Supporting Information

Near-infrared fluorescent probe for SO_3^{2-}/HSO_3^- and amines detection: integrated sensing tag/film with self-developed mobile app for visual fish freshness assessment

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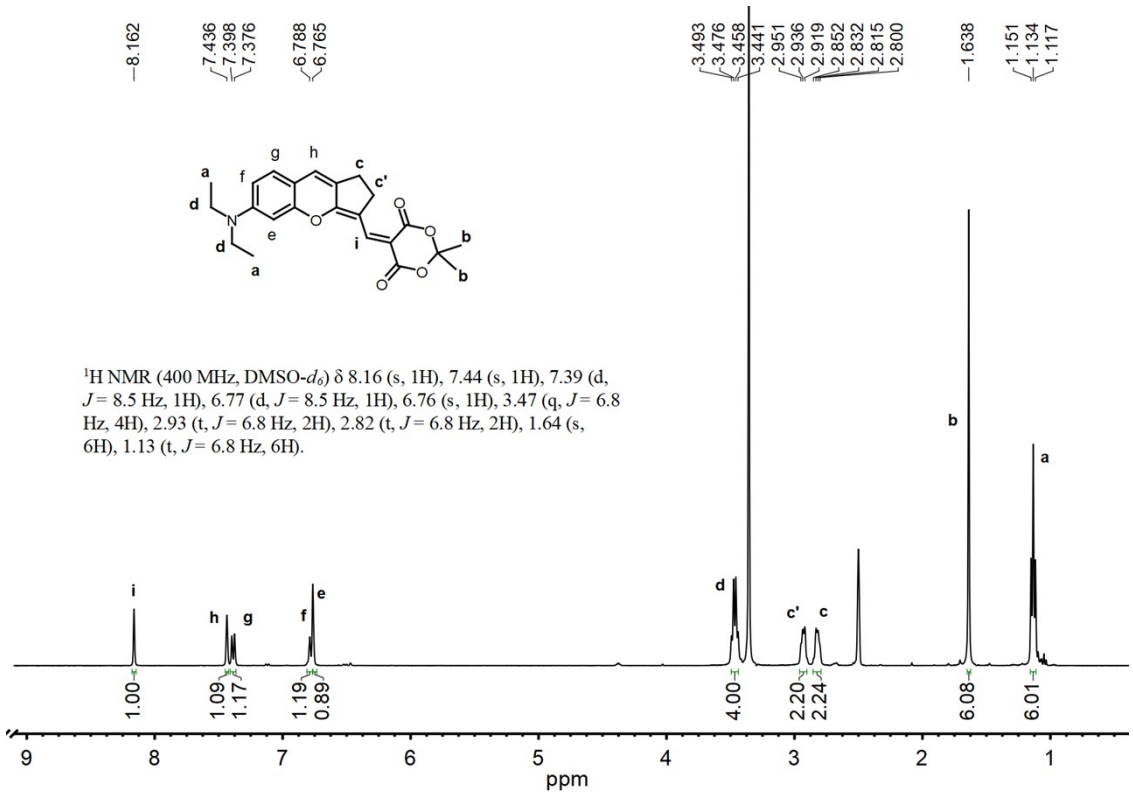

Figure S1. [1]H NMR spectrum of compound **Dma** in DMSO-d_6.

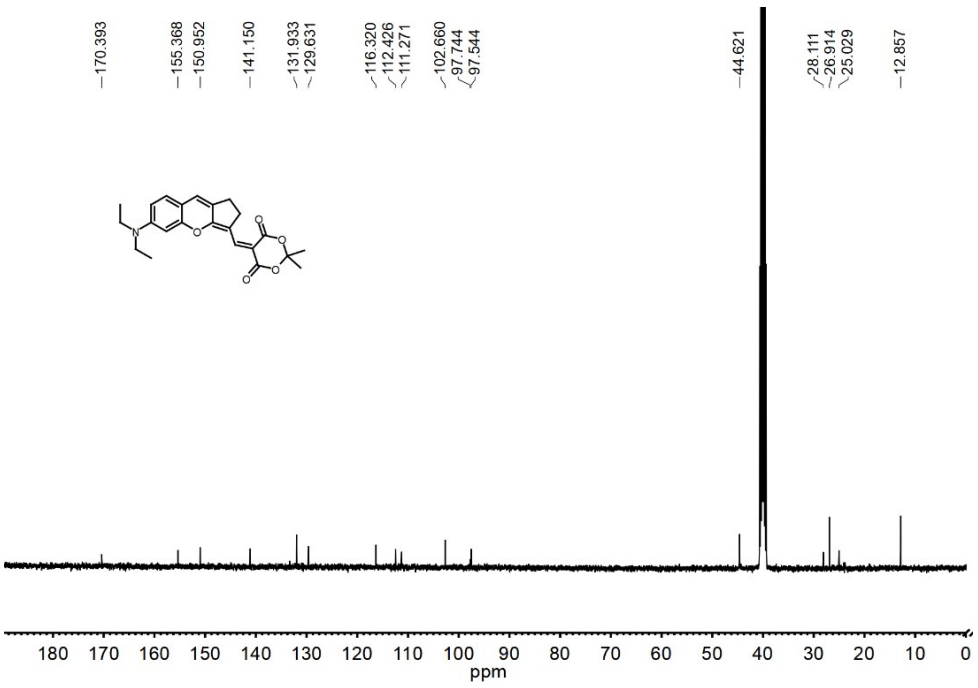

Figure S2. [13]C NMR spectrum of compound **Dma** in DMSO-d_6.

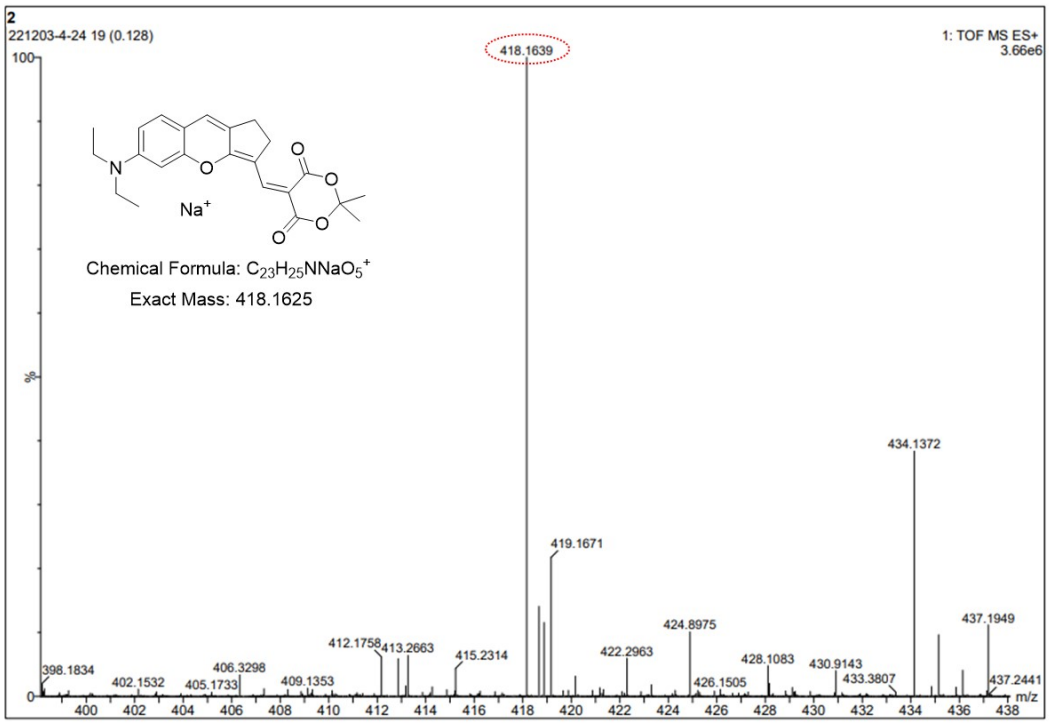

Figure S3. HRMS spectrum of probe **Dma** in MeOH. ($[M+Na]^+$ calcd: 418.1625, found: 418.1639)

Figure S4. Color of **Dma** solution under daylight illumination after the addition of various analytes (1: Blank, 2: CO_3^{2-}, 3: HCO_3^-, 4: $C_2O_4^{2-}$, 5: CH_3COO^-, 6: PPI, 7: HPO_4^{2-}, 8: SO_4^{2-}, 9: $S_2O_3^{2-}$, 10: SCN^-, 11: HS^-, 12: N_3^-, 13: NO_2^-, 14: F^-, 15: Cl^-, 16: Br^-, 17: I^-, 18: Cys, 19: Hcy, 20: GSH, 21: S^{2-}, 22: SO_3^{2-}, 23: HSO_3^-).

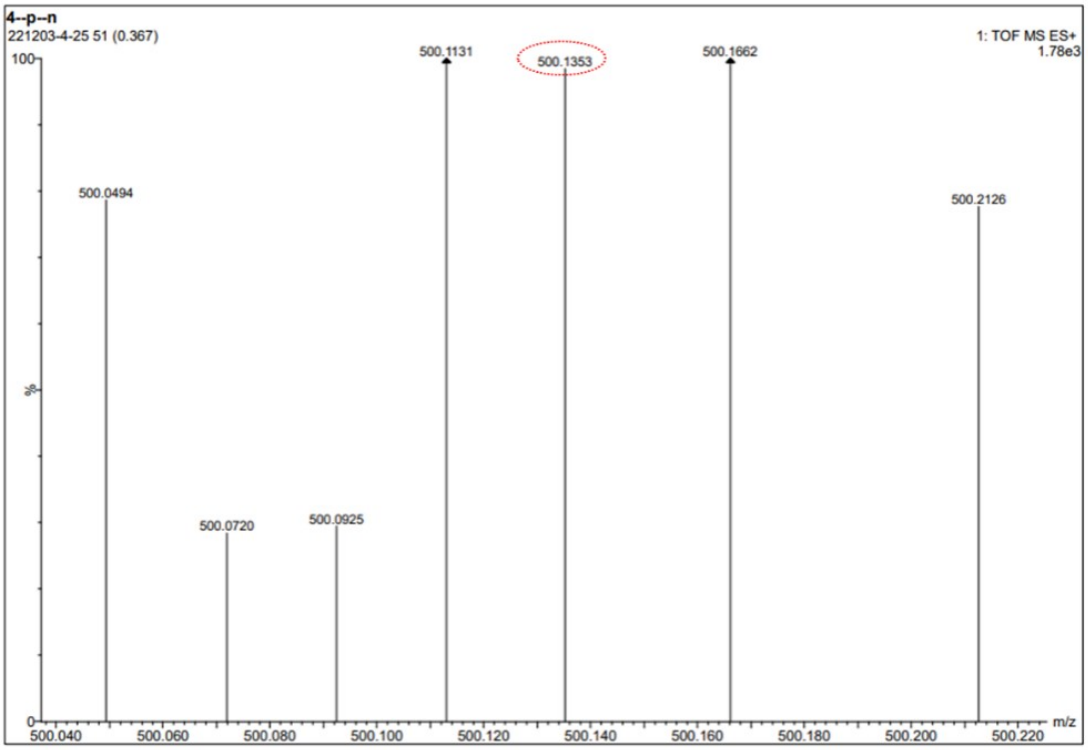

Figure S5. HRMS spectrum of compound **Dma**+HSO_3^- in DMSO. ($[M+HSO_3^-+Na]^+$ calcd: 500.1350, found: 500.1353)

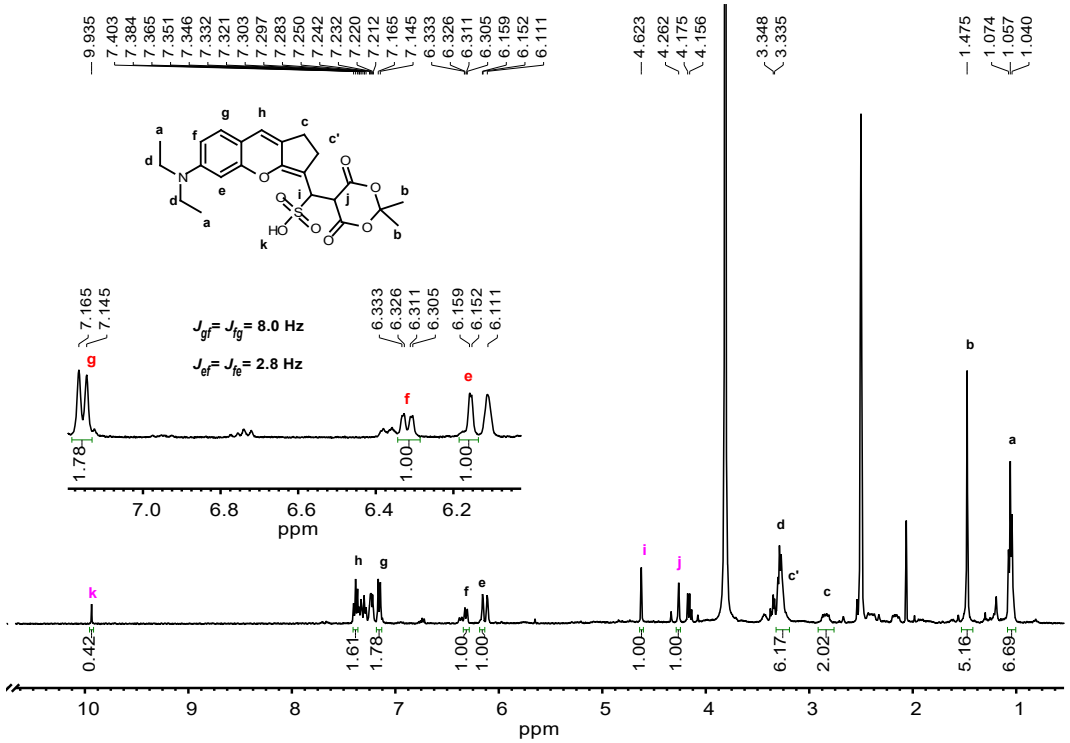

Figure S6. ^{1}H-NMR spectra of **Dma** after adding HSO_3^- (DMSO-d_6+D_2O).

Figure S7. Daylight (above) and Fluorescent (below) color changes of **Dma** (10 μM) on the addition of various amines in DMSO/H_2O (4/6, v/v, pH=6.4). (1: Blank, 2: ANI, 3: TMA, 4: TYA, 5: PEA, 6: DEA, 7: TPA, 8: CHA, 9: PPA, 10: TEA, 11: DEA, 12: SPE, 13: PUT, 14: CAD).

Figure S8. Photographs of **Dma** (10 μM) solution following the addition of varying concentrations of TEA (0-400 μM) under (a) daylight and (b) UV light.

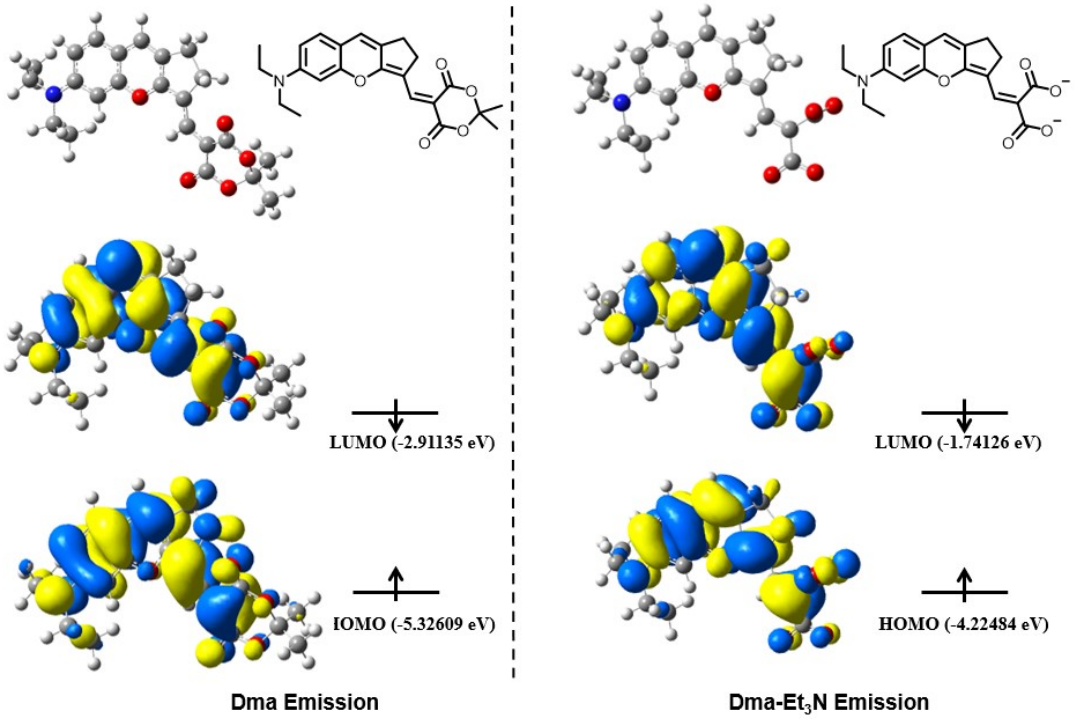

Figure S9. Optimized configurations in the S_1 state and the frontier molecular orbital transition illustrations of **Dma** and **Dma**-Et_3N based on CAMB3LYP/6-31G(d), respectively.

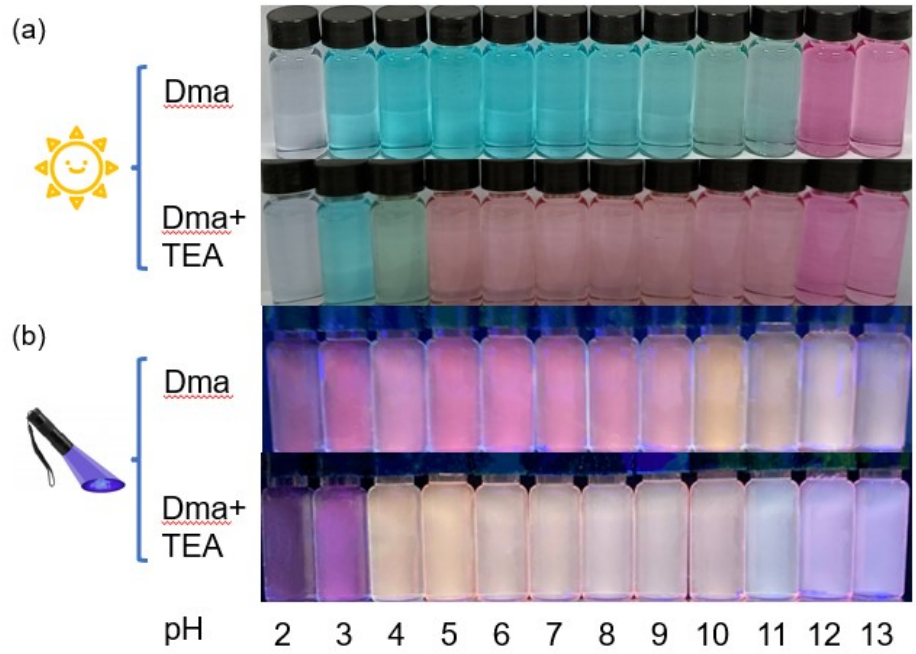

Figure S10. Sunlight (a) and fluorescence (b) photographs of **Dma** solutions at different pH levels with and without the addition of TEA.

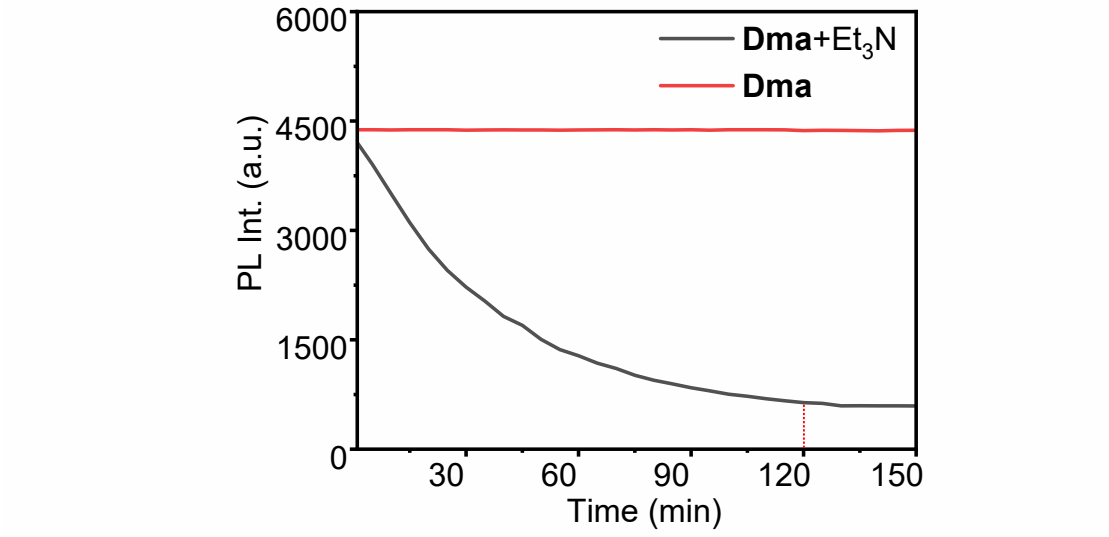

Figure S11. The change in fluorescence intensity at 675 nm of **Dma** (10 μM) and **Dma** + TEA over time in DMSO/H_2O (4/6, v/v, pH=6.4).

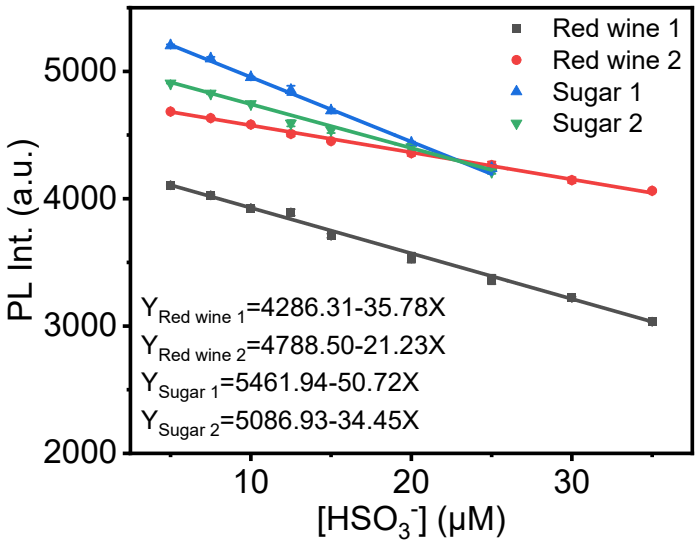

Figure S12. The relationship between the fluorescence intensity of probe **Dma** (10 μM) and the concentration of HSO_3^- in food samples.

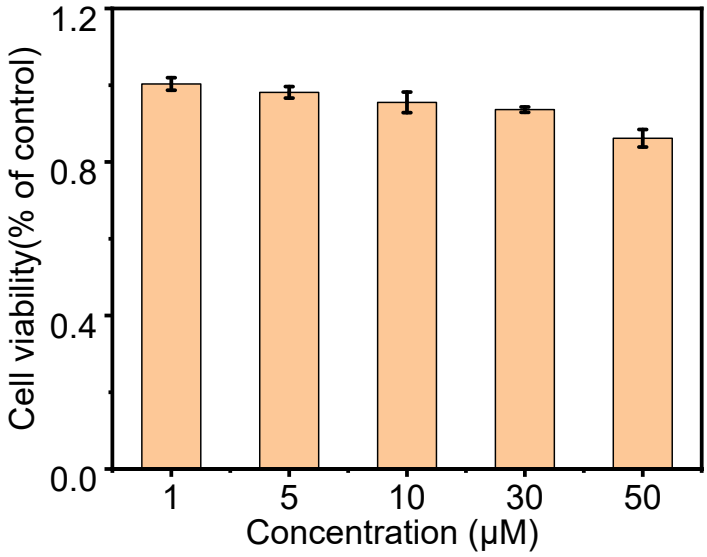

Figure S13. The cell viability of MCF-7 cells treated with **Dma** for 24 hours was assessed at concentrations of 1, 5, 10, 30, and 50 μM, respectively (The error bar indicates the standard deviation (SD) of three independent replicates).

Figure S14. The TVB-N content detecting fish meat utilizing a fitting curve generated in Figure 8(a).

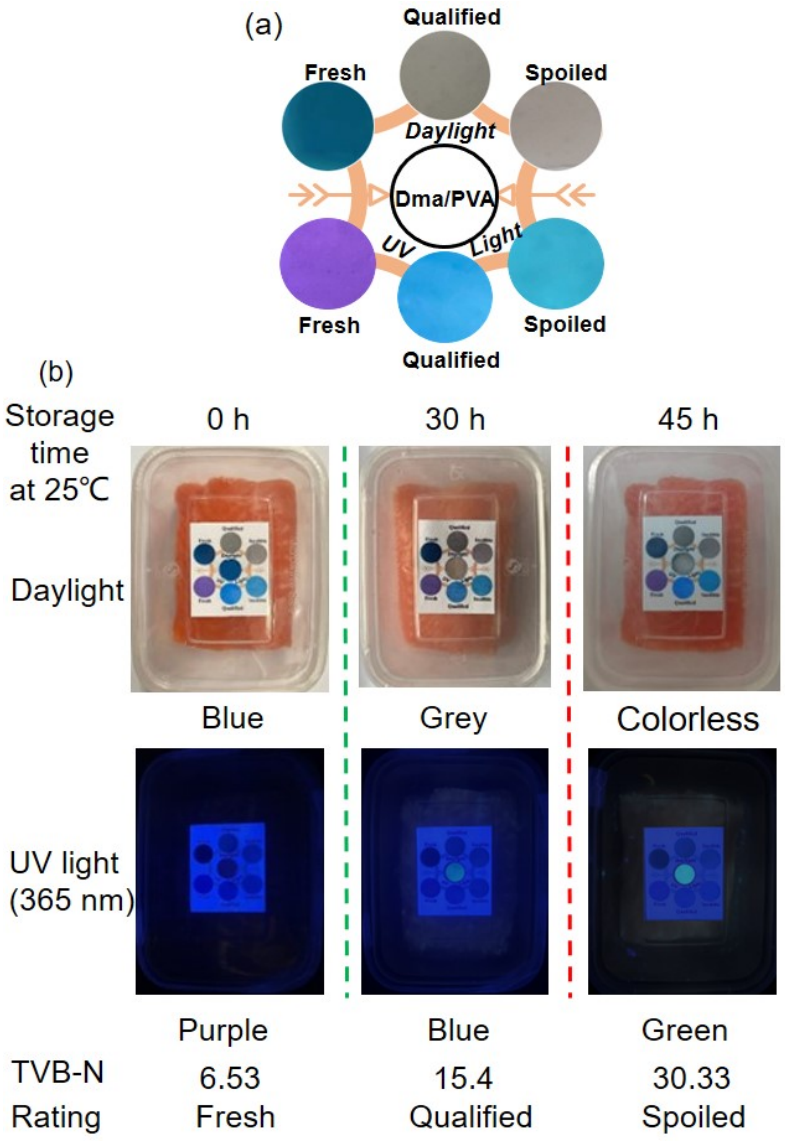

Figure S15. (a) The design of the indicator label integrating colorimetric card and **Dma/FPS,** (b) the storage time at 25 ◦C, the color of the integrated label**,** rating evaluated by indicator labels, TVB-N determined according to GB5009.34-2022.

Table S1. Smartphone platform test parameters.

Projects	Test condition
Phone model	OnePlus ACE3
Camera settings	No special settings
Shooting environment（Fluorescence）	Camera obscura-type UV analyzer (Shanghai Jiapeng ZF-7 with camera stand)
Smartphone software	Visual Evaluation App

Reagents and instruments

Reagents: phosphorus tribromide, cyclopentanone, chloroform, cesium carbonate, 4-diethylaminosalicylaldehyde, 2,2-Dimethyl-1,3-dioxane-4,6-dione, polyvinyl alcohol. All of them are purchased from Energy Chemical and can be used directly without purification. The silica gel (100~200 mesh) used in column chromatography is the product of the Qingdao Yuming Chemical Plant. The test water is deionized, and the reagents used are Tianjin Yongda chemical reagents.

Instruments: heat collecting constant temperature heating magnetic stirrer (DF-101S), vacuum drying oven (DZF-1B), high-speed homogenizer (FJ200-S), Haineng semi-automatic nitrogen determinator (K9840), color difference instrument, pH meter, 400 MHz nuclear magnetic resonance instrument F-4700 fluorescence spectrophotometer, U-T1810DS ultraviolet spectrophotometer.

General procedure for preparation of probe test solutions

Analytical grade solvents were used for entire experiments. **Dma** (3.95 mg, 0.01 mmol) was dissolved in DMSO to obtain a stock solution of probe (1.0 mM). The 1 mM **Dma** stock solution was diluted to 10 μM with DMSO/PBS (2/8, v/v, pH=7.4) solution for UV and fluorescence spectroscopy of SO_3^{2-}/HSO_3^-. A stock solution of **Dma** (20 μL) was added to the DMSO/H_2O (4/6, v/v, pH=6.4) in a cuvette (2.0 mL), to make a 2.0 mL solution for spectroscopic measurement. The UV–Vis or fluorescence spectra were recorded upon the addition of amine analytes. All spectroscopic experiments were carried out at room temperature. For all measurements, the excitation slit/emission width was set as 5 nm/10 nm.

Preparation of anion solutions and biological mercaptan solutions, taking the preparation of HSO_3^- solution as an example: $NaHSO_3$ (52.03 mg, 0.5 mmol) was dissolved in secondary distilled water and diluted to 10mL to prepare 50 mM HSO_3^- stock solutions, which were further diluted with secondary distilled water to make any lower concentration of HSO_3^- solution. Similarly, other anions and biological mercaptans, including SO_3^{2-}, S^{2-}, CO_3^{2-}, HCO_3^-, $C_2O_4^{2-}$, CH_3COO^-, PPI, HPO_4^{2-}, SO_4^{2-},

$S_2O_3^{2-}$, SCN^-, HS^-, N_3^-, NO_2^-, F^-, Cl^-, Br^-, I^-, glutathione (GSH), L-cysteine (Hcy) and homocysteine (Cys) were used to prepare 50 mM stock solution using the same method.

Preparation of various biogenic amines solutions (1,2-cyclohexanediamine, diethylamine, n-propylamine, triethylamine, spermine, cadaverine, putrescine, 2-phenylethylamine, tyramine, tryptamine, aniline, trimethylamine, dimethylamine), taking the preparation of triethylamine solution as an example: Triethylamine (50.60 mg, 0.5 mmol) was dissolved in the secondary distilled water and diluted to 10 mL to prepare 50 mM Et_3N stock solutions which were further diluted by the secondary distilled water to afford any lower concentration of Et_3N solutions. Similarly, other biogenic amines were used to prepare 50 mM stock solution by the same method, except that tryptamine was diluted to 50 mM with ethanol. All solutions were protected against light and stored at 4 °C before use.

Preparation of food samples testing solution

Red wine and sugar were purchased from the local supermarket. 1 mL of red wine was diluted 100 times with PBS (pH=7.4) buffer solution, and then a mixed solution of DMSO/red wine (2/8, v/v) was prepared. With this solution, the **Dma** stock solution (250 μL) was diluted to 25 mL to obtain the required test solution. 0.5 g of sugar was diluted with DMSO/PBS (2/8, v/v, pH=7.4) solution, and 1 mM of **Dma** solution (250 μL) was added to make a 25mL test solution.

Colorimetric measurements

The color parameters (L^*, a^*, b^*) of **Dma/FPS** and **Dma/PVA** were measured by using a colorimeter, where L^* represents lightness, a^* redness or greenness, and b^* yellowness or blueness, respectively. For total color difference (ΔE^*) indicates:

$$\Delta E^*=[(L^*-L_0^*)^2+(a^*-a_0^*)^2+(b^*-b_0^*)^2]^{1/2}$$

Where L^*, a^*, and b^* are the color parameters after **Dma/FPS** and **Dma/PVA** detection, and L_0^*, a_0^*, and b_0^* are the initial color parameters of **Dma/FPS** and **Dma/PVA**. Each indicator was measured three times and averaged.