

Synthesis, Spectral, Thermal and Biological Studies of 4-Cyclohexyl-3-(4-nitrophenyl)methyl-1,2,4-triazolin-5-thione and Its Copper(II) Coordination Compound, [CuCl₂(H₂O)₂L₂]

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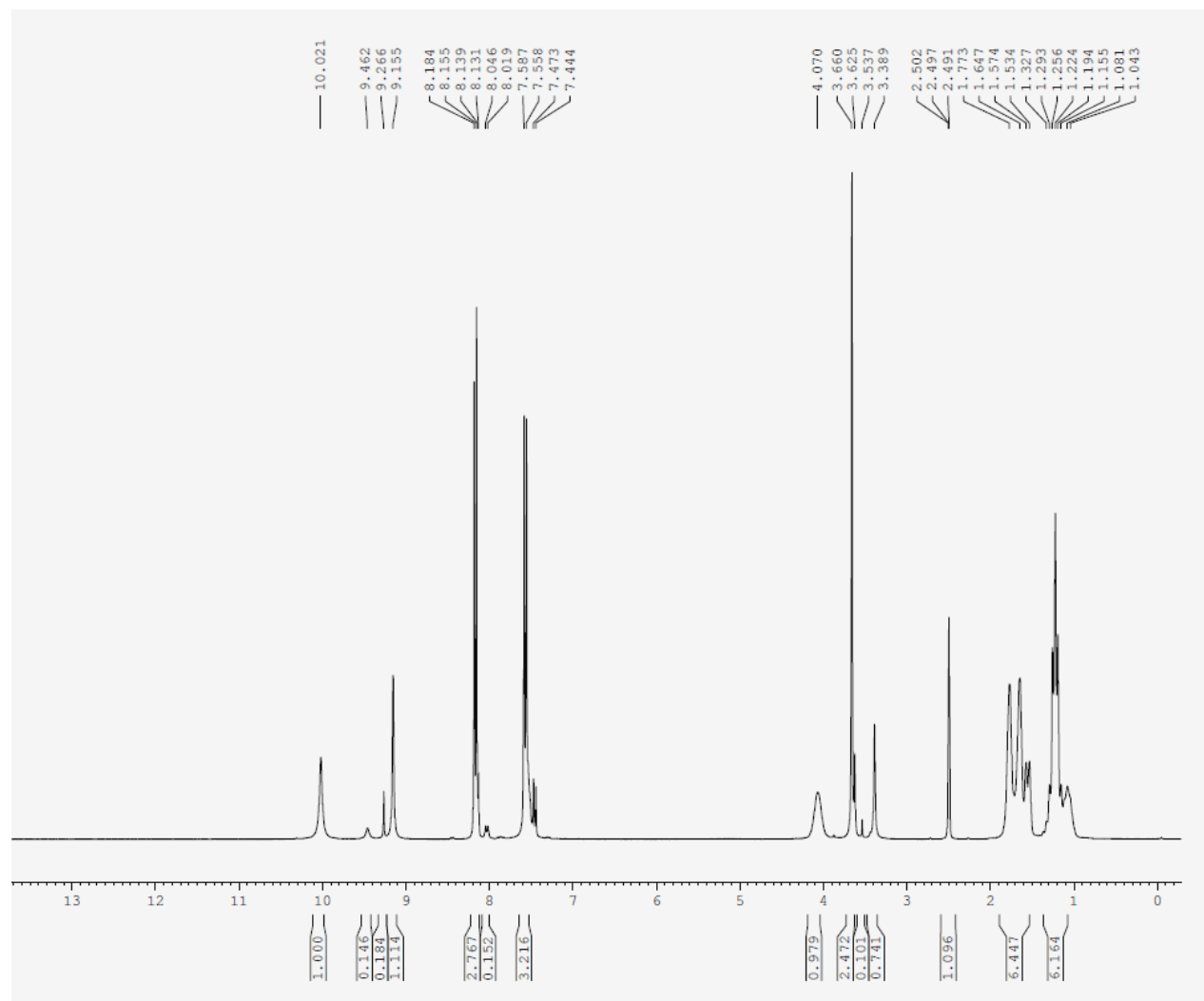


Figure S1. ¹H NMR spectrum for compound 2.

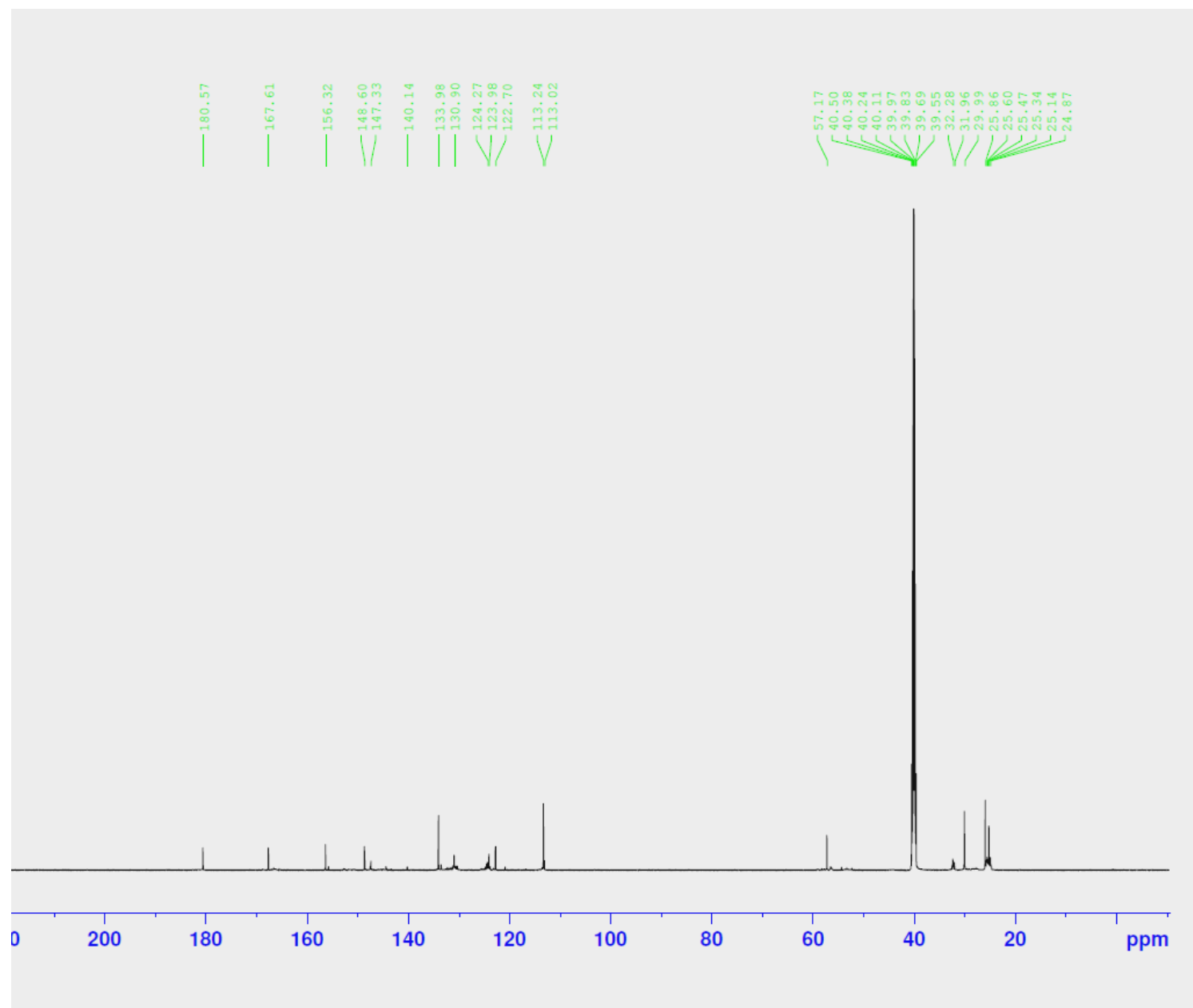


Figure S2. ^{13}C NMR spectrum for compound 2.

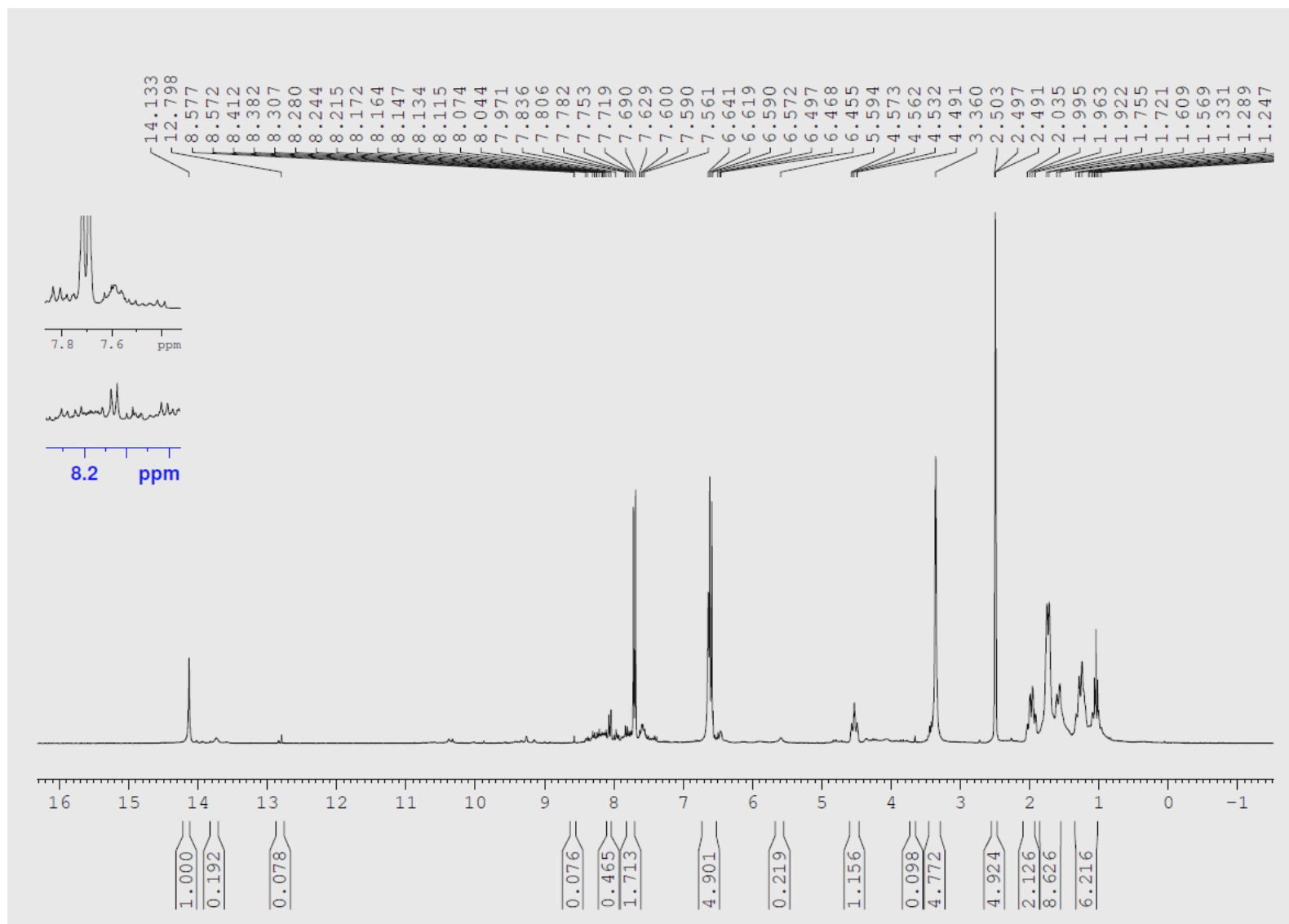


Figure S3: ¹H NMR spectrum for compound 3.

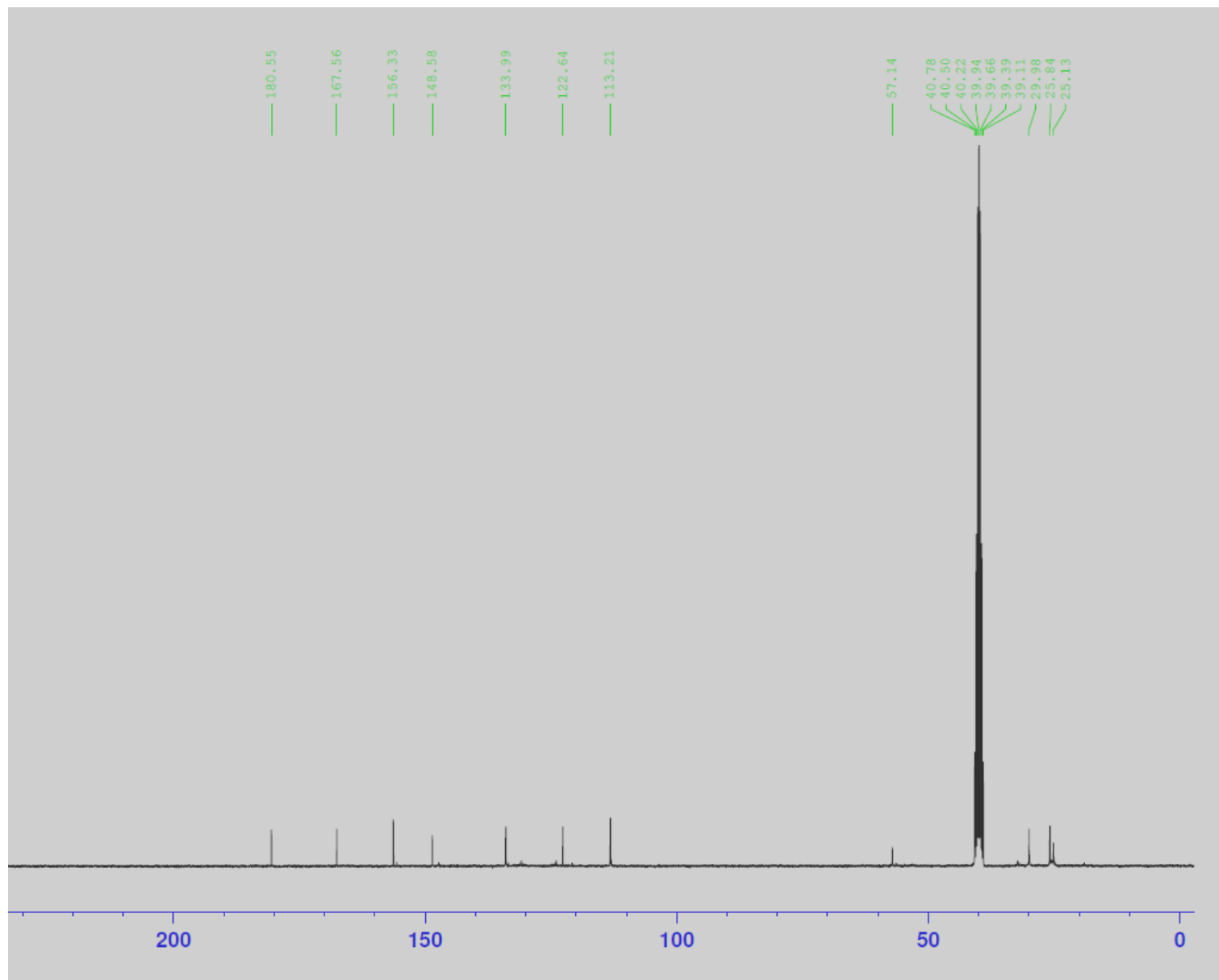
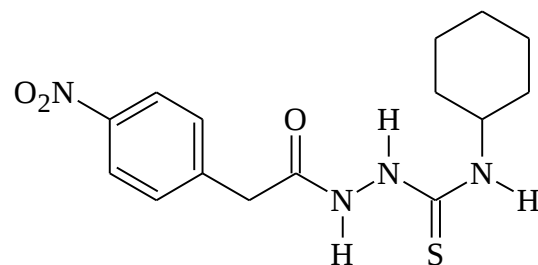


Figure S4: ^{13}C NMR spectrum for compound 3.



$C_{15}H_{20}N_4O_3S$

Calculated monoisotopic mass: 336.1256

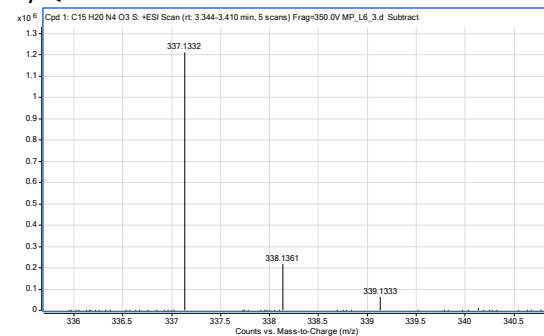
Measured monoisotopic mass: 336.1260

Mass error: 1.24 ppm

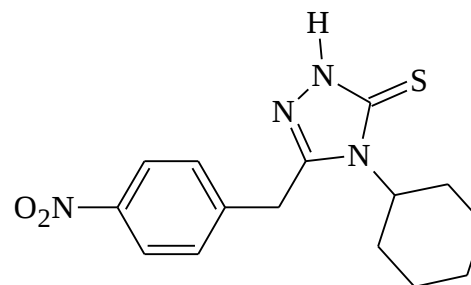
(a)

Theoretical monoisotopic mass of $[M+H]^+$:
337.1329

LC/QTOF MS scan



(c)



$C_{15}H_{18}N_4O_2S$

Calculated monoisotopic mass: 318.1150

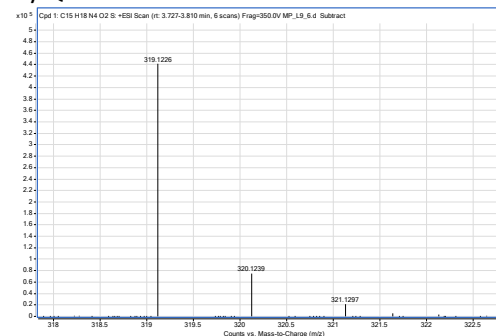
Measured monoisotopic mass: 318.1155

Mass error: 1.36 ppm

(b)

Theoretical monoisotopic mass of $[M+H]^+$:
319.1223

LC/QTOF MS scan



(d)

Figure S5. (a) The structure of compound 2; (b) The structure of compound 3; (c) MS spectrogram for compound 2; (d) MS spectrogram for compound 3.



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