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Supporting Information

C(5) Site-Selective Functionalization of (S)-Cotinine

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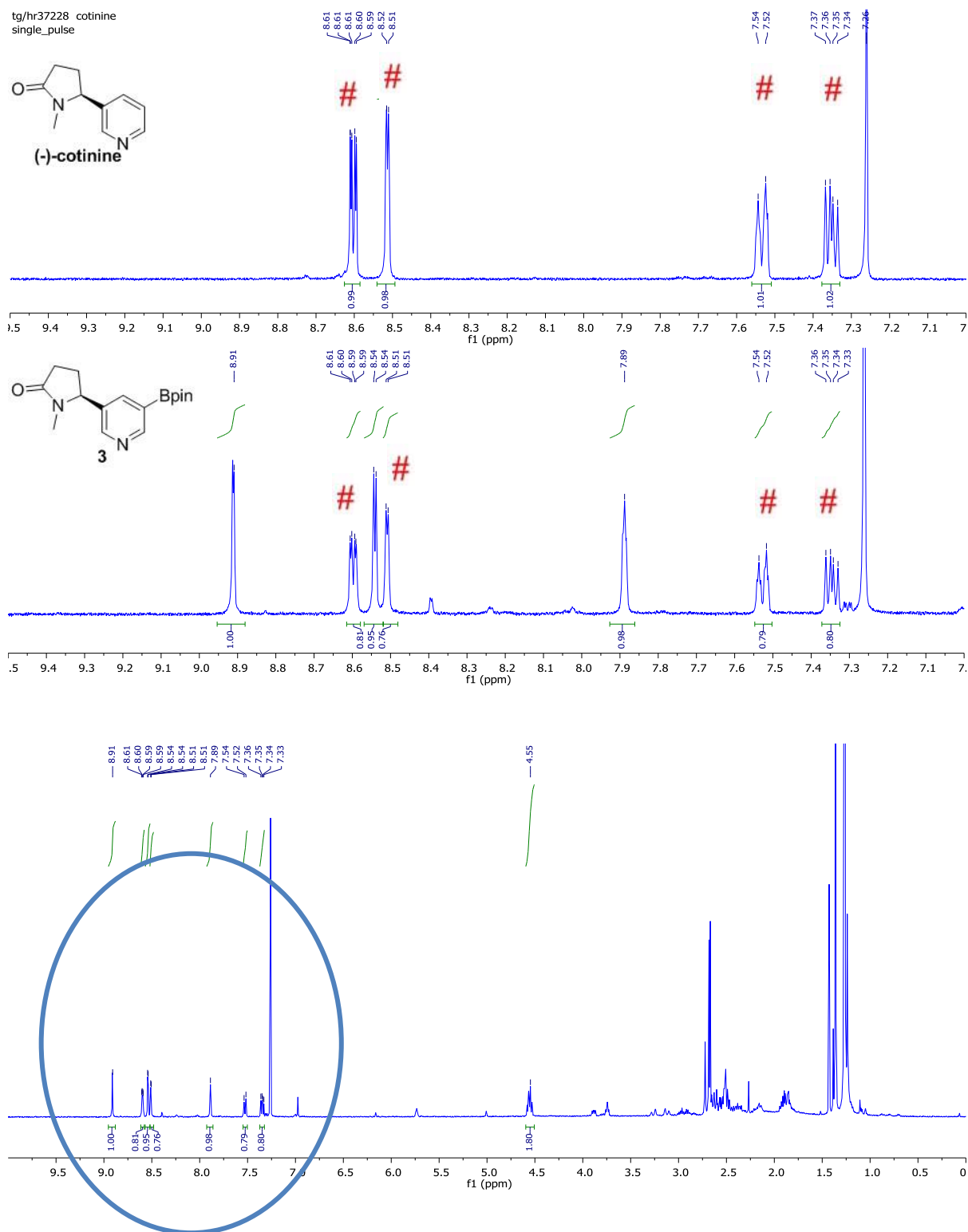
Contents:

Page 2: ^1H NMR of crude borylation reaction mixture comprising cotinine **2** and boronate ester **3**

Page 3-12: ^1H and ^{13}C NMR spectra of compounds **4** and **5a-h**.

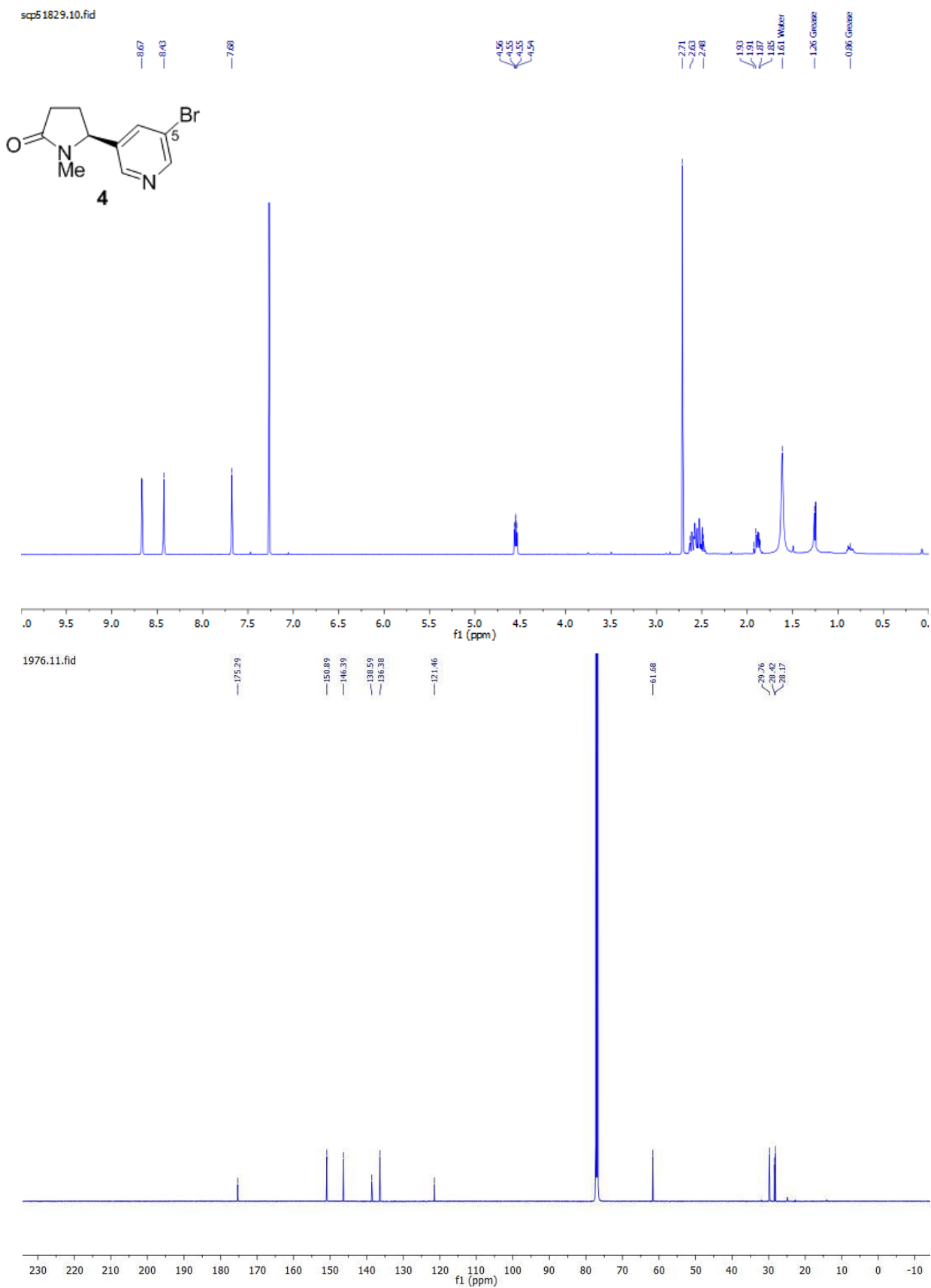
5-(4,4,5,5-Tetramethyl-1,3,2-dioxaborolan-2-yl)cotinine (**3**).

¹H-NMR (400 MHz): ¹H NMR of the crude borylation reaction mixture arising from Ir-catalysed borylation of (-)-cotinine **2** leading to **3**. ¹H NMR of (-)-cotinine **2** (starting material and marked by #) is shown for comparison alongside the reaction mixture containing the borylated product **3** with residual **2**. The aromatic region shown inside the blue circle has been amplified for clarity. Crude **3** was converted directly, without any purification, to **4**, which was then subjected to chromatography.



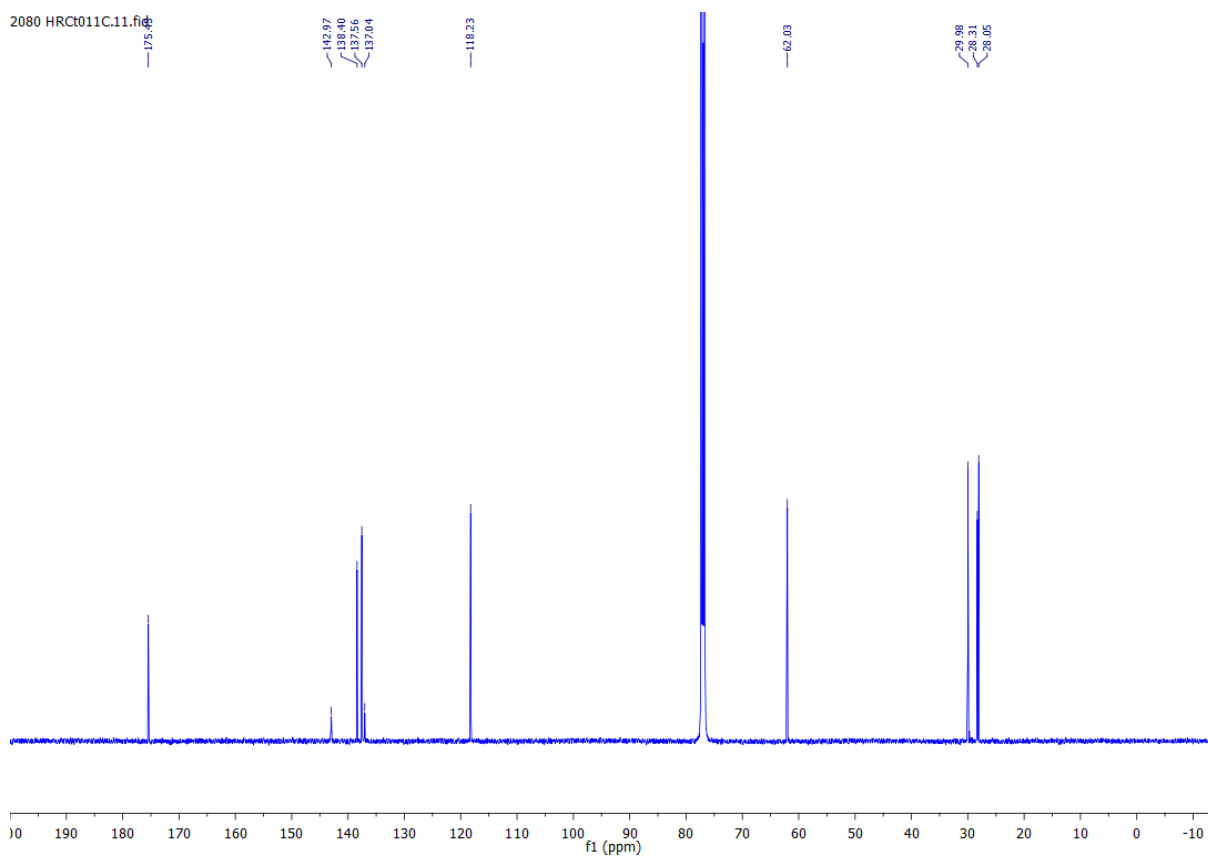
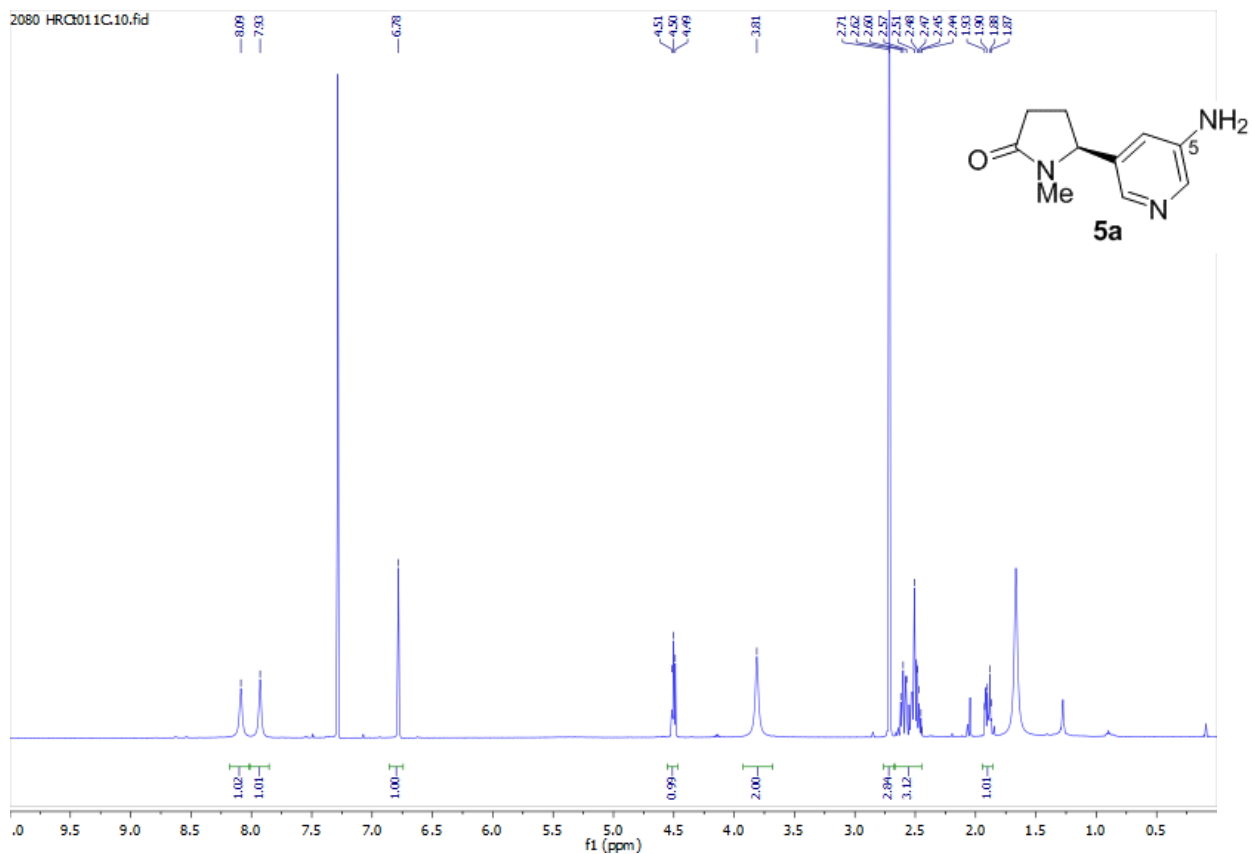
(-)-5-Bromocotinine (4).

$^1\text{H-NMR}$ (500 MHz), $^{13}\text{C-NMR}$ (125 MHz): CDCl_3



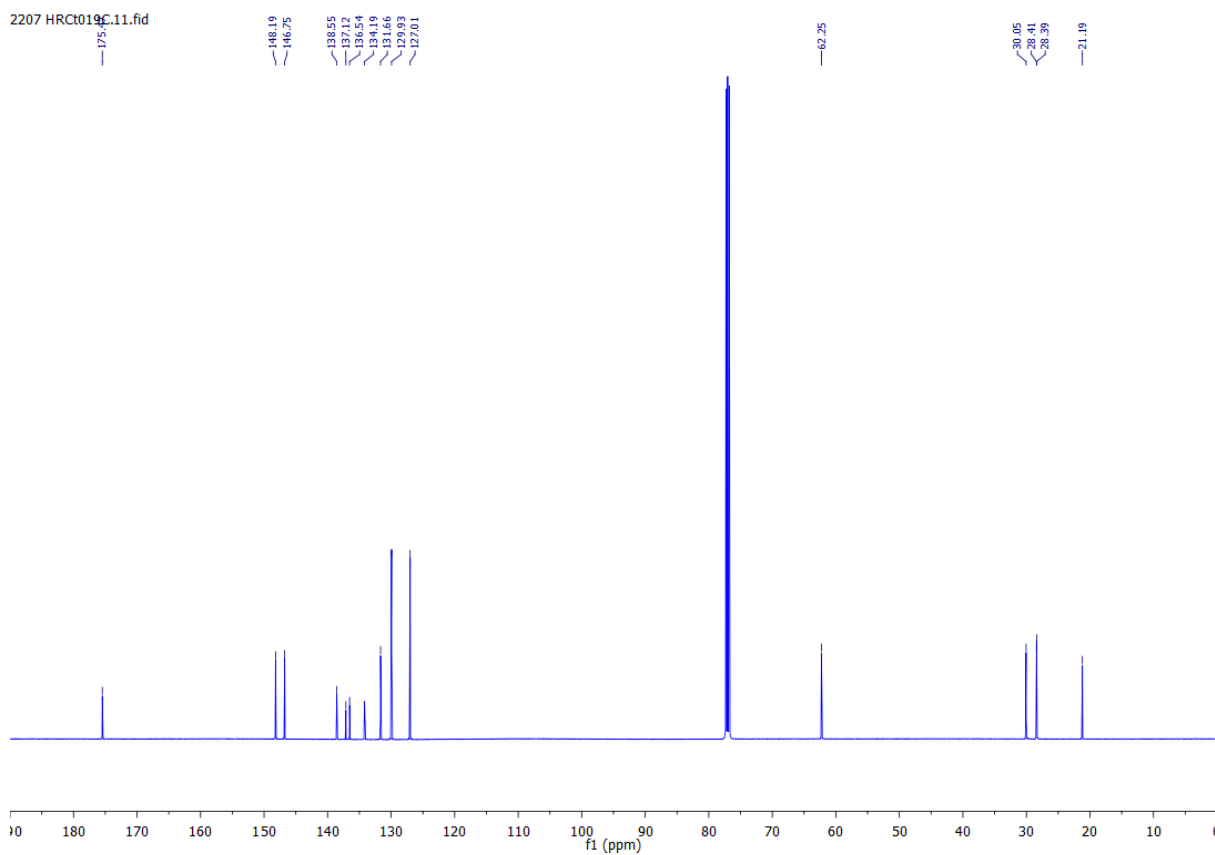
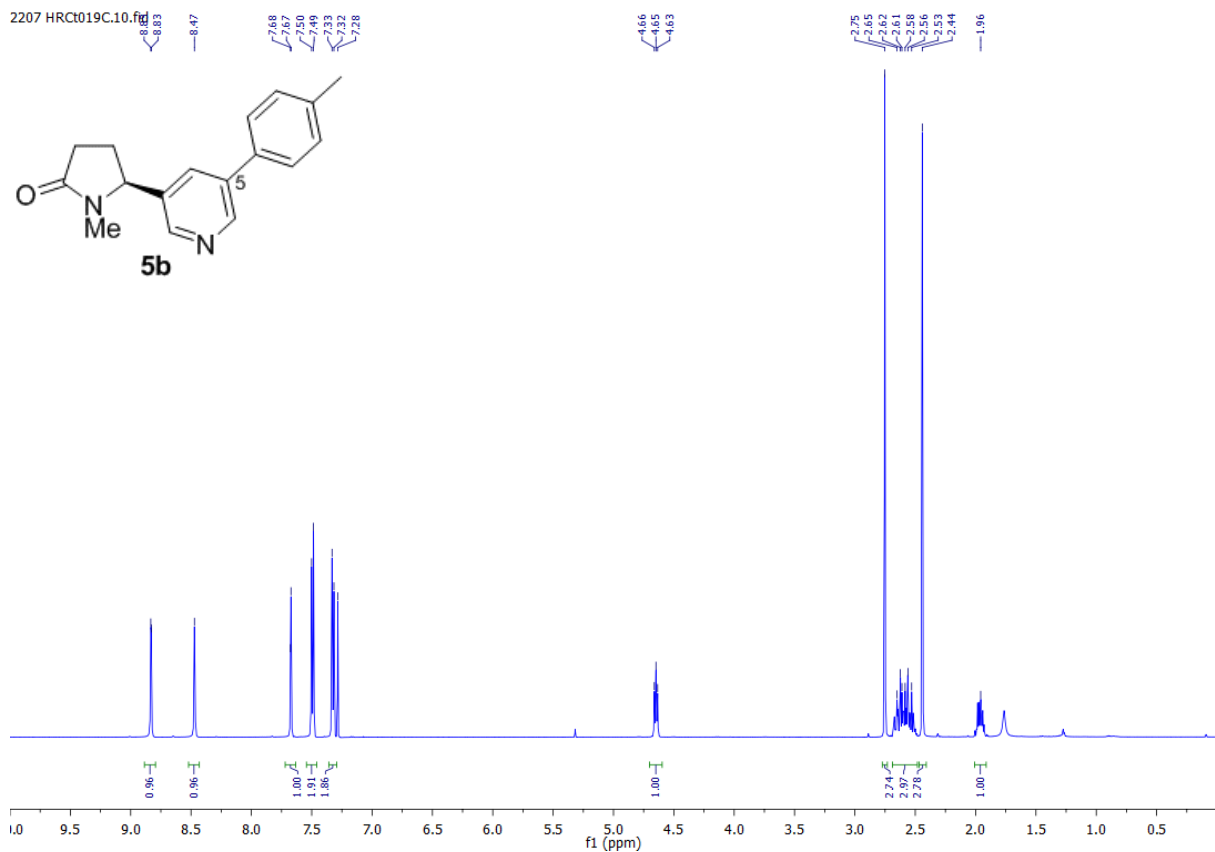
(-)-5-Aminocotinine (5a).

$^1\text{H-NMR}$ (500 MHz), $^{13}\text{C-NMR}$ (125 MHz): CDCl_3



(-)-5-(4-Tolyl)cotinine (5b).

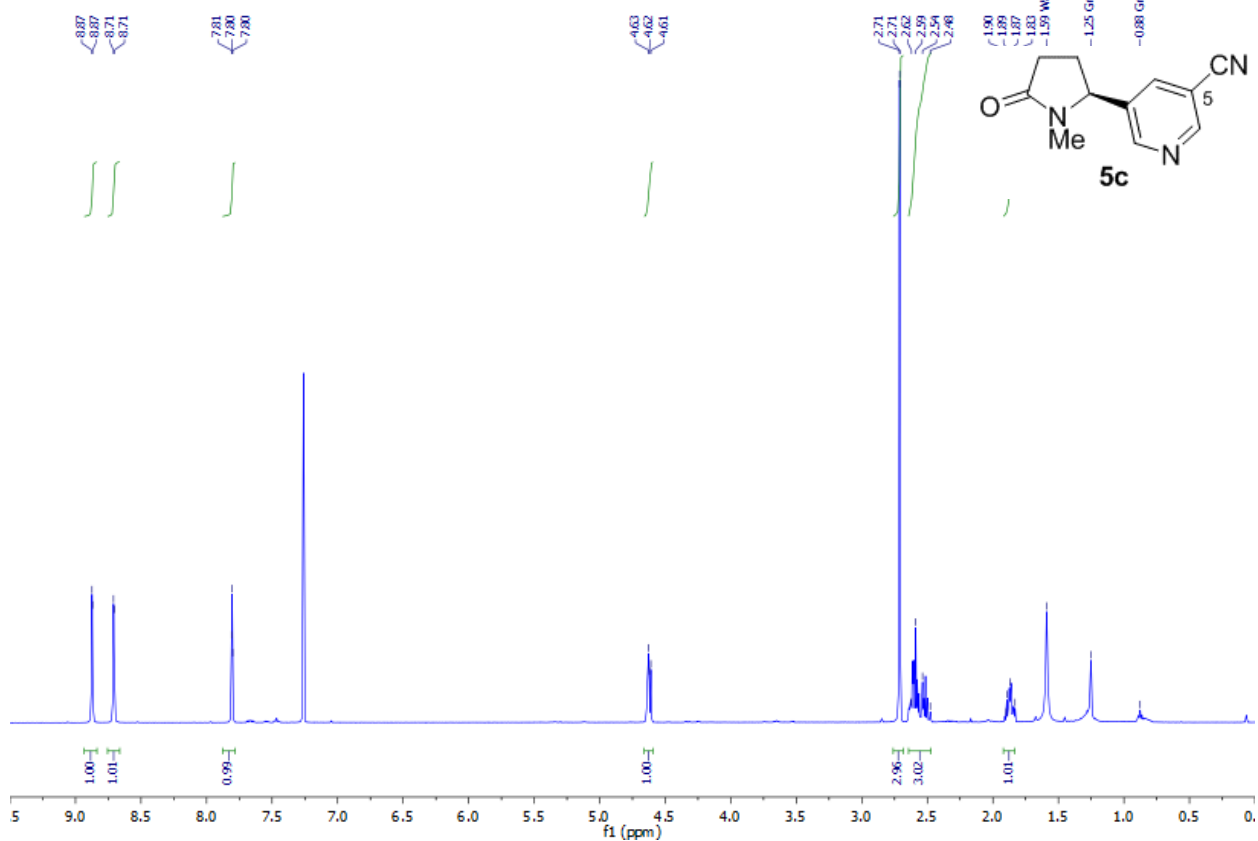
¹H-NMR (500 MHz), ¹³C-NMR (125 MHz): CDCl₃



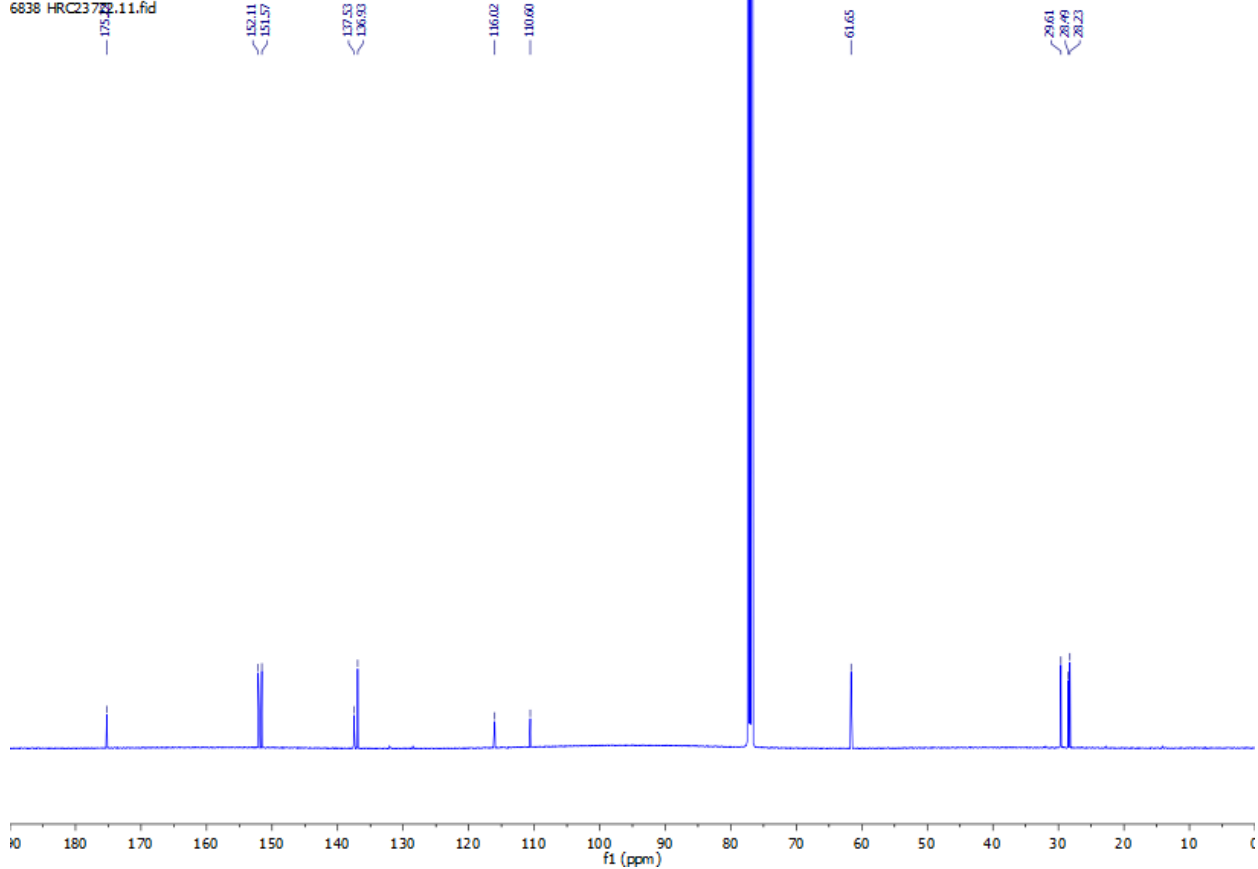
(-)-5-Cyanocotinine (5c).

¹H-NMR (500 MHz), ¹³C-NMR (125 MHz): CDCl₃

6838_HRC23722.10.fid



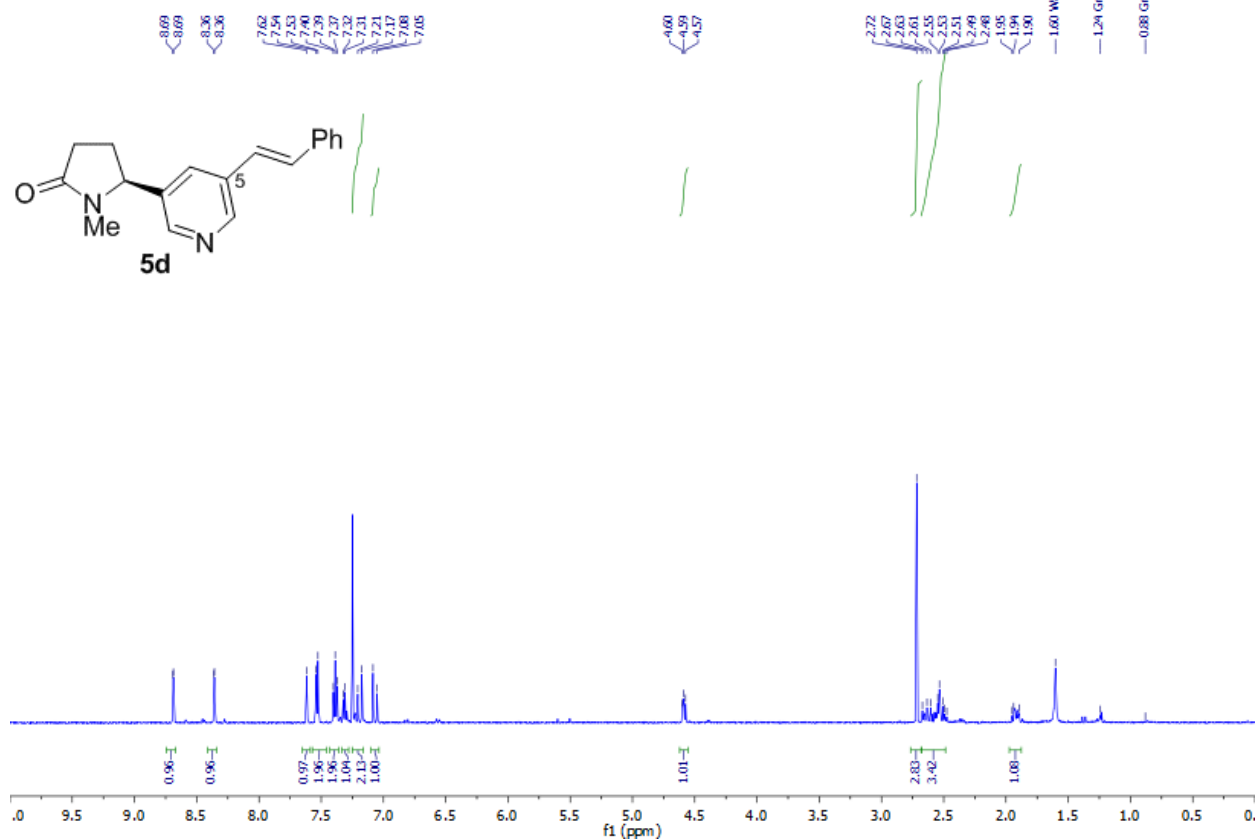
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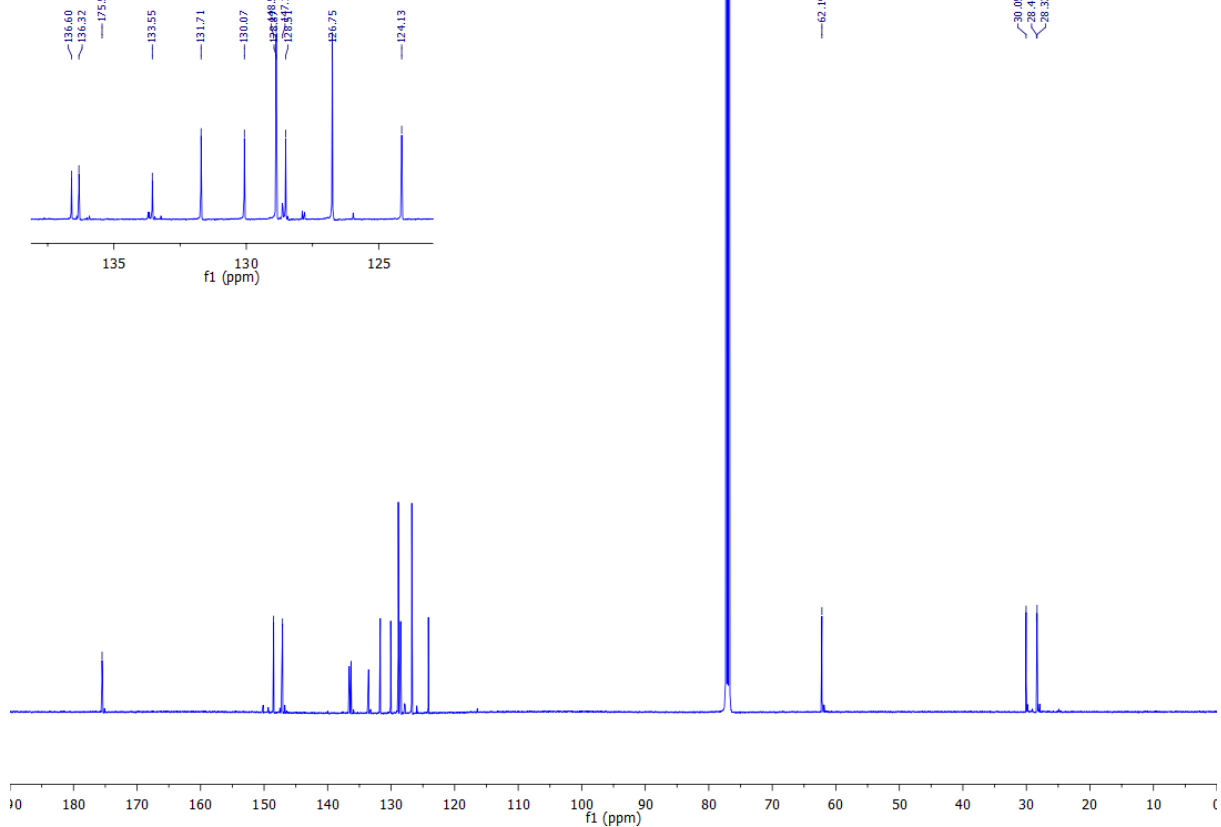
(-)-5-(E-2-Phenylethenyl)cotinine (5d).

¹H-NMR (500 MHz), ¹³C-NMR (125 MHz): CDCl₃

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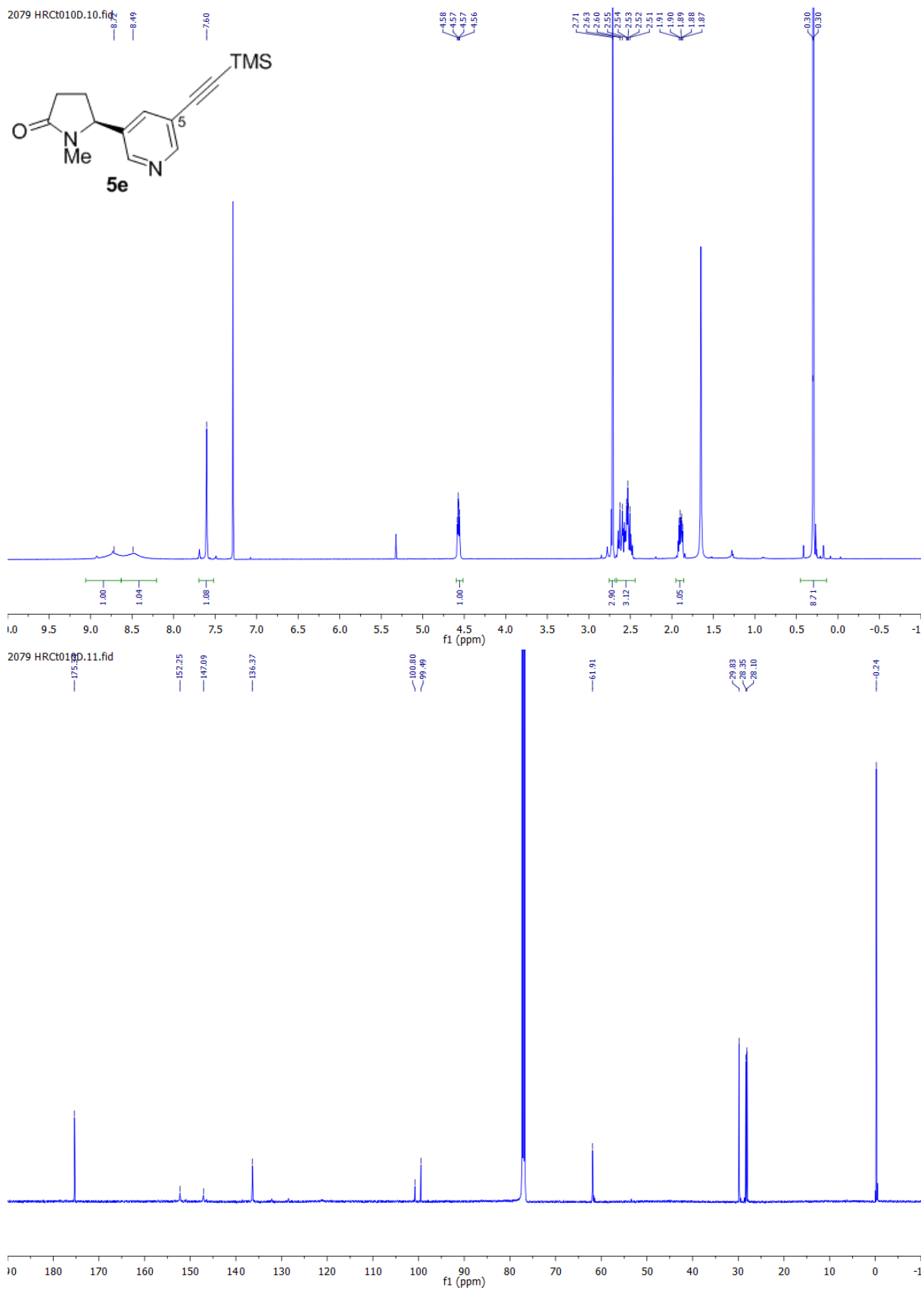


2217 HRC018C.11.fid



(-)-5-(2-Trimethylsilylethynyl)cotinine (5e).

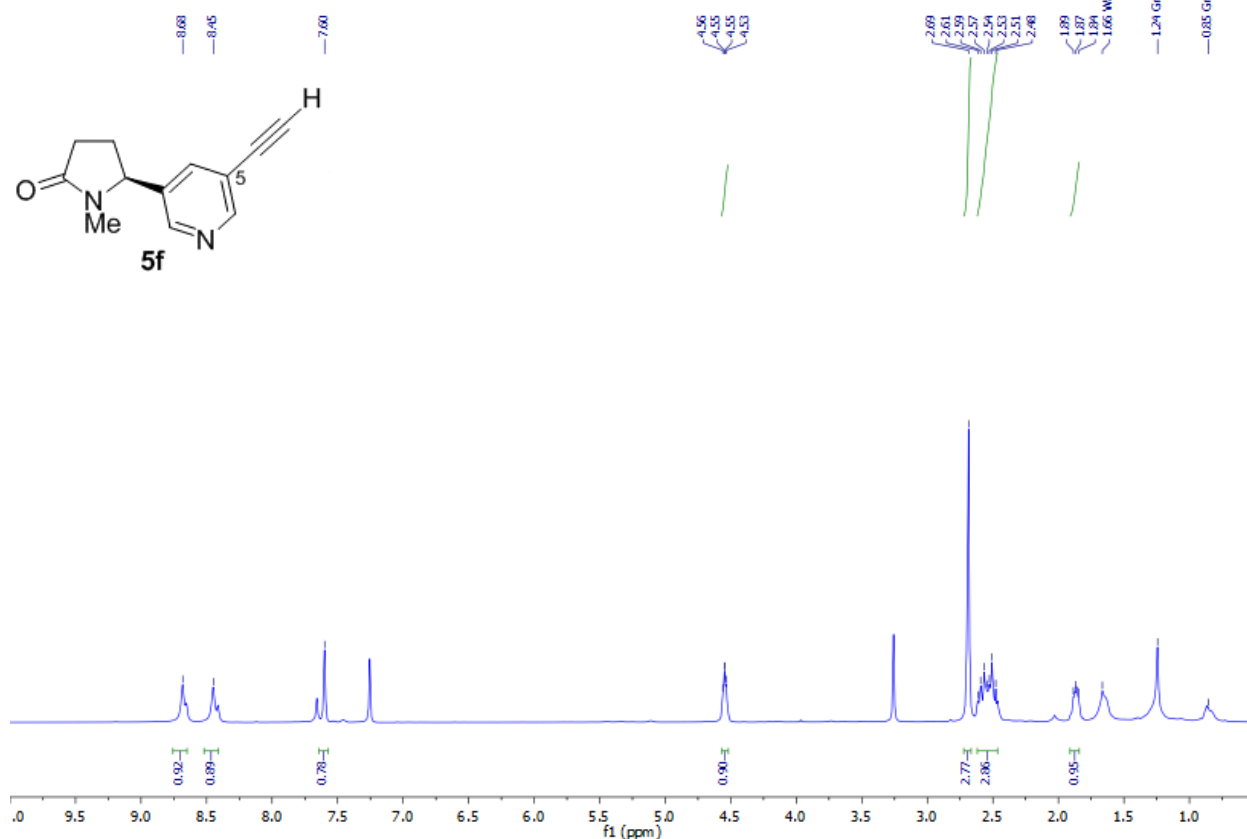
¹H-NMR (500 MHz), ¹³C-NMR (125 MHz): CDCl₃



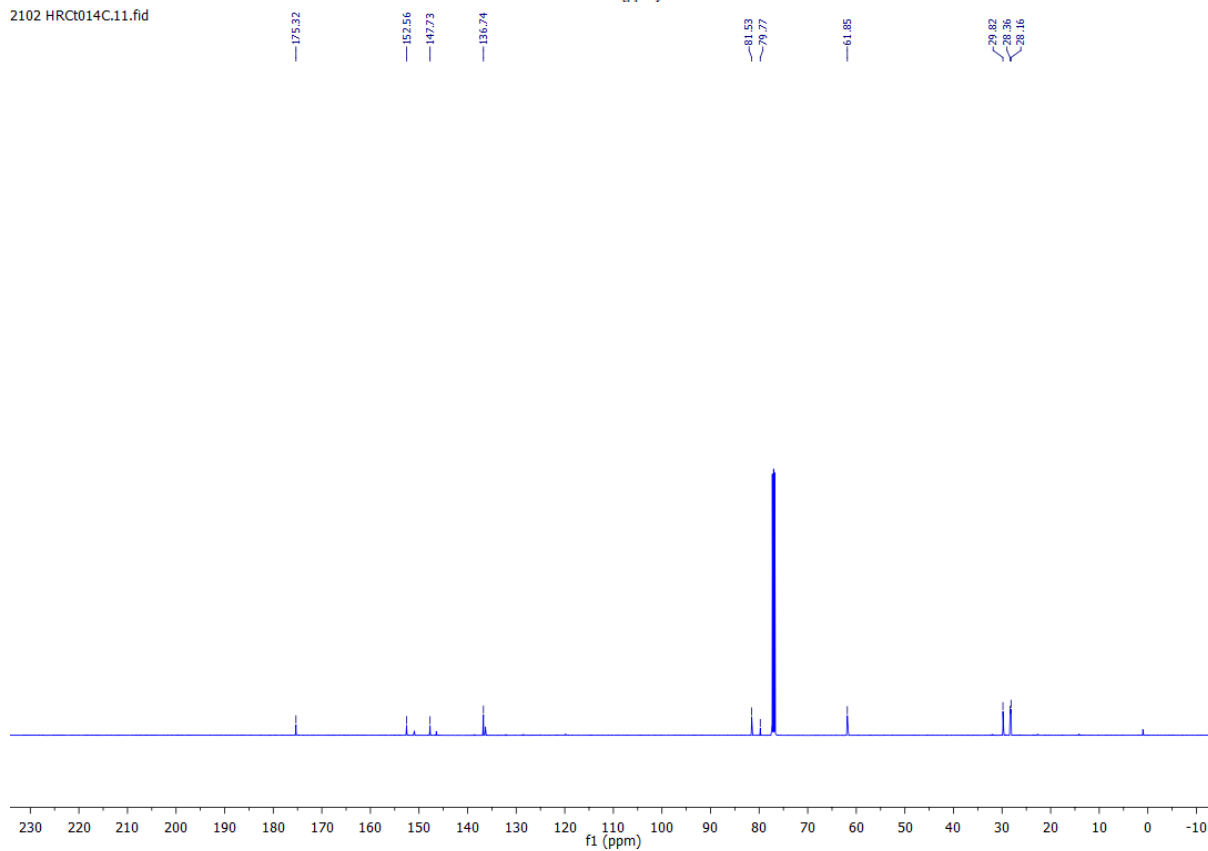
(-)-5-Ethynylcotinine (5f).

¹H-NMR (500 MHz), ¹³C-NMR (125 MHz): CDCl₃

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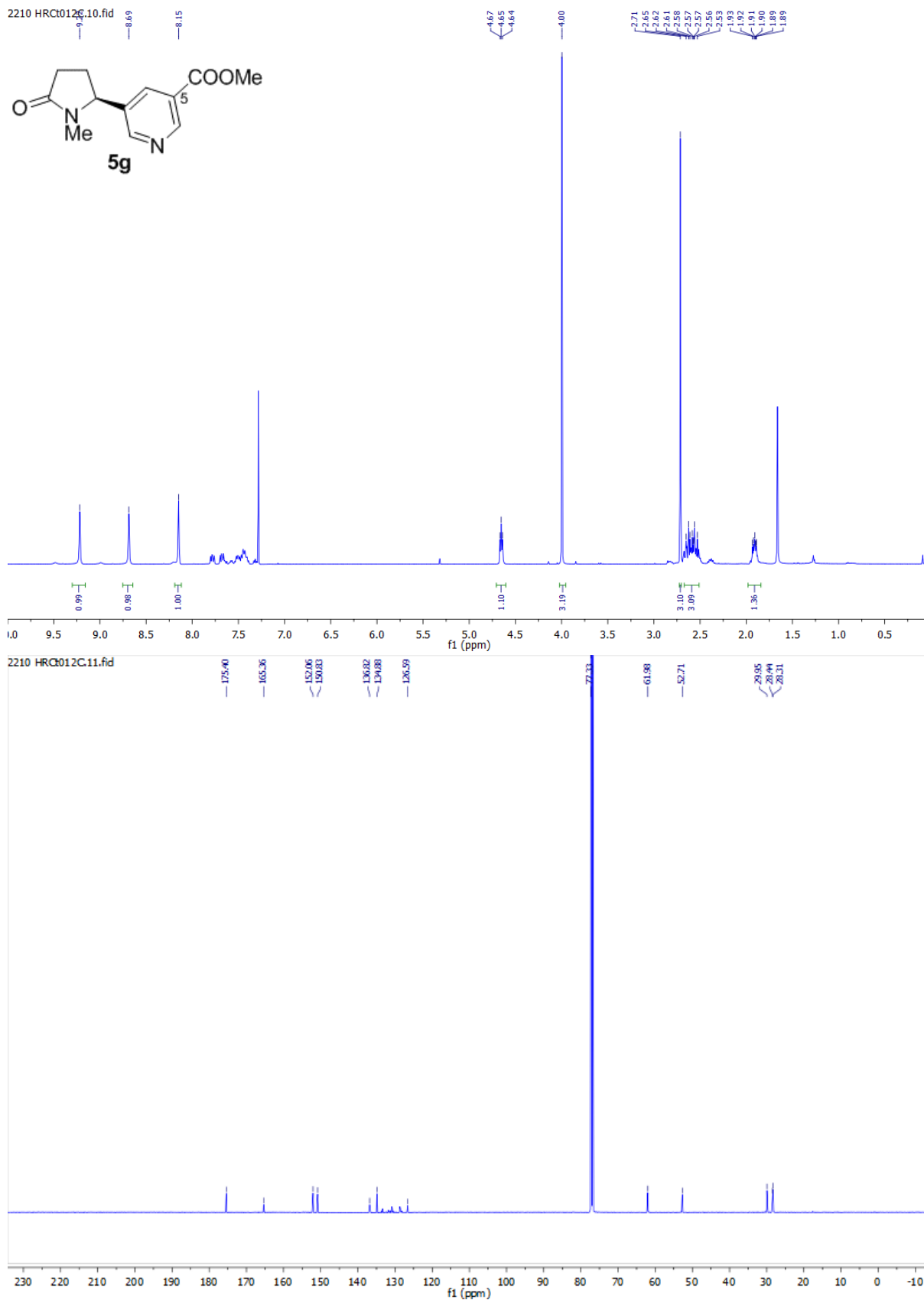


2102 HRC014C.11.fid



(+)-Methyl cotinine-5-carboxylate (5g).

¹H-NMR (500 MHz), ¹³C-NMR (125 MHz): CDCl₃



(+)-5-(Cotinin-5-yl)-cotinine (5h).

¹H-NMR (500 MHz), ¹³C-NMR (125 MHz): CDCl₃

