Analytical Methods

Electronic Supplementary Information

Activatable molecular rotor based on bithiophene quinolinlium toward viscosity detection in liquid

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The Förster–Hoffmann equation

According to the previous studies,¹ the relationship between the fluorescence intensity of the molecular rotor DPADQ and the viscosity can be determined by the following Förster–Hoffmann equation:

$$\log I = C + x \log \eta \tag{1}$$

where η represents the viscosity, *I* represents the fluorescence intensity of the molecular rotor DPADQ at 725 nm, C is a constant, and x represents the sensitivity of the molecular rotor towards viscosity.



Fig. S2 ¹³C-NMR spectrum of Compound 1 in DMSO-d₆.



Fig. S3 HR mass spectrum of Compound 1. MS (ESI): m/z 194.99271 [M+H]⁺.



Fig. S4 Partial enlargement of the spectrum focusing on Compound 1 [M+H]⁺.



Fig. S5 ¹H-NMR spectrum of the molecular rotor BTPEQ in CDCl₃.



Fig. S6 ¹³C-NMR spectrum of the molecular rotor BTPEQ in CDCl₃.



Fig. S7 HR mass spectrum of molecular rotor BTPEQ. MS (ESI): m/z 348.08763

 $[M]^{+}$.



Fig. S8 Partial enlargement of the spectrum focusing on molecular rotor BTPEQ

[M]⁺.



Fig. S9 Detection limit of the rotor BTPEQ.

The calibration curve was first obtained from the plot of log (I_{648}) as a function of log

(η). Then the regression curve equation was obtained for the lower viscosity part.

The detection limit = $3 \times S.D./k$

Where k is the slope of the curve equation, and S.D. represents the standard deviation

for the log (I_{648}) of molecular rotor DPPBQD.

$$\log (I_{648}) = 1.583 + 0.357 \times \log (\eta) (R^2 = 0.991)$$

 $\log (LOD) = 3 \times 0.002/0.357 = 0.017$

LOD =10^0.036 =1.040 cP



Fig. S10 Fluorescence spectra of the rotor BTPEQ (10 μ M) in glycerol under different temperature, including the ambient temperature (25 °C), higher storage temperature (37 °C), and lower storage temperature (5 °C).



Fig. S11 (a) Normalized absorption spectra of molecular rotor BTPEQ in six kinds of common solvents. (b) Normalized fluorescence emission spectra in six kinds of common solvents.



Fig. S12 Fluorescence images of the rotor BTPEQ in various solvents.



Fig. S13 Normalized dual emission spectra of the rotor BTPEQ in various solvents.



Fig. S14 Fluorescence emission intensity of the molecular rotor BTPEQ (10 μ M) at 648 nm under various pH values (containing 1% DMSO) in low viscosity water and in high viscosity glycerol, λ_{ex} =488 nm.



Fig. S15 Photostability analysis of the molecular rotor BTPEQ in water (containing 1% DMSO) and other eight kinds of common liquid food (containing 1% DMSO). All upon samples were tested under continuous light irradiation with 488 nm UV lamp.



Fig. S16 Fluorescence spectra of the molecular rotor BTPEQ (10 μ M, containing 1% DMSO) in nine kinds of common liquid food, including the water, rose tea, cranberry tea, mango juice, lemon juice, milk, jasmine tea juice, watermelon juice and edible oil, λ_{ex} =488 nm.



Fig. S17 Digital images of the mango juice (a) and cranberry tea (b) that stored under ambient temperature and lower temperature which containing Escherichia Coli for varying time (from 0 to 3 days), corresponding fluorescence spectra and viscosity values at different time intervals. Concentration of BTPEQ = $10 \ \mu$ M, λ_{ex} =488 nm.

Probe	λ_{ab}^{*}	λ_{em}^{**}	Stokes shift ^{***}	Applicatio n	Reference
	511 nm	583 nm	72 nm	Biological system, living cells.	2
	530 nm	620 nm	90 nm	Biological system, living cells.	3
$ \begin{array}{c} \circ (& \circ)_{g_{11}} \\ \circ &$	560 nm	580 nm	20 nm	Biological system, living cells.	4
S N S N N O N	600 nm	635 nm	35 nm	Biological system, living cells, in vivo.	5
	580 nm	635 nm	55 nm	Biological system, living cells.	б
	678 nm	698 nm	20 nm	Biological system, living cells, rat slice.	7
t-But	545 nm	628 nm	83 nm	Biological system, living cells.	8

Table S1. Comparison of the representative fluorescence-based dyes for viscosity

 detection reported in recent years.

N+ ST + F	525 nm	595 nm	70 nm	Biological system, living cell.	9
	520 nm	610 nm	90 nm	Biological system, living cell, zebra fish, mice.	10
	470 nm	560 nm	90 nm	Biological system, living cell.	11
	520 nm	580 nm	60 nm	Biological system, living cell.	12
	488 nm	648 nm	160 nm	Liquid food, food spoilage analysis.	This work

* Absorption peak. The absorption was measured in the glycerol.

** Emission peak. The fluorescence emission was measured in the glycerol.

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

Solvents	Dielectric	η (cP)	Absorption	Emission
	constant (ϵ)		λ_{ab} (nm)	λ_{em} (nm)
Toluene	2.4	0.6	448.2	632.3
DCM	8.9	0.4	452.3	641.1
THF	7.4	0.5	453.2	642.1
Acetonitrile	37.5	0.4	458.4	645.6
DMF	36.7	0.8	460.1	646.2
Methanol	32.6	0.6	463.2	650.7
DMSO	46.8	2.1	465.3	651.3
Water	78.5	1.0	466.1	653.1
Glycerol	45.8	956.0	488.3	648.3

Table S2. Photo-physical properties of the molecular rotor BTPEQ in different solvents.

 Table S3. Viscosity values of the beverages determined by viscometer.

Beverages	Viscosity (cP)	Calculated (cP)
Water	1.00	1.01
Rose Tea	1.71	1.73
Cranberry Tea	1.85	1.88
Mango Juice	4.22	4.25
Lemon Juice	3.50	3.54
Milk	2.82	2.85
Jasmine Tea Juice	6.20	6.14
Watermelon Juice	7.50	7.45
Edible Oil	68.10	68.25

References

- I. E. Steinmark, P.-H. Chung, R. M. Ziolek, B. Cornell, P. Smith, J. A. Levitt, C. Tregidgo, C. Molteni, G. Yahioglu, C. D. Lorenz and K. Suhling, *Small*, 2020, 16, 1907139.
- 2 B. Chen, C. Li, J. Zhang, J. Kan, T. Jiang, J. Zhou and H. Ma, *Chem. Commun.*, 2019, **55**, 7410–7413.
- 3 G. Zhang, Y. Sun, X. He, W. Zhang, M. Tian, R. Feng, R. Zhang, X. Li, L. Guo, X. Yu and S. Zhang, *Anal. Chem.*, 2015, **87**, 12088–12095.
- 4 L.-L. Li, K. Li, M.-Y. Li, L. Shi, Y.-H. Liu, H. Zhang, S.-L. Pan, N. Wang, Q. Zhou and X.-Q. Yu, *Anal. Chem.*, 2018, **90**, 5873–5878.
- 5 M. Ren, L. Wang, X. Lv, J. Liu, H. Chen, J. Wang and W. Guo, *J. Mater. Chem. B*, 2019, **7**, 6181–6186.
- 6 L. Zhu, M. Fu, B. Yin, L. Wang, Y. Chen and Q. Zhu, *Dye. Pigment.*, 2020, **172**, 107859.
- 7 S. J. Park, B. K. Shin, H. W. Lee, J. M. Song, J. T. Je and H. M. Kim, *Dye. Pigment.*, 2020, **174**, 108080.
- 8 K. Zhou, M. Ren, B. Deng and W. Lin, *New J. Chem.*, 2017, **41**, 11507–11511.
- 9 Y. Baek, S. J. Park, X. Zhou, G. Kim, H. M. Kim and J. Yoon, *Biosens. Bioelectron.*, 2016, **86**, 885–891.
- 10 J. Yin, M. Peng and W. Lin, Anal. Chem., 2019, 91, 8415–8421.
- 11 Z. Zou, Q. Yan, S. Ai, P. Qi, H. Yang, Y. Zhang, Z. Qing, L. Zhang, F. Feng and R. Yang, *Anal. Chem.*, 2019, **91**, 8574–8581.
- 12 L. He, Y. Yang and W. Lin, Anal. Chem., 2019, 91, 15220–15228.