Supplementary information

Fluorometric probing lipase levels as acute pancreatitis biomarker based on interfacial controlled aggregation-induced emission (AIE)

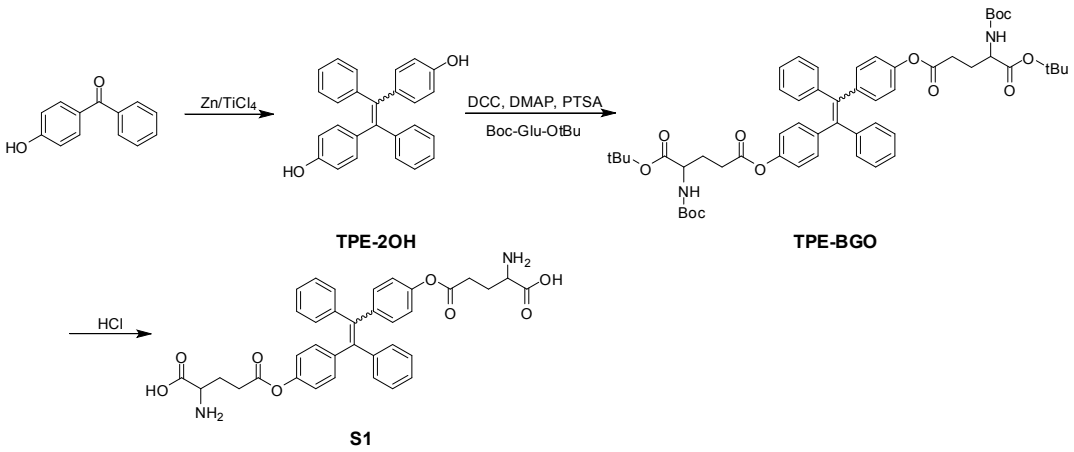
Jie Shi,[a] Qianchun Deng,[a] Chuyun Wan,[a] Mingming Zheng,[a] Fenghong Huang[a] and Bo Tang*[b]*

[a]Hubei Key Laboratory of Lipid Chemistry and Nutrition, Oil Crops and Lipids Process Technology National & Local Joint Engineering Laboratory, Key Laboratory of Oilseeds Processing, Ministry of Agriculture, Oil Crops Research Institute, Chinese Academy of Agricultural Sciences, Wuhan 430062, China

[b]College of Chemistry, Chemical Engineering and Materials Science, Collaborative Innovation Center of Functionalized Probes for Chemical Imaging in Universities of Shandong, Key Laboratory of Molecular and Nano Probes, Ministry of Education, Shandong Normal University, Jinan 250014, China

* Corresponding author. Phone: 86-27-86827874; E-mail: shij@whu.edu.cn

* Corresponding author. Phone: 86-531-86182545; E-mail: tangb@sdnu.edu.cn



Scheme S1. Synthetic route for the probe **S1**.

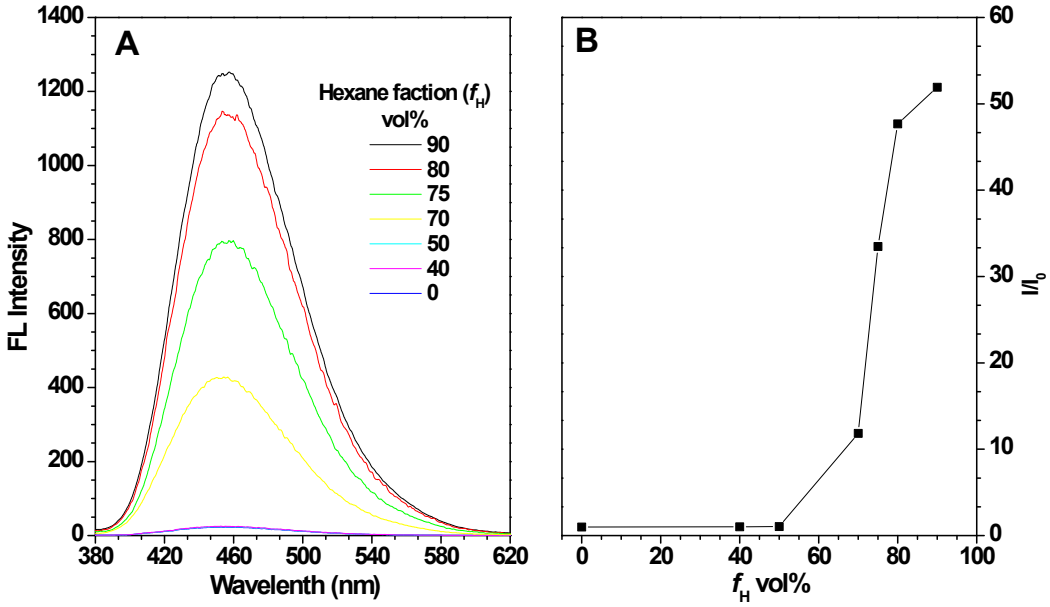


Fig. S1 (A) fluorescence emission spectra of **TPE-2OH** (10 μM) in THF-hexane mixtures with different fractions of hexane (f_H). (B) Plot of I/I_0 at 453 nm versus f_H, where I_0 is the fluorescence intensity in pure THF solution. Excitation wavelength: 360 nm.

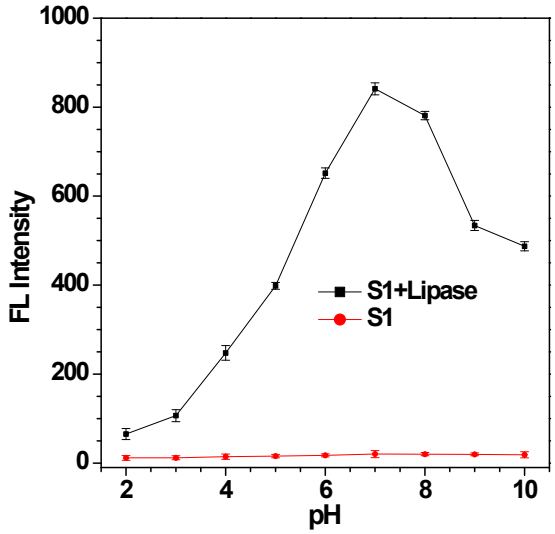


Fig. S2 Fluorescent emission spectra of **S1** and **S1** + lipase at different pH value in PBS buffer, excited at 360 nm.

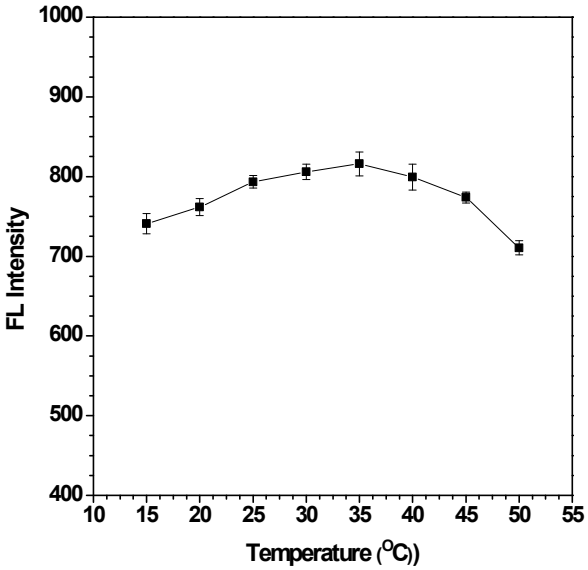


Fig. S3 Fluorescent emission spectra of **S1** (10 μM) after incubation with lipase at different temperatures in PBS buffer, excited at 360 nm.

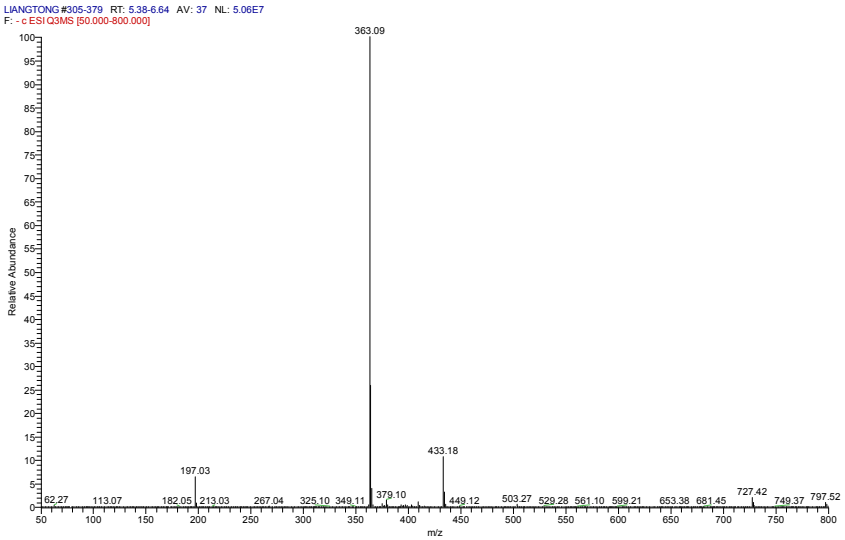


Fig. S4 Mass spectrum of the enzymatic reaction product. The probe (10 μM) with lipase (80 U/L) at 37 °C in PBS-buffered water (pH 7.4, 0.1 M) was incubated for 20 min. MS (ESI): the enzymatic reaction product m/z 363.09 $[M-H]^-$. It is indicated that the product of the enzymatic reaction has the same molecular structure as **TPE-2OH**.

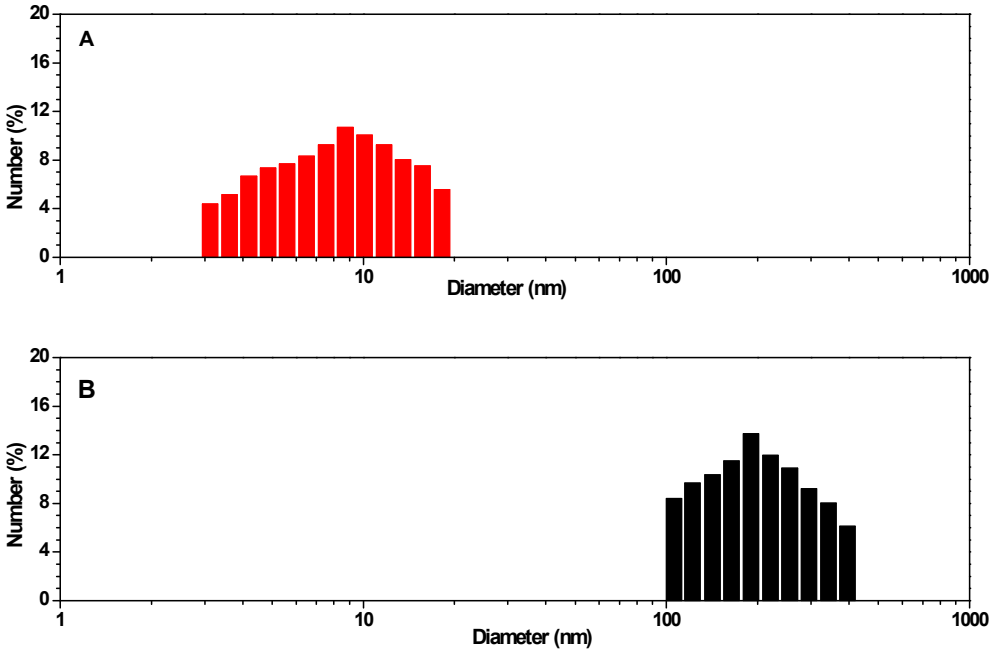


Fig. S5 Dynamic light scattering (DLS) results for the solution of probe **S1** in the absence and presence of lipase: (a) probe **S1** (10 μM) in hexane solution; (b) probe **S1** (10 μM) in hexane solution after incubated with lipase (80 U/L) for 20 min.

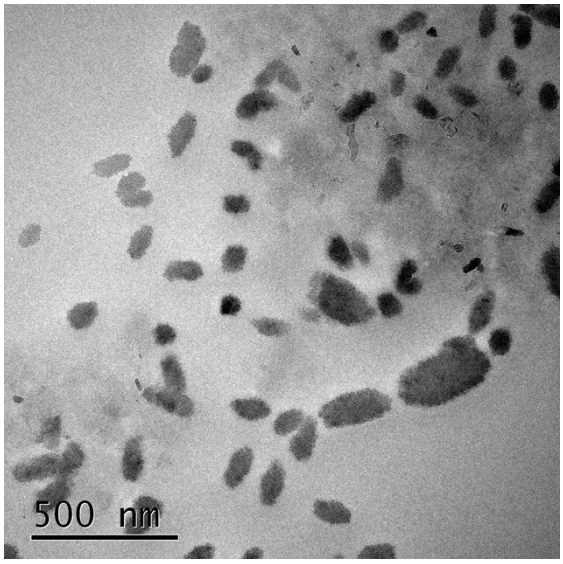


Fig. S6 TEM image of the enzymatic reaction product in hexane after incubated with lipase (80 U/L) for 20 min.

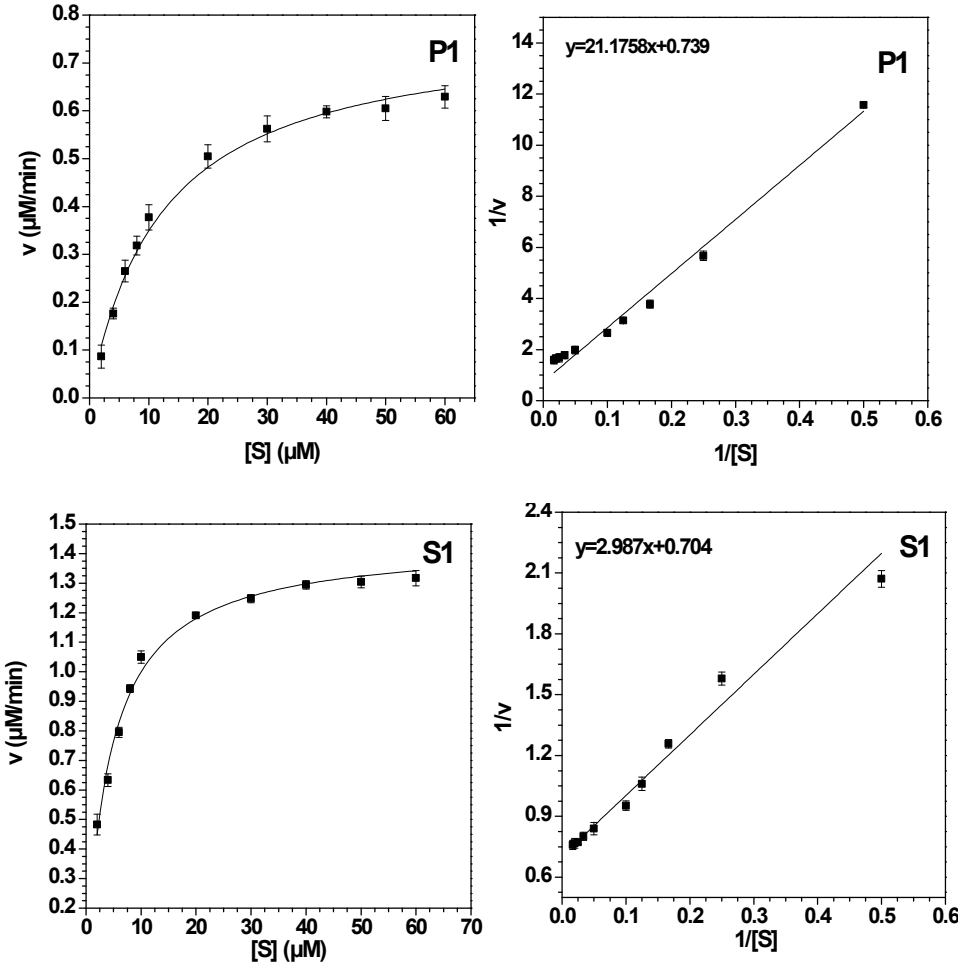


Fig. S7 Substrate dependence of the initial degradation velocities for Lipase. Initial

velocities were plotted against the substrate concentrations and fit to the Michaelis-Menten model.

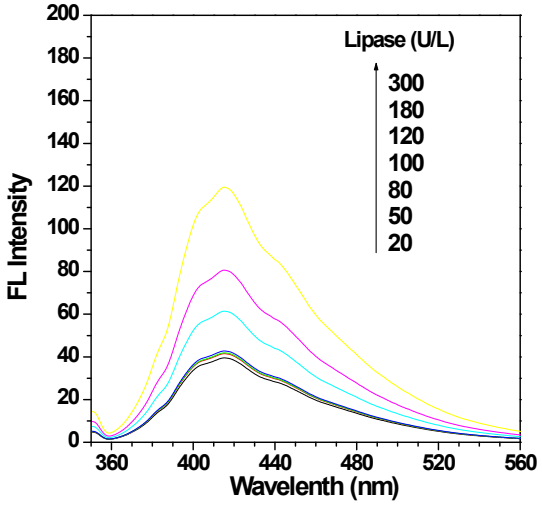


Fig. S8 The fluorescence emission spectra of probe **P1** (10 μM) after incubation with different concentrations of lipase-buffer (0.1 M PBS) solution at 25 °C.

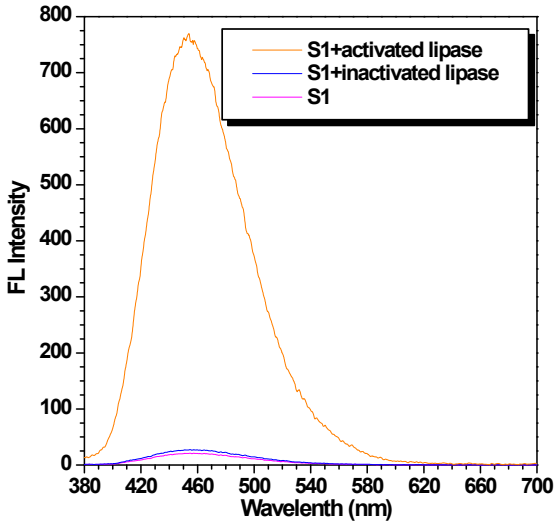


Fig. S9 Fluorescence spectra of the probe **S1**, probe **S1**/activited lipase and probe **S1**/inactivited lipase. Concentration: probe **S1** (10 μM); activited lipase (80 U/L); inactivited lipase (80 U/L). Excitation wavelength: 360 nm.

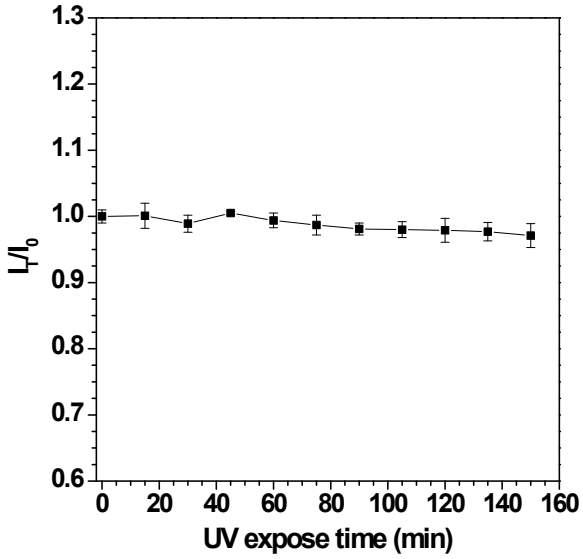


Fig. S10 Photostability of the reaction product aggregates. I_t/I_0 is the fluorescence intensity ratio at 453 nm, excited at 254 and 365 nm after T-minute light irradiation and before light irradiation. Excitation wavelength: 360 nm.

Table S1 Use of **S1** as substrate in pH-stat method for detecting the hydrolytic activity of commerical lipases. All assays were performed with 0.01 g lipase at 37 °C and pH 7.4 for 20 min.

Lipase	PCL	CALB	RFL	ANL	CRL	PPL

V_{NaOH} (mL)	1.61	3.64	2.39	4.59	2.99	8.31
V_{error} (mL)	0.117	0.365	0.209	0.142	0.197	0.322
Activity (U/g)	39.69	89.48	58.91	113.02	73.54	204.53

Method	Sample	Lipase amount (U/L)		Recovery (%)	SD (%)
		Added	Found		
Lipase Assay Kit	1	10.00	9.75	97.50	4.3
	2	20.00	20.04	100.20	5.1
	3	30.00	29.63	98.77	4.9
	4	40.00	39.13	97.83	3.6
	5	50.00	48.71	97.42	3.4
	6	60.00	60.09	100.15	3.5
	7	70.00	69.38	99.11	2.7
	8	80.00	81.24	101.55	3.3
	9	90.00	88.97	98.86	4.1
	10	100.00	102.44	102.44	1.8
Probe **S1**	1	10.00	9.89	98.90	2.9
	2	20.00	19.31	96.55	4.8
	3	30.00	28.79	95.97	2.2
	4	40.00	39.22	98.05	1.9
	5	50.00	51.25	102.5	3.7
	6	60.00	59.67	99.45	3.5
	7	70.00	68.54	97.91	4.2
	8	80.00	81.69	102.11	4.6
	9	90.00	87.71	97.46	3.4
	10	100.00	98.59	98.59	2.5

Table S2. Comparison of lipase levels detection by using lipase assay kit and probe **S1**. Standard recovery experiments were performed by adding a known quantity of lipase to diluted human serum samples of healthy people.