RSC Advances

Supplementary Information

Turn-on mode probe based on the sustainable xanthohumol extract for the efficient viscosity response in liquid system

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Experimental section

1 Materials and apparatus

The hops (female flowers of Humulus lupulus L.) were kindly supplied by the Shandong Fengtai Biotech. Co., Ltd. Tetrahydrofuran (THF), toluene, dimethylsulfoxide (DMSO), N, N-dimethylformamide (DMF), methanol, ethyl acetate (EA), glycerol and various metal salts were purchased from Shanghai Aladdin Bio-Chem Technology Co., Ltd. The glucose, D-mannitol, acesulfame, sorbitol, sodium carboxymethyl cellulose (SCC), pectin (Pec), xanthan gum (XG), trisodium citrate dehydrate (TCD), vitamin C (VC), sodium benzoate (SB) and beet molasses (BM) 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:

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

where η represents the viscosity, I represents the fluorescence intensity of the natural molecular probe XTH at 425 nm, C is a constant, and x represents the sensitivity of the natural molecular probe XTH toward viscosity.

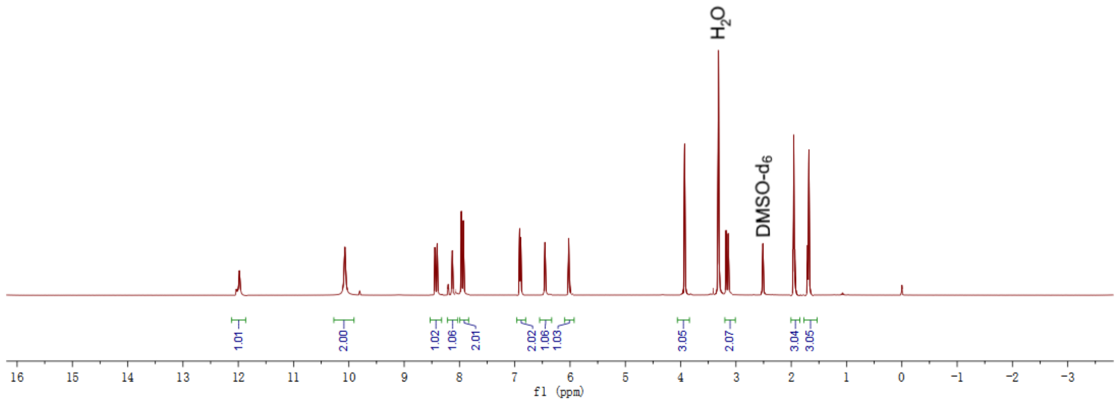


Figure S1 ^{1}H NMR spectrum of the extracted molecular probe xanthohumol (XTH).

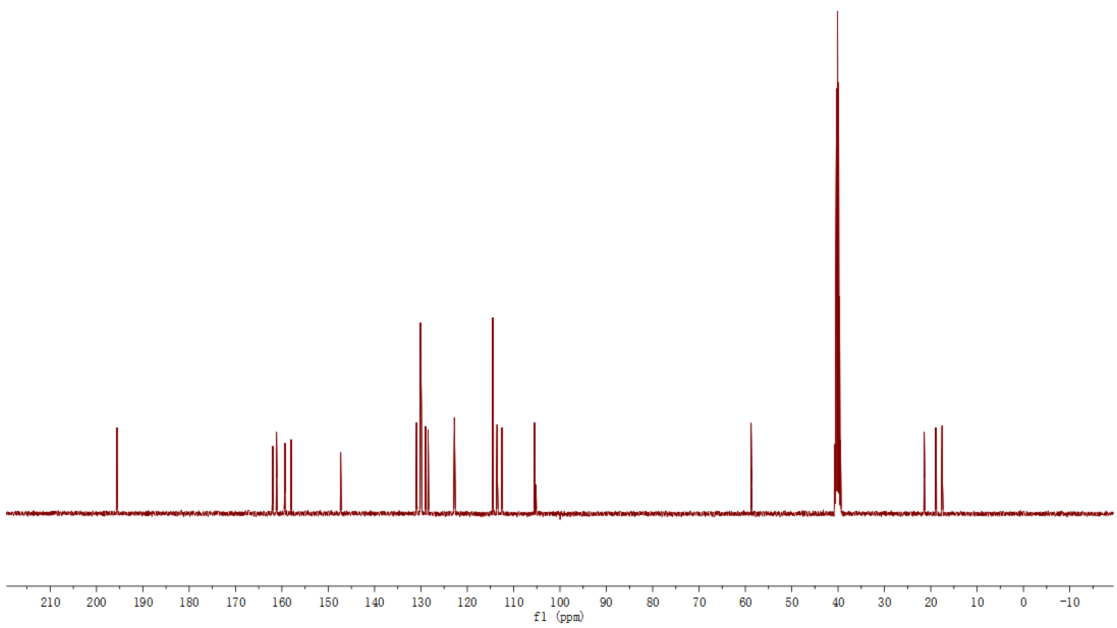


Figure S2 ^{13}C NMR spectrum of the extracted molecular probe xanthohumol (XTH).

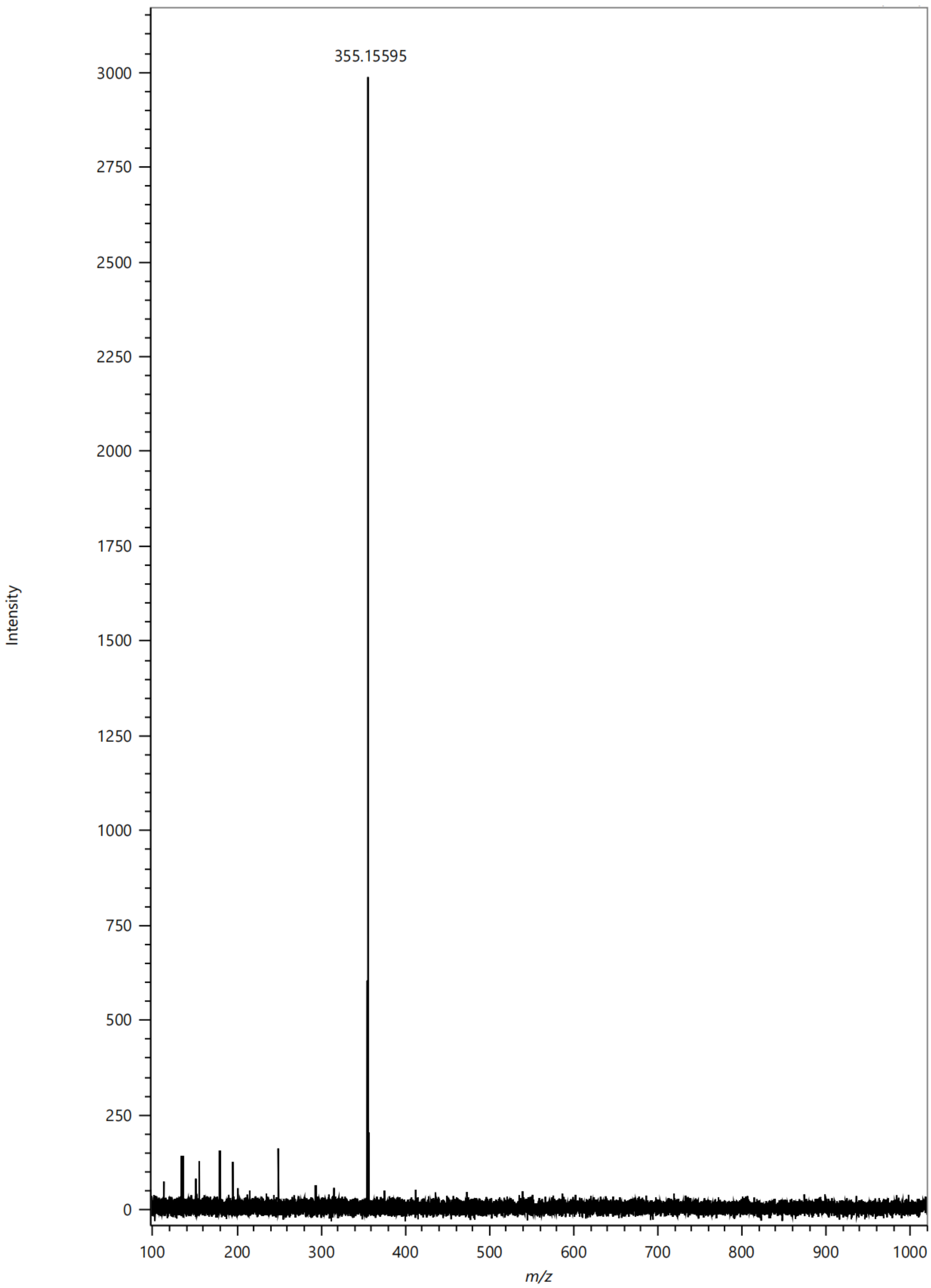


Figure S3 HR mass spectrum of the extracted molecular probe xanthohumol (XTH).

MS (ESI): m/z 355.15595 $[M+H]^+$.

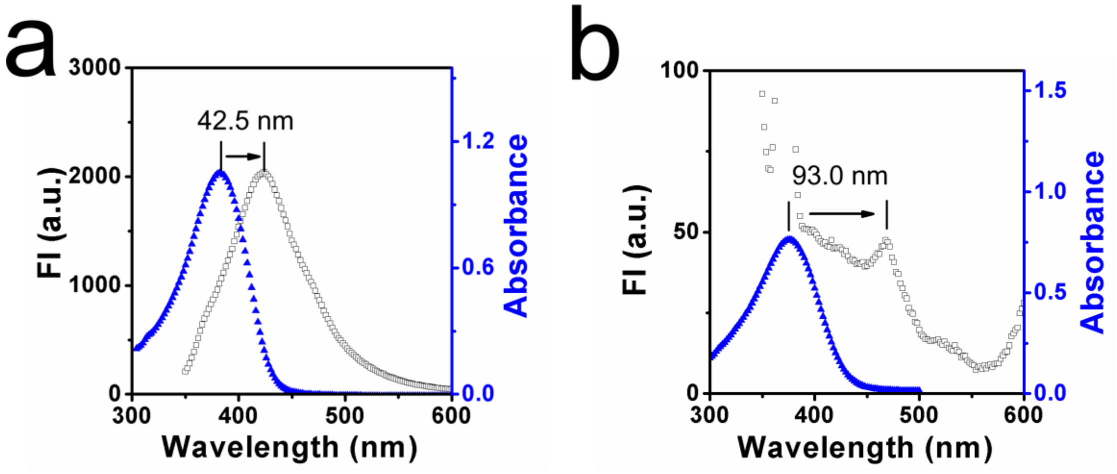


Figure S4 (a) Recorded absorption and emission spectra of XTH in glycerol. (b) Recorded absorption and emission spectra of XTH in distilled water.

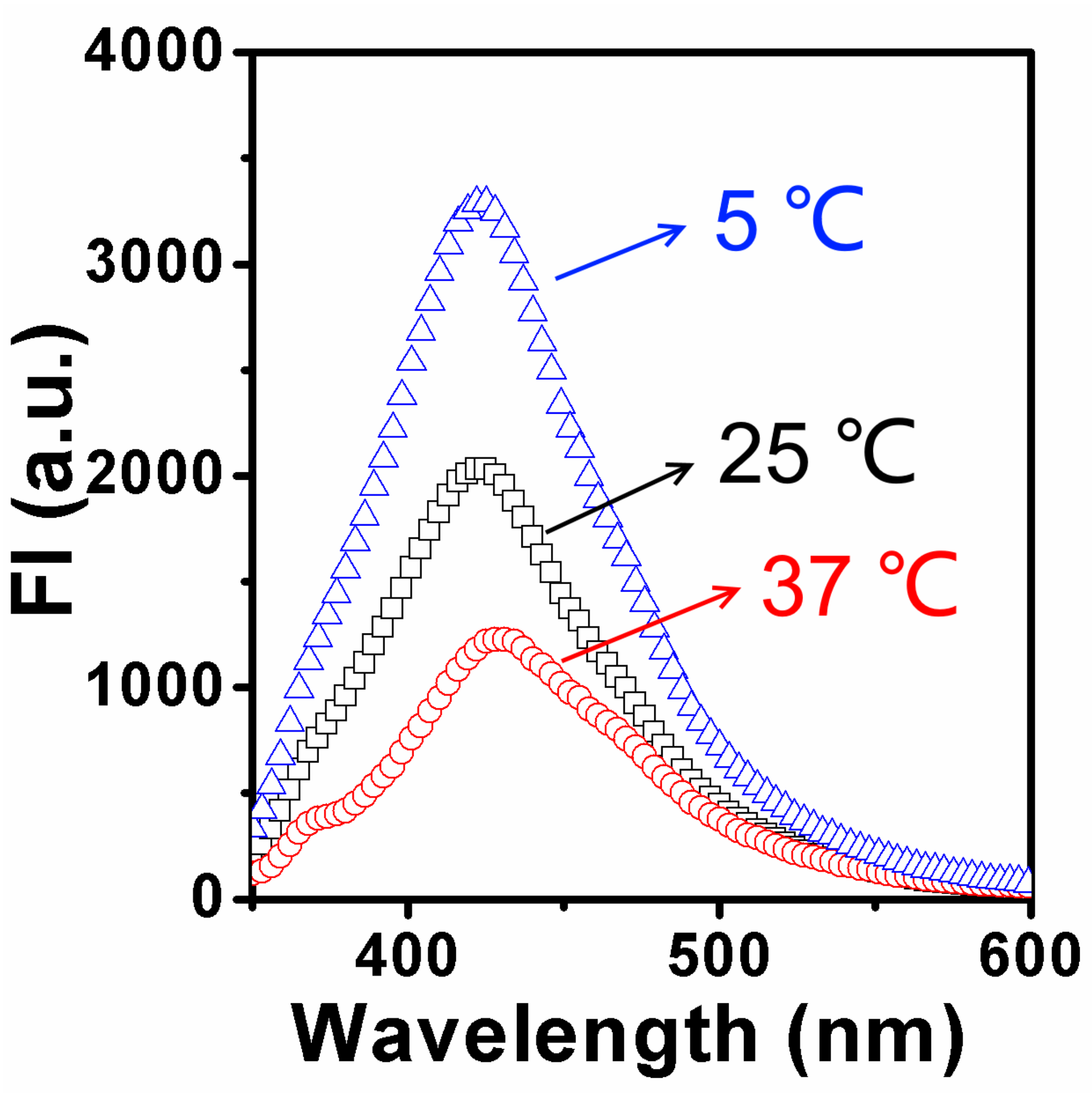


Figure S5 Fluorescence spectra of the natural molecular probe XTH (10 μM) in glycerol under different temperature, including the ambient temperature (25 °C), higher storage temperature (37 °C), and lower-maintenance temperature (5 °C).

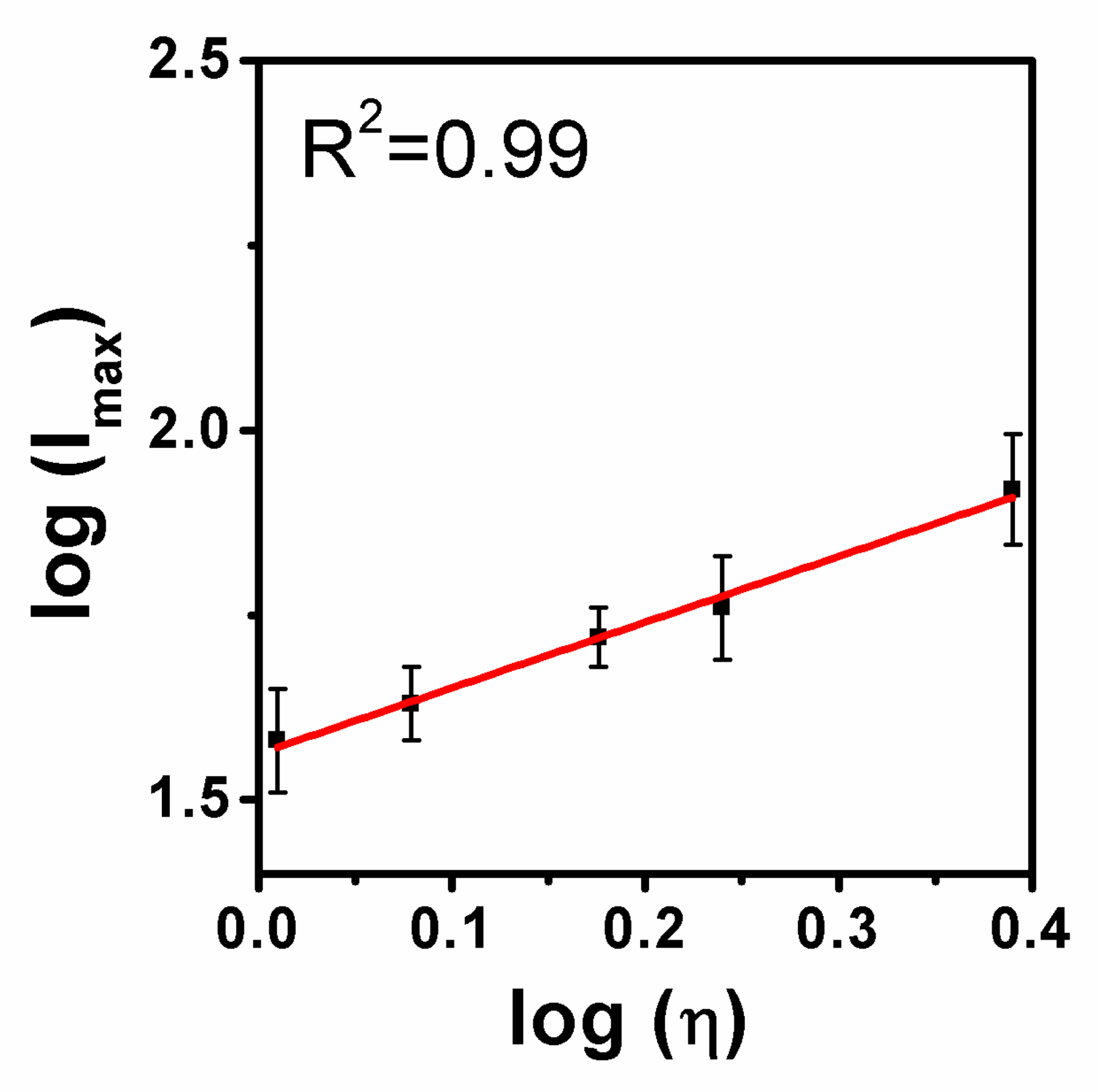


Figure S6 Detection limit of the natural molecular probe xanthohumol (XTH).

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 molecular probe XTH.

log (I_{max}) = 1.562 + 0.890 × log (η) (R^2 = 0.990)

log (LOD) = 3 × 0.036/0.890 = 0.121

LOD =10^0.121 =1.321 cP

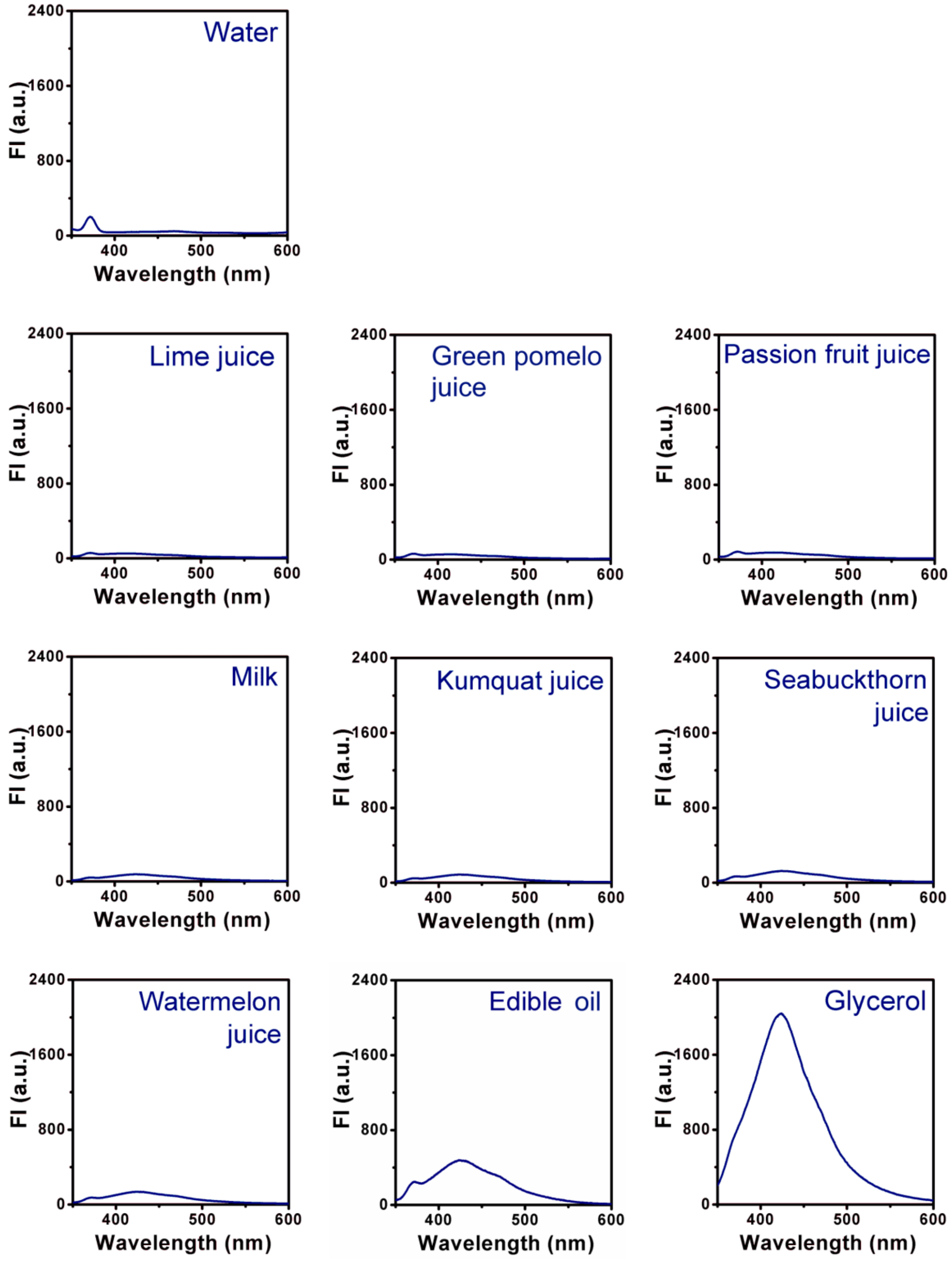


Figure S7 Fluorescence spectra of the natural molecular probe XTH (10 μM) in ten kinds of common liquids, including the distilled water, lime juice, green pomelo juice, passion fruit juice, milk, kumquat juice, seabuckthorn juice, watermelon juice, edible oil and glycerol, λ_{ex}=320 nm.

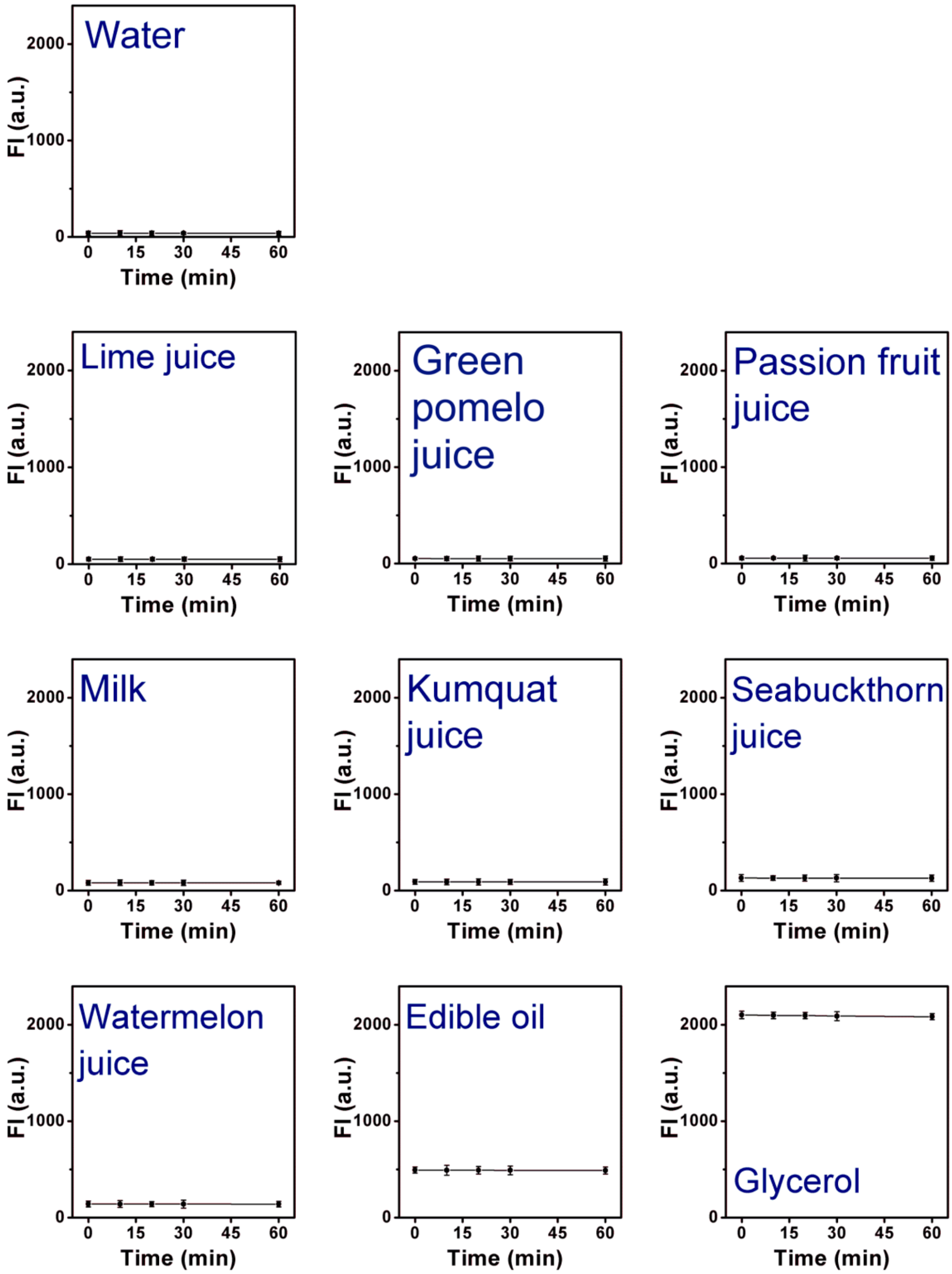


Figure S8 Photo-stability analysis of the natural molecular probe XTH in the glycerol and other eight kinds of common liquids. All upon samples were tested under continuous light irradiation with 320 nm UV lamp.

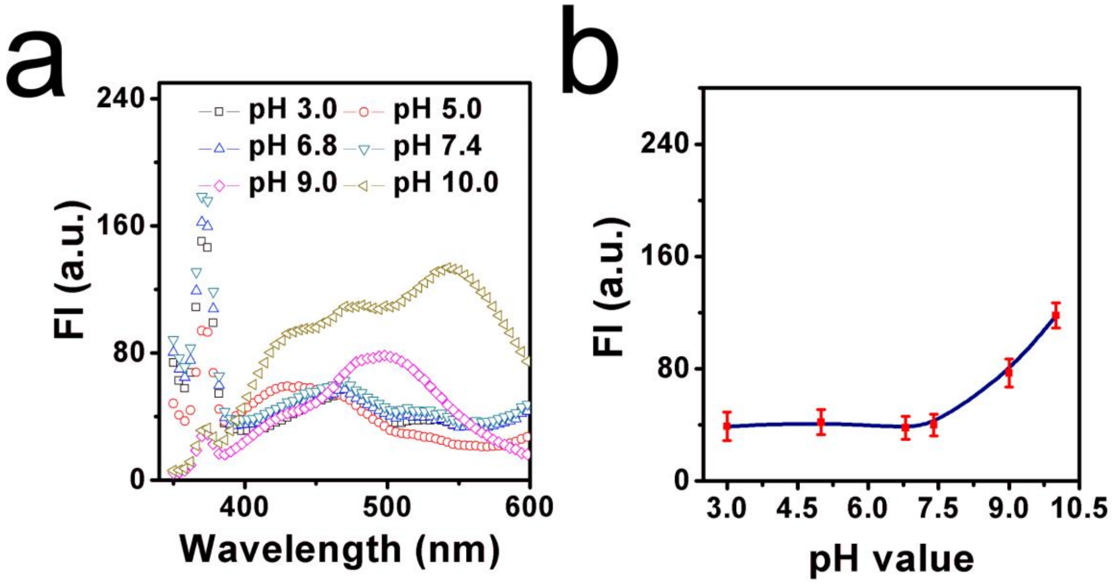


Figure S9 Fluorescence emission intensity of the natural molecular probe XTH (10 μM) under various pH values in the distilled viscosity water, λ_{ex}=320 nm.

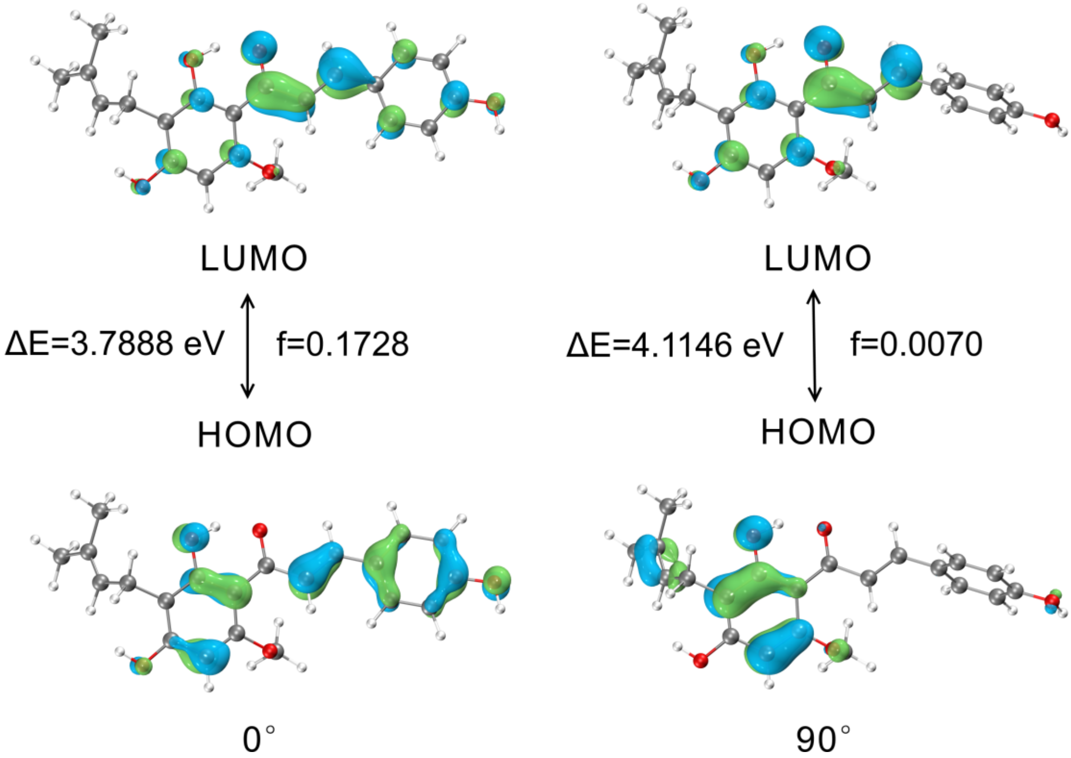


Figure S10 Optimized molecular structure and calculated molecular orbital energy levels of the LUMOs and HOMOs of XTH based on B3LYP/6-31G basis set.

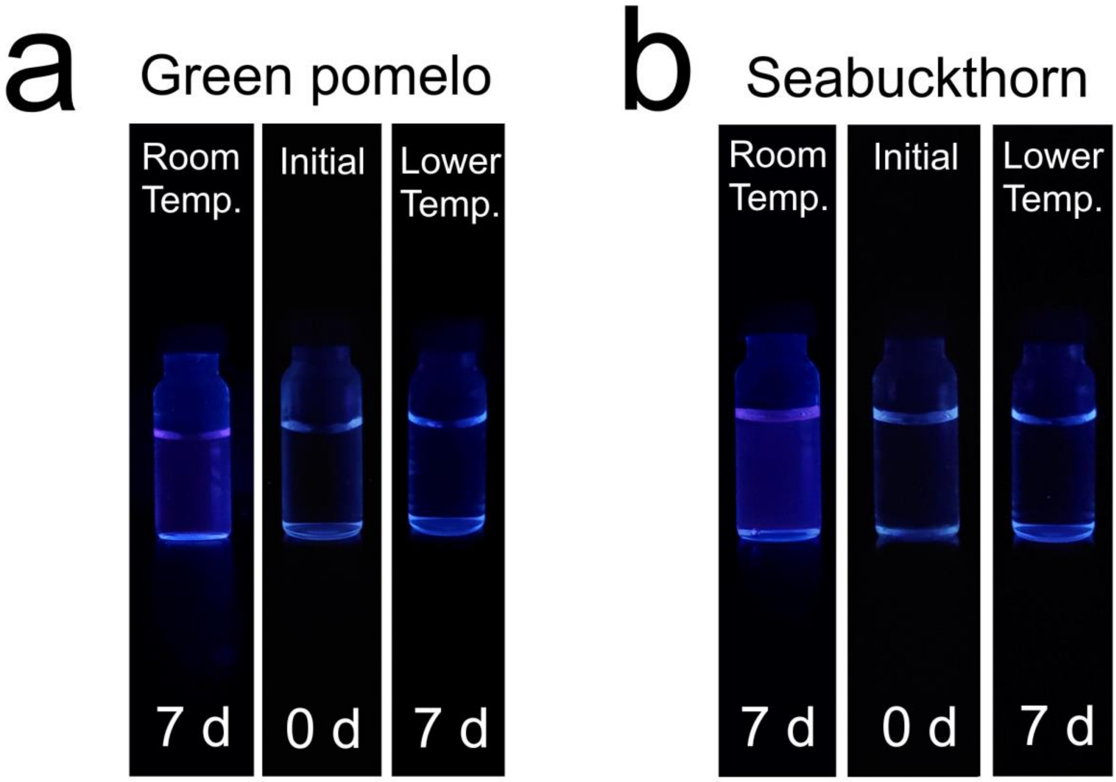
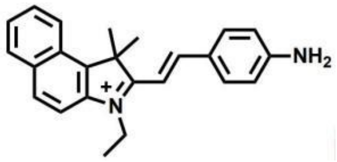
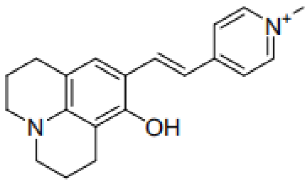
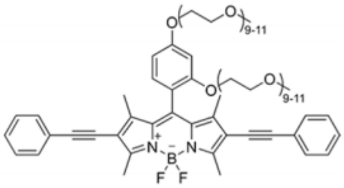
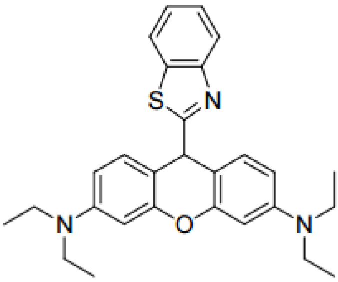
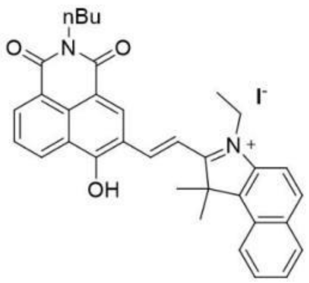
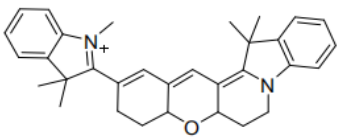
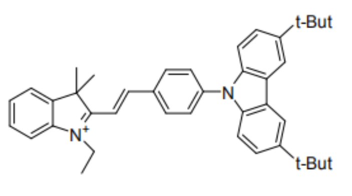
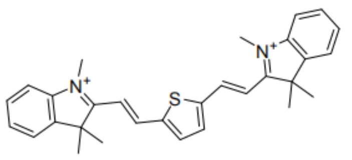
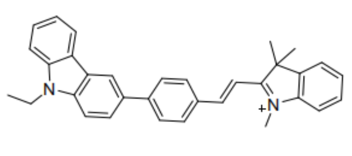
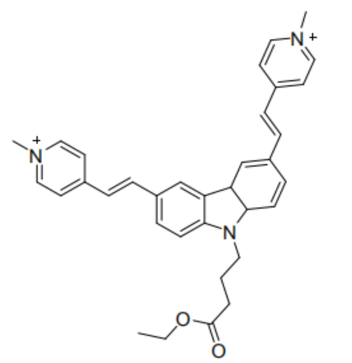
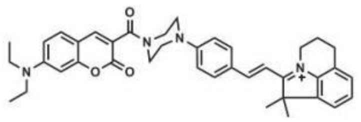
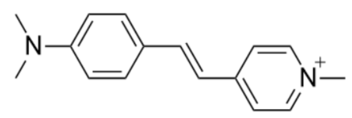
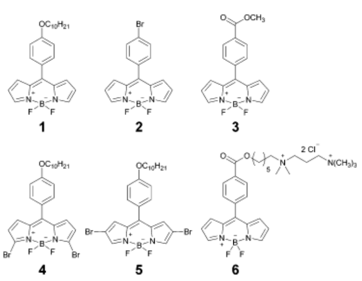
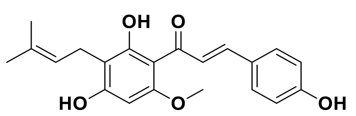


Figure S11 Emission fluorescence signal of green pomelo juice and seabuckthorn juice under different storage temperatures for 7 days from the naked eye.

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

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

	Artificial synthesis	83 nm	Biological system, living cells.	[7]
	Artificial synthesis	70 nm	Biological system, living cell.	[8]
	Artificial synthesis	90 nm	Biological system, living cell, zebra fish, mice.	[9]
	Artificial synthesis	90 nm	Biological system, living cell.	[10]
	Artificial synthesis	60 nm	Biological system, living cell.	[11]
	Artificial synthesis	148 nm	Polymer solutions	[12]
	Artificial synthesis	20 nm	Cellular imaging	[13]
	Natural product	42.5 nm	Liquid system, food spoilage 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 **XTH** in different solvents.

Emitter	Quantum yield	
XTH	Quantum yield in water (Φ)*	Quantum yield in glycerol (Φ)*
	0.06%	2.61%
	Fluorescence lifetime	
	In water	In glycerol
	1.131 ns	1.623 ns

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

Table S3. Fluorescence intensity of commercial liquids with the molecular probe **XTH**.

Liquids	Fluorescence intensity
Lime juice	50.81
Green pomelo juice	54.98
Passion fruit juice	73.45
Milk	79.43
Kumquat juice	90.01
Seabuckthorn juice	129.21
Watermelon juice	140.22
Edible oil	490.34
Glycerol	2087.20

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

Liquids	Viscosity (cP)	Calculated (cP)
Lime juice	1.18	1.32
Green pomelo juice	1.38	1.42
Passion fruit juice	2.37	2.48
Milk	2.79	2.99
Kumquat juice	3.32	3.03
Seabuckthorn juice	6.52	6.63
Watermelon juice	7.48	7.62
Edible oil	68.00	68.79
Glycerol	956.00	963.60

Table S5. Photo-physical properties of the molecular probe **XTH** in different solvents.

Solvents	Dielectric constant (ε)	η (cP)	Absorption λ_{ab} (nm)	Emission λ_{em} (nm)
Glycerol	45.8	956.0	382.5	425.0
Water	78.5	1.0	375.5	468.5
Toluene	2.4	0.6	365.1	408.1
DMSO	46.8	2.1	374.8	458.9
Methanol	32.6	0.6	369.3	440.2
Acetonitrile	37.5	0.4	368.4	433.7
DMF	36.7	0.8	368.1	431.7
EA	6.1	0.4	321.8	418.6

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