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Supplementary Information

Optimized erucic acid-based extract as a natural probe for viscosity detection of liquid safety

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Experimental section

1 Materials and apparatus

The natural rosemary were kindly supplied by the Shandong Fengtai Biotech. Co., Ltd. Tetrahydrofuran (THF), toluene, dimethylsulfoxide (DMSO), N,N-dimethylformamide (DMF), methanol, ethyl acetate (EtOAc), glycerol and various metal salts were purchased from Shanghai Aladdin Bio-Chem Technology Co., Ltd. The gallic acid, acesulfame, sorbic acid, vitamin C, erythorbic acid, sodium benzoate (SB), beet molasses (BM) and trisodium citrate dehydrate (TCD) were obtained from Shanghai Macklin Biochemical Company. All the chemical reagents used in this work were of analytical grade and used as received.

2 The Förster–Hoffmann equation

Förster–Hoffmann equation:

$$\log I = C + x \log \eta \qquad (1)$$

where η represents the viscosity, I represents the fluorescence intensity of the natural molecular rotor EAd at maximum, C is a constant, and x represents the sensitivity of the natural molecular rotor EAd toward viscosity.

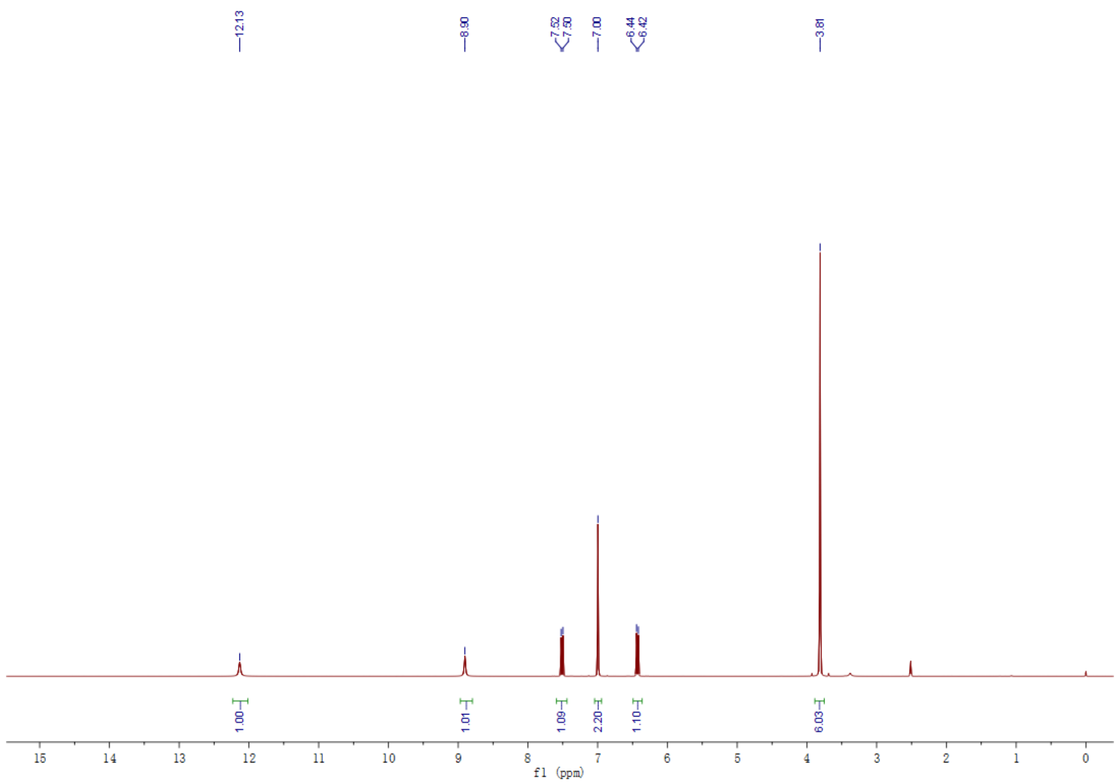


Figure S1 ^{1}H NMR spectrum of the extracted molecular probe erucic acid (EAd).

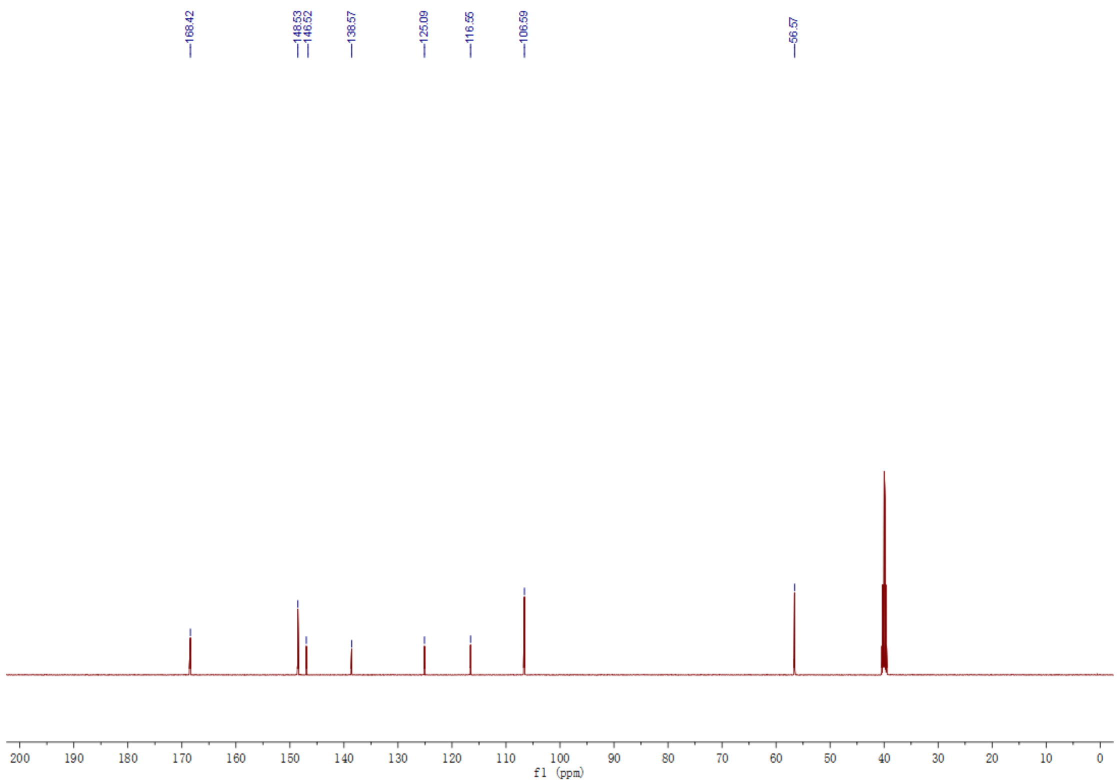


Figure S2 ^{13}C NMR spectrum of the extracted molecular probe erucic acid (EAd).

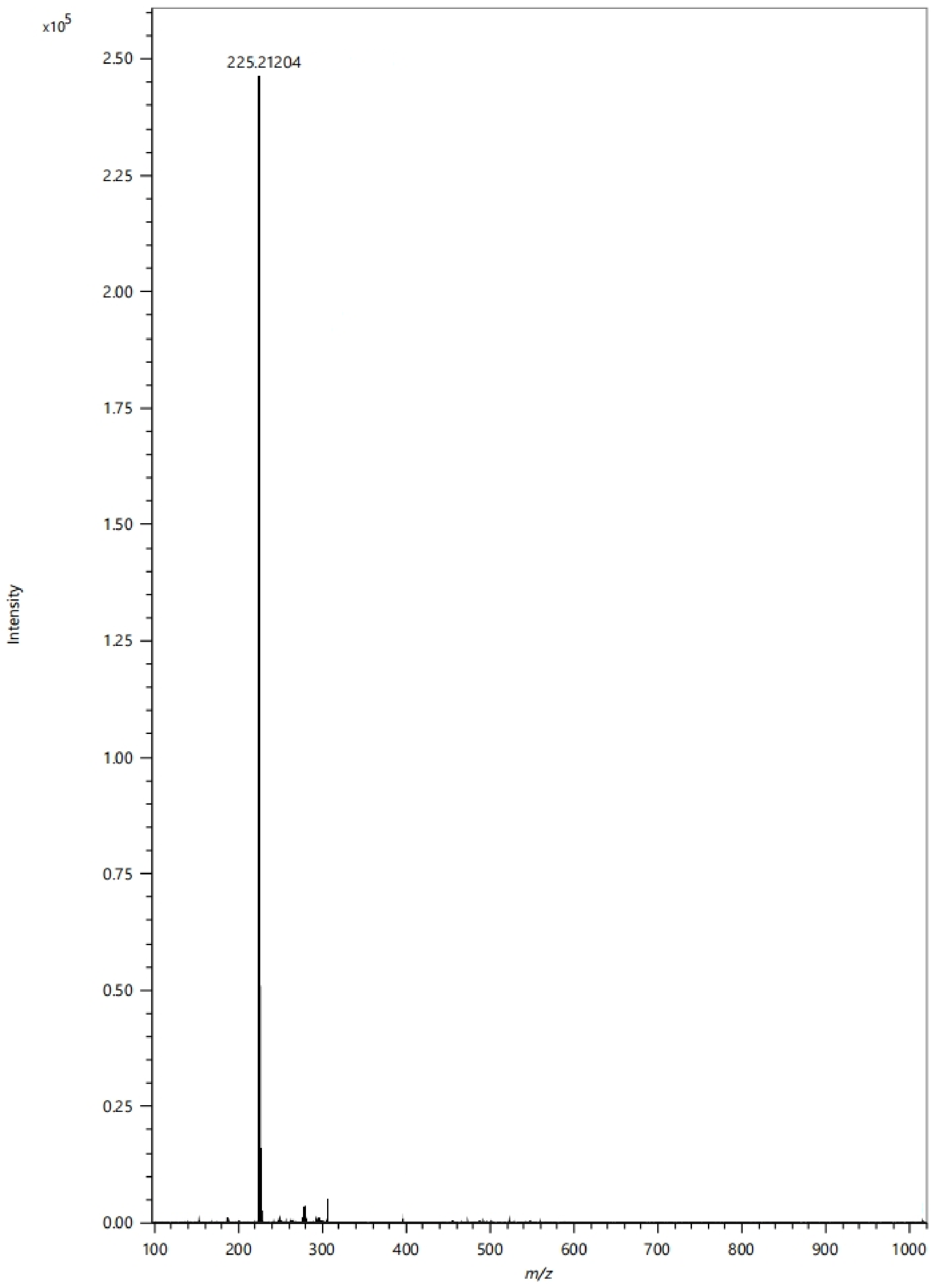


Figure S3. HR mass spectrum of the extracted molecular probe erucic acid (EAd). MS (ESI): m/z 225.21204 $[M+H]^+$.

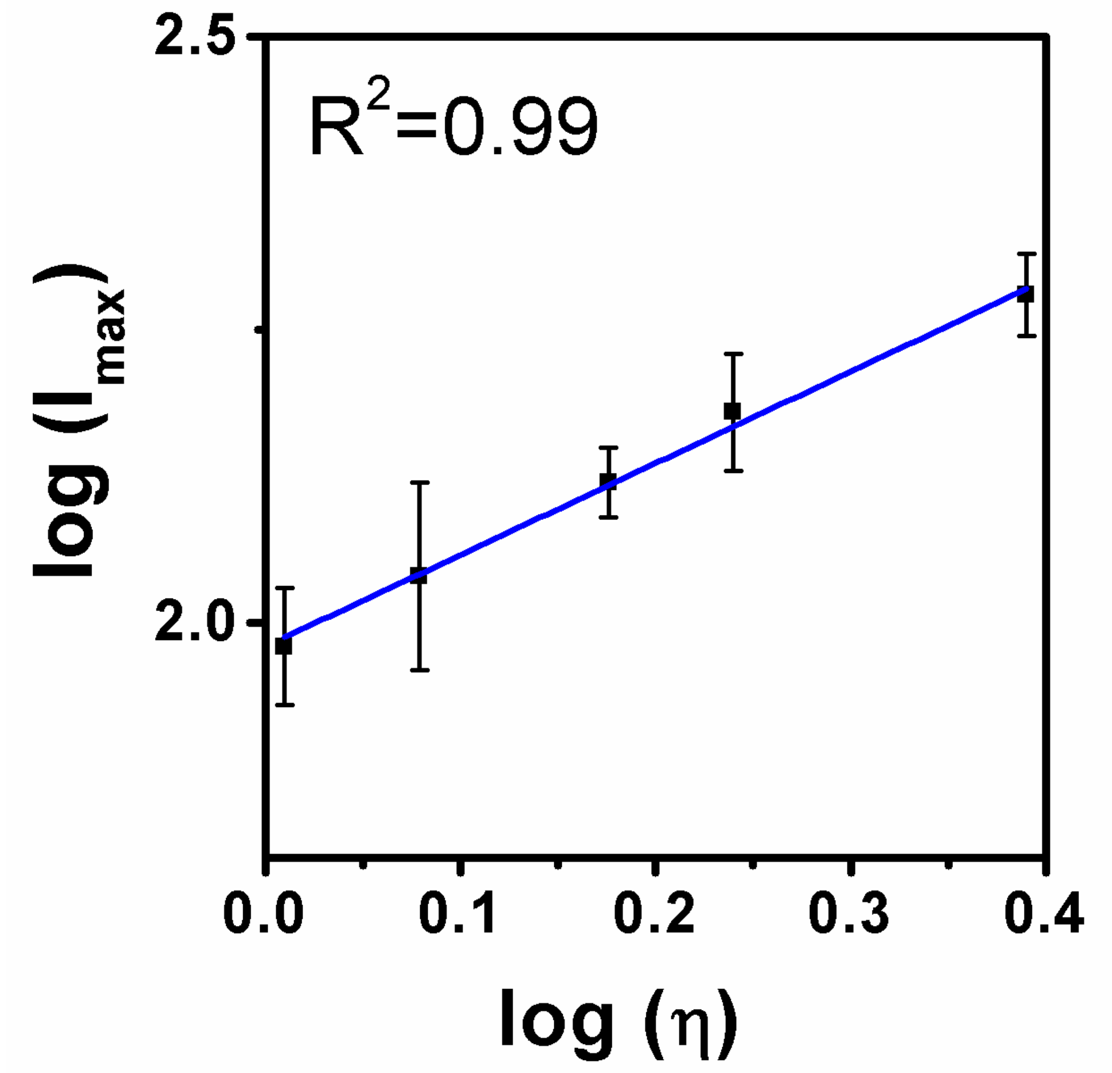


Figure S4 Detection limit of the natural probe erucic acid (EAd).

The calibration curve was first obtained from the plot of log (I_{max}) as a function of log (η). Then the regression curve equation was obtained for the lower viscosity part.

The detection limit = 3 × *S.D.*/*k*

Where *k* is the slope of the curve equation, and *S.D.* represents the standard deviation for the log (I_{max}) of natural probe erucic acid (EAd).

log (I_{486}) = 1.980 + 0.781 × log (η) (R^2 = 0.990)

log (LOD) = 3 × 0.031/0.781 = 0.119

LOD =10^0.119 =1.315 cP

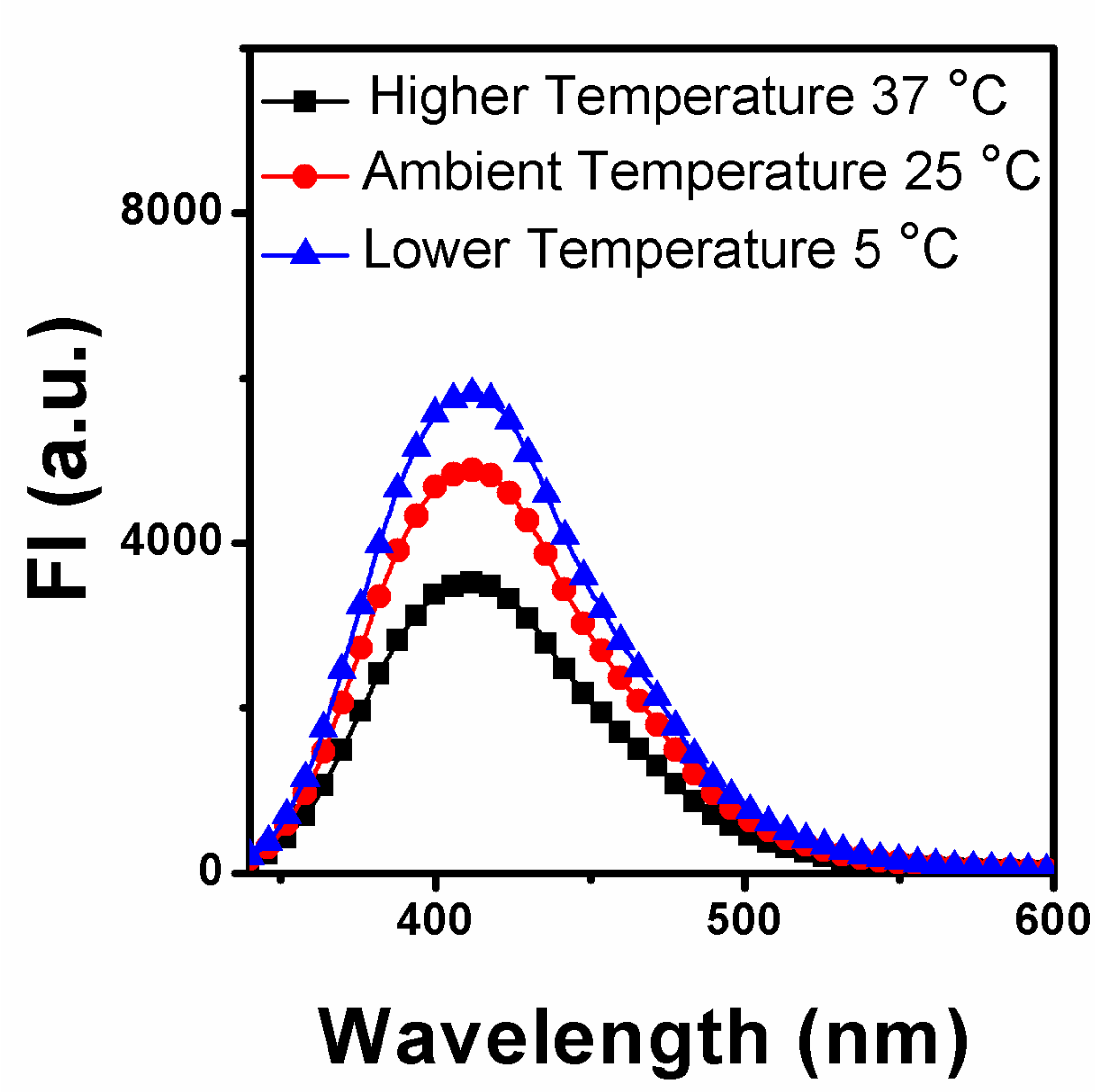


Figure S5 Emission spectra of the natural probe erucic acid (EAd) (10 μM) in glycerol under different temperature, including the higher storage temperature (37 °C), ambient temperature (25 °C), and lower storage temperature (5 °C).

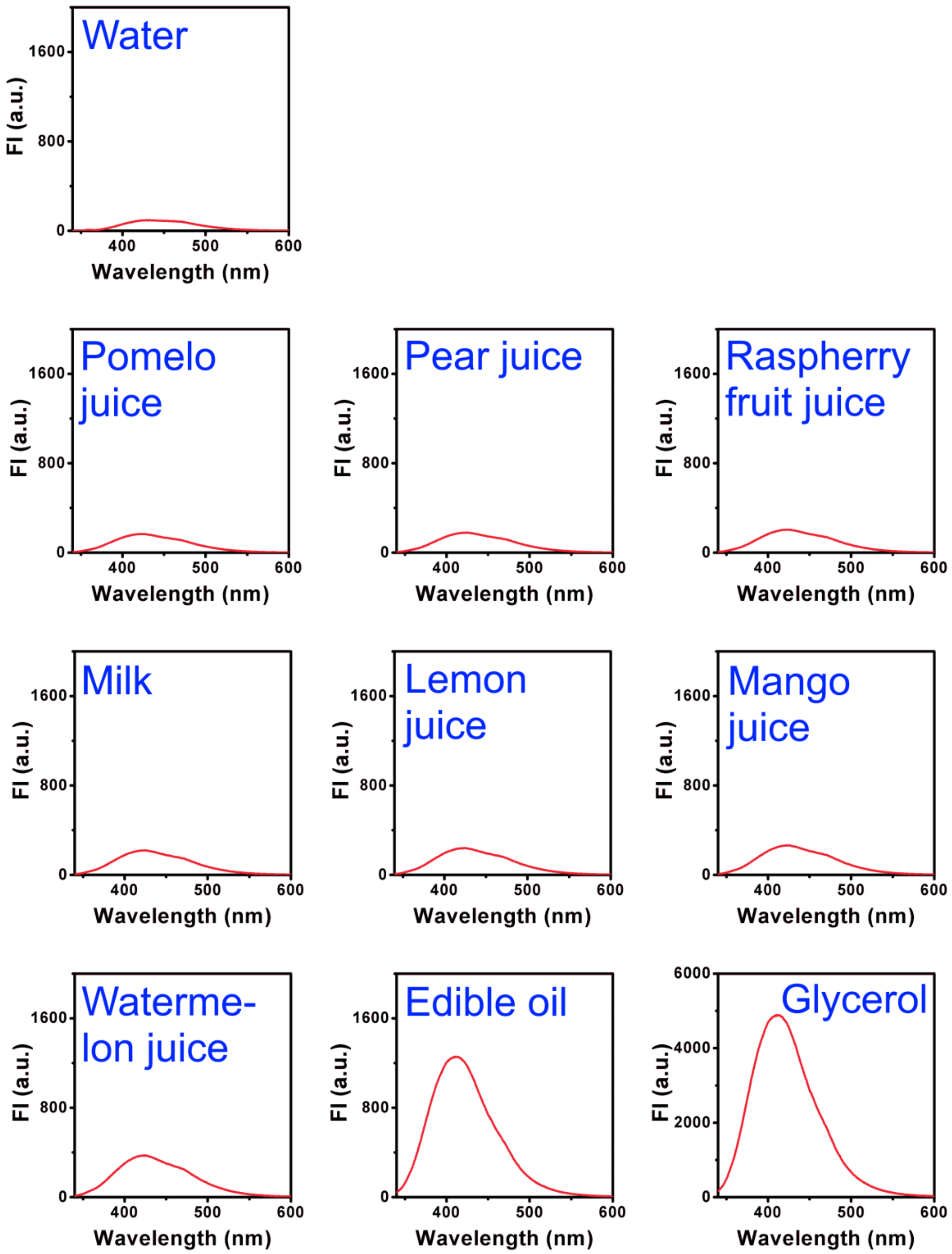


Figure S6 Fluorescence spectra of the natural probe erucic acid (EAd) (10 μM) in ten kinds of commercial liquid system, including the water, pomelo juice, pear juice, raspherry fruit juice, milk, lemon juice, mango juice, watermelon juice, edible oil, and glycerol, λ_{ex}=320 nm.

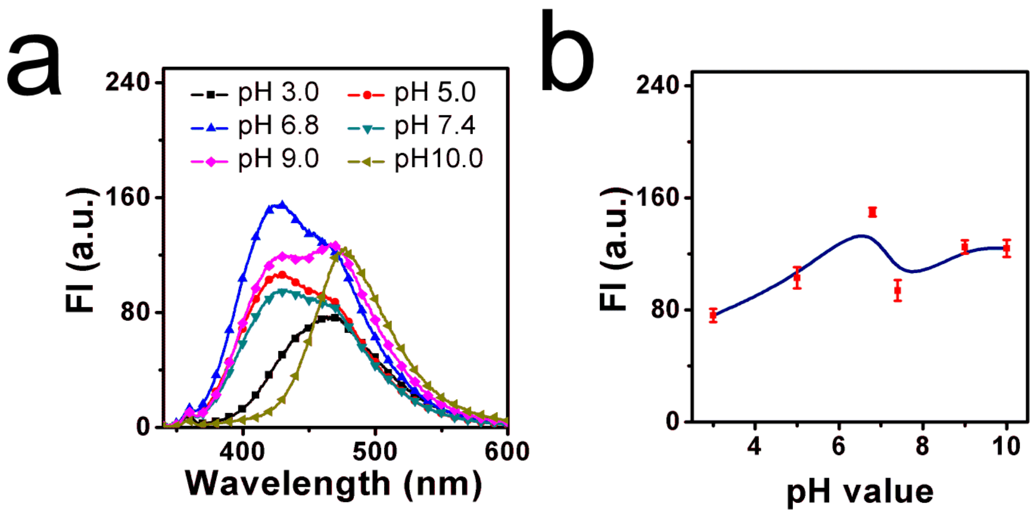


Figure S7 Fluorescence emission intensity of natural probe erucic acid (EAd) under various pH values (containing 1% DMSO), λ_{ex}=320 nm.

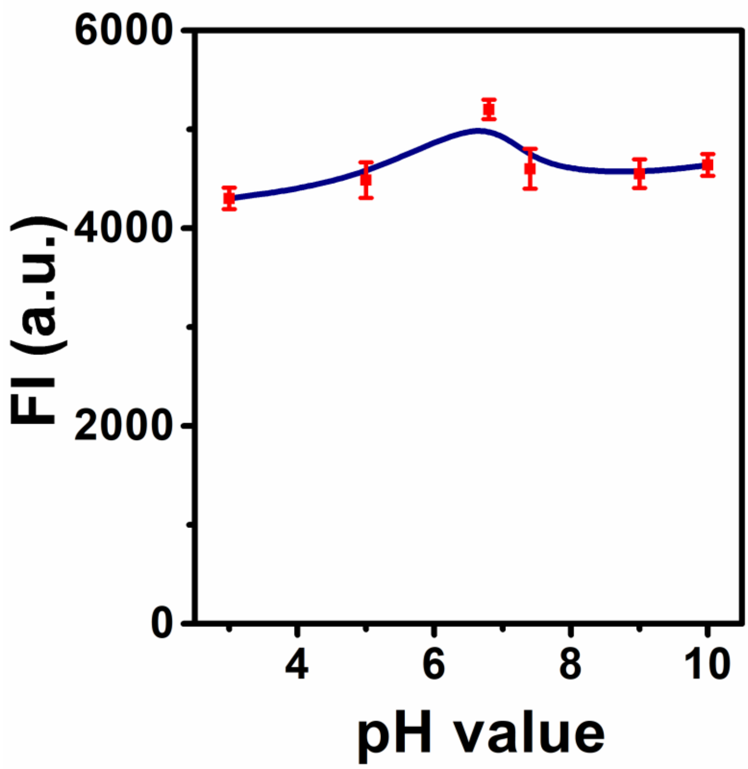


Figure S8 Fluorescence emission intensity of natural probe erucic acid (EAd) under high viscous common pH range, λ_{ex}=320 nm.

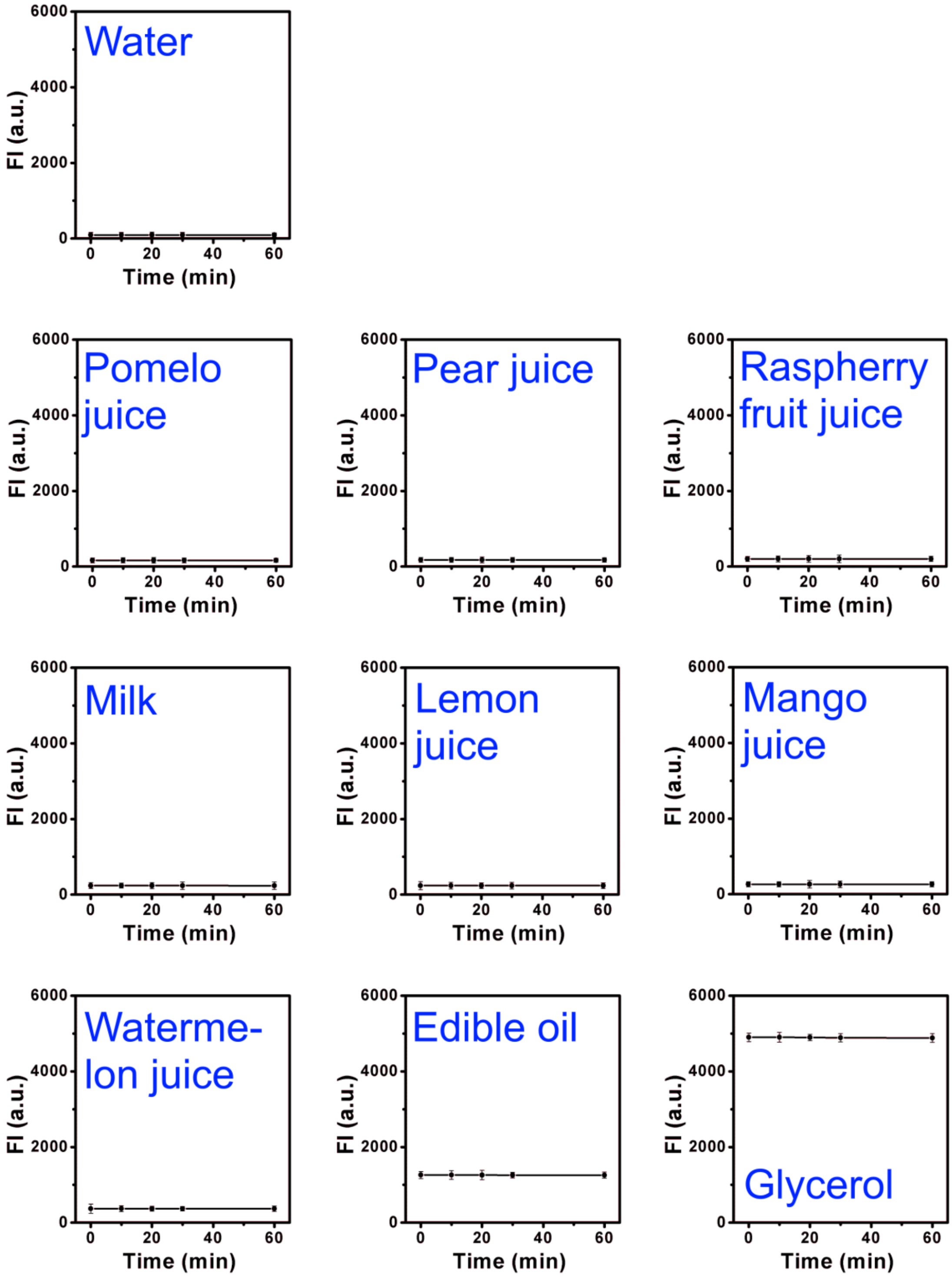


Figure S9 Photostability analysis of the natural probe EAd in water, glycerol and other eight kinds of common liquid food (containing 1% DMSO). All upon samples were tested under continuous light irradiation with 320 nm UV lamp.

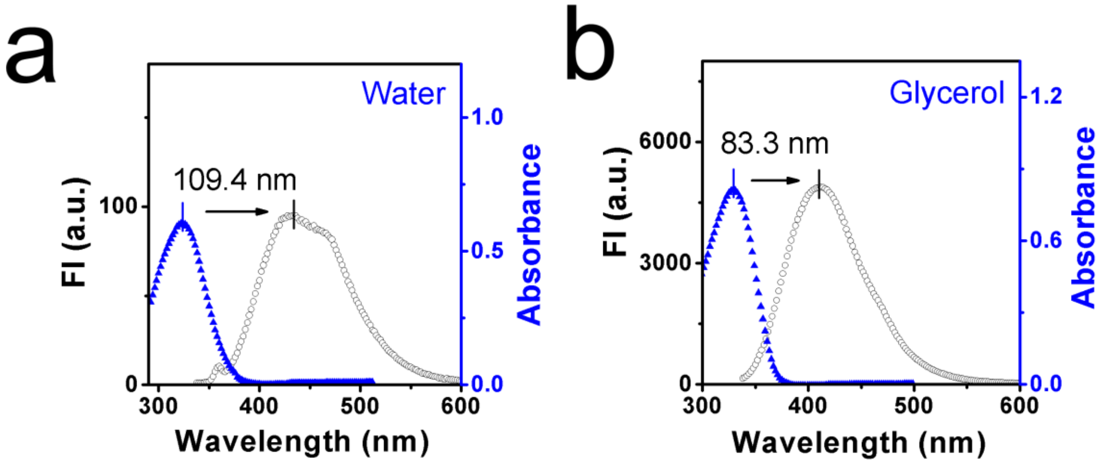


Figure S10 (a) Stokes shift of EAd in the water. (b) Stokes shift of EAd in the glycerol.

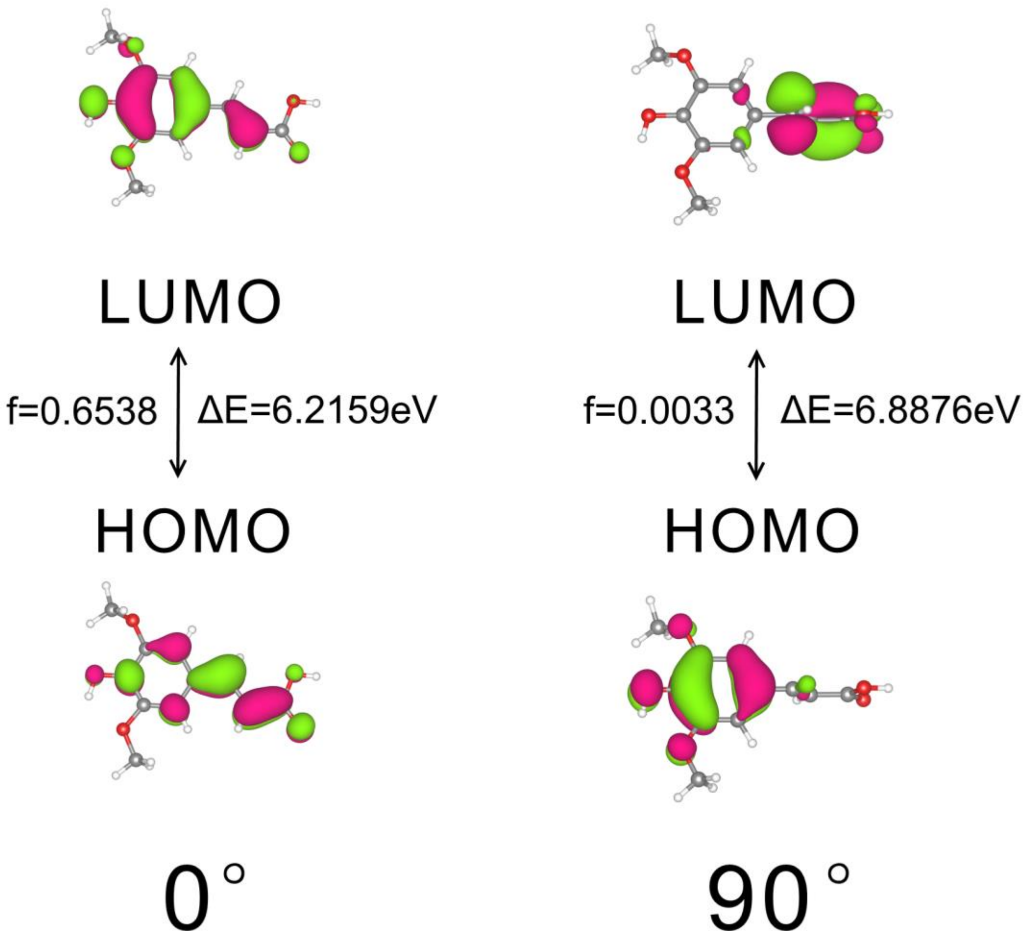


Figure S11 Optimized molecular structure and calculated molecular orbital energy levels of the LUMO and HOMO of EAd based on B3LYP/6-31G basis set.

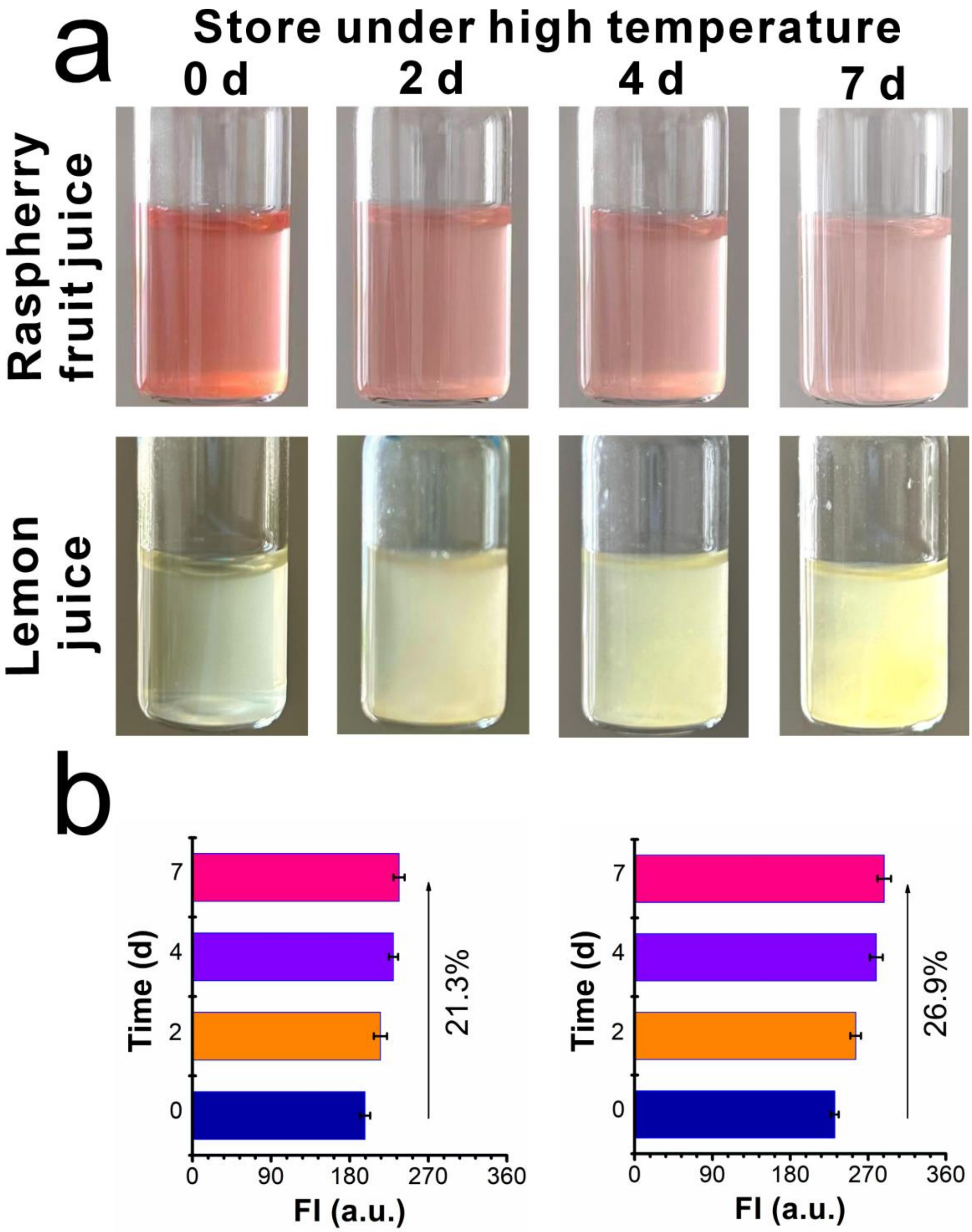
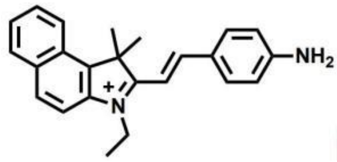
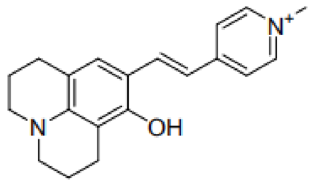
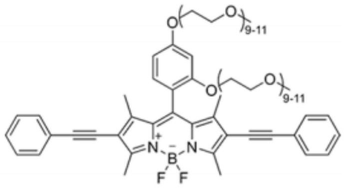
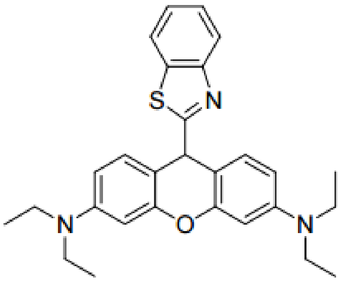
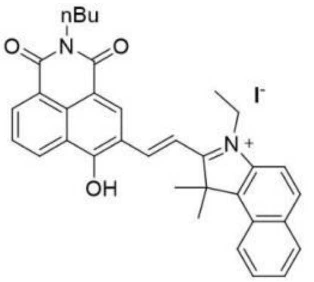
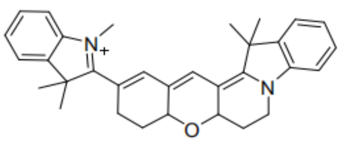
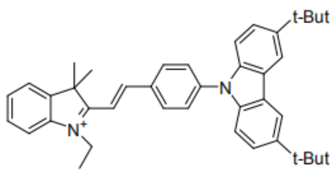
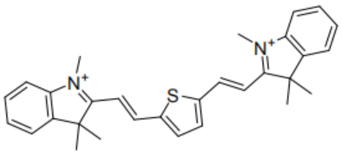
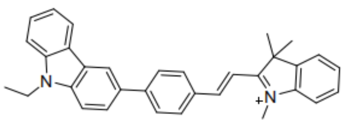
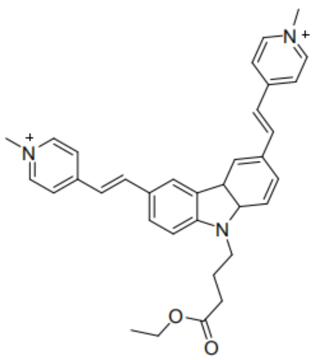
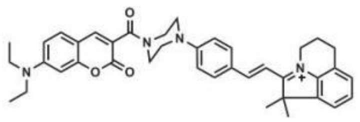
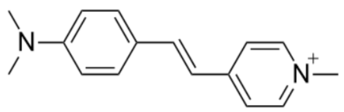
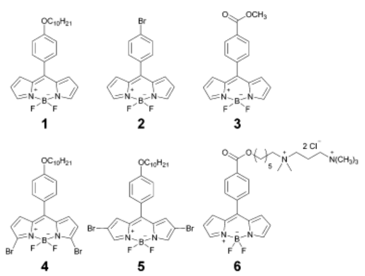
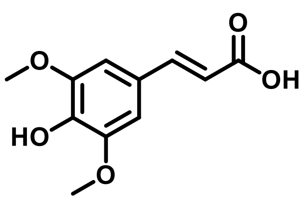


Figure S12 (a) Digital images of the raspberry fruit juice and lemon juice stored under high temperature within 7 days. (b) Emission intensity enhancement of raspberry fruit juice and lemon juice during the 7 days under high temperature.

Table S1. Comparison of the representative fluorescence-based dyes for viscosity detection reported in recent years.

Probe	Sources	Sensitive coefficient	Stokes shift*	Application	Reference
	Artificial synthesis	0.58	72 nm	Biological system, living cells.	[1]
	Artificial synthesis	/	90 nm	Biological system, living cells.	[2]
	Artificial synthesis	0.26	20 nm	Biological system, living cells.	[3]
	Artificial synthesis	0.41	35 nm	Biological system, living cells, in vivo.	[4]
	Artificial synthesis	0.45	55 nm	Biological system, living cells.	[5]
	Artificial synthesis	0.38	20 nm	Biological system, living cells, rat slice.	[6]

	Artificial synthesis	0.43	83 nm	Biological system, living cells.	[7]
	Artificial synthesis	0.59	70 nm	Biological system, living cell.	[8]
	Artificial synthesis	0.52	90 nm	Biological system, living cell, zebra fish, mice.	[9]
	Artificial synthesis	0.53	90 nm	Biological system, living cell.	[10]
	Artificial synthesis	0.46	60 nm	Biological system, living cell.	[11]
	Artificial synthesis	0.45	148 nm	Polymer solutions	[12]
	Artificial synthesis	0.25	20 nm	Cellular imaging	[13]
	Natural extract	0.56	83.3 nm	Liquid system, food safety analysis.	This work

* The stokes shift herein was obtained from the absorption and emission measured in the glycerol.

Table S2. Optical properties of the molecular probe **EAd** in different solvents.

Emitter	Quantum yield	
EAd	Quantum yield in water (Φ)*	Quantum yield in glycerol (Φ)*
	0.05%	1.98%
	Fluorescence lifetime	
	In water	In glycerol
	1.112 ns	1.556 ns

* Estimated using Fluorescein as the standard (in 0.1 M NaOH solution).

Table S3. Fluorescence intensity of commercial liquids with the natural probe EAd.

Liquids	Fluorescence intensity
Water	95.5
Pomelo juice	165.96
Pear juice	177.80
Raspherry fruit juice	204.22
Milk	217.81
Lemon juice	238.32
Mango juice	263.20
Watermelon juice	371.52
Edible oil	1258.91
Glycerol	4899.02

Table S4. Viscosity values of the liquids determined by viscometer and fluorescent spectrometer.

Liquids	Viscosity (cP)	Calculated (cP)
Water	1.00	1.01
Pomelo juice	1.90	1.94
Pear juice	2.12	2.05
Raspherry fruit juice	2.64	2.53
Milk	3.00	2.94
Lemon juice	3.50	3.43
Mango juice	4.25	4.33
Watermelon juice	7.50	7.41
Edible oil	68.10	68.26

Table S5. Photo-physical properties of the molecular sensor EAd in different solvents.

Solvents	Dielectric constant (ε)	η (cP)	Absorption λ_{ab} (nm)	Emission λ_{em} (nm)
Glycerol	45.8	956.0	329.3	412.6
Water	78.5	1.0	324.9	434.3
Toluene	2.4	0.6	311.2	389.0
Methanol	32.6	0.6	322.9	420.5
THF	7.4	0.5	321.6	402.7

DCM	9.1	0.4	313.2	391.8
DMSO	46.8	2.1	323.7	424.6
EtOAc	6.1	0.4	313.5	417.5

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