Electronic Supplementary Information for

# A fluoride activated methylene blue releasing platform for imaging and antimicrobial photodynamic therapy of human dental plaque

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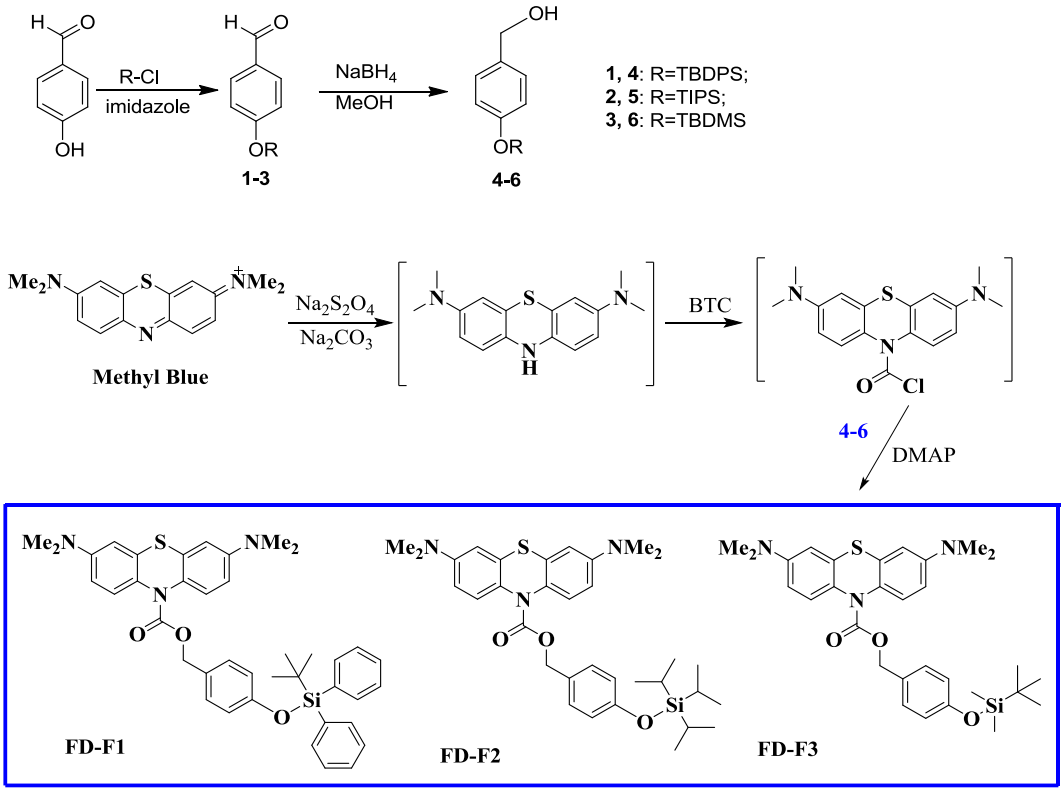
## 1. Experimental section

### 1.1 Materials and Instruments

All the starting materials were obtained from commercial suppliers and used as received. $^{1}$H NMR (400 MHz) and $^{13}$C NMR (100 MHz) spectra were taken on a Bruker AV400 nuclear magnetic resonance spectrometer, using DMSO-$d_6$ or $CD_3CN$ as solvent. Proton chemical shifts are reported in parts per million downfield from tetramethylsilane (TMS), with tetramethylsilane ($\delta$ = 0.0 ppm) or the solvent residue peak $CD_3CN$ (1.94 ppm for $^{1}$H, 1.32 ppm for $^{13}$C), or DMSO-$d_6$ (2.50 ppm for $^{1}$H, 39.52 ppm for $^{13}$C) as the chemical shift standard. High-resolution mass spectra (HRMS) were measured on a Bruker Micro TOF II 10257 instrument with electro-spray ionization (ESI) technique and direct injection method. UV-visible spectra were recorded on a Shimadzu UV-2550 spectrometer. Steady-state fluorescent spectra at room temperature were measured on an Edinburgh instrument FLS-920 spectrometer with a Xe lamp as an excitation source.

### 1.2 Synthesis of the compounds




**Scheme S1.** Synthesis route of compounds **FD-F1 ~ FD-F3**

### 1.2.1 General procedure for the synthesis of 1-3

4-Hydroxybenzaldehyde (2.0 g, 16.38 mmol, 1.0 eq) and imidazole (3.35 g, 49.14 mmol, 3.0 eq) were dissolved in 30 mL of dichloromethane, the resulting mixture was stirred in an ice-water bath. R-Cl (19.66 mmol, 1.2 eq) was dissolved in 10 mL of dichloromethane and added dropwise. After addition, the mixture was stirred at room temperature until the reaction completed as indicated by TLC analysis which was conducted at 1 h intervals. The reaction mixture was poured into 300 mL of ice-water while stirring, and the resulting mixture was extracted with three 150 mL portions of dichloromethane. The combined extracts were washed with brine, dried over anhydrous sodium sulfate and evaporated on a rotary evaporator to afford an oily residue, which was purified by column chromatography (ethyl acetate/petroleum ether = 1/20) to yield the pure product **1-3**.

**4-((tert-butyldiphenylsilyl)oxy)benzaldehyde (1)**

White solid. Yield, 5.37 g, 91%. $^1$H NMR (400 MHz, DMSO-*d6*) δ 9.80 (s, 1H), 7.75 – 7.65 (m, 6H), 7.53 – 7.42 (m, 6H), 6.90 (d, *J* = 8.4 Hz, 2H), 1.05 (s, 9H).

**4-((triisopropylsilyl)oxy)benzaldehyde (2)**

Colorless oil. Yield, 4.38 g, 96%. $^1$H NMR (400 MHz, DMSO-*d6*) δ 9.87 (s, 1H), 7.84 (d, *J* = 8.4 Hz, 2H), 7.05 (d, *J* = 8.4 Hz, 2H), 1.34-1.25(m, 3H), 1.07 (d, *J* = 7.6 Hz, 18H).

**4-((tert-butyldimethylsilyl)oxy)benzaldehyde (3)**

Colorless oil. Yield, 3.64 g 94%. $^1$H NMR (400 MHz, DMSO-*d6*) δ 7.18 (d, *J* = 8.4 Hz, 2H), 6.79 (d, *J* = 8.4 Hz, 2H), 5.05 (t, *J* = 5.8 Hz, 1H), 4.40 (d, *J* = 6.0 Hz, 2H), 0.94 (s, 9H), 0.17 (s, 6H).

### 1.2.2 General procedure for the synthesis of 4-6

To a solution of **1-3** (3.87 mmol, 1.0 eq) in 150 mL of MeOH, cooled with an ice-water bath, $NaBH_4$ (0.63 g, 16.64 mmol, 1.2 eq) was added in batches. After addition, the reaction mixture was stirred at this temperature for 30 min and then at room temperature until the reaction completed as indicated by TLC analysis (typically within 1-3 h). The reaction mixture was poured into 200 mL of ice-water while stirring, and the resulting mixture was extracted with three 100 mL portions of dichloromethane. The combined extracts were washed with brine, dried over anhydrous sodium sulfate and evaporated on a rotary evaporator to afford an oily residue, which was purified by column chromatography (ethyl acetate/petroleum ether = 1/20) to yield the pure product **4-6**.

**(4-((tert-butyldiphenylsilyl)oxy)phenyl)methanol (4)**

White solid. Yield, 1.36 g, 97%. $^1$H NMR (400 MHz, DMSO-*d6*) δ 7.69 – 7.63 (m, 5H), 7.47 – 7.42 (m, 5H), 7.07 (d, *J* = 8.8 Hz, 2H), 6.68 (d, *J* = 8.4 Hz, 2H), 4.99 (t, *J* = 5.6 Hz, 1H), 4.33 (d, *J* = 5.2 Hz, 2H), 1.03 (s, 9H).

**(4-((triisopropylsilyl)oxy)phenyl)methanol (5)**

Colorless oil. Yield, 1.07 g, 99%. $^1$H NMR (400 MHz, DMSO-*d6*) δ 7.18 (d, *J* =

8.4 Hz, 2H), 6.81 (d, *J* = 8.4 Hz, 2H), 5.05 (t, *J* = 5.8 Hz, 1H), 4.40 (d, *J* = 6.0 Hz, 2H), 1.27 – 1.18 (m, 3H), 1.05 (d, *J* = 8.4 Hz, 18H).

**(4-((tert-butyldimethylsilyl)oxy)phenyl)methanol (6)**

Colorless oil. Yield, 0.9 g, 98%. $^{1}$H NMR (400 MHz, DMSO-*d6*) δ 7.18 (d, *J* = 8.4 Hz, 2H), 6.79 (d, *J* = 8.4 Hz, 2H), 5.05 (t, *J* = 5.8 Hz, 1H), 4.40 (d, *J* = 6.0 Hz, 2H), 0.94 (s, 9H), 0.17 (s, 6H).

### 1.2.3 General procedure for the synthesis of FD-F1 ~ FD-F3

To an aqueous solution (3 mL) of MB (1.11 g, 3.75 mmol, 1.0 eq), dichloromethane (10 mL) and $Na_2CO_3$ (2.38 g, 22.50 mmol, 6.0 eq) were added and stirred at 60 ℃ under a nitrogen atmosphere. Sodium dithionite (2.61 g, 15.00 mmol, 4.0 eq) was dissolved in 7 mL of water and added dropwise. After addition the mixture was stirred at 60 ℃ under nitrogen atmosphere until the solution became yellow (typically within 15-30 min). The mixture was cooled with an ice-water bath, to which a dichloromethane solution (5 mL) of bis(trichloromethyl)carbonate (1.11 g, 3.75 mmol, 1.0 eq) was added dropwise. After addition, the mixture was stirred for another 1 h. The dichloromethane layer was separated from the water layer and quickly dried with anhydrous sodium sulfate. After sodium sulfate was removed by filtration, the solution was added dropwise to a mixture of **4 - 6** (0.8 eq), DMAP (0.92 g, 7.50 mmol, 2.0 eq), $Na_2CO_3$ (1.19 g, 11.25 mmol, 3.0 eq) and 5 mL dichloromethane. After addition, the mixture was stirred in an ice-water bath for 1 h and then at room temperature until the reaction was completed as indicated by TLC analysis.

After the undissolved substance was removed by filtration, the solution was poured into 200 mL of ice-water while stirring, and the resulting mixture was extracted with three 100 mL portions of dichloromethane. The combined extracts were washed with brine, dried over anhydrous sodium sulfate and evaporated on a rotary evaporator to afford an oily or solid residue, which was purified by column chromatography (ethyl acetate/n-hexane = 1/10 then 1/5) to yield **FD-F1~ FD-F3** as white solids.

**FD-F1.** Yield, 0.51 g, 20%. $^{1}$H NMR (400 MHz, $CD_3CN$) $\delta$ 7.72 (dd, *J* = 8.0, 1.2 Hz, 4H), 7.49 – 7.45 (m, 2H), 7.42 – 7.39 (m, 4H), 7.26 (d, *J* = 8.8 Hz, 2H), 7.07 (d, *J* = 8.4 Hz, 2H), 6.74 (d, *J* = 8.8 Hz, 2H), 6.68 (d, *J* = 2.8 Hz, 2H), 6.62 (m, 2H), 5.00 (s, 2H), 2.90 (s, 12H), 1.07 (s, 9H). $^{13}$C NMR (100 MHz, $CD_3CN$) $\delta$ 156.42, 155.12, 150.11, 136.44, 133.64, 133.56, 131.21, 130.38, 129.05, 128.94, 128.13, 120.58, 120.36, 111.90, 110.86, 68.12, 40.84, 26.89, 19.92. HRMS (ESI), calculated for $C_{40}H_{44}N_3O_3SSi$ ($[M+H]^+$) 674.2867, found 674.2871.

**FD-F2.** Yield, 0.52 g, 23%. $^{1}$H NMR (400 MHz, $CD_3CN$) $\delta$ 7.30 (d, *J* = 8.8 Hz, 2H), 7.21 (d, *J* = 8.4 Hz, 2H), 6.88 (d, *J* = 8.4 Hz, 2H), 6.69 (d, *J* = 2.8 Hz, 2H), 6.64 (m, 2H), 5.07 (s, 2H), 2.90 (s, 12H), 1.31 – 1.22 (m, 3H), 1.09 (d, *J* = 7.6 Hz, 18H). $^{13}$C NMR (100 MHz, $CD_3CN$) $\delta$ 156.96, 155.16, 150.07, 133.62, 130.64, 130.21,

129.02, 128.15, 120.77, 111.88, 110.84, 68.25, 40.83, 18.32, 13.46. HRMS (ESI), calculated for $C_{33}H_{46}N_3O_3SSi$ ($[M+H]^+$) 592.3024, found 592.3021.

**FD-F3.**Yield, 0.37 g, 18%. $^1$H NMR (400 MHz, $CD_3CN$) $\delta$ 7.31 (d, $J$ = 9.2 Hz, 2H), 7.22 (d, $J$ = 8.8 Hz, 2H), 6.84 (d, $J$ = 8.4 Hz, 2H), 6.69 (d, $J$ = 2.4 Hz, 2H), 6.65 (dd, $J$ = 8.8, 2.8 Hz, 2H), 5.08 (s, 2H), 2.90 (s, 12H), 0.98 (s, 9H), 0.19 (s, 6H). $^{13}$C NMR (100 MHz, $CD_3CN$) $\delta$ 150.56, 155.14, 150.06, 133.60, 130.59, 130.44, 128.95, 128.13, 120.97, 118.29, 110.82, 68.21, 40.81, 26.01, 18.58, −4.26. HRMS (ESI), calculated for $C_{30}H_{40}N_3O_3SSi$ ($[M+H]^+$) 550.2554, found 550.2567.

### 1.3 Preparation of probes and analytes

Stock solutions of **FD-F1~FD-F3** (1 mM or 2.5 mM for imaging; 5 mg/mL for aPDT) were prepared in DMSO. The test solution for each probe (10 μM) was prepared by placing stock solutions in a 10-mL volumetric flask, and diluting with DMSO-HEPES buffer solution (3/2, v/v, 10 mM HEPES, pH = 7.2). The resulting solutions were shaken well and incubated at room temperature before recording the spectra.

Sodium fluoride (NaF) was used as a fluoride source for the fluoride ion sensing test. The stock solution of NaF was prepared in deionized water. Other analytes were prepared in dd$H_2O$.

### 1.4 Preparation of toothpastes

Selected toothpastes were dispersed in 10 mL of distilled water. The obtained mixture was stirred at 70 ℃ for 3 h, and then filtered. The filtrate was used for the analysis of $F^-$. The test solution of **FD-F3** (10 μM) to measure $F^-$ from different toothpastes in 10 mM DMSO-HEPES solution (3/2, v/v, 10 mM HEPES, pH = 7.2) was prepared by placing **FD-F3** stock solutions (100 μL) and different toothpaste stock solutions in 10-mL volumetric flasks, diluting with buffer solution to volume, and mixing. The resulting solution were shaken well and incubated at room temperature before recording the spectra.

For comparison, the fluoride concentration was also measured by FISE which is a type of ion selective electrode that is sensitive to the concentration of $F^-$ (detailed described in U.S. Environmental Protection Agency Website https://www.epa.gov/sites/production/files/2015-12/documents/9214.pdf).

### 1.5 Procedure for fluorescence imaging of fluoride uptake in plaque biofilm.

Human subjects (aged 20 to 30 years old) were enrolled in the study according to the inclusion criteria (Turesky Plaque Index Score 2 to 3). Hydroxyapatite (HA) discs

used as plaque biofilm accumulators were worn by the subjects for 48 hours before harvesting the natural plaque biofilm. After removal, the HA discs were randomly assigned to a 2-minute treatment with phosphate-buffered saline (PBS, blank control), 25% slurry of a marketed non-fluoride toothpaste (NFT) or 25% slurry of a marketed sodium fluoride toothpaste (SFT), and then washed with PBS for three times to remove the excess toothpaste ingredients.

HA discs were incubated in PBS solution with 0.2%(v/v) DMSO containing 5 μM **FD-F3** and 5 μM SYTO® 9 Green Fluorescent Nucleic Acid Stain at 37°C for 30 min in the dark, washed with PBS three times to remove the excess probes and bathed in PBS (2 mL) before imaging.

Confocal laser scanning microscopy (CLSM) images were obtained with Leica™ TCS SP8 AOBS spectral confocal microscope and Leica™ Confocal software LAS AF3.3.0 (Leica Mikroskopie GmbH, Wetzlar, Germany). The following parameters were used: XYZ-scan mode with dual-channel excitation and emission filters for SYTO® 9 (λex = 488 nm, λ em = 500-550 nm) and **FD-F3** (λex = 633 nm, λem = 670-720 nm), 20x objective lens, and scanning from the biofilm surface to a total depth of 60 μm with a step size of 5 μm.

### 1.6 Procedure for PDT in plaque biofilm.

Natural plaque biofilms were obtained according to the above method and divided into six groups as follows. (1) without any treatment as control; (2) treated only with free **FD-F3** (50 μg/mL) for 30 min; (3) treated only with NaF (50 μg/mL) for 60 min; (4) treated with **FD-F3** (50 μg/mL) for 30 min then NaF (50 μg/mL) for 60 min; (5) treated only with light (100 mW/cm$^2$) for 5 min; (6) treated with **FD-F3** (50 μg/mL) for 30 min then NaF (50 μg/mL) for 60 min then light (100 mW/cm$^2$) for 5 min.

The distribution of dead/live bacterial cells in biofilms were observed under confocal laser scanning microscope (CLSM). Live and dead biofilm bacteria were simultaneously viewed using the reagents SYTO 9 stain and propidium iodide in the LIVE/DEAD BacLight Bacterial Viability Kit according to the manufacturer's instructions. All data analysis was performed using SPSS 13.0 software package.

## 2. Additional Tables

**Table S1**

**Table S1** Other Photophysical Parameters of **the probes** before and after treated with NaF[a]

| | ε[b] ($M^{-1}$ $cm^{-1}$) | $\Phi$[c] | Brightness[d] ($M^{-1}$ $cm^{-1}$) |
|---|---|---|---|
| **FD-F1** (10 μM) | 200 | - | - |
| **FD-F1** (10 μM) + NaF (500 μM)[e] | 6000 | 0.11 | 660 |
| **FD-F2** (10 μM) | 100 | - | - |
| **FD-F2** (10 μM) + NaF (500 μM)[e] | 2400 | 0.13 | 312 |
| **FD-F3** (10 μM) | 300 | - | - |
| **FD-F3** (10 μM) + NaF (500 μM)[e] | 49900 | 0.10 | 4990 |

[a] The data was recorded in DMSO-HEPES solution (3/2, v/v, 10 mM HEPES, pH = 7.2)

[b] Molar absorption coefficient at 667 nm

[c] Φ: absolute fluorescence quantum yield

[d] Brightness = ε × $\Phi$, at 667 nm[1]

[e] The data was recorded 50 min later after adding NaF

**Table S2** The quantitative analysis of different probes (10 μM) after reacted with NaF (500 μM) for 50 min

| | MB detection concentration (μM) | MB release efficiency (%) |
|---|---|---|
| **FD-F1 + NaF** | 4.59 | 45.9 |
| **FD-F2 + NaF** | 3.69 | 36.9 |
| **FD-F3 + NaF** | 9.69 | 96.9 |

**Table S3** Determination of $F^-$ content in water with different fluoride sources.

| $F^-$ source | Spiked (μM) | Recovered (μM) | Recovery (%) | RSD |
|---|---|---|---|---|
| NaF | 7 | 7.4 | 105.7 | 0.09 |
| NaF | 18 | 17.1 | 95 | 0.03 |
| NaF | 31 | 28 | 90.3 | 0.06 |
| SMFP | 185 | 193.3 | 104.5 | 0.03 |
| SMFP | 570 | 580.7 | 101.9 | 0.05 |

The data presented has been converted into the concentiation of NaF or SMFP

## 3. Additional images and figures

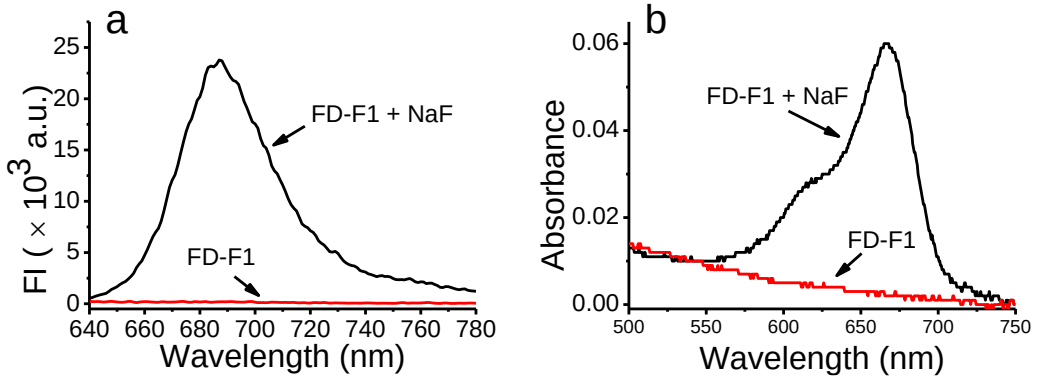



**Fig. S1** (a) Fluorescence spectra of **FD-F1 (10 μM)** before/after treated with 500 μM NaF; (b) the absorption spectra of **FD-F1 (10 μM)** before/after treated with 500 μM NaF (incubated for 50 min, DMSO-HEPES solution. (3/2, v/v, 10 mM HEPES, pH=7.2), λex =620 nm)

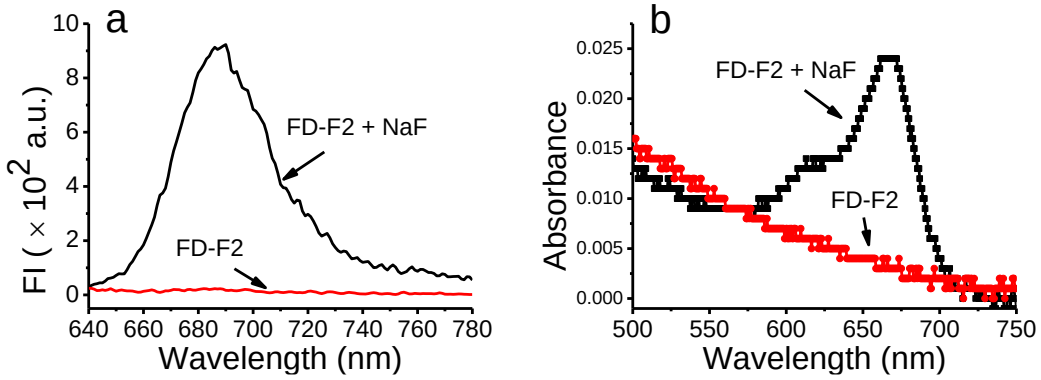



**Fig. S2** (a) Fluorescence spectra of **FD-F2 (10 μM)** before/after treated with 500 μM NaF; (b) the absorption spectra of **FD-F2 (10 μM)** before/after treated with 500 μM NaF. (incubated for 50 min, DMSO-HEPES solution (3/2, v/v, 10 mM HEPES, pH = 7.2), λex = 620 nm)

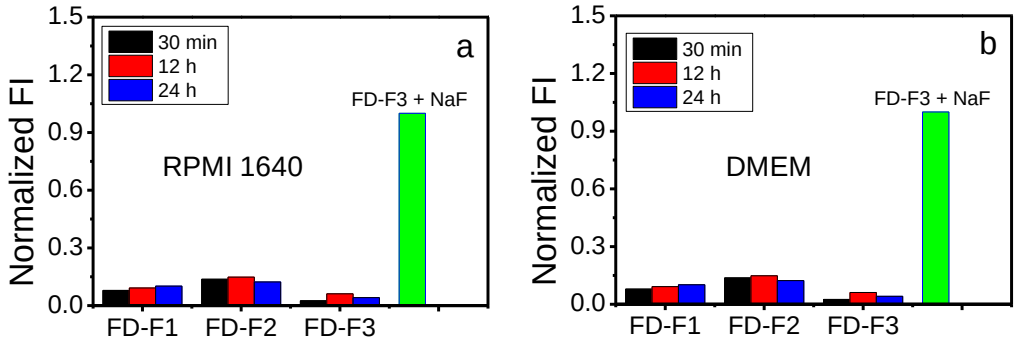



**Fig. S3** Fluorescence intensity changes at 690 nm of probes (50 μM) were incubated in different cell medium (a) Dulbecco's modified essential medium (RPMI 1640) and (b) Dulbecco's Modified Eagle's medium (DMEM) for different time. (The green bar is

the fluorescence intensity of 10 μM **FD-F3** and 20 μM NaF reacted for 50 min as reference)

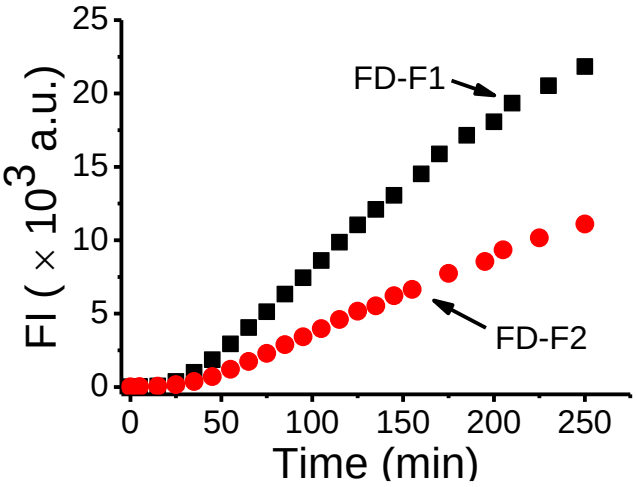



**Fig. S4** Fluorescence intensity enhancement at 690 nm for **FD-F1 (10 μM)** and **FD-F2 (10 μM)** with time increase after treated with 500 μM NaF. (DMSO-HEPES solution (3/2, v/v, 10 mM HEPES, pH = 7.2), λex = 620 nm)

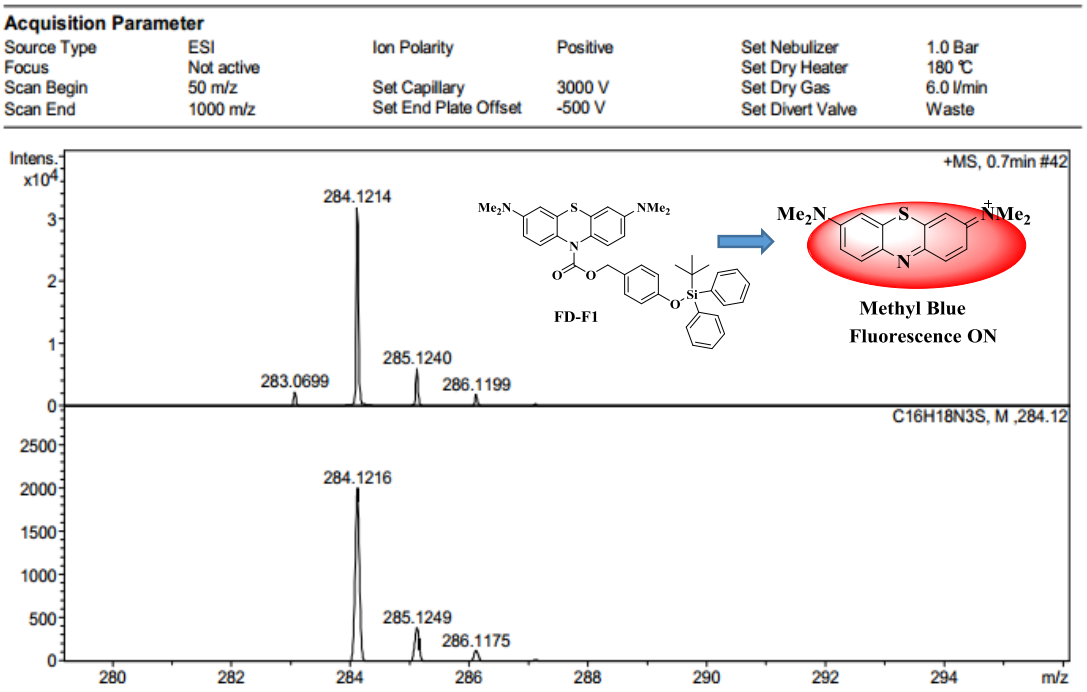



**Fig. S5** HRMS analysis of compound **FD-F1** after reacted with NaF (the theoretical molecular mass of the MB is 284.1216, $[M - Cl^-]^+$ )

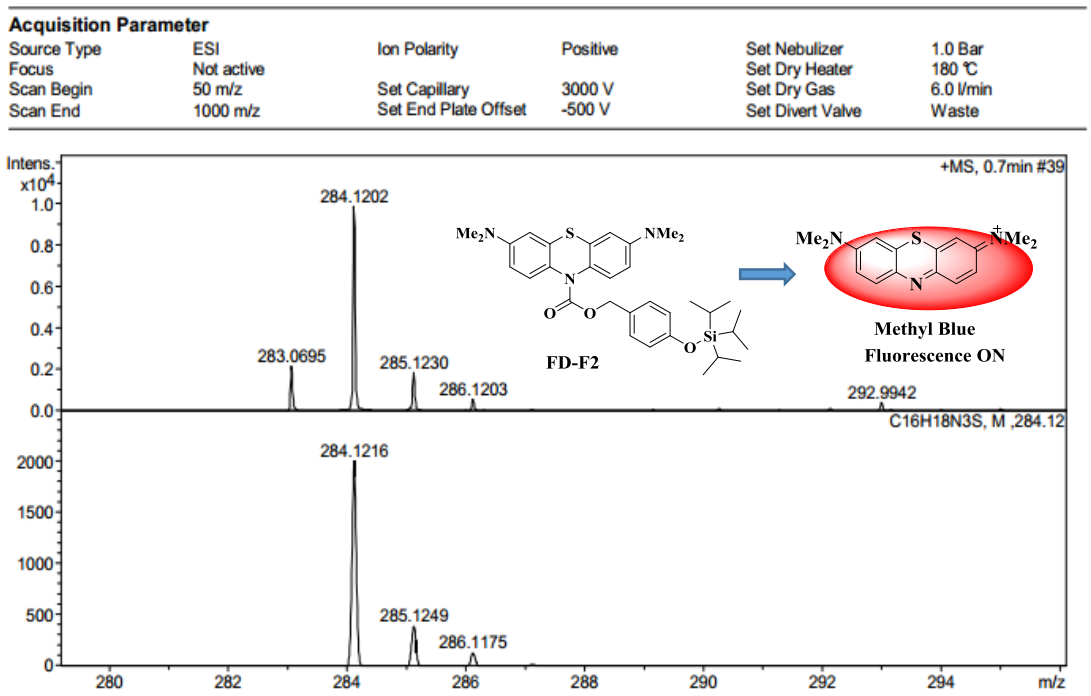



**Fig. S6** HRMS analysis of compound **FD-F2** after reacted with NaF (the theoretical molecular mass of the MB is 284.1216, $[M - Cl^{-}]^{+}$ )

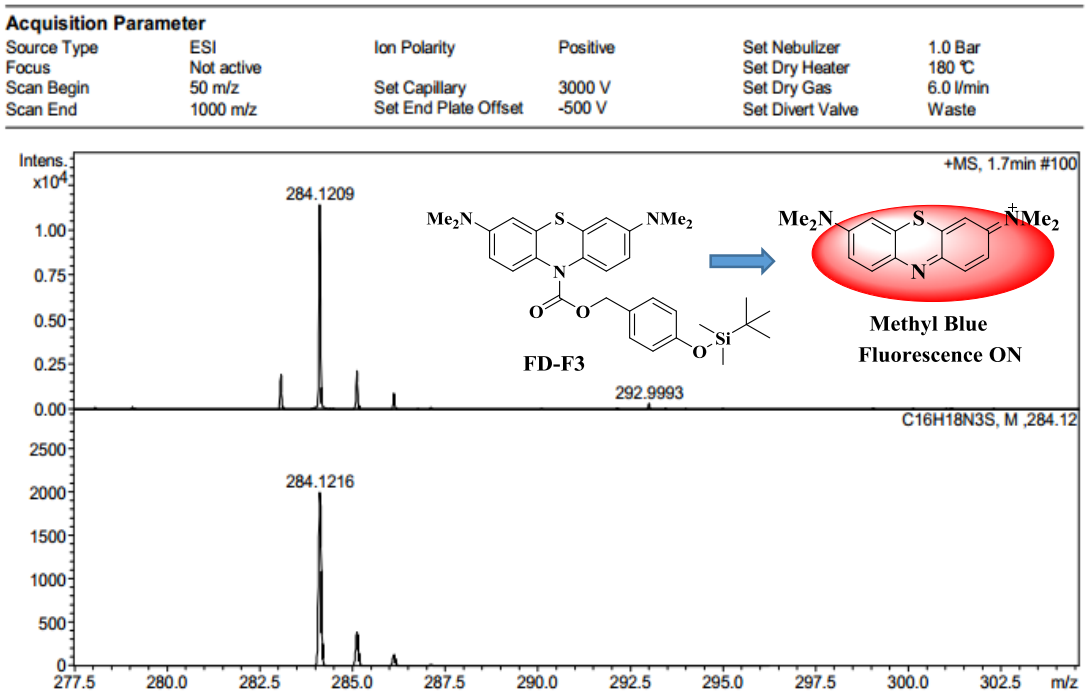



**Fig. S7** HRMS analysis of compound **FD-F3** after reacted with NaF (the theoretical molecular mass of the MB is 284.1216, $[M - Cl^{-}]^{+}$ )

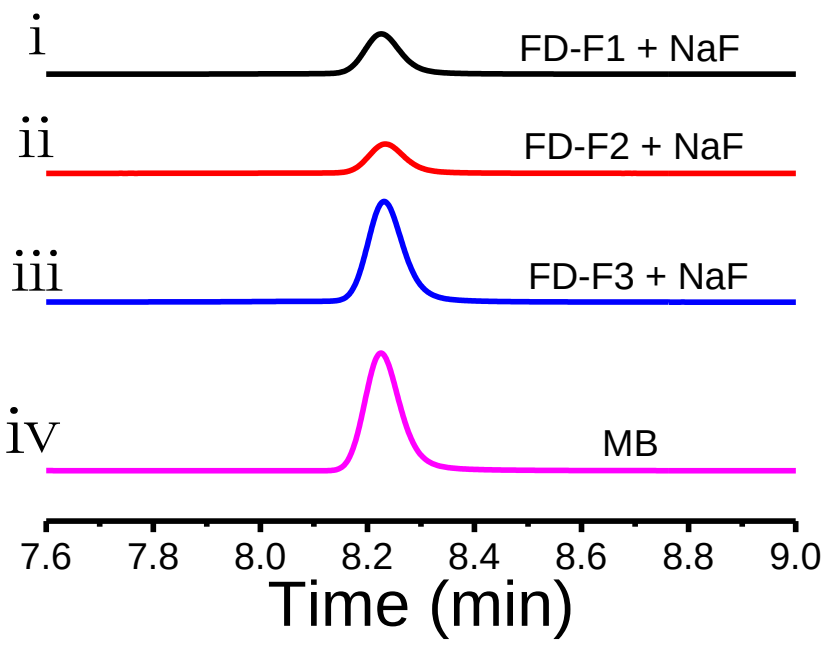



**Fig. S8** HPLC analysis of MB (10 μM) and different probes (10 μM) after reacted with NaF (500 μM) for 50 min.

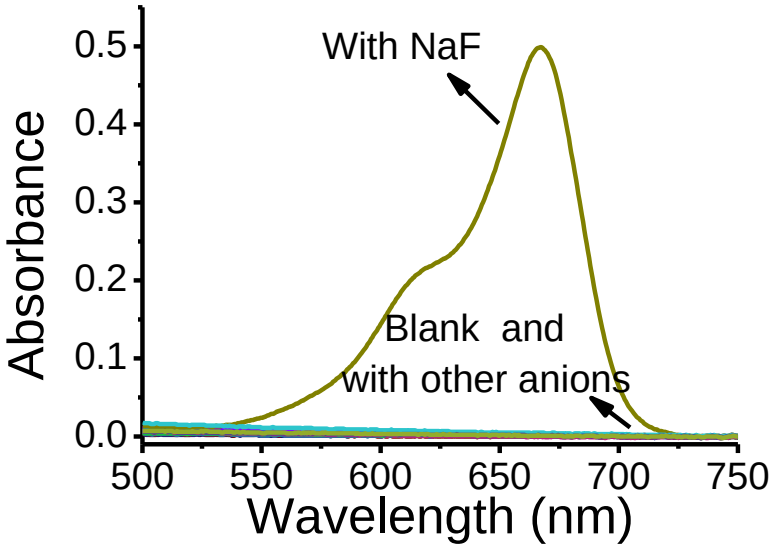



**Fig. S9** The absorption spectra of probe **FD-F3** (10 μM) when treated with 500 μM various tested analytes (incubated for 50 min, DMSO-HEPES solution (3/2, v/v, 10 mM HEPES, pH=7.2), λex=620nm)

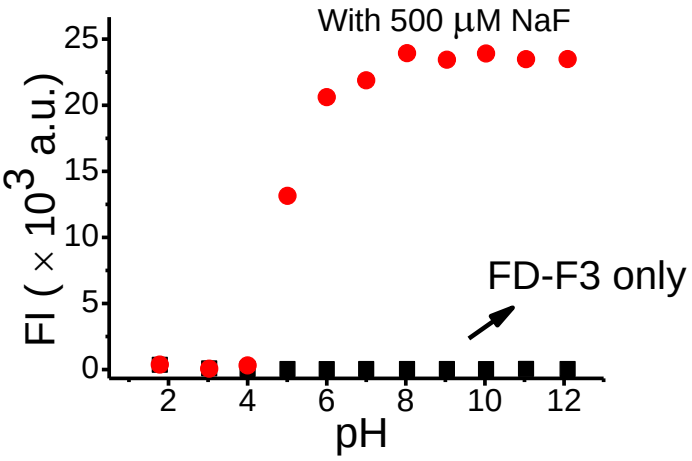



**Fig. S10** Fluorescence intensity at 690 nm at different pH levels before and after treatment with 500 μM NaF for 50 min. (DMSO-HEPES solution, 3/2, v/v, 10 mM HEPES, pH = 7.2; λex = 620 nm)

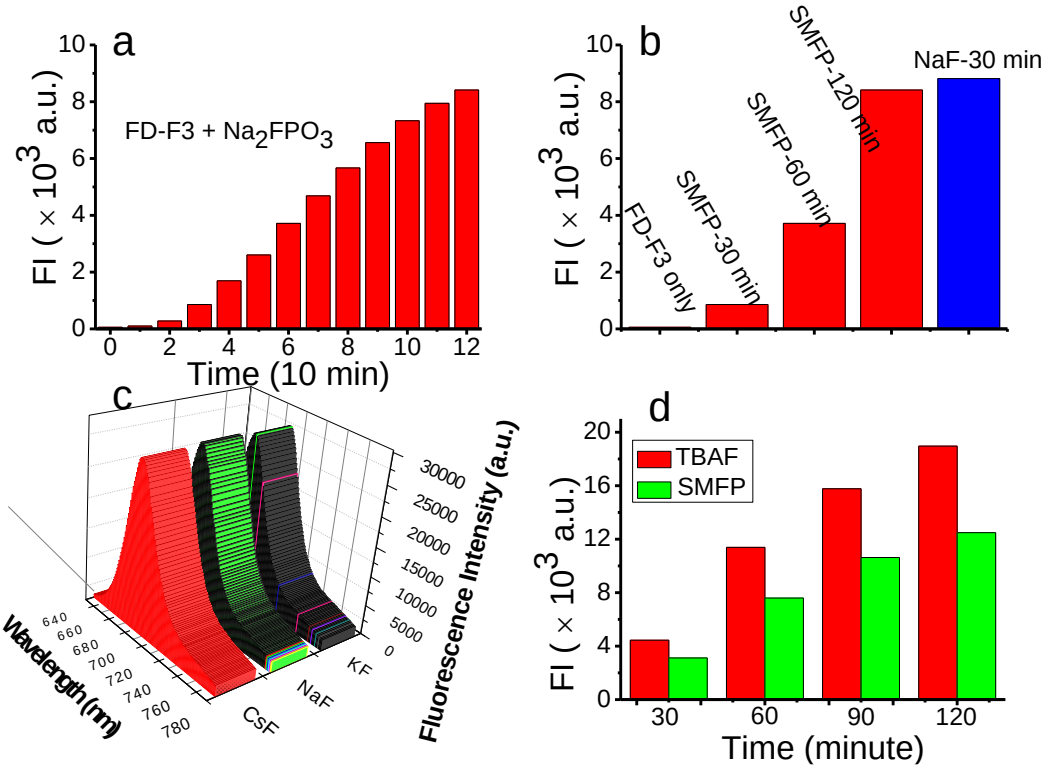



**Fig. S11** Fluorescence intensity of **FD-F3** (10 μM) at 690 nm (a) with different incubation times after treatment with 500 μM SMFP; (b) with different incubation times after treatment with 500 μM SMFP and incubated for 30 min after treatment with 500 μM NaF. (c) Fluorescence spectra of **FD-F3** after adding 500 μM different inorganic fluoride. (d) Fluorescence intensity of **FD-F3** with different incubation time after treated with 500 μM SMFP and TBAF. (DMSO-HEPES solution, 3/2, v/v, 10 mM HEPES, pH = 7.2; λex = 620 nm)

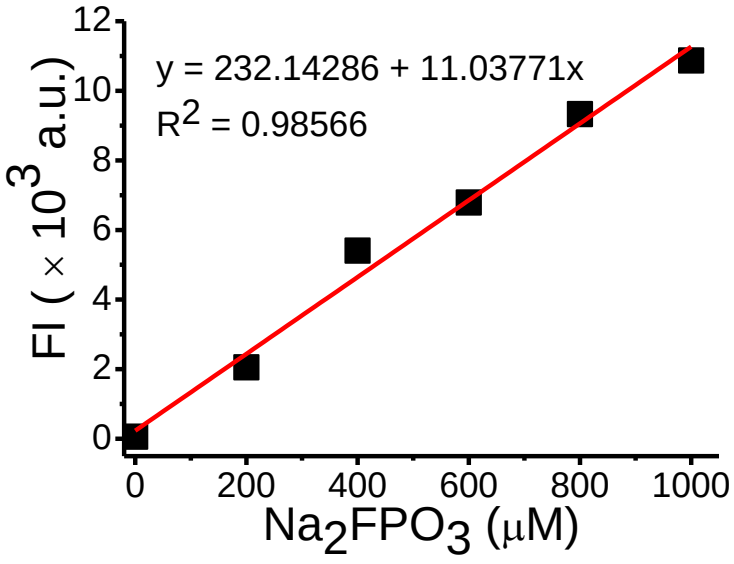



**Fig. S12** Fluorescence intensity of **FD-F3** (10 μM) at 690 nm with different concentrations of SMFP incubated for 50 min. (DMSO-HEPES solution, 3/2, v/v, 10 mM HEPES, pH = 7.2; λex = 620nm)

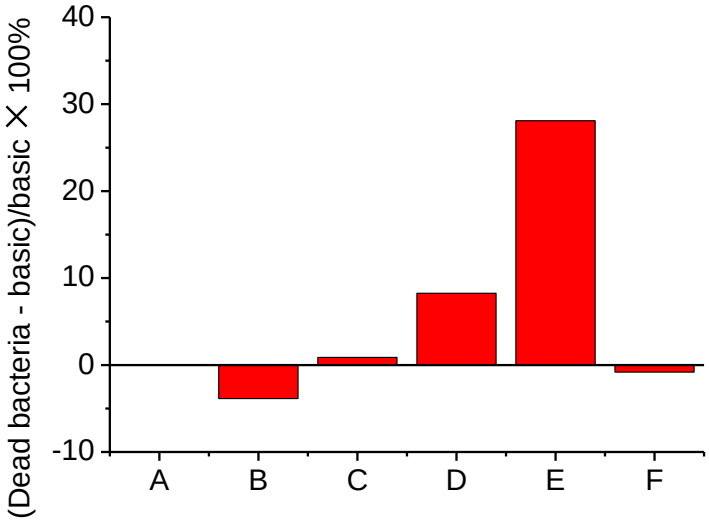



**Fig. S13** Proportion of dead bacteria after treated with (A) either no drug as control; (B) treated only with free **FD-F3** (50 μg/mL) for 30 min; (C) treated only with NaF (50 μg/mL) for 60 min; (D) treated with **FD-F3** (50 μg/mL) for 30 min then NaF (50 μg/mL) for 60 min (E) treated with **FD-F3** (50 μg/mL) for 30 min then NaF (50 μg/mL) for 60 min then light (100 mW/cm$^2$) for 5 min; (F) treated only with light (100 mW/cm$^2$) for 5 min. ( The light was using laser at 655 nm. )

## 4. NMR and HRMS spectra of the compounds

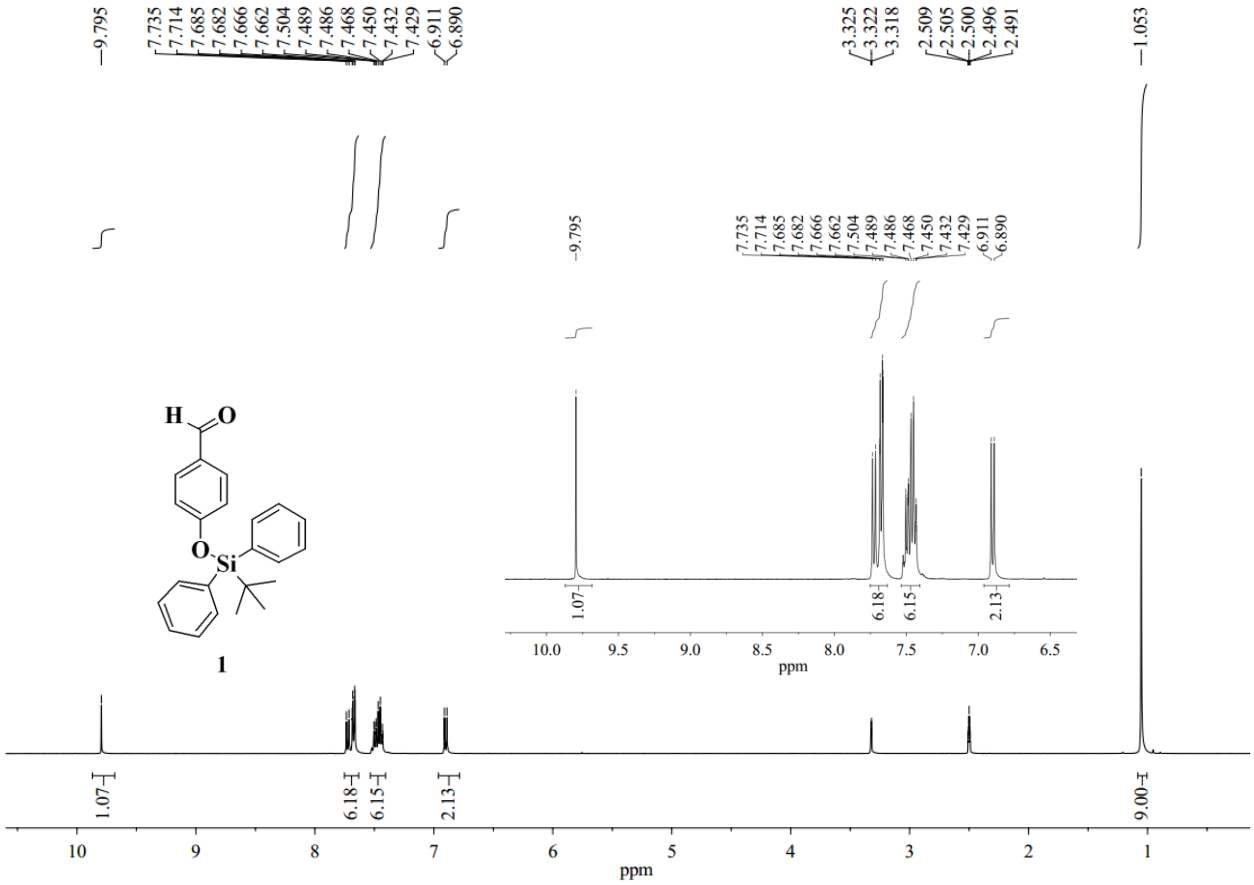



**Fig. S14** $^{1}$H-NMR of compound 1 in DMSO-*d6*

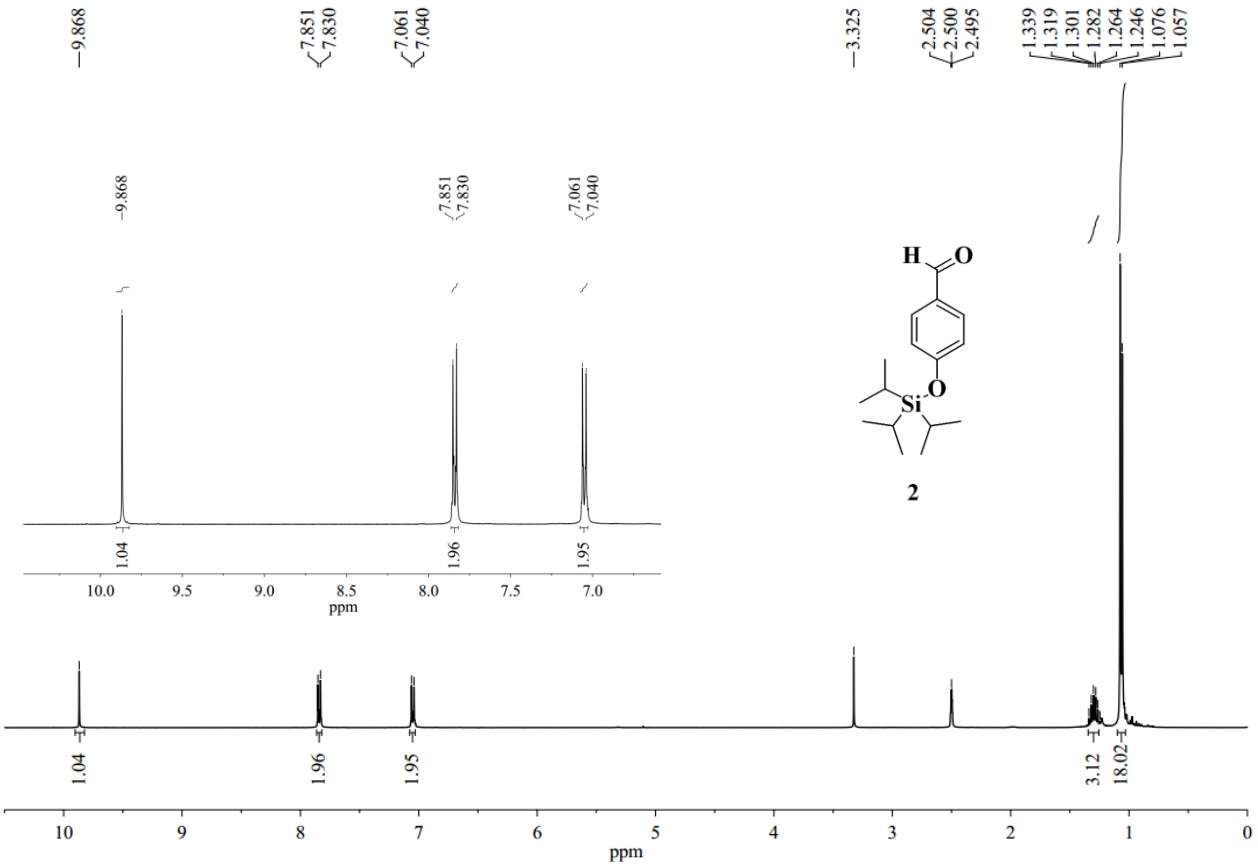



**Fig. S15** $^{1}$H-NMR of compound 2 in DMSO-*d6*

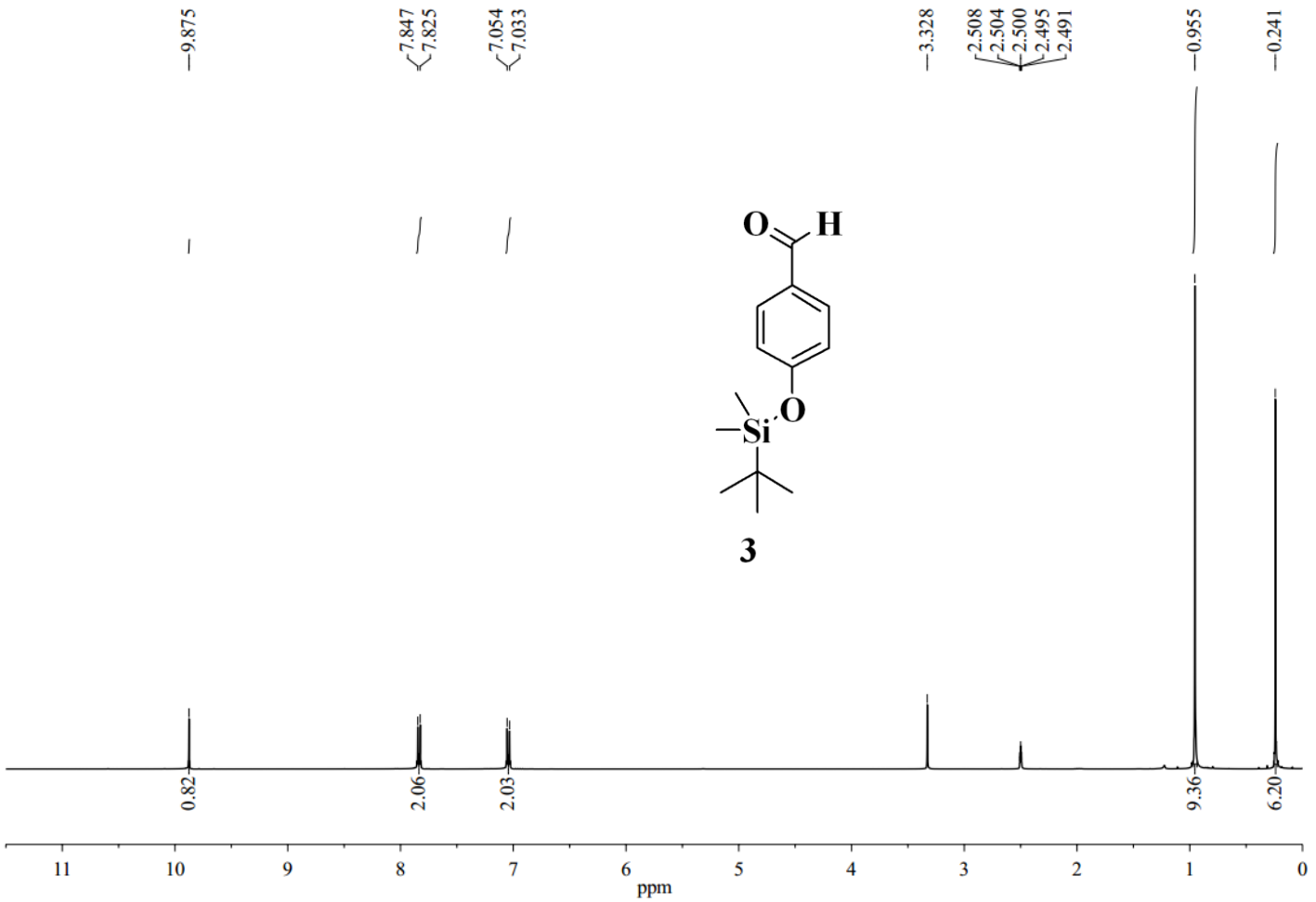



**Fig. S16** [1]H-NMR of compound 3 in DMSO-*d6*

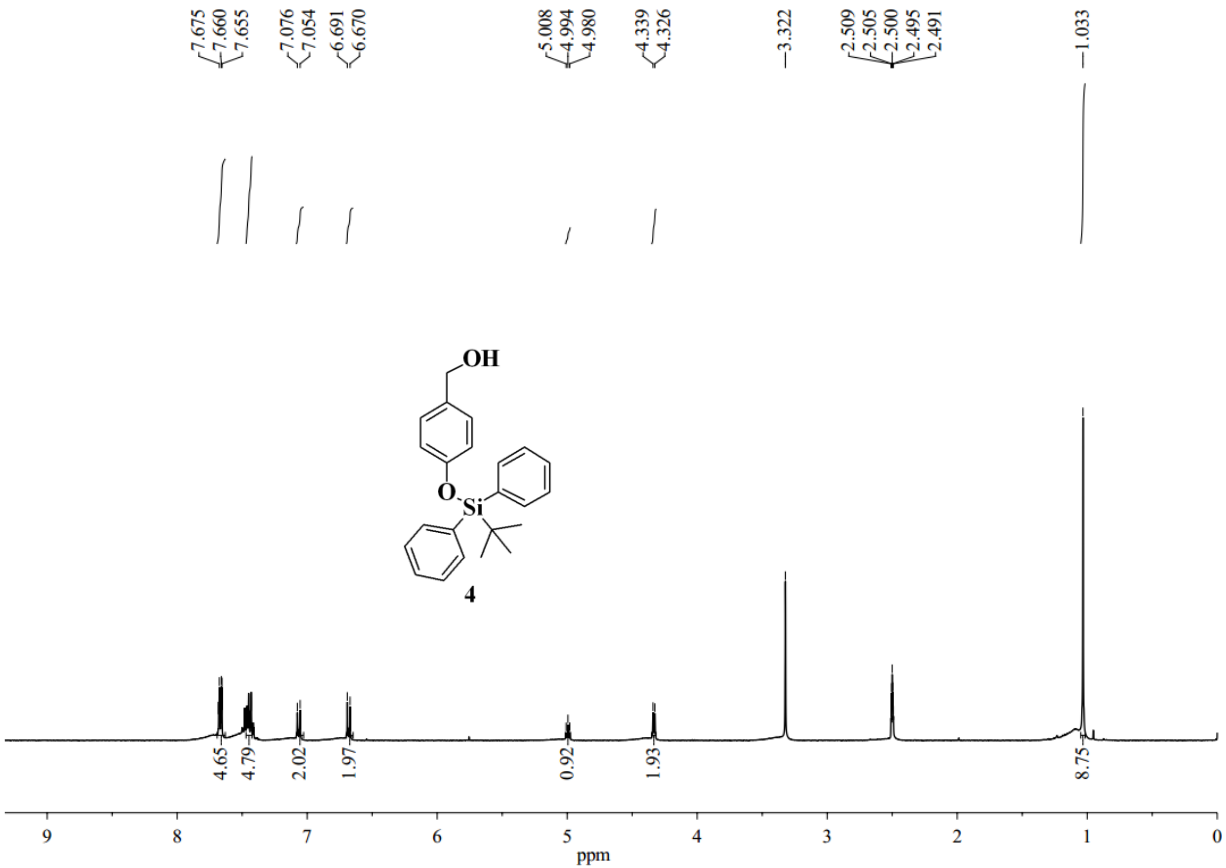



**Fig. S17** $^{1}$H-NMR of compound 4 in DMSO-*d6*

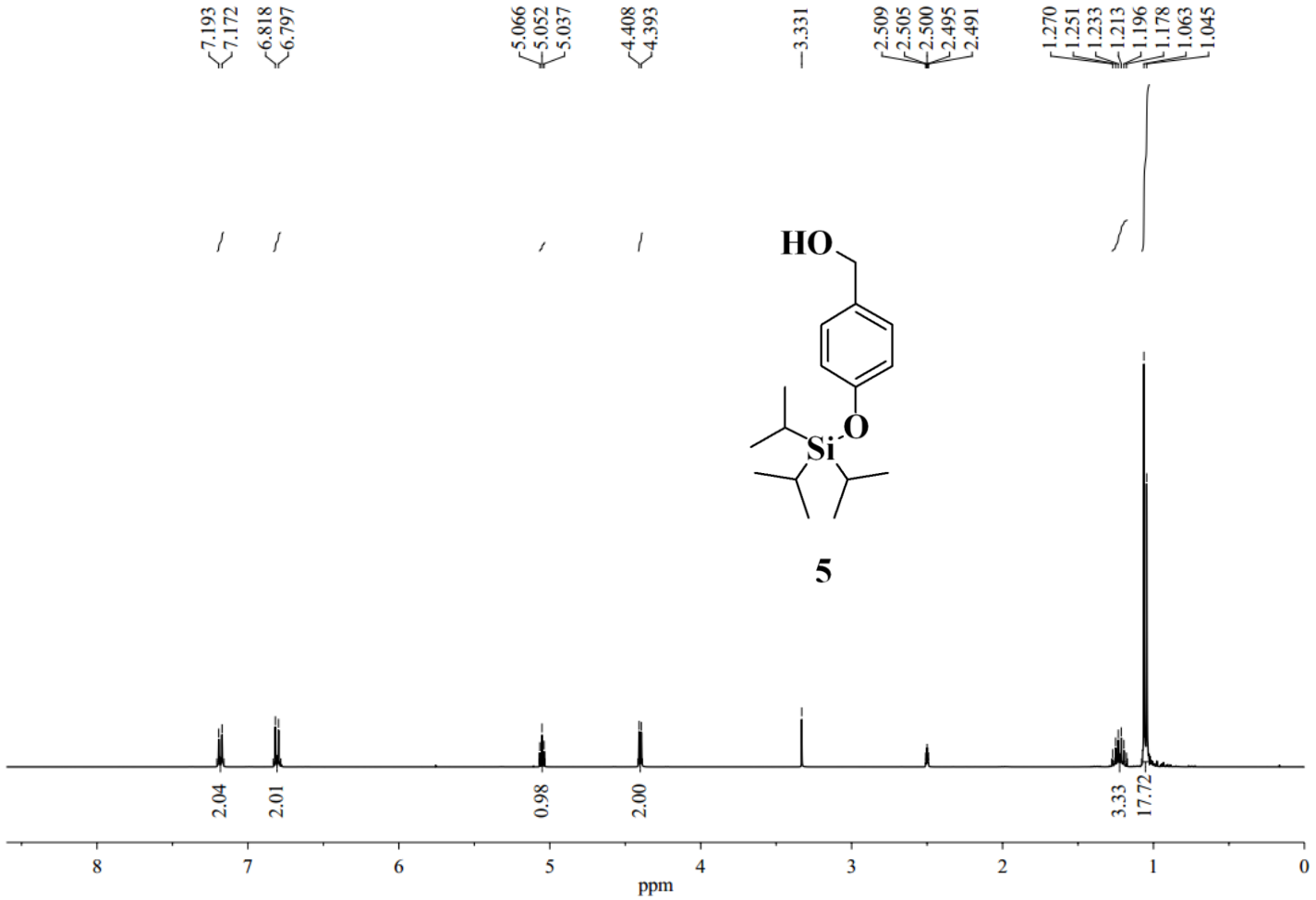



**Fig. S18** [1]H-NMR of compound 5 in DMSO-*d6*

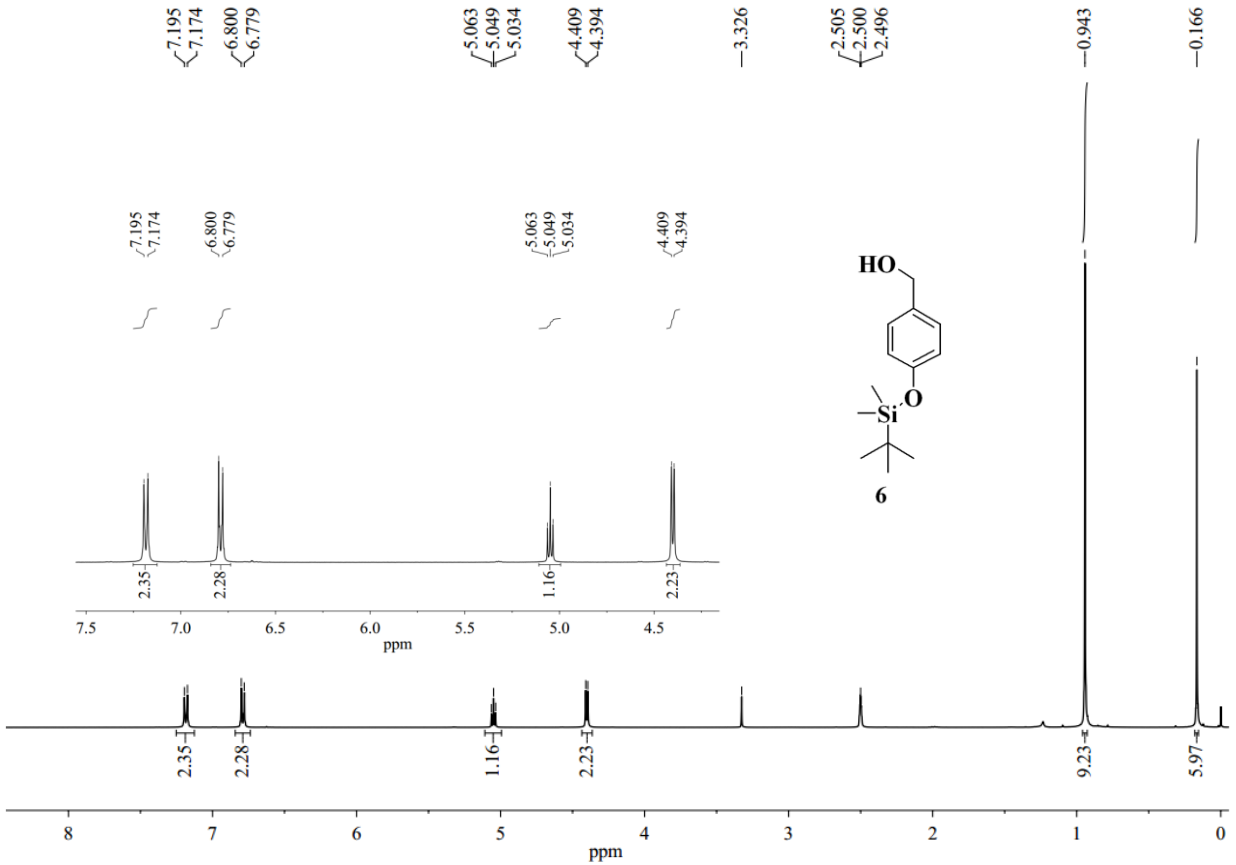



**Fig. S19** $^{1}$H-NMR of compound **6** in DMSO-*d6*

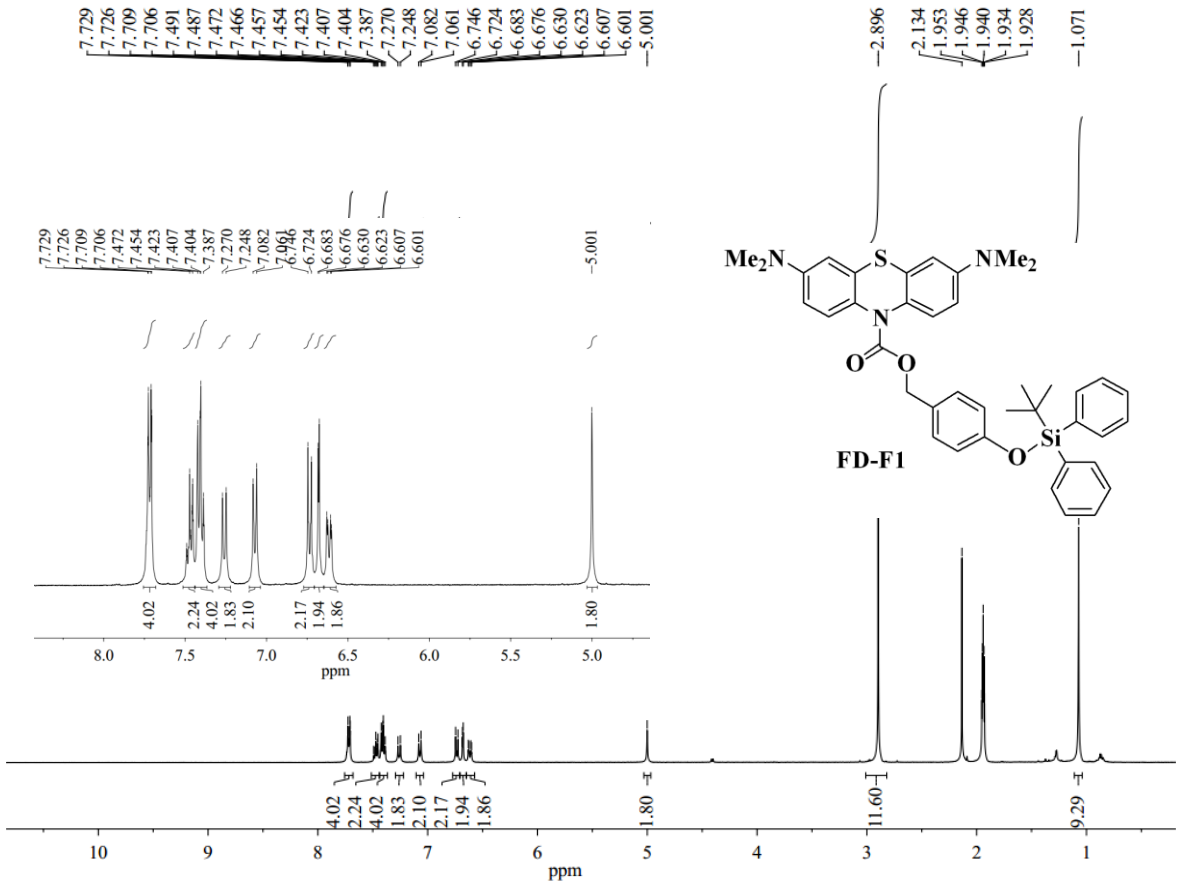



**Fig. S20** $^{1}$H-NMR of compound **FD-F1** in $CD_3CN$

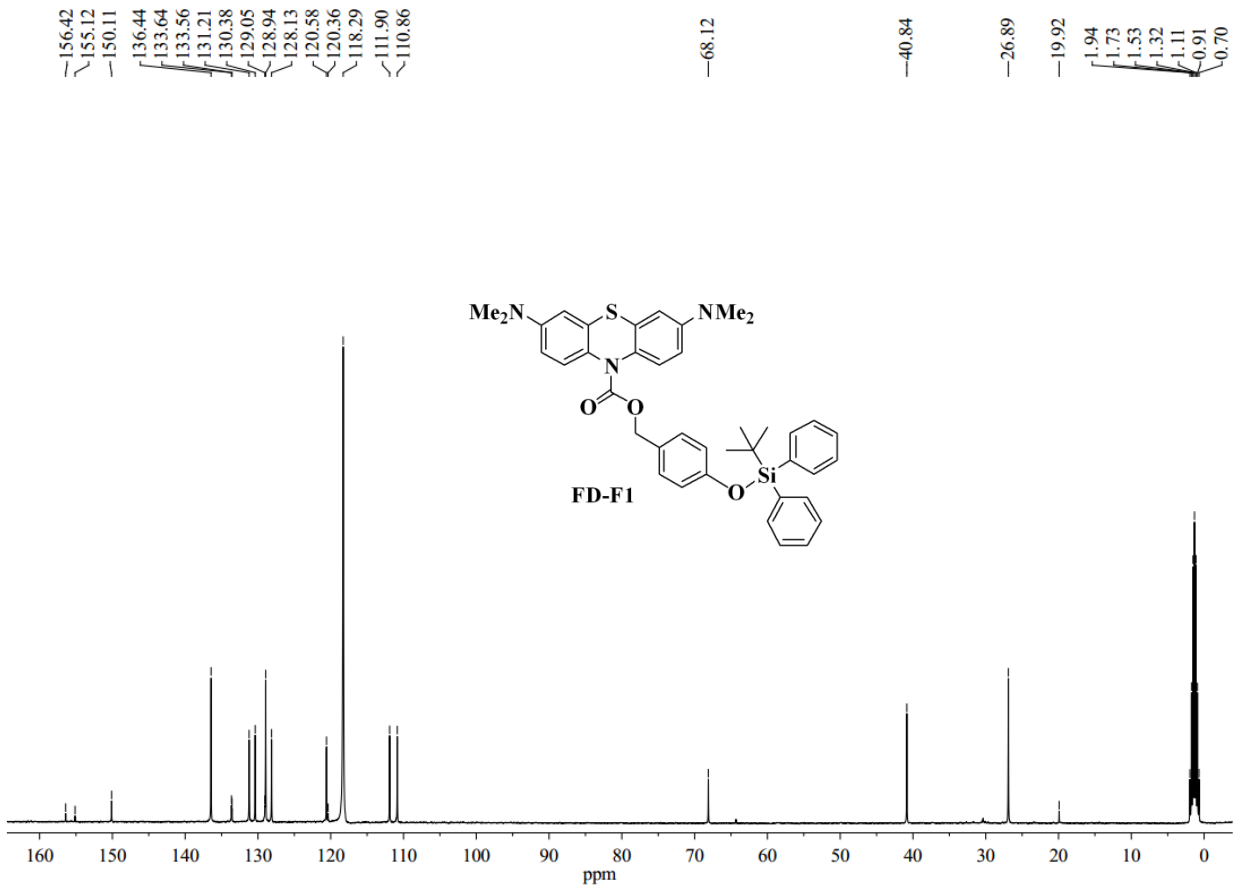



**Fig. S21** $^{13}$C-NMR of compound **FD-F1** in $CD_3CN$

| Acquisition Parameter | | | | | |
|---|---|---|---|---|---|
| Source Type | ESI | Ion Polarity | Positive | Set Nebulizer | 1.0 Bar |
| Focus | Not active | | | Set Dry Heater | 180 ℃ |
| Scan Begin | 50 m/z | Set Capillary | 3000 V | Set Dry Gas | 6.0 l/min |
| Scan End | 1000 m/z | Set End Plate Offset | -500 V | Set Divert Valve | Waste |

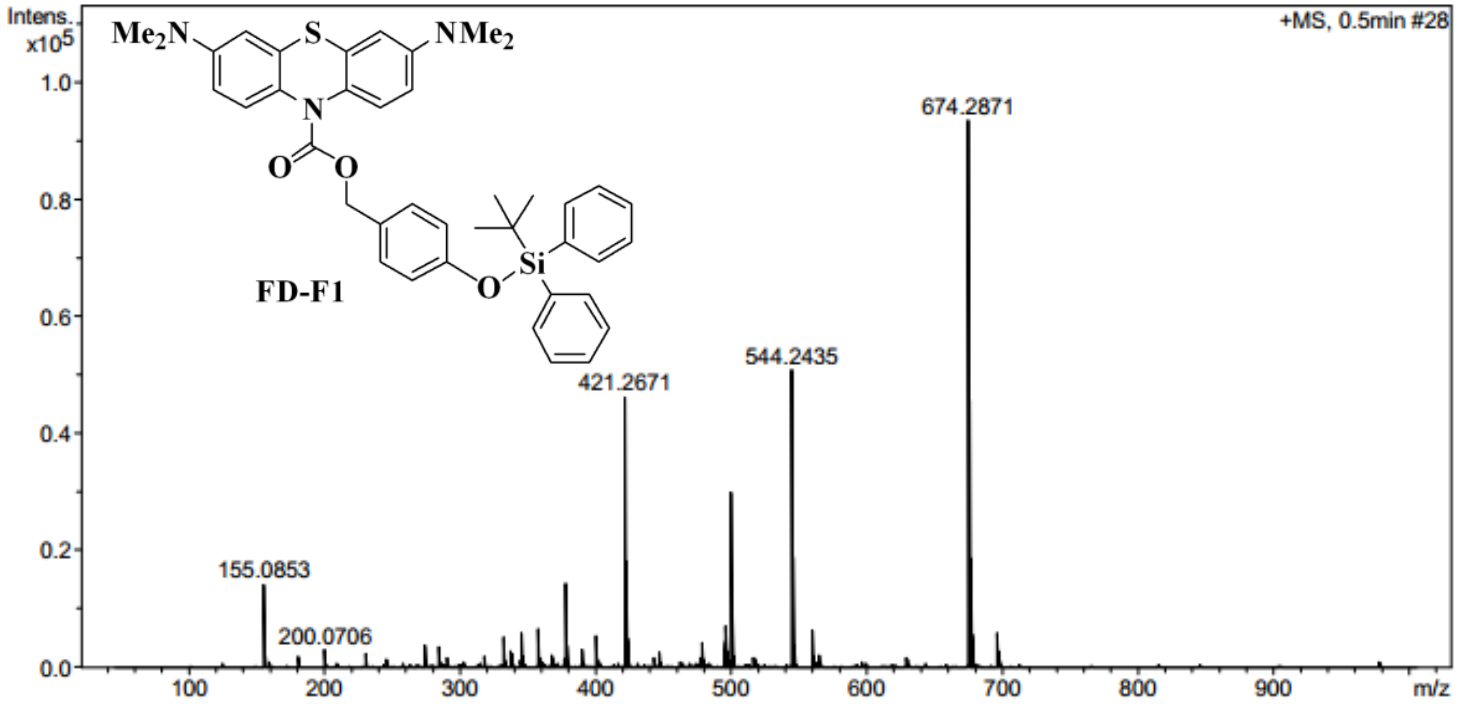



**Fig. S22** HRMS of compound **FD-F1**

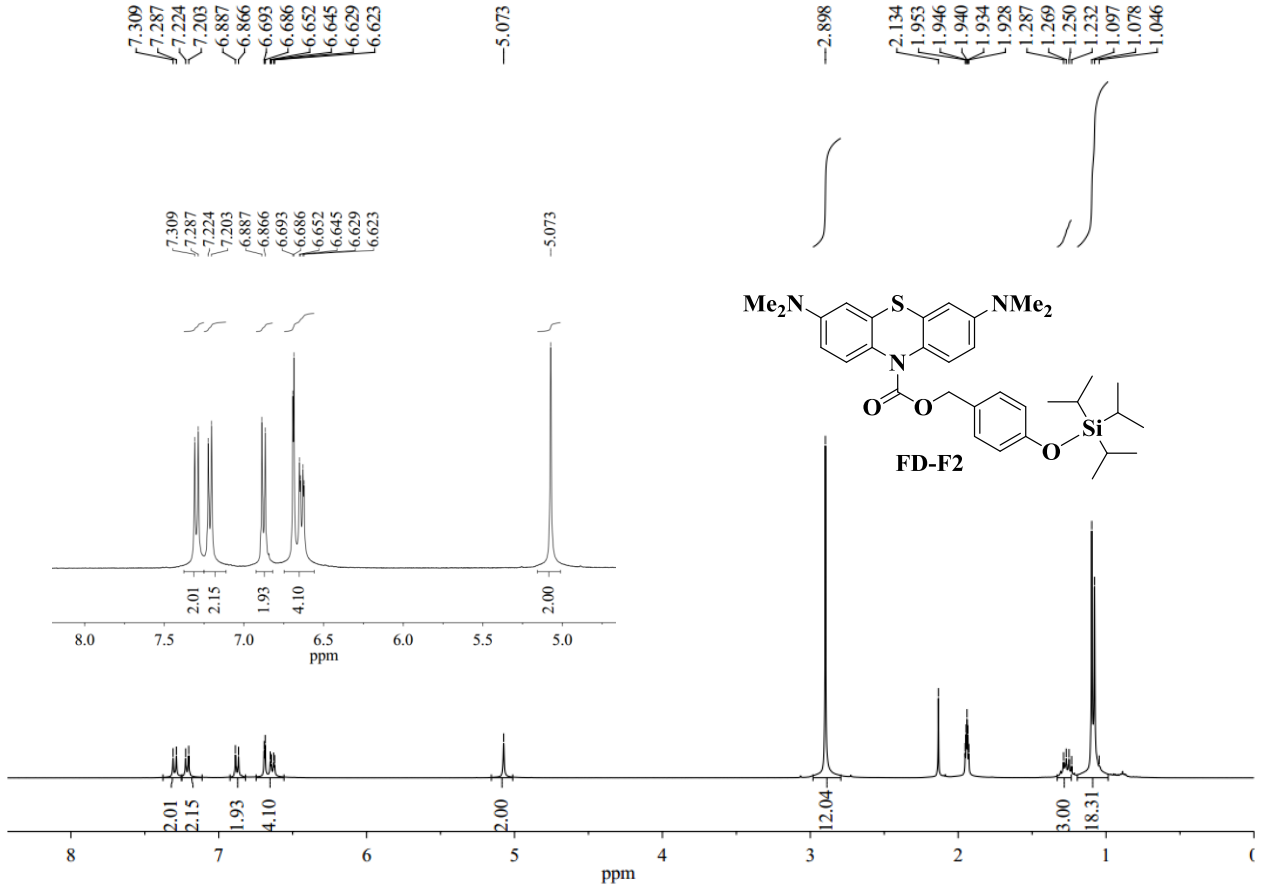



**Fig. S23** $^{1}$H-NMR of compound **FD-F2** in $CD_3CN$

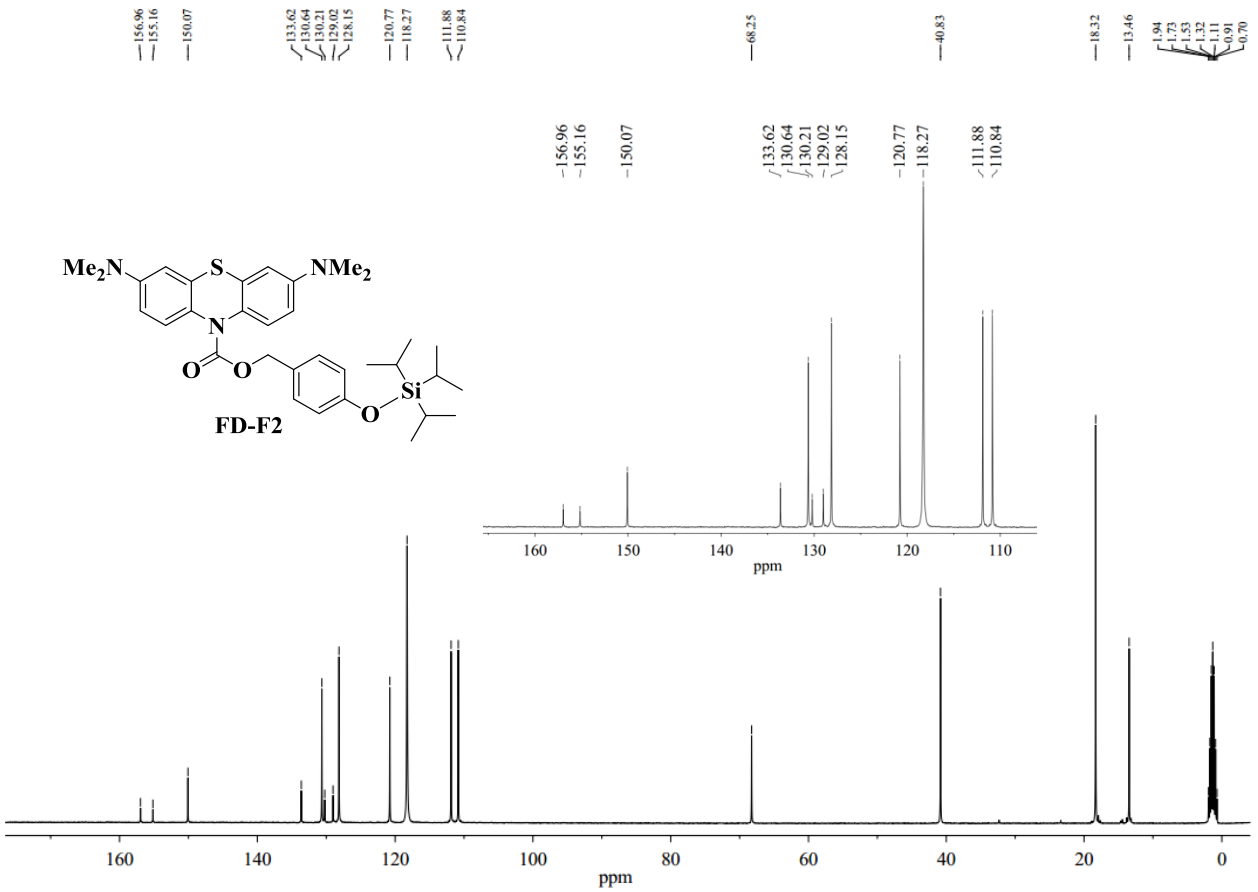



**Fig. S24** $^{13}$C-NMR of compound **FD-F2** in $CD_3CN$

| Acquisition Parameter | | | | | |
|---|---|---|---|---|---|
| Source Type | ESI | Ion Polarity | Positive | Set Nebulizer | 1.0 Bar |
| Focus | Not active | | | Set Dry Heater | 180 ℃ |
| Scan Begin | 50 m/z | Set Capillary | 3000 V | Set Dry Gas | 6.0 l/min |
| Scan End | 1000 m/z | Set End Plate Offset | -500 V | Set Divert Valve | Waste |

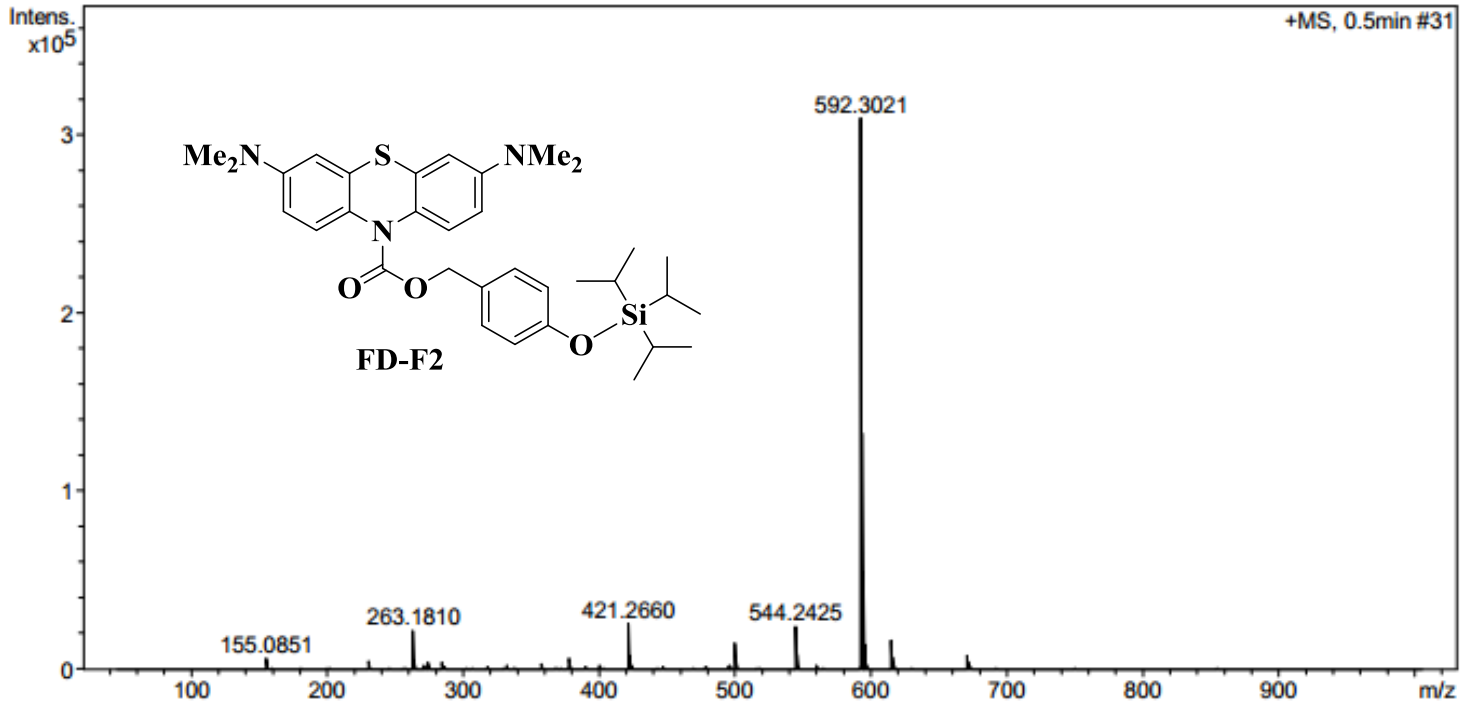



**Fig. S25** HRMS of compound **FD-F2**

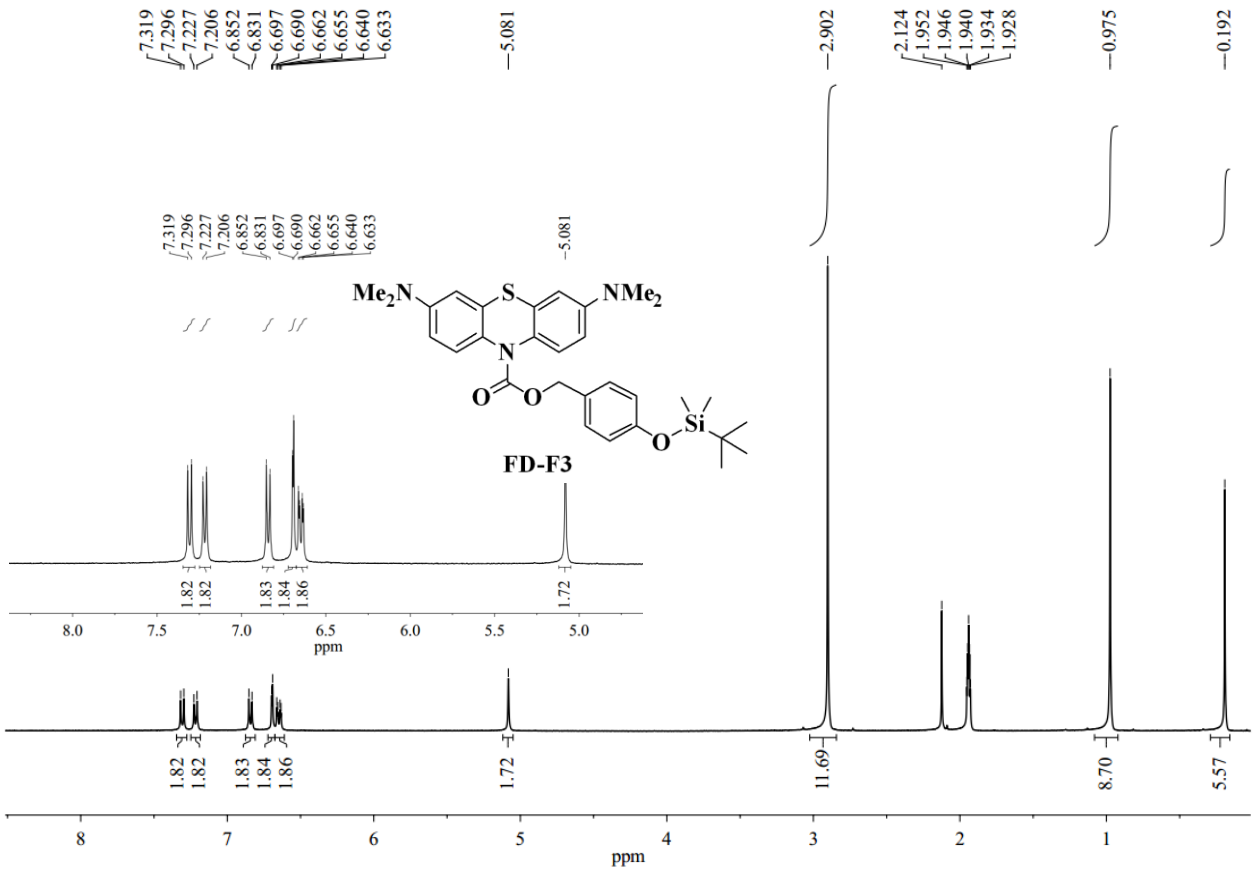



**Fig. S26** $^{1}$H-NMR of compound **FD-F3** in $CD_3CN$

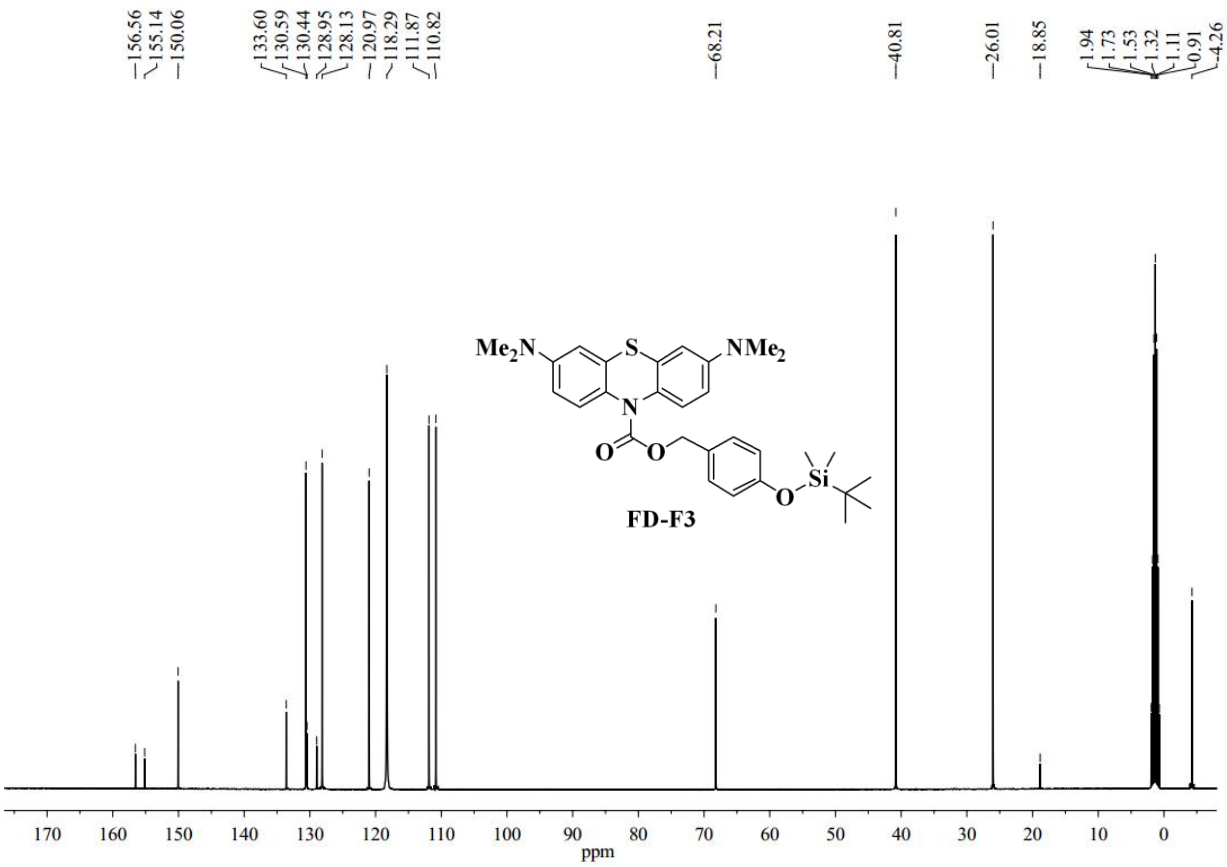



**Fig. S27** $^{13}$C-NMR of compound **FD-F3** in $CD_3CN$

| Acquisition Parameter | | | | | |
|---|---|---|---|---|---|
| Source Type | ESI | Ion Polarity | Positive | Set Nebulizer | 1.0 Bar |
| Focus | Not active | | | Set Dry Heater | 180 ℃ |
| Scan Begin | 50 m/z | Set Capillary | 3000 V | Set Dry Gas | 6.0 l/min |
| Scan End | 1000 m/z | Set End Plate Offset | -500 V | Set Divert Valve | Waste |

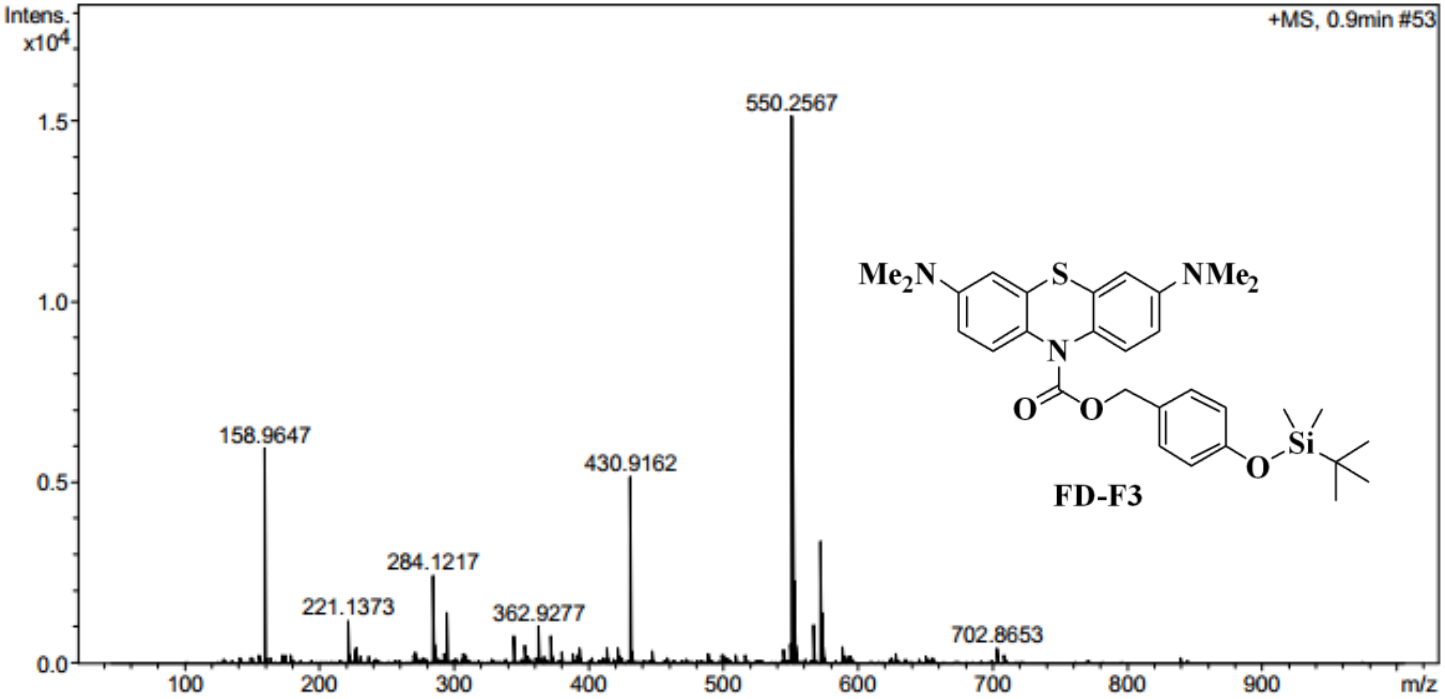



**Fig. S28** HRMS of compound **FD-F3**

## 5. Reference

1. Y. Zhang, S. Swaminathan, S. Tang, J. Garcia-Amorós, M. Boulina, B. Captain, J. D. Baker and F. M. Raymo, *J. Am. Chem. Soc.*, 2015, **137**, 4709-4719.