Supporting Information

A simple terephthalaldehyde-based AIE fluorescent probe for highly sensitive and selective detection of bisulfites in food samples

Wanmeng Li[a], Lingxiao Xiong[a], Bo Wang[b,*], Guodong Feng[a,*]

[a] College of Chemistry, Jilin University, Changchun, Jilin,130021, China

[b] State key Laboratory of Supramolecular Structure and Materials, Jilin University, Changchun, Jilin 130012, China

Table of contents

Characterization of FPB

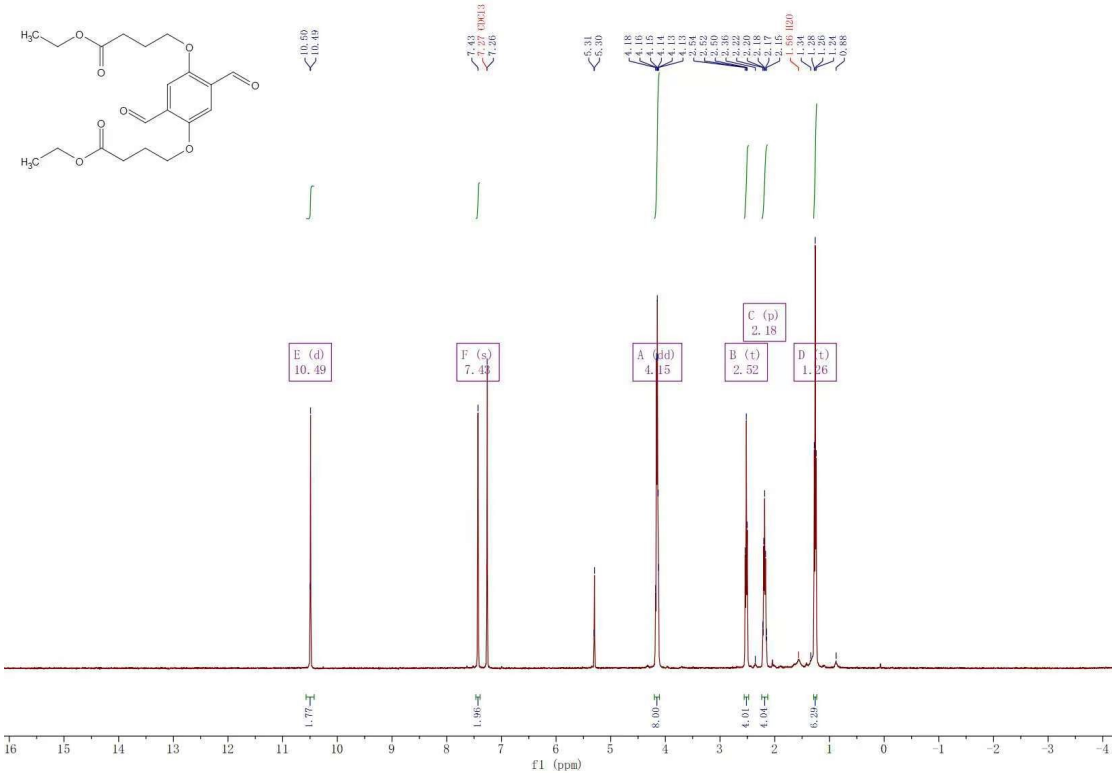

Fig. S1 ^{1}H NMR of FPB in $CDCl_3$

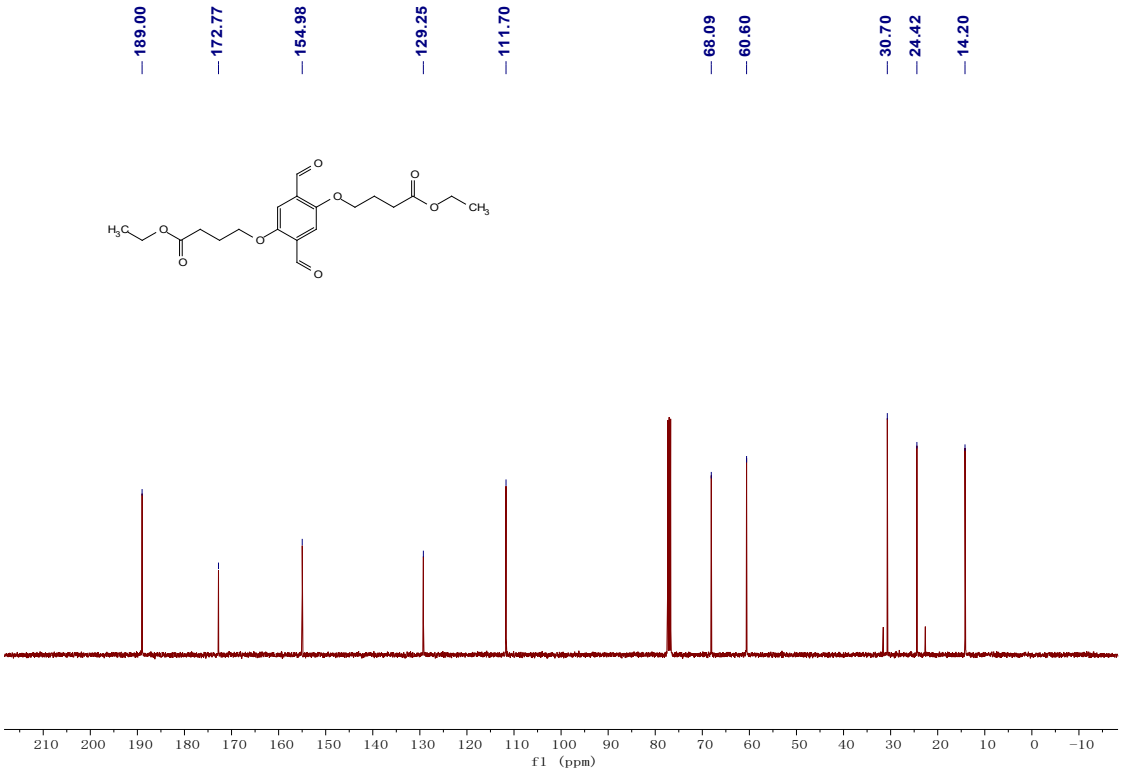

Fig. S2 ^{13}C NMR of FPB in $CDCl_3$

Spectra data

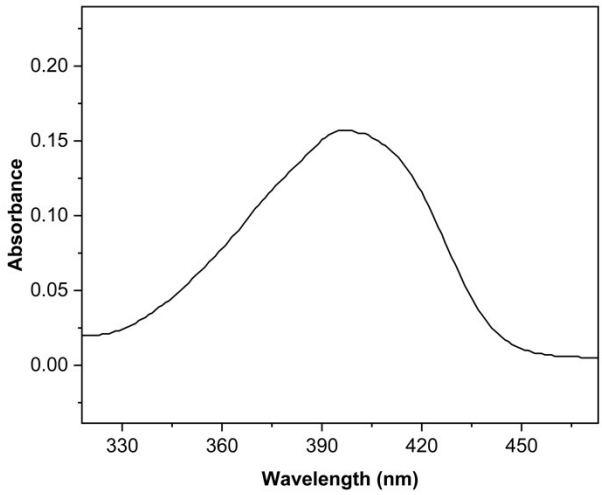

Fig. S3 Absorbance spectra of FPB (30 μM) in DMSO.

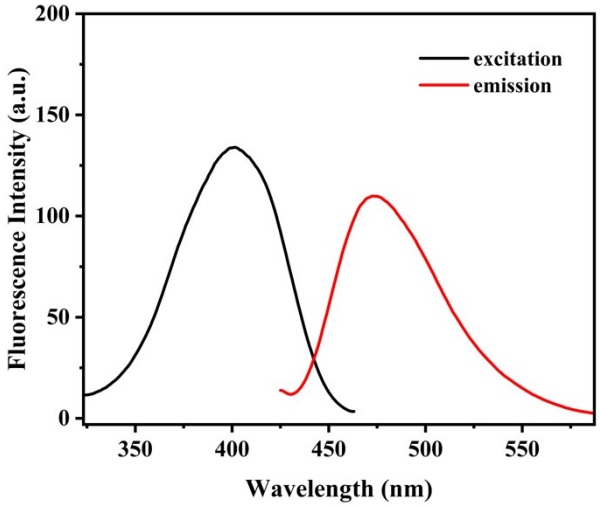

Fig. S4 The fluorescent excitation and emission spectra of FPB (10 μM) in DMSO solution, λex =405 nm.

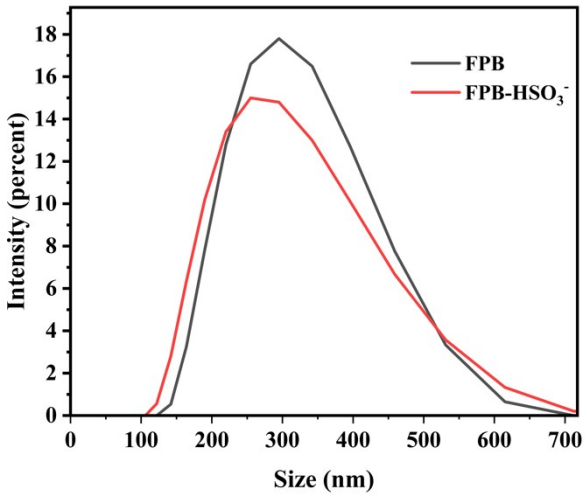

Fig. S5 The average diameter of FPB (10 μM) or FPB (10 μM) with HSO_3^- (5 μM) in BR solution.

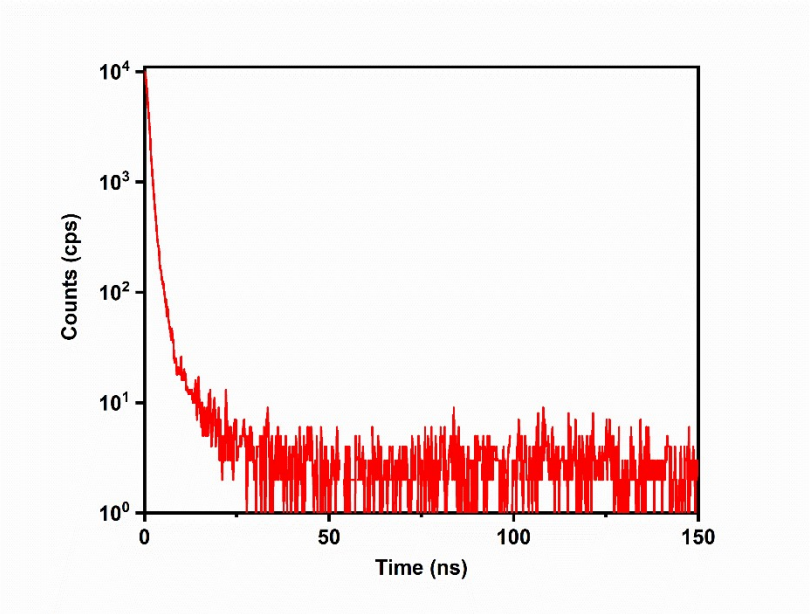

Fig. S6 Fluorescent lifetime of FPB (10 μM) in DMSO solution

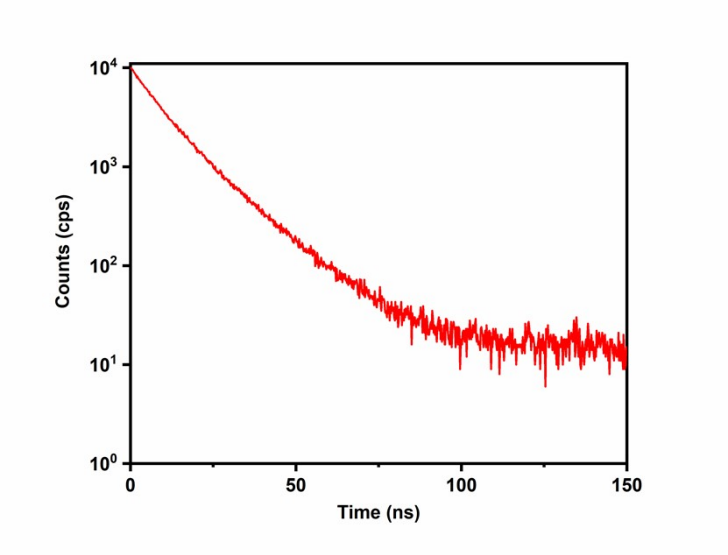

Fig. S7 Fluorescent lifetime of FPB (10 μM) in BR butter solution (pH = 6)

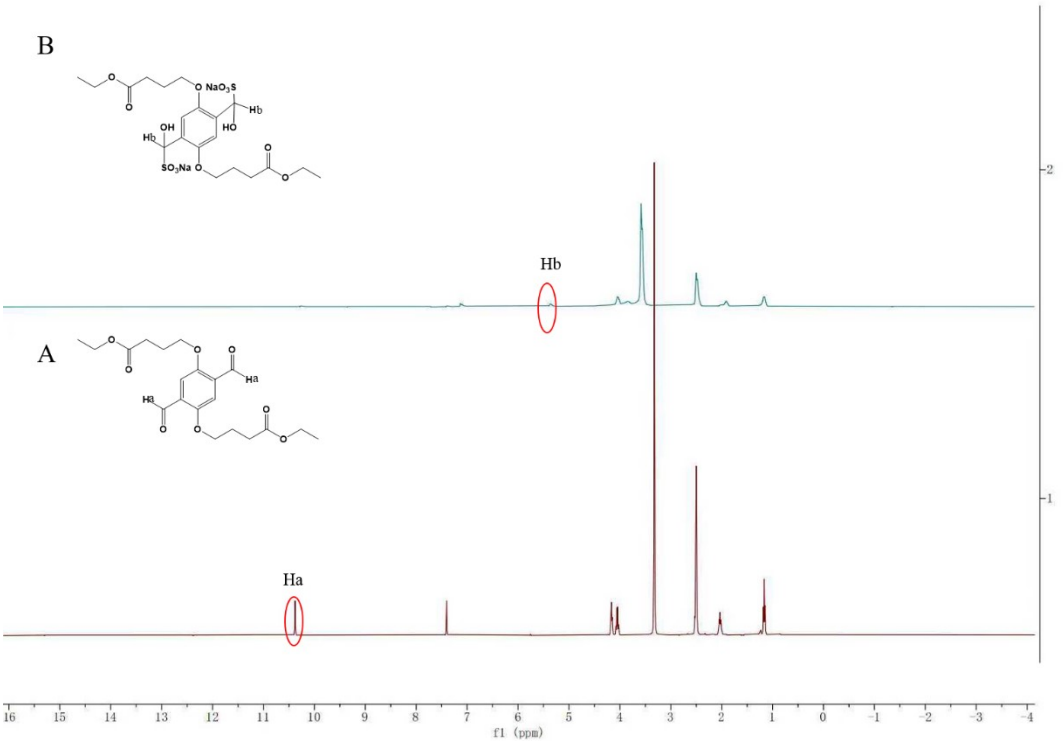

Fig. S8 (A)^{1}H NMR of FPB in *d*-DMSO;(B) ^{1}H NMR of FPB in the presence of HSO_3^- in *d*-DMSO and D_2O.

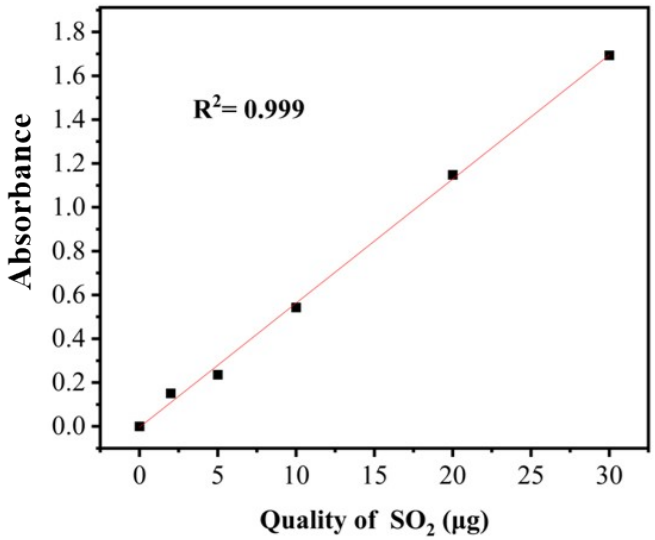

Fig. S9 Spectrophotometric standard curve of SO_2 standard solution (0, 2.5, 5.0, 10.0, 20.0, 30.0 μg),according to GB 5009.34-2022.

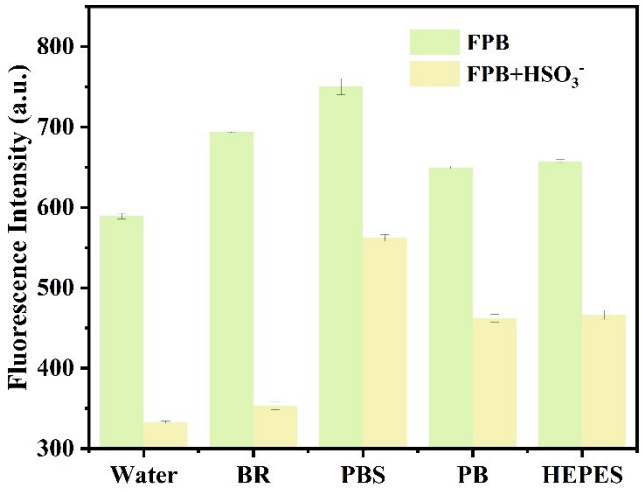

Fig. S10 The fluorescence emission intensity of FPB with or without HSO_3^- in different buffer solutions (BR: Britton-Robison buffer solution; PBS: Phosphate buffer saline; PB: Phosphate buffer; HEPES: 2-[4-(2-hydroxyethyl)piperazin-1-yl]ethanesulfonic acid).

Structural parameters for single crystals of FPB

Table S1 Crystal data and structure refinement for FPB

Phase data	
Identification	FPB
CCDC NO.	2397701
Empirical formula	$C_{20}H_{26}O_8$
Formula weight	394.41
Crystal system,	Triclinic,
Space group	P-1
Cell dimensions	a = 4.7164(4) Å alpha = 76.335(2) deg. b = 10.1972(8) Å beta = 84.552(3) deg. c = 10.9556(7) Å gamma = 77.787(3) deg.
Calculated density	11.310 mg/m^3
Crystal size	0.24 x 0.21 x 0.17 mm

Table S2 Bond lengths [Å] for FPB

Atoms 1,2	**d 1,2 [Å]**	**Atoms 1,2**	**d 1,2 [Å]**
O(1)-C(1)	1.364(2)	C(5)-C(6)	1.515(3)
O(1)-C(4)	1.4404(19)	C(5)-H(5A)	0.9700
O(2)-C(7)	1.333(2)	C(5)-H(5B)	0.9700
O(2)-C(8)	1.455(2)	C(6)-C(7)	1.501(2)
O(3)-C(7)	1.198(2)	C(6)-H(6A)	0.9700
O(4)-C(10)	1.193(2)	C(6)-H(6B)	0.9700
C(1)-C(2)	1.383(2)	C(8)-C(9)	1.484(3)
C(1)-C(3)#1	1.405(2)	C(8)-H(8A)	0.9700
C(2)-C(3)	1.389(2)	C(8)-H(8B)	0.9700
C(2)-H(2)	0.9300	C(9)-H(9A)	0.9600
C(3)-C(10)	1.475(2)	C(9)-H(9B)	0.9600
C(4)-C(5)	1.506(2)	C(9)-H(9C)	0.9600
C(4)-H(4A)	0.9700	C(10)-H(10)	0.9300
C(4)-H(4B)	0.9700		

Table S3 Bond angles [°] for FPB

Atoms 1,2,3	Angle 1,2,3 [°]	Atoms 1,2,3	Angle 1,2,3 [°]
C(1)-O(1)-C(4)	119.24(13)	C(7)-C(6)-H(6A)	108.8
C(7)-O(2)-C(8)	116.51(14)	C(5)-C(6)-H(6A)	108.8
O(1)-C(1)-C(2)	124.94(15)	C(7)-C(6)-H(6B)	108.8
O(1)-C(1)-C(3)#1	115.82(15)	C(5)-C(6)-H(6B)	108.8
C(2)-C(1)-C(3)#1	119.24(15)	H(6A)-C(6)-H(6B)	107.7
C(1)-C(2)-C(3)	120.18(15)	O(3)-C(7)-O(2)	123.23(17)
C(1)-C(2)-H(2)	119.9	O(3)-C(7)-C(6)	125.40(17)
C(3)-C(2)-H(2)	119.9	O(2)-C(7)-C(6)	111.37(15)
C(2)-C(3)-C(1)#1	120.58(15)	O(2)-C(8)-C(9)	107.43(17)
C(2)-C(3)-C(10)	119.26(15)	O(2)-C(8)-H(8A)	110.2
C(1)#1-C(3)-C(10)	120.14(15)	C(9)-C(8)-H(8A)	110.2
O(1)-C(4)-C(5)	105.91(14)	O(2)-C(8)-H(8B)	110.2
O(1)-C(4)-H(4A)	110.6	C(9)-C(8)-H(8B)	110.2
C(5)-C(4)-H(4A)	110.6	H(8A)-C(8)-H(8B)	108.5
O(1)-C(4)-H(4B)	110.6	C(8)-C(9)-H(9A)	109.5
C(5)-C(4)-H(4B)	110.6	C(8)-C(9)-H(9B)	109.5
H(4A)-C(4)-H(4B)	108.7	H(9A)-C(9)-H(9B)	109.5
C(4)-C(5)-C(6)	113.44(15)	C(8)-C(9)-H(9C)	109.5
C(4)-C(5)-H(5A)	108.9	H(9A)-C(9)-H(9C)	109.5
C(6)-C(5)-H(5A)	108.9	H(9B)-C(9)-H(9C)	109.5
C(4)-C(5)-H(5B)	108.9	O(4)-C(10)-C(3)	124.63(18)
C(6)-C(5)-H(5B)	108.9	O(4)-C(10)-H(10)	117.7
H(5A)-C(5)-H(5B)	107.7	C(3)-C(10)-H(10)	117.7
C(7)-C(6)-C(5)	113.95(15)		

Table S4 Hydrogen bonds for FPB [A and deg.].

D-H...A	d(D-H)[Å]	d(H...A) [Å]	d(D...A) [Å]	<(DHA)
C(4)-H(4B)...O(3)#2	0.97	2.653	3.453(2)	140.1
C(8)-H(8A)...O(4)#2	0.97	2.576	3.505(3)	162.7