Supplementary Information for

A rationally designed MALDI-TOF MS probe for rapid quantitative analysis of carboxylesterase activity

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^{1}H NMR (500 MHz, Methanol-*d*4) δ 8.35 – 8.28 (m, 2H), 7.86 (ddd, *J* = 7.9, 2.7, 1.3 Hz, 2H), 7.80 (dd, *J* = 1.8, 0.8 Hz, 1H), 7.69 (ddd, *J* = 8.4, 6.9, 1.4 Hz, 1H), 7.48 (ddd, *J* = 8.1, 6.9, 1.1 Hz, 1H), 7.38 (dd, *J* = 3.5, 0.8 Hz, 1H), 6.68 (dd, *J* = 3.5, 1.8 Hz, 1H).

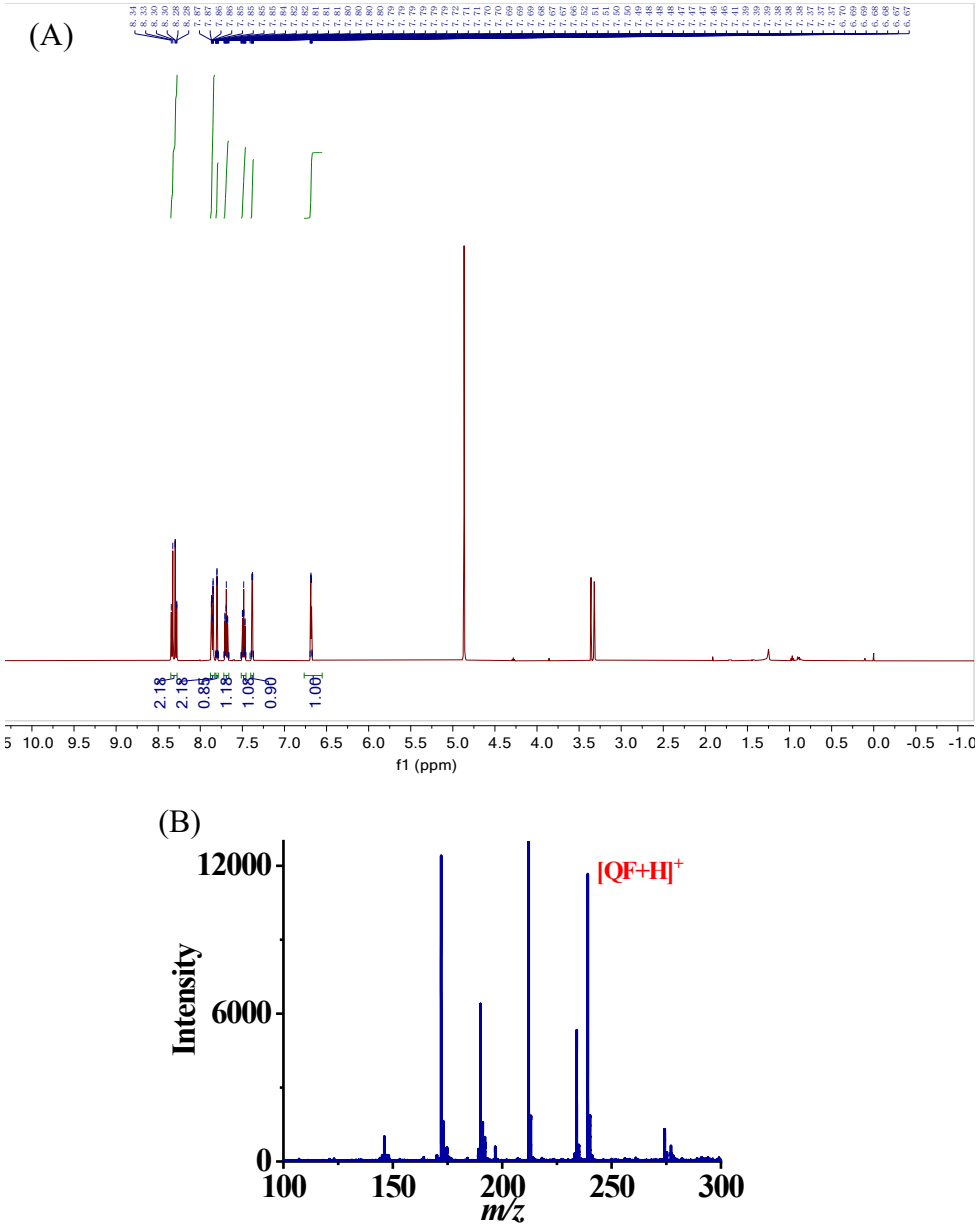

Figure S1. A) 1H NMR spectrum of compound QF and B) MALDI-TOF MS spectrum of QF.

^{1}H NMR (500 MHz, Methanol-*d*4) δ 8.13 (s, 1H), 7.92 (dq, *J* = 8.5, 0.9 Hz, 1H), 7.87 (dd, *J* = 8.2, 1.4 Hz, 1H), 7.73 (ddd, *J* = 8.5, 6.9, 1.4 Hz, 1H), 7.59 (ddd, *J* = 8.2, 6.9, 1.2 Hz, 1H), 3.20 (s, 3H), 3.04 (s, 3H).

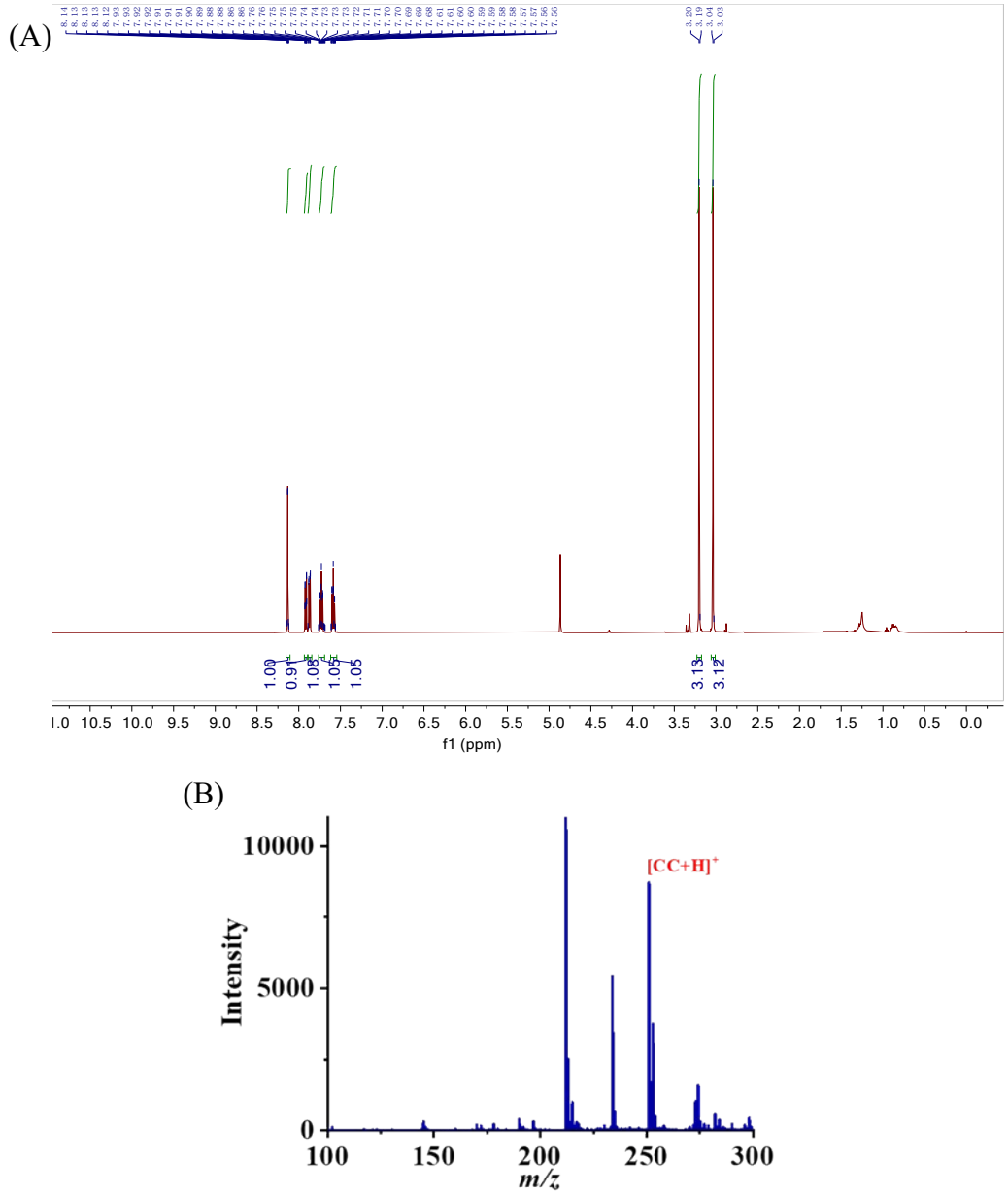

Figure S2. A) ^{1}H NMR spectrum of compound CC and B) MALDI-TOF MS spectrum of CC.

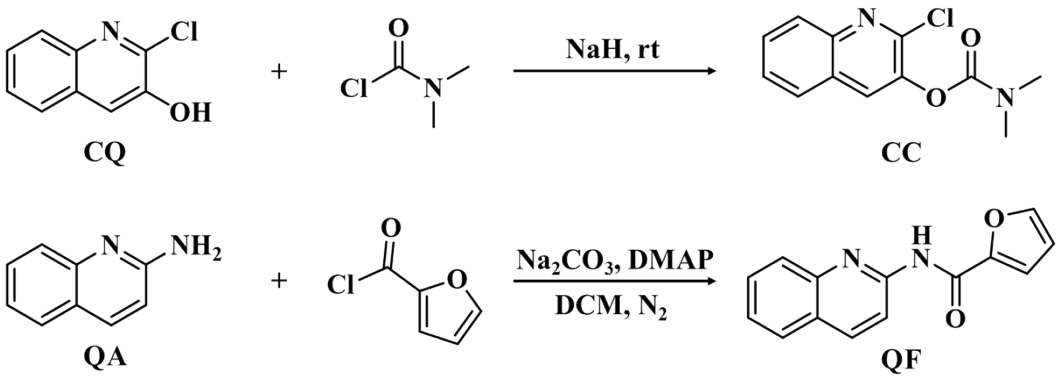

Figure S3. The detailed chemical formula of CC and QF.

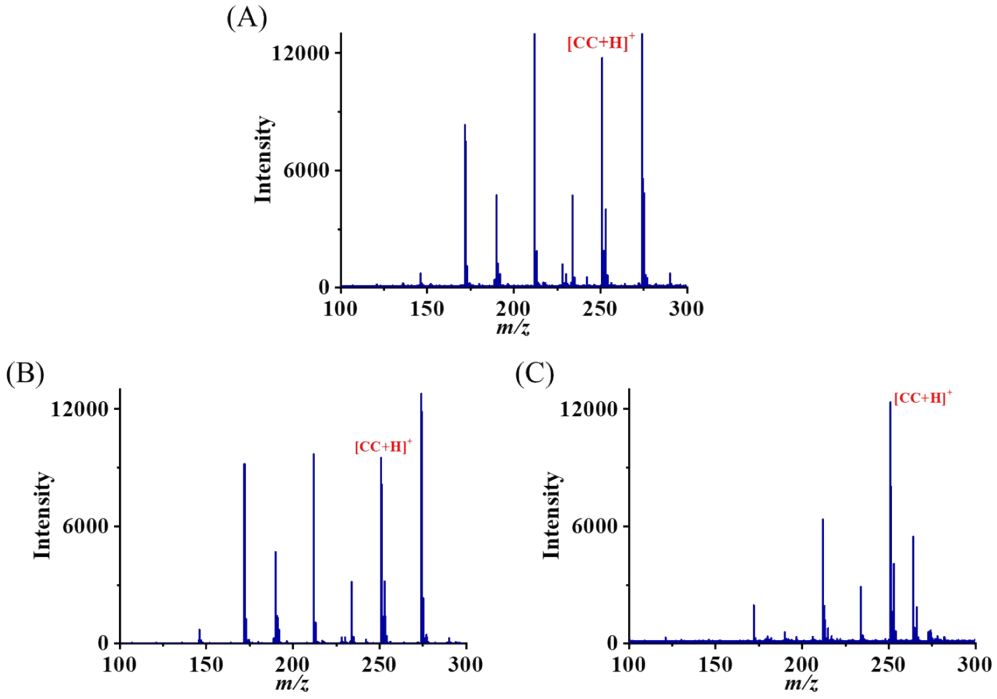

Figure S4. MALDI-TOF MS spectra of A) CC, B) BChE hydrolysis with CC, C) AChE hydrolysis with CC.

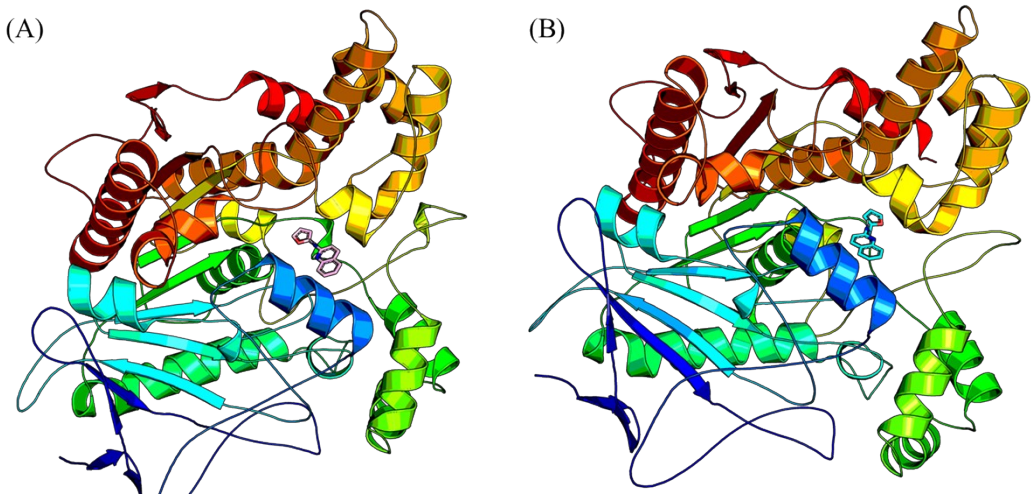

Figure S5. The molecular docking between CES A) from human or B) from porcine and QF.

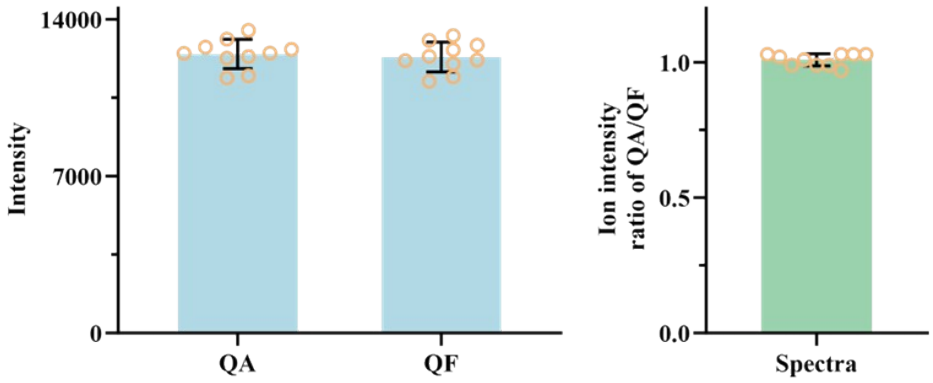

Figure S6. The reproducibility of MALDI-TOF MS detection for QF and QA.

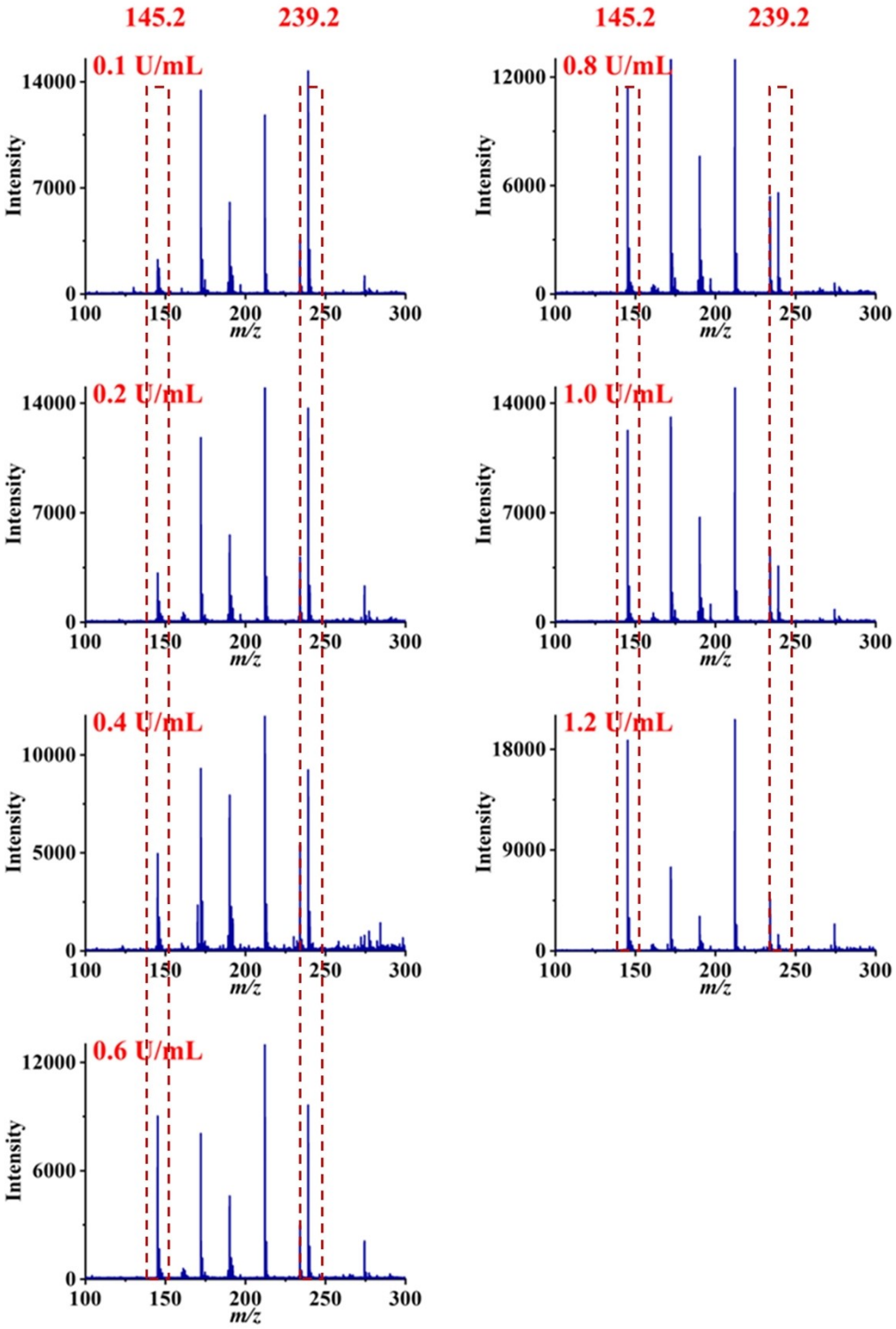

Figure S7. MALDI-TOF MS spectra of different concentrations of CES.

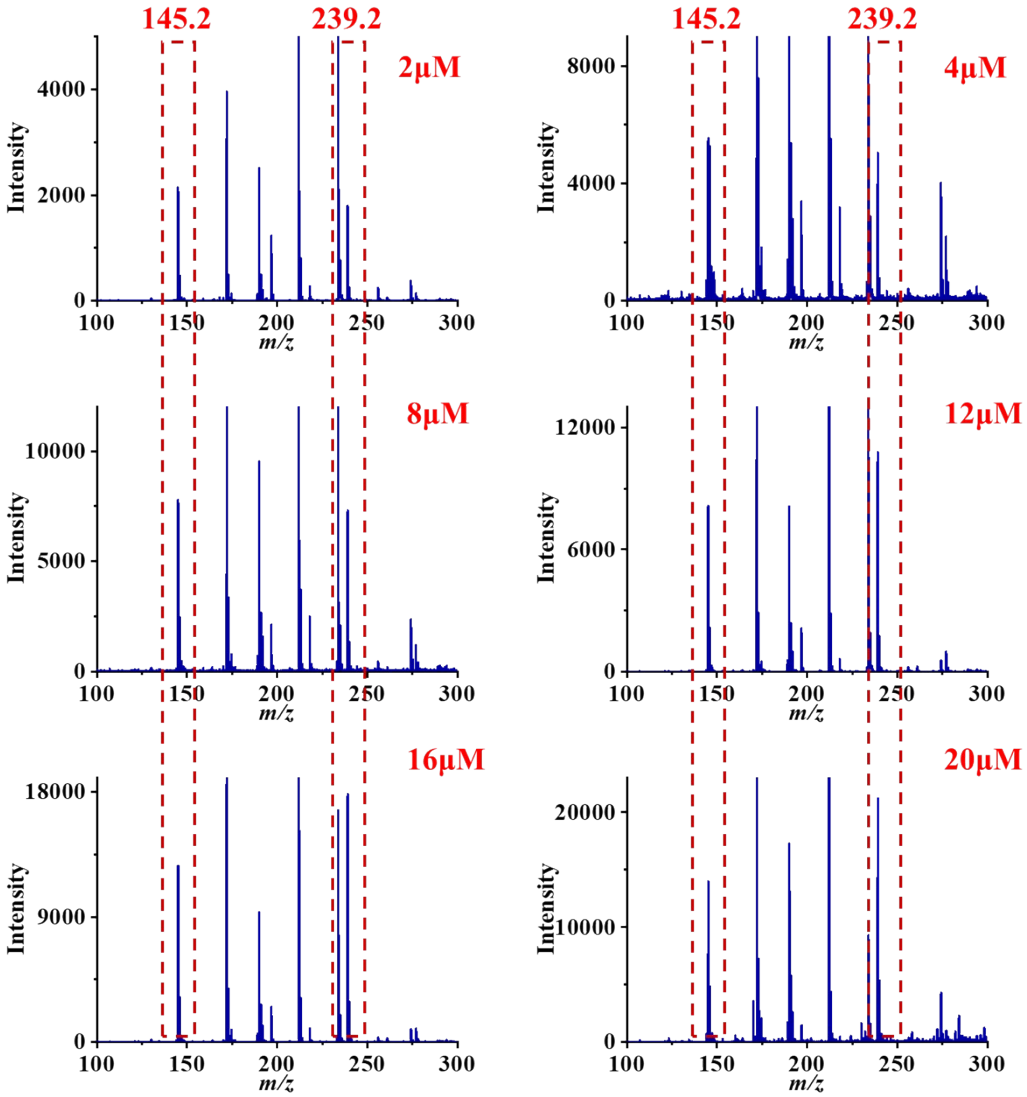

Figure S8. MALDI-TOF MS spectra of different concentrations of QF (0.6 U/mL CES).

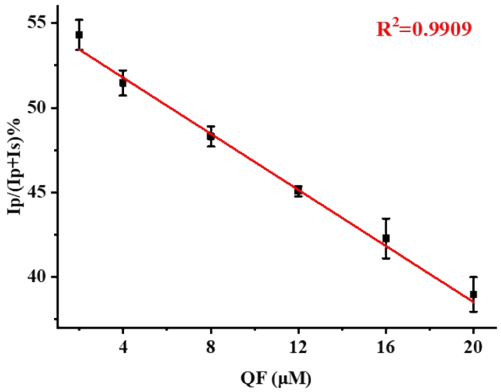

Figure S9. The calibration curve between the concentrations of QF and Ip/(Is + Ip).

The recovery test:

The different concentrations CES (0.5, 0.8 and 1.2 U/mL) were added in 20-fold diluted fetal bovine serum samples. Then the QF was added in these samples, respectively. After reaction, the observer concentration could be calculated by calibration curve. The recovery is calculated by Observed Conc./Spiked Conc..

Table S1. Results of CE determination in serum sample (n=3).

Spiked Conc. (U/mL)	Observed Conc. (U/mL)	Recovery (%)	Precision (RSD, %)
0.50	0.47	94	0.65
0.80	0.84	105	1.92
1.20	1.12	93	0.38