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Identify fatty liver diverse stage by a two-photon absorption triphenylamine-based BODIPY analogues

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Animal experiment

All procedures involving animals were approved by and conformed to the guidelines of the Anhui University Animal Care Committee, School of life science. We have taken great efforts to reduce the number of animals used in these studies and also taken effort to reduce animal suffering from pain and discomfort.

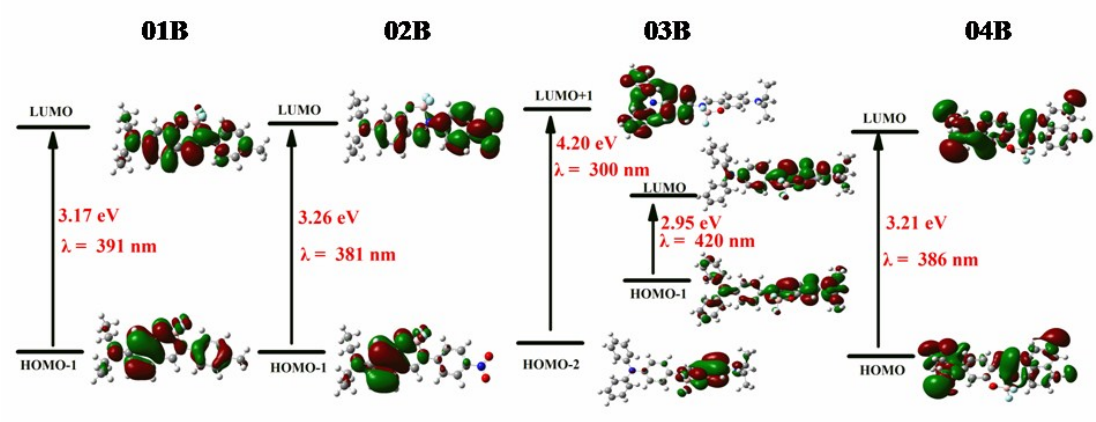

Fig. S1. Molecular orbital energy diagrams of all the **BODIPYs** analogues.

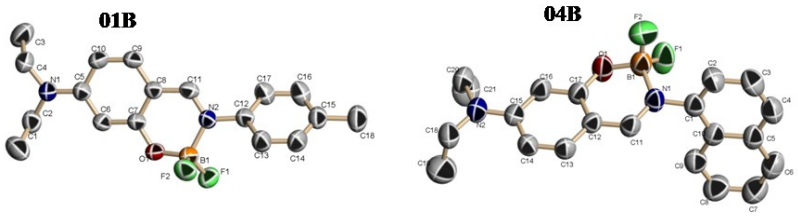

Fig. S2. ORTEP drawings for **0 1B** (left) and **04B** (right); Thermal ellipsoids are shown at the 50% probability level; H atoms are omitted for clarity.

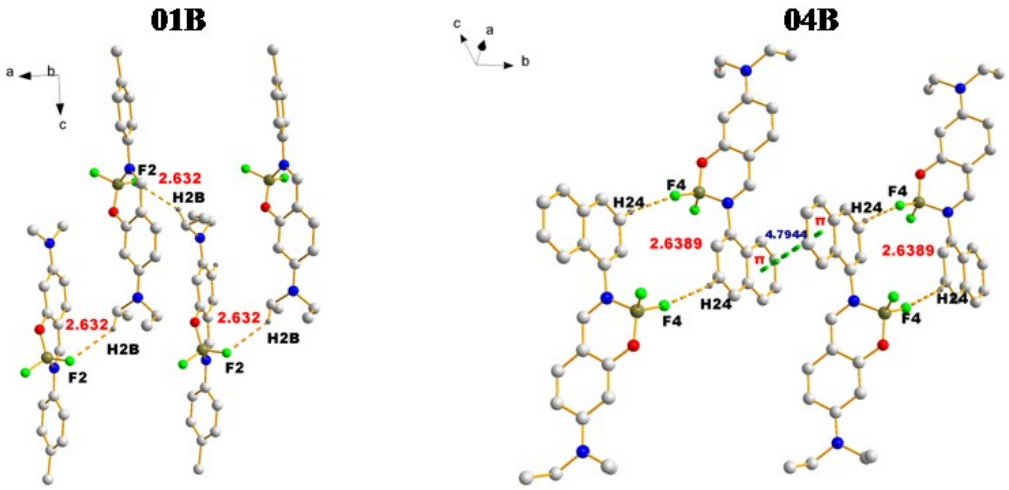

Fig. S3. Crystal packing mode of **01B** and **04B**, the intermolecular interactions are shown as dashed lines.

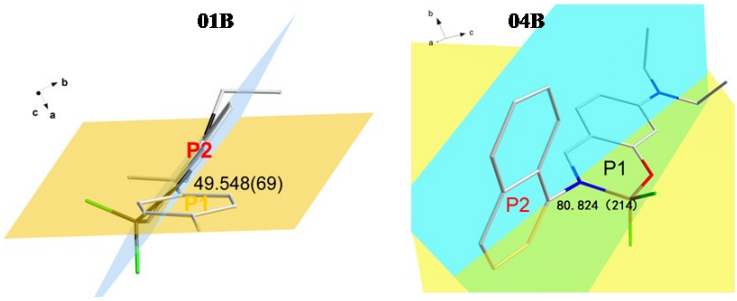

Fig. S4. Dihedral angle of **01B** and **04B**.

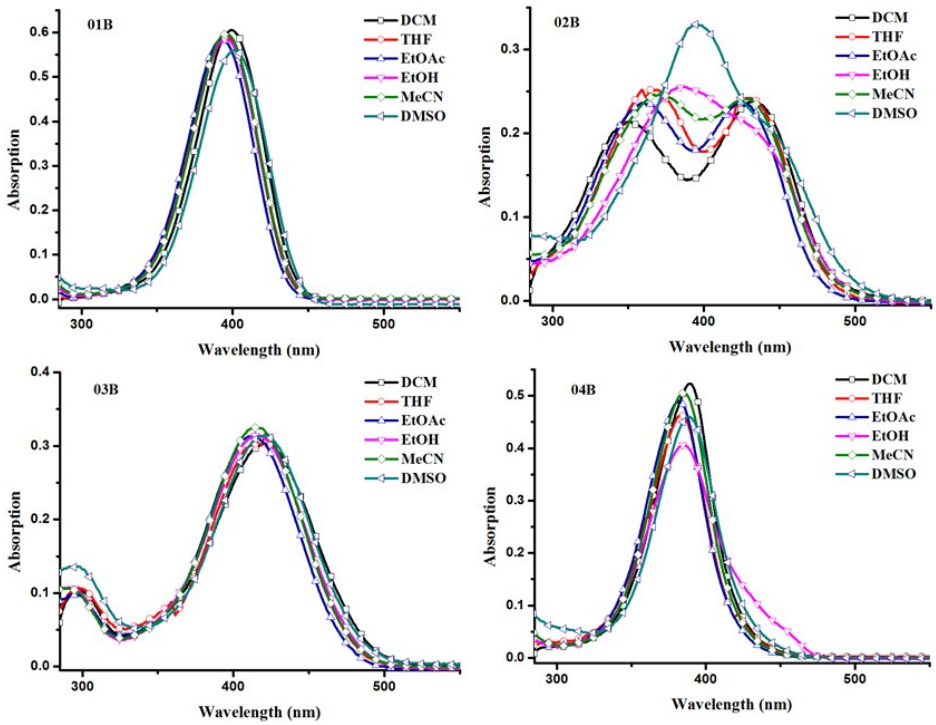

Fig. S5. UV-*vis* absorption spectra of **01B**~**04B** in different solvent (1.0×10^{-5}M).

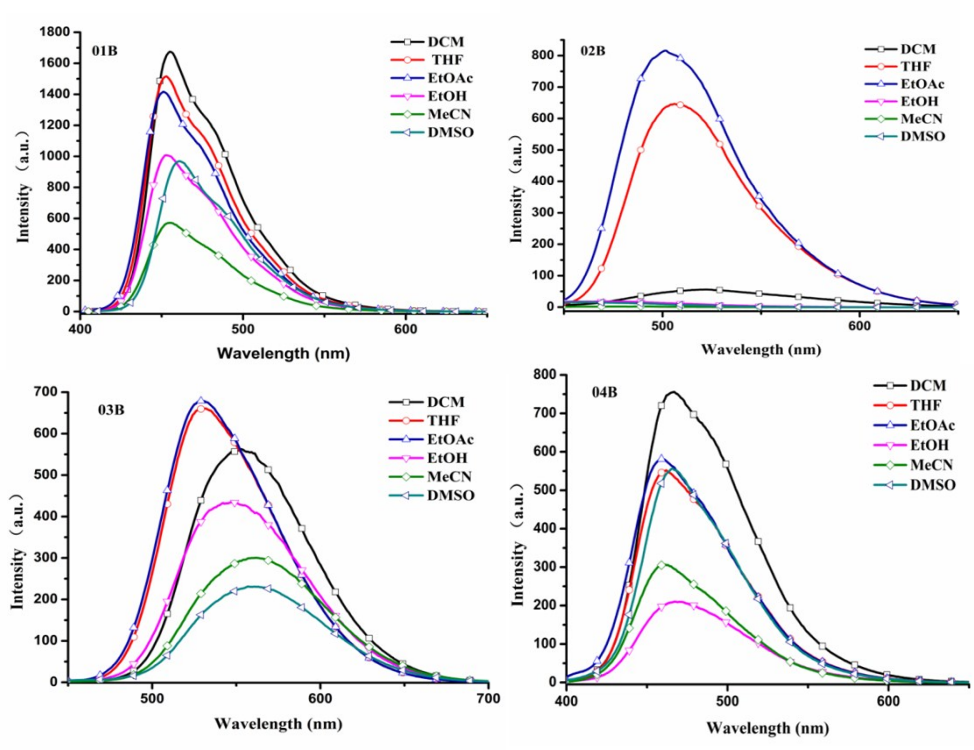

Fig. S6. Fluorescence emission spectra of **01B**~**04B** in different solvents (1.0×10^{-5} M).

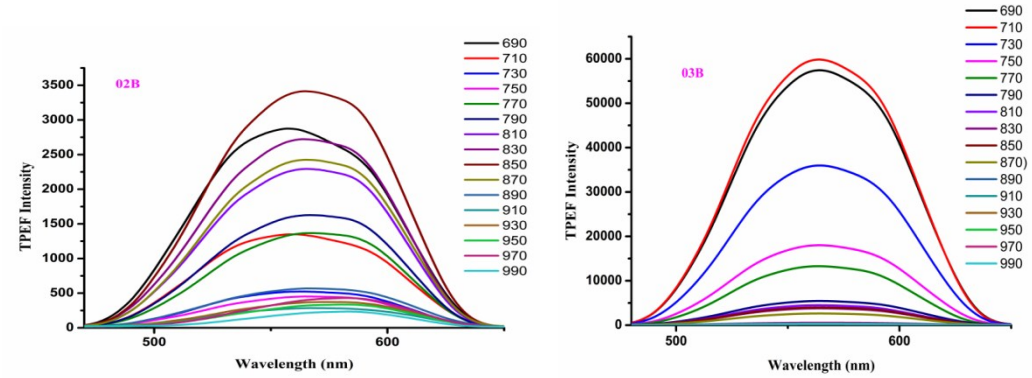

Fig. S7. Two-photon excited fluorescence of **02B** and **03B.**

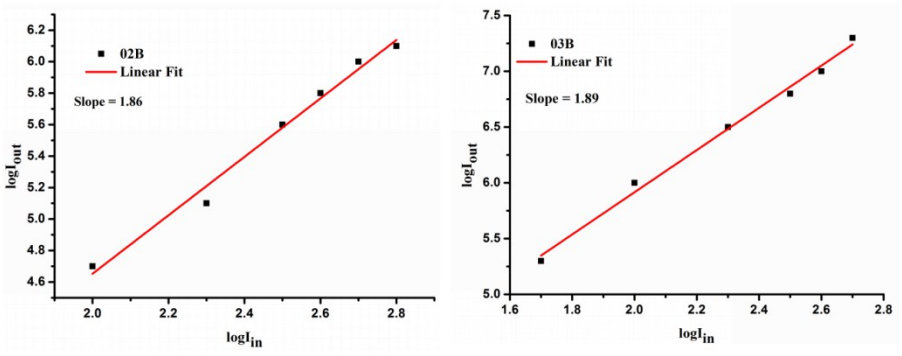

Fig. S8 The logarithmic plots of power-squared dependence of the 2PA-induced fluorescence

intensity on the input intensity of these compounds in corresponding solvents.

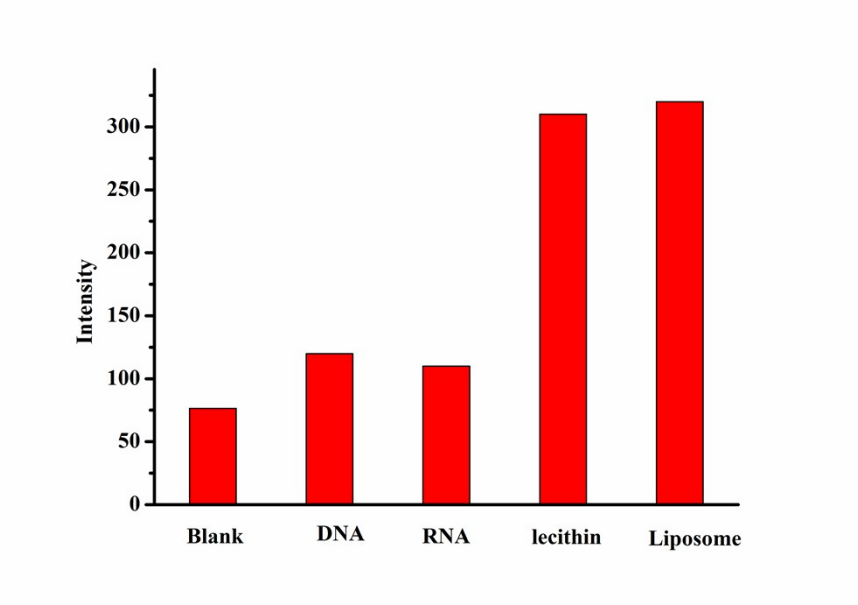

Fig. S9. One-photon fluorescence emission spectra of **03B** (10 μM in PBS buffer, pH = 7.4) in treated with liposome, calf thymus DNA, RNA or Lecithin (100 μg/mL).

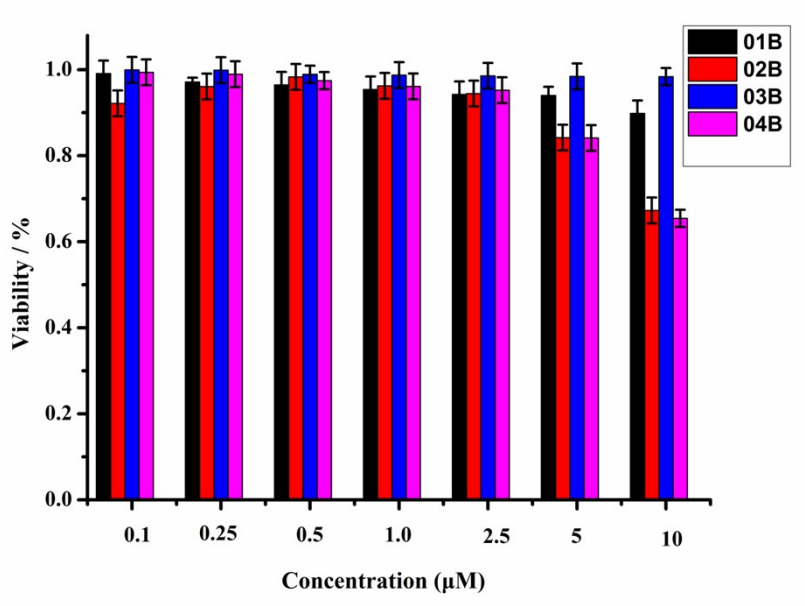

Fig. S10. Cytotoxicity data results obtained from the MTT assay.

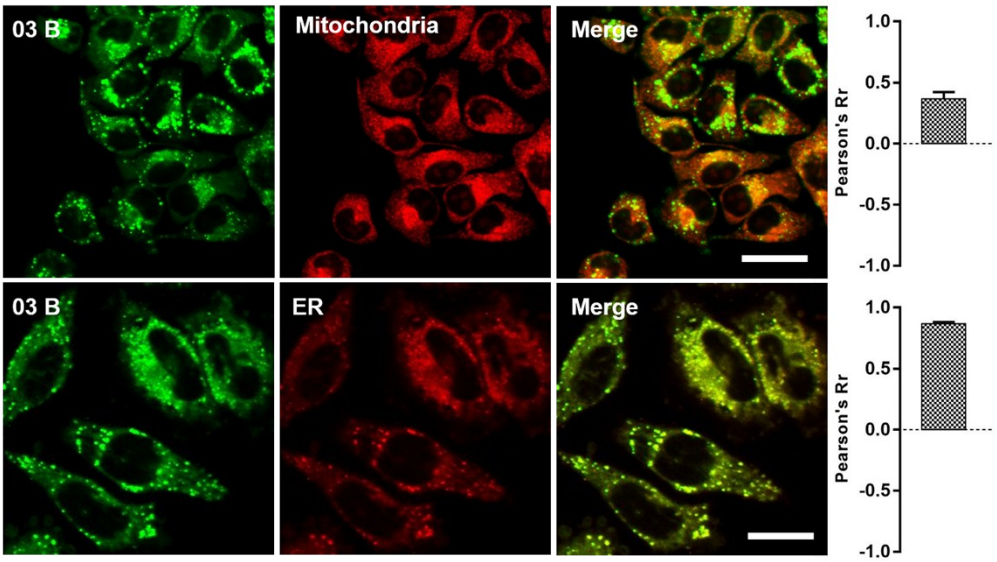

Fig. S11. Colocalization experiments of **03B** (10 μM) and Mito-Tracker Deep Red, ER-Tracker green in HepG2 cells. (Scale bar=5μm. λex = 710 nm, λem = 550 nm).

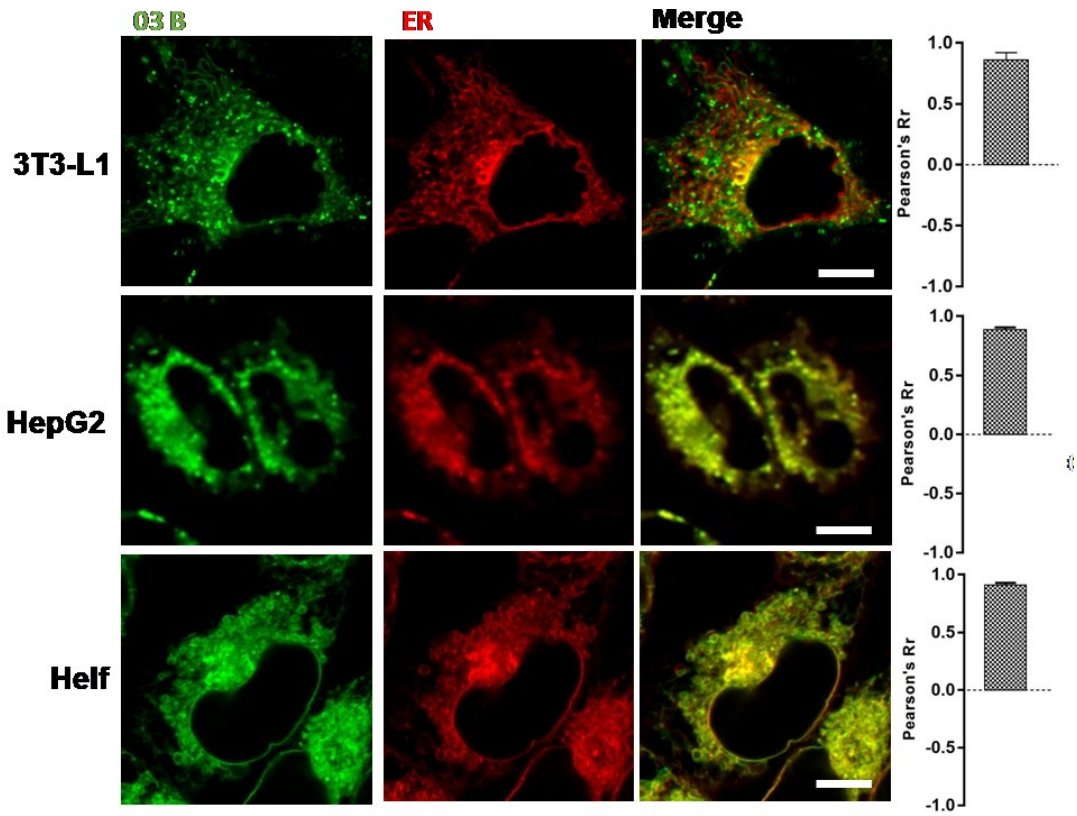

Fig. S12. Colocalization experiments involving **03B** (10 μM, λex = 710 nm, λem = 550 nm) and ER-Tracker green in different cells. Scale bar=10 μm.

Table. S1 Crystal data and structure refinement for **01B** and **04B**

Comp	**01B**	**04B**
CCDC No.	1520258	1567226
Empirical formula	$C_{18}H_{21}BF_2N_2O$	$C_{21}H_{21}BF_2N_2O$
Formula weight	330.18	366.21
T/K	296(2)	298 (2)
Crystal system	Orthorhombic	Triclinic
Space group	$P2_12_12_1$	$P\bar{1}$
Crystal size/mm	0.30 × 0.26 × 0.24	0.30×0.20×0.20
a/Å	7.863 (2)	10.8533 (14)
b/Å	12.769 (4)	11.2855 (15)
c/Å	16.939 (5)	15.709 (2)
α/(º)	90.00	101.368 (2)
β /(º)	90.00	91.808 (2)
γ/(º)	90.00	96.518 (2)
V/Å^3	1700.6 (9)	1871.3 (4)
Z	4	4
D_c/Mg m^{-3}	1.290	1.300
μ/mm^{-1}	0.09	0.09
F(000)	696	768
Final R indices[I > 2σ(I)]	R_1 = 0.036, wR_2 = 0.083	R_1 = 0.057, wR_2 = 0.184
Goodness-of-fit on F^2	1.20	1.05

Table. S2 Main bond lengths (Å), angles (°) and dihedral angles (°) of single crystal structure of **01B**

Bond lengths of 01B					
C(6)–C(7)	1.368(2)	C(7)–O(1)	1.343(2)	C(17)–O(16)	1.380(3)
C(6)–C(5)	1.410(2)	C(11)–N(2)	1.314(2)	C(16)–O(15)	1.328(3)
C(8)–C(11)	1.397(2)	C(5)–C(10)	1.417(3)	C(15)–O(18)	1.520(3)

C(8)–C(9)	1.404(2)	C(12)–C(17)	1.373(3)	N(2)–B(1)	1.574(3)
C(8)–C(7)	1.412(2)	C(12)–N(2)	1.440(2)	O(1)–B(1)	1.437(3)

Bond angles of **01B**			
C(11)–C(8)–C(9)	122.83(17)	C(9)–C(10)–C(5)	120.74(18)
C(9)–C(8)–C(7)	117.52(16)	C(17)–C(12)–C(13)	118.98(18)
C(1)–C(7)–C(8)	119.41(15)	C(16)–C(15)–C(18)	121.2(2)
C(6)–C(7)–C(8)	121.26(16)	C(11)–C(2)–B(1)	119.29(15)
C(6)–C(5)–C(10)	117.90(16)	C(10)–C(9)–C(8)	121.75(18)
C(12)–N(2)–B(1)	120.51(15)	C(5)–N(1)–C(2)	121.84(16)
C(5)–N(1)–C(4)	121.77(17)	F(1)–B(1)–F(2)	109.68(17)
C(7)–O(1)–B(1)	123.81(15)	O(1)–B(1)–N(2)	110.83(16)

Dihedral angles of **01B**					
$P_{1,2}$	4.576(49)	$P_{2,3}$	47.499(53)	$P_{1,3}$	51.421(59)

Bond lengths of 04B					
F3—B2	1.390 (3)	C26—C27	1.436 (5)	N1—C11	1.317 (3)
F2—B1	1.381 (4)	N1—C1	1.447 (3)	C31—C30	1.437 (4)
N1—B1	1.568 (4)	C27—C28	1.333 (6)	C33—C32	1.393 (3)
C27—H27	0.9300	C33—C38	1.410 (3)	C4—C3	1.348 (4)
C33—C34	1.414 (3)	C4—H4	0.9300	C12—C11	1.401 (3)

Dihedral angles of **04B**					
$P_{3,4}$	4.43	$P_{1,2}$	2.25	$P_{1,3}$	81.81

Table. S3 Experiment and theoretical calculation of spectral data of the **BODIPYs**

Compd.	**OI[a]**	**ΔE [b]**	**λ_{max}(nm)[c]**	**f[d]**	**Character**

01B	H-1→L	3.1723	391	0.0766	π→π*
02B	H-1→L	3.2572	381	0.0339	ICT
03B	H-2→L+1	4.1988	300	0.0044	ICT
	H-1→L	2.9535	420	0.7216	π→π*/ICT
04B	H→L	3.2147	386	1.2970	π→π

[a] Orbitals involved in the excitations.

[b] Excitation energies (eV).

[c] Calculated peak position of the longest absorption band in ethanol.

[d] Oscillator Strengths, H represents HOMO, L represents LUMO.

Table. S4 Photophysical properties of **01B**, **02B**, **03B** and **04B**.

Compounds	Solvents	λ_{max}[a](ε_{max}[b])	λ_{max}[c]	Δ_v[d]	Φ[e]
01B	Dichloromethane	399(6.05)	455	56	0.113
	Tetrahydrofuran	395(5.93)	453	58	0.104
	Ethyl acetate	393(5.84)	451	58	0.097
	Ethanol	395(5.86)	453	58	0.071
	Acetonitrile	395(5.97)	456	61	0.039
	DMSO	401(5.60)	461	60	0.070
02B	Dichloromethane	351(2.13)			
		431(2.38)	522	91	0.016
	Tetrahydrofuran	367(2.53)			
		429(2.42)	506	77	0.142
	Ethyl acetate	360(2.36)			
		424(2.37)	502	78	0.181
	Ethanol	385(2.55)	473	88	0.003
	Acetonitrile	371(2.47)			
		428(2.41)	-	-	
	DMSO	394(3.28)			
		433(3.30)	-	-	
	Dichloromethane	421(3.03)	553	132	0.112

03B	Tetrahydrofuran	421(3.18)	530	109	0.117
	Ethyl acetate	414(3.13)	529	115	0.123
	Ethanol	416(3.15)	547	131	0.088
	Acetonitrile	415(3.25)	562	147	0.062
	DMSO	421(3.14)	561	140	0.049
04B	Dichloromethane	389(5.23)	467	78	0.079
	Tetrahydrofuran	382(4.63)	462	80	0.062
	Ethyl acetate	382(4.90)	459	77	0.063
	Ethanol	384(4.06)	467	83	0.029
	Acetonitrile	385(5.06)	461	76	0.030
	DMSO	388(4.60)	466	78	0.059

[a] Absorption peak position in nm.

[b] Maximum molar extinction coefficient in 10^4 mol^{-1}. $L.cm^{-1}$.

[c] Peak position of SPEF, exited at the maximum wavelength of absorption.

[d] Stokes shift in nm.

[e] Fluorescence quantum yield.

Table. S5 Octanol/water partition coefficients (log Po/w) of **01B**~**04B**

01B	02B	03B	04B
2.8785	**0.865**	**1.5478**	**1.3695**