

## Supplementary Information 2

### **In Search of Herbistasis: COT-Metsulfuron Methyl Displays Rare Herbistatic Properties**

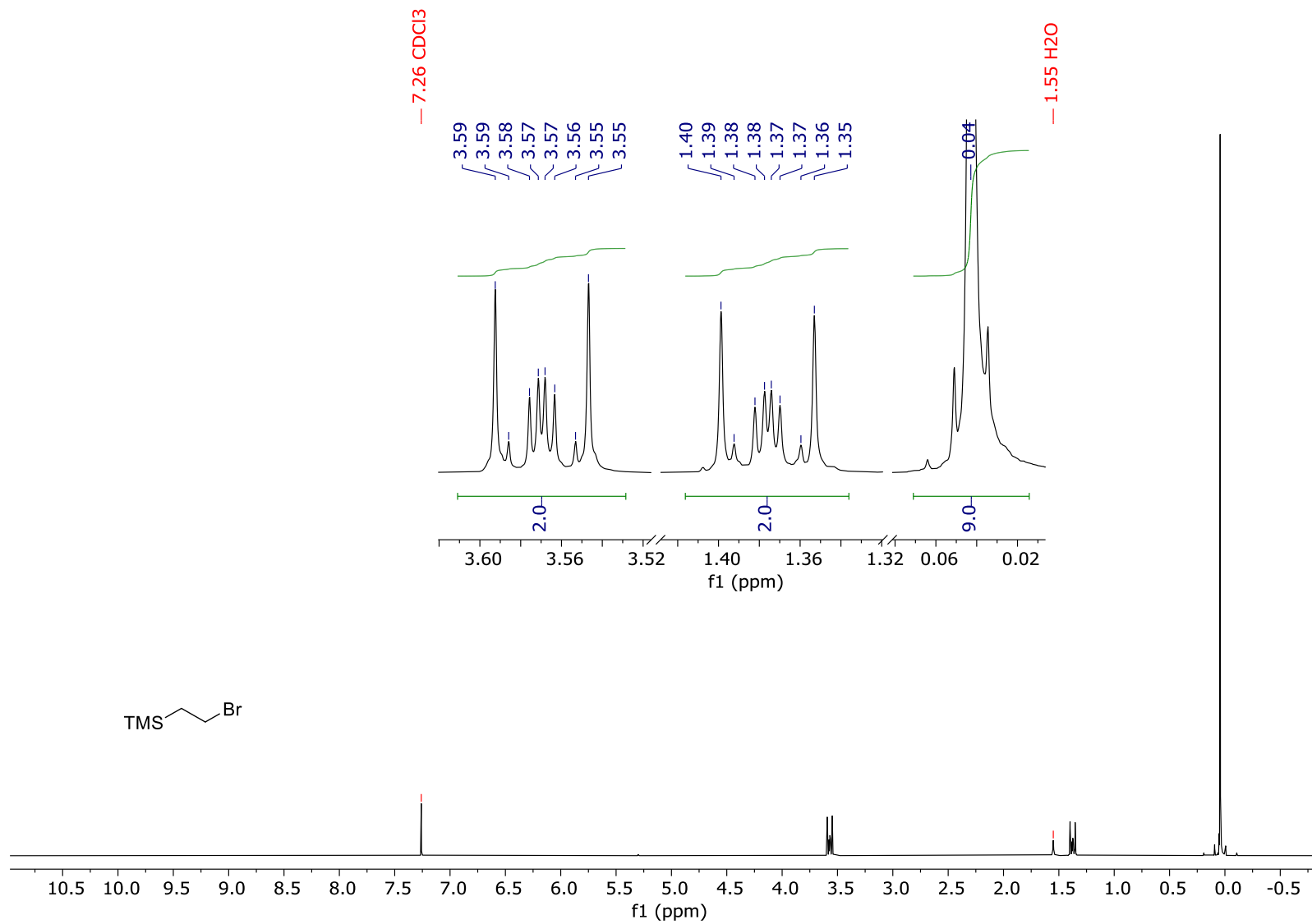
Hui Xing, Sarah K. M. McGregor, Bruna D. Batista, Cassidy Whitefield, Isobella S. J. Stone, Cody-Ellen Murray, Rebecca M. Hurst, Yizhou Liu, Sharon Chow, Tyler Fahrenhorst-Jones, Qi Zhao, Sevan D. Houston, Shu-Hong Hu, Thierry Lonhienne, Amanda Nouwens, Jed M. Burns, G. Paul Savage, Gimme H. Walter, Luke W. Guddat, Michelle A. Rafter and Craig M. Williams\*

## Characterisation Spectra

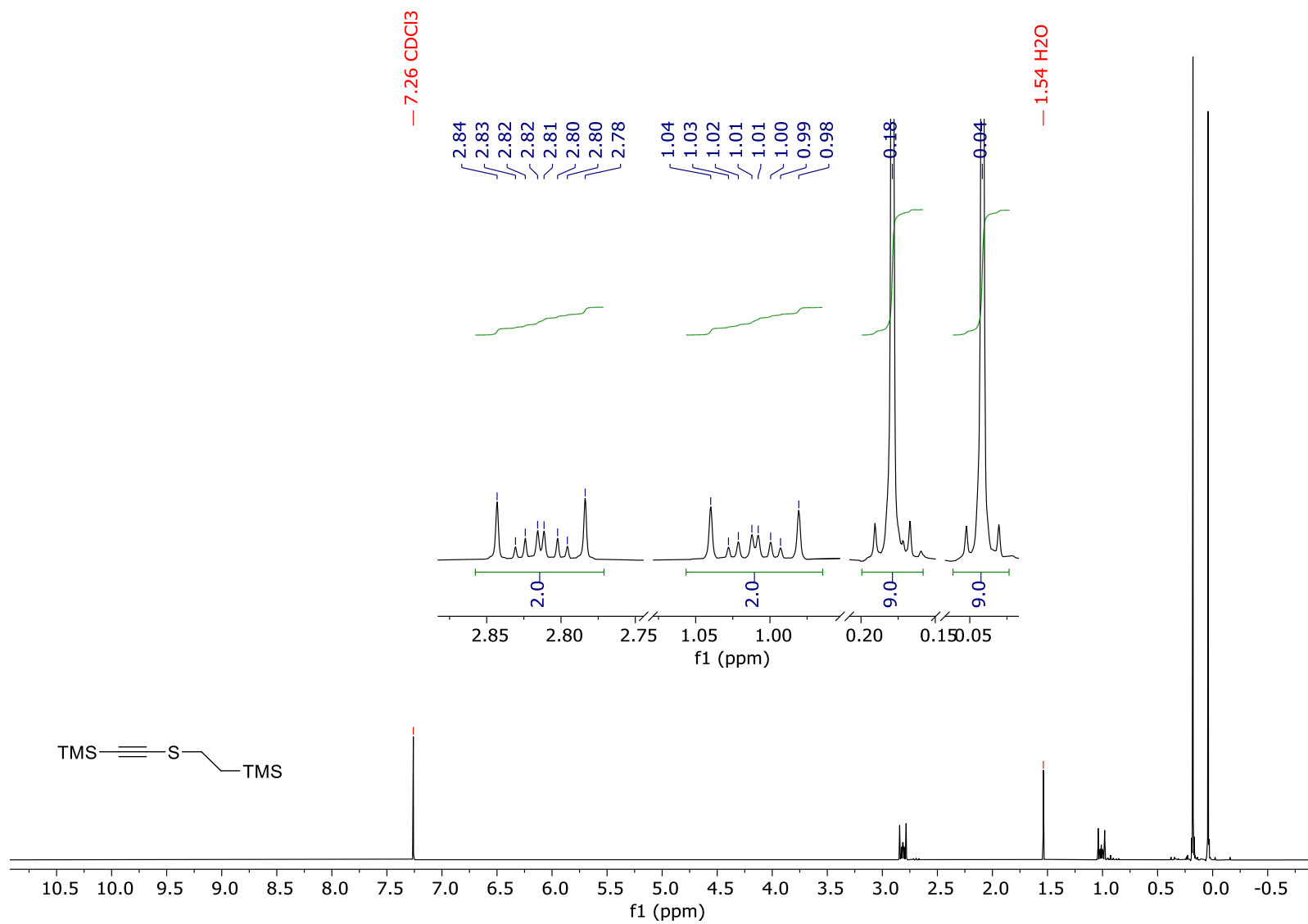
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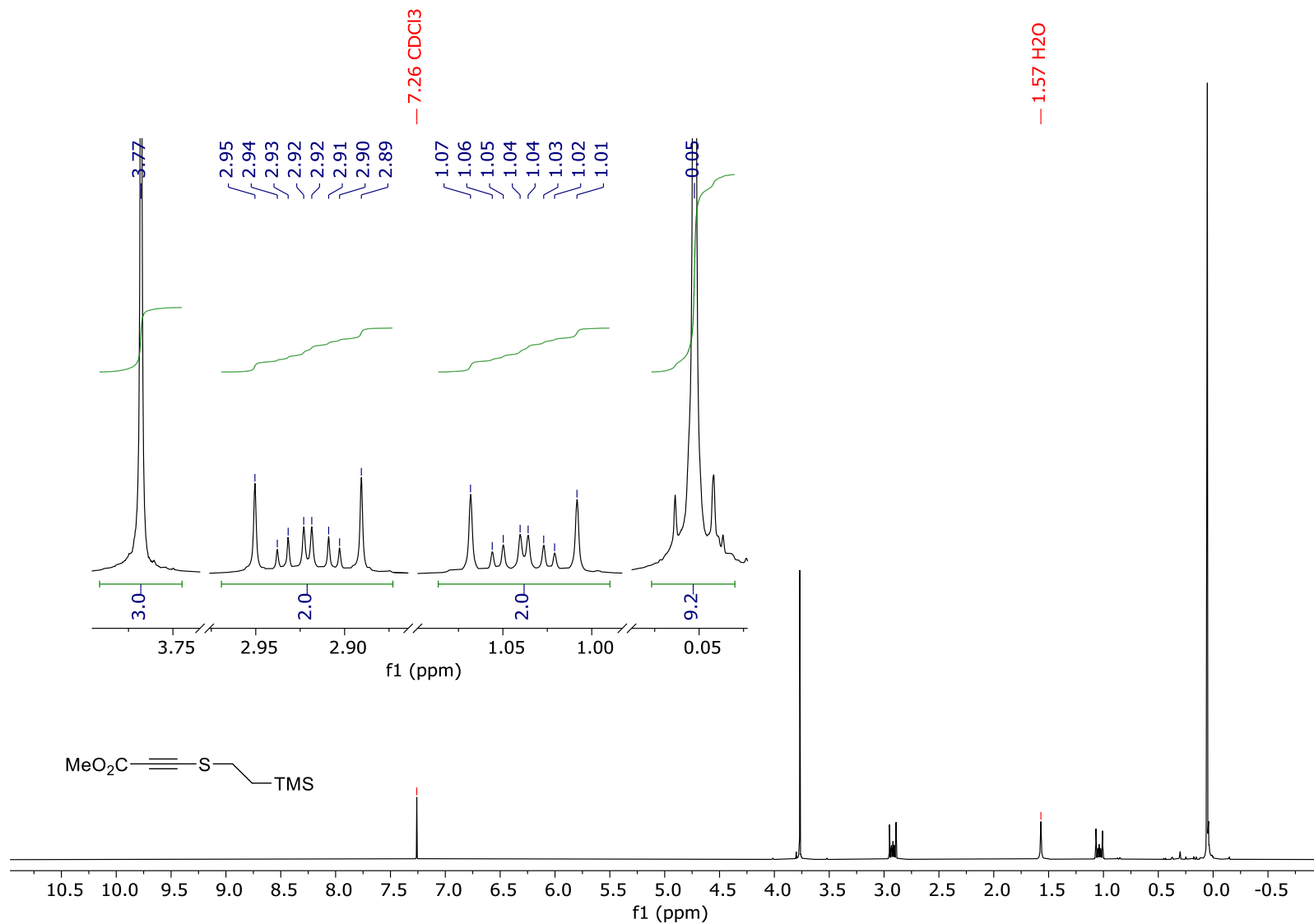
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) of (2-Bromoethyl)trimethylsilane (18)



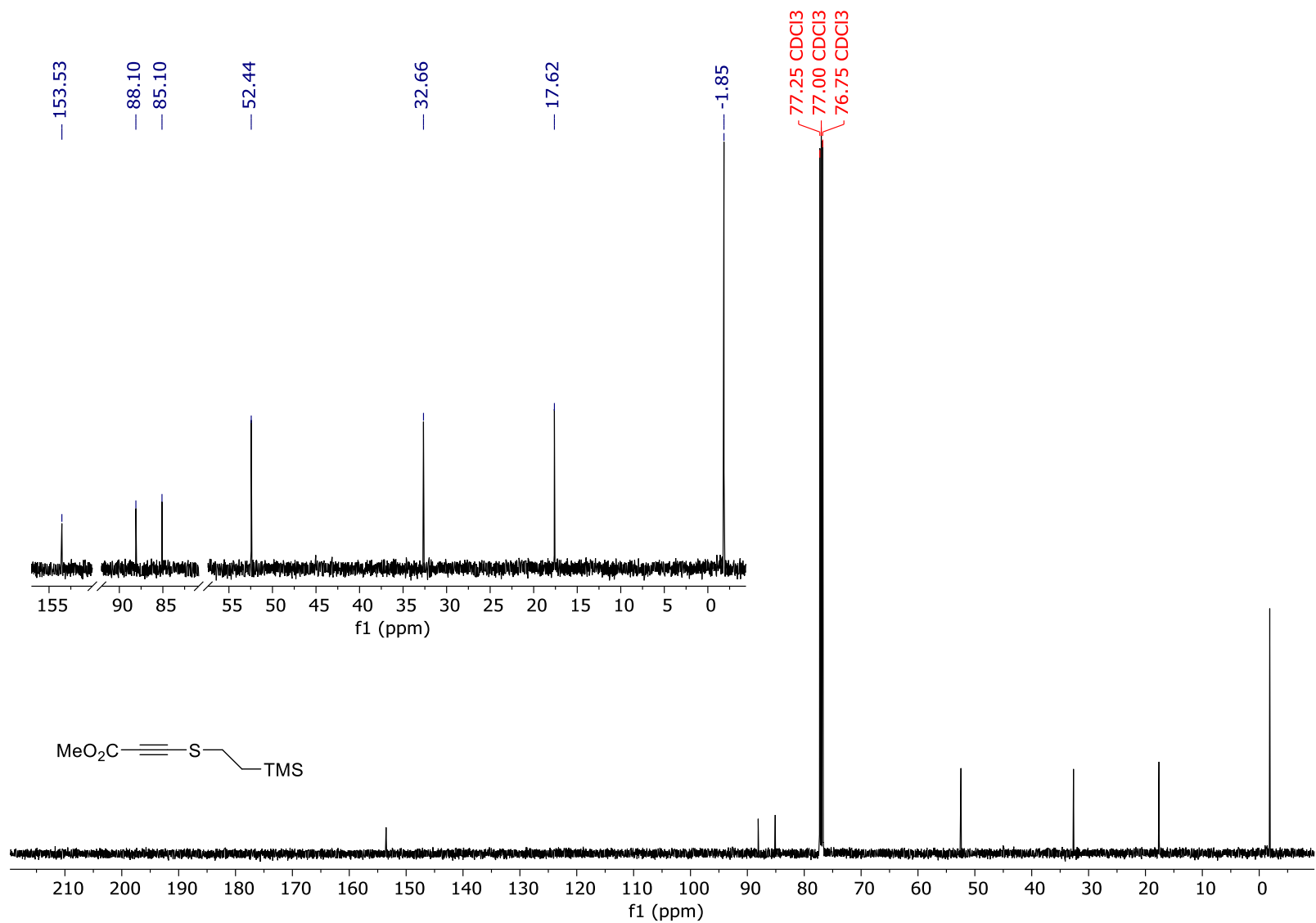
$^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ ) of Trimethyl(((2-(trimethylsilyl)ethyl)thio)ethynyl)silane (21)



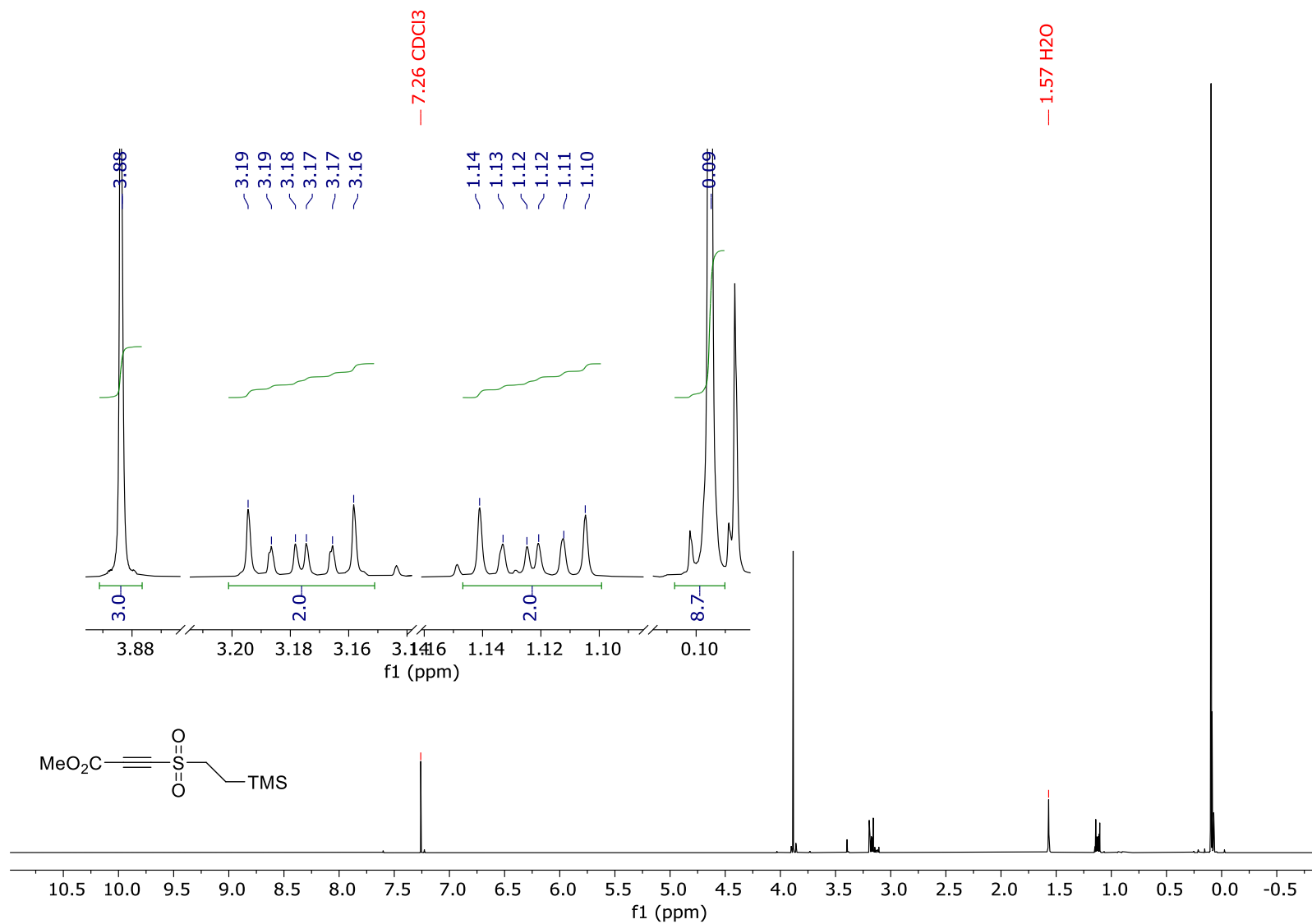
$^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ ) of Methyl 3-((2-(trimethylsilyl)ethyl)thio)propiolate (22)



<sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) of Methyl 3-((2-(trimethylsilyl)ethyl)thio)propiolate (22)

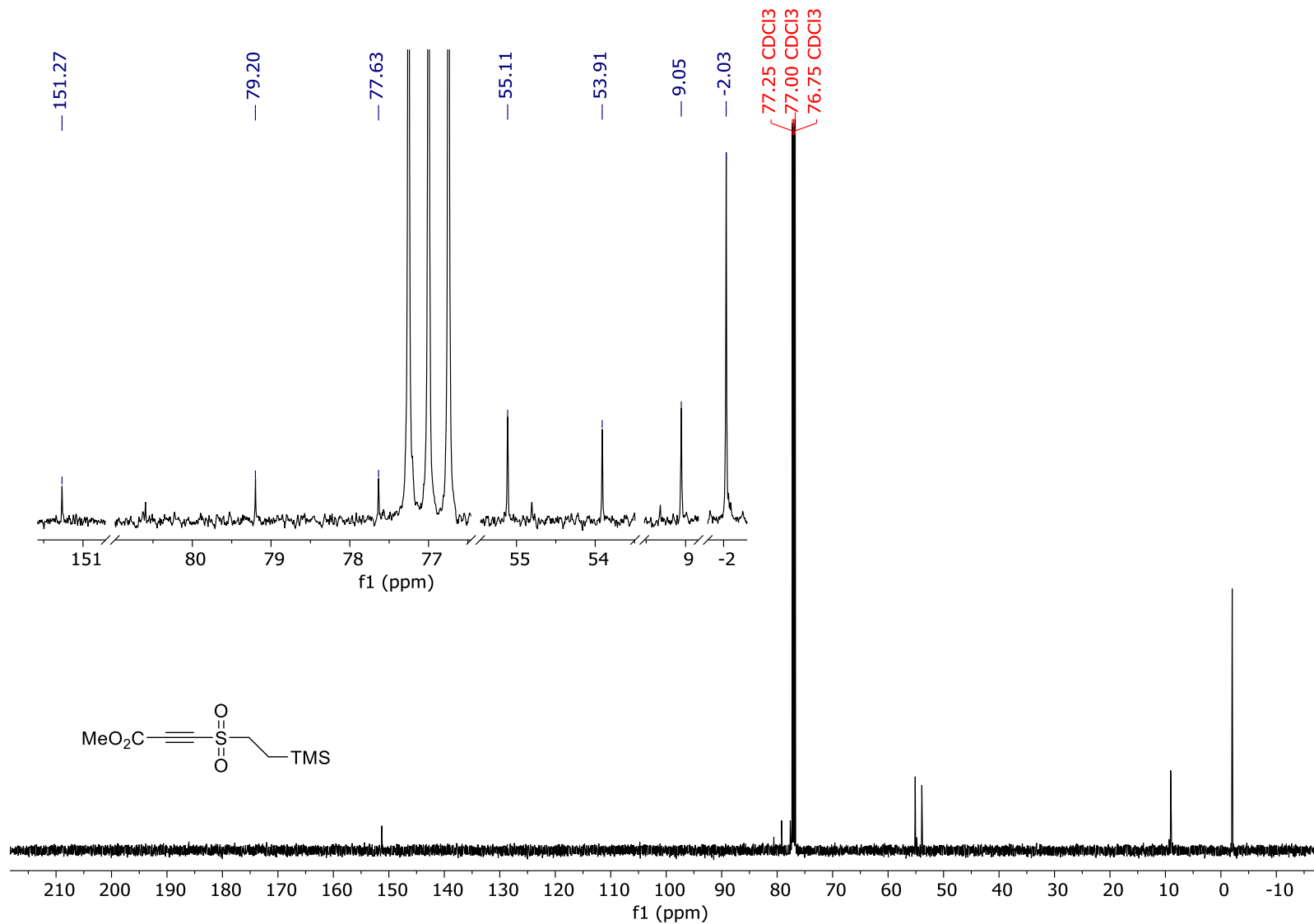


$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) of Methyl 3-((2-(trimethylsilyl)ethyl)sulfonyl)propiolate (15)

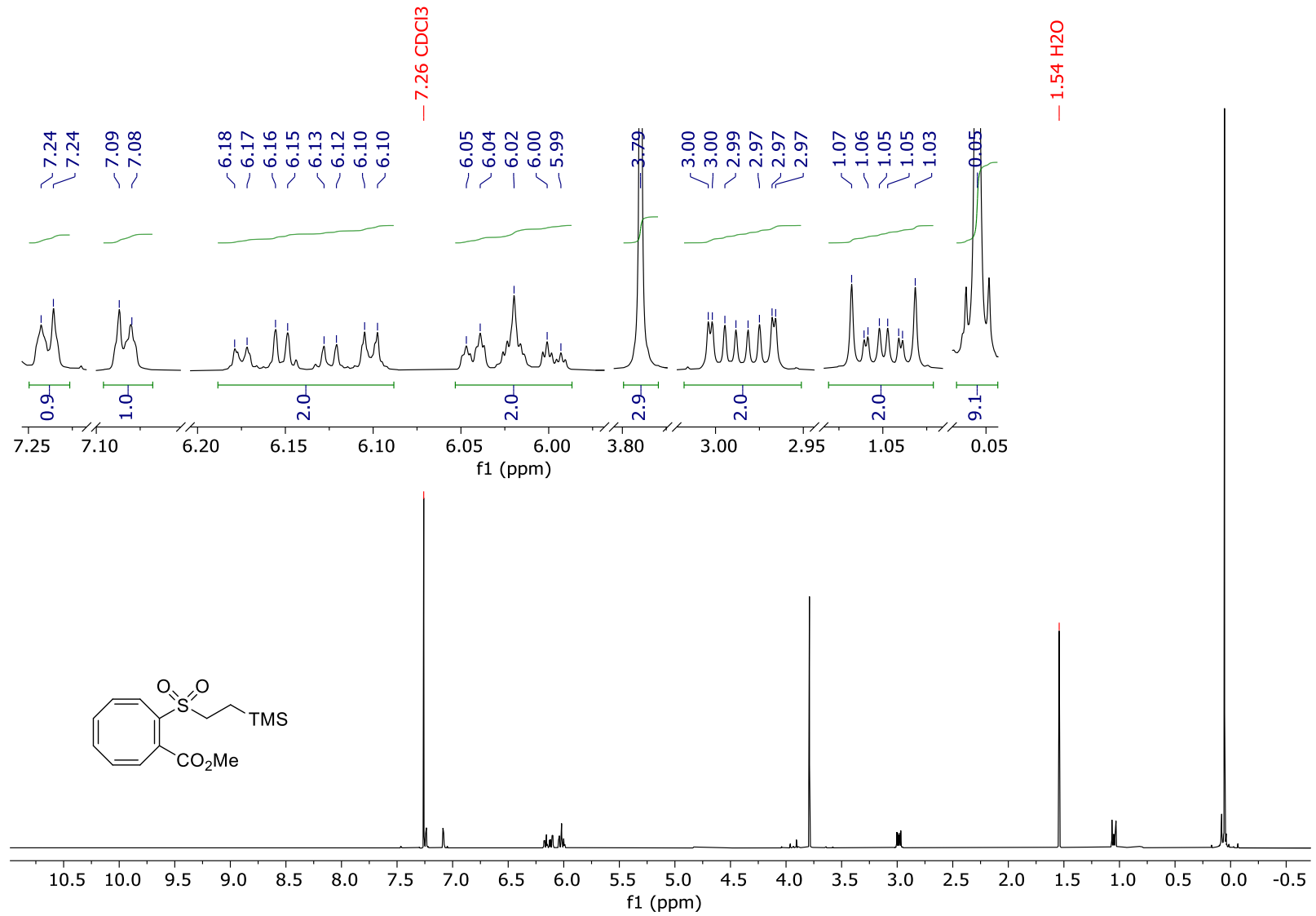




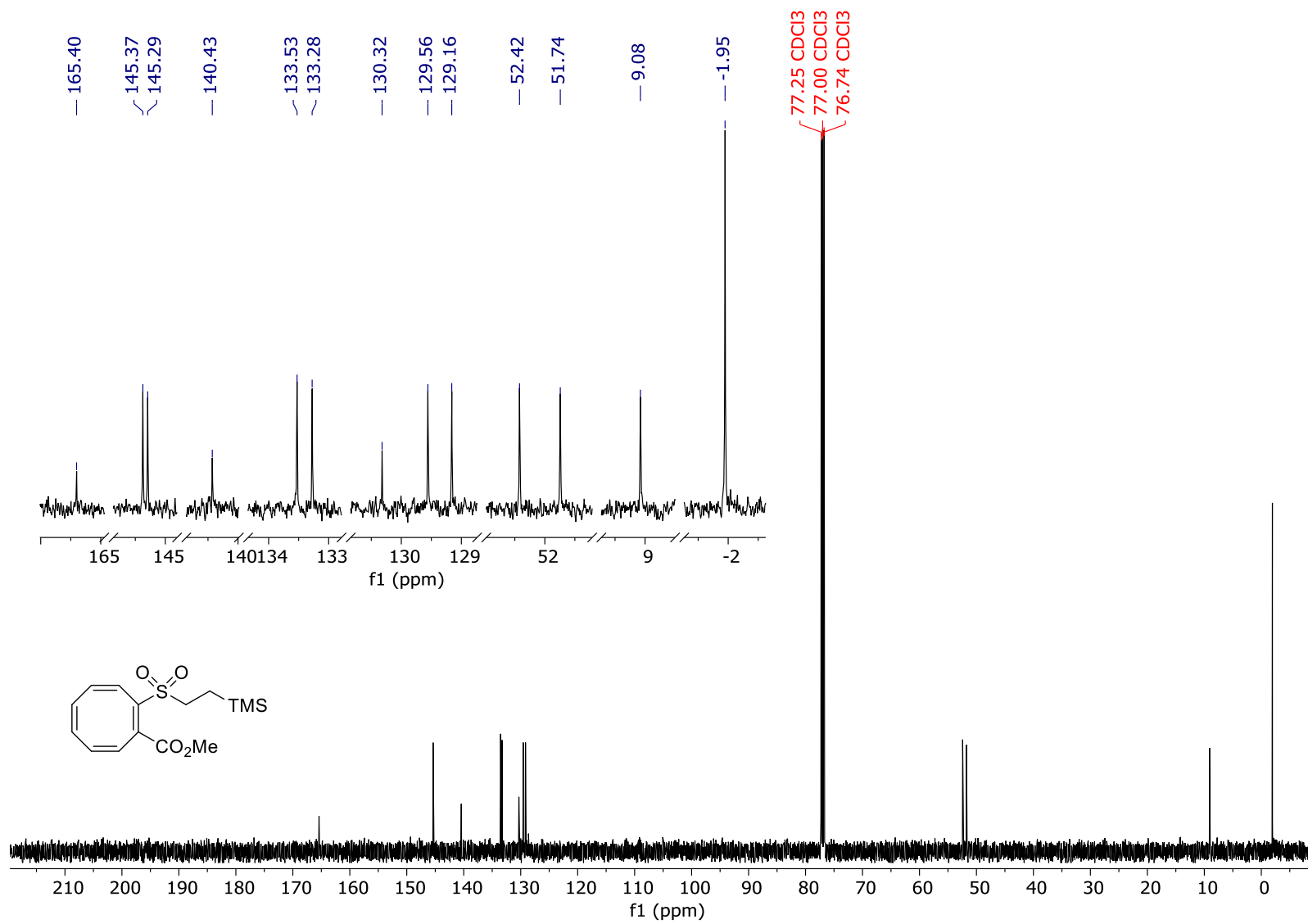
<sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) of Methyl 3-((2-(trimethylsilyl)ethyl)sulfonyl)propiolate (15)



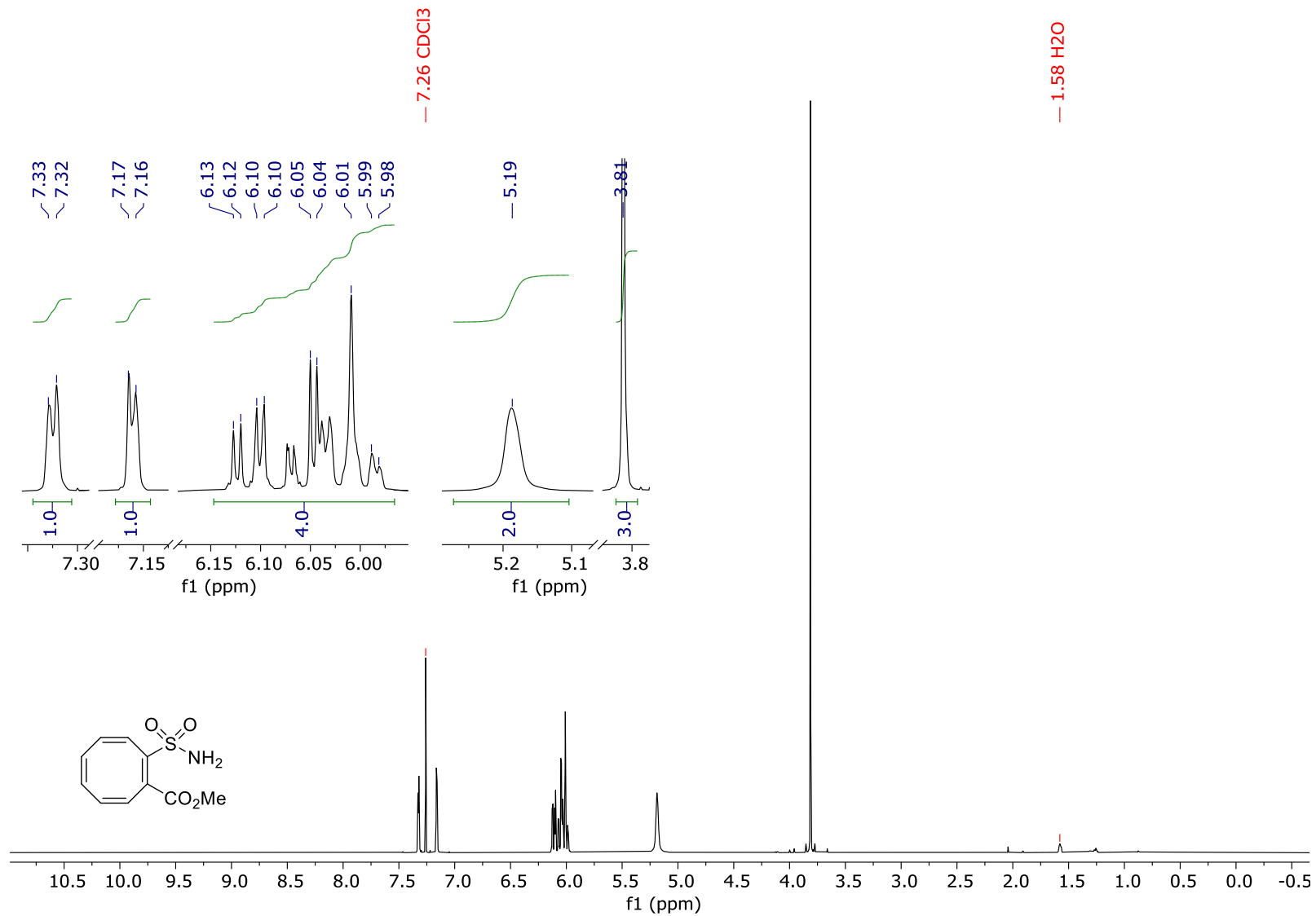
<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) of Methyl 2-((2-(trimethylsilyl)ethyl)sulfonyl)cycloocta-1,3,5,7-tetraene-1-carboxylate (23)



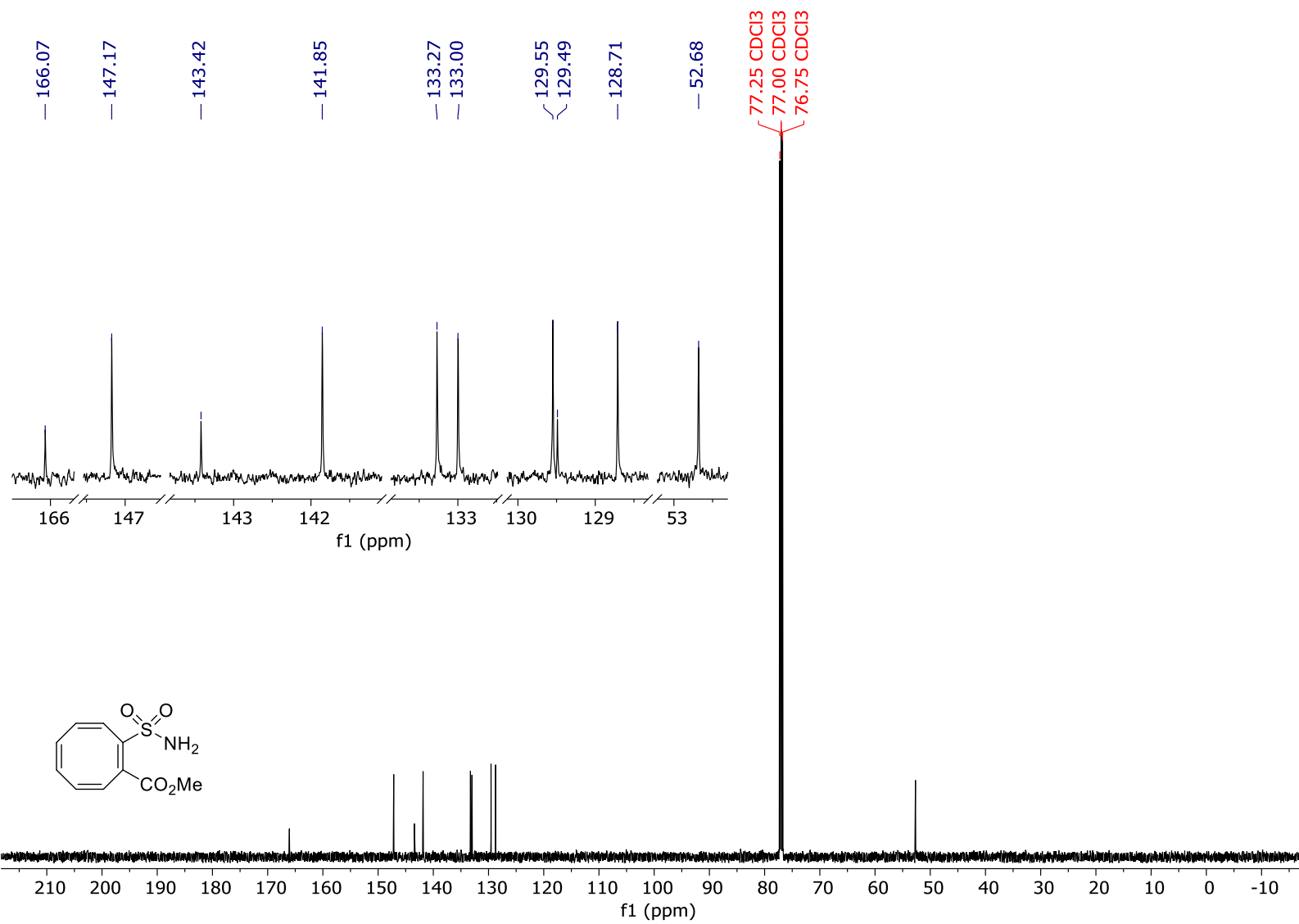
<sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) of Methyl 2-((2-(trimethylsilyl)ethyl)sulfonyl)cycloocta-1,3,5,7-tetraene-1-carboxylate (23)



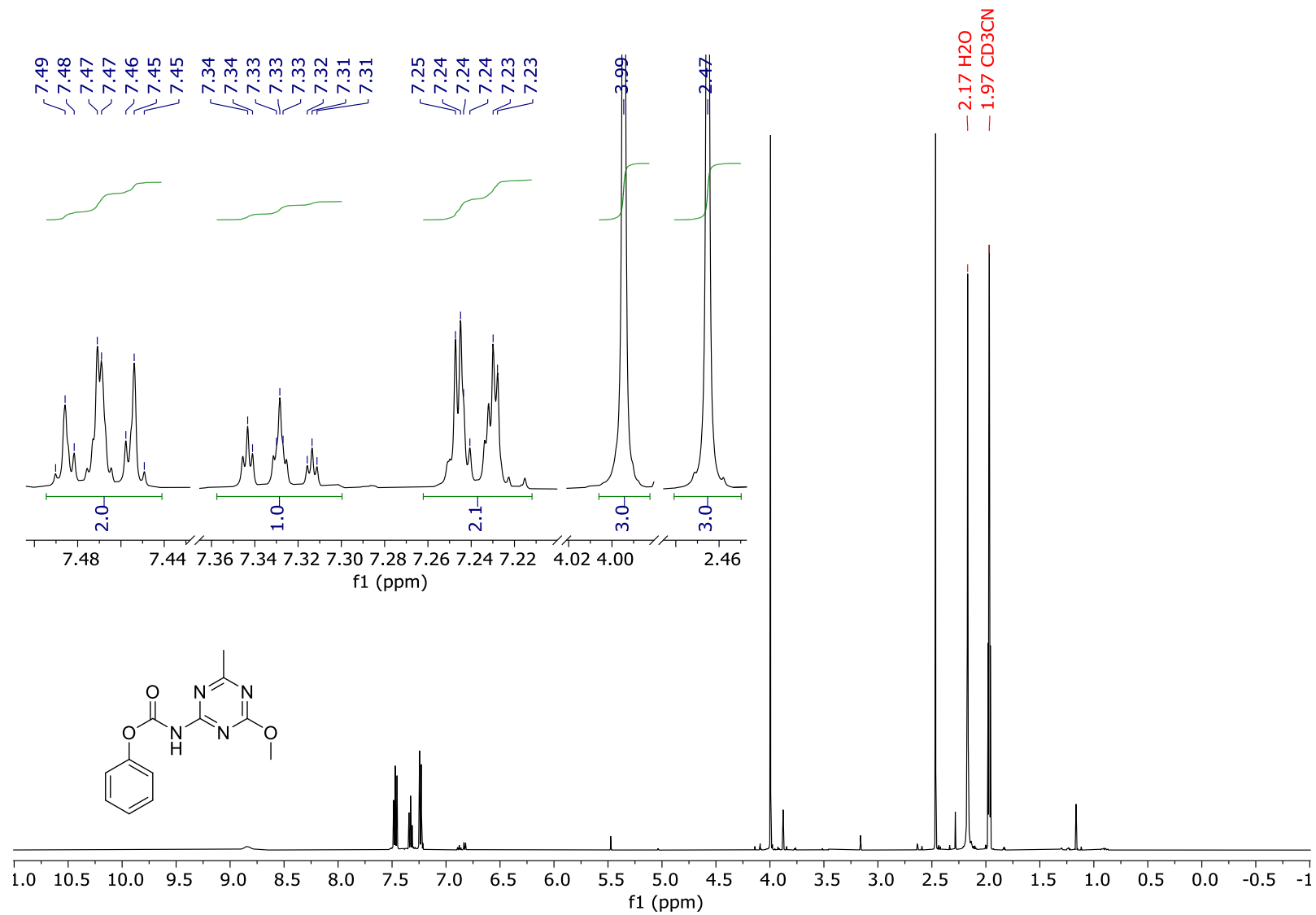
$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) of Methyl 2-sulfamoylcycloocta-1,3,5,7-tetraene-1-carboxylate (24)



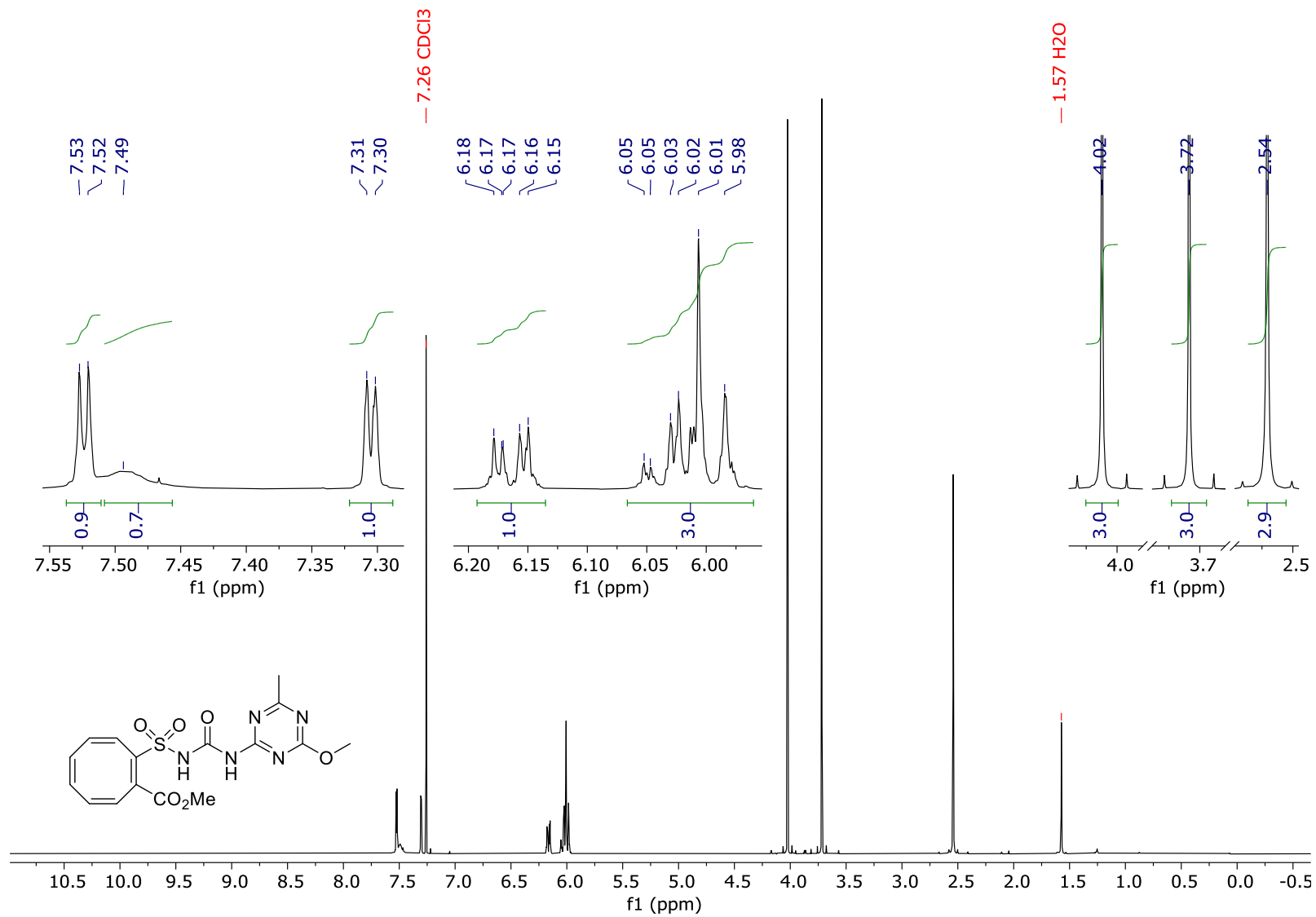
<sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) of Methyl 2-sulfamoylcycloocta-1,3,5,7-tetraene-1-carboxylate (24)



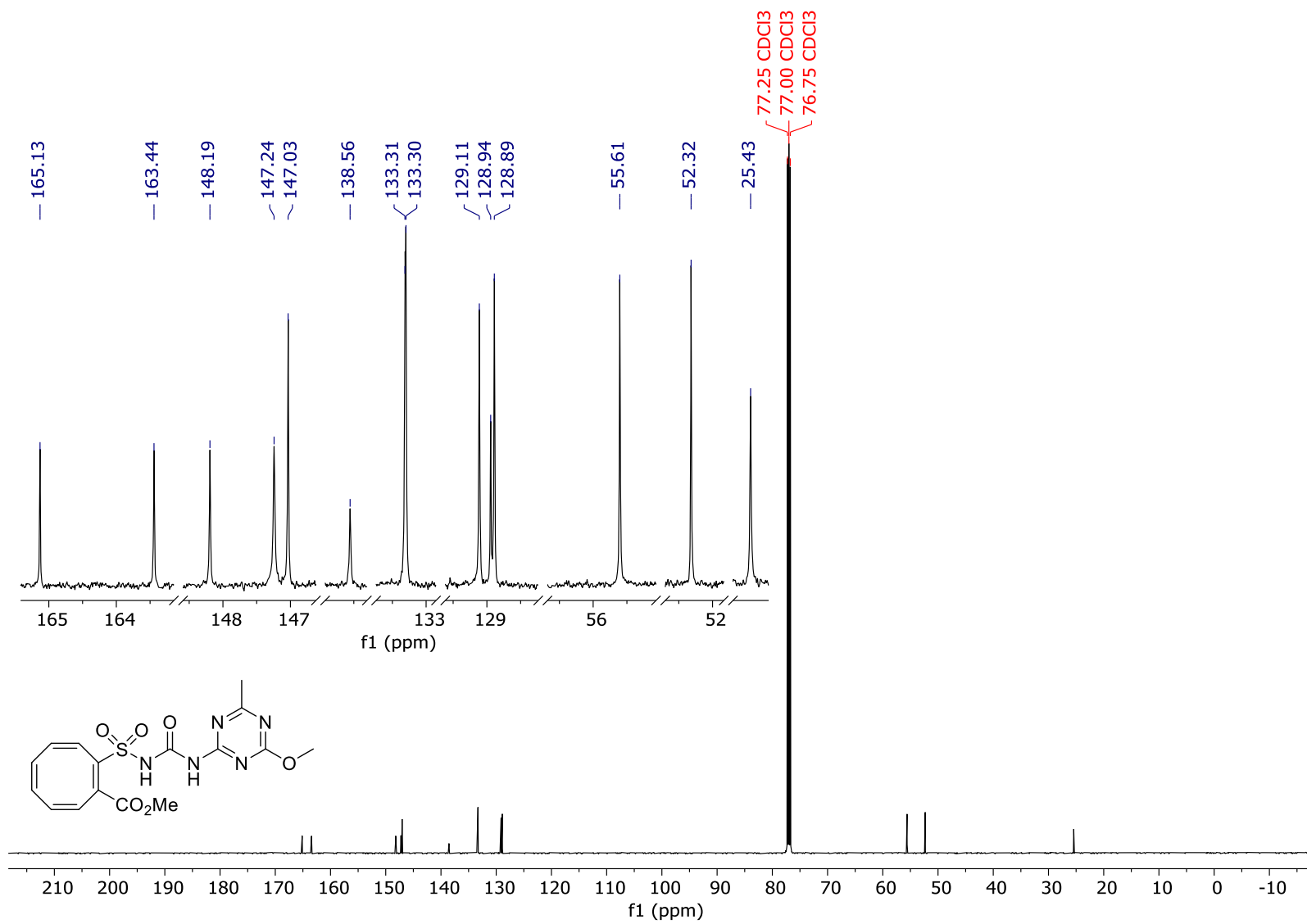
<sup>1</sup>H NMR (500 MHz, CD<sub>3</sub>CN) of Phenyl *N*-(4-methoxy-6-methyl-1,3,5-triazin-2-yl) (26)



<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) of COT-MM (10)

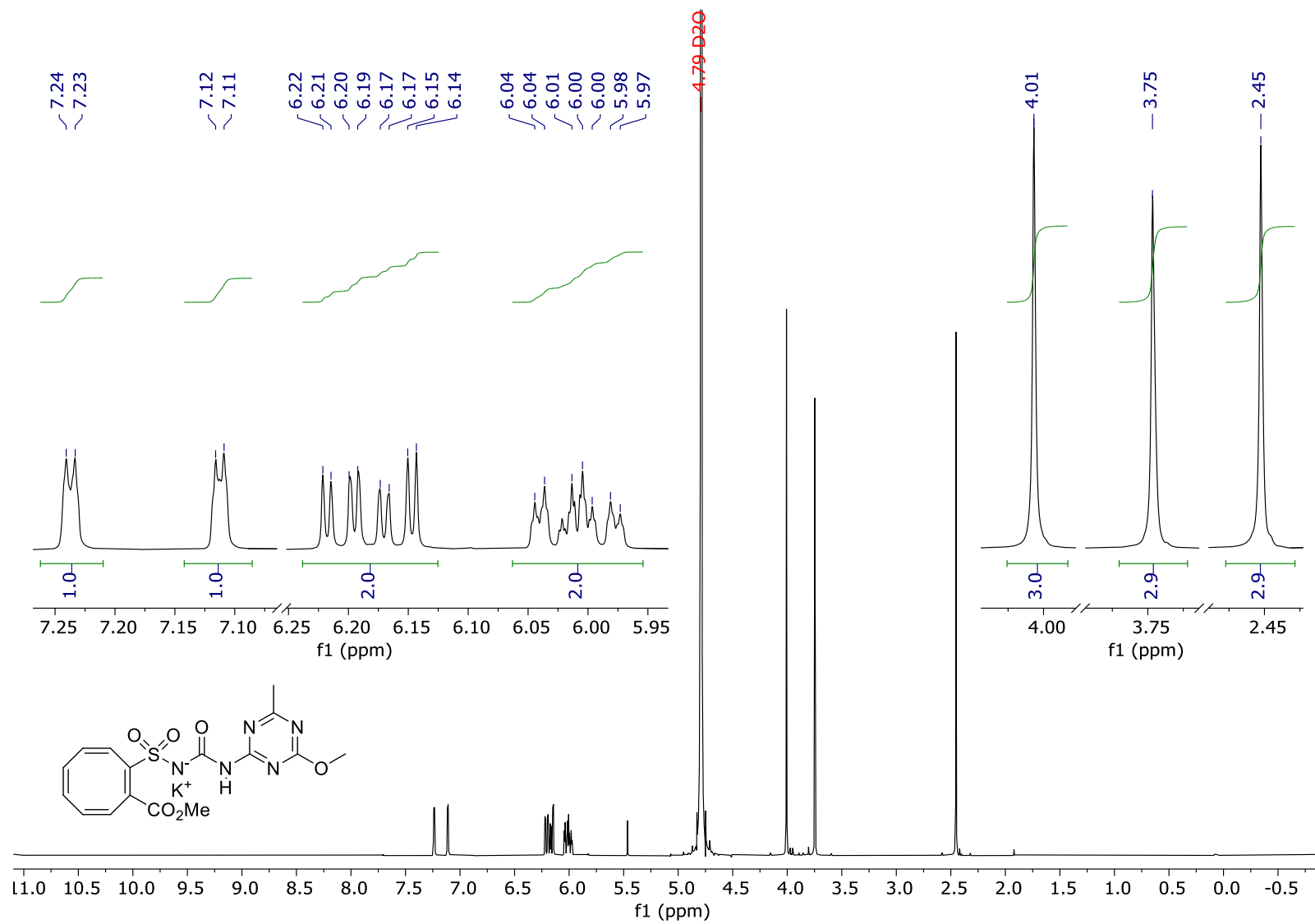


<sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) of COT-MM (10)

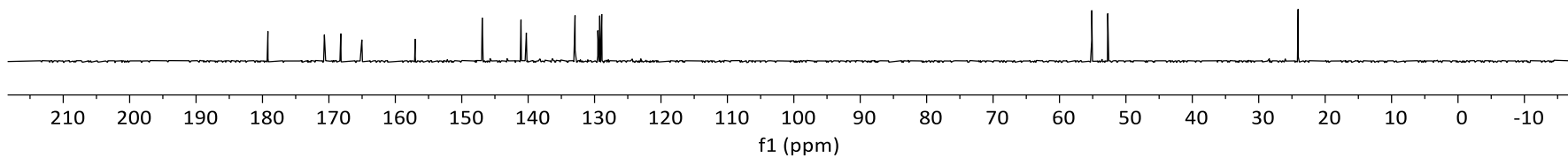
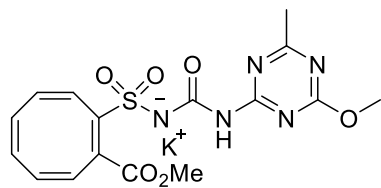
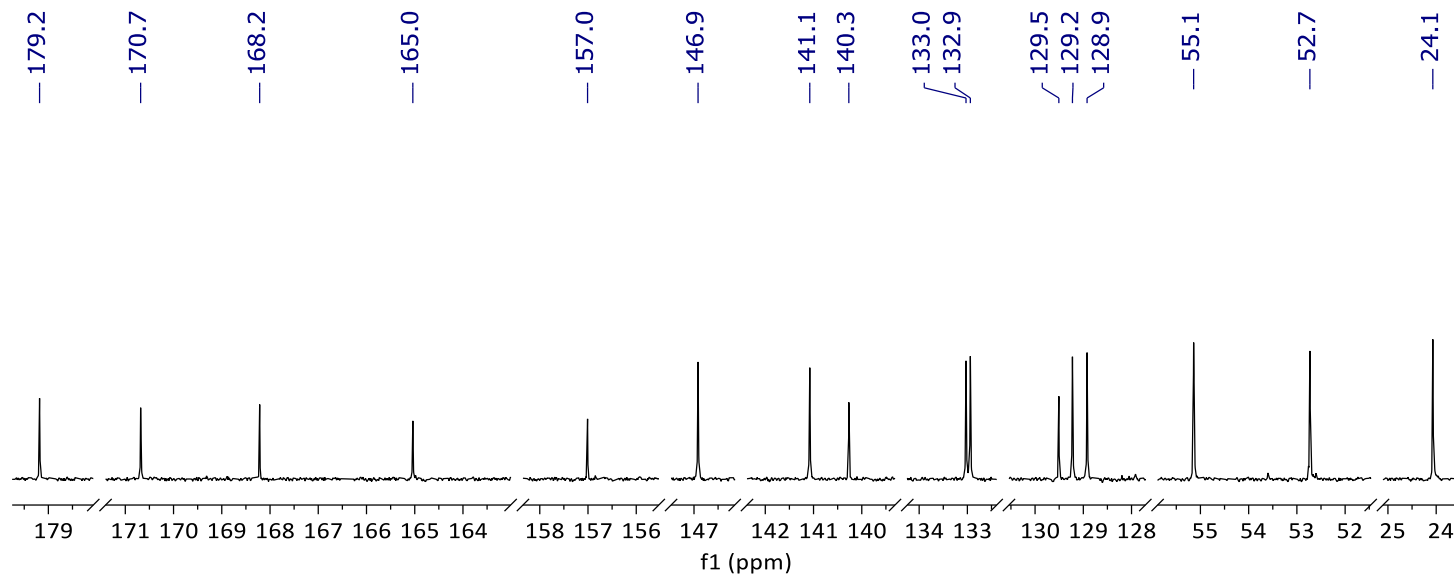




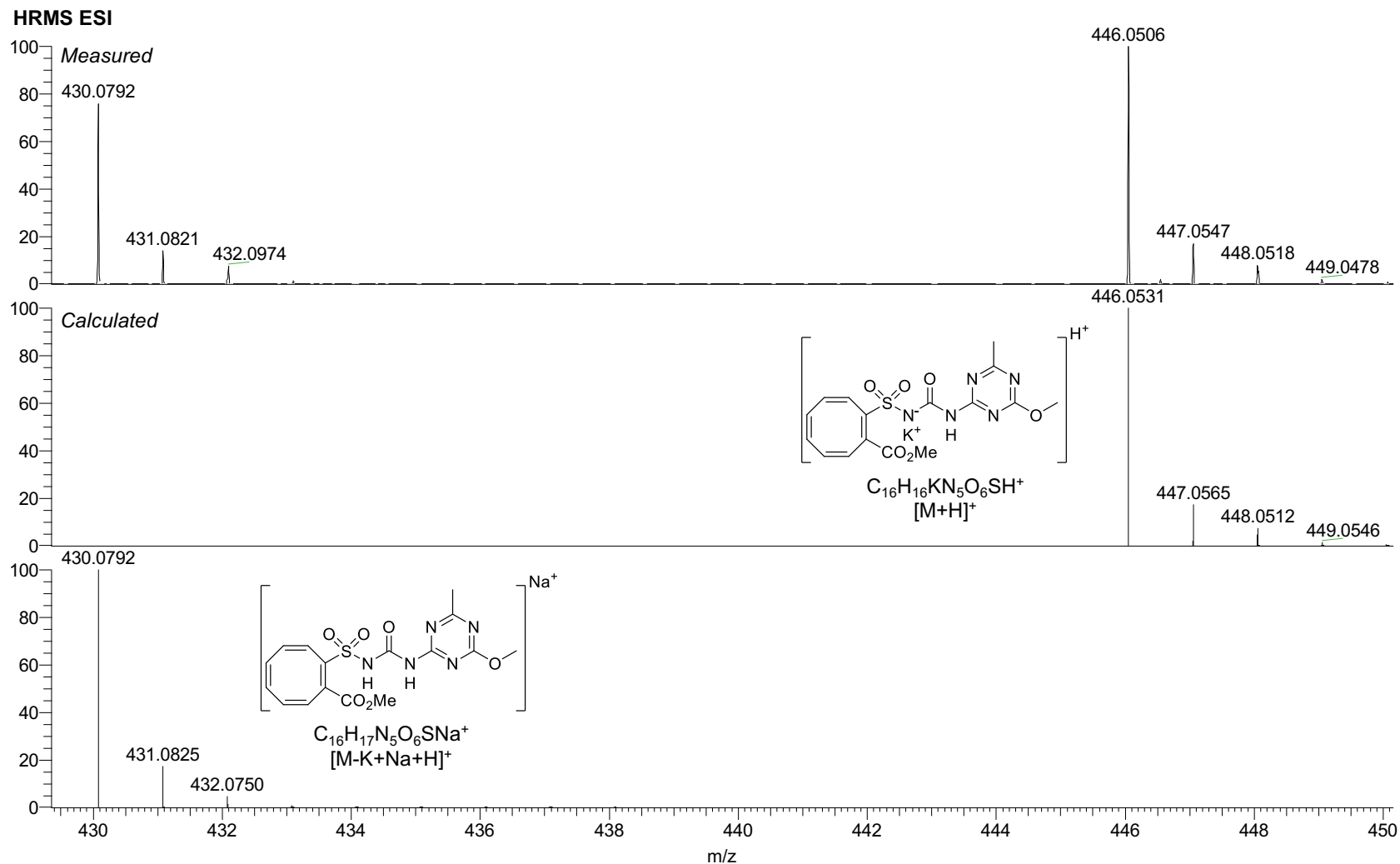
$^1\text{H}$  NMR (500 MHz,  $\text{D}_2\text{O}$ ) of COT-MM  $\text{K}^+$



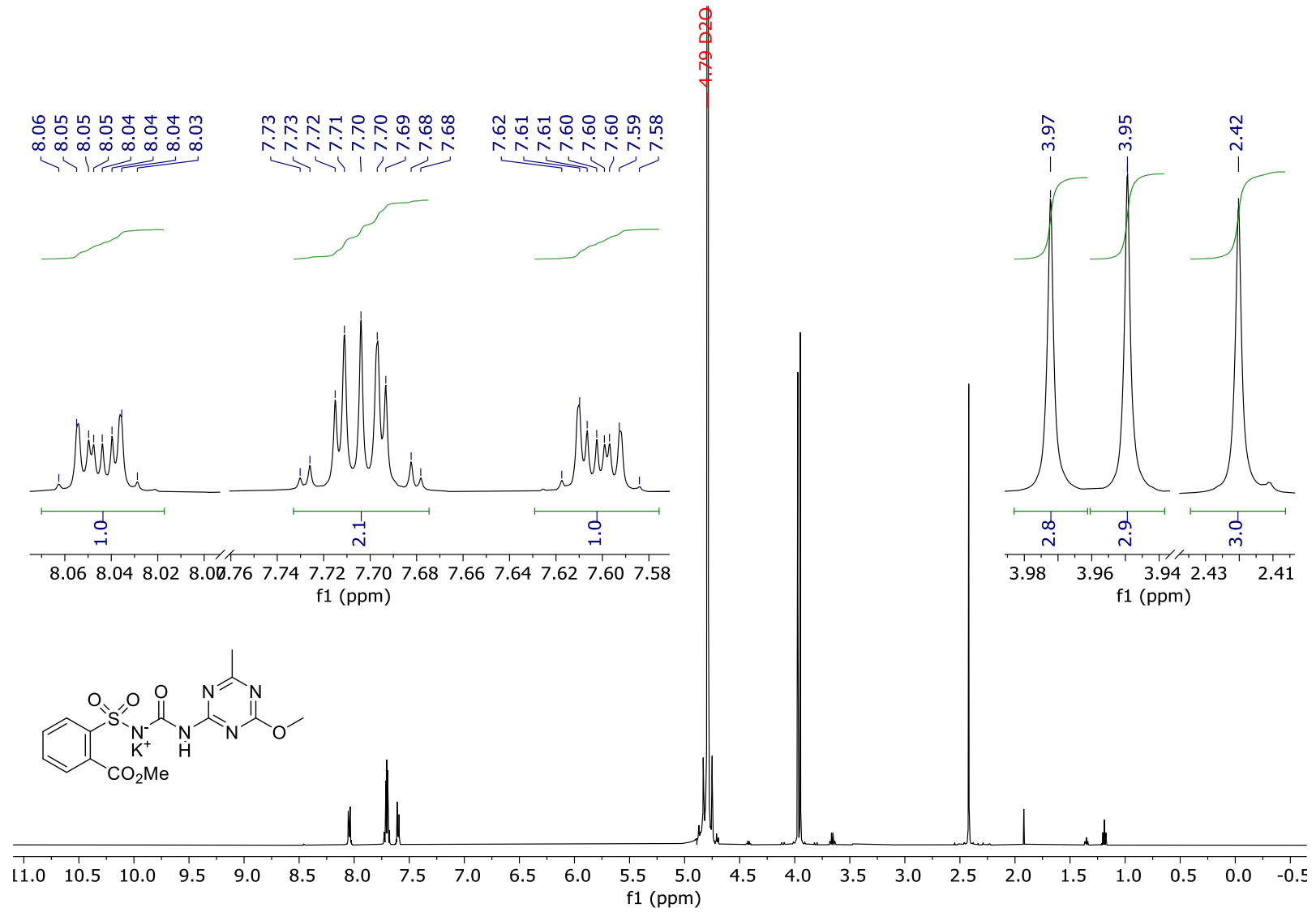
$^{13}\text{C}$  NMR (125 MHz,  $\text{D}_2\text{O}$ ) of **COT-MM K<sup>+</sup>**



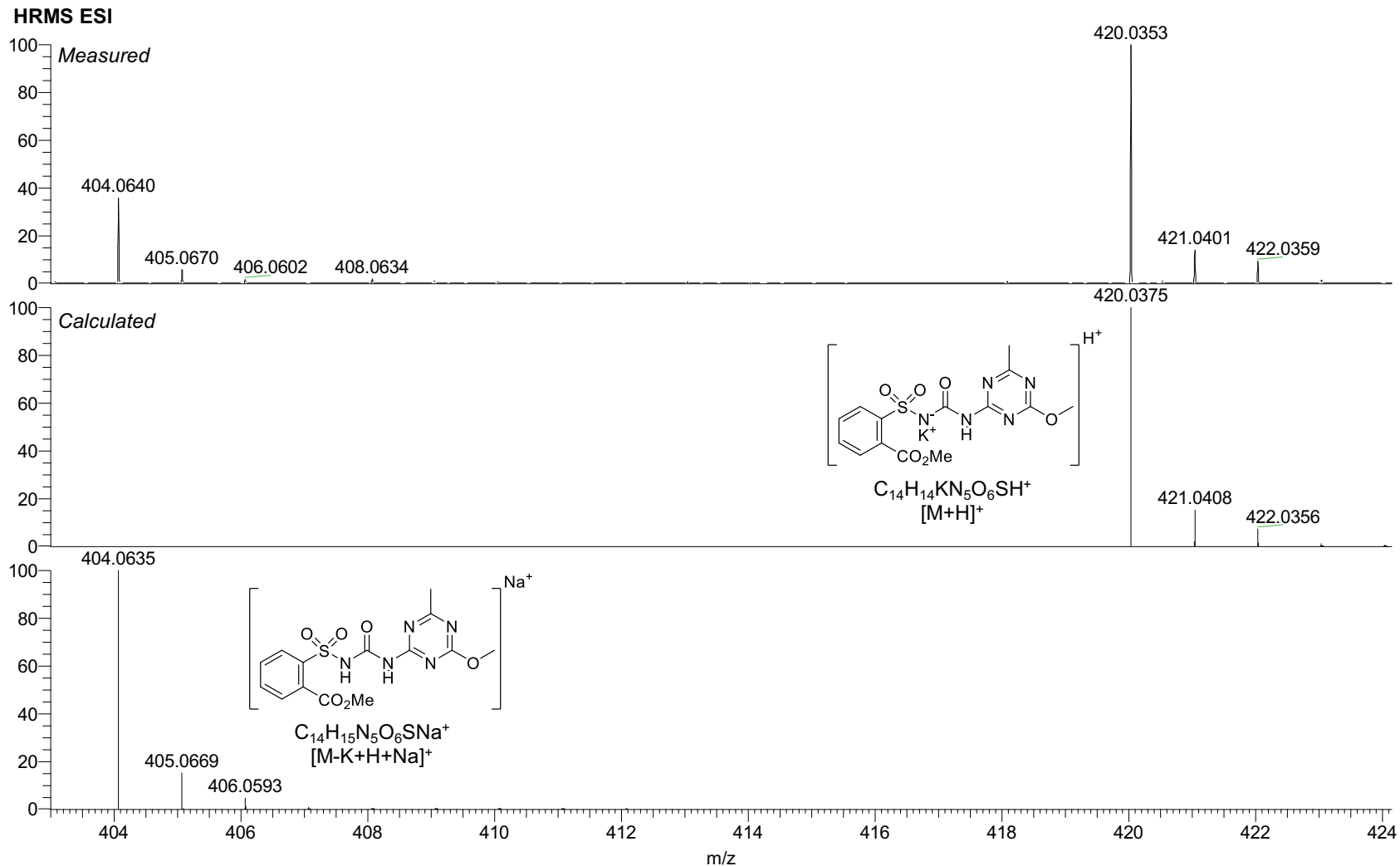
HRMS ESI of COT-MM K<sup>+</sup>



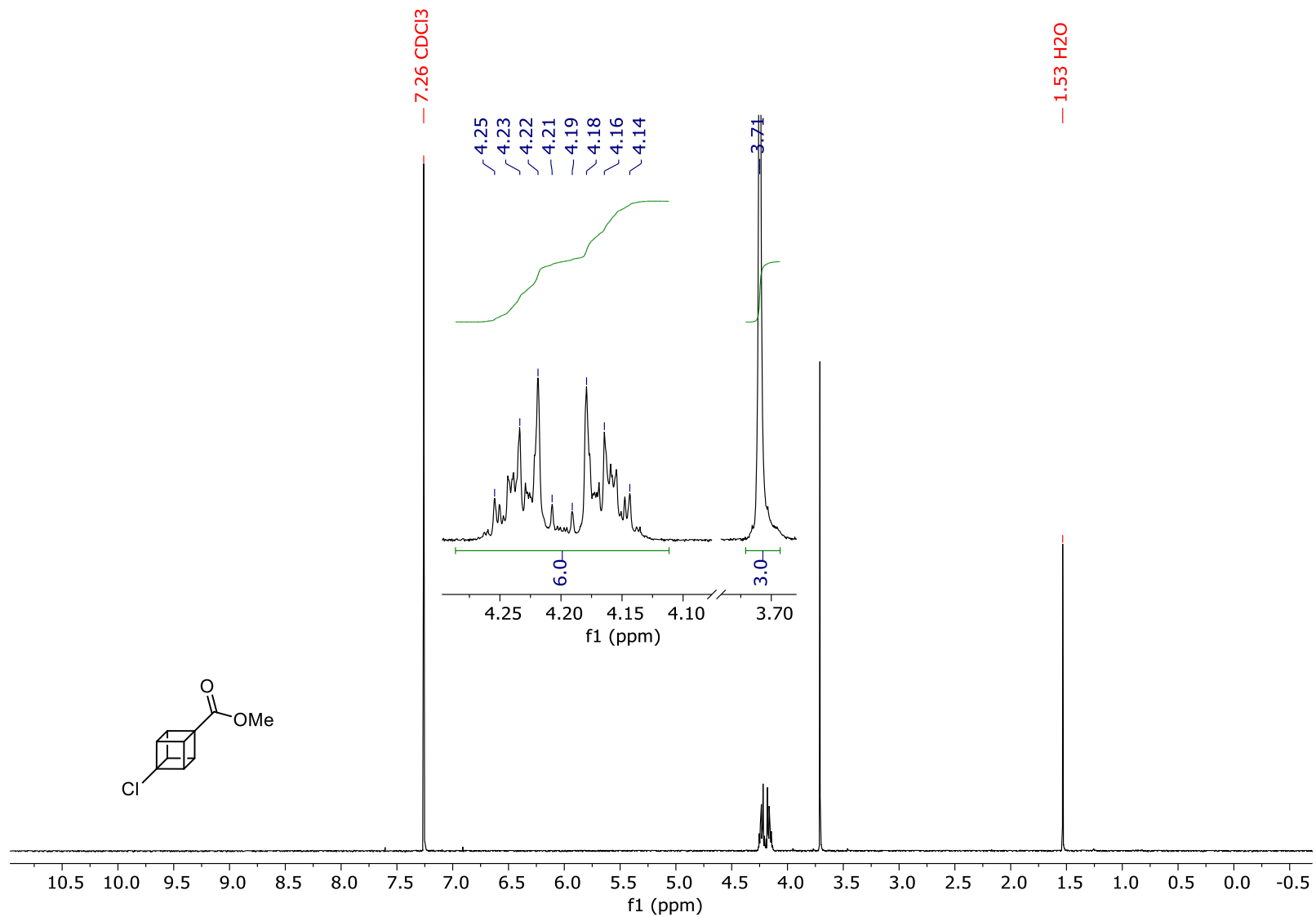
$^1\text{H}$  NMR (500 MHz,  $\text{D}_2\text{O}$ ) of  $\text{MM K}^+$



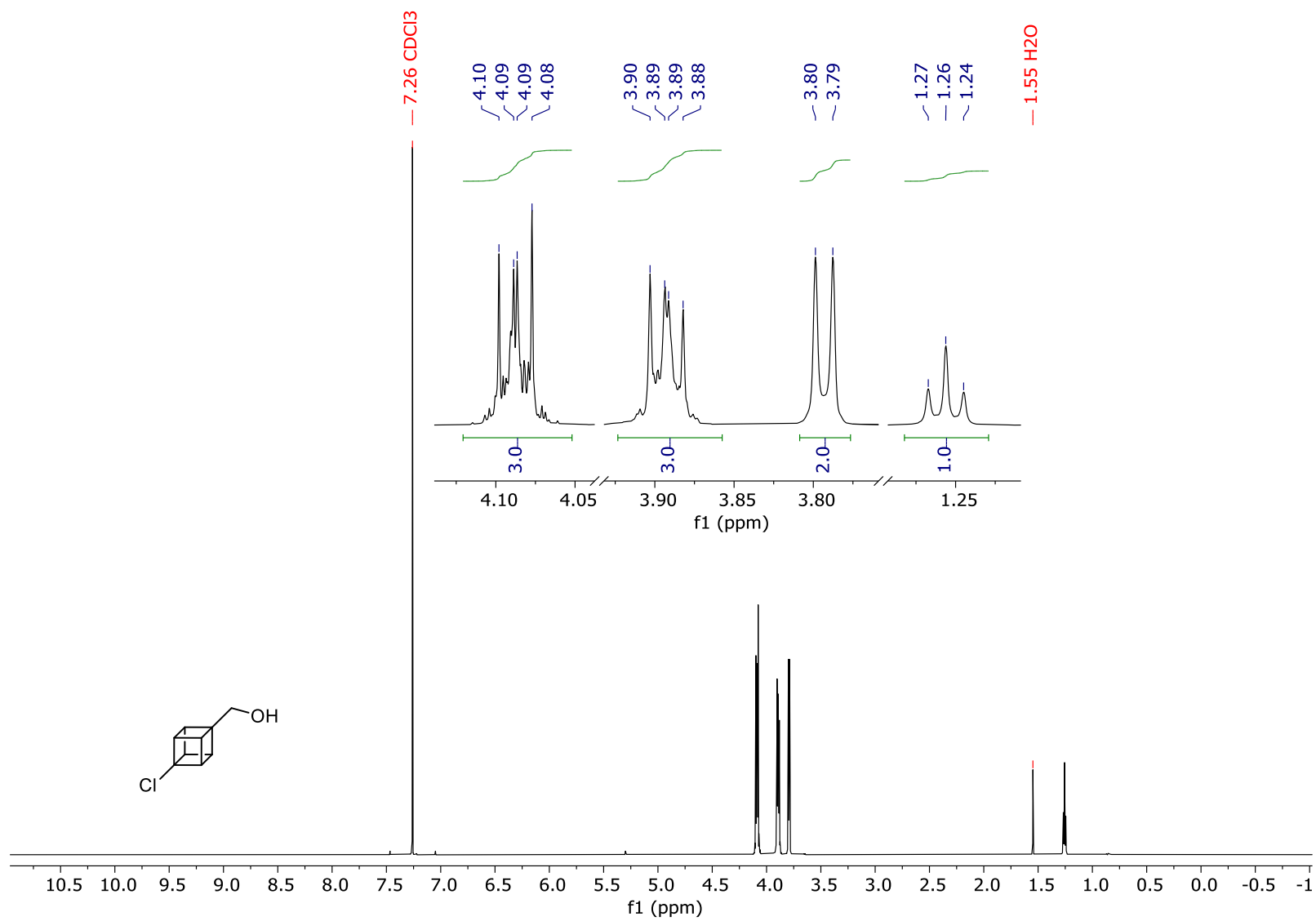
HRMS ESI of MM K<sup>+</sup>



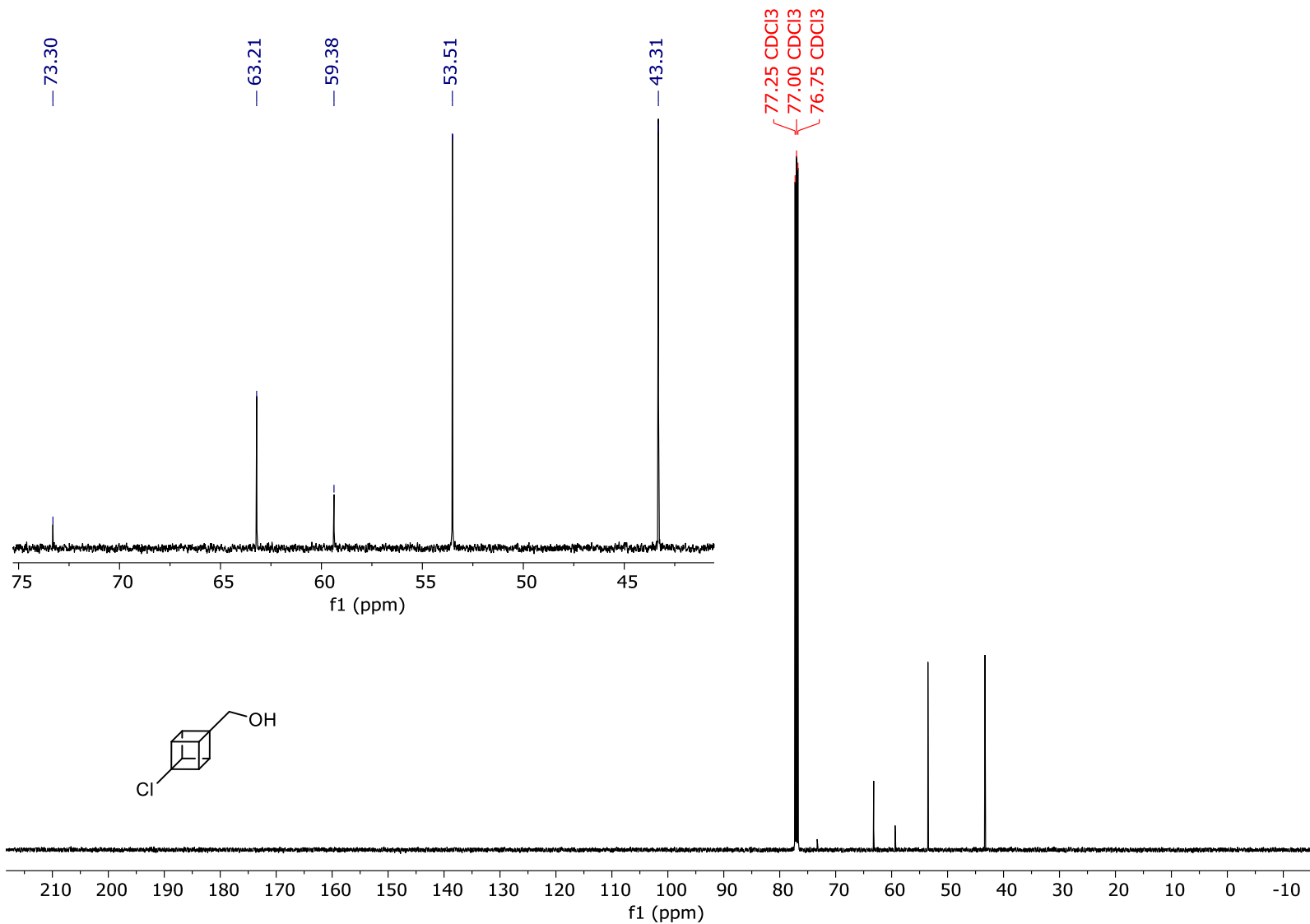
$^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ ) of Methyl 4-chlorocubane-1-carboxylate (33)



<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) of (4-chlorocuban-1-yl)methanol (34)

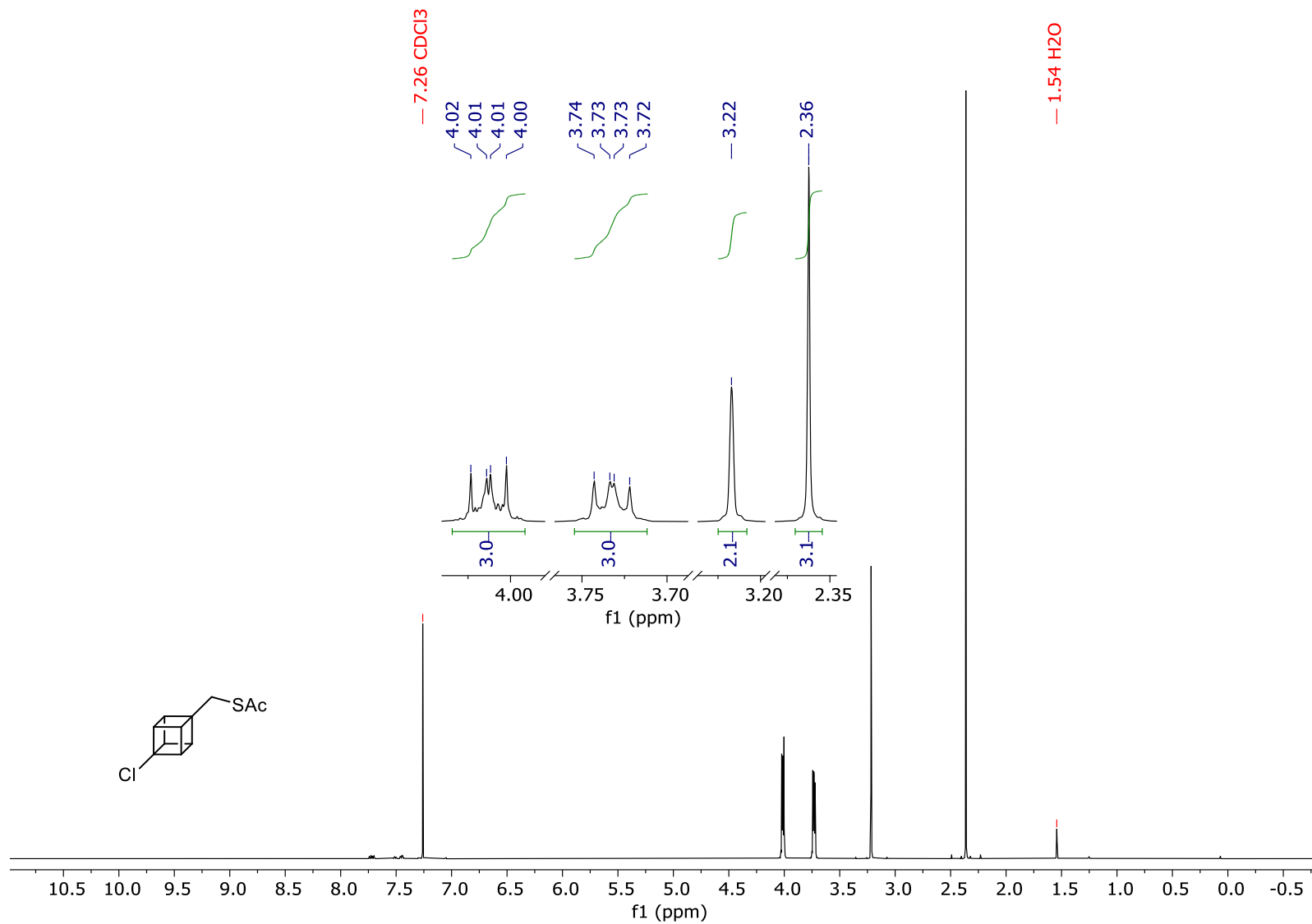


$^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) of (4-chlorocuban-1-yl)methanol (34)

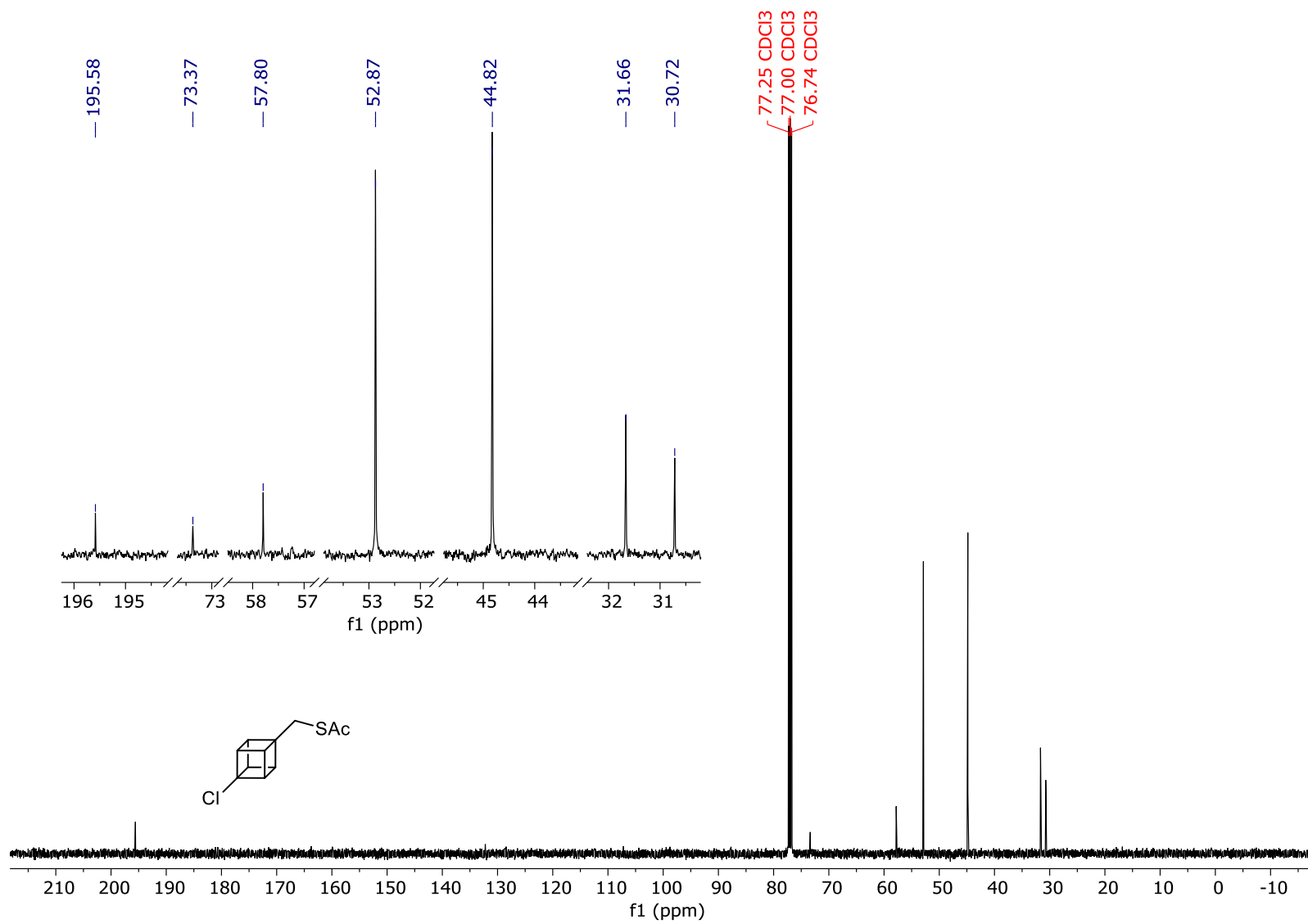




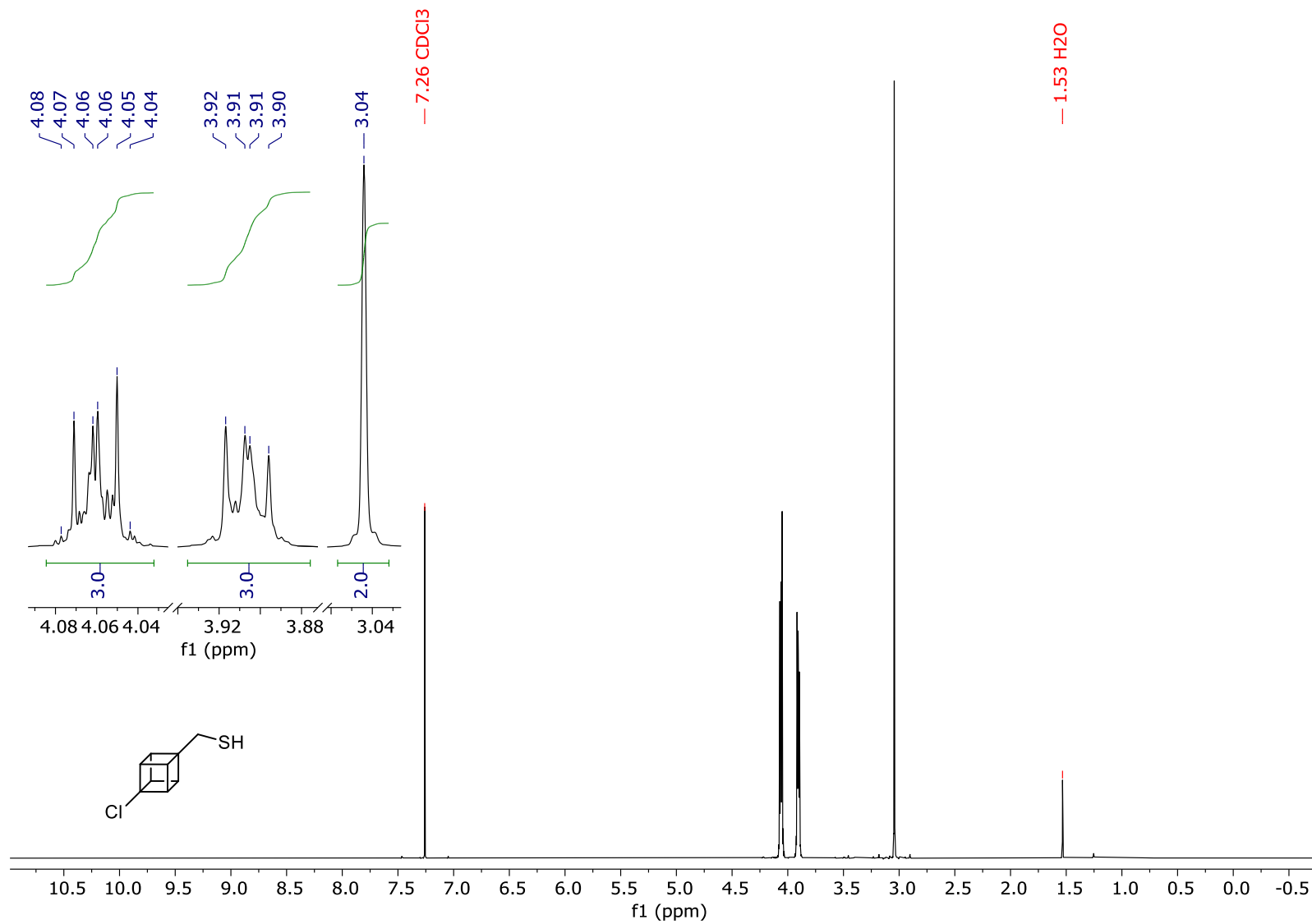
<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) of ((4-Chlorocuban-1-yl)methyl) ethanethioate (35)



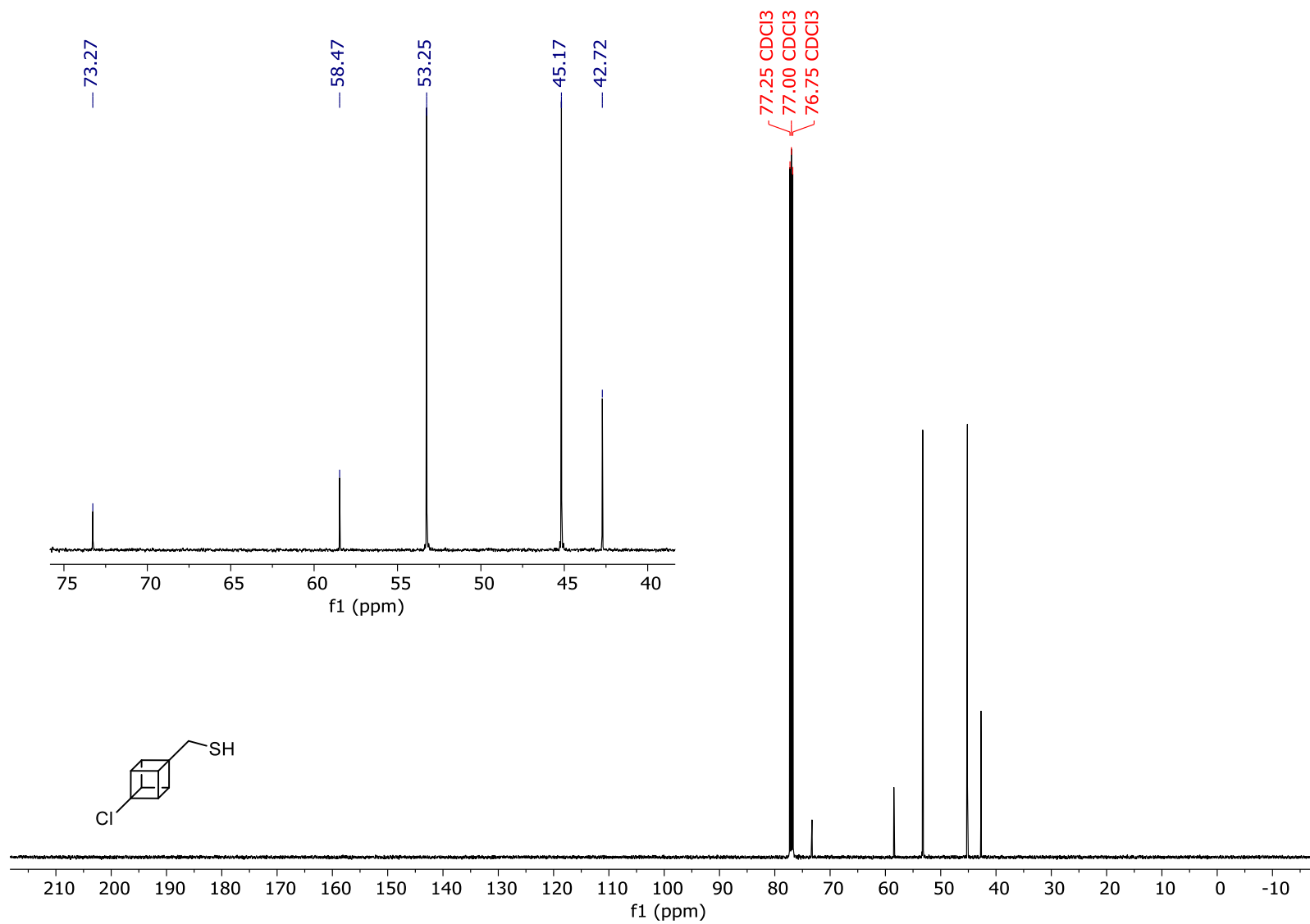
$^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) of ((4-Chlorocuban-1-yl)methyl) ethanethioate (35)



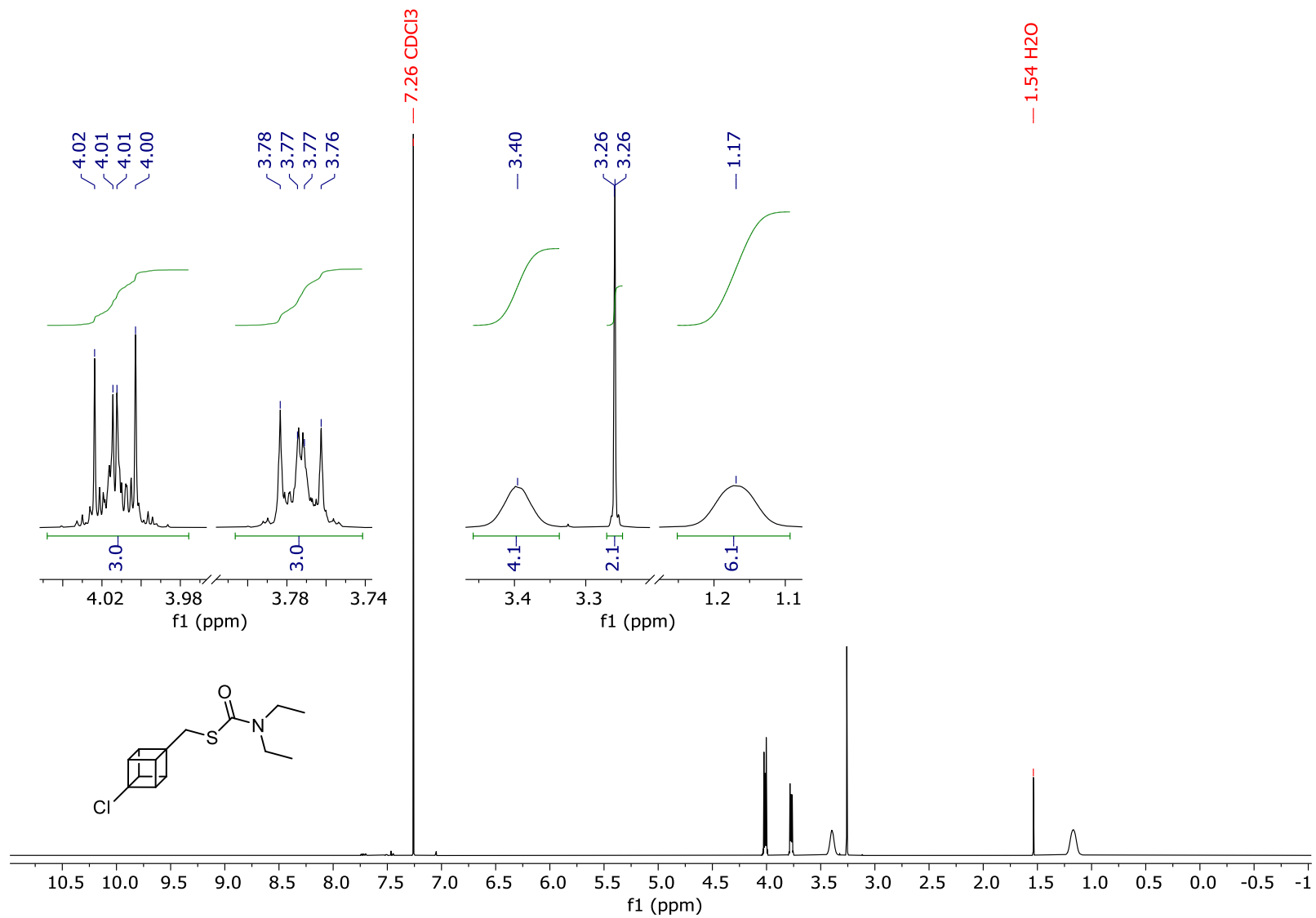
<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) of (4-chlorocuban-1-yl)methanethiol (36)



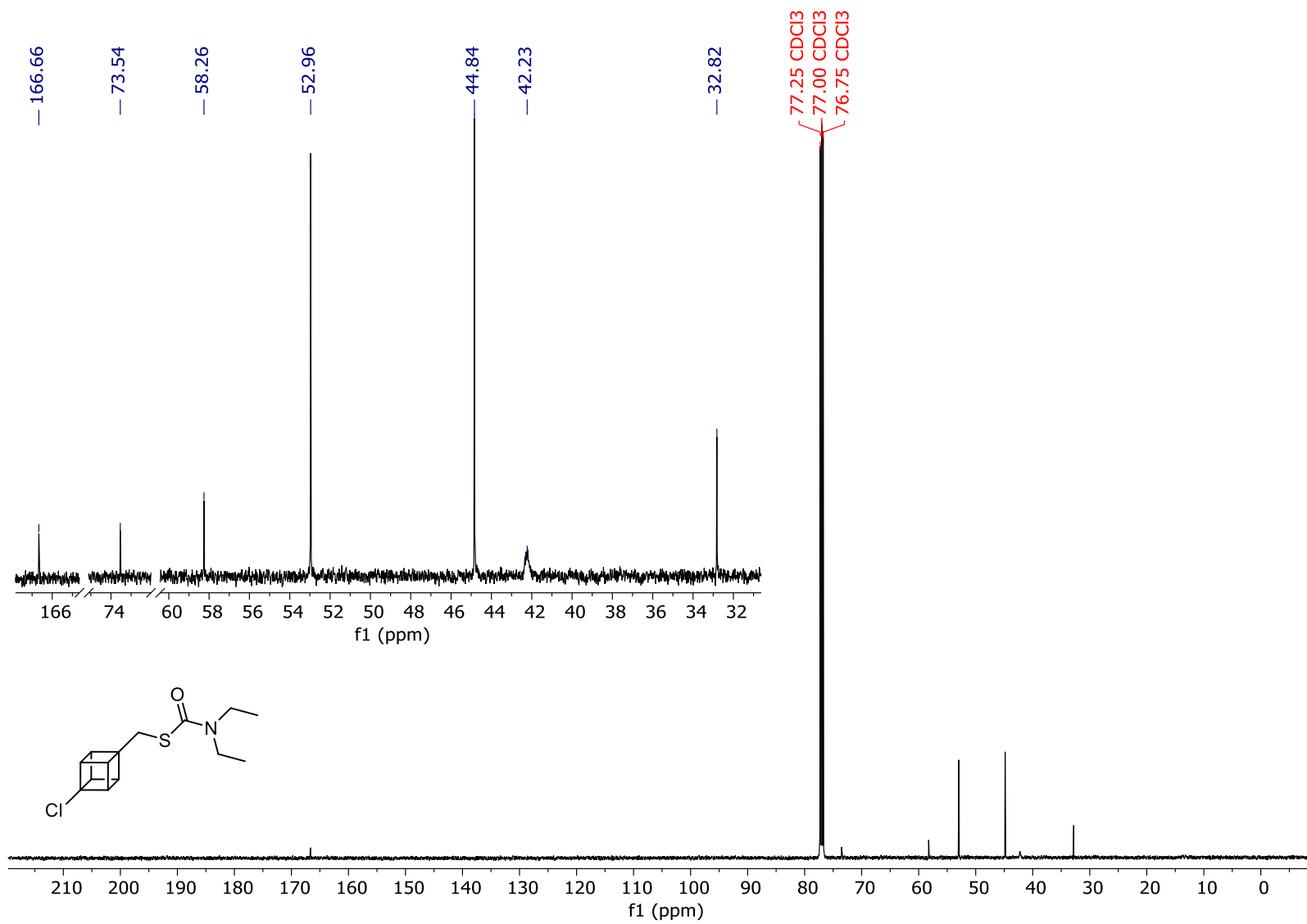
$^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) of (4-chlorocuban-1-yl)methanethiol (36)



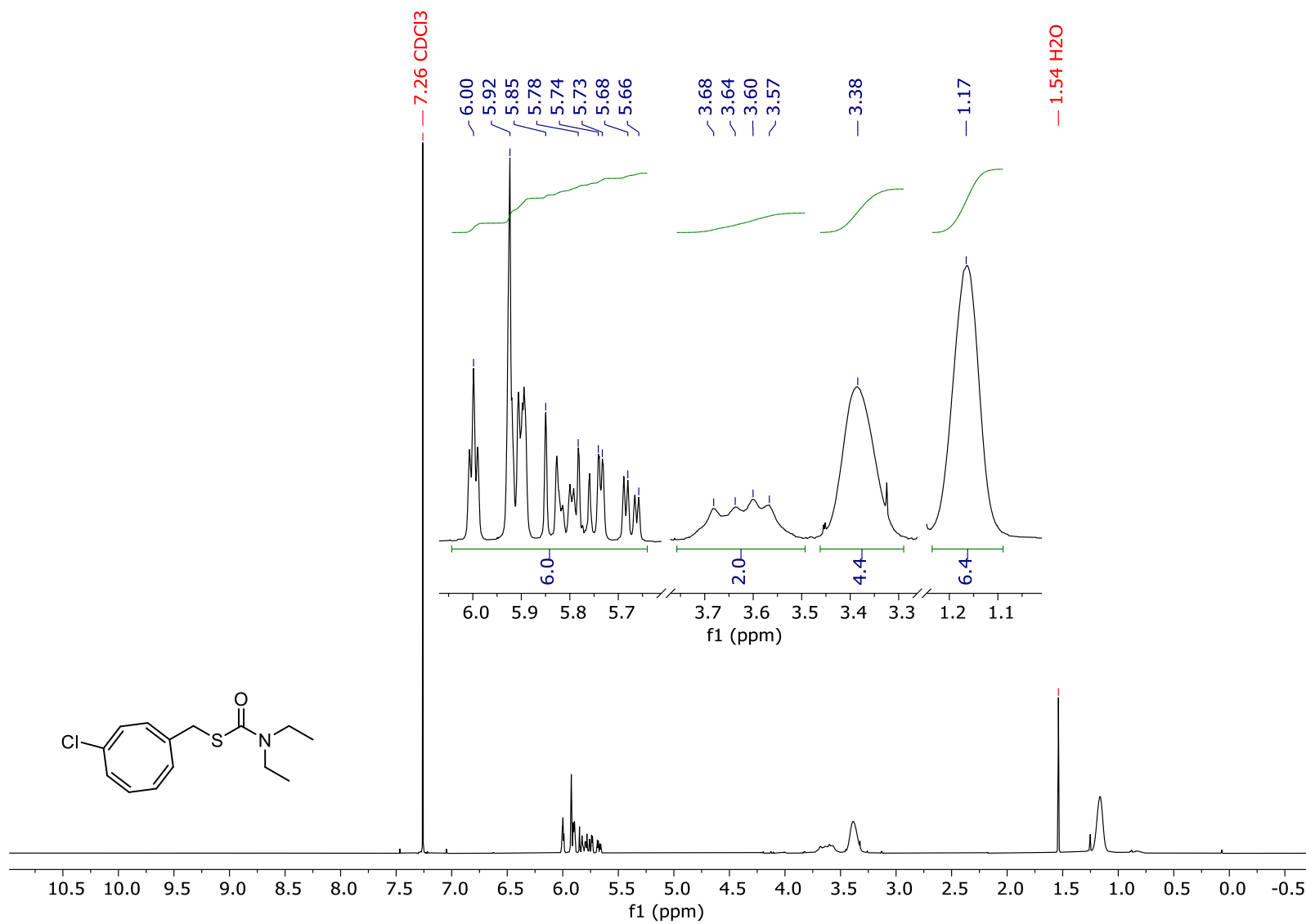
<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) of ((4-Chlorocuban-1-yl)methyl)diethylcarbamothioate (38)



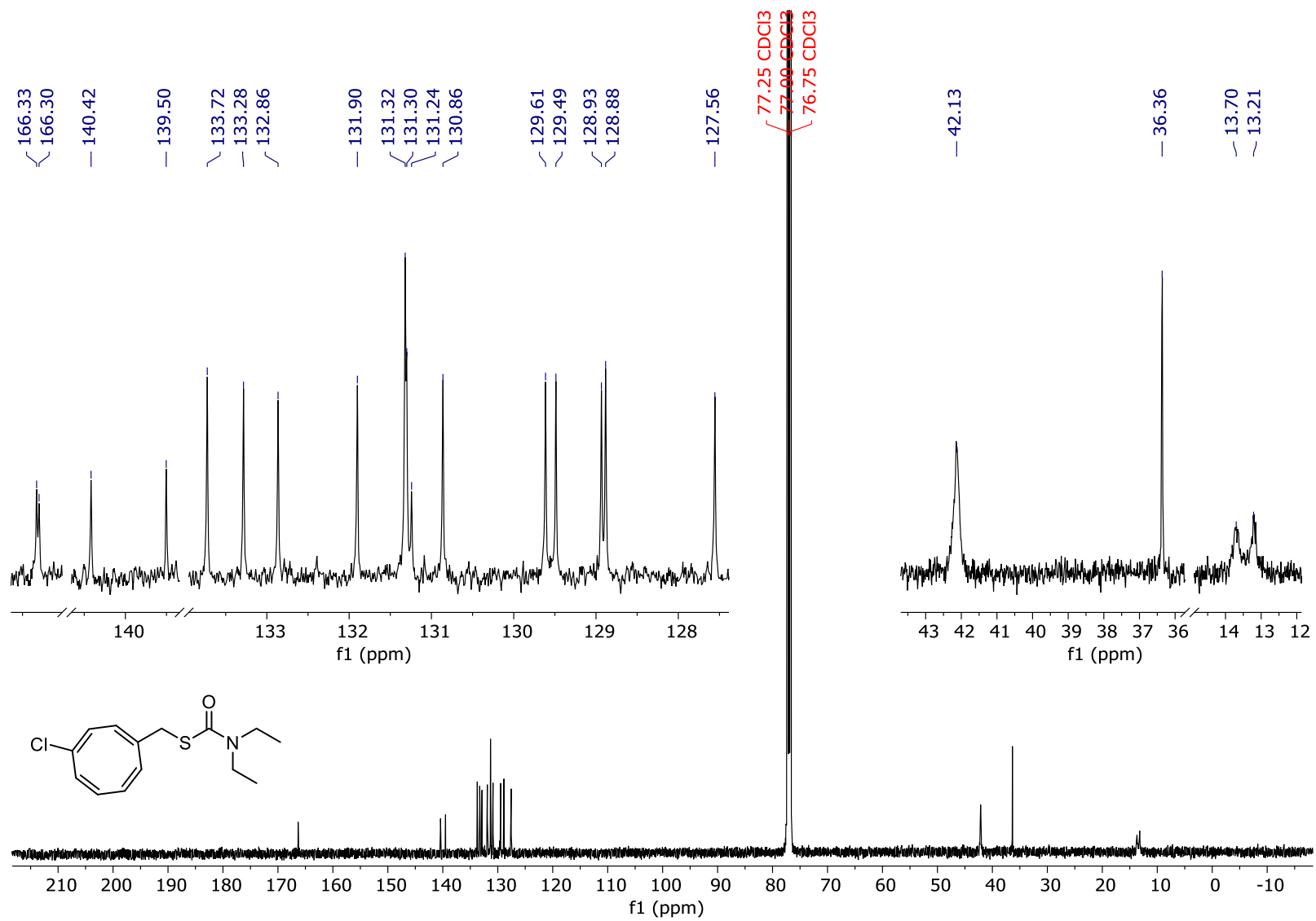
$^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) of ((4-Chlorocuban-1-yl)methyl)diethylcarbamothioate (38)



$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) of COT-BT (28)



$^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) of COT-BT (28)





$^1\text{H}$ - $^{13}\text{C}$  HSQC NMR (500 MHz,  $\text{CDCl}_3$ ) of COT-BT (28)

