

Supporting Information for:

A novel homolateral and dicationic AIEgen for the sensitive detection of casein

Zenghe Li,^a Lianying Wang,^a Weijiang Guan,^a Caifeng Ding,^b Zhiqin Yuan^{*ac} and Chao Lu^{*a}

^a *State Key Laboratory of Chemical Resource Engineering, Beijing University of Chemical Technology, Beijing 100029, China. Fax/Tel: 86 010 64411957*

^b *Laboratory of Optic-electric Sensing and Analytical Chemistry for Life Science, Ministry of Education; Qingdao University of Science and Technology, Qingdao 266042, China.*

^c *State Key Laboratory of Chemo/Biosensing and Chemometrics, Hunan University, Changsha 410082, China.*

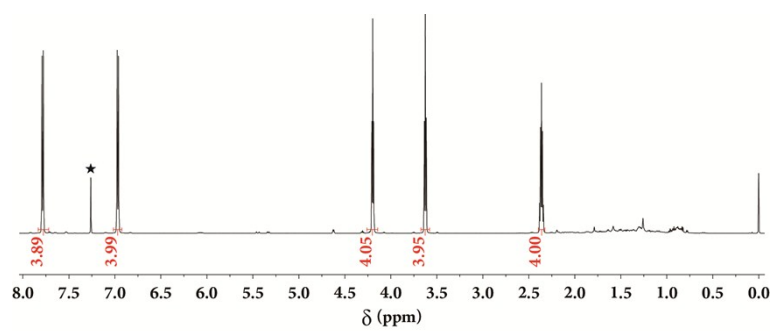


Fig. S1. ^1H NMR spectrum of compound **1** in CDCl_3 (asterisks represent solvent peaks).

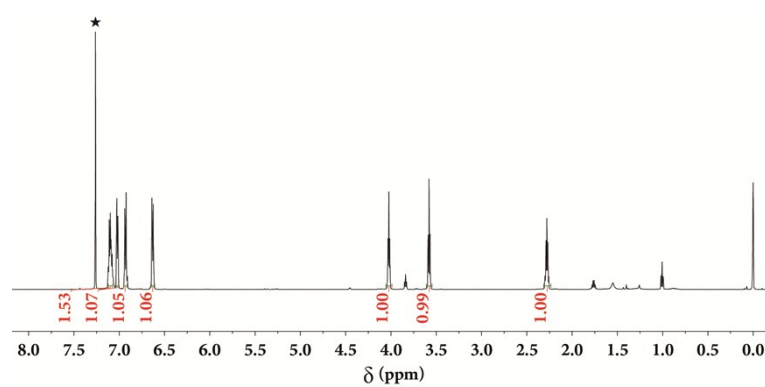


Fig. S2. ^1H NMR spectrum of compound **2** in CDCl_3 (asterisks represent solvent peaks).

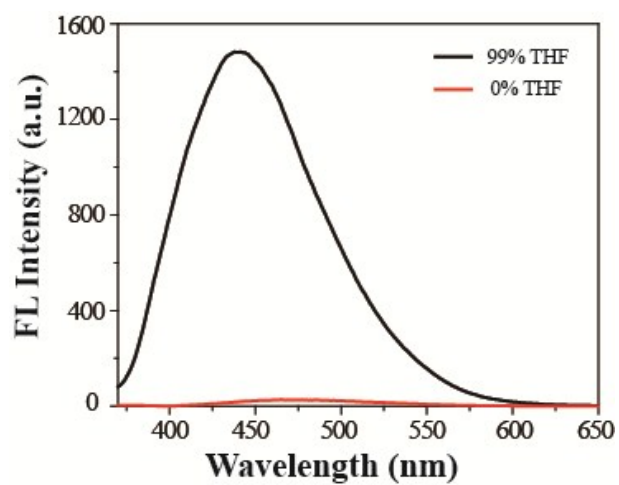


Fig. S3. Fluorescence spectra ($\lambda_{\text{exc}} = 350$ nm) of 20 μM *o*-TPEDTA in water-THF mixtures.

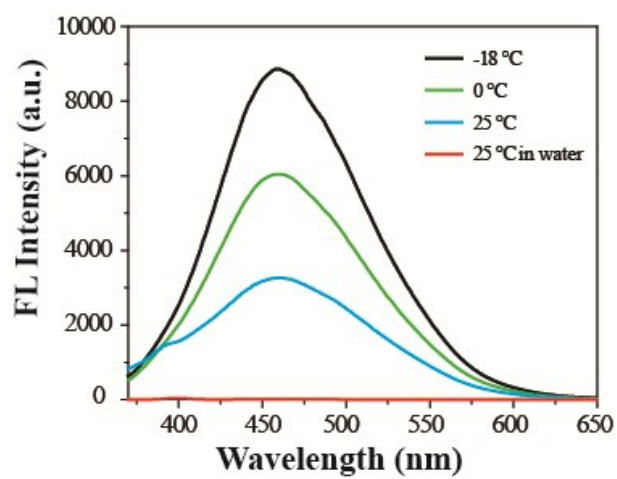


Fig. S4. Fluorescence emission spectra of 20 μM *o*-TPEDTA in glycerol-H₂O mixture (99% glycerol) at different temperatures.

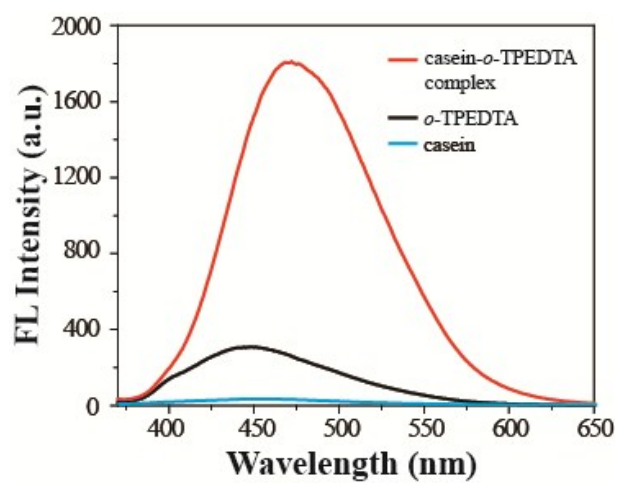


Fig. S5. Fluorescence emission spectra of 100 $\mu\text{g/mL}$ casein, 20 μM *o*-TPEDTA and casein-*o*-TPEDTA complex solution.

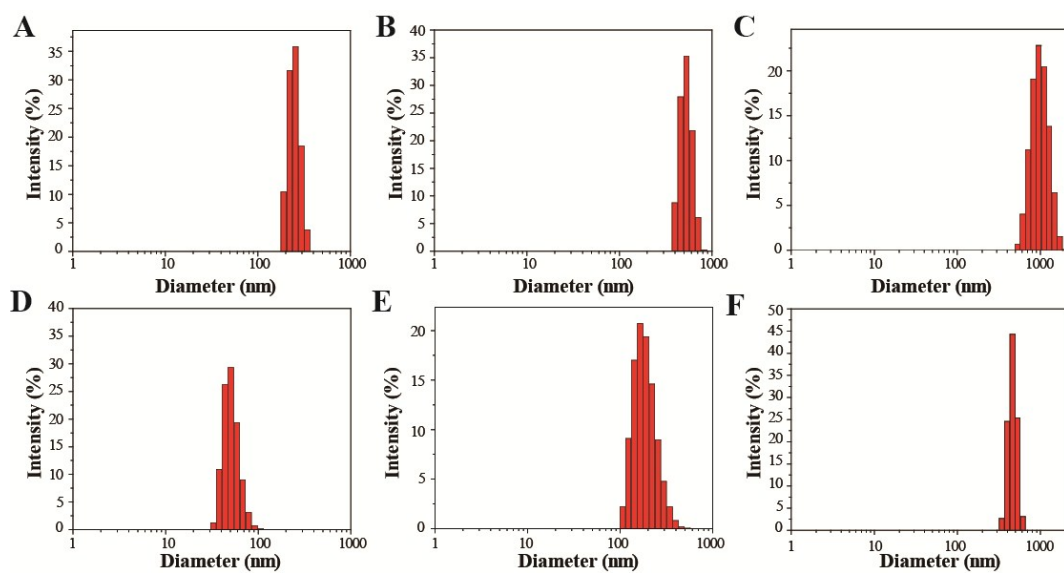


Fig. S6. Hydrodynamic size distribution of (A) 50 μ M, (B) 100 μ M, and (C) 200 μ M *o*-TPEDTA solution and upon adding 100 μ g/mL casein (E, D and F).

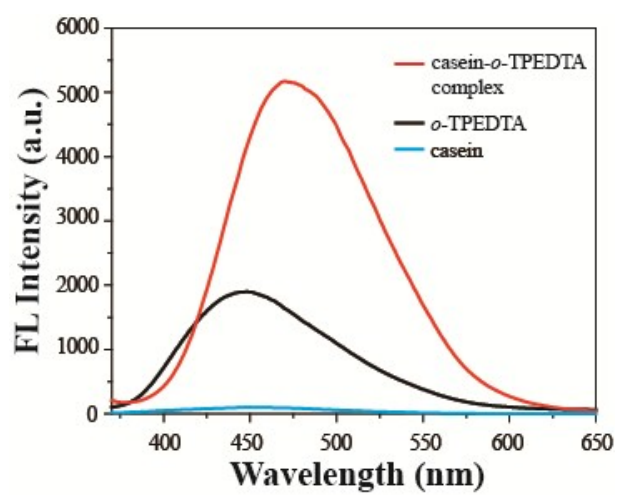


Fig. S7. Fluorescence emission spectra of 100 $\mu\text{g/mL}$ casein, 100 μM *o*-TPEDTA and casein-*o*-TPEDTA complex solution.

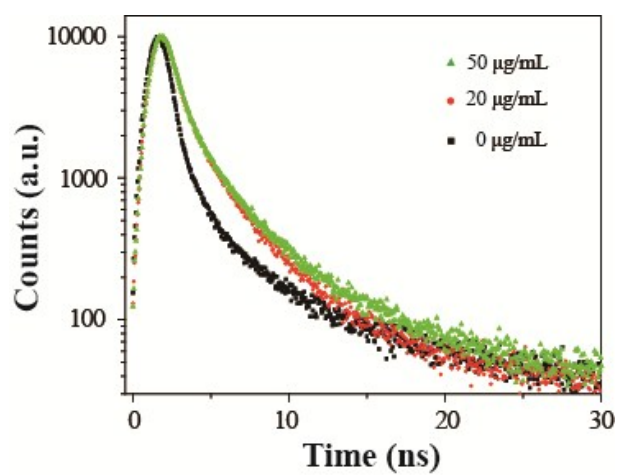


Fig. S8. The fluorescence decay curves of *o*-TPEDTA with different concentration of casein.

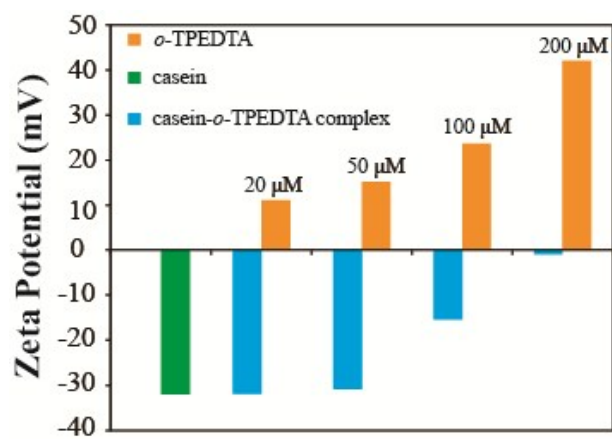


Fig. S9. Zeta potential measurements of 100 μ g/mL casein without (green histogram) and with (blue histogram) the addition of different concentrations of *o*-TPEDTA, and *o*-TPEDTA only (yellow histogram).

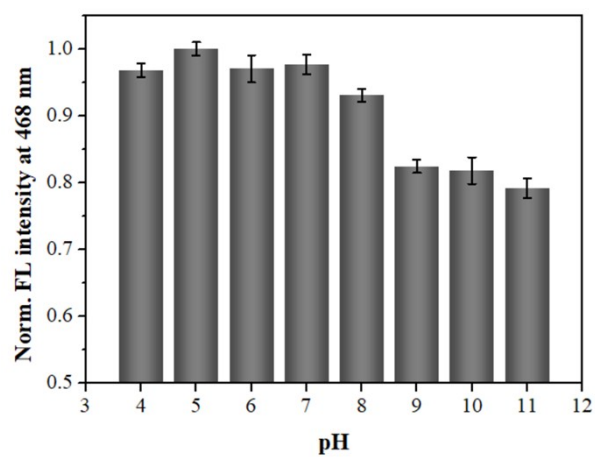


Fig. S10. Normalized fluorescent intensities of 20 μM *o*-TPEDTA solution in the presence of 100 $\mu\text{g/mL}$ casein with different pH values.

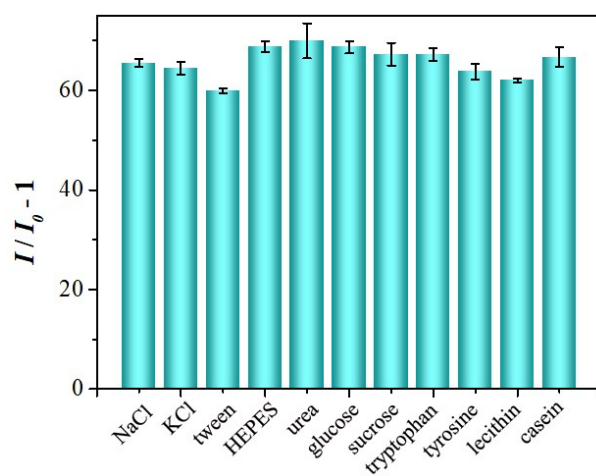


Fig. S11. Fluorescence intensity increment ($I/I_0 - 1$) of o-TPEDTA solution upon adding 60 $\mu\text{g/mL}$ casein in the presence of various interferents.

Table S1. The milk powder samples information.

Remarks	Total protein (label) (g)/100 g	Casein (g)/100 g
Full milk first stage 1	2.30	1.84 ~ 2.07
Full milk third stage 2	15.30	12.24 ~ 13.77
Full milk third stage 3	17.50	14.00 ~ 15.75
Full milk for female 4	23.80	19.04 ~ 21.42

Table S2. The multiexponential decay fitting results of fluorescence lifetimes of *o*-TPEDTA upon adding casein.

Conc. ($\mu\text{g/mL}$)	τ_1 (ns)	$A_1\%$	τ_2 (ns)	$A_2\%$	τ_3 (ns)	$A_3\%$	τ_{ave} (ns)
0	0.23	63.64	1.22	22.63	6.15	13.73	1.26
20	0.43	41.83	1.57	39.23	4.90	18.93	1.72
50	0.45	42.51	1.68	37.09	5.70	20.40	1.98

Table S3. Comparison of this work with some established spectroscopic casein detection methods.

No.	Probe	Strategy	LOD ($\mu\text{g/mL}$)	Linear range ($\mu\text{g/mL}$)	Ref
1	BSPOTPE	Fluorescence	10	20–1250	33
2	fluorescent microspheres	Fluorescence	0.1	0.1–10	44
3	2,2',4,4'-tetrahydroxybenzophenone azine	Fluorescence	5.7	0–300	45
4	immunomagnetic beads	Colorimetry	0.4	2–128	46
5	polyclonal antibodies raised against a casein fining agent	Colorimetry	0.2	0.49–60	47
6	anti-bovine β -casein monoclonal antibody	Colorimetry	10	10–8000	48
7	phosphomolybdic acid	SERS	1.5	2.5–25	49
8	nanoMIPs	SPR	0.13	0–150	50
9	gold nanoparticles	Colorimetry	0.03	0.08–250	51
10	<i>o</i> -TPEDTA	Fluorescence	0.05	0.1–10	This study