Supplementary Information for:

Highly selective fluorescent OFF-ON thiol probes based on dyads of BODIPY and potent intramolecular electron sink 2,4-dinitrobenzenesulfonyl subunits

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Index

General information .................................................................................................................. S2
Figure S1. $^1$H NMR of BODIPY 1 .......................................................................................... S3
Figure S2. $^{13}$C NMR of BODIPY 1 ...................................................................................... S3
Figure S3. TOF ESI MS of BODIPY 1 .................................................................................. S4
Figure S4. $^1$H NMR of probe 1 ........................................................................................... S4
Figure S5. $^{13}$C NMR of probe 1 .......................................................................................... S5
Figure S6. TOF ESI MS of probe 1 ...................................................................................... S5
Figure S7. $^1$H NMR of BODIPY 2 ....................................................................................... S5
Figure S8. $^{13}$C NMR of BODIPY 2 ...................................................................................... S6
Figure S9. TOF ESI MS of BODIPY 2 .................................................................................. S6
Figure S10. $^1$H NMR of probe 2 ........................................................................................ S7
Figure S11. $^{13}$C NMR of probe 2 ........................................................................................ S7
Figure S12. TOF ESI MS of probe 2 ................................................................................... S7
Scheme S1. The reaction mechanism of the probe 2 with R-SH ........................................... S8
Figure S13. API-ES MS of probe 2 after adding L-cysteine ....................................................... S9
Figure S14. UV-vis absorption of BODIPY 2 and probe 2 before and after addition of L-cysteine ................................................................. S9
Figure S15. Emission-pH relation of BODIPY 1 and probe 1 ................................................... S10
Figure S16. Response of probe 1 and probe 2 toward cysteine and glutathione (kinetic study) . . . S10
Figure S17. Fluorescence images of NCI-H446 cells for probe 2 ............................................. S11
Figure S18. Cyclic voltammograms of BODIPY and Probe 2 .................................................... S12
Table S1. Electrochemical properties of BODIPY and Probe 2 .............................................. S13
Table S2. TDDFT calculation result of BODIPY 2 and probe 2 .......................................... S14
Figure S19. Frontier Molecular Orbitals of Probe 3 and Probe 3 + MeSH .............................. S14
Table S3. TDDFT calculation result of 3 and 3 + MeSH ....................................................... S15
Z-matrix of BODIPY 1 ................................................................................................. S16
Z-matrix of probe 1 ........................................................................................................ S20
Z-matrix of BODIPY 2 ..................................................................................................... S25
Z-matrix of probe 2 ........................................................................................................ S29
Experimental

General methods

NMR spectra were taken on a 400 MHz Varian Unity Inova spectrophotometer. Mass spectra were recorded with a Q-TOF Micro MS spectrometer. UV-Vis spectra were taken on a HP8453 UV-visible spectrophotometer. Fluorescence spectra were recorded on a JASCO FP-6500 or a Sanco 970 CRT spectrofluorometer. Luminescence quantum yields were measured with BIDIPY (see the following molecular structure) as the reference ($\Phi = 48$ % in acetonitrile).\(^1\) The generation of the ROS species, such as such as $\text{O}_2^{-}$ and $\text{OH}^\cdot$, are carried out with literature methods.\(^2\) The detection limits of probe 1 and 2 were determined with analytes concentration for which the probes give a signal equal to the blank signal plus three times the standard deviation of the blank measurements (n= 8). The cells luminescence images were obtained using a Nikon ECLIPSE-Ti confocal laser scanning microscopy.

All voltammograms were obtained in a three-electrode cell under Ar atmosphere and room temperature. The working electrode was a Pt microdisk (2 mm\(^2\)). The experimental reference electrode was $\text{Ag/Ag}^+$ prepared by anodizing a silver wire in CH\(_3\)CN solution of 0.01 M AgNO\(_3\). The counter electrode was platinum wire. All potentials are reported relative to the normal hydrogen electrode (NHE) using $\text{Fc/Fc}^-$ as internal reference $E_{1/2}$ ($\text{Fc/Fc}^-$)= 0.08 V. All reversible redox steps result from one electron processes.

The structures of the complexes were optimized using density functional theory (DFT) with B3LYP functional and 6-31G(d)/LanL2DZ basis set. The excited state related calculations were carried out with the time dependent DFT (TD-DFT) with the ground state geometry. The 6-31G(d) basis set was employed for C, H, N, O, S. There are no imaginary frequencies for all optimized structures. All these calculations were performed with Gaussian 09.\(^3\)

References
Figure S1. $^1$H NMR of BODIPY 1 (CDCl$_3$, 400 MHz).

Figure S2. $^{13}$C NMR of BODIPY 1 (CDCl$_3$, 100 MHz).
Figure S3. TOF ESI MS of BODIPY 1.

Figure S4. $^1$H NMR of probe 1 (CDCl$_3$, 400 MHz).
Figure S5. $^{13}$C NMR of probe 1 (CDCl$_3$, 100 MHz).

Figure S6. TOF ESI MS of probe 1.

Figure S7. $^1$H NMR of BODIPY 2 (CDCl$_3$, 400 MHz).
**Figure S8.** $^{13}$C NMR of BODIPY 2 (CDCl$_3$, 100 MHz).

**Figure S9.** TOF ESI MS of BODIPY 2.
Figure S10. $^1$H NMR of probe 2 (CDCl$_3$, 400 MHz).

Figure S11. $^{13}$C NMR of probe 2 (CDCl$_3$, 100 MHz).
Figure S12. TOF ESI MS of probe 2.

Scheme S1. The reaction mechanism of the probe 2 with R-SH.
Figure S13. API-ES MS of probe 2 after adding L-Cysteine.

Figure S14. UV-vis absorption of BODIPY 2 and probe 2 before and after addition of L-cysteine. In MeOH/water (4:1, v/v) solution at room temperature. $c$ (probe) = $1.0 \times 10^{-5}$ mol dm$^{-3}$, $c$ (L-cysteine) = $2.0 \times 10^{-3}$ mol dm$^{-3}$. 20 °C.
**Figure S15.** pH titration curve of BODIPY 2 and probe 2. λem= 512 nm. c = 1.0 × 10\(^{-5}\) mol/L. The quench of the fluorescence of BODIPY 1 and BODIPY 2 at basic pH can be rationalized by DFT/TDDFT calculations, please refer to page S13 and S23 of the Supporting Information.

**Figure S16.** Reaction kinetics of Probes against cysteine and glutathione. (a) Response of Probe 1 against cysteine and glutathione. 20 μM probe 1. 2 mM analytes. The emission intensity was measured at 514 nm (λex = 450 nm). pH 7.4, methanol/water (4/1, v/v) solution. 37 °C. (b) Response of probe 2 to cysteine and glutathione. 10 μM probe, 2 mM analytes. The emission was monitored at 512 nm (λex = 450 nm). pH 7.4, methanol/water (4:1, v/v) solution. 37 °C.
Figure S17. Fluorescence images of NCI-H446 cells. (a) Fluorescence images of cell; (d) Fluorescence images of cells incubated with probe 2 (20 μM) for 10 min. (g) Fluorescence images of cells pretreated with N-methylmaleimide (0.5 mM) for 1 h and then incubated with probe 2 (20 μM) for 10 min; (b, e, h) are the corresponding bright field images of (a, d, g); (c), (f) and (i) are the overlay of respective fluorescent and bright images. 37 °C.
Figure S18. Cyclic voltamograms of BODIPY (black trace), Probe 2 (red trace) and Ferrocene (cyan trace) as the internal Reference in acetonitrile, containing 0.1M TBAPF$_6$, at room temperature. $c = 1.0 \times 10^{-3}$ mol/L. The reversible Fc/Fc$^+$ redox couple at 0.08 V corresponds to genuine ferrocene.

Table S1. Electrochemical properties of BODIPY and Probe 2. $^a$

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<th>$E_{red}^a$ (Ep mV)</th>
<th>HOMO (eV)</th>
<th>LUMO (eV)</th>
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<td>−2.45 (LUMO+2)</td>
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<td>−1756</td>
<td>−5.42</td>
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$^a$ Potentials determined by cyclic voltammetry in CH$_2$CN solution, containing 0.1 M TBAPF$_6$, [electrochemical window from 1.5 to -1.9 V], at a solute concentration of 1.0 mM, using a scan rate of 200 mV/s.
Table S2. Electronic Excitation Energies (eV) and corresponding Oscillator Strengths ($f$), main configurations and CI coefficients of the Low-lying Electronically Excited States Calculated by TDDFT//B3LYP/6-31G(d) for BODIPY 2 and thiol probe 2, based on the DFT//B3LYP/6-31G(d) Optimized Ground State Geometries.

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<th>Main configurations</th>
<th>CI coefficients</th>
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<td>Energy (eV) $^a$</td>
<td>$f^b$</td>
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<td>$^c$</td>
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<td>0.0000 HOMO$\rightarrow$LUMO</td>
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<td>HOMO$\rightarrow$LUMO+2</td>
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<td>3.33 eV 373 nm</td>
<td>0.0002 HOMO$\rightarrow$LUMO</td>
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$^a$ Only the selected low-lying excited states are presented. $^b$ Oscillator strength. $^c$ Only the main configurations are presented. $^d$ The CI coefficients are in absolute values.

Herein the S1 state of probe 2 is a dark state because the oscillator strength $f = 0.0000$ and the HOMO$\rightarrow$LUMO transition is an electron transfer transition (no overlap between the initial and the destination molecular orbitals). Thus the S1 state cannot be directly populated by photo-excitation, i.e. S0$\rightarrow$S1 is a forbidden transition. Thus S1$\rightarrow$S0 is also forbidden, and probe 2 is non-fluorescent.

For BODIPY 2, however, the S0$\rightarrow$S1 is allowed, indicated by the $f$ value and the locally-excited feature of the transition (LE). Thus S1 is probably an emissive state and BODIPY 2 is fluorescent.
Figure S19. The frontier molecular orbitals of probe 3 before and after reaction with thiols (the thiol was simplified as MeSH). (a) HOMO and LUMO of probe 3. (b) HOMO and LUMO of probe-thiol adduct 3-MeSH (i.e. the cleavage product of probe 3 in the presence of thiols. Calculated based on ground state geometry by DFT at the B3LYP/6-31G(d)/ LanL2DZ level using Gaussian 09.

Probe 3 was reported, please refer to: Matsumoto, T.; et al.; Nagano, T. *Org. Lett.* 2007, 9, 3375.

For probe 4 and 5, similar calculation results were observed. The discrepancy between the calculation results and the experiment results (which indicated that probe 4 and 5 are fluorescent, but calculation predicts non-fluorescent) is probably due to the free energy changes of the electron transfer ($\Delta G^\circ$). In the DFT calculations, the distance between the electron donor and the acceptor is not considered. But this distance is important for the ($\Delta G^\circ$) values (Rehm-Weller equation).
**Table S3.** Electronic Excitation Energies (eV) and corresponding Oscillator Strengths (f), main configurations and CI coefficients of the Low-lying Electronically Excited States Calculated by TDDFT//B3LYP/6-31G(d) for thiol probe 3 and its thiol adduct (Probe 3 + MeSH), based on the DFT//B3LYP/6-31G(d) Optimized Ground State Geometries.

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<th>Oscillator strength</th>
<th>Main configurations</th>
<th>CI coefficients</th>
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<td><strong>Probe 3 + MeSH</strong></td>
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* Only the selected low-lying excited states are presented. * Oscillator strength. * Only the main configurations are presented. * The CI coefficients are in absolute values.

For the discussion of the property of the $S_1$ state, please refer to page S14.
**BODIPY 1 (DFT//B3LYP/6-31G(d))**

No imaginary frequencies.

Symbolic Z-matrix:

- **Charge = 0**
- **Multiplicity = 1**

```
  C  1  B1
  C  2  B2  1  A1
  C  2  B3  1  A2  3  D1
  C  4  B4  2  A3  1  D2
  C  5  B5  4  A4  2  D3
  C  6  B6  5  A5  4  D4
  C  7  B7  6  A6  5  D5
  C  8  B8  7  A7  6  D6
  H  8  B9  7  A8  6  D7
  N  1  B10  3  A9  2  D8
  B  11  B12  1  A11  3  D10
  F  13  B13  11  A12  1  D11
  F  13  B14  11  A13  1  D12
  C  2  B15  1  A14  11  D13
  H  16  B16  2  A15  1  D14
  H  16  B17  2  A16  1  D15
  H  16  B18  2  A17  1  D16
  C  9  B19  8  A18  7  D17
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  H  20  B21  9  A20  8  D19
  H  20  B22  9  A21  8  D20
  C  7  B23  6  A22  5  D21
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  H  24  B26  7  A25  6  D24
  C  1  B27  11  A26  4  D25
  H  28  B28  1  A27  11  D26
  H  28  B29  1  A28  11  D27
  H  28  B30  1  A29  11  D28
  C  5  B31  4  A30  2  D29
  C  32  B32  5  A31  4  D30
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  C  33  B34  32  A33  5  D32
  C  34  B35  32  A34  5  D33
  H  34  B36  32  A35  5  D34
  H  35  B37  33  A36  32  D35
  H  36  B38  34  A37  32  D36
  H  3  B39  2  A38  1  D37
  C  35  B40  33  A39  32  D38
  H  41  B41  35  A40  33  D39
  O  33  B42  32  A41  5  D40
  H  43  B43  33  A42  32  D41
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No imaginary frequencies.

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No imaginary frequencies.

Symbolic Z-matrix:
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B 11  B12  1  A11  3  D10
F 13  B13  11  A12  1  D11
# Electronic Supplementary Material (ESI) for Organic and Biomolecular Chemistry

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Electronic Supplementary Material (ESI) for Organic and Biomolecular Chemistry
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N  7     B7  6     A6  1     D5
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C 15     B15  14    A14  13    D13
C 16     B16  15    A15  14    D14
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C  9     B19  8     A18  7     D17
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