Electronic supplementary information (ESI)

A colorimetric and ratiometric NIR fluorescent turn-on fluoride chemodosimeter based on BODIPY derivatives: high selectivity via specific Si-O cleavage

Jian Cao,[a,b] Chunchang Zhao,*[a] Peng Feng,[a] Yulin Zhang,[a] Weihong Zhu*[a]

[a]*Shanghai Key Laboratory of Functional Materials Chemistry, Key Laboratory for Advanced Materials and Institute of Fine Chemicals, East China University of Science & Technology, Shanghai 200237, P. R. China. E-mail: zhaocchang@ecust.edu.cn; whzhu@ecust.edu.cn*

[b]*Shanghai University of Engineering Science, Shanghai 201620, P. R. China.*

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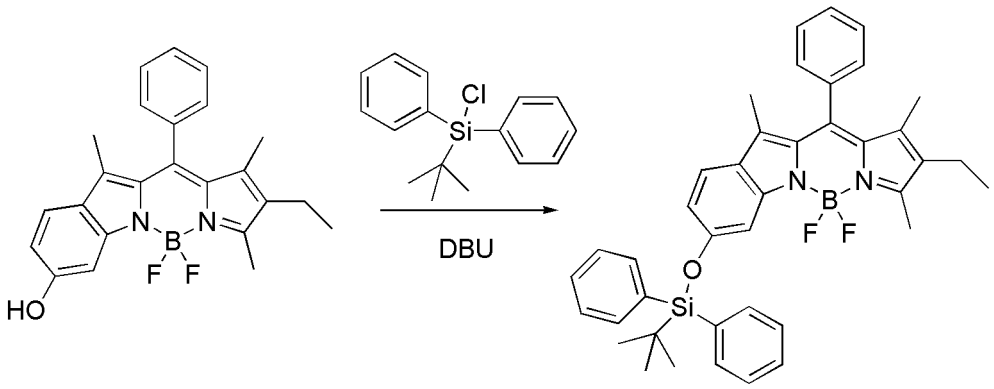
1. General Methods

All chemical reagents and solvents for synthesis were purchased from commercial suppliers and were used without further purification. ^{1}H NMR and ^{13}C NMR spectra were recorded on a Bruker AV-400 spectrometer with chemical shifts reported in ppm (in $CDCl_3$, TMS as internal standard) at room temperature. Mass spectra were measured on a HP 1100 LC-MS spectrometer.

UV-vis absorption spectra were recorded on a Varian Cary 100 spectrophotometer. Fluorescence spectra were measured with a Varian CARY Eclipse Fluorescence spectrophotometer. Spectral-grade solvents were used for measurements of UV-vis absorption and fluorescence.

2. Synthesis of BODIPY-OSi

Scheme S1



BODIPY-OH **BODIPY-OSi**

To a solution of **BODIPY-OH** (500 mg, 1.24mmol) in CH_2Cl_2 (25 mL) was added DBU (234 mg, 1.24 mmol) at -15 °C, the resulted solution was stirred for another 15 min at room temperature, the resulted solution was stirred for another 15 min at -15 °C, followed by the addition of *tert*-butyldiphenylchlorosilane (681 mg, 2.48

mmol). The resulting mixture was stirred for 10 min at -15 °C, quenched with 0.1M HCl (1.0 mL), extracted with CH_2Cl_2, washed with H_2O. The combined organic extracts were dried with anhydrous Na_2SO_4, and the solvent was removed in vacuo. The crude product was purified by flash chromatography to afford 557 mg (70%). **BODIPY-OSi**: ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.00-1.04 (t, J = 7.6 Hz, 3H, -$CH_2C\boldsymbol{H}_3$), 1.11 (s, 9H, -CH_3), 1.36 (s, 3H, -CH_3), 1.49 (s, 3H, -CH_3), 2.33-2.38 (q, J = 7.6 Hz, 2H, -$C\boldsymbol{H}_2CH_3$), 2.67 (s, 3H, -CH_3), 6.29-6.31 (dd, J_1 = 2.4 Hz, J_1 = 2 Hz, 1H), 7.02-7.04 (d, J = 8.8 Hz, 1H), 7.29-7.31 (m, 3H), 7.34-7.42 (m, 6H), 7.50-7.51 (m, 3H), 7.75-7.77 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 11.27, 12.15, 13.39, 14.26, 17.20, 19.57, 26.55, 103.98, 115.90, 121.54, 127.17, 127.78, 128.29, 129.10, 129.23, 129.67, 129.86, 132.52, 133.01, 133.42, 134.81, 135.18, 135.39, 135.53, 135.70, 136.73, 141.37, 141.51, 146.69, 157.68, 161.78; HRMS (ESI) calcd for $C_{40}H_{40}BF_2N_2OSi$: 641.2971; found: 641.2986. $[M - H]^-$.

Kinetics of fluorescence enhancement profile

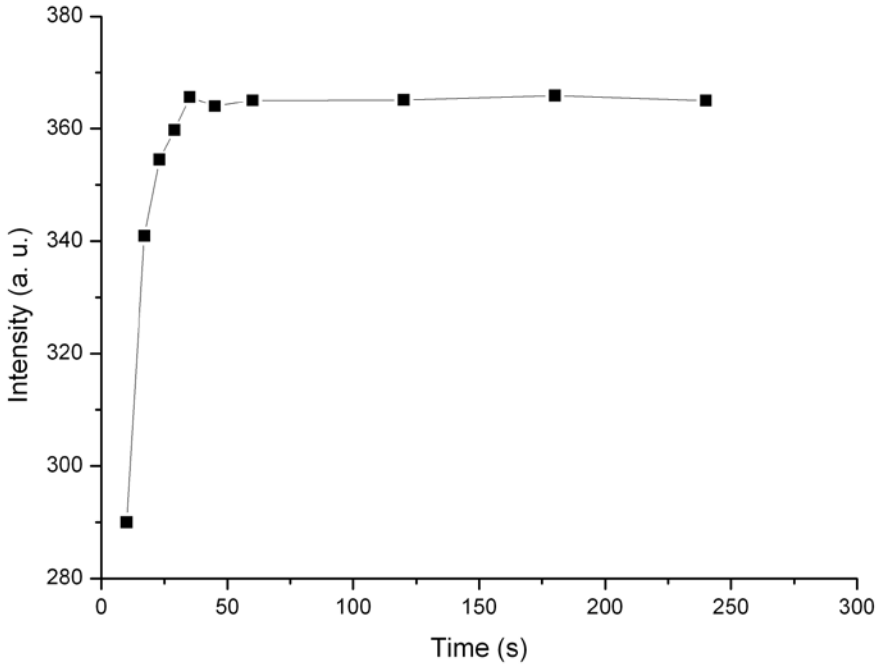


Fig. S1. Kinetics of fluorescence enhancement profile of **BODIPY-OSi** (5×10^{-6} M) at 676 nm in the presence of F^- (50 equiv), λ_{ex} = 644 nm. The spectra data were obtained at room temperature.

3. UPLC-Mass spectra of BODIPY-OSi and BODIPY-OSi + TBAF

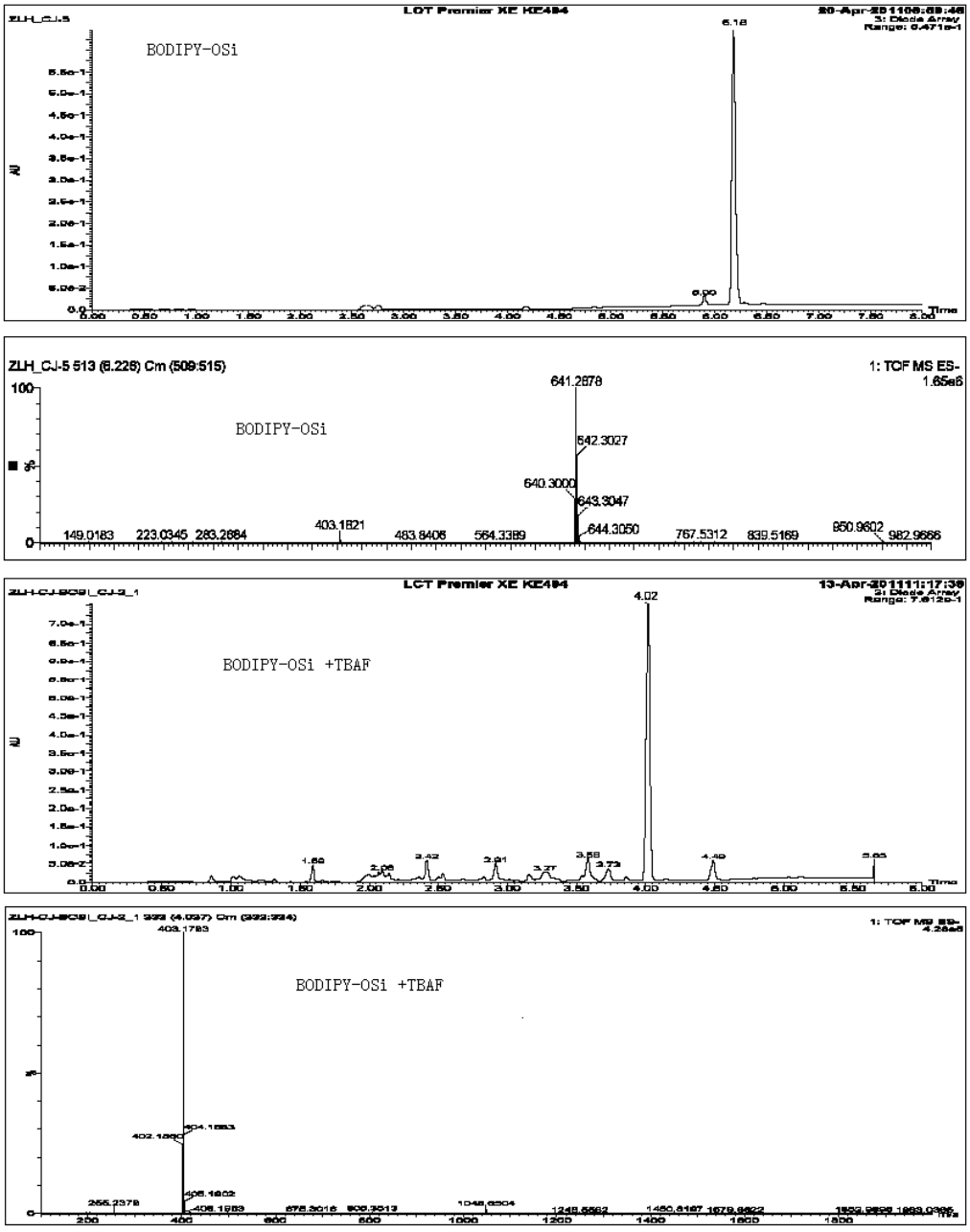


Fig. S2. UPLC-Mass spectra of **BODIPY-OSi** and **BODIPY-OSi** + TBAF.

4. ^{1}H NMR and ^{13}C NMR spectra

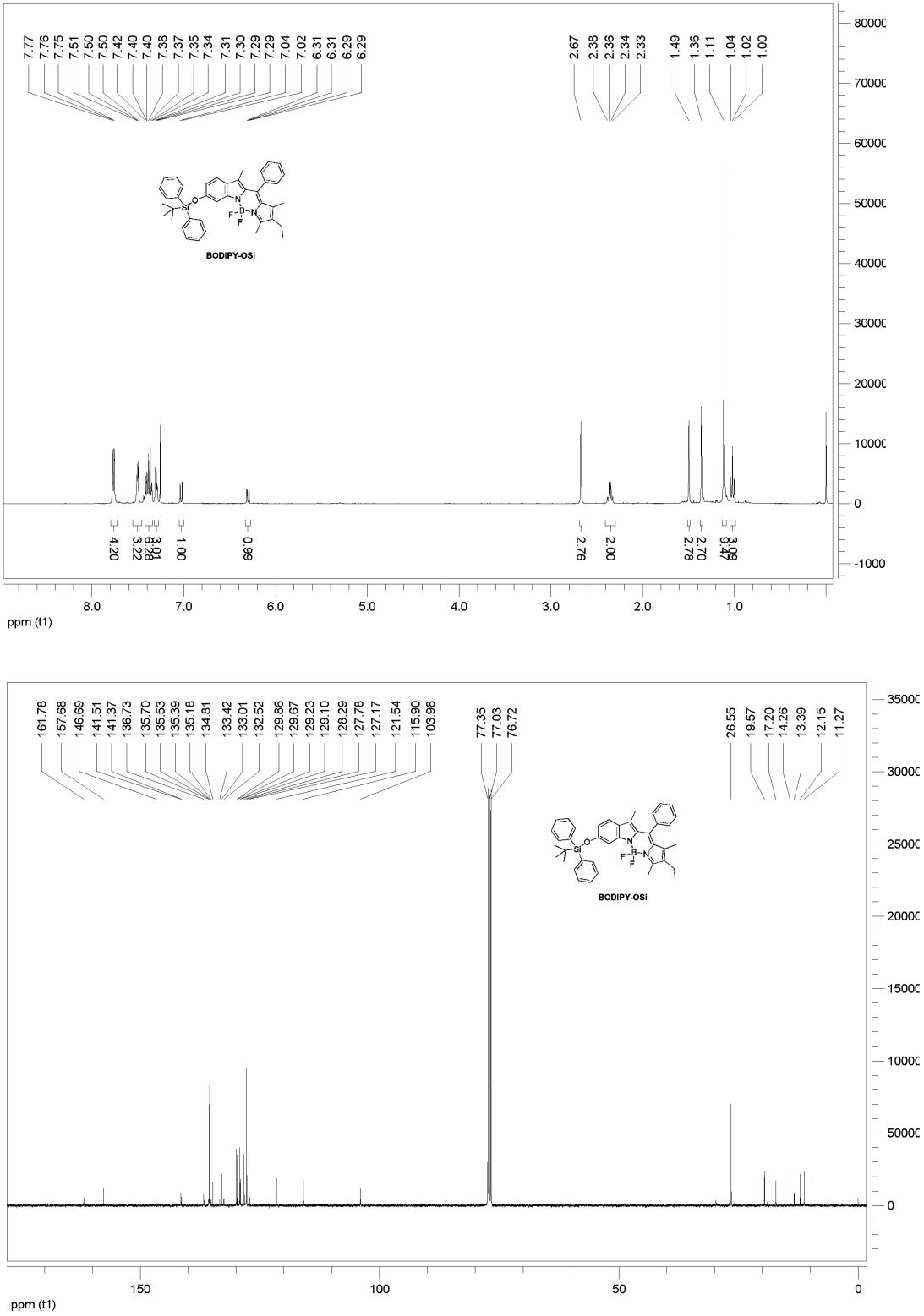


Fig. S3. ^{1}H NMR and ^{13}C NMR spectra of **BODIPY-OSi** (in $CDCl_3$)

5. HRMS spectrum

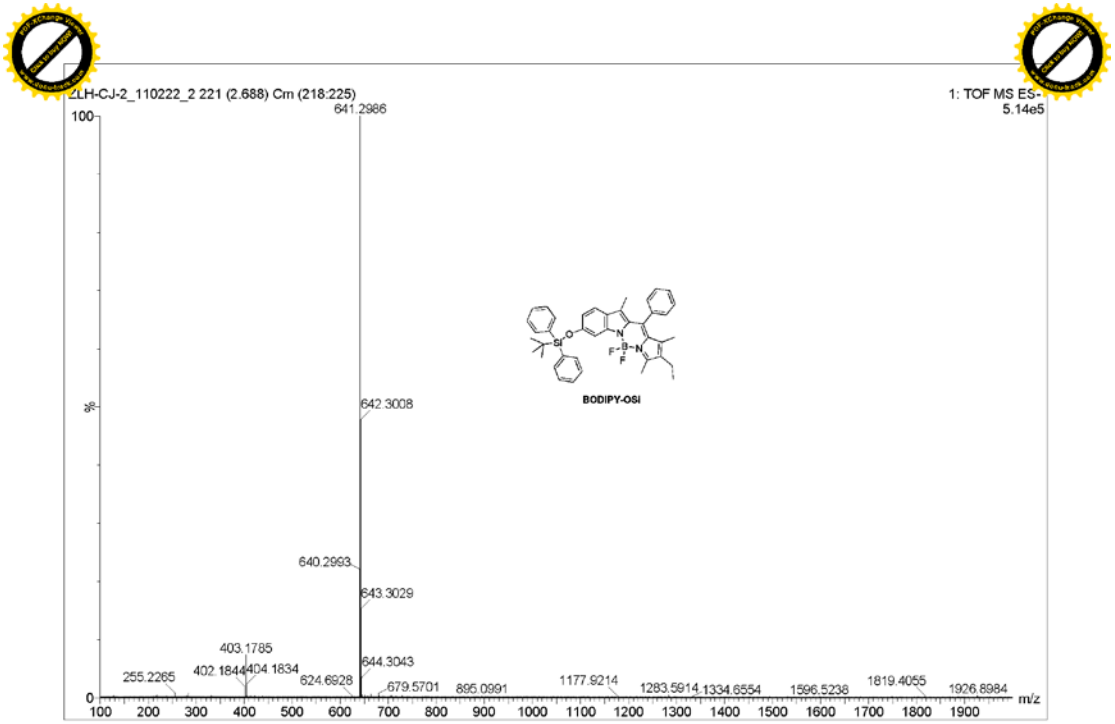


Fig. S4. HRMS spectrum of **BODIPY-OSi**