Electronic Supplementary Material (ESI) for RSC Advances.

Recurrent Neural Network (RNN) Model Accelerates the Development of Metronidazole Derivatives Antibacterial

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Bioassay Conditions

Stock solutions of the synthesized compounds (100 μg/mL) in DMSO were prepared, and graded quantities of the test compounds were incorporated in specified quantity of sterilized liquid MH medium. A specified quantity of the medium containing the test compound was poured into microtitration plates. Suspension of the microorganism was prepared to contain approximately 10^5 cfu/mL and applied to microtitration plates with serially diluted compounds in DMSO to be tested and incubated at 37 °C for 24 h. After the MICs were visually determined on each of the microtitration plates, 50 μL of PBS (phosphate buffered saline 0.01 mol/L, pH 7.4, $Na_2HPO_4 \cdot 12H_2O$ 2.9 g, KH_2PO_4 0.2 g, NaCl 8.0 g, KCl 0.2 g, distilled water 1000 mL) containing 2 mg of MTT/mL was added to each well. Incubation was continued at room temperature for 4–5 h. The content of each well was removed, and 100μL of isopropanol containing 5% 1 mol/L HCl was added to extract the dye. After 12 h of incubation at room temperature, the optical density (OD) was measured with a microplate reader at 550 nm.

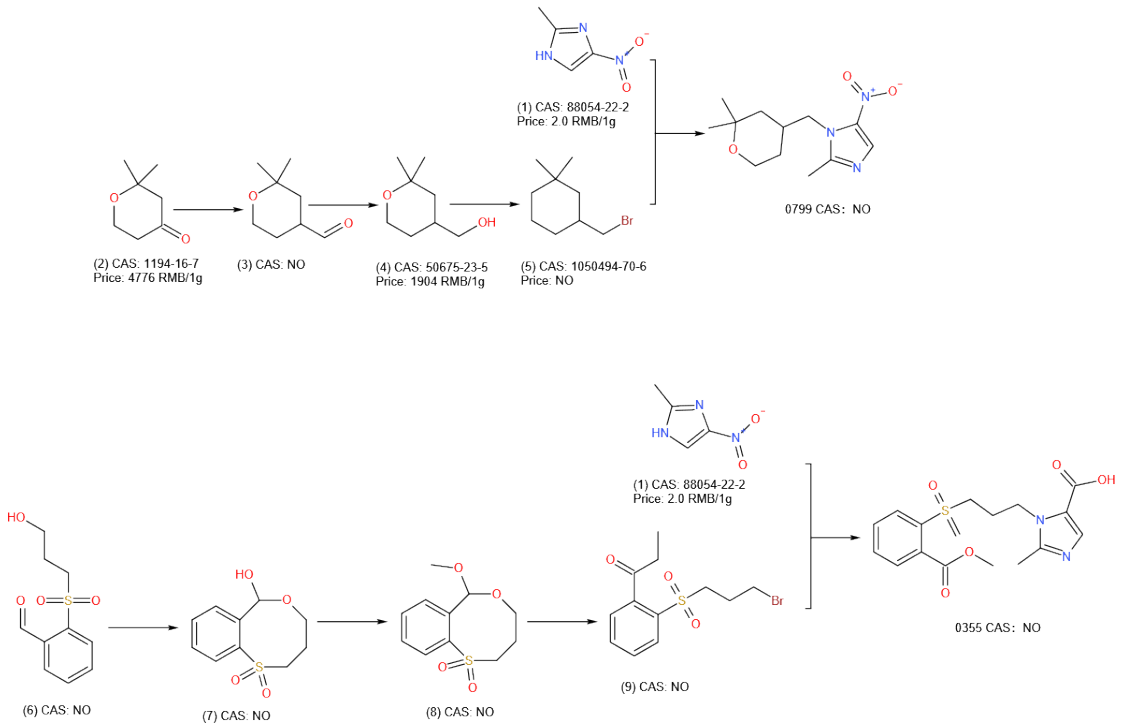

Fig. S1. The synthetic routes of 0355 and 0799 predicted by chemical.ai.

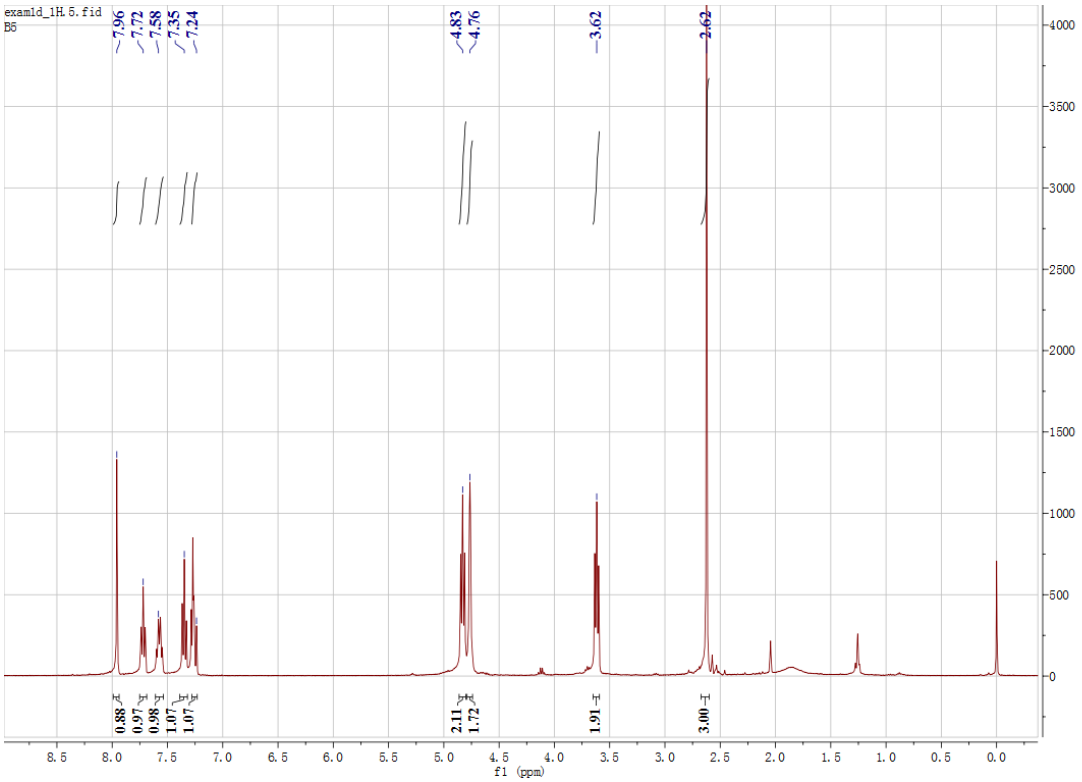

Fig. S2 ^{1}H NMR spectrum of **8a**.

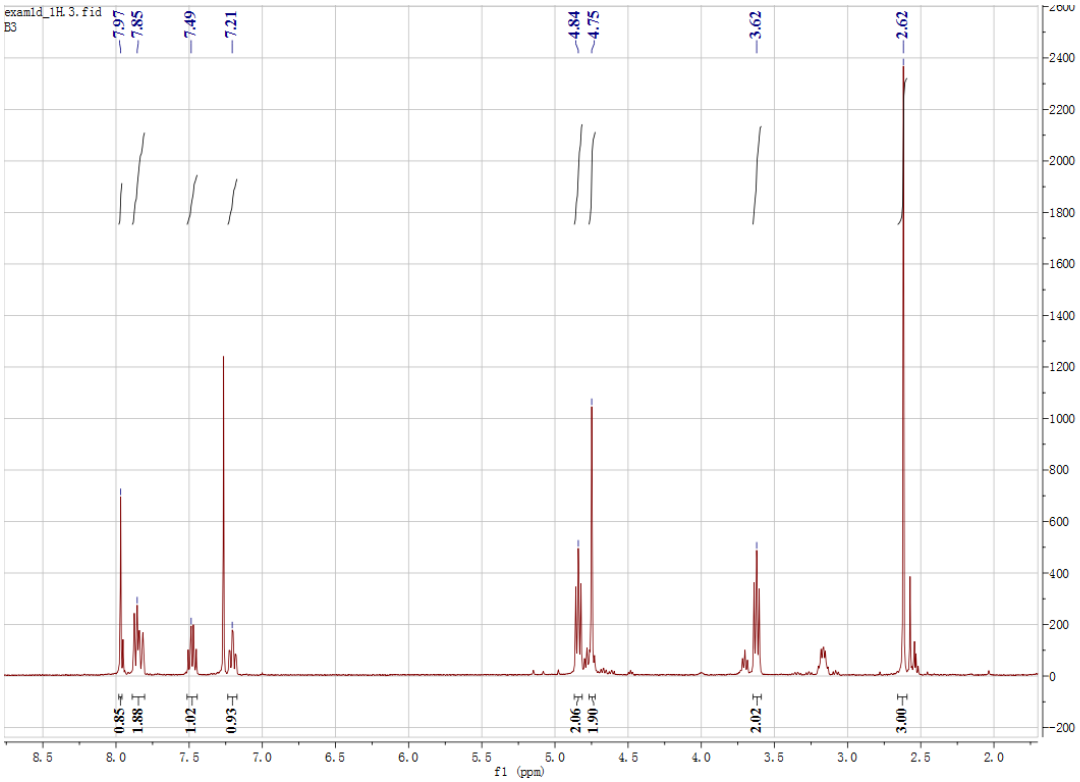

Fig. S3 ^{1}H NMR spectrum of **8b**.

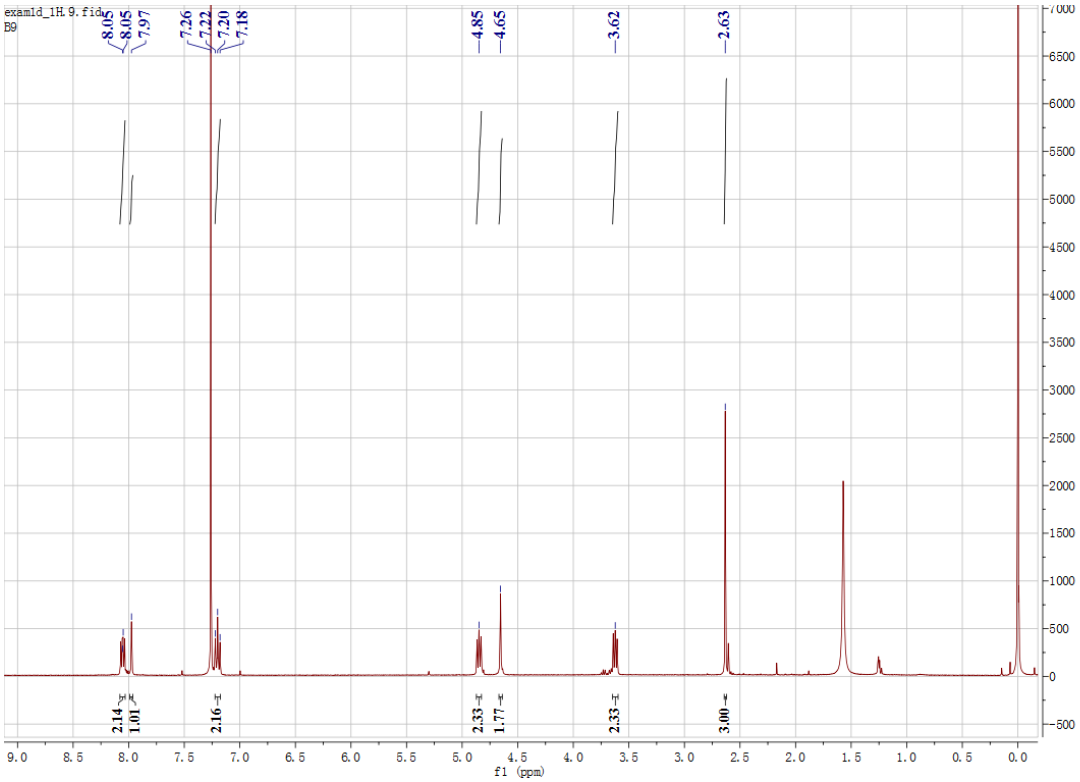

Fig. S4 ^{1}H NMR spectrum of **8c**.

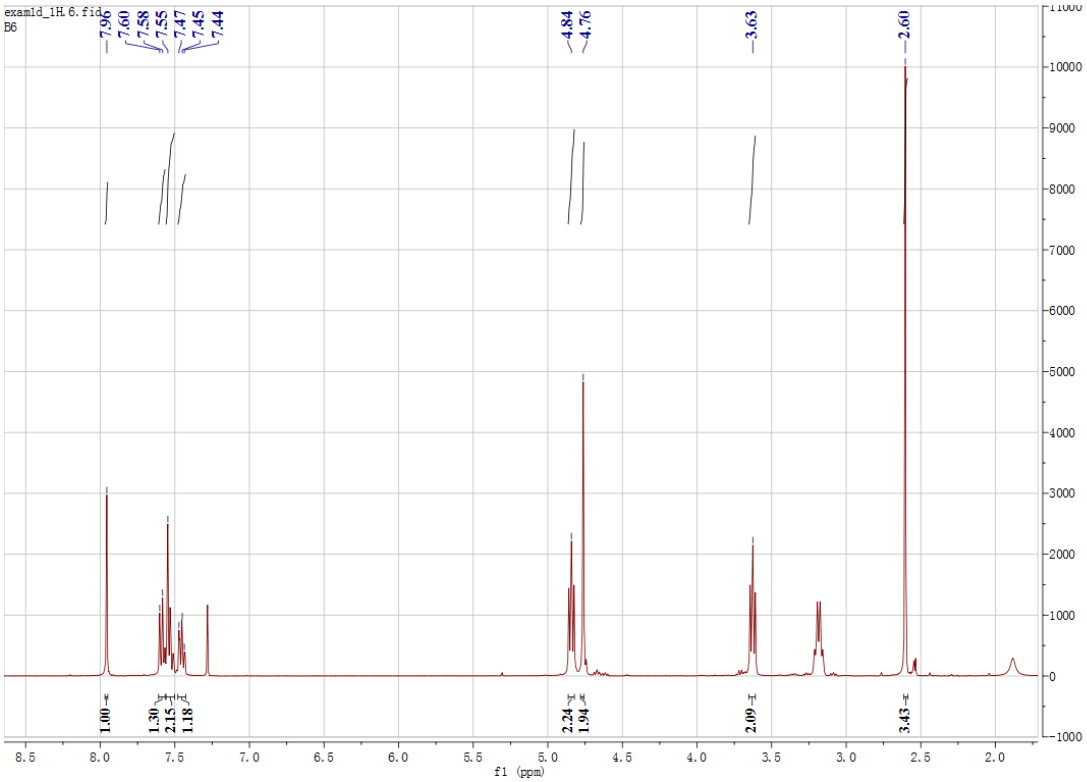

Fig. S5 ^{1}H NMR spectrum of **8d**.

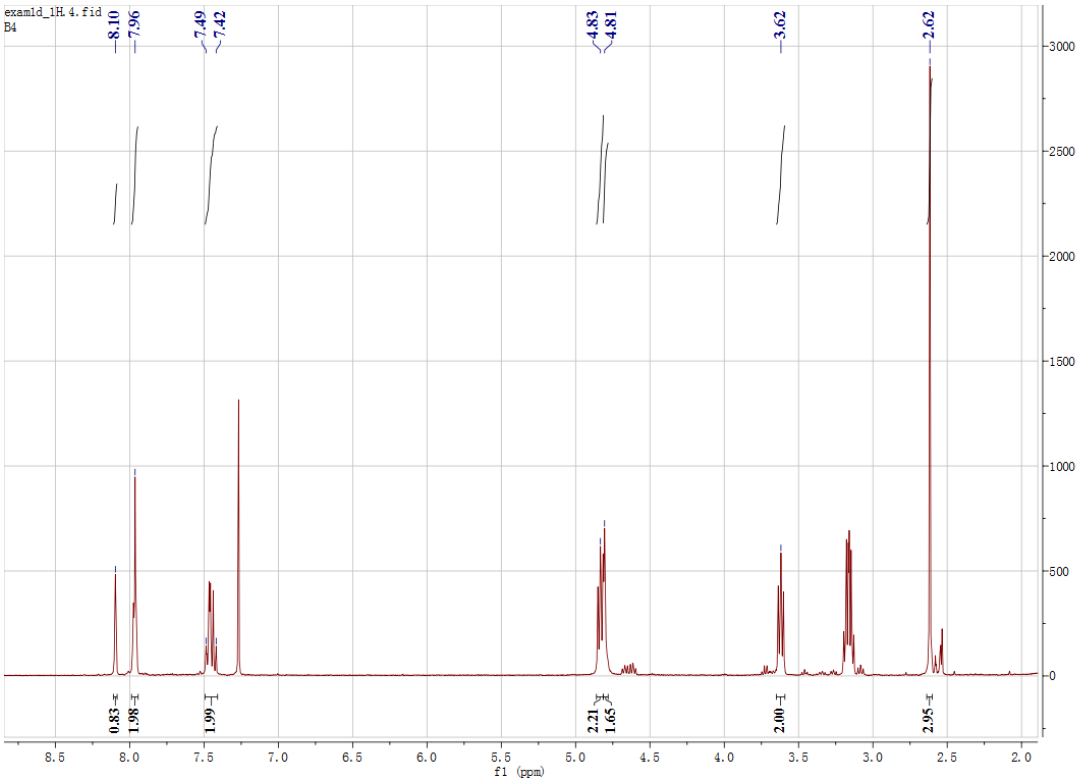

Fig. S6 ^{1}H NMR spectrum of **8e**.

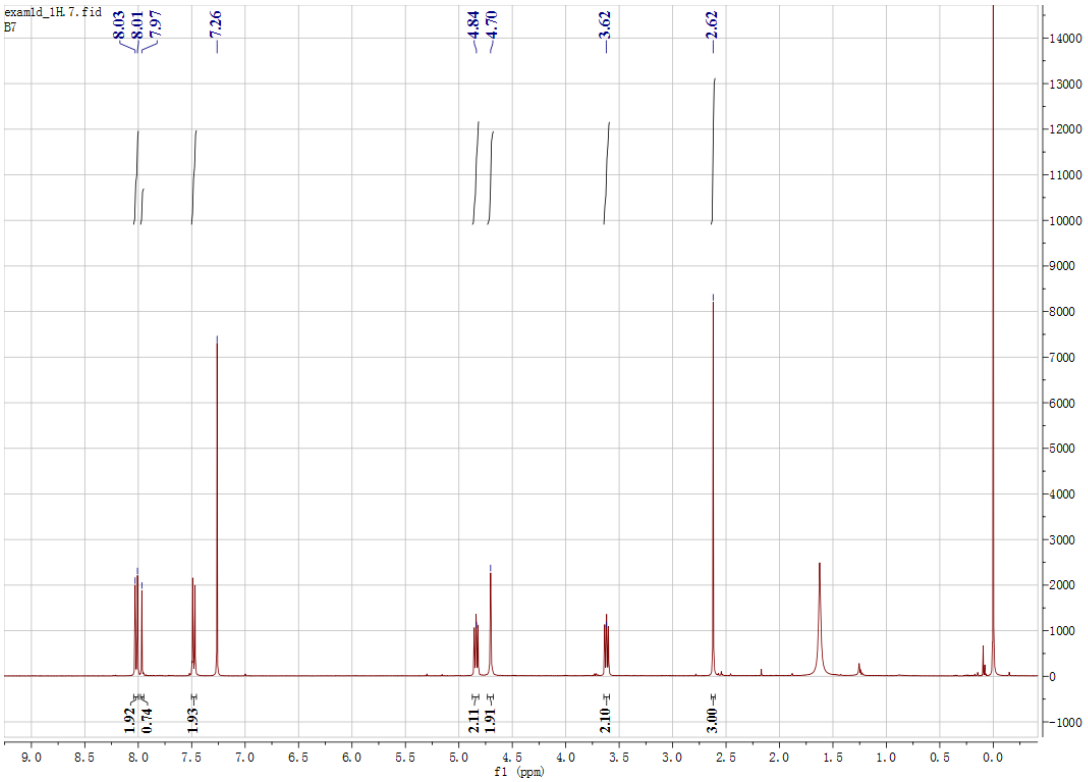

Fig. S7 ^{1}H NMR spectrum of **8f**.

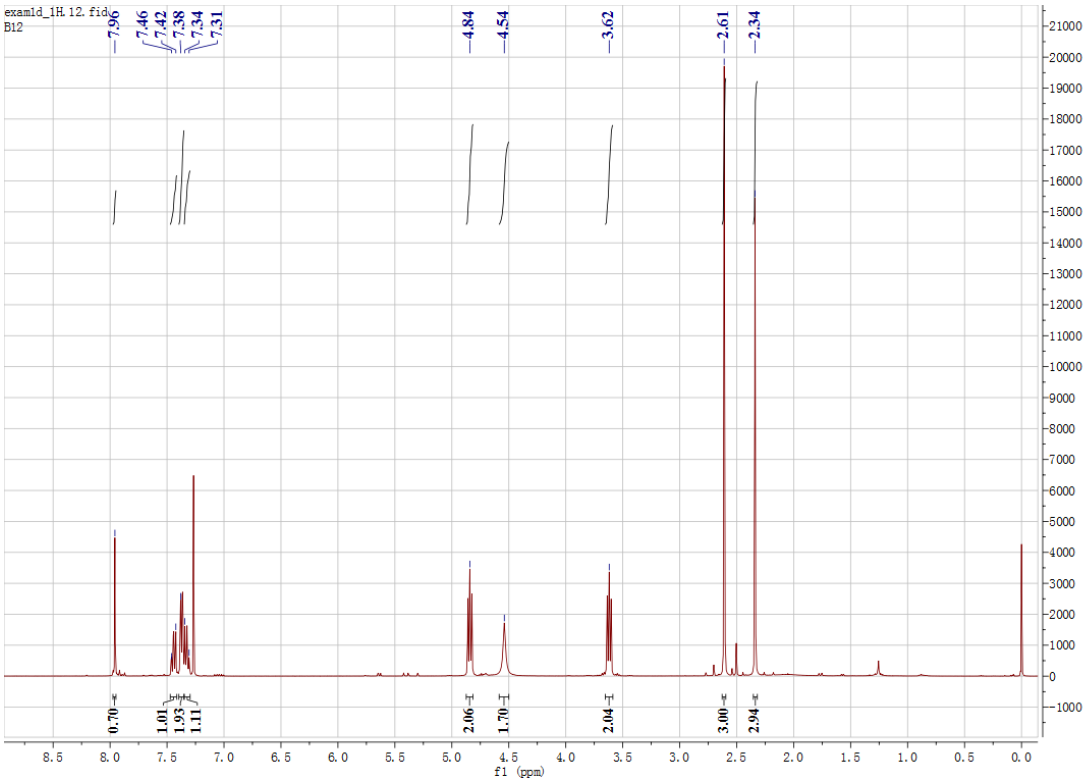

Fig. S8 ^{1}H NMR spectrum of **8g**.

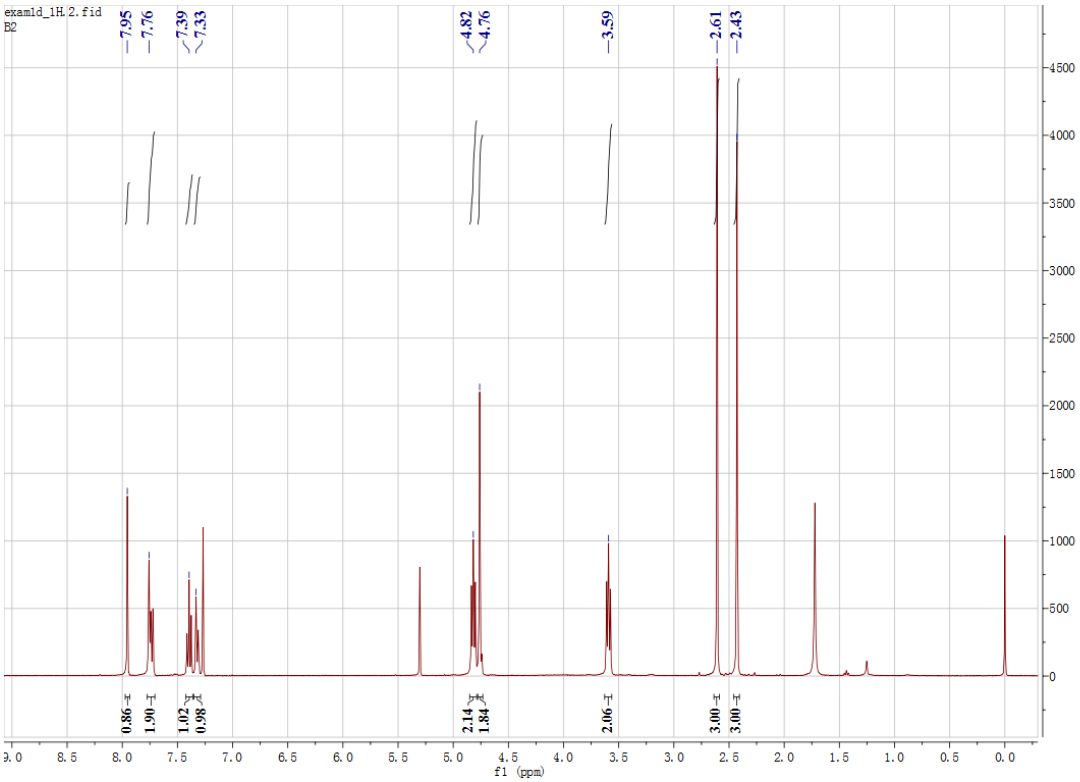

Fig. S9 ^{1}H NMR spectrum of 8h.

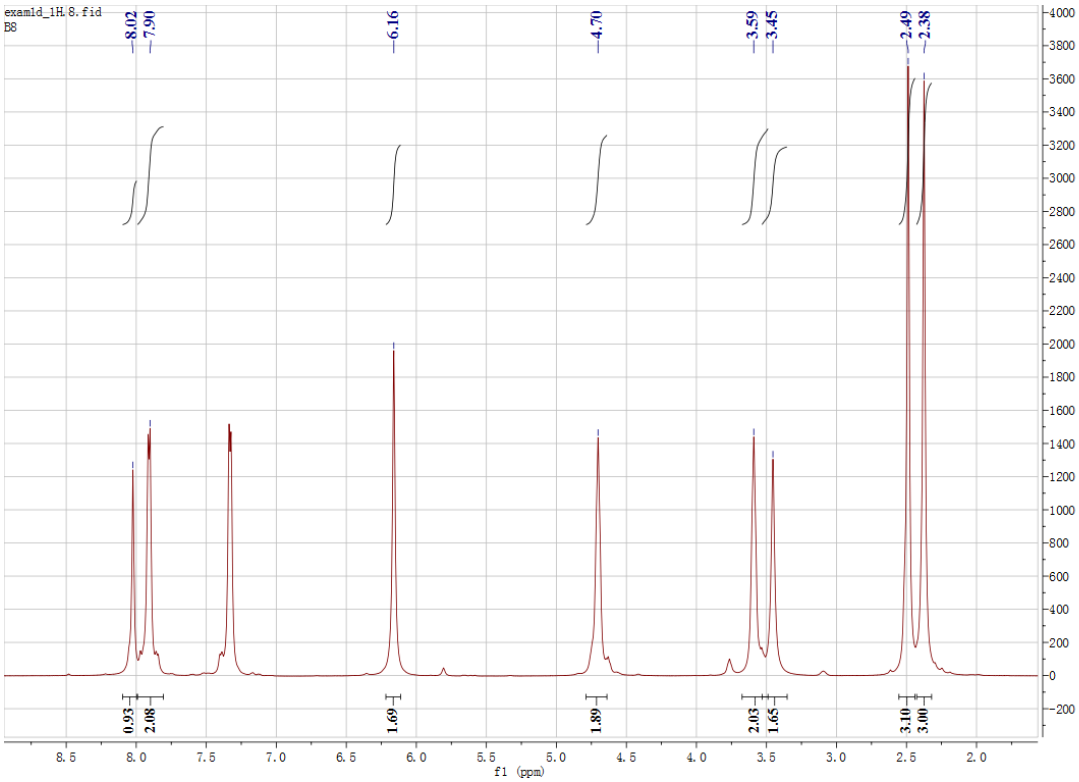

Fig. S10 ^{1}H NMR spectrum of **8i**.

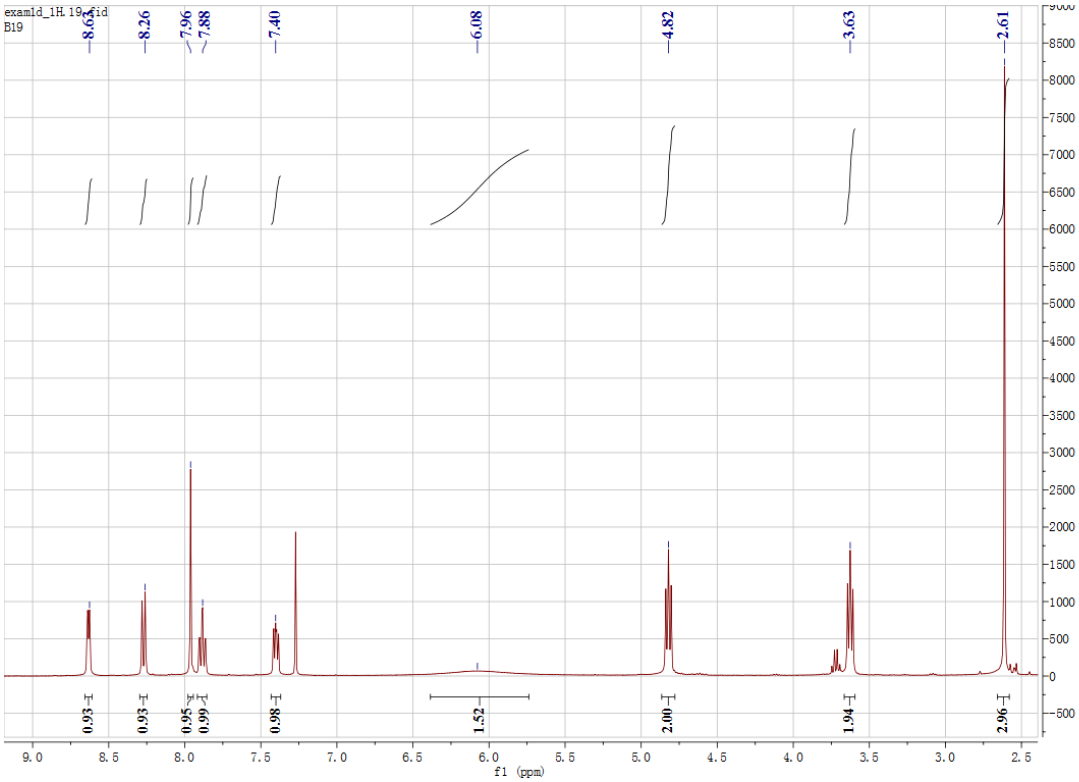

Fig. S11 ^{1}H NMR spectrum of **8j**.

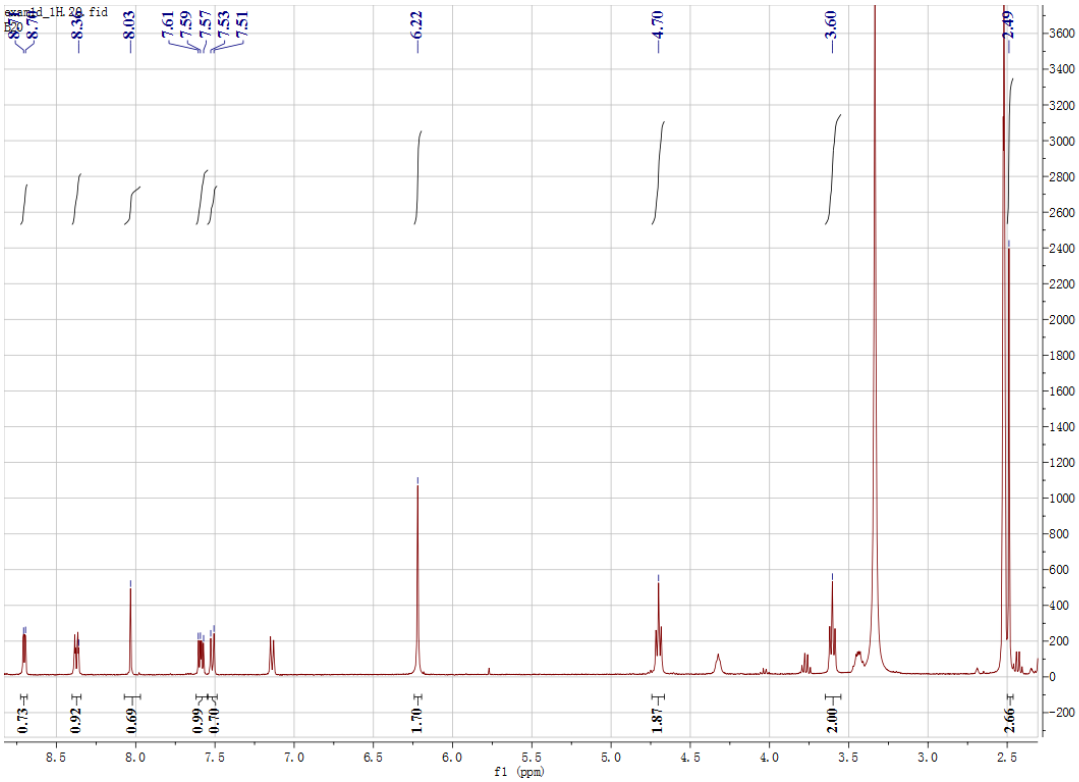

Fig. S12 ^{1}H NMR spectrum of **8k**.

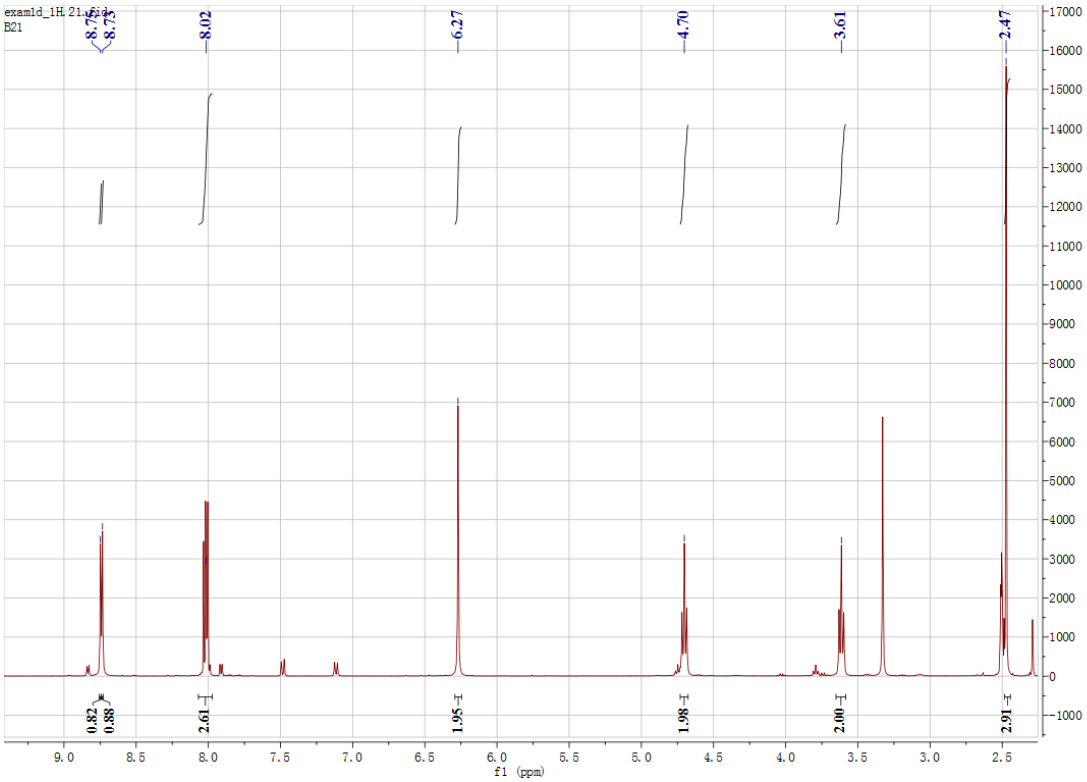

Fig. S13 ^{1}H NMR spectrum of **8l**.

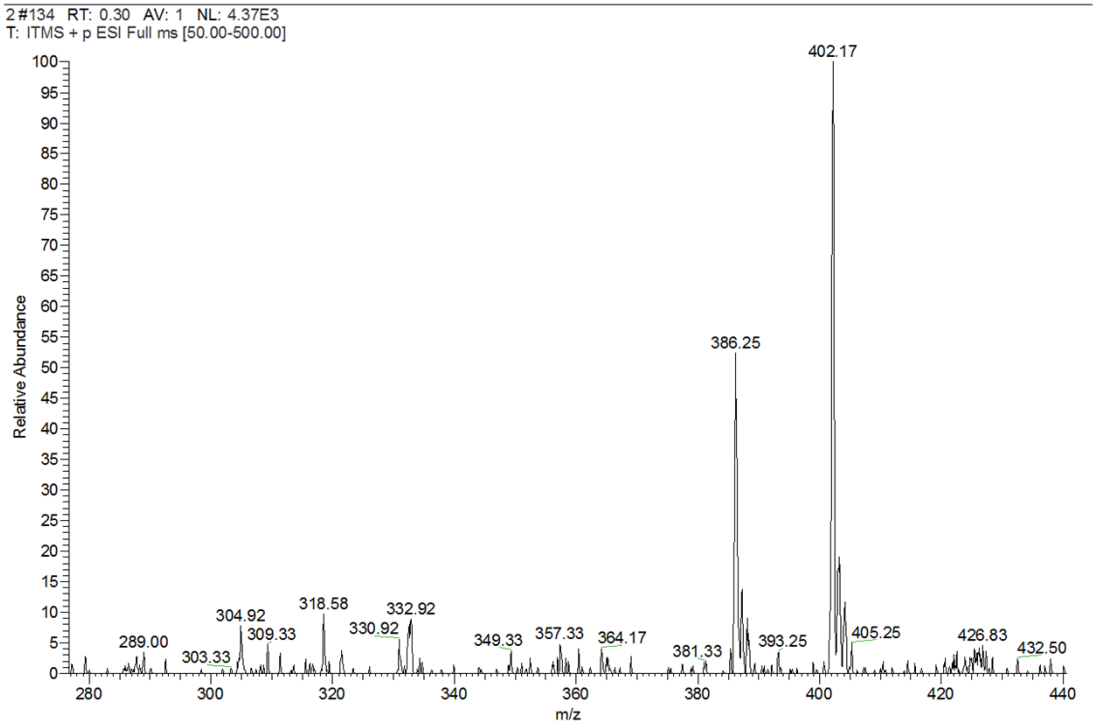

Fig. S14 ESI-MS spectrum of **8a**.

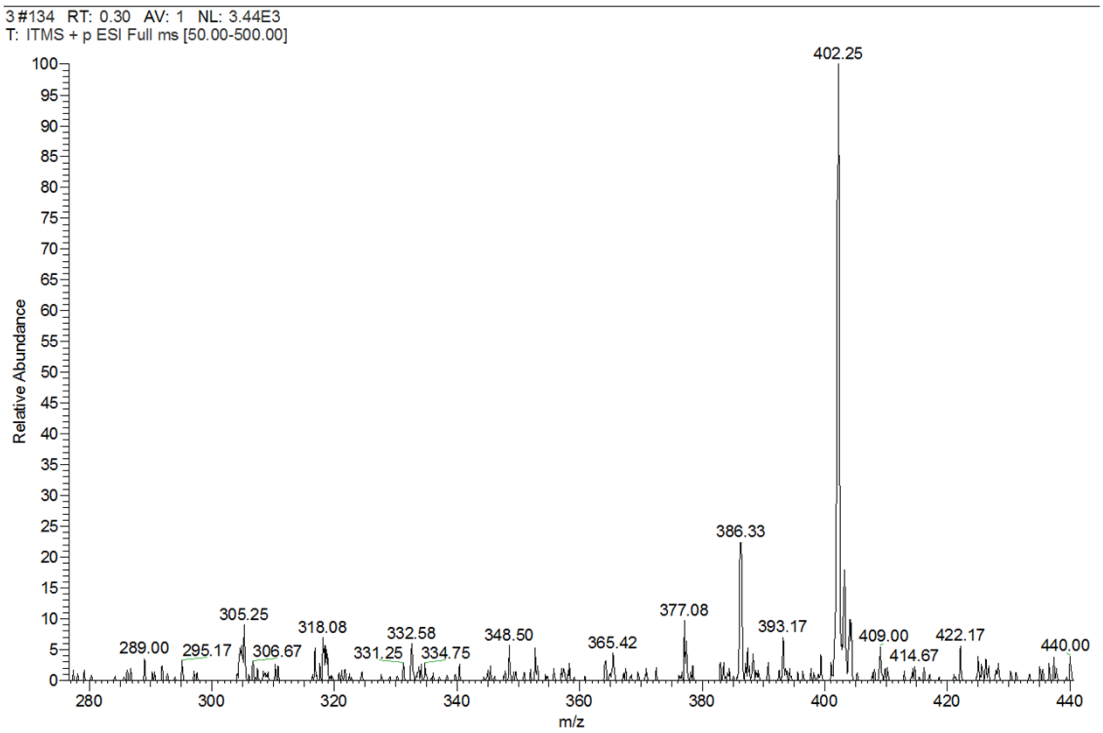

Fig. S15 ESI-MS spectrum of **8b**.

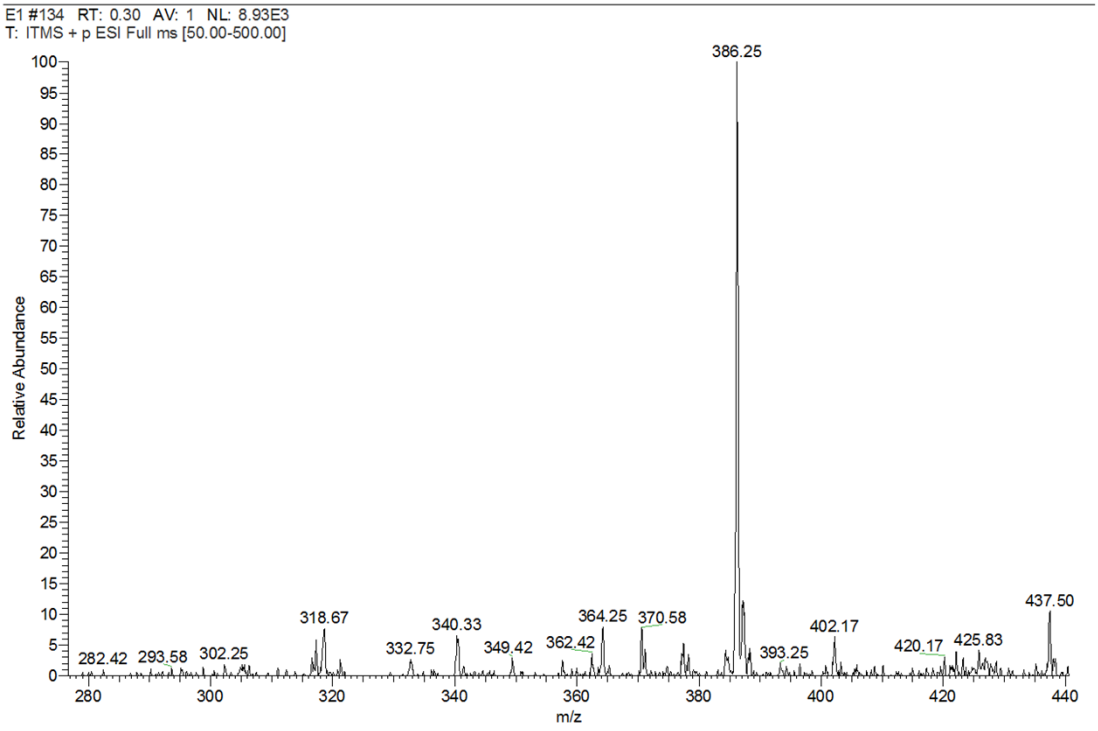

Fig. S16 ESI-MS spectrum of **8c**.

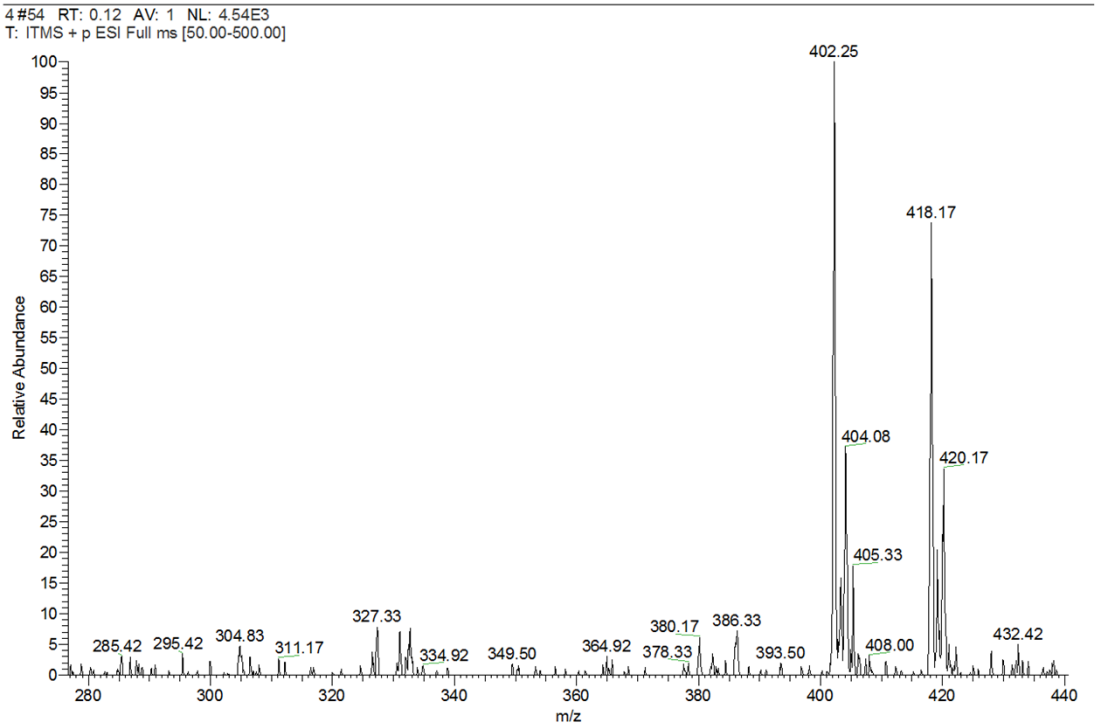

Fig. S17 ESI-MS spectrum of **8d**.

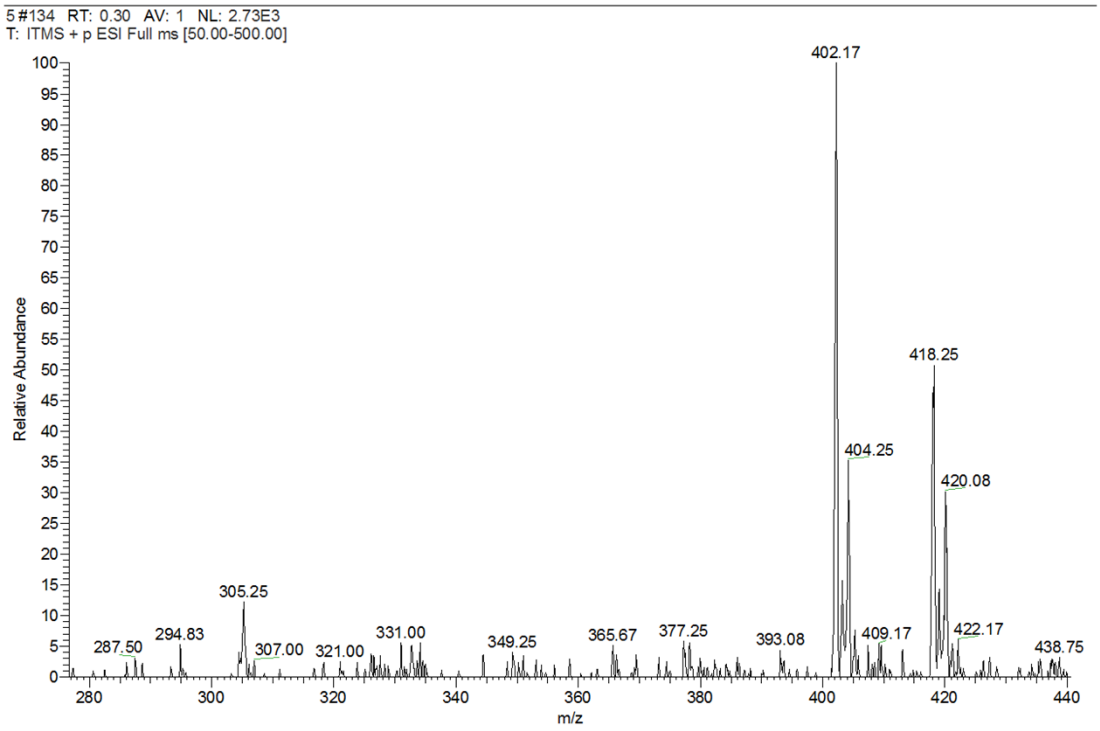

Fig. S18 ESI-MS spectrum of **8e**.

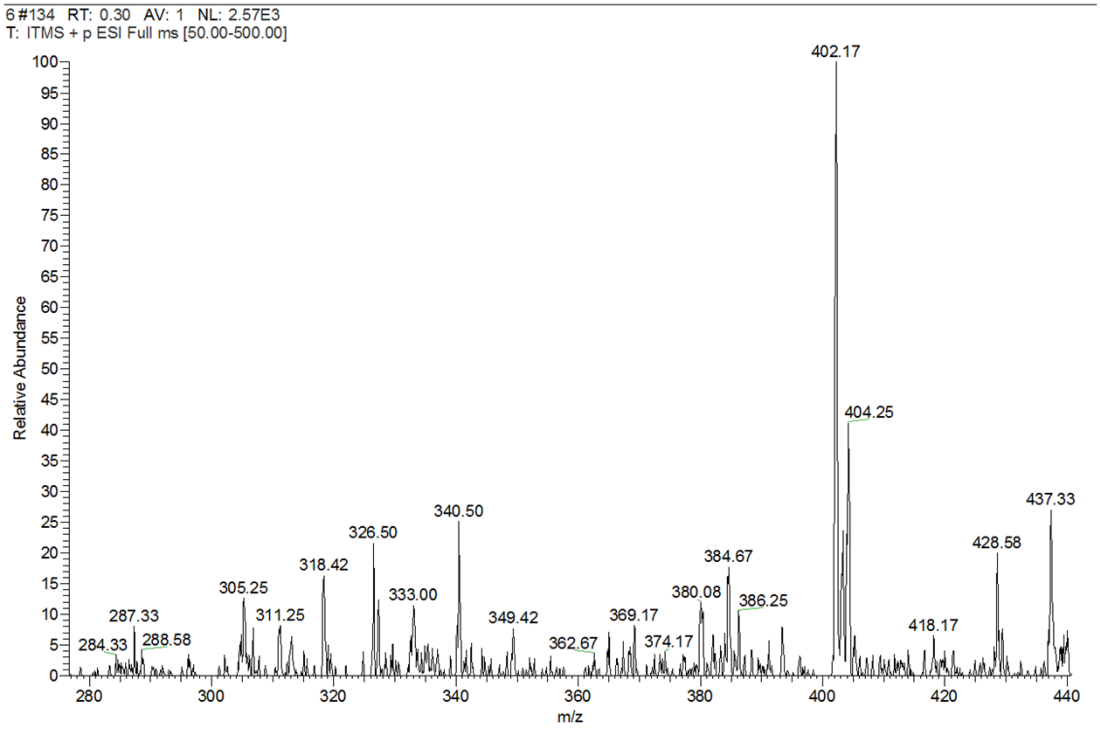

Fig. S19 ESI-MS spectrum of **8f**.

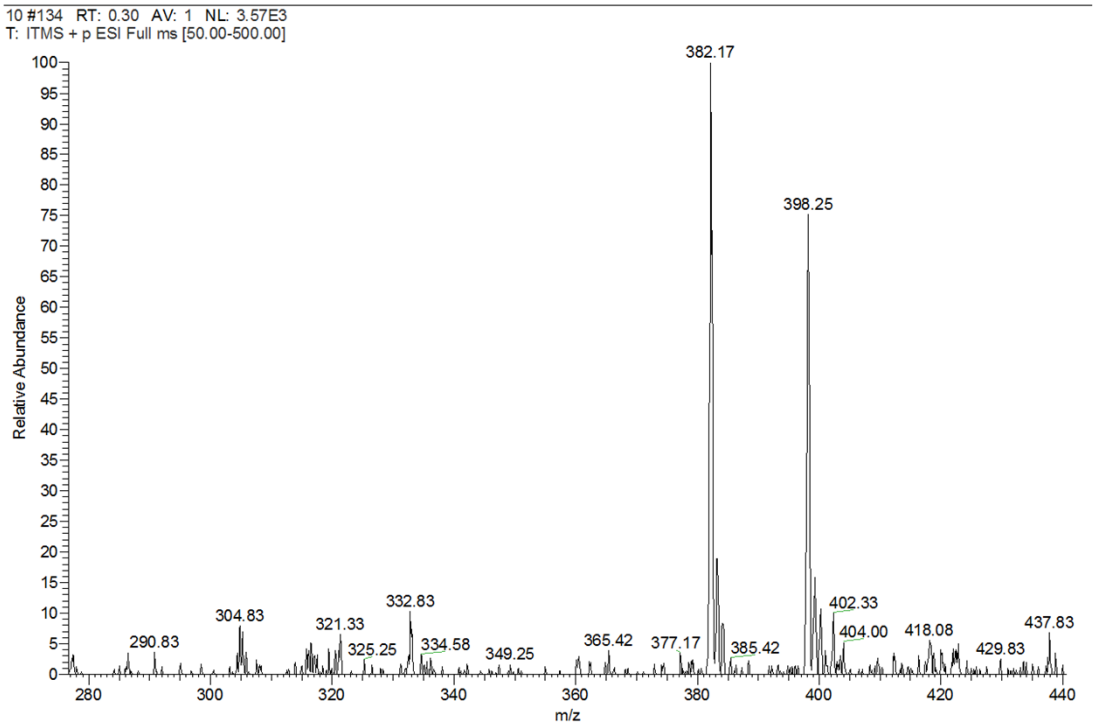

Fig. S20 ESI-MS spectrum of **8g**.

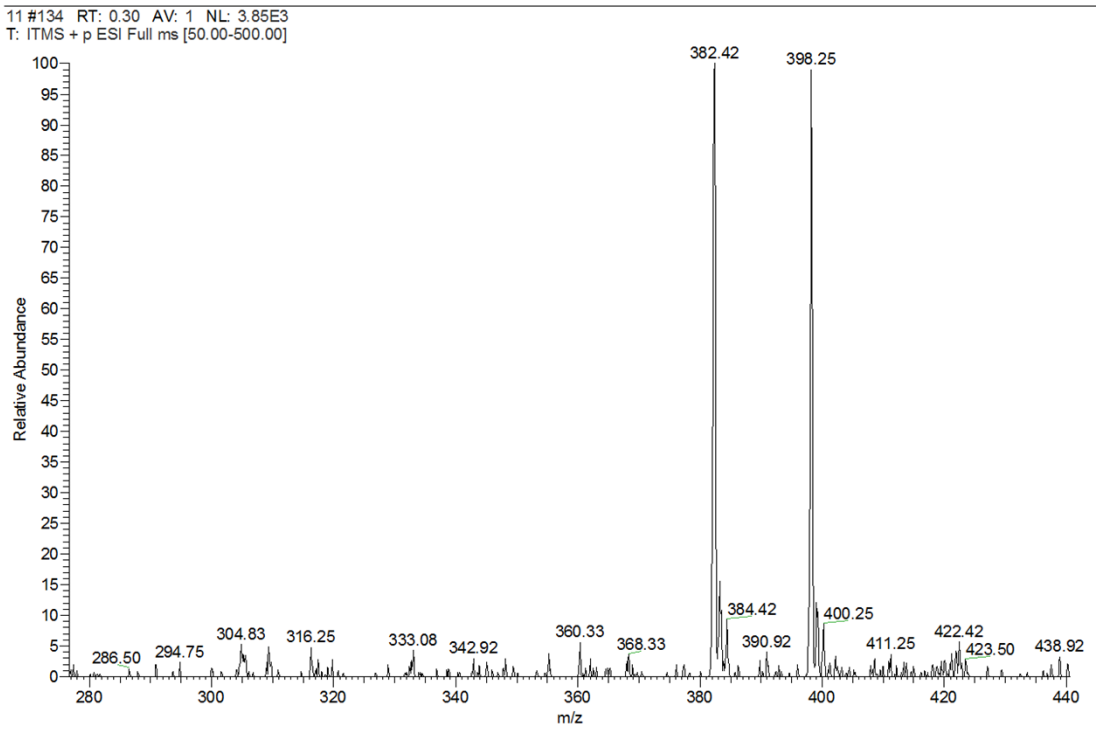

Fig. S21 ESI-MS spectrum of **8h**.

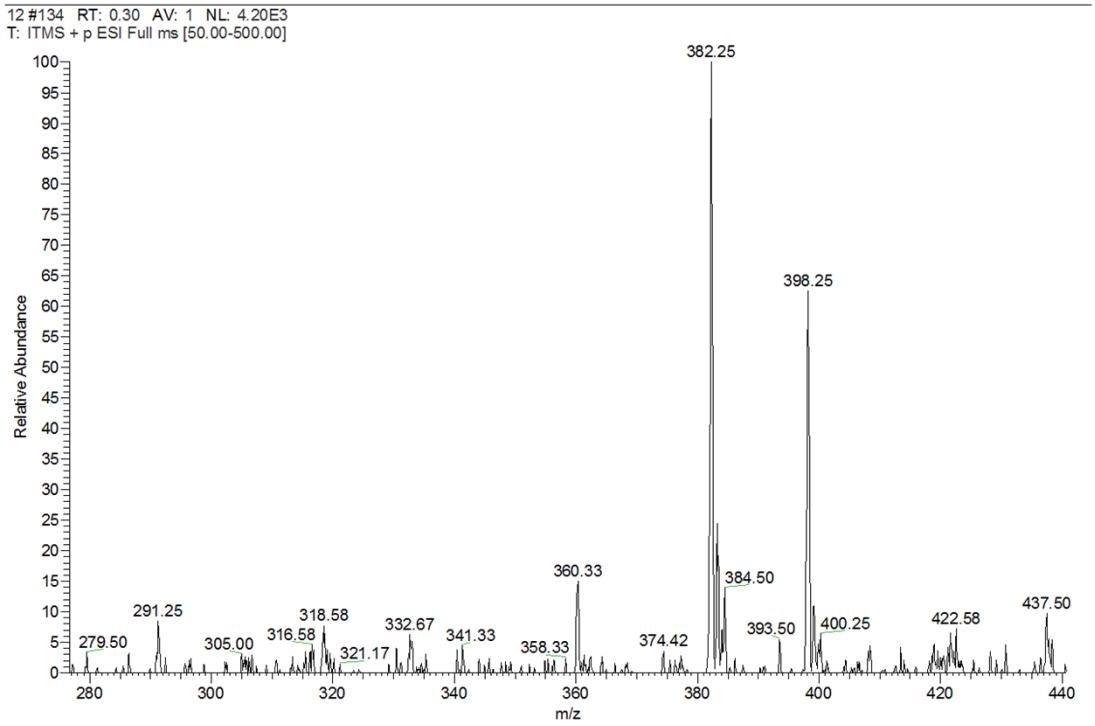

Fig. S22 ESI-MS spectrum of **8i**.

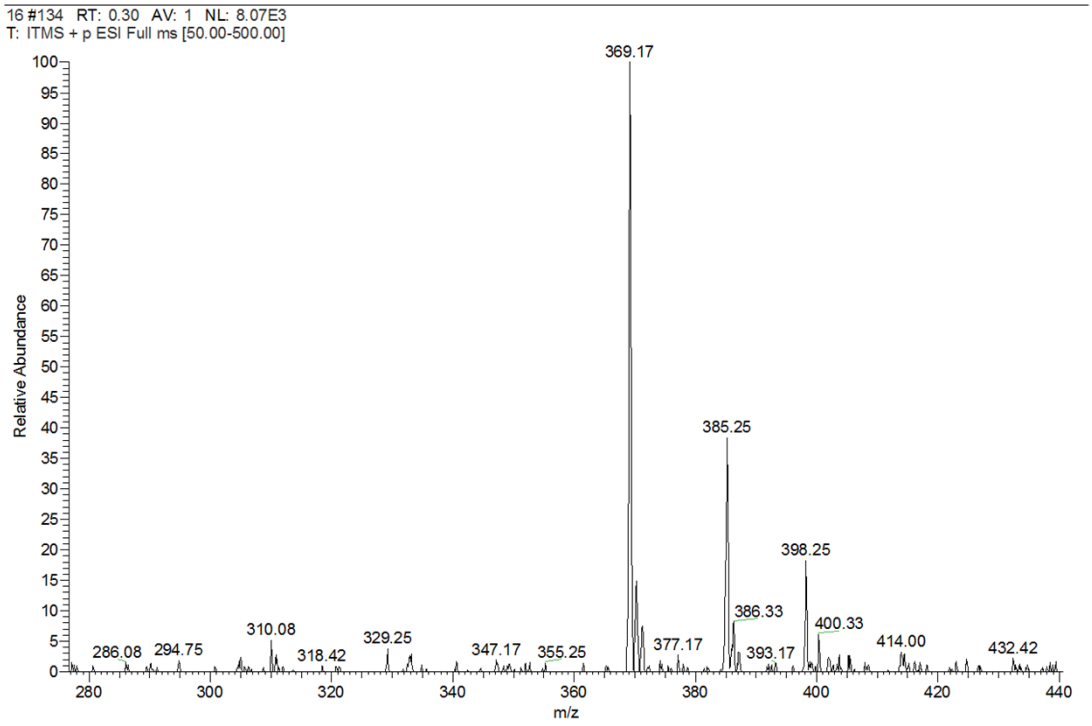

Fig. S23 ESI-MS spectrum of **8j**.

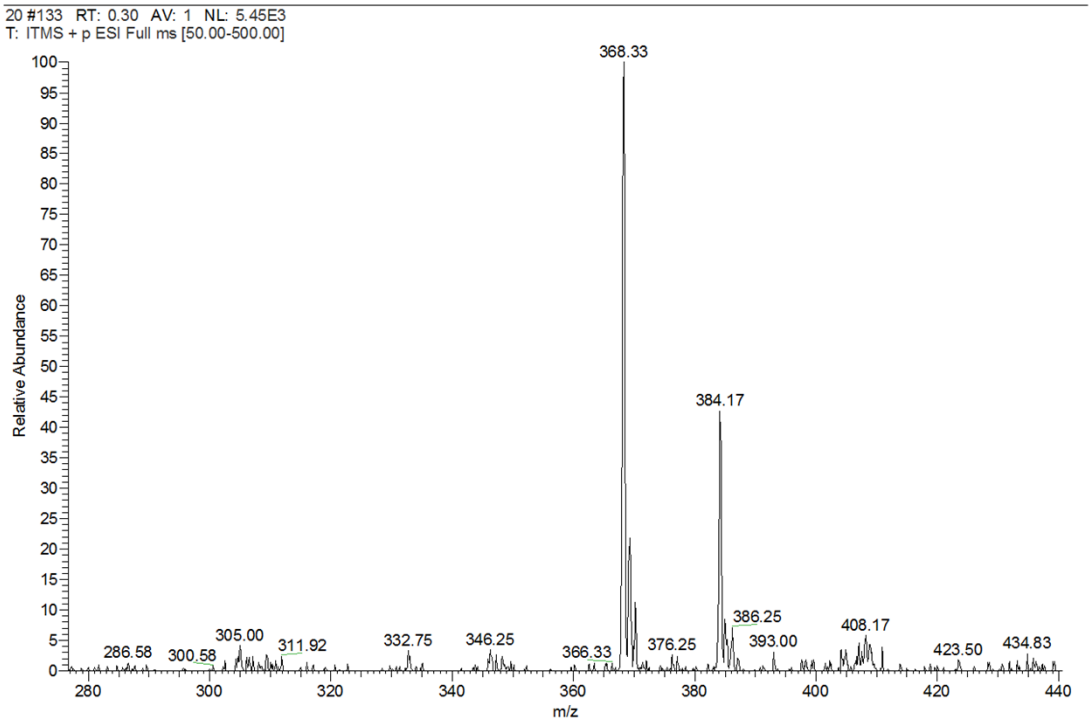

Fig. S24 ESI-MS spectrum of **8k**.

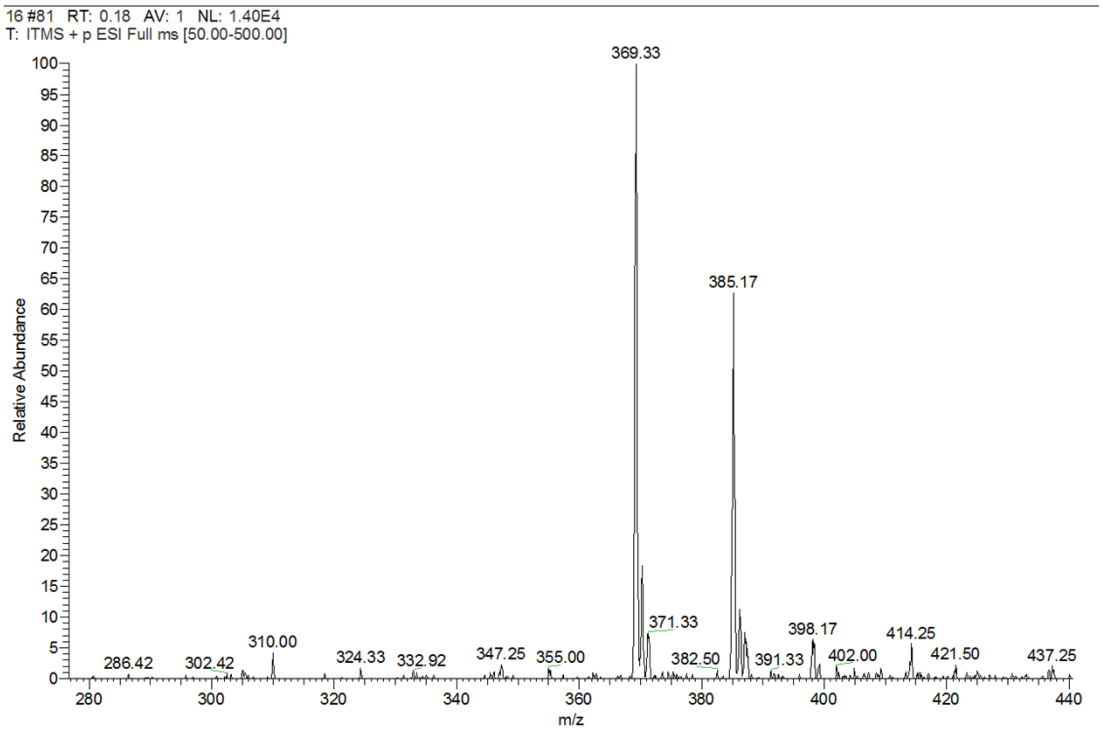

Fig. S25 ESI-MS spectrum of **8l**.