

## Supporting Information

### Highly Sensitive Detection of Hg<sup>2+</sup> in Aqueous Solution with Cationic Polythiophene Derivatives

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#### 3-[1-(2-dimethyl butyryl)piperidine-4-methylene]thiophene (2)

Compound **1** (0.28 g, 1.56 mmol) and N,N-dimethylaminobutyryl chloride hydrochloride (0.29 g, 1.56 mmol) were mixed in 10 mL methylene chloride, and the mixture was stirred at room temperature under the nitrogen atmosphere. Then a mixture of triethylamine (0.46 g, 4.50 mmol) in dichloromethane (10 mL) was added dropwise over 30 min at room temperature, then the reaction liquid was kept stirring for 1 h. The relatively pure product (0.36 g, 78.8%) was obtained from the organic mixture after separation. Ms (ESI):  $m/z = 293.1[M^+]$ . FTIR (KBr,  $\text{cm}^{-1}$ ): 1645 (C=O), 1438 (CH=C), 1209 (C-N). <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz, ppm):  $\delta = 7.24\text{-}7.26$  (d, 1H,  $J = 8$  Hz), 7.02 (s, 1H), 6.96-6.98 (d, 1H,  $J = 8$  Hz), 6.25 (s, 1H), 3.39-3.46 (m, 4H), 2.21 (s, 6H), 2.29-2.39 (m, 4H), 1.77-1.84(m, 2H)

#### 3-[1-(2-trimethylammonium butyryl)piperidine-4-methylene]thiophene bromide (3)

Compound **2** (0.20 g, 0.68 mmol) was dissolved in 10 mL acetonitrile, and then 3 mL 33% bromomethane was added. The reaction was kept at room temperature for 20 h. The final compound **3** was resulted as white solid (0.22 g, 83.0%) after the removal of solvent. Ms (ESI):  $m/z =$

307.2[M<sup>+</sup>-Br]. FTIR (KBr, cm<sup>-1</sup>): 1632 (C=O), 1470 (CH=C), 1165 (C-N). <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz, ppm): δ = 7.38-7.41 (d, 1H, *J* = 12 Hz), 7.19 (s, 1H), 7.17-7.18 (d, 1H, *J* = 4 Hz), 6.39 (s, 1H), 6.39 (s, 1H), 3.47-3.75 (m, 4H), 3.29-3.31 (s, 9H), 2.38-2.58 (m, 4H).

**poly{3-[1-(2-trimethylammonium butyryl)piperidine-4-methylene]thiophene-2,5-diyl chloride}**  
**(PTBPT-Cl)**

Compound **3** (0.12 g, 0.31 mmol) and sodium lauryl sulfate (SLS) (89.2 mg, 0.31 mmol) were added to 20 mL dry acetone, then the mixture was smashed in an ultrasonic vessel for 30 min. The acetone was removed by rotary evaporation, and then the white solid was obtained as compound **3**/SLS complex. This complex was dissolved in dry chloroform (20 mL) to give a translucent liquid. Anhydrous ferric chloride (0.25 g, 1.54 mmol) was suspended in 20 mL dry chloroform and stirred for 30 min under nitrogen, and then the above resulting translucent liquid was added dropwise. The mixture was stirred at room temperature for 24 hours. Treatment of the reaction mixture with methanol (10 mL) resulted in a red precipitate. The precipitate, 30 mL methanol and 1 mL hydrazine were mixed and stirred for 2 h, and then the solution was filtered and evaporated to dryness. The crude polymer was obtained after being washed six times with a solution of tetrabutylammonium chloride in methanol. Then the crude solid material was purified in a Soxhlet extractor with methanol/acetone (1:7). Finally, claret-colored solid material **PTBPT-Cl** (85.1 mg, 71.4%) was obtained after evaporation of the Soxhlet extract. FTIR (KBr, cm<sup>-1</sup>): 1628 (C=O), 1427 (CH=C), 1165 (C-N). <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz, ppm): δ = 4.51-5.12 (m, 8H), 3.47-3.75(m, 4H), 3.29-3.31(s, 9H), 2.38-2.58 (m, 4H). GPC: *M<sub>n</sub>* = 8328 g/mol, PDI = 1.42.

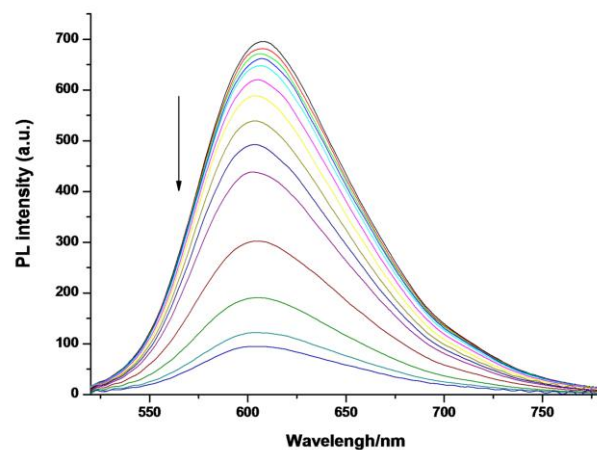


Fig. S1 Fluorescence intensity changes of **PDPMT-Cl** ( $5 \times 10^{-5}$  M,  $\lambda_{\text{ex}} = 450$  nm) in aqueous solution upon addition of  $0 \sim 2 \times 10^{-5}$  M  $\text{Hg}^{2+}$  at pH 3.

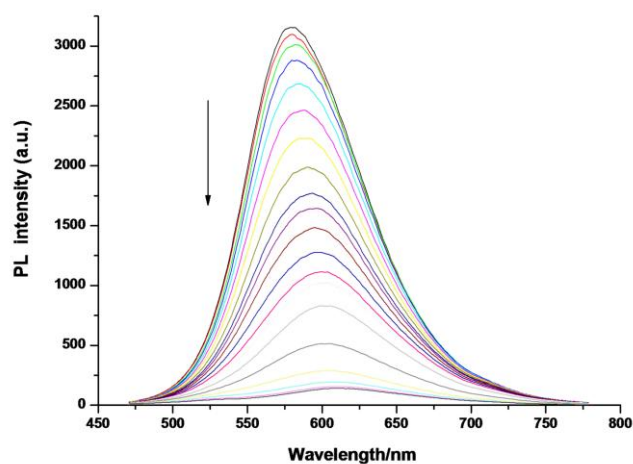


Fig. S2 Fluorescence intensity changes of **PTCA-Cl** ( $5 \times 10^{-5}$  M,  $\lambda_{\text{ex}} = 450$  nm) in aqueous solution upon addition of  $0 \sim 5 \times 10^{-5}$  M  $\text{Hg}^{2+}$  at pH 3.

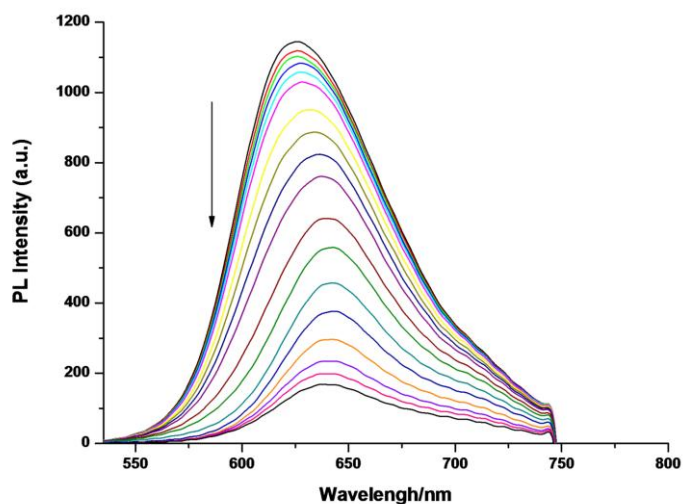


Fig. S3 Changes in fluorescence emission spectra of **PTAPT-Cl** ( $5 \times 10^{-5} \text{ mol L}^{-1}$ ,  $\lambda_{\text{ex}} = 512 \text{ nm}$ ) upon addition of  $\text{Hg}^{2+}$  (0.0005, 0.0009, 0.0025, 0.004, 0.008, 0.01, 0.03, 0.05, 0.1, 0.15, 0.25, 0.5, 3, 10, 15, 25,  $40 \times 10^{-5} \text{ M}$ ).

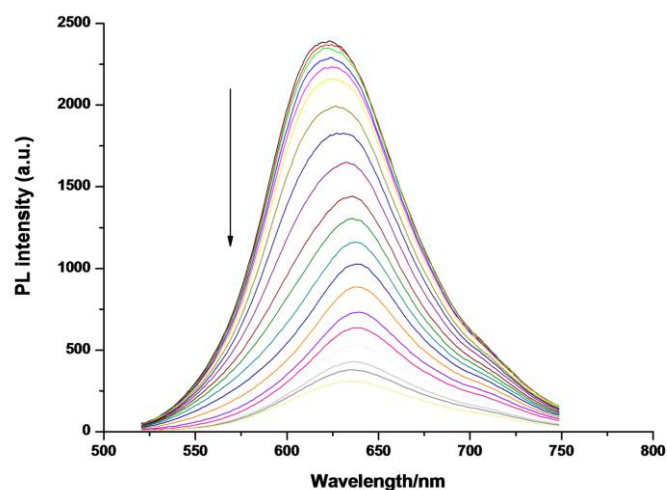
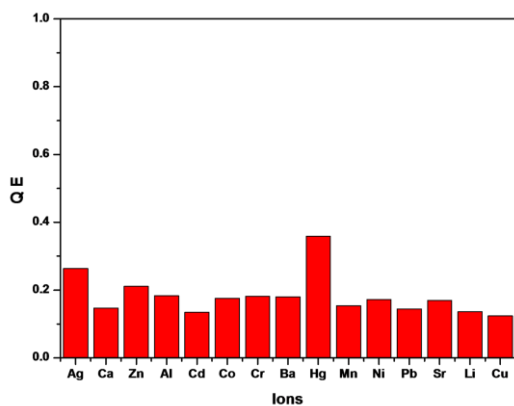
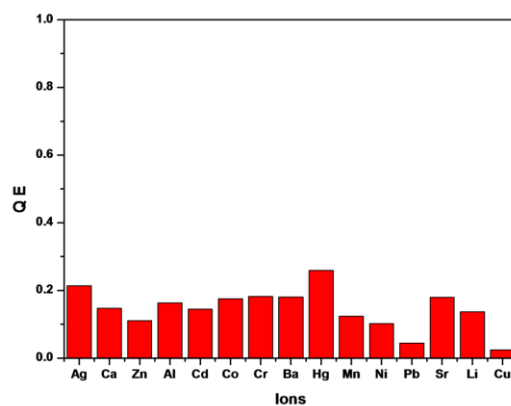


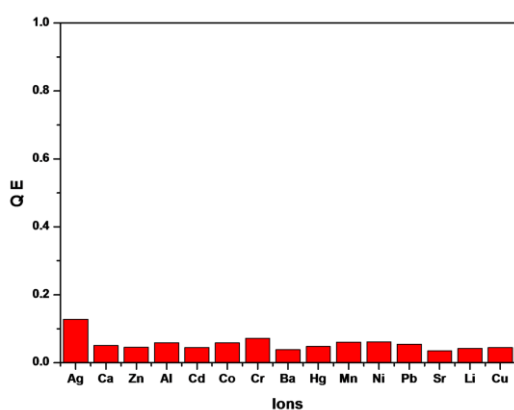
Fig. S4 Fluorescence spectra of **PTBPT-Cl** ( $5 \times 10^{-5} \text{ mol L}^{-1}$ ,  $\lambda_{\text{ex}} = 504 \text{ nm}$ ) with increasing amounts of  $\text{Hg}^{2+}$  (0.0001, 0.0005, 0.001, 0.005, 0.01, 0.03, 0.07, 0.15, 0.25, 0.5, 1, 2, 5, 10, 20, 35, 50, 70,  $100 \times 10^{-5} \text{ M}$ ) in aqueous solution.



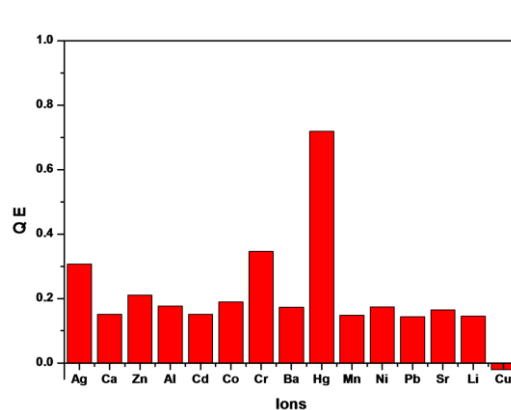
**PDPMT-CI**



**PTCA-CI**

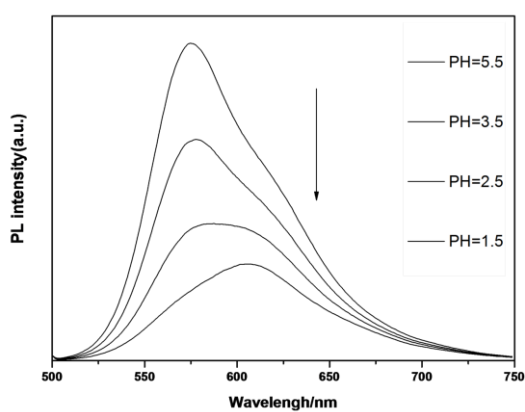


**PTAPT-CI**

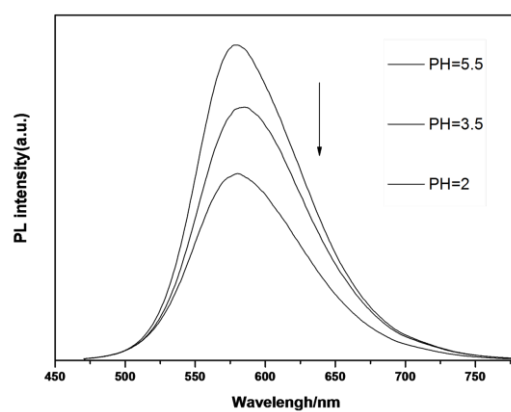


**PTBPT-CI**

Fig. S5 The relative fluorescence quenching efficiency of the polymers as a function of various added metal ions ( $5 \times 10^{-5}$  M).



**PDPMT-CI**



**PTCA-CI**

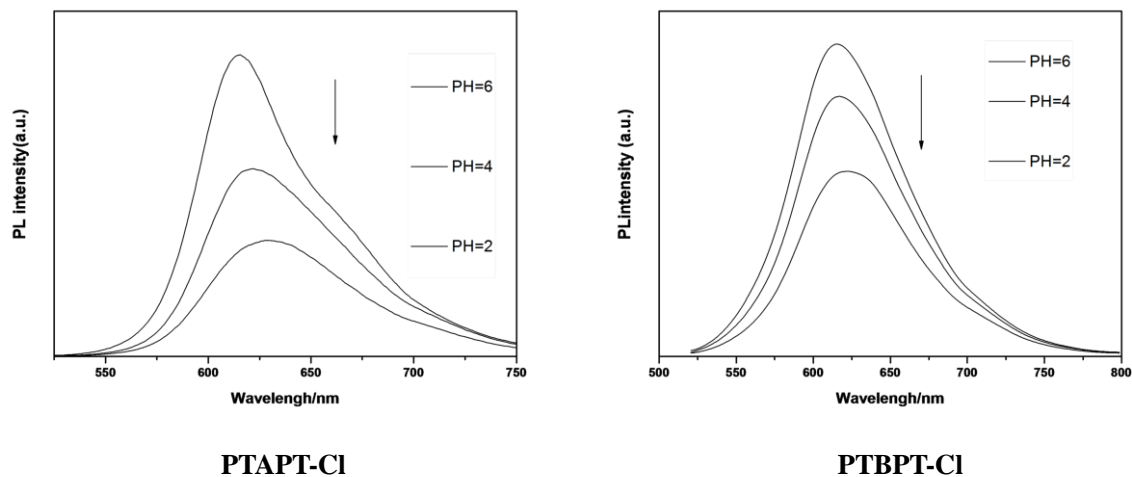


Fig. S6 Fluorescence emission spectra changes of  $5 \times 10^{-5}$  M polymer solution at 25 °C in the pH range of 2~6.

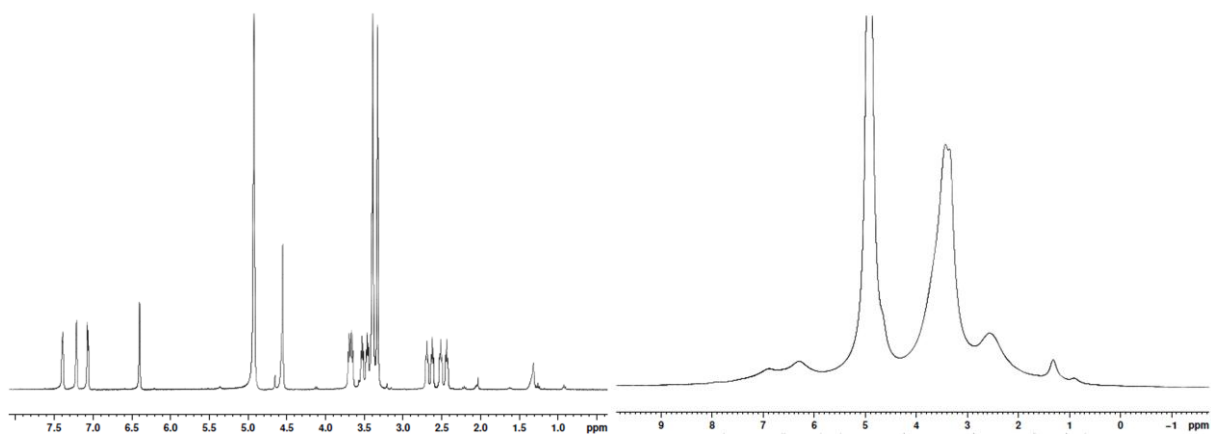


Fig. S7 The <sup>1</sup>H NMR spectrum of polymer **PTAPT-Cl**(right) and its monomer (left).

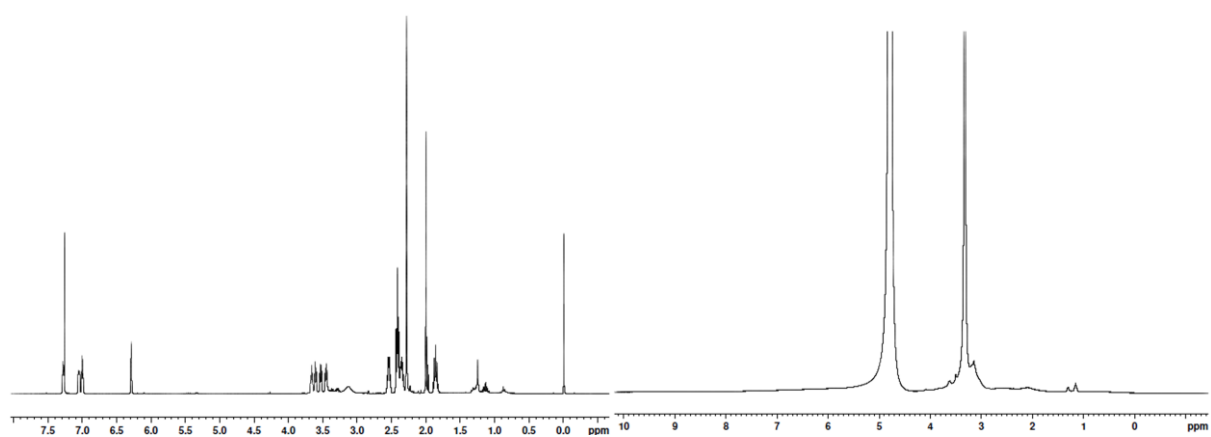


Fig. S8 The <sup>1</sup>H NMR spectrum of polymer **PTBPT-Cl**(right) and its monomer (left).

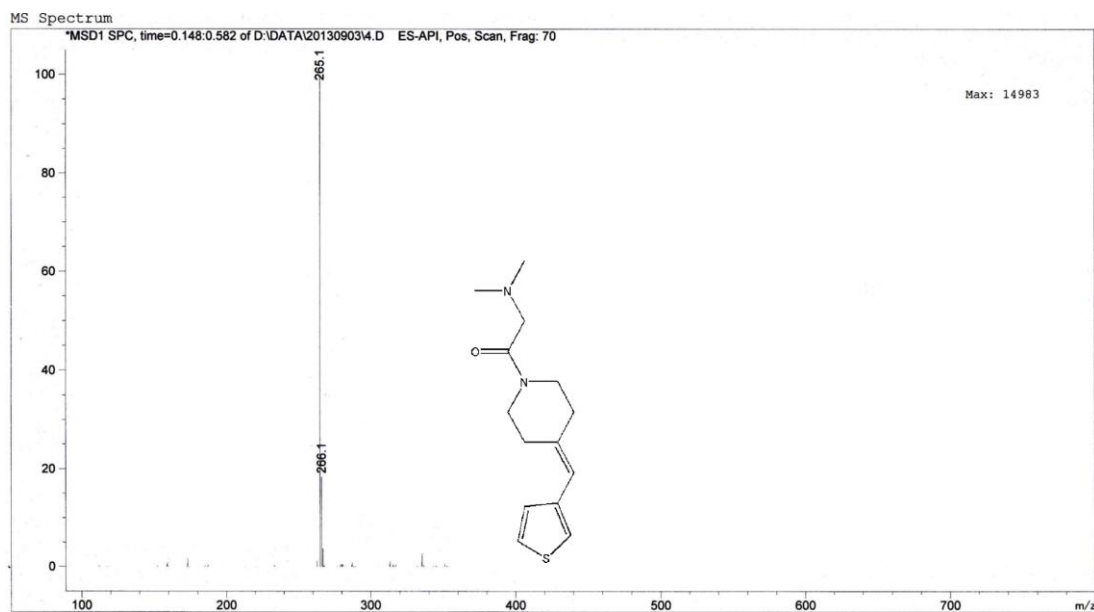


Fig. S9 The mass spectrum of 3-[1-(2-dimethylglycyl) piperidine-4-methylene]thiophene (2).

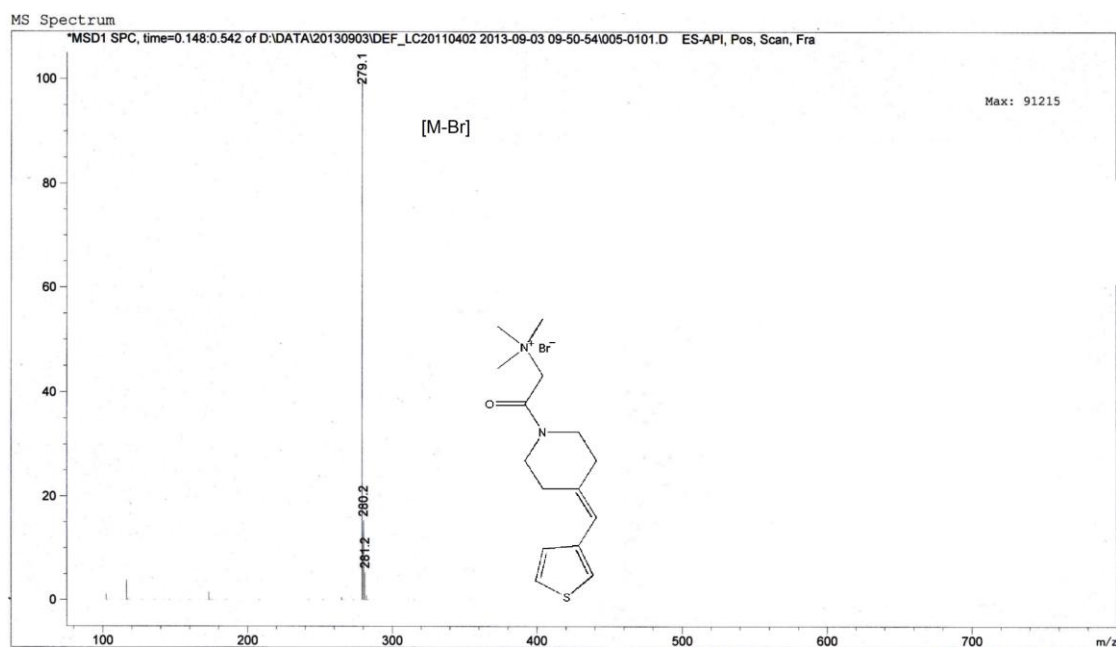


Fig. S10 The mass spectrum of 3-[1-(2-trimethylammoniumacetyl) piperidine-4-methylene]thiophene bromide (3).

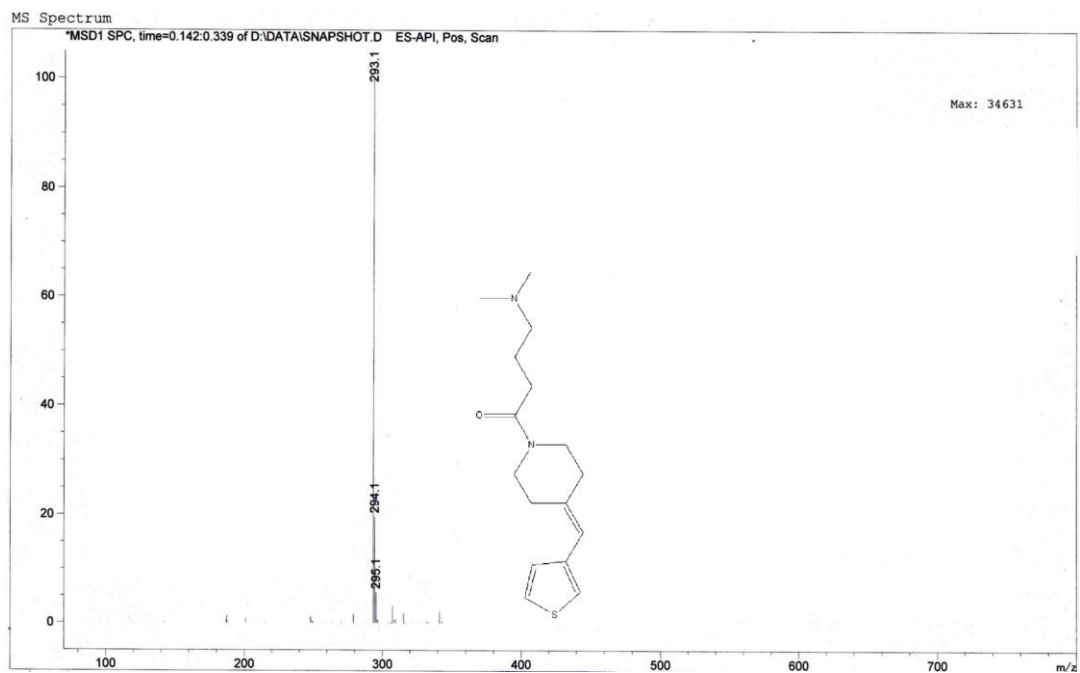


Fig. S11 The mass spectrum of 3-[1-(2-dimethyl butyryl)piperidine-4-methylene]thiophene (2).

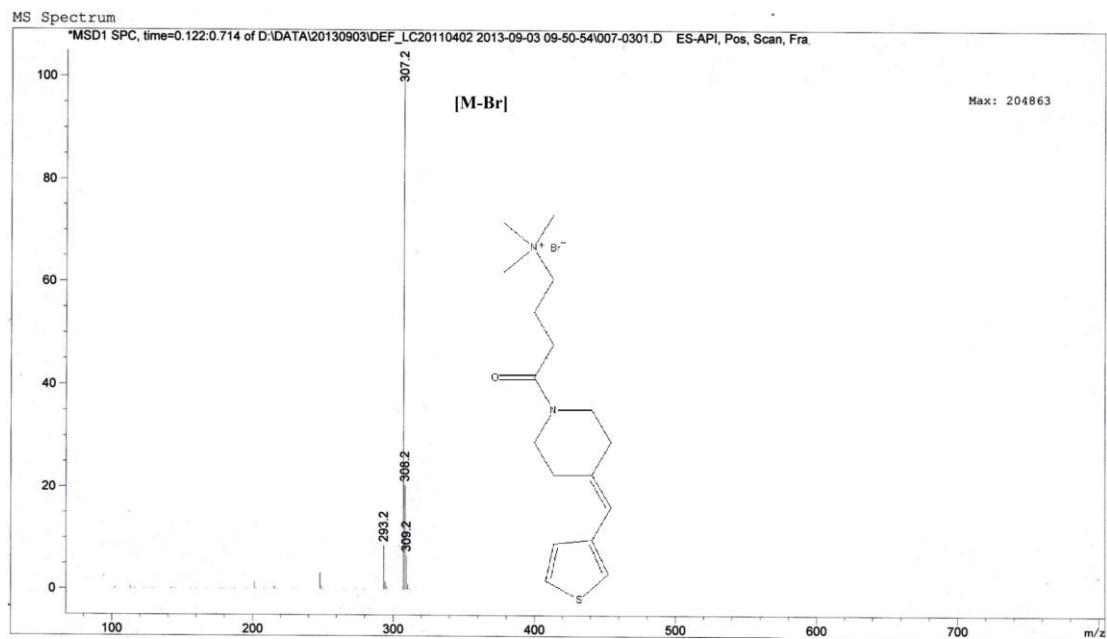


Fig. S12 The mass spectrum of 3-[1-(2-trimethylammonium butyryl)piperidine-4-methylene]thiophene bromide (3).