Electronic Supplementary Information

A novel "turn-on" fluorogenic probe for sensing hypochlorous acid based on BODIPY

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Synthesis of BODIPY and BODIPY-AL

BODIPY was synthesized according to the literature procedure[1]. BODIPY-AL was synthesized from BODIPY by using well known Vismeier Haack's formylation reaction[2].

BODIPY: The mixed solution of 2,4-dimethylpyrrole (19.0 mmol, 2mL), benzoyl chloride (9.5 mmol, 1.15 mL) and DCM (50 mL) was stirred overnight at room temperature under N_2 atmosphere. Then triethylamine (10 mL) was added drop-by-drop in ice water bath. After stirred about 30 min under N_2 atmosphere, drop-by-drop addition of boron fluoride ethyl ether (10 mL) was begun. The mixture was stirred overnight again at room temperature under N_2 atmosphere. The organic phase was washed with saturated $NaHCO_3$ solution (100 mL), and then washed with water for three times and dried with anhydrous sodium sulfate. The product was purified by column chromatography (petroleum ether-dichloromethane, v:v, 5:1) to give a orange solid (1.2 g, 38%).

BODIPY-AL: To a 100 mL round-bottomed flask, $POCl_3$ (3 mL) was added in a solution of DMF (3 mL) in ice water bath under N_2 atmosphere. After stirred about 30 min, viscid liquid with yellow was appeared. When the temperature rise to 50 ^oC, drop-by-drop addition of 30 mL DCE solution of BODIPY (3.1 mmol, 1 g) was begun. The mixture was stirred for 8 h at 55 °C under N_2 atmosphere. Following the completion of the reaction, saturated $NaHCO_3$ solution (200 mL) was added in ice water bath, then stirred for 30 min. The organic phase was washed with 100 mL water for three times and dried with anhydrous sodium sulfate. The product was purified by column chromatography (dichloromethane-methanol, v:v, 10:1) to give a orange solid (0.9 g, 81%).

Reference

1. M. Emrullahoglu, M. Ucuncu and E. Karakus, Chem. Commun., 2013, 49, 7836-7838.

2. M. Isik, T. Ozdemir, I. S. Turan, S. Kolemen and E. U. Akkaya, Org. Lett., 2013, 15, 216-219.

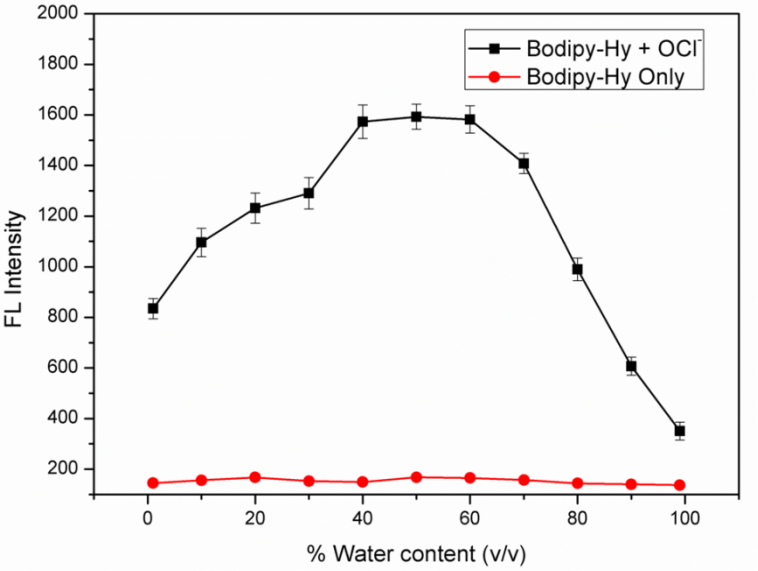

Fig. S1. Effect of fraction of water on the interaction of Bodipy-Hy (10 μM) with HOCl (200 μM, 20 equiv.) in 0.1 M phosphate buffer-ethanol (pH 7.20) solution (λ_{ex}=465 nm, λ_{em}=510 nm at 25 °C).

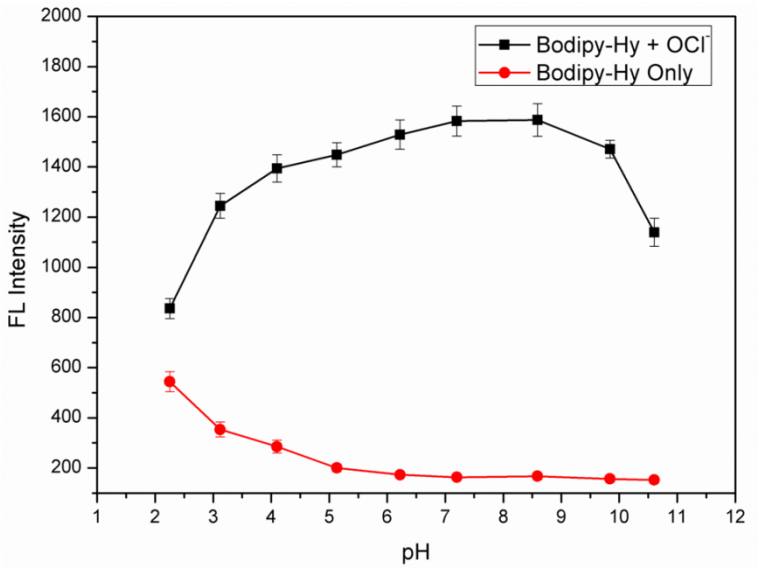

Fig. S2. Effect of pH on the interaction of Bodipy-Hy (10 μM) with HOCl (200 μM, 20 equiv.) in 0.1 M phosphate buffer-ethanol (v/v, 1:1) solution (λ_{ex}=465 nm, λ_{em}=510 nm at 25 °C)

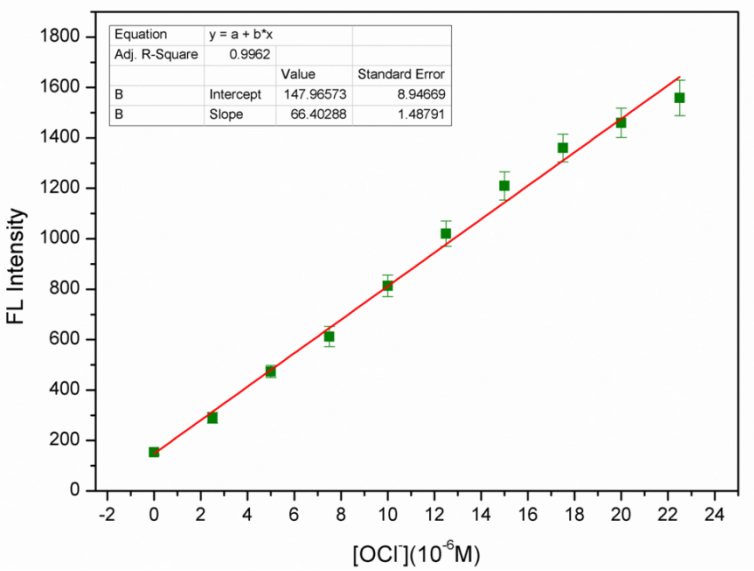

Fig. S3. Fluorescence intensity changes of Bodipy-Hy (10 μM) against HOCl concentration from 0 to 22.5 μM in 0.1 M phosphate buffer-ethanol (pH 7.20, v/v, 1:1) solution (λ_{ex}=465 nm, λ_{em}=510 nm at 25 °C)

Fig. S4. TLC image of the reaction of Bodipy-Hy with HOCl (100/50/1, v/v/v, dichloromethane/ petroleum ether/ triethylamine).

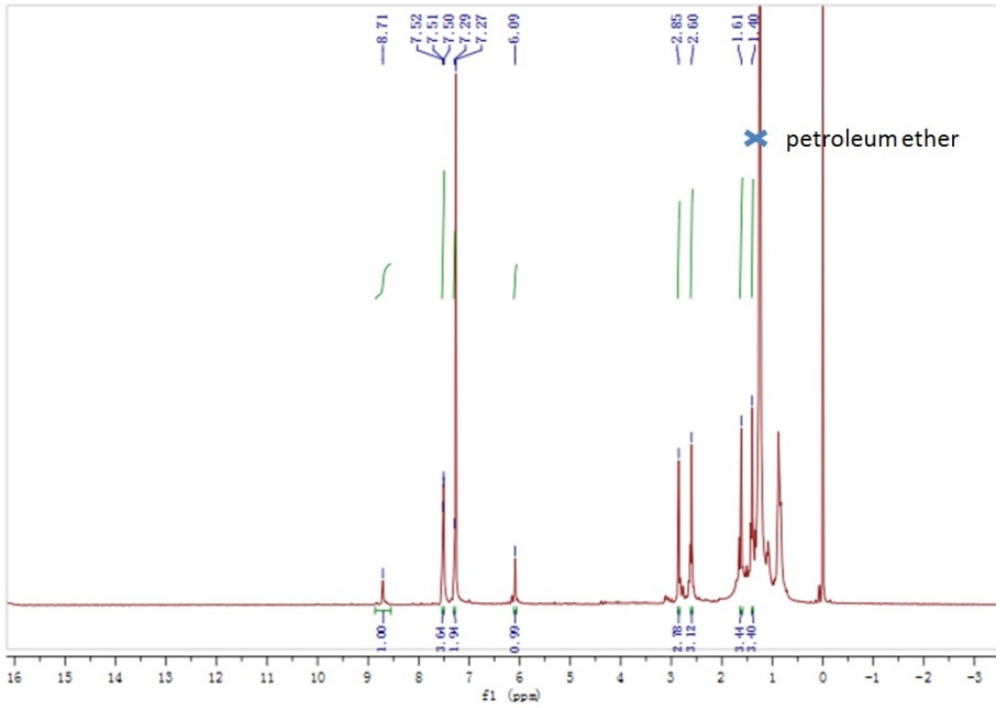

Fig. S5. ^{1}H NMR of Bodipy-Hy. ($CDCl_3$)

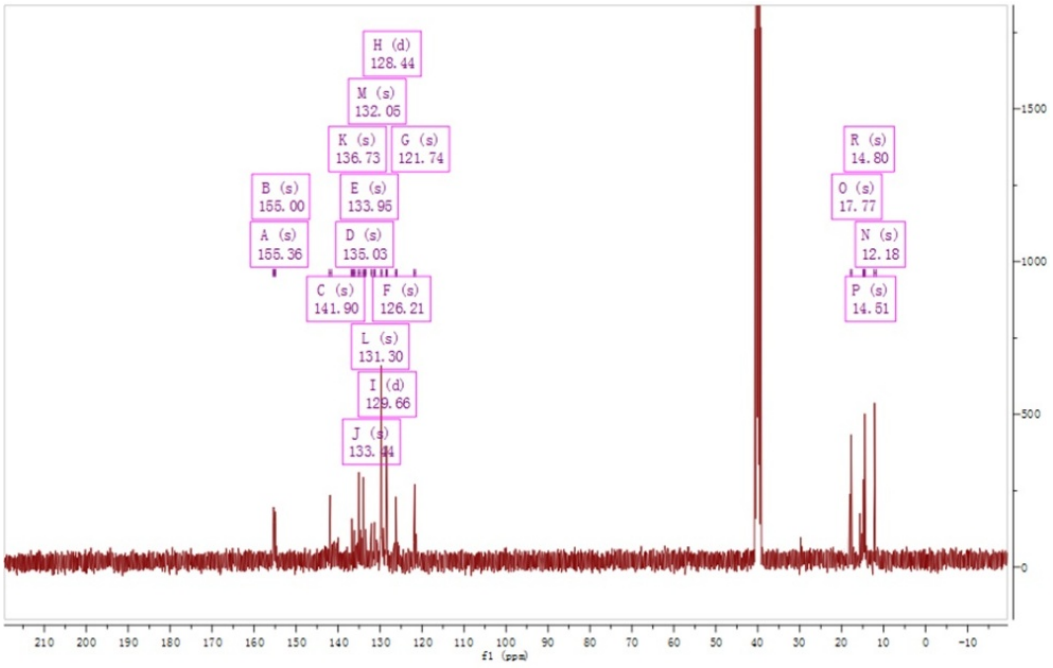

Fig. S6. ^{13}C NMR of Bodipy-Hy. (DMSO-d_6)

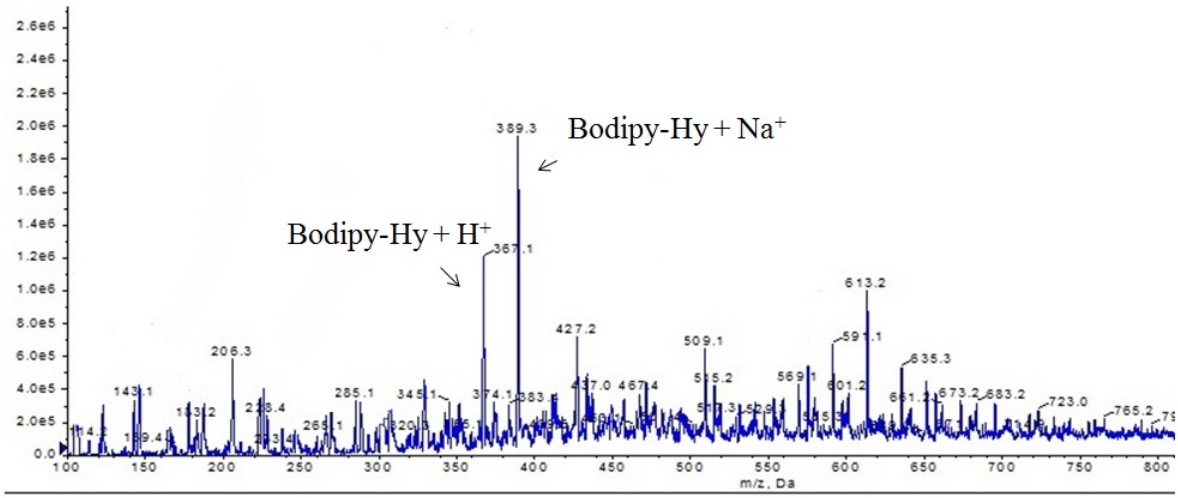

Fig. S7. Mass spectrometry of Bodipy-Hy

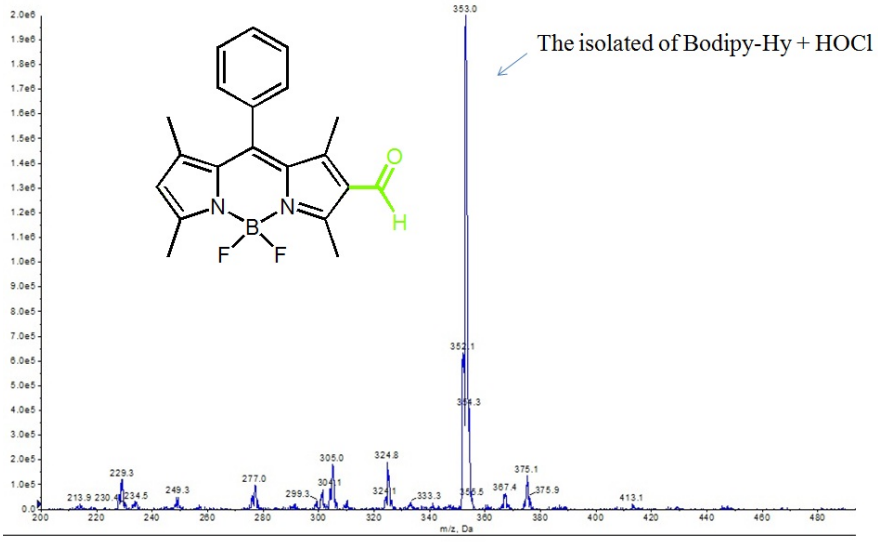

Figure S8. Mass spectrometry of isolated Bodipy-Hy + HOCl