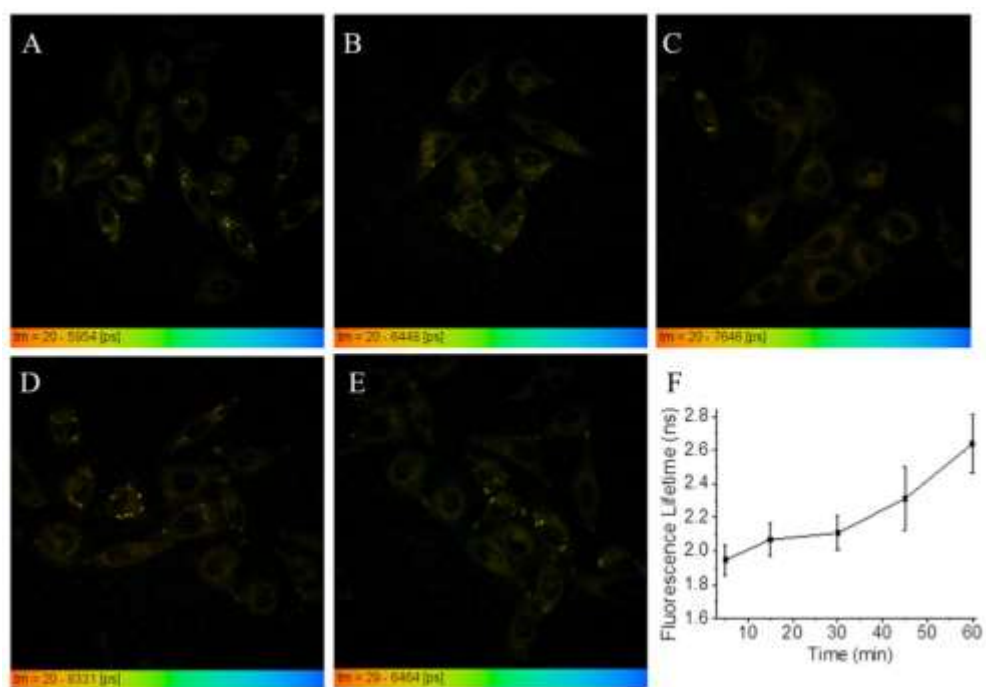


Figure S29. Cell viability of **1b** at different concentrations.

## 9. Viscosity determination in real-time during apoptosis

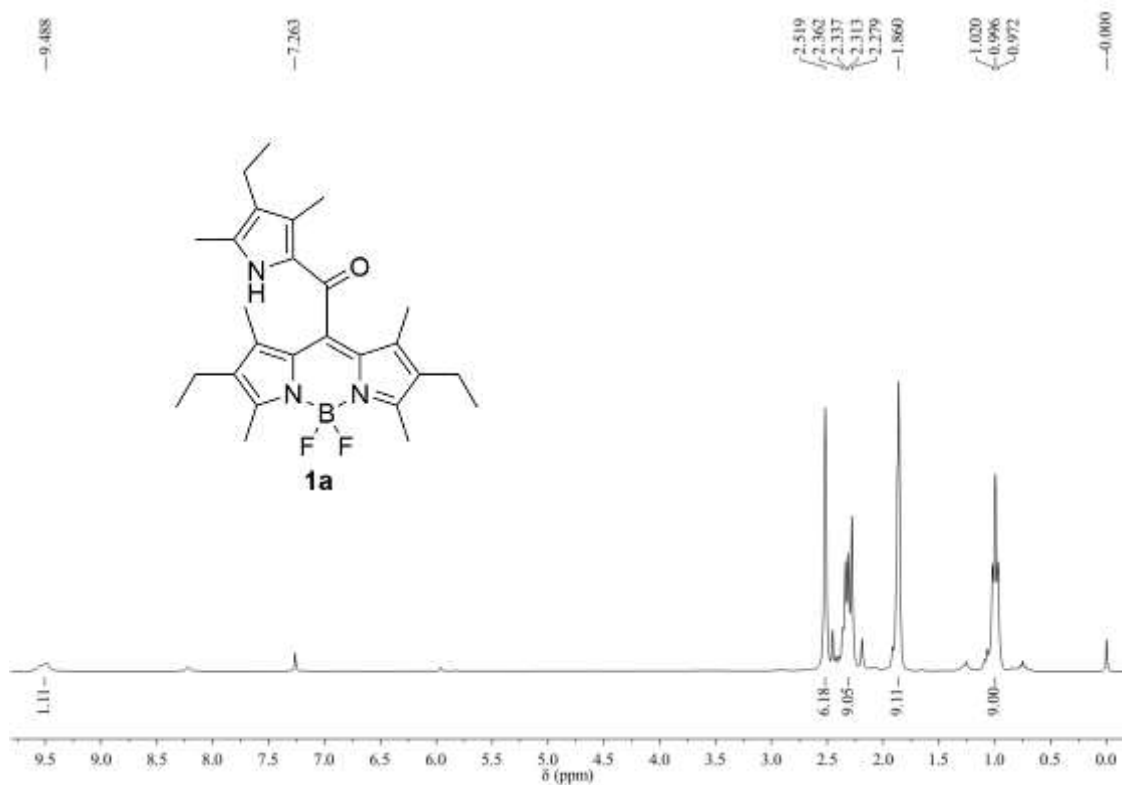


**Figure S30.** FLIM of MCF-7 cells in the absence and presence of etoposide for 0-60 min (A-E); (G) Plots of fluorescence lifetimes of **1a** ( $5 \mu\text{M}$ ) stimulate for different times using etoposide.

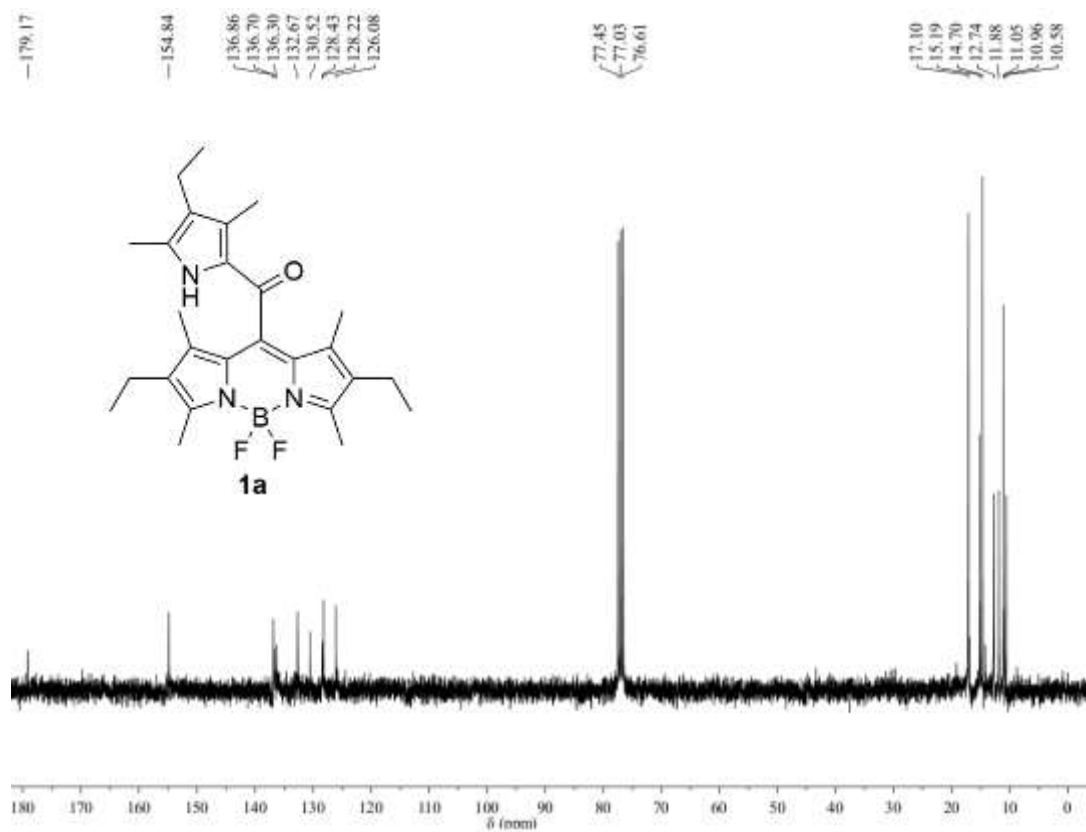


**Figure S31.** FLIM of MCF-7 cells in the absence and presence of etoposide for 0-60 min (A-E); (G) Plots of fluorescence lifetimes of **1b** ( $5 \mu\text{M}$ ) stimulate for different times using etoposide.

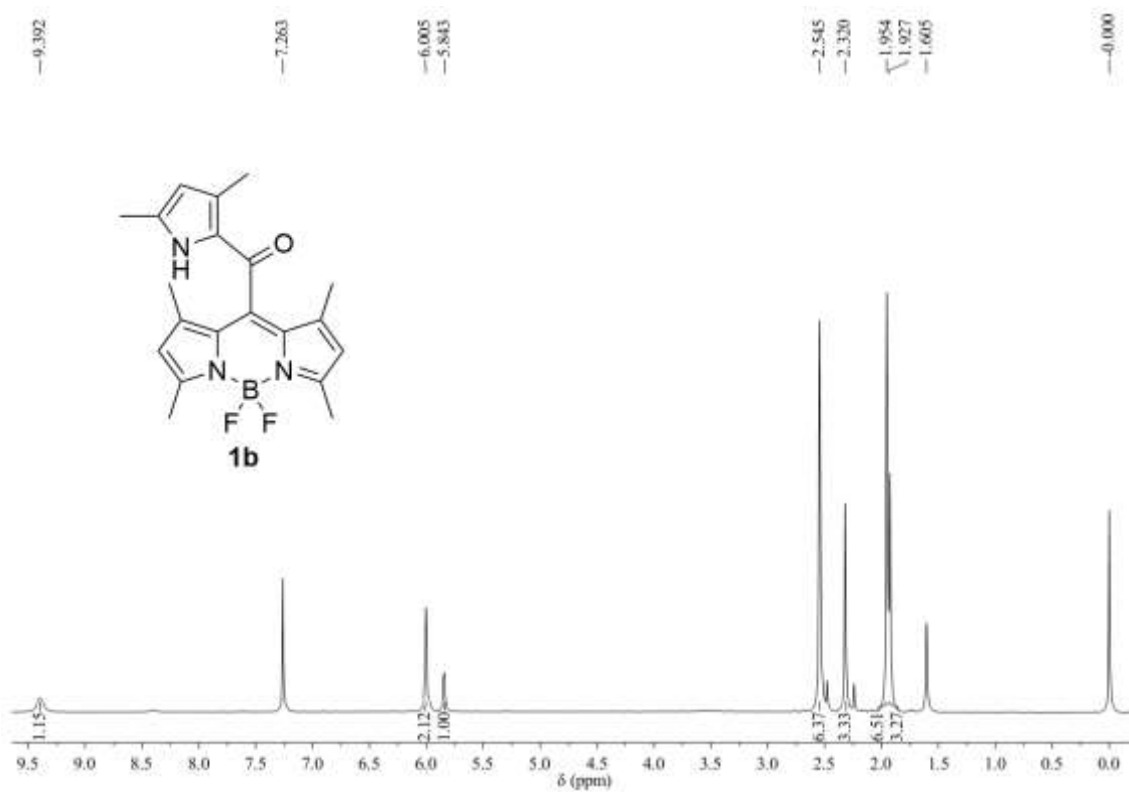
## 10. NMR spectra for *meso*-2-ketopyrrolyl BODIPYs



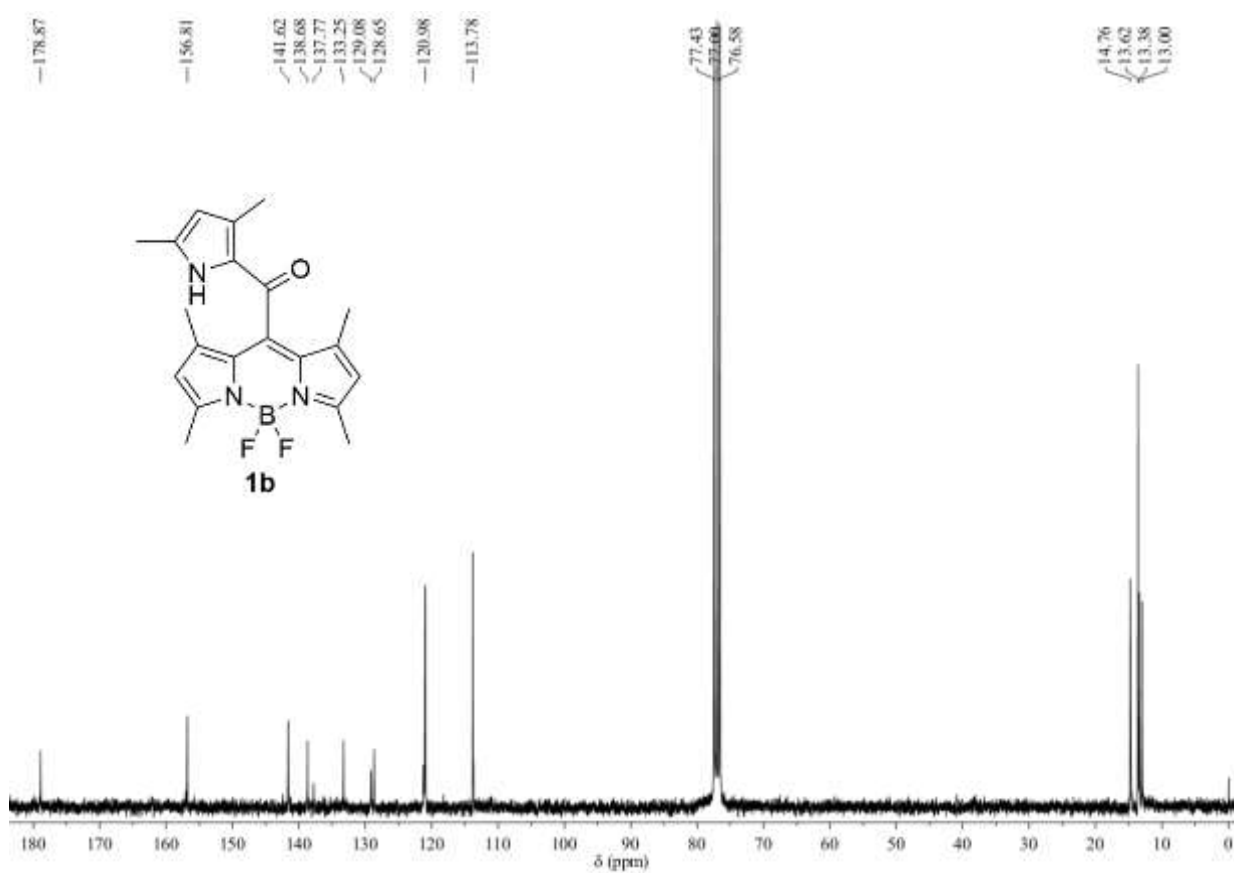
<sup>1</sup>H NMR spectrum of *meso*-2-ketopyrrolyl derived BODIPY **1a** in CDCl<sub>3</sub>



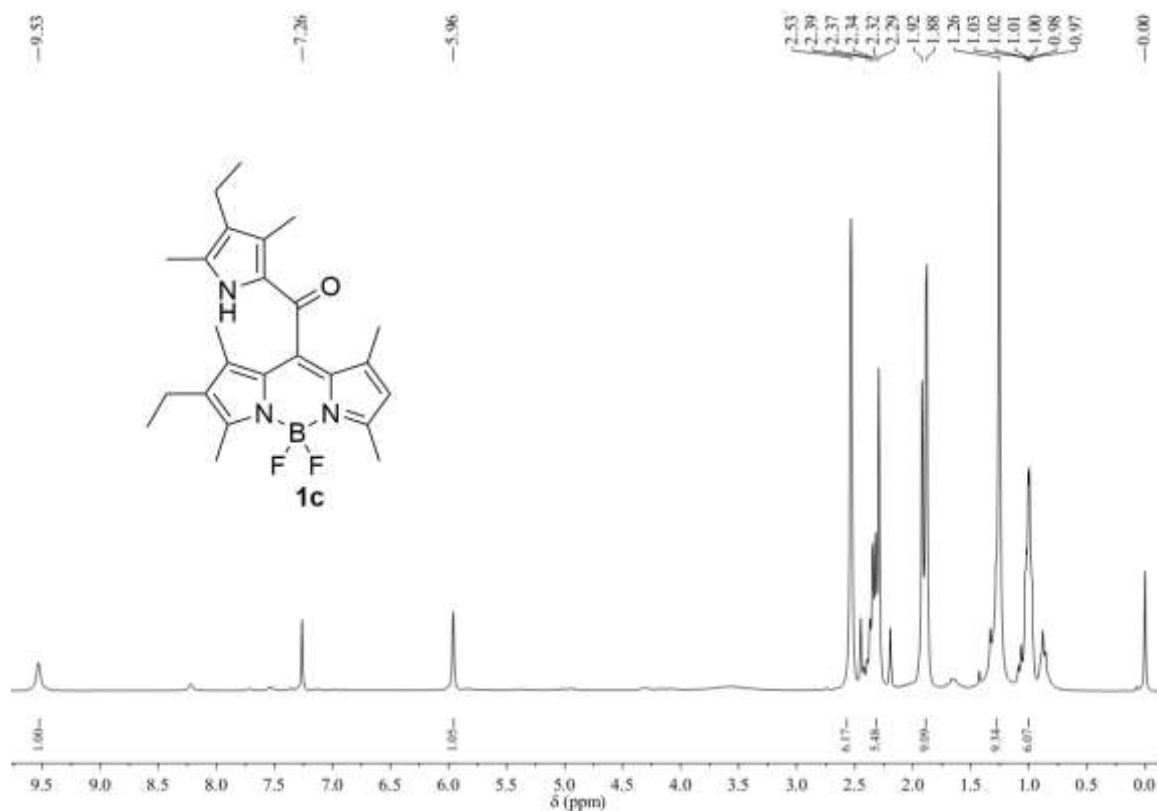
<sup>13</sup>C NMR spectrum of *meso*-2-ketopyrrolyl derived BODIPY **1a** in CDCl<sub>3</sub>



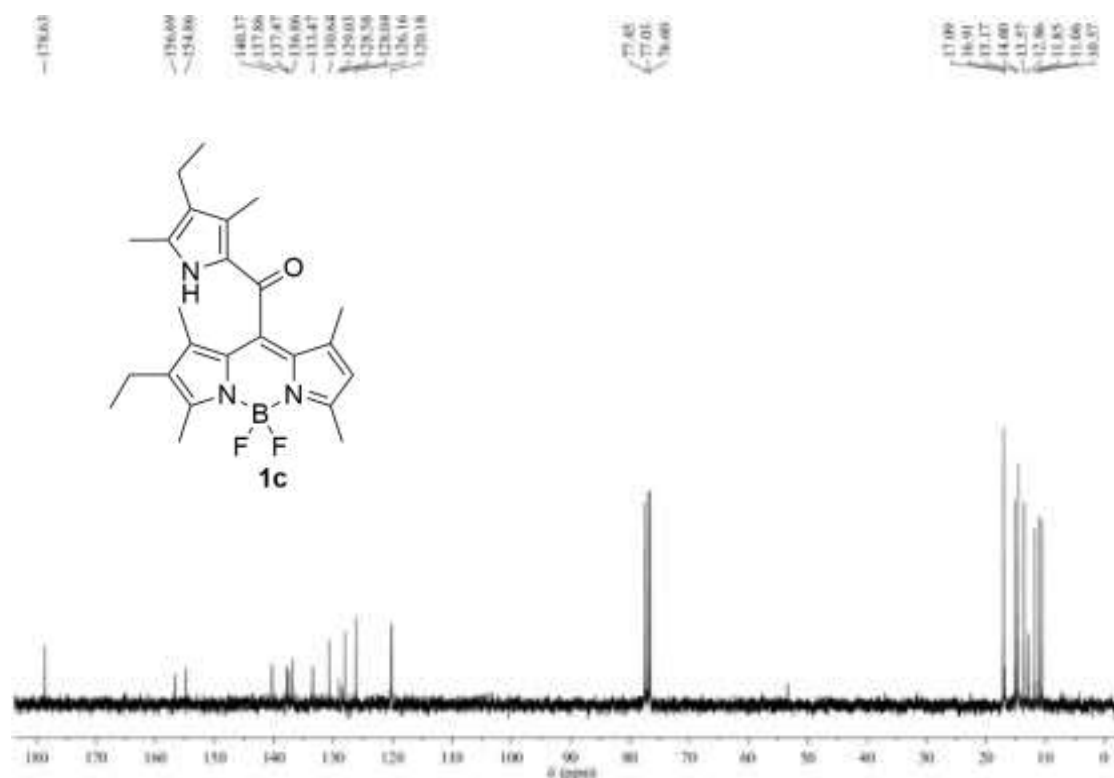
<sup>1</sup>H NMR spectrum of *meso*-2-ketopyrrolyl derived BODIPY **1b** in CDCl<sub>3</sub>



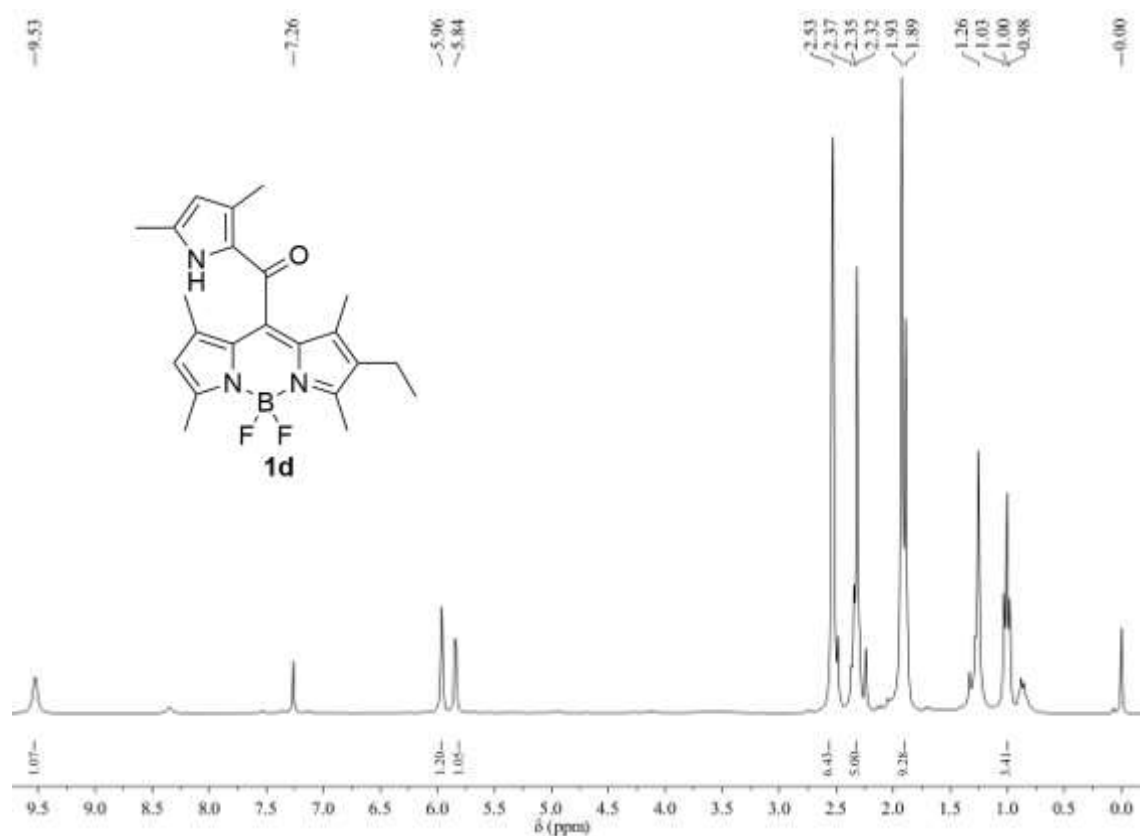
<sup>13</sup>C NMR spectrum of *meso*-2-ketopyrrolyl derived BODIPY **1b** in CDCl<sub>3</sub>



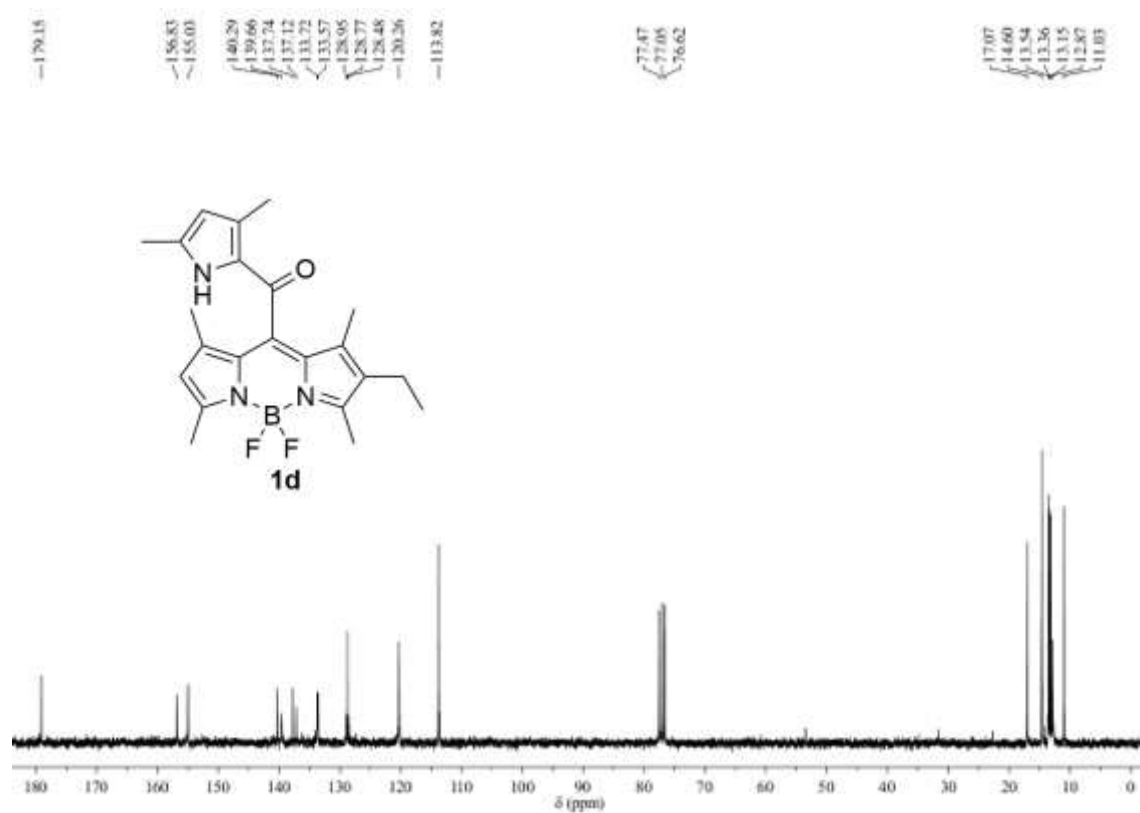
<sup>1</sup>H NMR spectrum of *meso*-2-ketopyrrolyl derived BODIPY **1c** in CDCl<sub>3</sub> solution



<sup>13</sup>C NMR spectrum of *meso*-2-ketopyrrolyl derived BODIPY **1c** in CDCl<sub>3</sub> solution



<sup>1</sup>H NMR spectrum of *meso*-2-ketopyrrolyl derived BODIPY **1d** in CDCl<sub>3</sub> solution

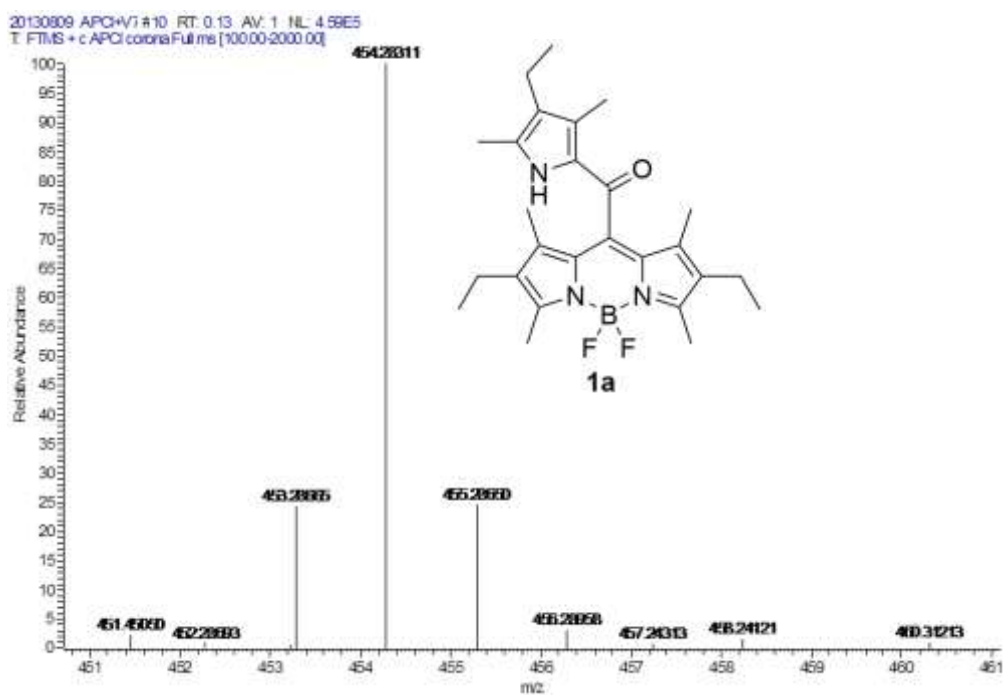


<sup>13</sup>C NMR spectrum of *meso*-2-ketopyrrolyl derived BODIPY **1d** in CDCl<sub>3</sub> solution

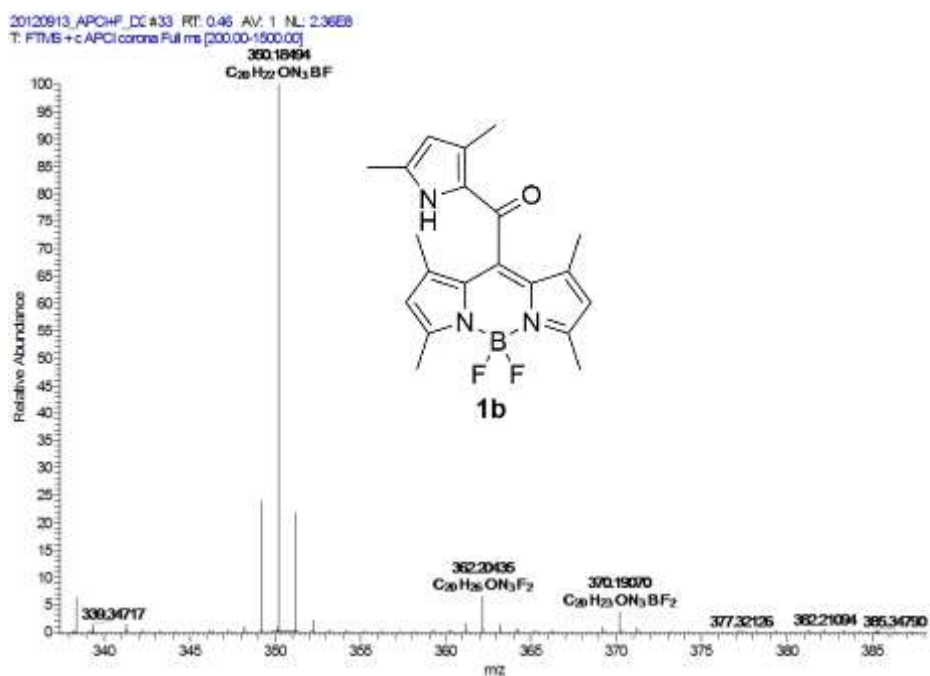


## 11. HRMS for *meso*-2-ketopyrrolyl derived BODIPYs

### HRMS of 1a

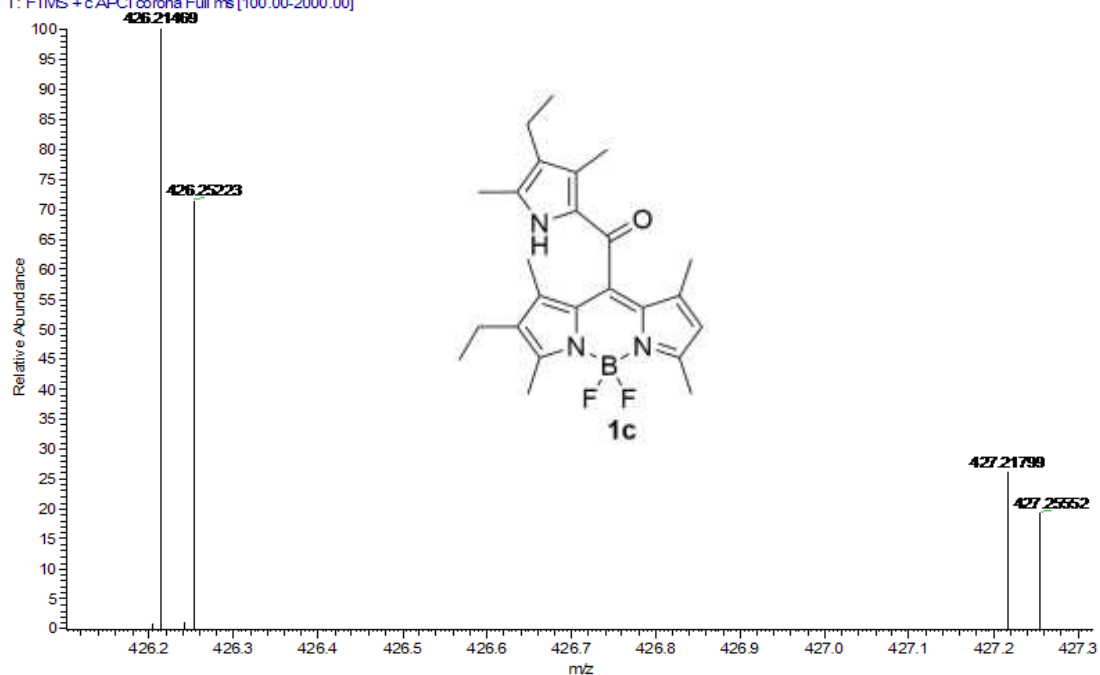


### HRMS of 1b



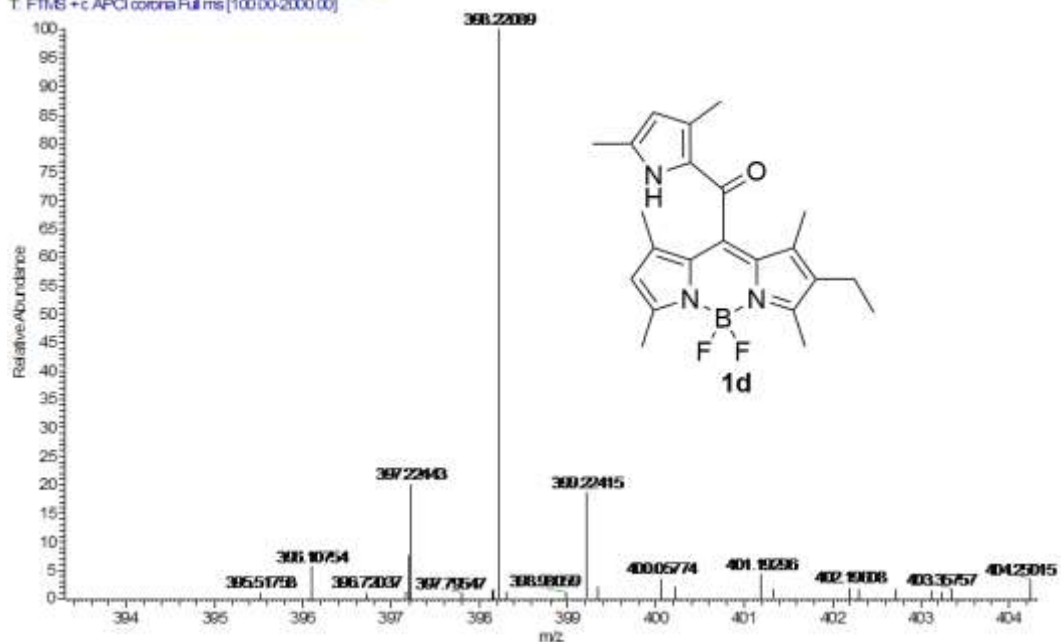
## HRMS of *meso*-2-ketopyrrolylBODIPY 1c

20130809\_APCI+VE #11 RT: 0.15 AV: 1 SB: 4 0.01-0.06 NL: 6.50E5  
T: FTMS +c APCI corona Full ms [100.00-2000.00]



## HRMS of *meso*-2-ketopyrrolylBODIPY 1d

20130809\_APCI+VE #11 RT: 0.15 AV: 1 NL: 3.54E5  
T: FTMS +c APCI corona Full ms [100.00-2000.00]



## 12. DFT computations

**Table S4.** Selected electronic excitation energies (eV) and oscillator strengths (f), configurations of the low-lying excited states of *meso*-2-ketopyrrolyl BODIPYs **1a** calculated by TDDFT//B3LYP/6-31+G(d,p), based on the optimized ground state geometries. The TDDFT calculations of all the molecules in dichloromethane were done by using the Self-Consistent Reaction Field method and the Polarizable Continuum Model.

Electronic transition	TD//B3LYP/6-31+G(d, p)			
	Energy/ eV [a] nm	<i>f</i> <sup>[b]</sup>	Composition [c]	CI [d]
S0→S1	2.6513 eV 467.63 nm	0.2725	HOMO -1 → LUMO	0.4533
			HOMO → LUMO	0.5334
S0→S2	2.7606 eV 449.12 nm	0.3296	HOMO -1 → LUMO	0.5403
			HOMO → LUMO	0.4408
S0→S3	3.2421 eV 382.42 nm	0.1056	HOMO -2 → LUMO	0.6879
			HOMO -1 → LUMO	0.1514

PCM-DFT optimized coordinates for *meso*-2-ketopyrrolyl BODIPY **1a**

F	-2.97442500	-0.05047800	2.04099400
F	-4.22904900	0.20534100	0.13134100
N	-2.23428600	-1.17516400	0.02409900
N	-2.07065300	1.30760100	0.24501900
N	2.06125800	-0.20249200	0.98092200
H	1.16226200	-0.15721300	1.43990700
O	1.28371000	0.05575600	-2.54643500
C	-0.80830300	1.25348100	-0.35506900
C	-0.96538300	-1.18203100	-0.56524500
C	-0.25739200	0.01784800	-0.72686800
C	-2.70208400	-2.44052900	0.04711100
C	-2.37462800	2.59955900	0.48729200
C	-0.65403000	-2.53316000	-0.92774900
C	2.24482900	-0.14368700	-0.39703200
C	-0.32693800	2.59647700	-0.49336200
C	-1.31497900	3.43295300	0.03731400
C	3.25856500	-0.32184500	1.61285000
C	1.14362900	-0.02013200	-1.32339800
C	4.26264300	-0.34849500	0.63372900
C	3.62766800	-0.23605400	-0.63117300
C	-1.75090600	-3.31312900	-0.54690500
B	-2.92916100	0.07254000	0.63692300
C	-4.03687600	-2.78720000	0.62400800
H	-4.14732800	-2.36807900	1.62871300
H	-4.16562100	-3.86960800	0.67810600
H	-4.84480400	-2.36746400	0.01481200
C	3.35451800	-0.37903400	3.10514000
H	3.51093200	0.61585200	3.54093100
H	4.19273000	-1.00784100	3.41791600

H	2.44275300	-0.79448900	3.54647100
C	-3.65821100	3.00859600	1.13436600
H	-4.50465500	2.82989500	0.46235100
H	-3.63902300	4.06856300	1.39476300
H	-3.84365900	2.42348100	2.03995700
C	0.57843400	-3.02931400	-1.62623700
H	0.70129900	-2.55829700	-2.60662000
H	0.52837300	-4.11066000	-1.77243800
H	1.48780600	-2.81611800	-1.05365500
C	0.95872300	3.04384700	-1.12620800
H	1.83484600	2.62555300	-0.61901900
H	1.04450400	4.13219900	-1.09286700
H	1.01910500	2.73217200	-2.17380000
C	5.74204100	-0.44856800	0.89770900
H	5.91016900	-0.98401000	1.84019900
H	6.21165900	-1.06259900	0.11975200
C	4.29192100	-0.22164900	-1.97579700
H	3.78153200	-0.88591700	-2.67816300
H	5.34009900	-0.52372100	-1.90008400
H	4.26020700	0.77836200	-2.42436000
C	-1.30475800	4.93770400	0.09541600
H	-1.81683300	5.27307500	1.00546900
H	-0.27242400	5.29281400	0.19175600
C	-1.95858000	5.61111200	-1.12698600
H	-3.00677400	5.31066500	-1.22927800
H	-1.44355800	5.33020700	-2.05168300
H	-1.92582200	6.70268600	-1.03618200
C	-1.91288800	-4.80149300	-0.71069300
H	-2.97341700	-5.04204700	-0.84837300
H	-1.41733900	-5.12274000	-1.63411600
C	6.45705300	0.91500800	0.96022400
H	6.04560200	1.53946900	1.76067100
H	6.33967000	1.46361100	0.01986100
H	7.52920400	0.78723400	1.14699400
C	-1.35778500	-5.62075200	0.47083000
H	-1.49927400	-6.69448900	0.30378700
H	-1.85992700	-5.35384300	1.40699900
H	-0.28685100	-5.43591400	0.60718000