Supporting Information

One-pot synthesis of hydrogen peroxide selective fluorogenic probe and its application in Parkinson's disease *in vitro* and *vivo* models

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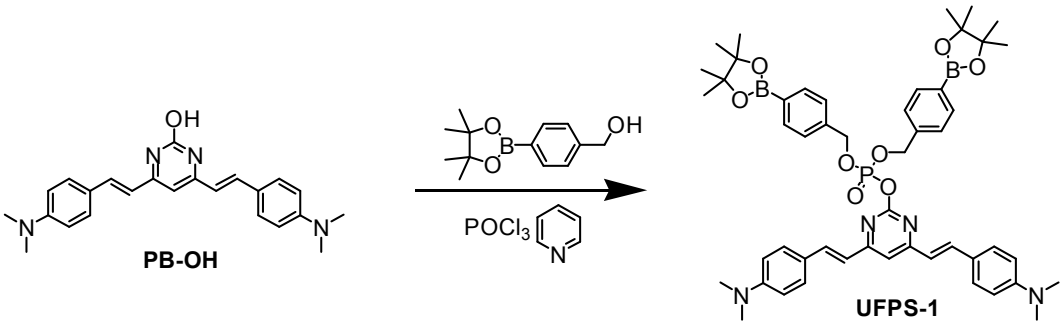


Figure S1. Synthesis method of **UFPS-1**.

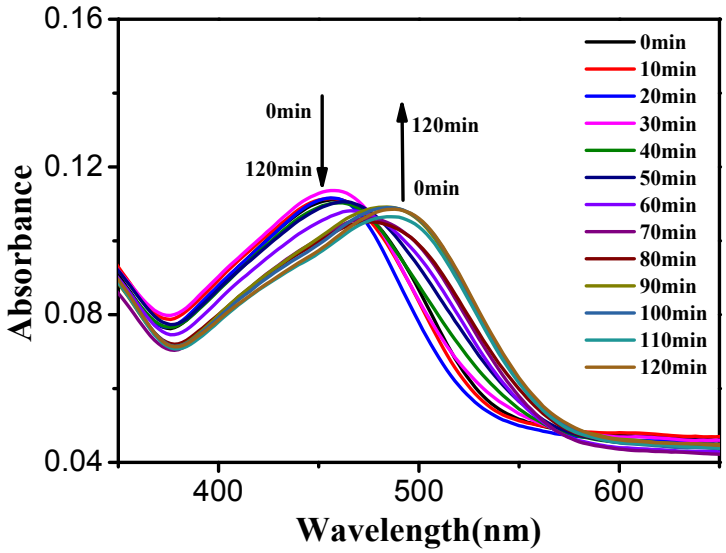


Figure S2. Absorbance spectra of **UFPS-1** (2 μM) in DMSO/PBS (1/500) buffer (pH=7.4, 10 mM) mixture in the presence of H_2O_2 (200 μM) at different time (0-120 min).

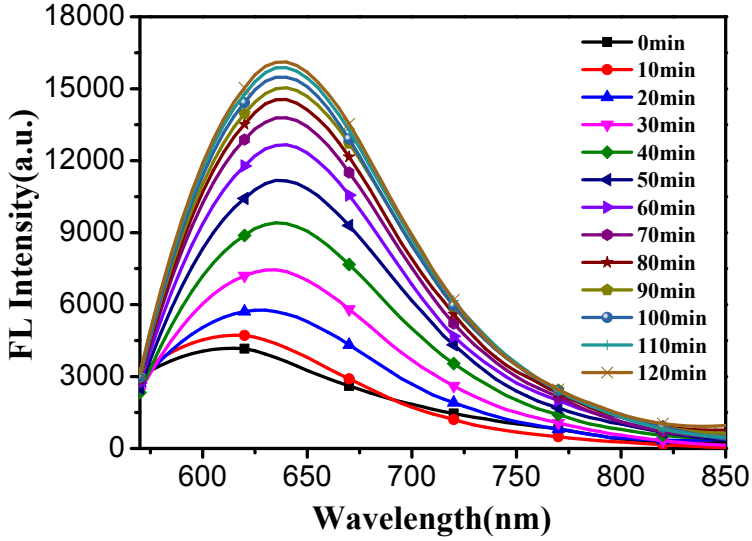
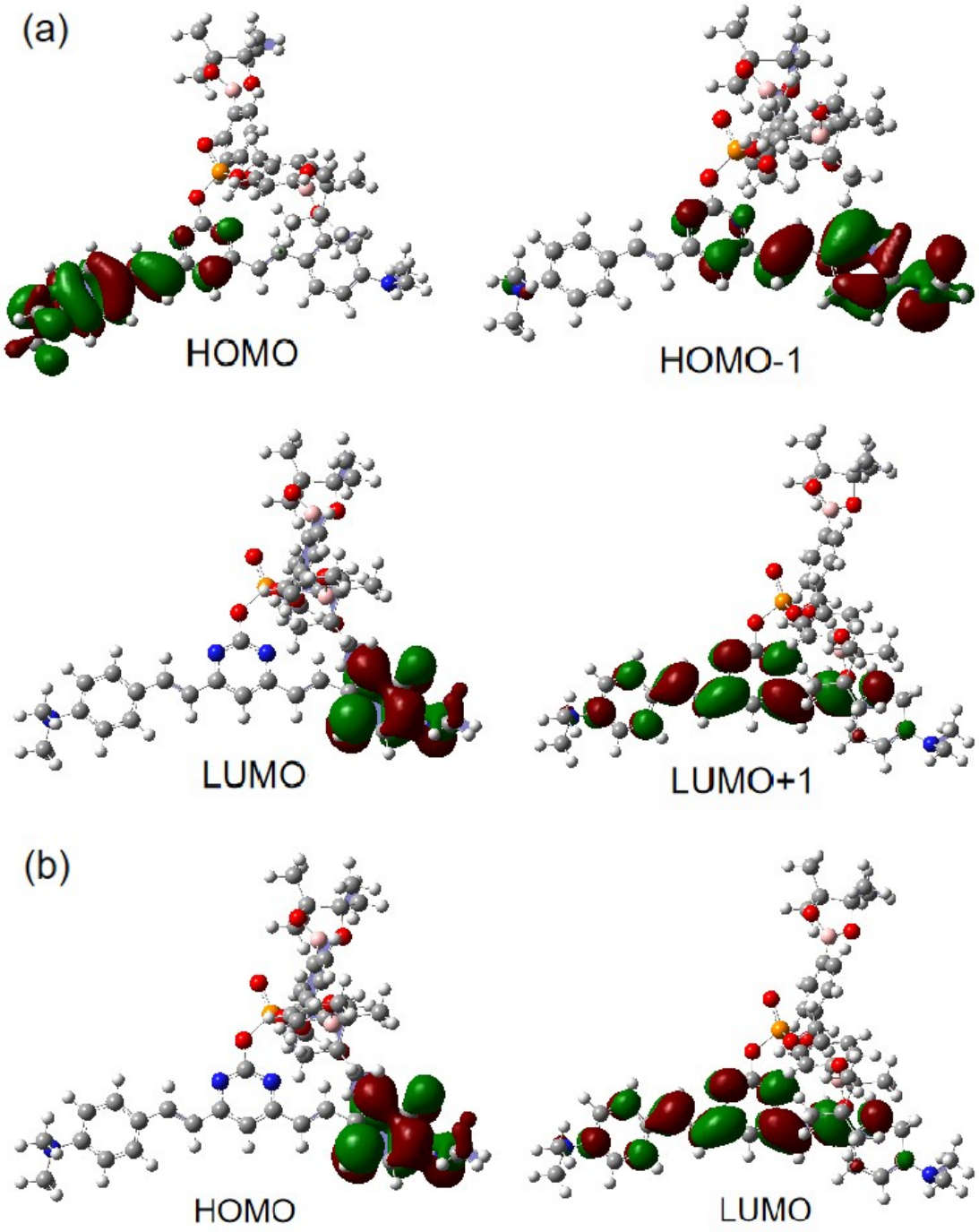


Figure S3. Fluorescence response of **UFPS-1** (2 μM) in DMSO/PBS (1/500) buffer (pH=7.4, 10 mM) mixture in the presence of H_2O_2 (200 μM) at different time (0-120 min).

Orbital energy level diagram of possible intermediates



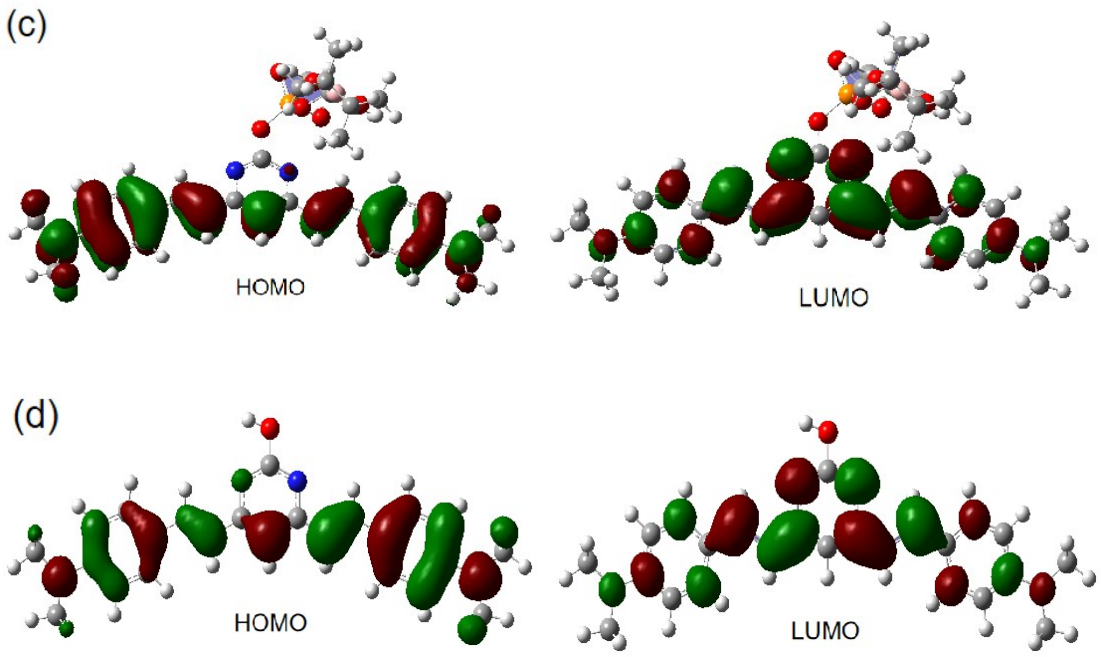


Figure S4. The orbital energy level map of intermediates that **UFPS-1** may produce during the detection of hydrogen peroxide. (a) **UFPS-1**; (b) and (c) possible intermediate; (d) **PB-OH**. In the ball-and-stick representation, carbon, hydrogen, nitrogen, oxygen, boron and phosphorus atoms are colored in gray, white, blue, red, pink and yellow, respectively.

Speculated reaction mechanism

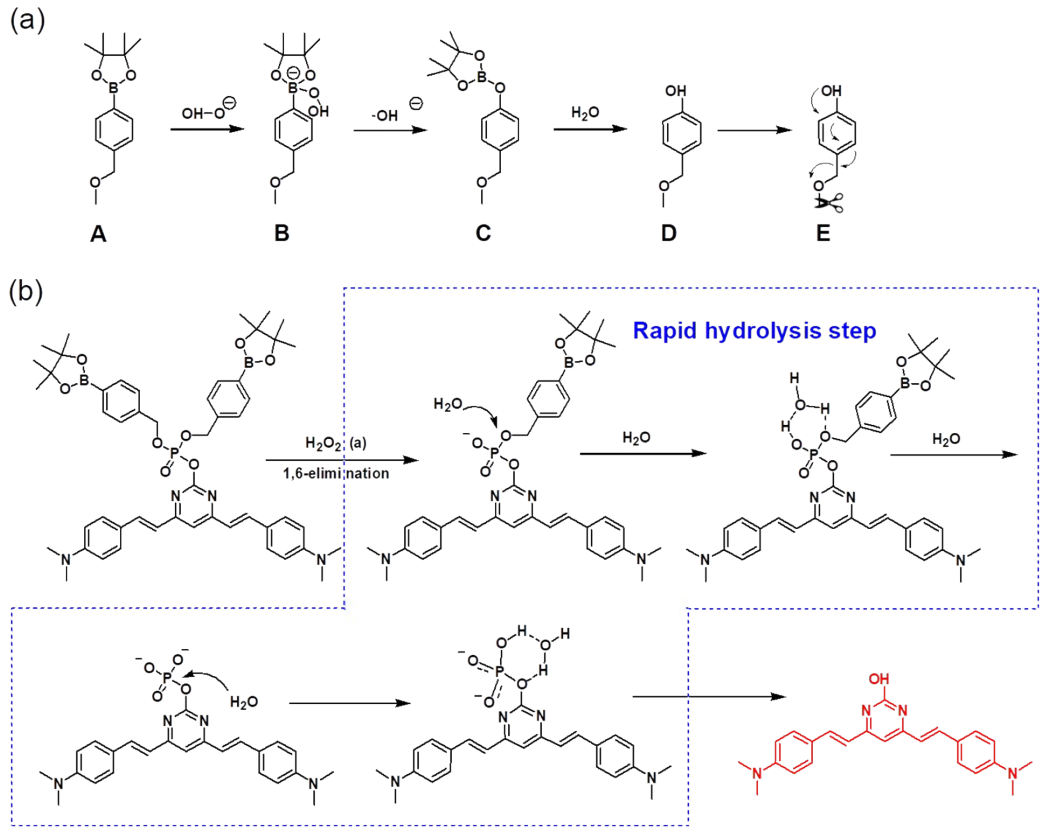


Figure S5. Proposed reaction mechanism of (a) borate ester and (b) **UFPS-1** upon H_2O_2 detection.

We propose the probe reaction mechanism as follow: first, when H_2O_2 nucleophilically attacks the boron atom, it will form an intermediate **B**, **B** will rearrange to form an unstable structure **C** that will be rapidly hydrolyzed, thus the borate ester group will be removed and form **D**. After that, the remaining 4-(hydroxymethyl)phenol group (**E**) will be further cleaved under the mechanism of 1,6-benzyl elimination and expose the phosphate group (a). It is reported that benzyl phosphate could be easily hydrolyzed under aqueous condition,[1] and finally released the deep-red fluorescent dye **PB-OH** (b).

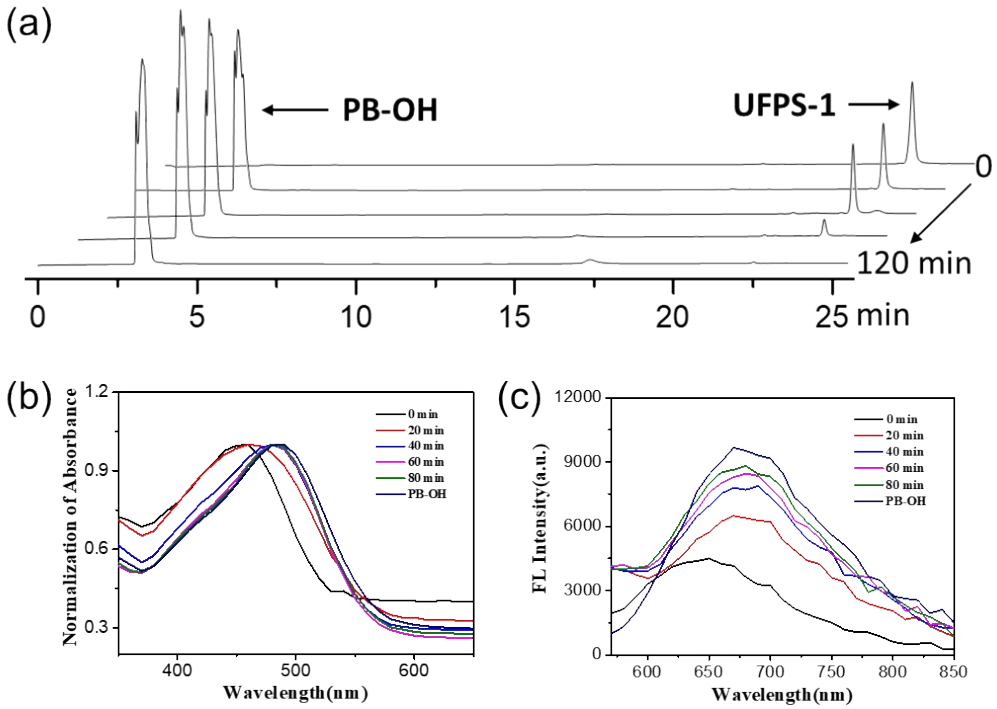


Figure S6. (a) The HPLC spectra (a), UV-vis (b) and fluorescence (c) spectra of the probe **UFPS-1** (5 μM) response to H_2O_2 (1 mM) from 0 to 120 min.

The method for determining the limit of detection (LOD)

As the H_2O_2 concentration increased from 0 to 20 μM, the fluorescence intensity at 640 nm was linearly fitted to obtain a calibration curve. As can be seen from Fig S3, the slope (S) of the curve is 101 μM^{-1} (R^2 = 0.974). The σ value in Table S1 is 3.0882. The detection limit of **UFPS-1** for H_2O_2 was calculated according to the formula (3σ/S) to be 92nM.[2]

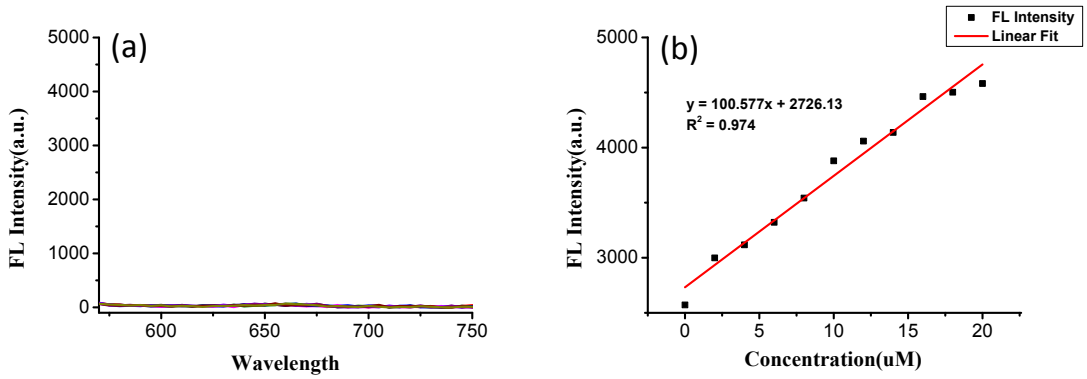


Figure S7. (a) Multi-recorded fluorescence spectra of blank measurement. (b) Calibration curve of emission intensity at 640 nm of **UFPS-1**. λ_{ex} = 540 nm.

Table S1. The data for standard deviation (σ) of blank measurement from **Figure S4**.

Emission Intensity at 640 nm					σ (F)
40	37	42	40	38	3.0882
31	44	40	43	38	
42	42	44	36	42	
39	40	40	37	41	

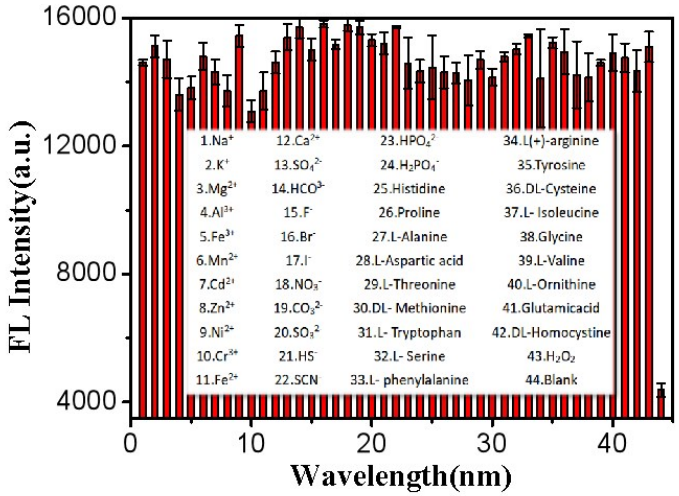


Figure S8. The effect of 43 analytes (100 equiv.) on the fluorescence response of **UFPS-1** (2 μM) to H_2O_2 (100 equiv.). λ_{ex} = 540 nm.

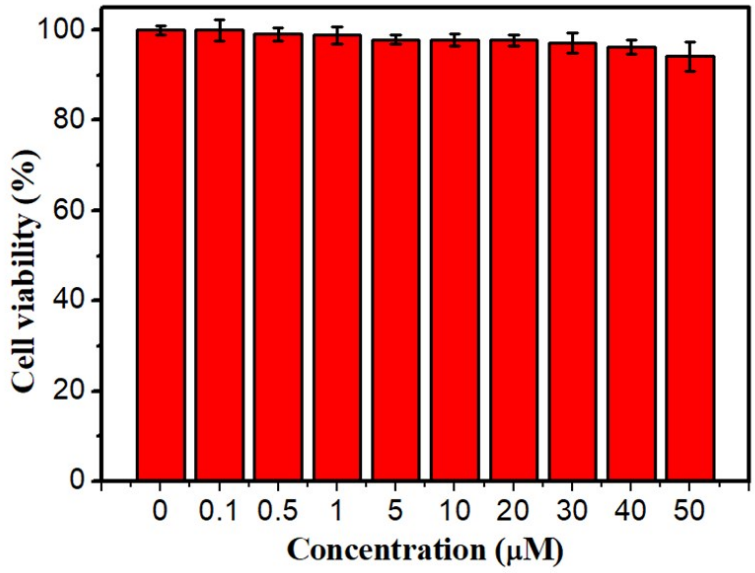


Figure S9. Survive rate of HepG-2 cells after incubated with various concentrations of **UFPS-1** for 24 h.

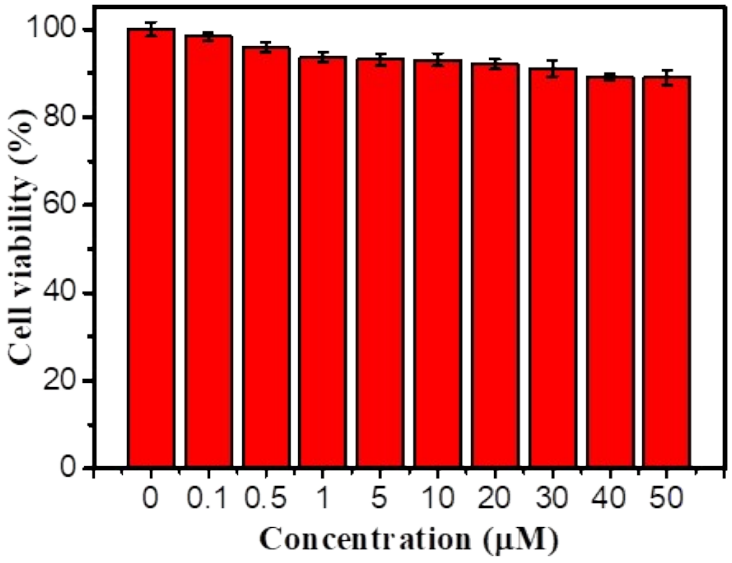


Figure S10. Survive rate of LO2 cells after incubated with various concentrations of **UFPS-1** for 24 h.

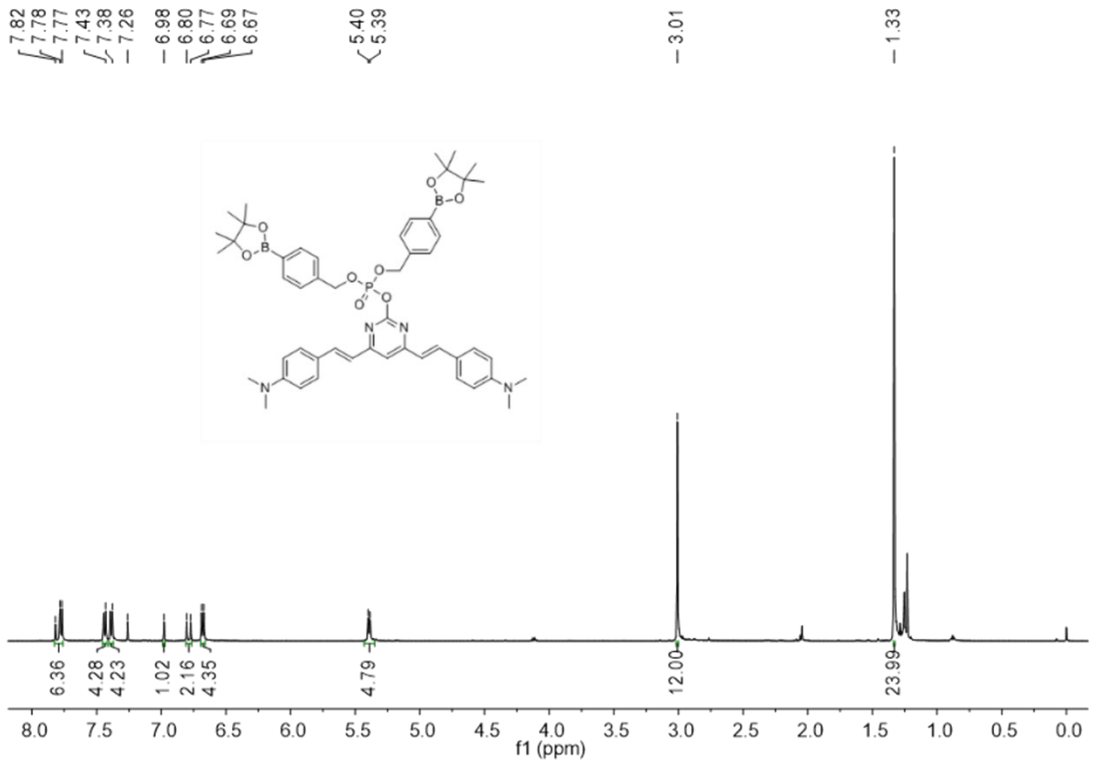


Figure S11. ^{1}H NMR spectrum of **UFPS-1**

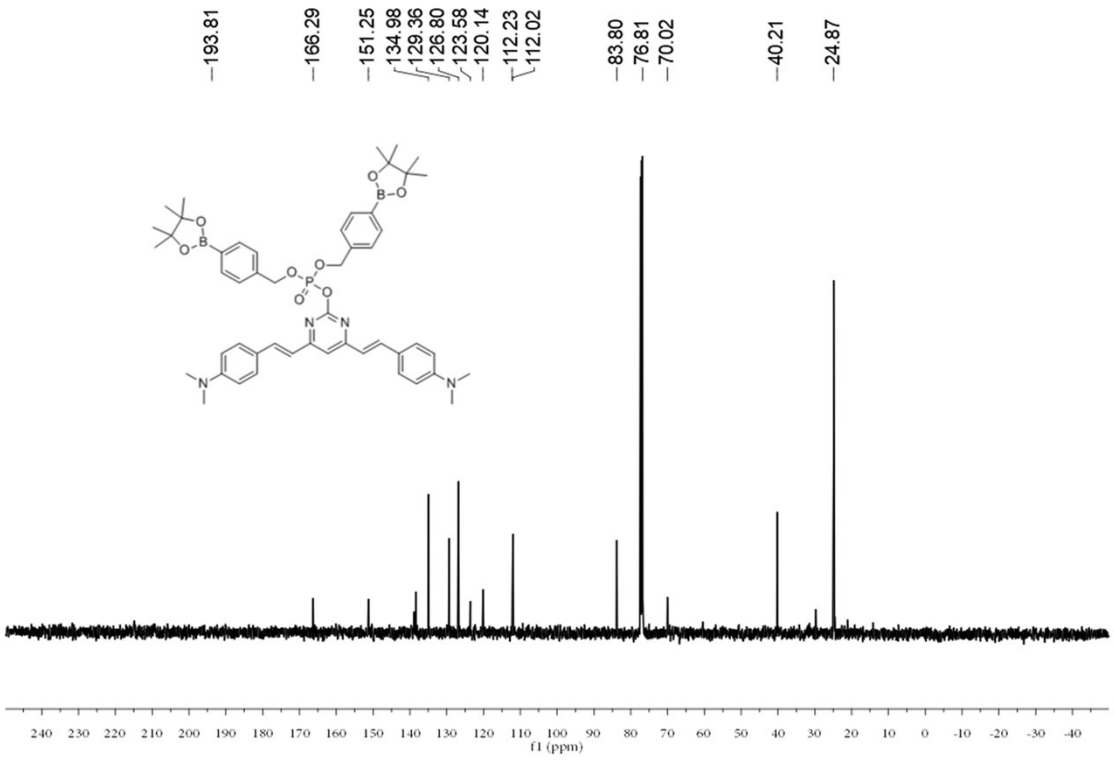


Figure S12. ^{13}C NMR spectrum of **UFPS-1.**

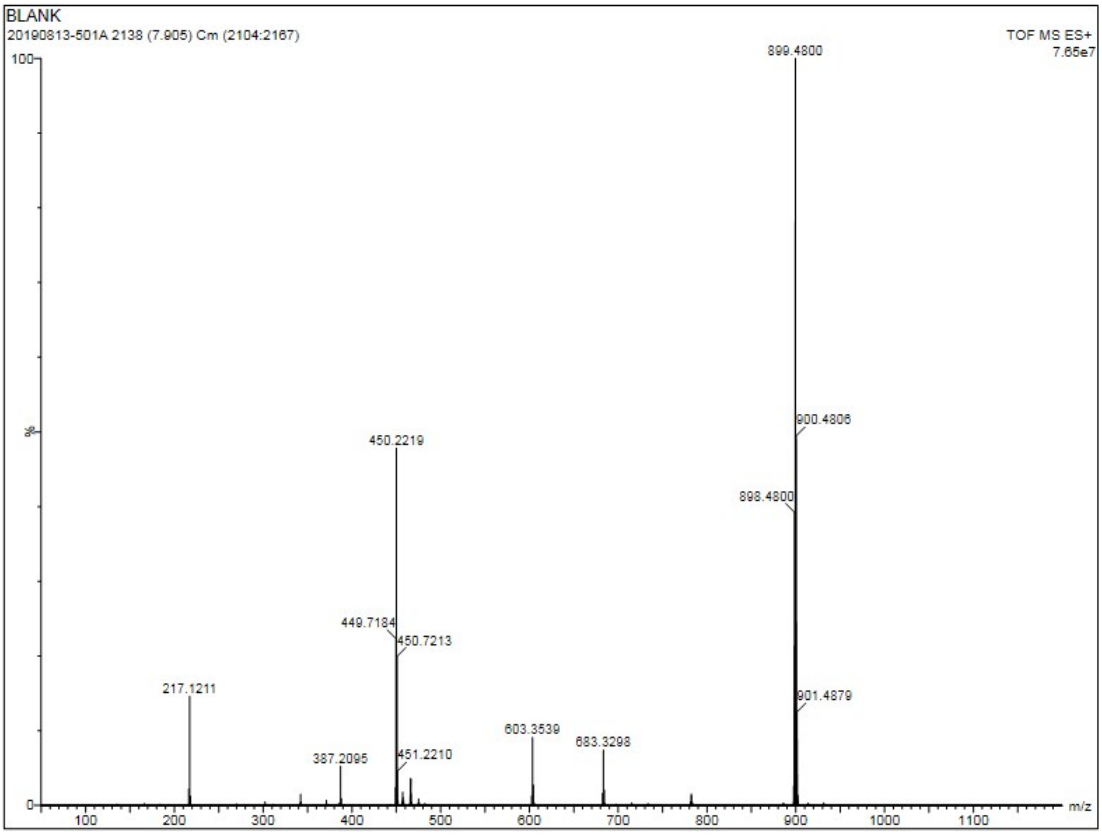


Figure S13. HRMS spectrum of **UFPS-1**

Reference

[1] J. Kumamoto and F. H. Westheimer, The Hydrolysis of Mono- and Dibenzyl Phosphates. J. Am. Chem. Soc.1955, 77, 2515-2518;

[2] Ma F, Liu M, Wang Z-y, Zhang C-y. Multiplex detection of histone-modifying enzymes by total internal reflection fluorescence-based single-molecule detection. Chem. Comm. 2016; 52:1218-21.