

*Electronic Supplementary Information (ESI)*

## **Broadening AIEgen application: rapid and portable sensing of foodstuff hazards in deep-frying oil†**

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## 1. Chemicals and instruments

$^1\text{H}$  and  $^{13}\text{C}$  NMR spectra in  $\text{CDCl}_3$  were determined by a Bruker AVANCE III 400 MHz Spectrometer with tetramethylsilane (TMS) as the internal standard. High-resolution mass spectra (HRMS) were obtained by a Waters LCT Premier XE spectrometer (ESI). Absorption and fluorescence spectra were carried out on a Varian Cary 100 spectrometer and a Varian Cary Eclipse spectrometer, respectively. Viscosity was determined by Anton Paar SVM 3000. Polymer was determined by Agilent 1260 Infinity II Prime LC. All chemicals used in this study were of analytical reagent grade. Deionized water was used to prepare all aqueous solutions. 4-(diphenylamino)benzaldehyde was purchased from Aladdin Reagent Co., Ltd. The starting material 2-(1-ethyl-2-methylquinolin-4(1*H*)-ylidene)malononitrile was prepared according to the established method (C. X. Shi, Z. Q. Guo, Y. L. Yan, S. Q. Zhu, Y. S. Xie, S. Z. Yong, W. H. Zhu, T. He, *ACS Appl. Mater. Interfaces*, 2013, **5**, 192-198).

A mixture of 2-(1-ethyl-2-methylquinolin-4(1*H*)-ylidene)malononitrile (200 mg, 0.85 mmol), 4-(diphenylamino)benzaldehyde (270 mg, 1 mmol), acetonitrile (30 mL) and piperidine (0.4 mL) was refluxed for 8 h under argon protection. The solvent was removed by vacuum, and the residua were purified by column chromatography on silica gel (DCM:PE = 2:1) to obtain the target probe QM-TPA (192 mg, yield 46%).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ , ppm):  $\delta$  = 1.54 (3H,  $-\text{CH}_2\text{CH}_3$ ), 4.37 (q,  $J$  = 7.2 Hz, 2H,  $-\text{CH}_2\text{CH}_3$ ), 6.90 (d,  $J$  = 16.0 Hz, 1H, alkene-H), 7.05-7.07 (2H, phenyl-H, quinoline-H), 7.11-7.16 (m, 7H, phenyl-H), 7.29-7.31 (m, 4H, phenyl-H and 1H, alkene-H), 7.41 (d,  $J$  = 8.0 Hz, 2H, phenyl-H), 7.46 (1H, phenyl-H), 7.60 (d,  $J$  = 8.4 Hz, 1H, phenyl-H), 7.75 (m, 1H, phenyl-H), 9.16 (d,  $J$  = 8.8 Hz, 1H, phenyl-H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ , ppm):  $\delta$  = 13.95, 43.86, 50.89, 107.49, 115.97, 116.33, 119.31, 120.41, 121.60, 121.82, 124.13, 124.56, 125.42, 127.04, 127.87, 128.81, 129.54, 133.12, 138.16, 140.00, 146.85, 148.25, 149.80, 153.38. MS (ESI positive ion mode for  $[\text{M} + \text{K}]^+$ ): Calcd. for  $\text{C}_{34}\text{H}_{26}\text{N}_4\text{K}$ : 529.1795; found: 529.1799.

## 2. Optical properties of QM-TPA

Table S1 Optical properties of QM-TPA

Emitter	$\lambda_{abs}$ (nm)	$\lambda_{em}$ (nm)		
		Soln ( $\Phi_F$ ) <sup>a</sup>	Aggr ( $\Phi_F$ ) <sup>a</sup>	Powder ( $\Phi_F$ ) <sup>b</sup>
QM-TPA	430	584 (0.1)	584 (42.9)	625 (8.6)

Abbreviations: Soln = solution (10  $\mu$ M in THF); Aggr = THF / water mixture with 90% water fraction for QM-TPA;  $\lambda_{abs}$  = absorption maximum;  $\lambda_{em}$  emission maximum; and  $\Phi_F$  fluorescence quantum yield. <sup>b</sup>Estimated using Rhodamine B as the standard ( $\Phi_F$  50% in ethanol). Note: the optical density of the solution is < 0.05, to avoid self-absorption. <sup>c</sup>Measured by an integrating sphere.

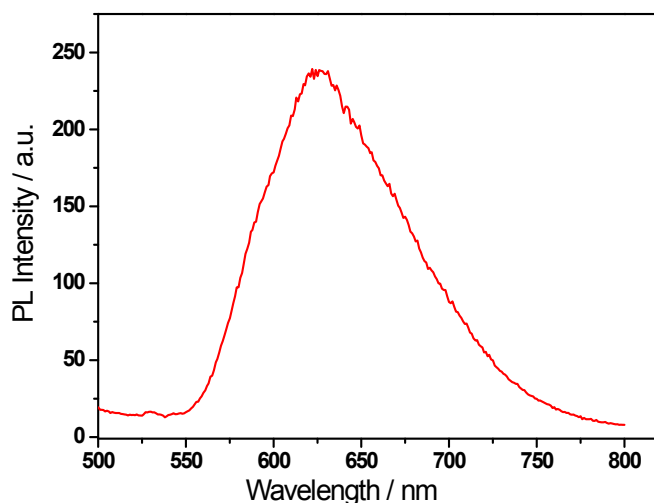


Fig. S1 PL spectrum from pristine powder of QM-TPA,  $\lambda_{ex}$  = 430 nm

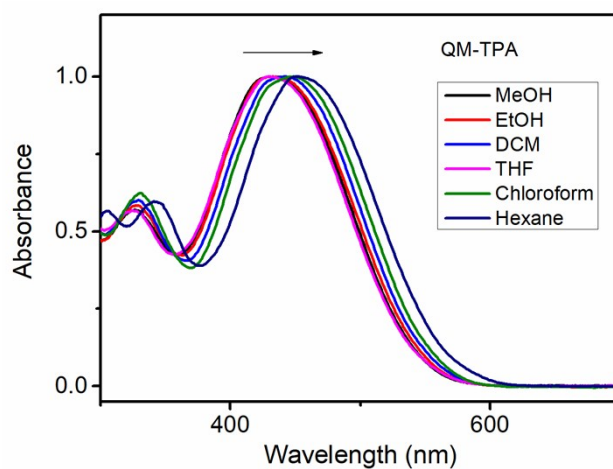
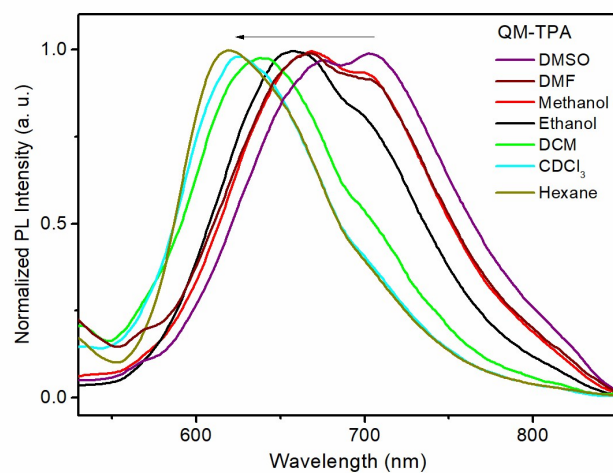
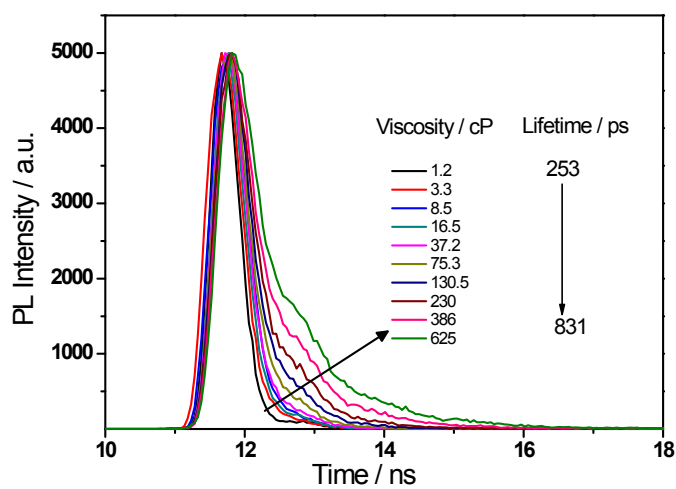


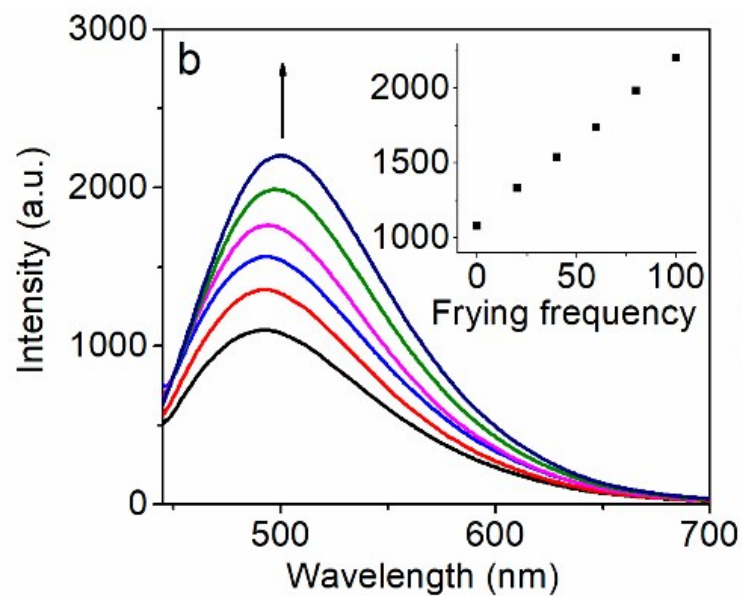
Fig. S2 Absorption spectra of QM-TPA in various solvents.



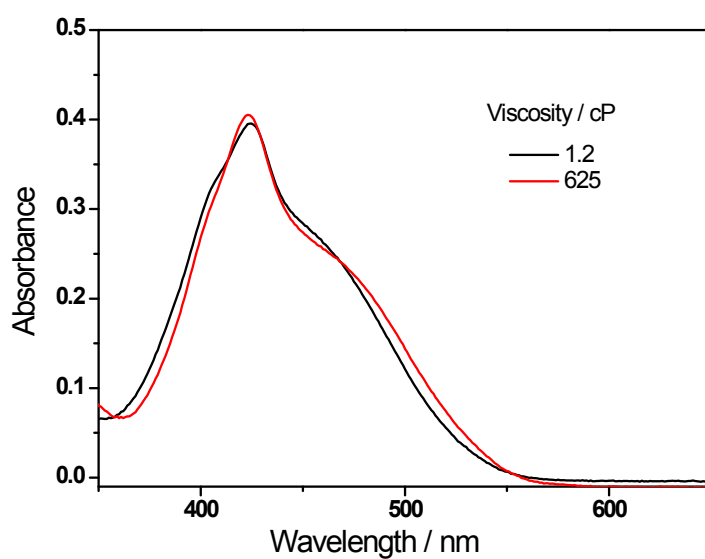
**Fig. S3** Normalized PL spectra in various solvents of QM-TPA,  $\lambda_{\text{ex}} = 430 \text{ nm}$



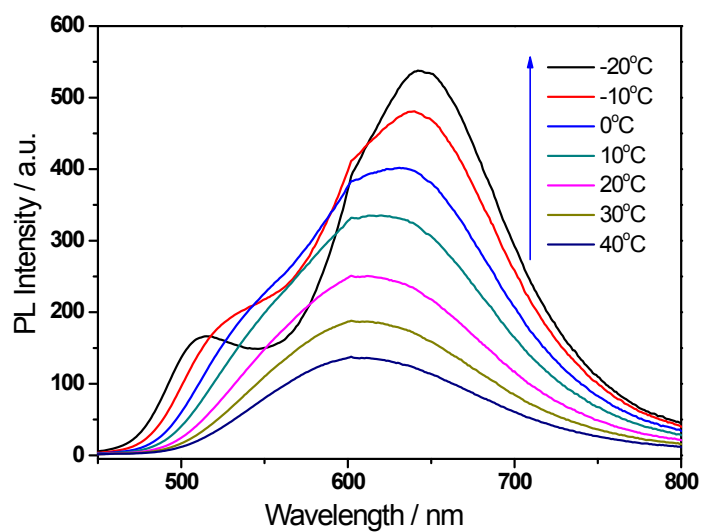
**Fig. S4** Fluorescence lifetime of QM-TPA ( $10^{-5} \text{ M}$ ) with different viscosity in mixed ethanol/glycerol mixtures.  $\lambda_{\text{ex}} = 441 \text{ nm}$ ,  $\lambda_{\text{em}} = 600 \text{ nm}$ .



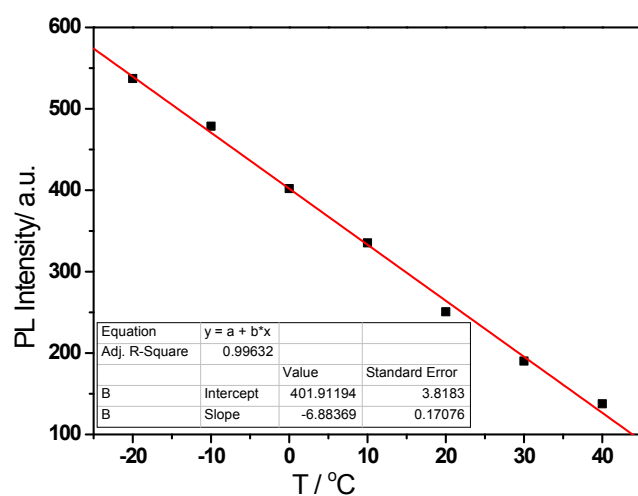
**Fig. S5** Fluorescence intensity of QM-TPA (10 μM) in oil/ethanol (1/1, v/v) mixed system with increasing frying frequencies from 0 to 100 times,  $\lambda_{ex} = 430$  nm. Inset: fluorescence intensity at 500 nm as a function of frying frequency.



**Fig. S6** Absorption spectra of QM-TPA (10<sup>-5</sup> M) in ethanol/glycerol mixtures of different viscosity. Note: the absorption of QM-TPA showed a negligible change in solvents with different viscosity.

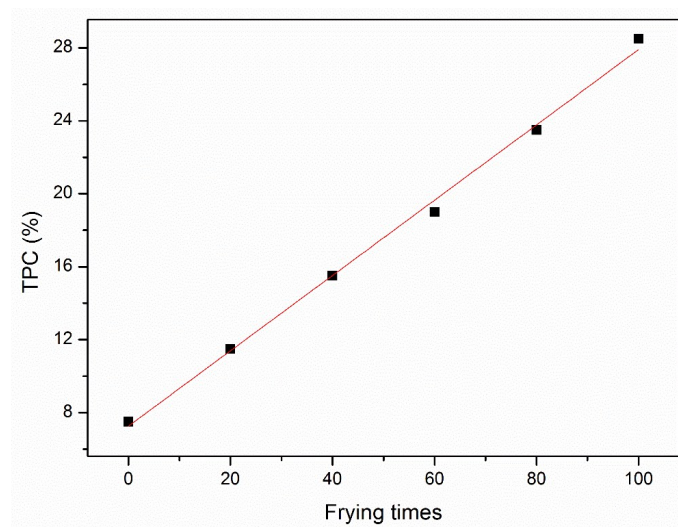


**Fig. S7** Fluorescence spectra of QM-TPA at different temperatures. Note: with temperature decreasing, the fluorescence intensity of QM-TPA exhibited a significant increase because the restriction of intramolecular motions will strengthen at the low temperature.



**Fig. S8** The linearity of  $I_{\max}$  versus temperature. Note: the fluorescence intensity showed an excellent linear relationship with temperature.

### 3. Relations between frying times and TPC



**Fig. S9** Frying frequency vs. total polar compound (TPC) level (0: 7.5%, 20: 11.5%, 40: 15.5%, 60: 19%, 80: 23.5%, 100: 28.5%). Note: with frying frequency increasing, the level of TPC gradually enhances in oil, demonstrating that the quality of oil degenerates.

4.  $^1\text{H}$ ,  $^{13}\text{C}$  NMR and HRMS data for QM-TPA.

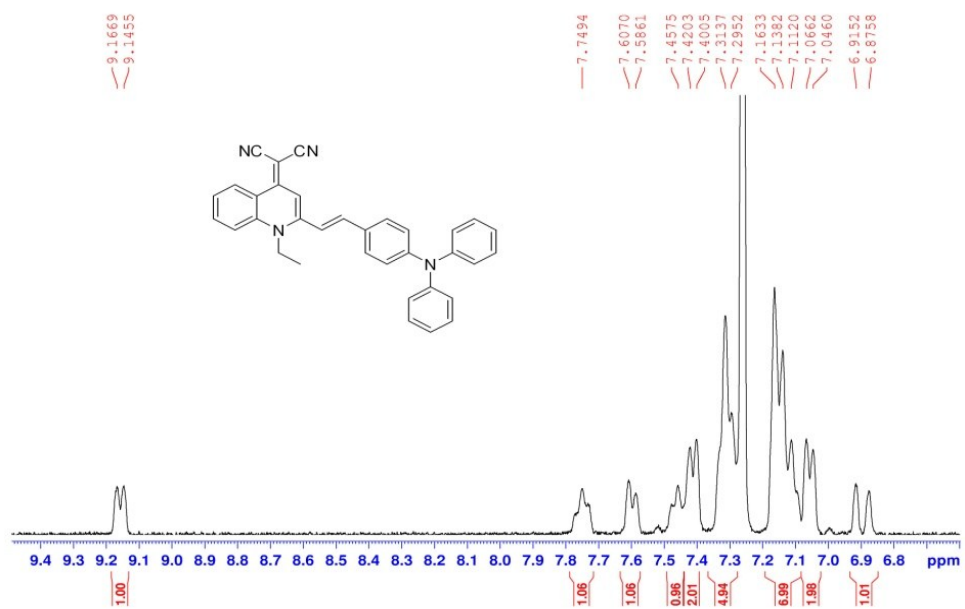
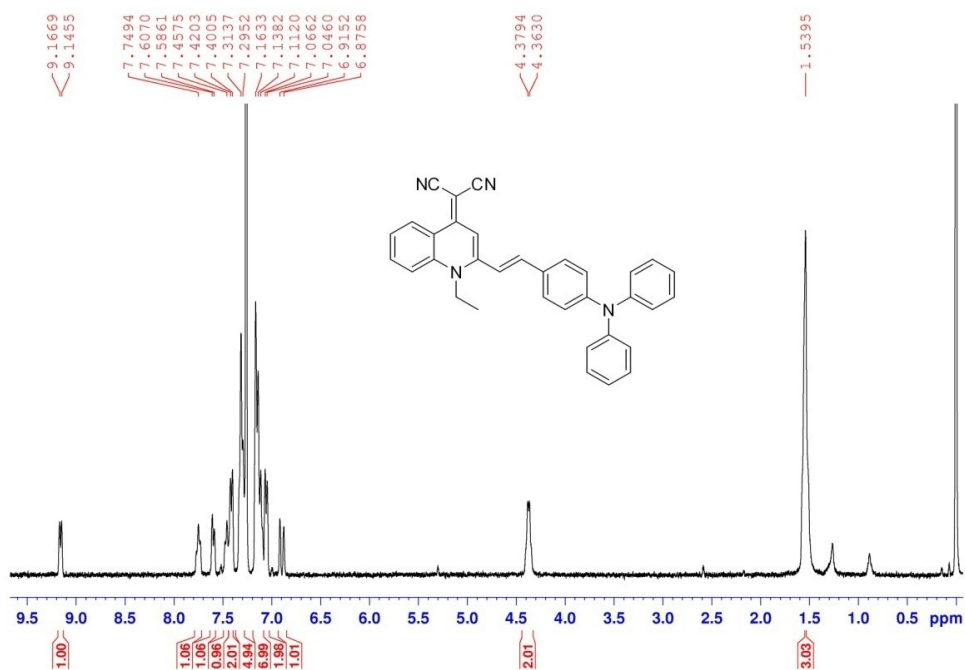


Fig. S10  $^1\text{H}$  NMR spectrum of compound QM-TPA in  $\text{CDCl}_3$



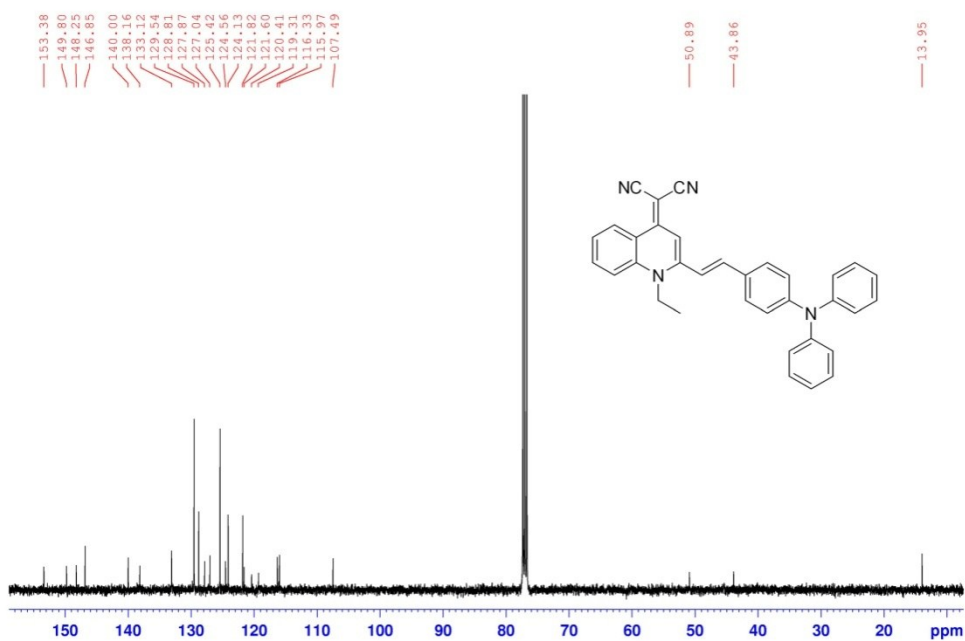


Fig. S11  $^{13}\text{C}$  NMR spectrum of compound QM-TPA in  $\text{CDCl}_3$

Elemental Composition Report

Single Mass Analysis

Tolerance = 3.0 mDa / DBE: min = -1.5, max = 50.0  
 Element prediction: Off  
 Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions  
 151 formula(e) evaluated with 1 results within limits (up to 1 best isotopic matches for each mass)  
 Elements Used:  
 C: 32-65 H: 0-1000 N: 0-200 K: 0-1

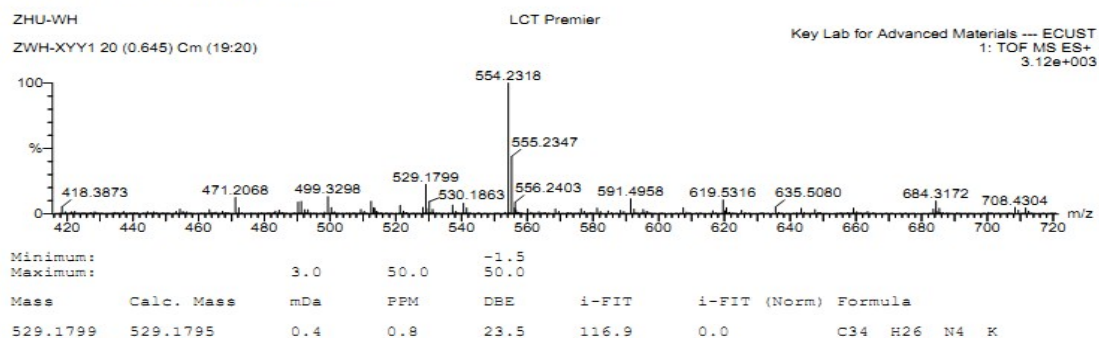


Fig. S12 HRMS spectrum of QM-TPA