## Supporting Information

# Design of a Quinoxalinone-based AIE probe for detection of ROS in *in vitro* and *in vivo* sepsis model

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**Preparation of 3**

To a solution of **1** (8.11 g, 33.9 mmol) in acetone (100 mL) was added $K_2CO_3$ (9.36 g, 67.8 mmol) and 3-bromoprop-1-ene (8.20 g, 67.8 mmol). The resulting solution was stirred at 50°C for 7 h. Then acetone was removed via rotary evaporator and the residue was suspended in water (100 mL) and ethyl acetate (EA) (300 mL). The organic layer was separated and dried over anhydrous $Na_2SO_4$, filtered, and then evaporated under reduced pressure. The residue was further purified by chromatography on a silica gel column using hexane/ethyl acetate (9:1, v/v) as the eluent to afford **3** (4.54 g, 48%) as a white solid. $^1$H NMR (400 MHz, $CDCl_3$): δ ppm 7.64 (d, $J$ = 8.0 Hz, 1H), 7.42 – 7.38 (m, 2H), 5.95 – 5.86 (m, 1H), 5.30 – 5.27 (m, 1H), 5.17 – 5.13 (m, 1H), 4.85 – 4.82 (m, 2H), 2.56 (s, 3H). $^{13}$C NMR (101.6 MHz, $CDCl_3$): δ ppm 158.85, 154.43, 133.50, 131.68, 130.79, 130.14, 126.87, 123.47, 118.43, 117.17, 44.57, 21.59. HRMS (ESI): m/z calculated for $C_{12}H_{12}BrN_2O$ $[M+H]^+$, 279.0127; found, 279.0118.

**Preparation of 5**

A mixture of **3** (1.30 g, 4.66 mmol) and **4** (1.92 g, 5.60 mmol) was dissolved in acetic acid (30 mL). Then a catalytic amount of concentrated sulfuric acid was added into the reaction mixture. The resulting solution was stirred at 50°C for 16 h. Then acetic acid was removed via rotary evaporator and the residue was supplemented with water (60 mL) and ethyl acetate (EA) (150 mL). The organic layer was separated and dried over anhydrous $Na_2SO_4$, filtered, and then evaporated under reduced pressure. The residue was further purified by chromatography on a silica gel column using hexane/ethyl acetate (30:1, v/v) as the eluent to afford **5** (2.09 g, 73%) as a red solid. $^1$H NMR (400 MHz, $CDCl_3$): δ ppm 8.27 (d, $J$ = 16.0 Hz, 1H), 7.69 (d, $J$ = 8.4 Hz, 1H), 7.48 – 7.37 (m, 5H), 7.30 – 7.23 (m, 5H), 7.17 – 7.11 (m, 5H), 7.07 – 7.03 (m, 4H), 5.97 – 5.89 (m, 1H), 5.28 (d, $J$ = 12.4 Hz, 1H), 5.18 (d, $J$ = 16.8 Hz, 1H), 4.88 (d, $J$ = 4.8 Hz, 2H). $^{13}$C NMR (101.6 MHz, $CDCl_3$): δ ppm 154.28, 152.33, 147.99, 147.30, 146.83, 140.70, 132.92, 132.60, 132.07, 131.72, 130.82, 130.18, 129.42, 127.57, 127.20, 126.70, 124.84, 123.45, 123.27, 123.14, 120.53, 118.40, 117.14, 44.71. HRMS (ESI): m/z calculated for $C_{35}H_{27}BrN_3OS$ $[M+H]^+$, 616.1052; found, 616.1023.

**Preparation of QuinoNS**

To a solution of **5** (616 mg, 1.0 mmol) and **6** (482 mg, 1.20 mmol) in 1, 4-dioxane/$H_2O$ (5:1 v/v, 18 mL) was added $K_2CO_3$ (276 mg, 2.0 mmol) followed by $Pd(PPh_3)_4$ (116 mg, 0.10 mmol). The resulting mixture was degassed with argon three times, and then was stirred at 70°C for 4 h. The mixture was cooled to room temperature and then diluted with ethyl acetate (EA) (100 mL), which was washed with distilled water (40 mL). The organic layer was dried over anhydrous $Na_2SO_4$, filtered, and then evaporated under reduced pressure. The residue was purified by chromatography on a silica gel column

with hexane/ethyl acetate (4:1, v/v) as the eluent to afford **QuinoNS** (121 mg, 15%) as a red solid. $^{1}$H NMR (400 MHz, DMSO-$d_6$): δ ppm 8.23 (d, $J$ = 16.0 Hz, 1H), 8.07 (d, $J$ = 8.4 Hz, 2H), 7.92 (d, $J$ = 8.4 Hz, 1H), 7.80 – 7.76 (m, 2H), 7.66 (d, $J$ = 8.4 Hz, 2H), 7.54 – 7.46 (m, 4H), 7.39 – 7.33 (m, 5H), 7.16 – 7.07 (m, 8H), 7.04 -6.97 (m, 4H), 6.95 – 6.90 (m, 2H), 6.41 – 6.38 (m, 2H), 6.08 – 5.99 (m, 1H), 5.23 – 5.09 (m, 4H). $^{13}$C NMR (101.6 MHz, DMSO-$d_6$): δ ppm 153.42, 150.53, 146.88, 146.07, 144.73, 142.70, 140.30, 139.69, 139.35, 137.69, 132.15, 132.08, 131.74, 131.21, 129.78, 129.11, 129.01, 126.81, 126.33, 126.19, 126.17, 124.05, 123.98, 123.48, 123.13, 122.59, 122.01, 121.90, 120.14, 119.84, 116.60, 116.37, 112.32, 43.23. HRMS (ESI): m/z calculated for $C_{53}H_{39}N_4OS_2$ $[M+H]^+$: 811.2559; found, 811.2515.

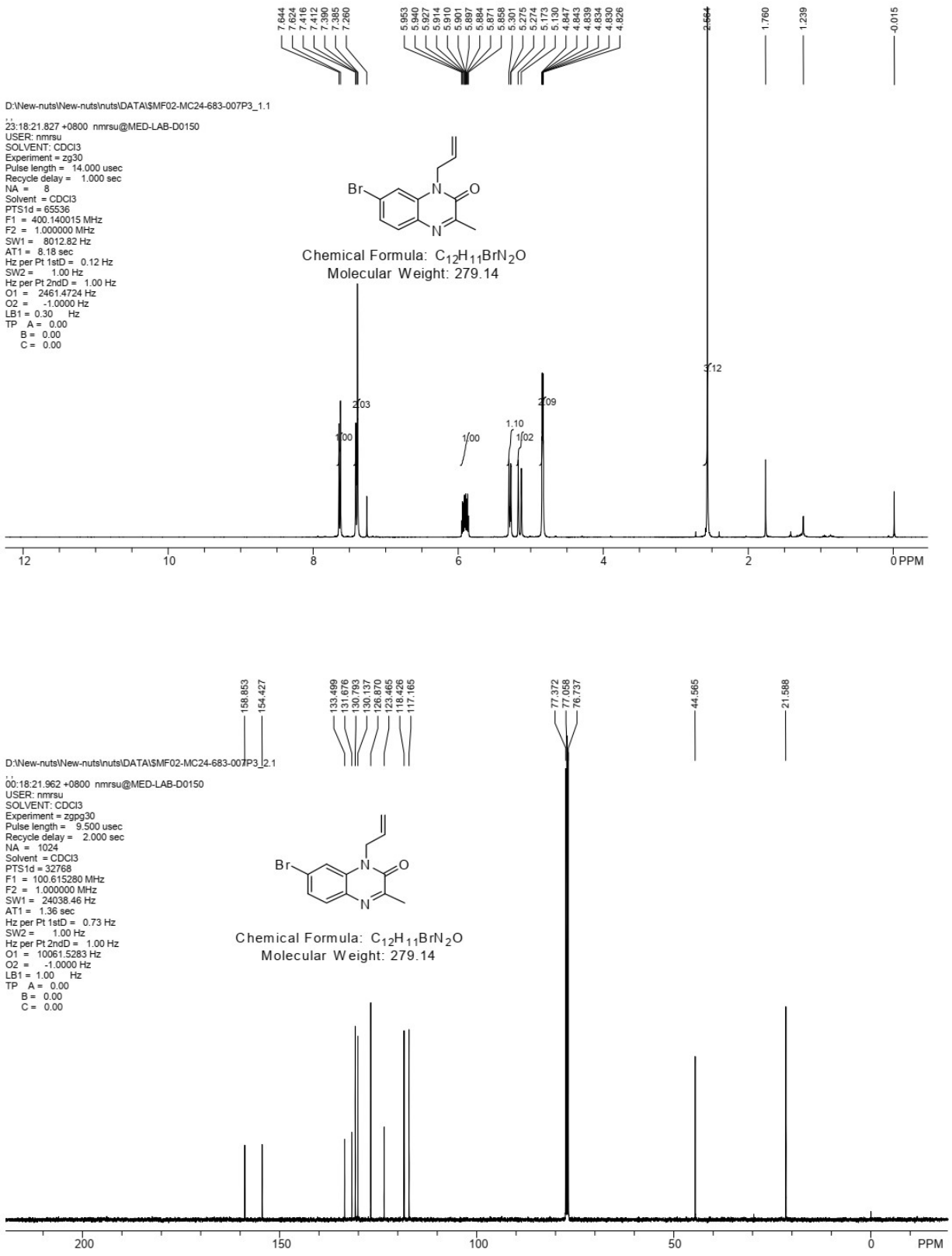



Fig.S1. $^{1}H$ (top) and $^{13}C\{^{1}H\}$ (bottom) NMR spectra of **3** in $CDCl_3$.

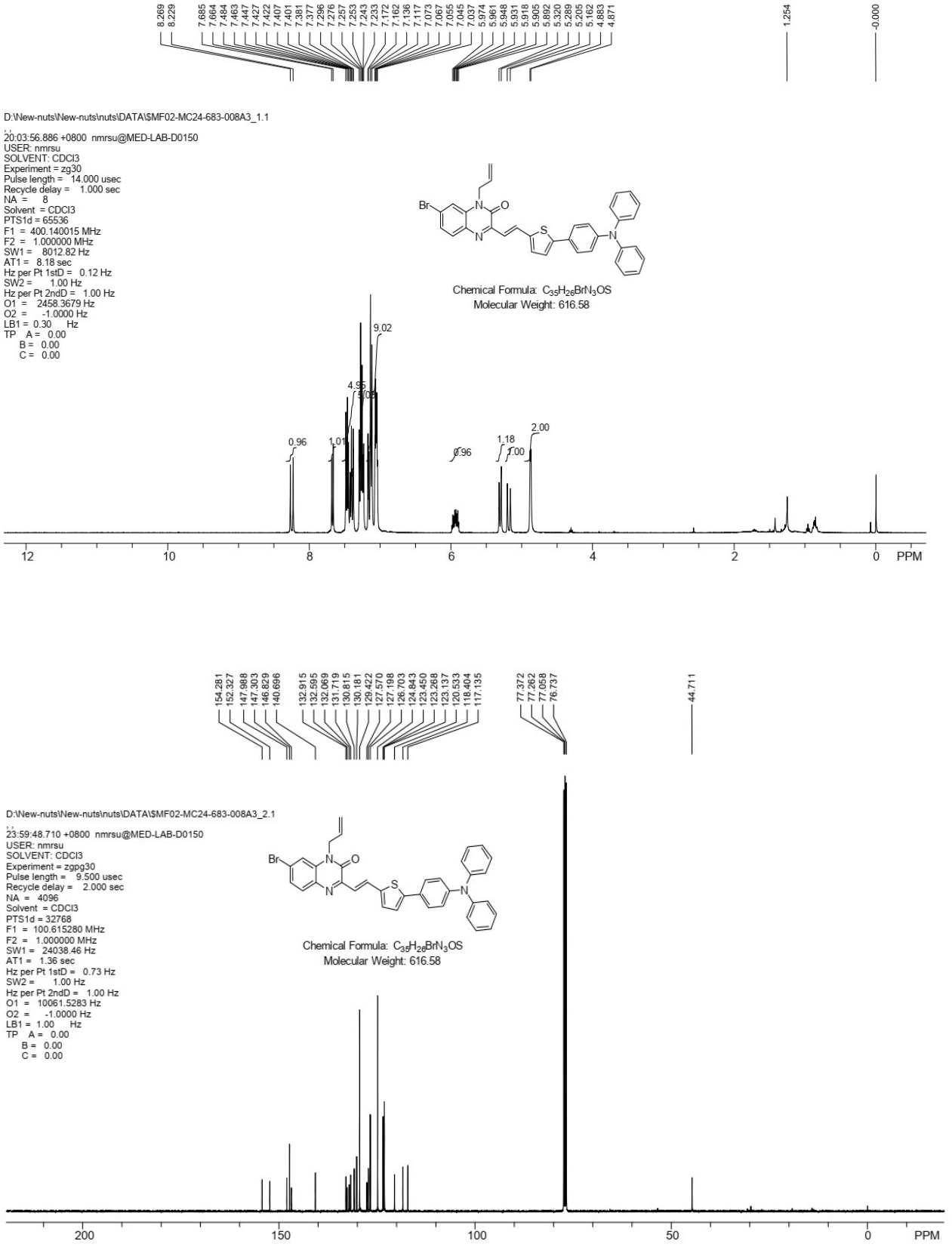
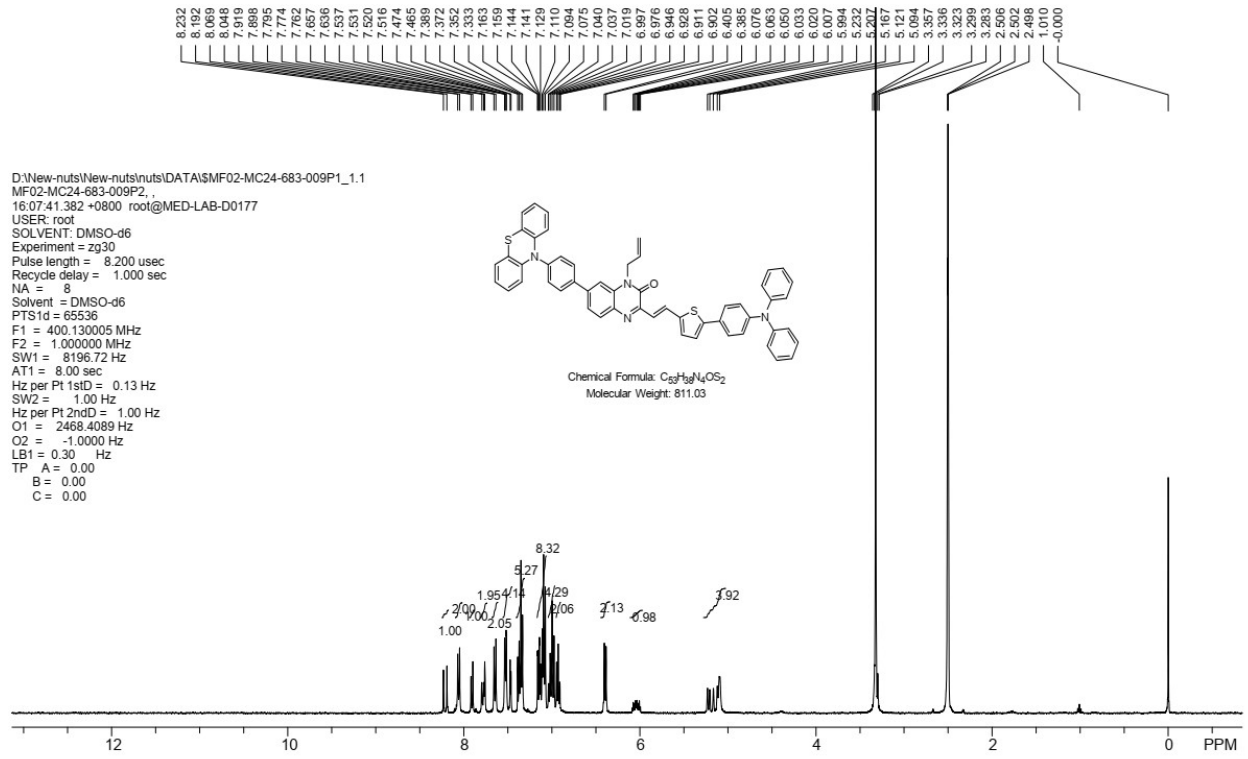



Fig.S2. $^{1}H$ (top) and $^{13}C\{^{1}H\}$ (bottom) NMR spectra of **5** in $CDCl_3$.



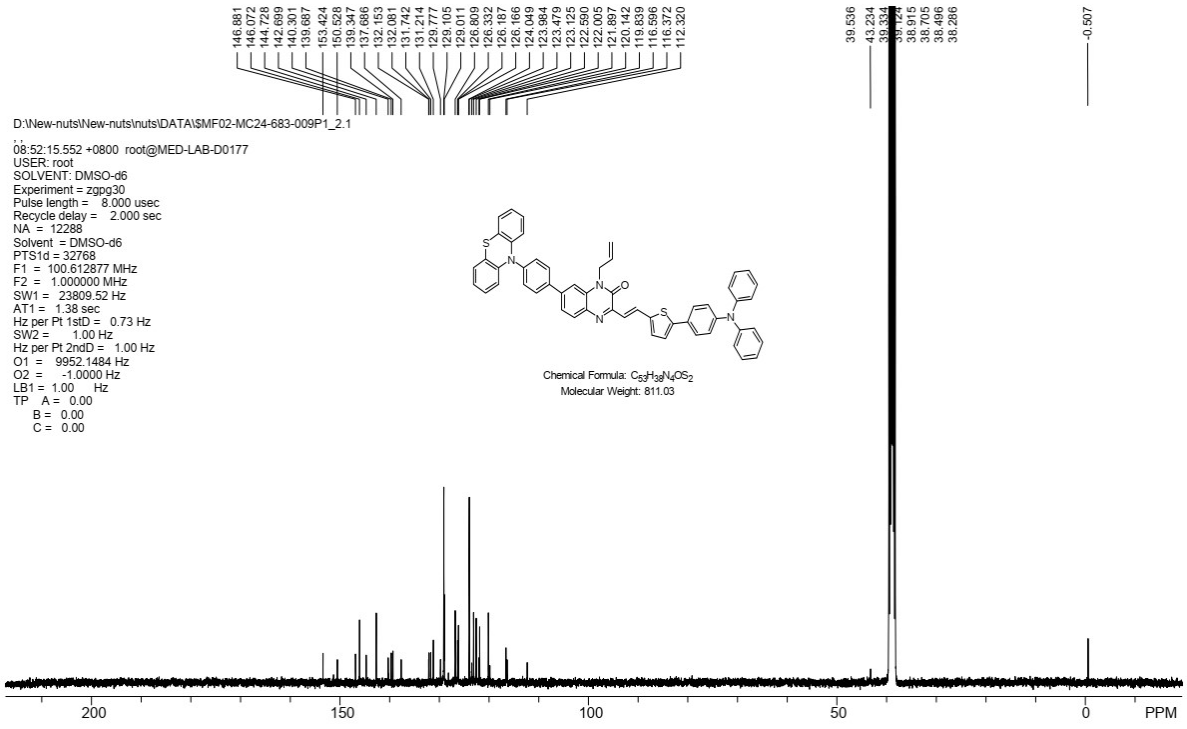




Fig.S3. $^{1}H$ (top) and $^{13}C\{^{1}H\}$ (bottom) NMR spectra of **QuinoNS** in DMSO-$d_6$.

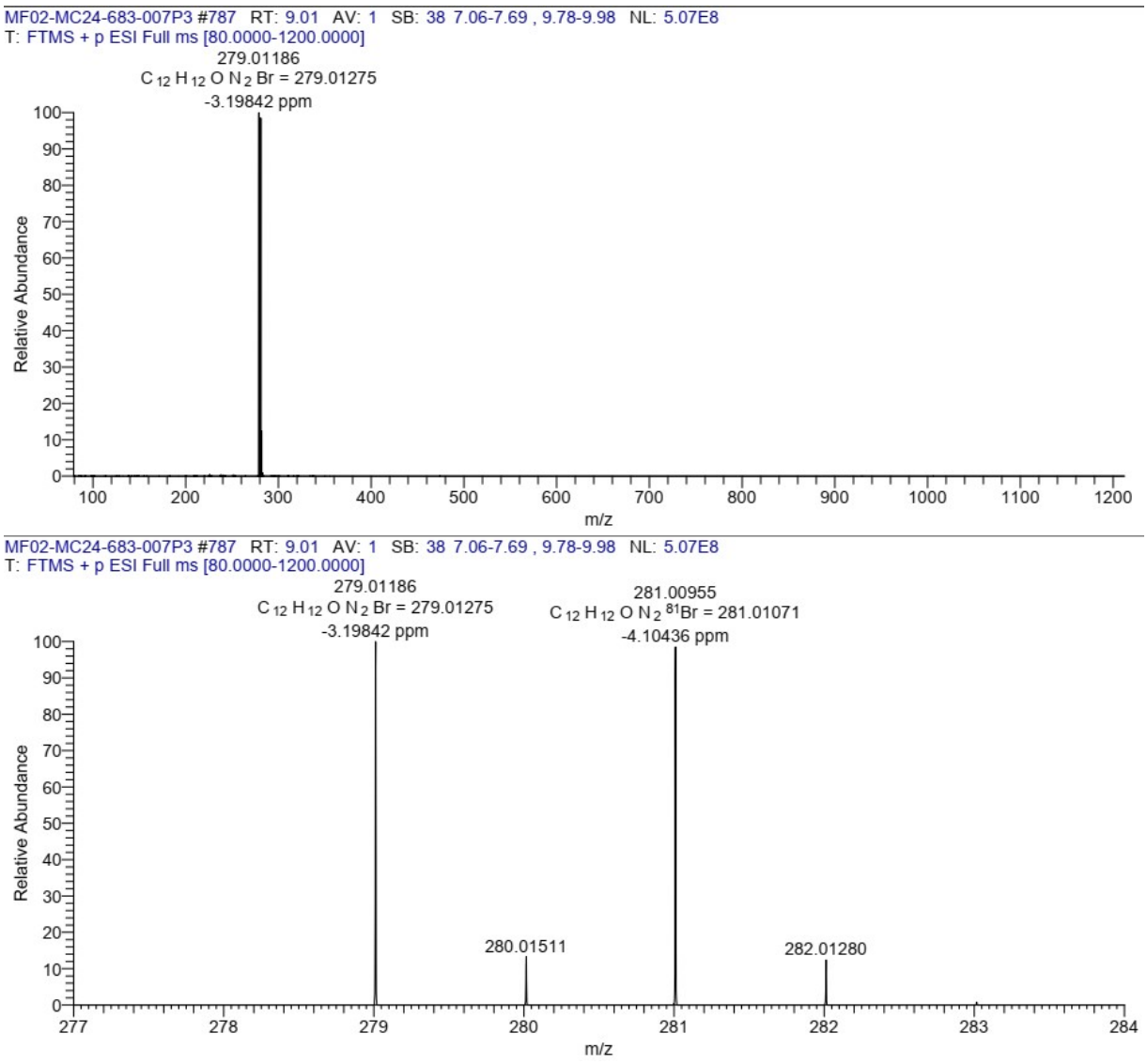



Fig.S4. ESI mass spectrum of **3**.

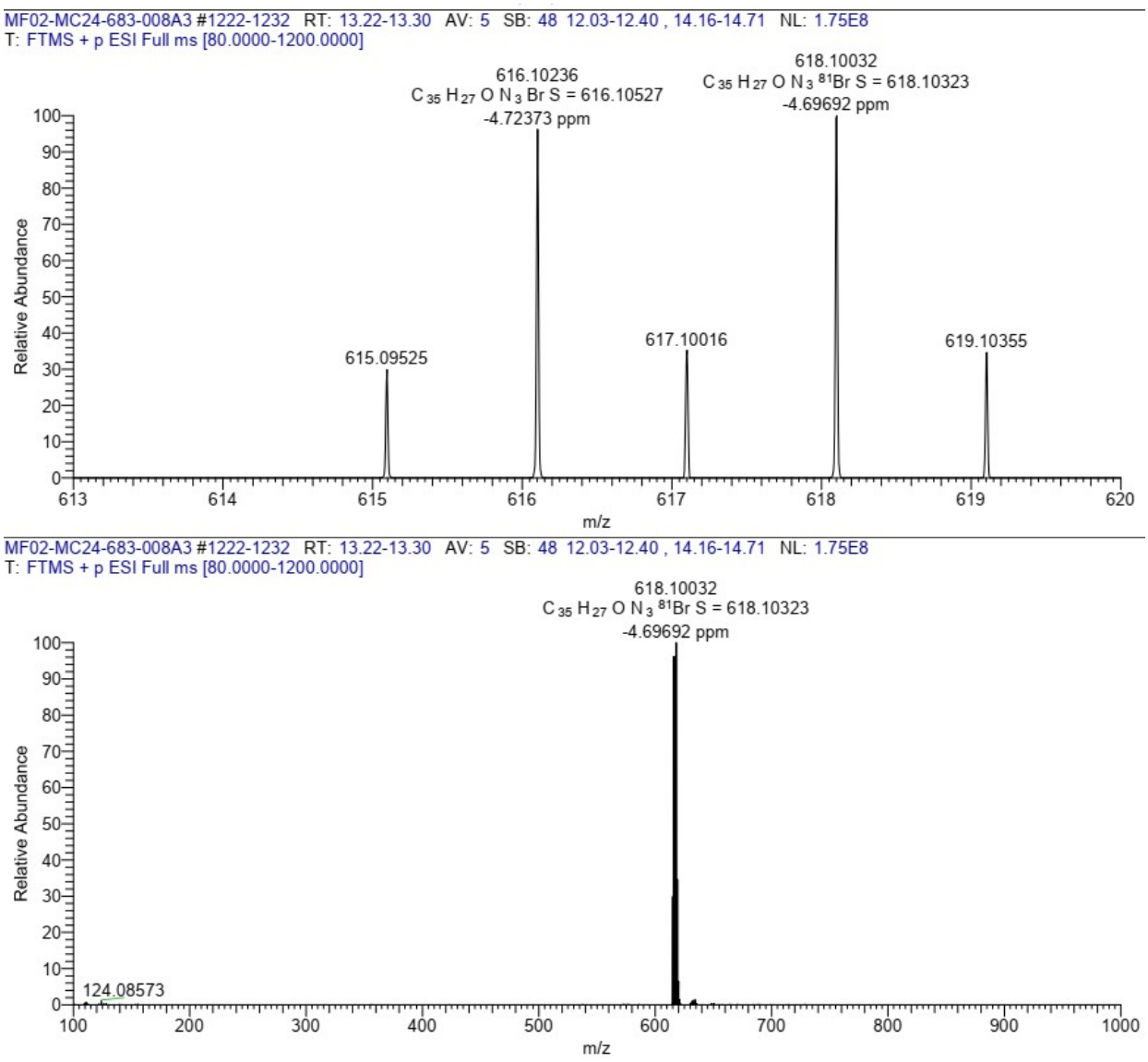



Fig.S5. ESI mass spectrum of **5**.

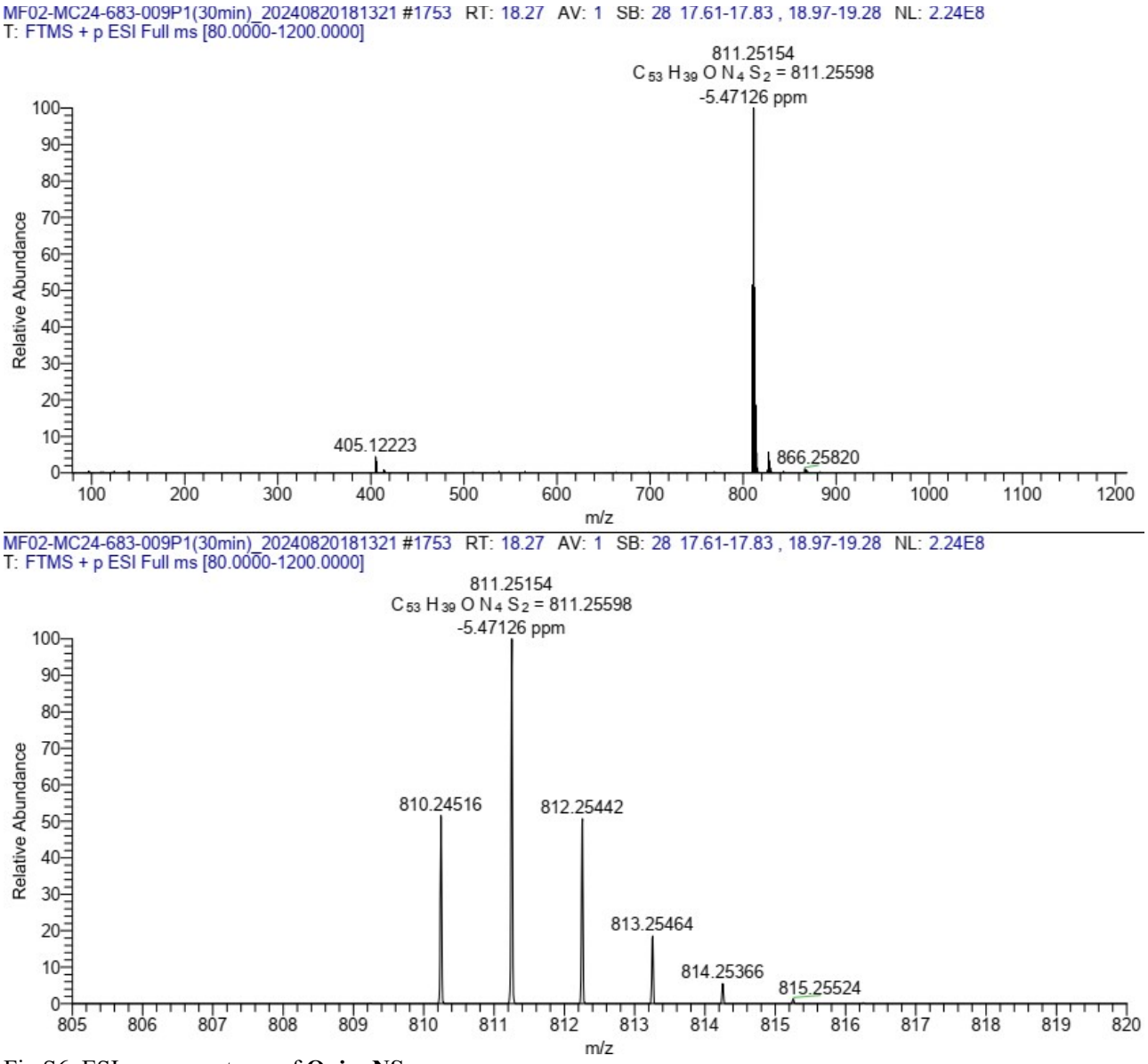



Fig.S6. ESI mass spectrum of **QuinoNS**.