

## **Supplementary information**

### **Use of novel haptens in the production of antibodies for the detection of tryptamines**

Michal Maryška<sup>a, d</sup>, Lucie Fojtíková<sup>a, c</sup>, Radek Jurok<sup>b, d</sup>, Barbora Holubová<sup>c</sup>, Oldřich Lapčík<sup>a</sup> and Martin Kuchar<sup>a, d, \*</sup>

<sup>a</sup> *Department of Chemistry of Natural Compounds, University of Chemistry and Technology, Technická 5, 166 28 Praha 6 - Dejvice, Czech Republic*

<sup>b</sup> *Department of Organic Chemistry, University of Chemistry and Technology, Technická 5, 166 28 Praha 6 - Dejvice, Czech Republic*

<sup>c</sup> *Department of Biochemistry and Microbiology, University of Chemistry and Technology, Technická 3, 166 28 Praha 6 - Dejvice, Czech Republic*

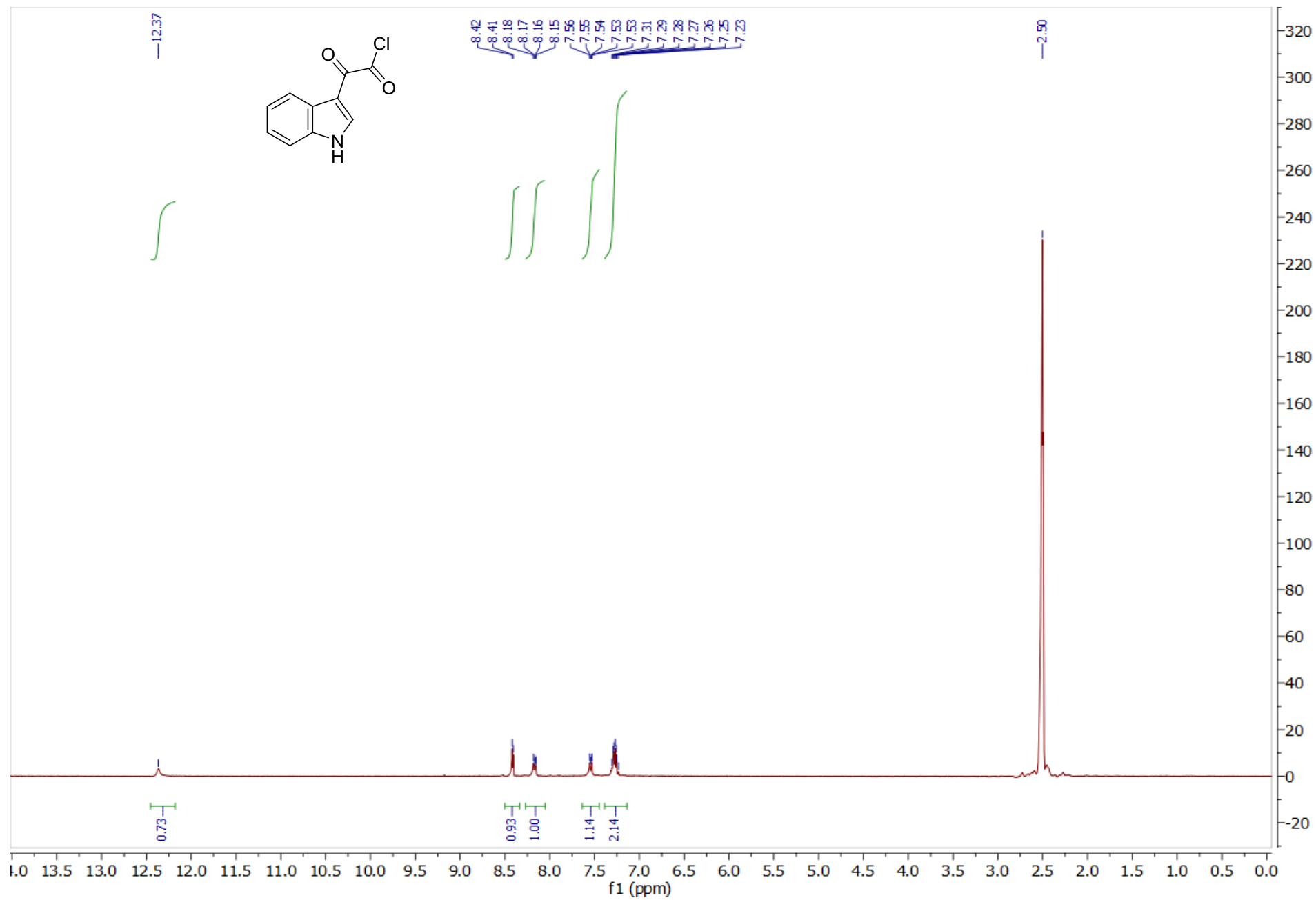
<sup>d</sup> *Forensic Laboratory of Biologically Active Substances, University of Chemistry and Technology, Technická 3, 166 28 Praha 6 - Dejvice, Czech Republic*

\* Corresponding author. Tel.: +420-220-444-432; fax: +420-220-444-422; e-mail: martin.kuchar@vscht.cz

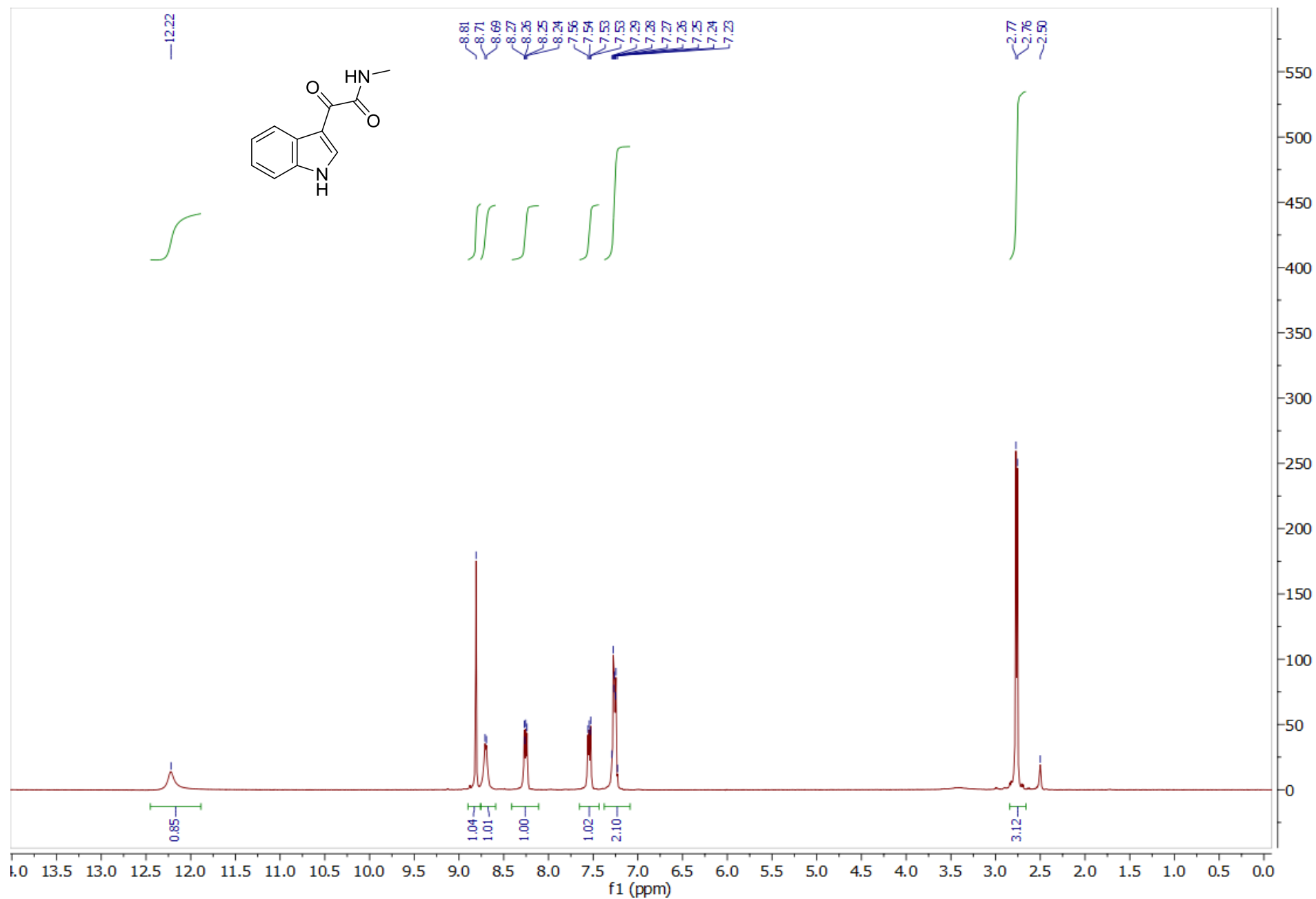
### **Table of contents**

<b><sup>1</sup>H and <sup>13</sup>C NMR spectra of prepared compounds .....</b>	<b>p2 - p31</b>
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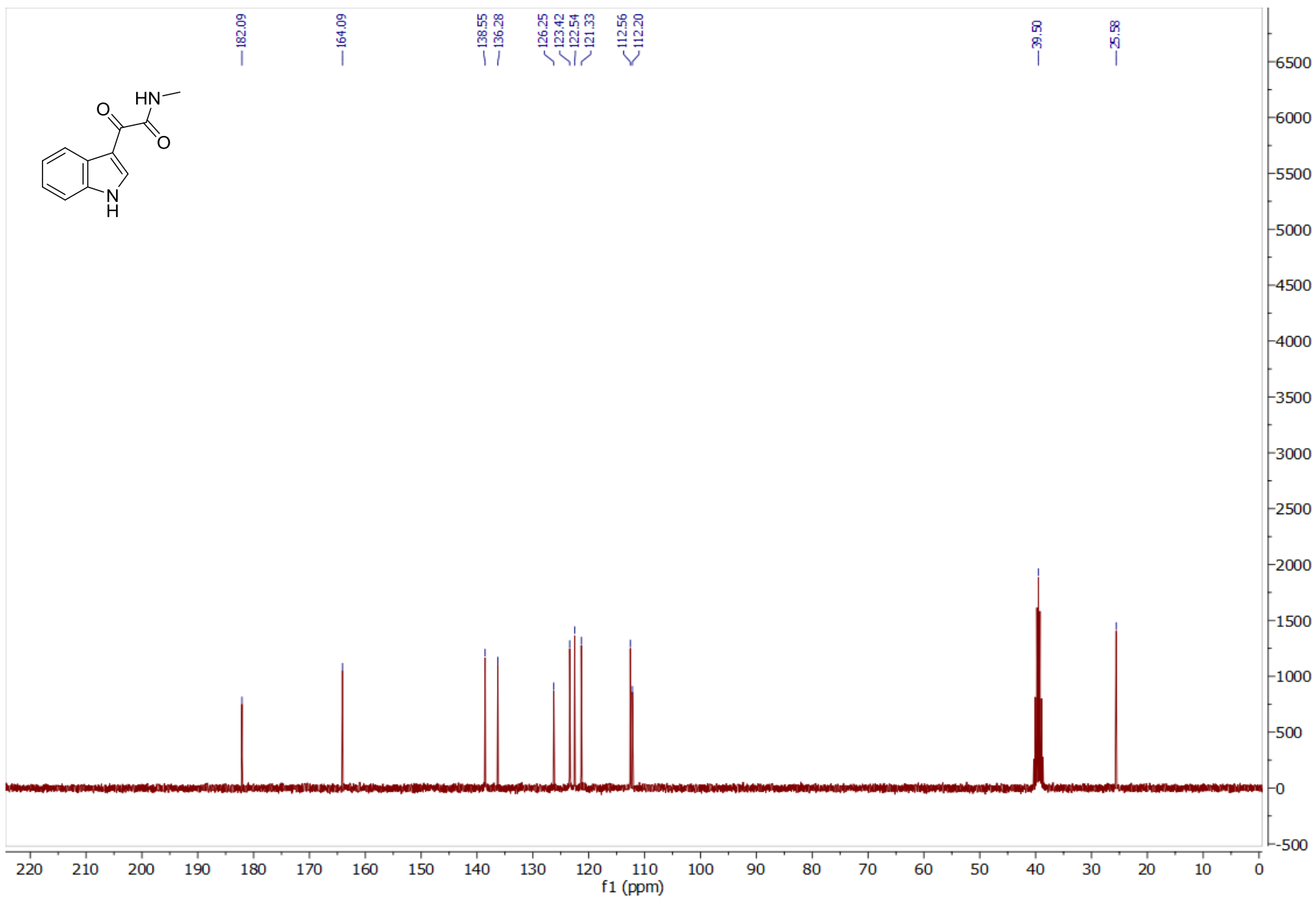
$^1\text{H}$  NMR of 2-(1*H*-indol-3-yl)-2-oxoacetyl chloride (**3**) (300 MHz, DMSO- $d_6$ )



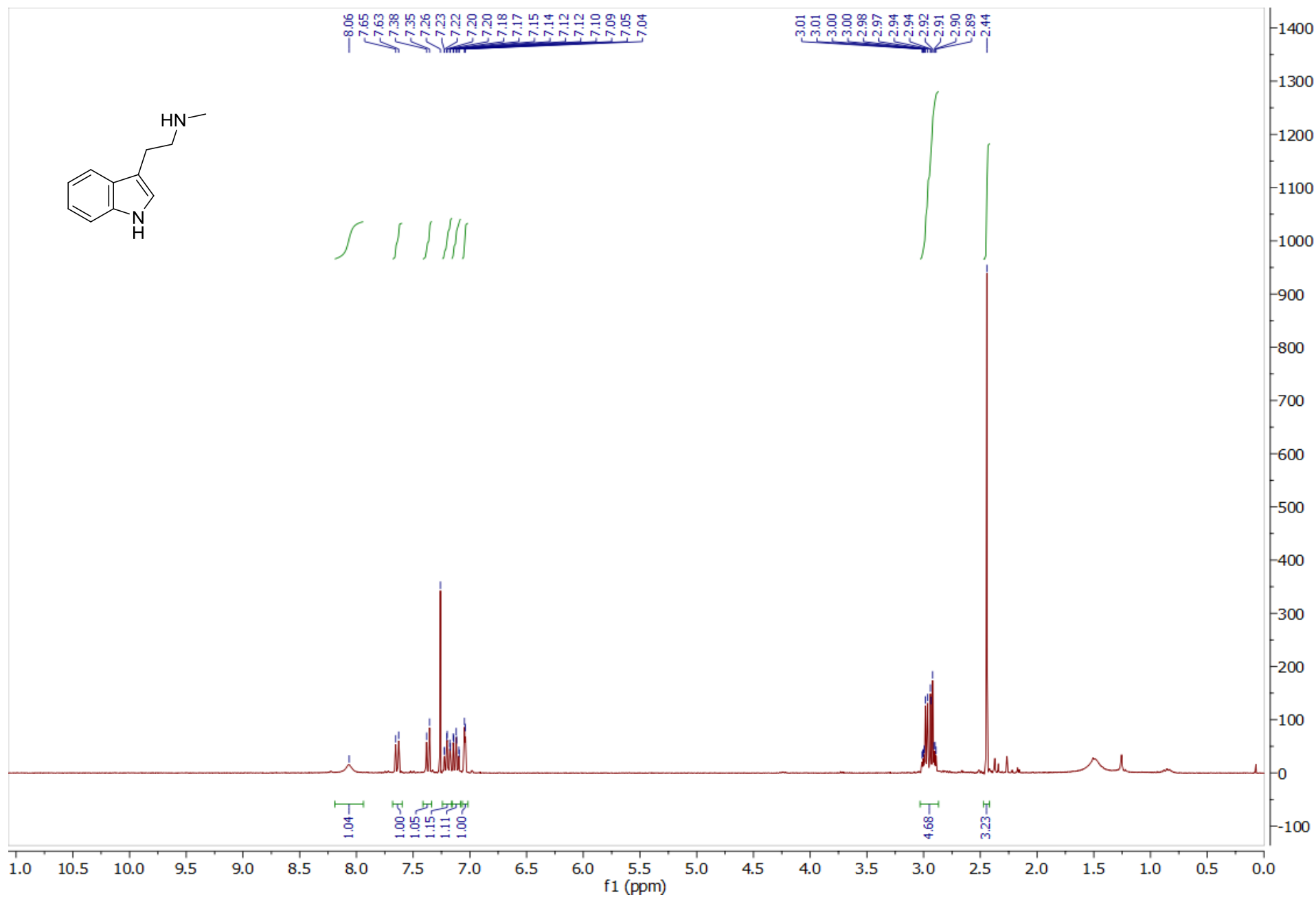
$^1\text{H}$  NMR of 2-(1*H*-indol-3-yl)-*N*-methyl-2-oxoacetamide (**4**) (300 MHz, DMSO- $\text{d}_6$ )



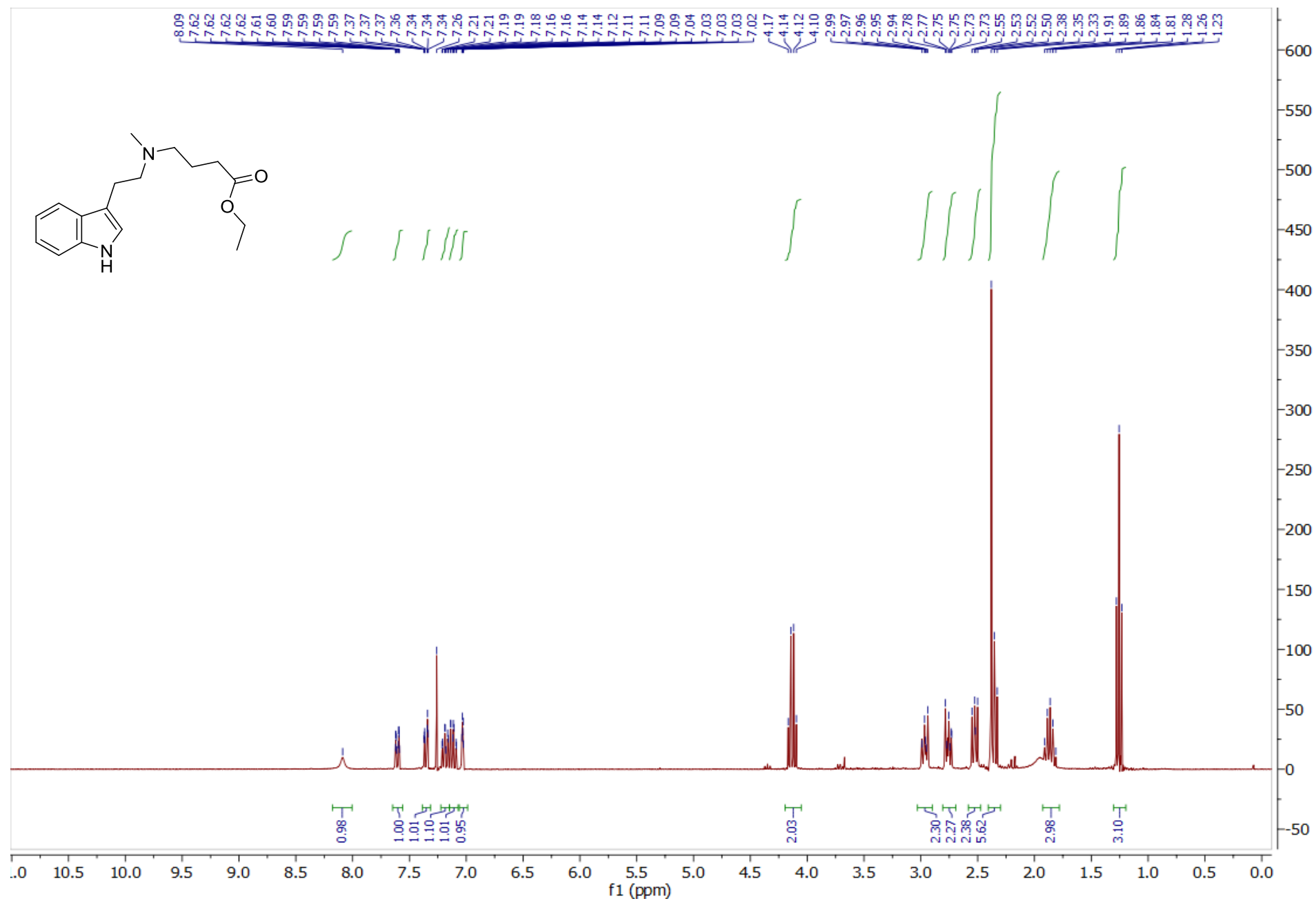
$^{13}\text{C}$  NMR of 2-(*1H*-indol-3-yl)-*N*-methyl-2-oxoacetamide (**4**) (75 MHz, DMSO- $\text{d}_6$ )



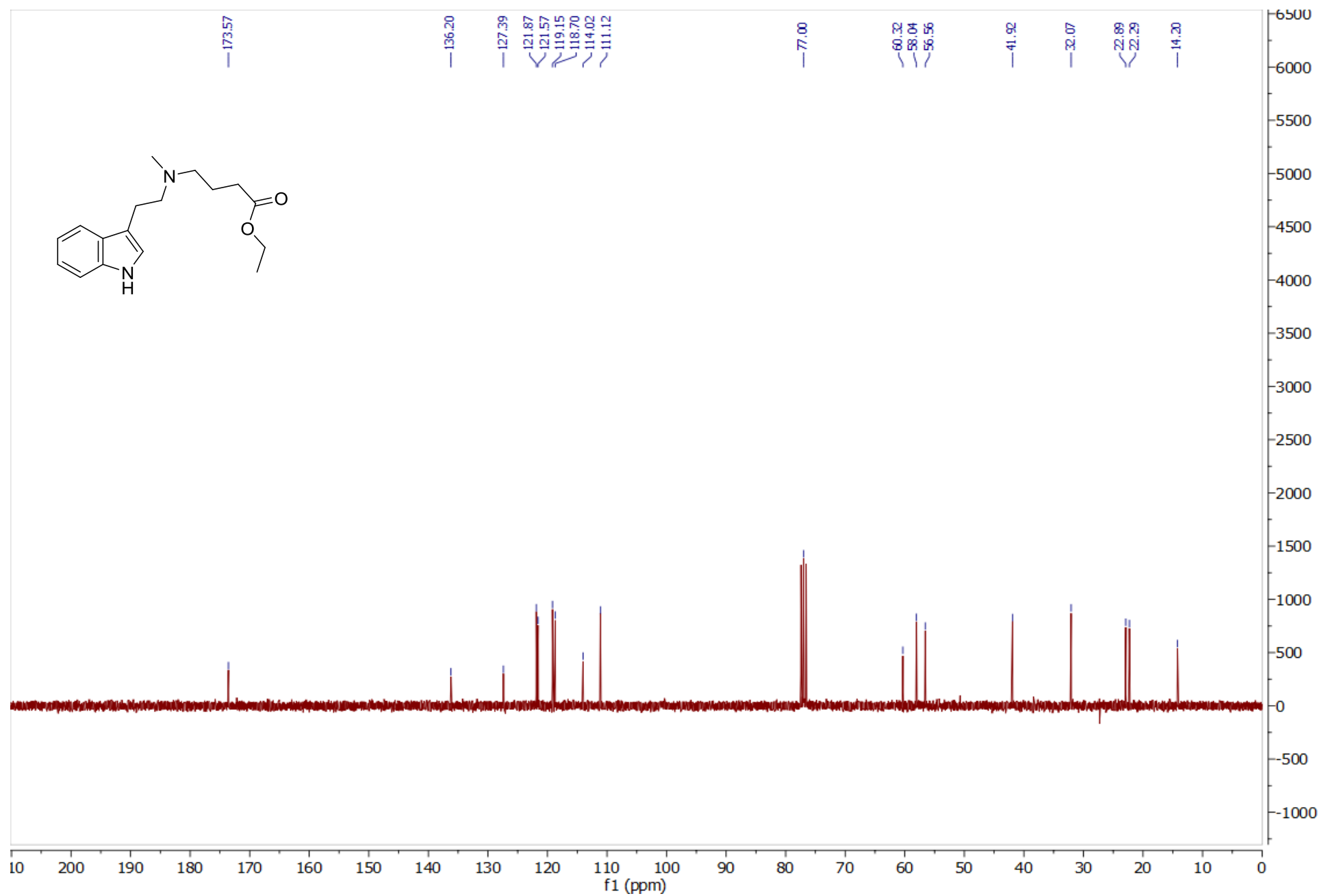
<sup>1</sup>H NMR of *N*-methyltryptamine (**5**) (300 MHz, CDCl<sub>3</sub>)



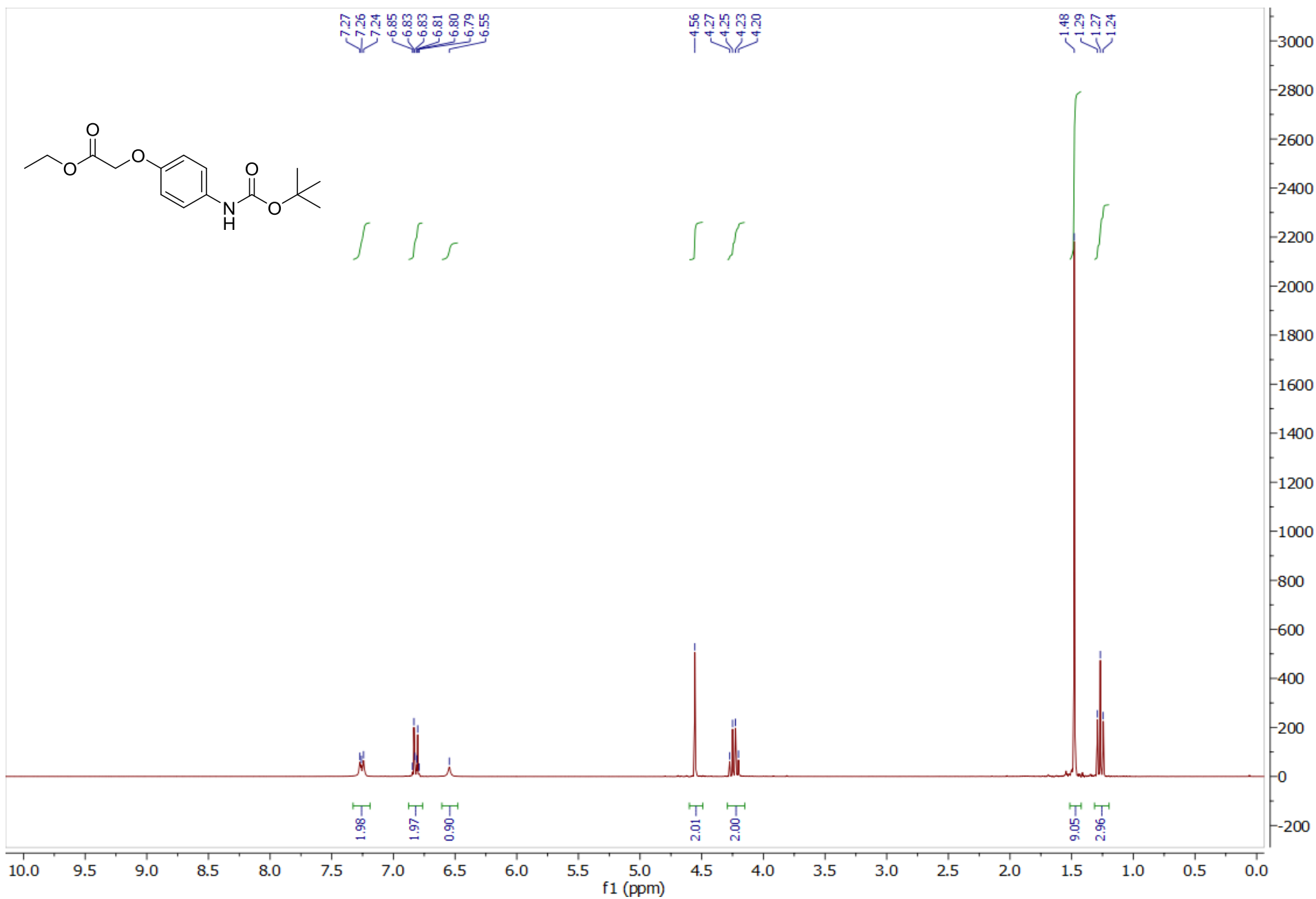
<sup>1</sup>H NMR of ethyl 4-[N-[2-(1*H*-indol-3-yl)ethyl]-*N*-methyl]aminobutanoate (**6**) (300 MHz, CDCl<sub>3</sub>)



$^{13}\text{C}$  NMR of ethyl 4-[*N*-[2-(*1H*-indol-3-yl)ethyl]-*N*-methyl]aminobutanoate (**6**) (75 MHz,  $\text{CDCl}_3$ )

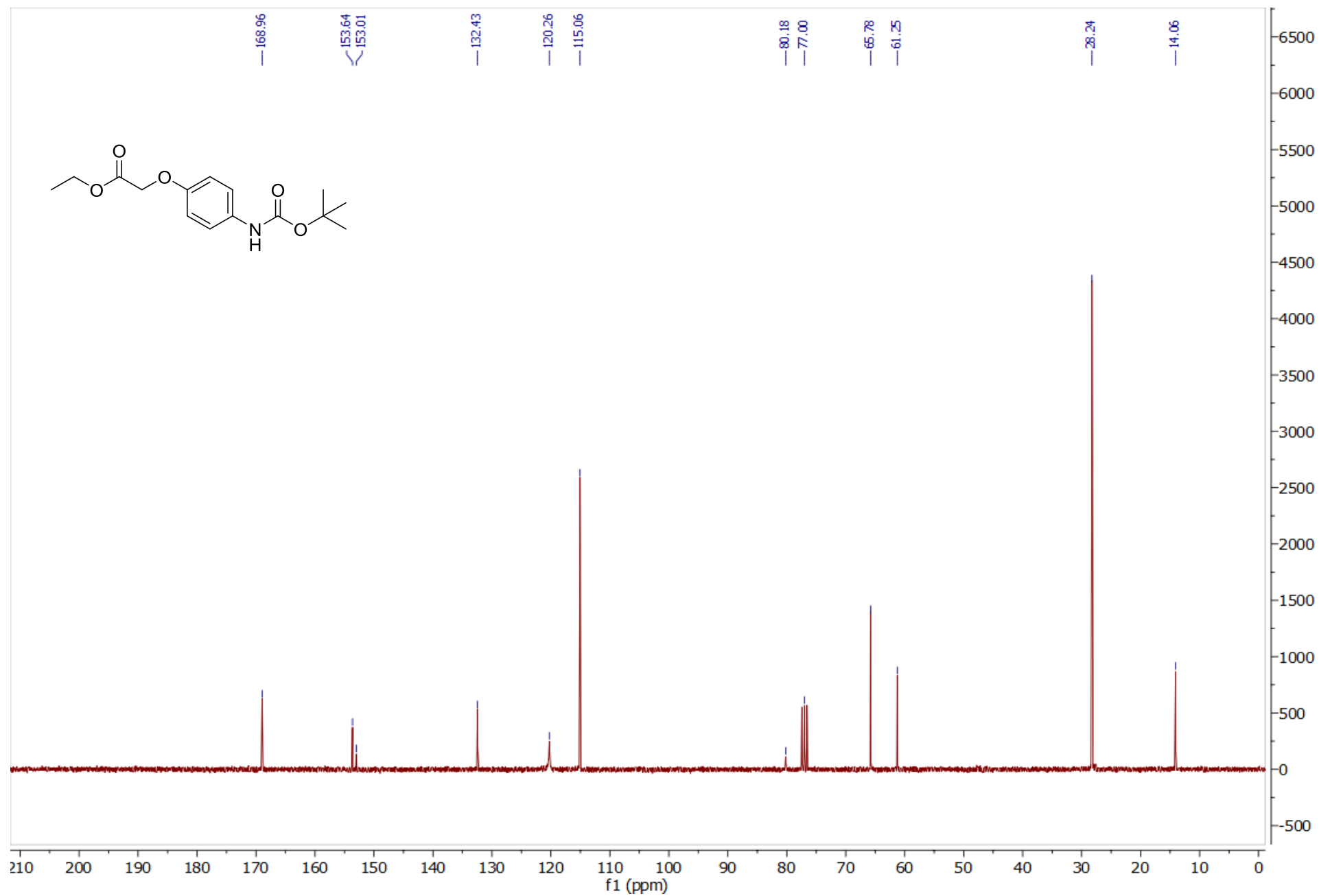


$^1\text{H}$  NMR of ethyl 2-[4-[(*tert*-butoxycarbonyl)amino]phenoxy]acetate (**16**) (300 MHz,  $\text{CDCl}_3$ )

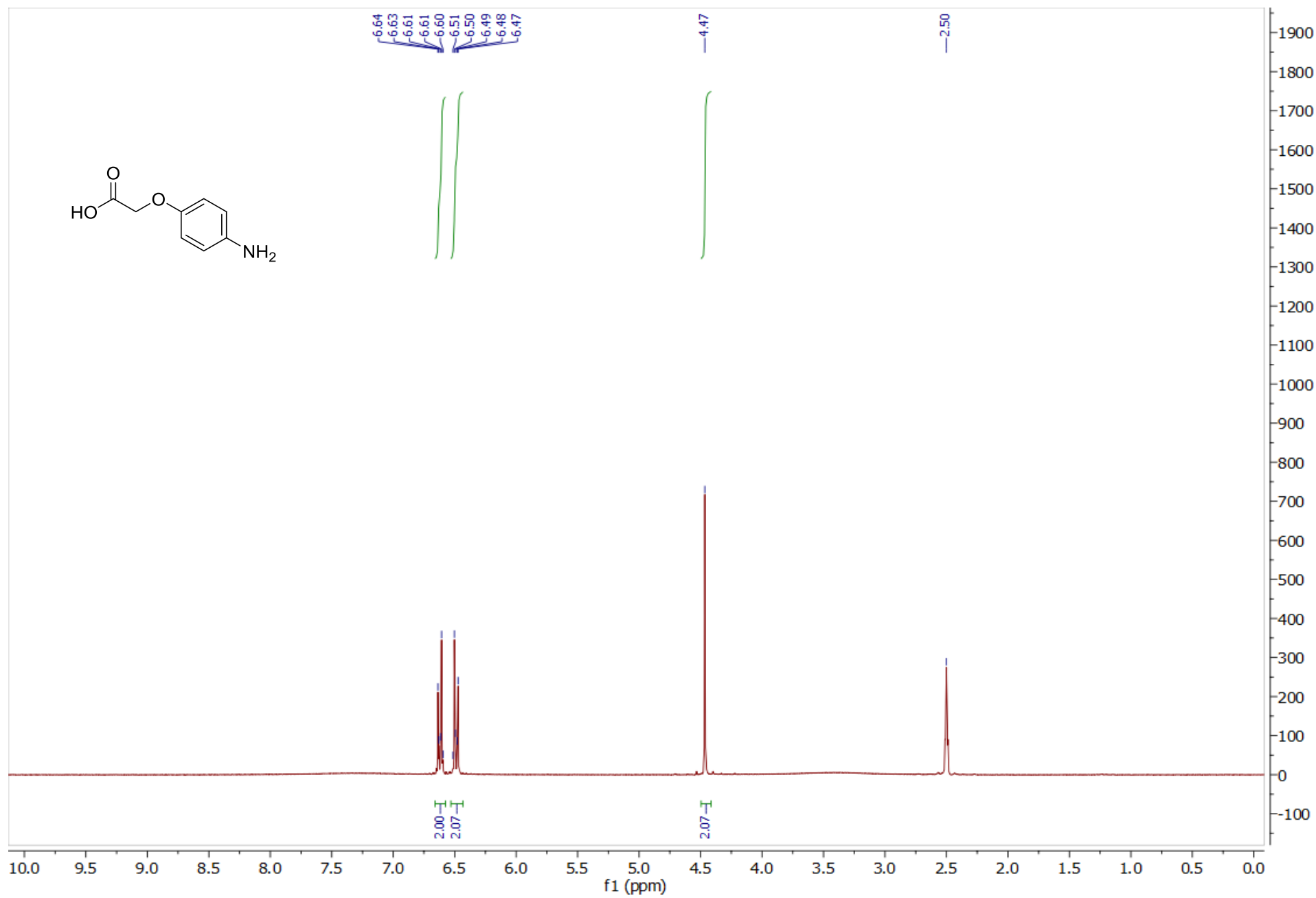




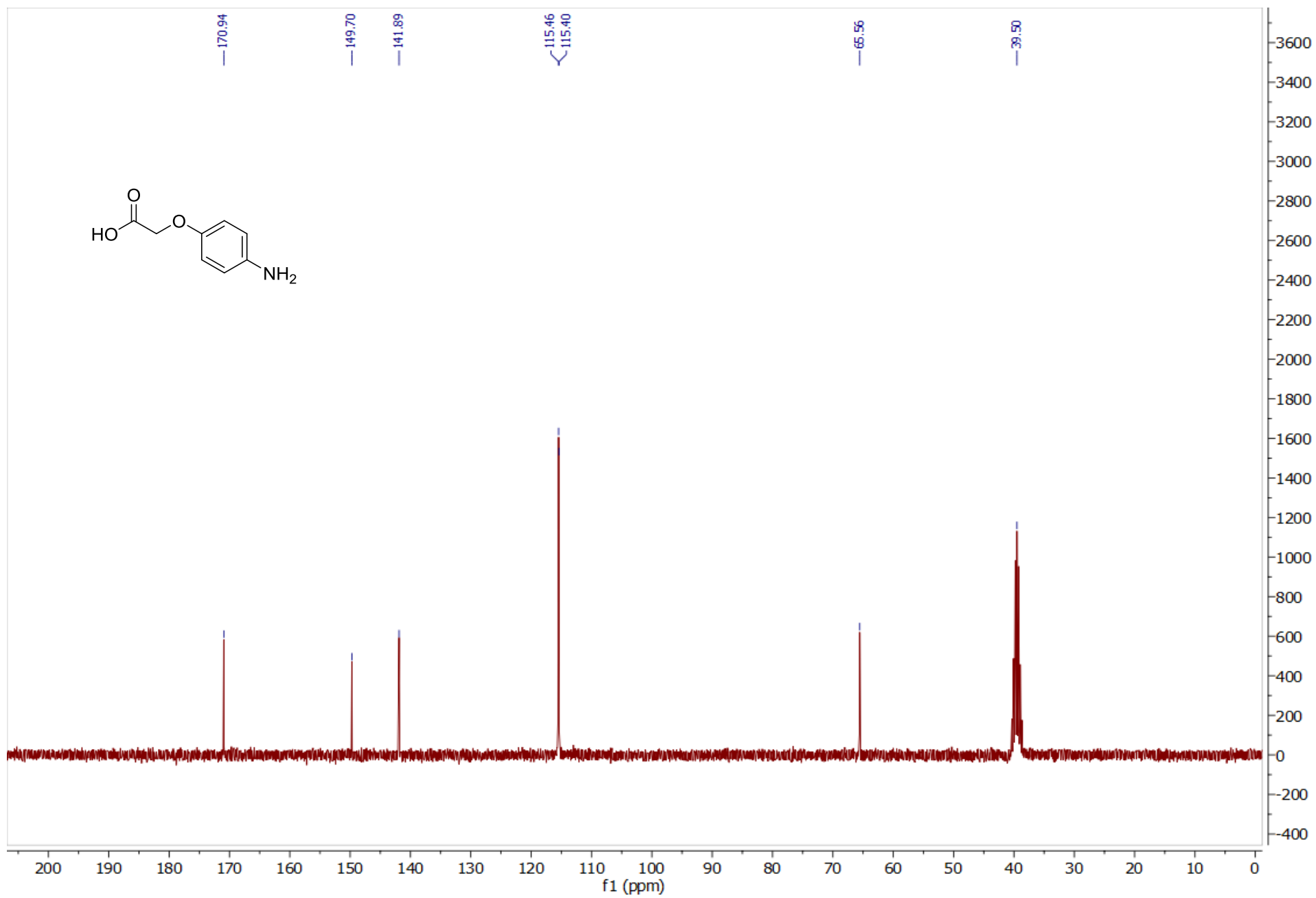
$^{13}\text{C}$  NMR of ethyl 2-[4-[(*tert*-butoxycarbonyl)amino]phenoxy]acetate (**16**) (75 MHz,  $\text{CDCl}_3$ )



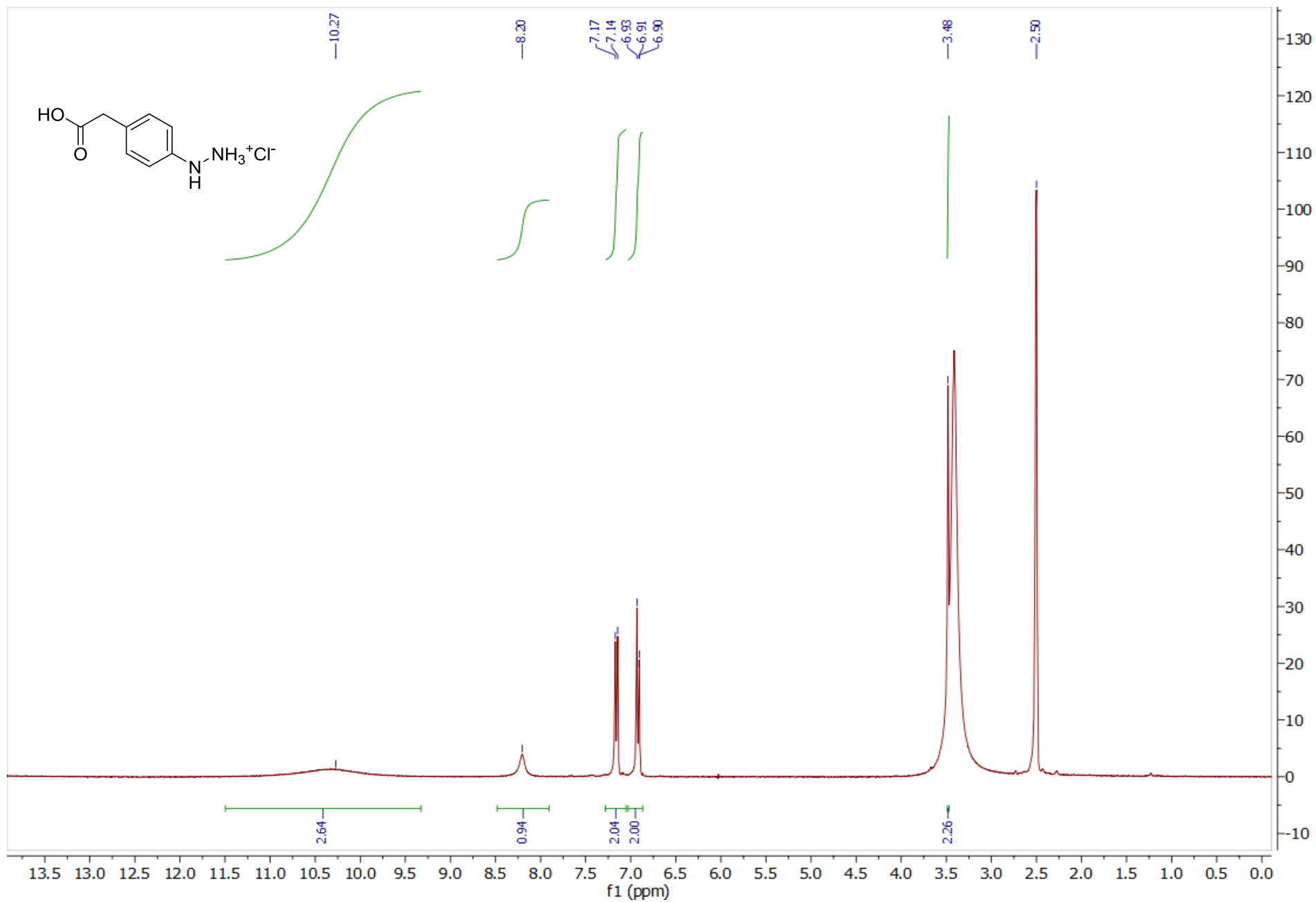
$^1\text{H}$  NMR of 2-(4-aminophenoxy)acetic acid (**8b**) (300 MHz,  $\text{DMSO-d}_6$ )



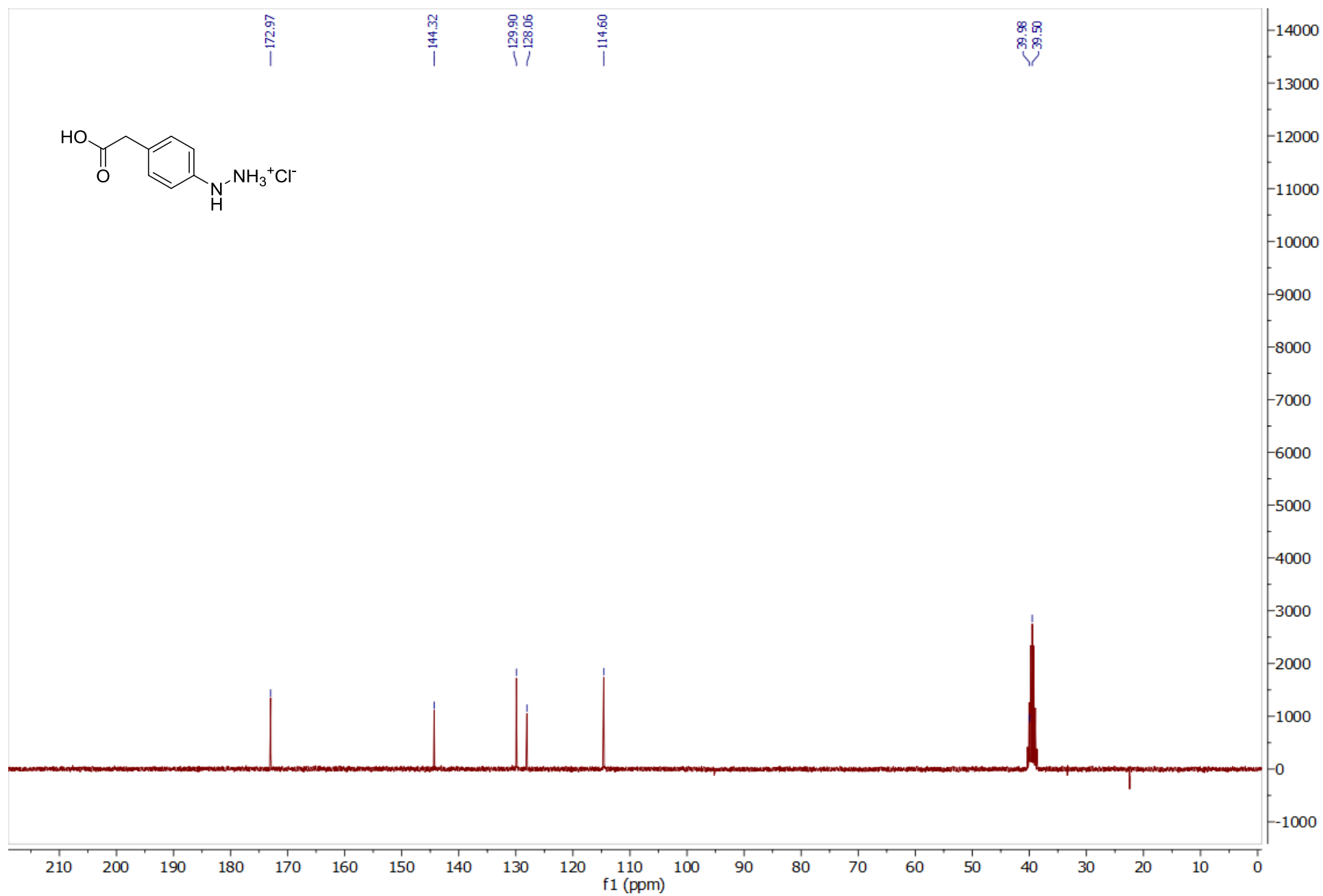
$^{13}\text{C}$  NMR of 2-(4-aminophenoxy)acetic acid (**8b**) (75 MHz, DMSO- $\text{d}_6$ )



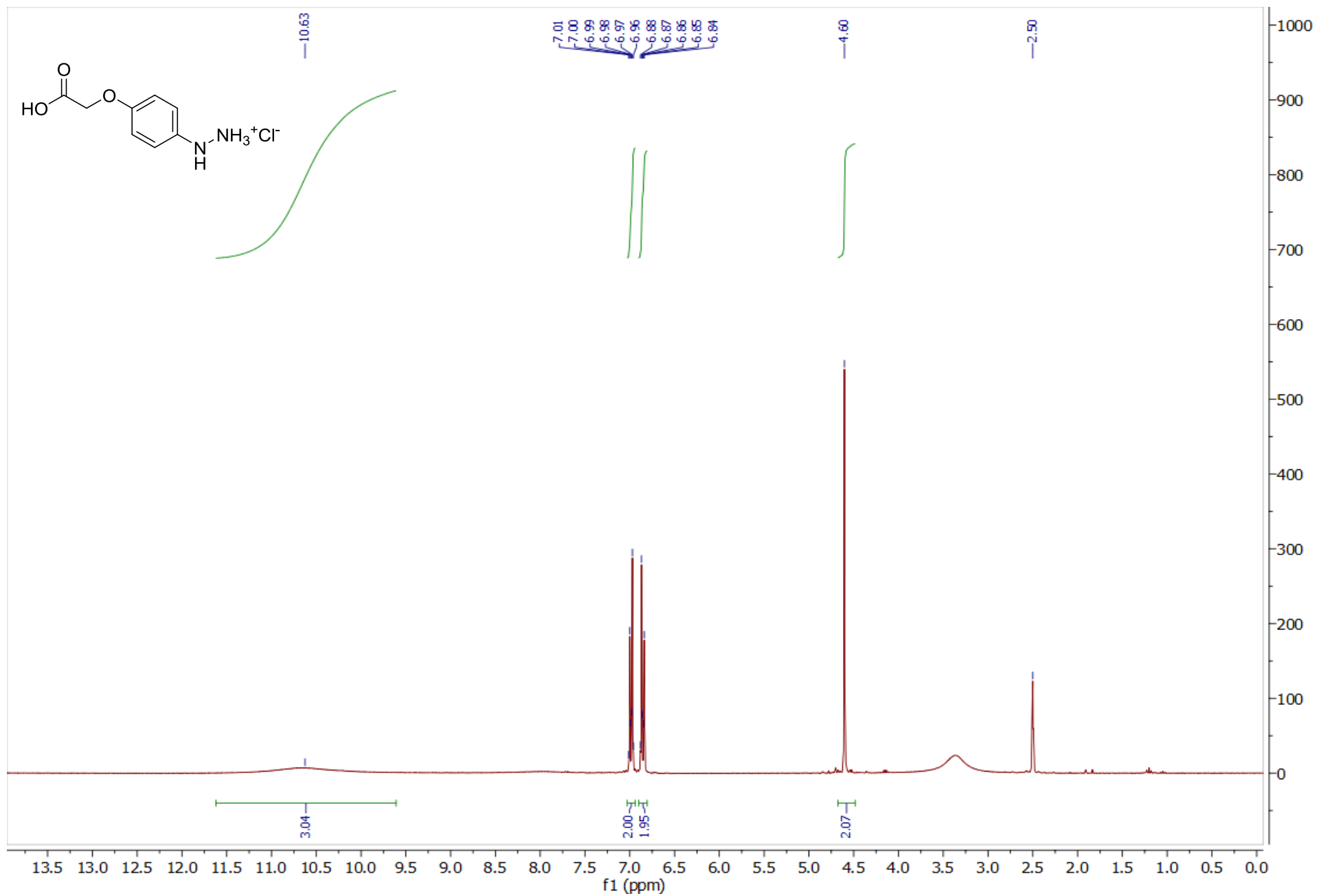
$^1\text{H}$  NMR of 4-(carboxymethyl)phenylhydrazinium chloride (**7a**) (300 MHz, DMSO- $d_6$ )



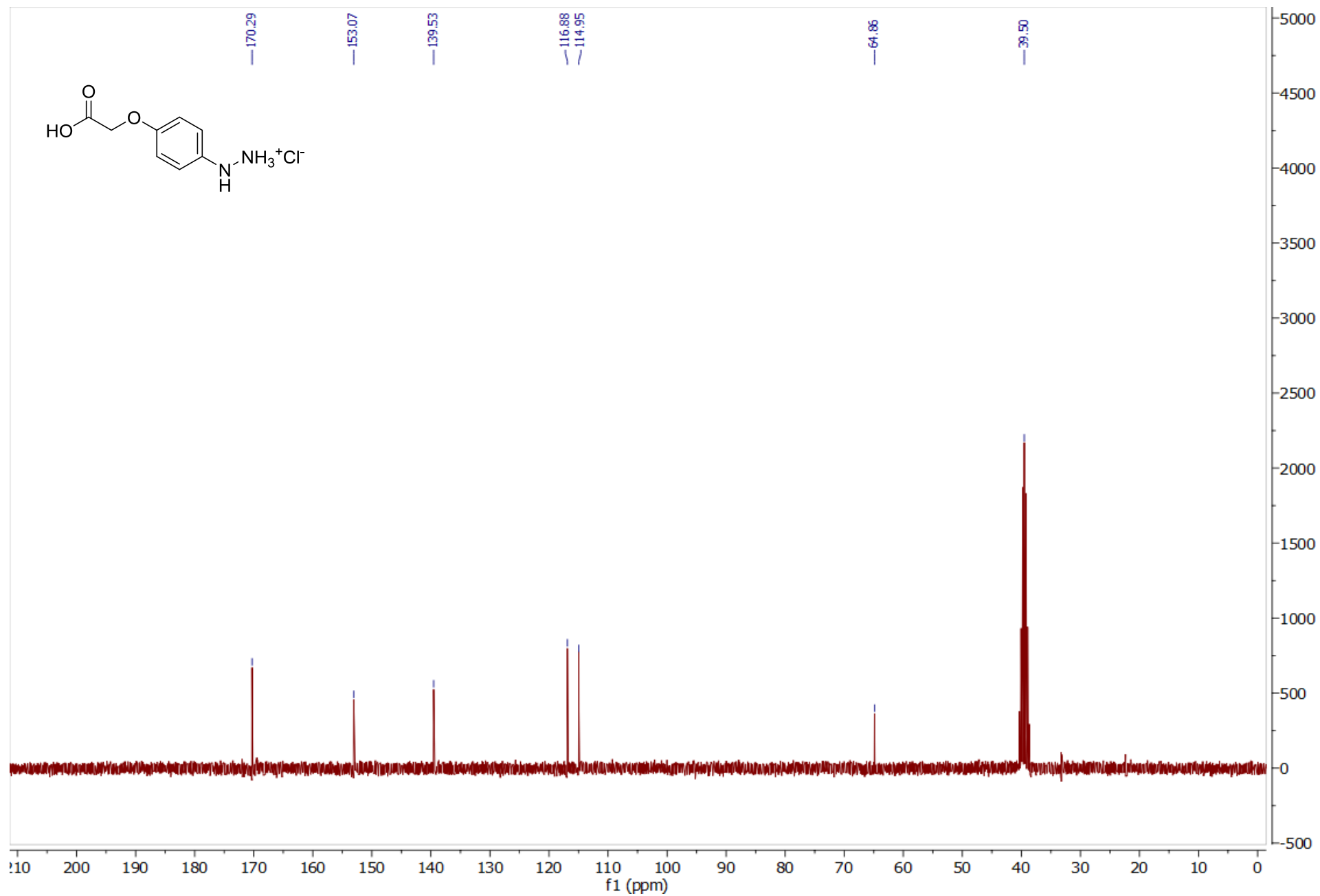
$^{13}\text{C}$  NMR of 4-(carboxymethyl)phenylhydrazinium chloride (**7a**) (75 MHz, DMSO- $\text{d}_6$ )



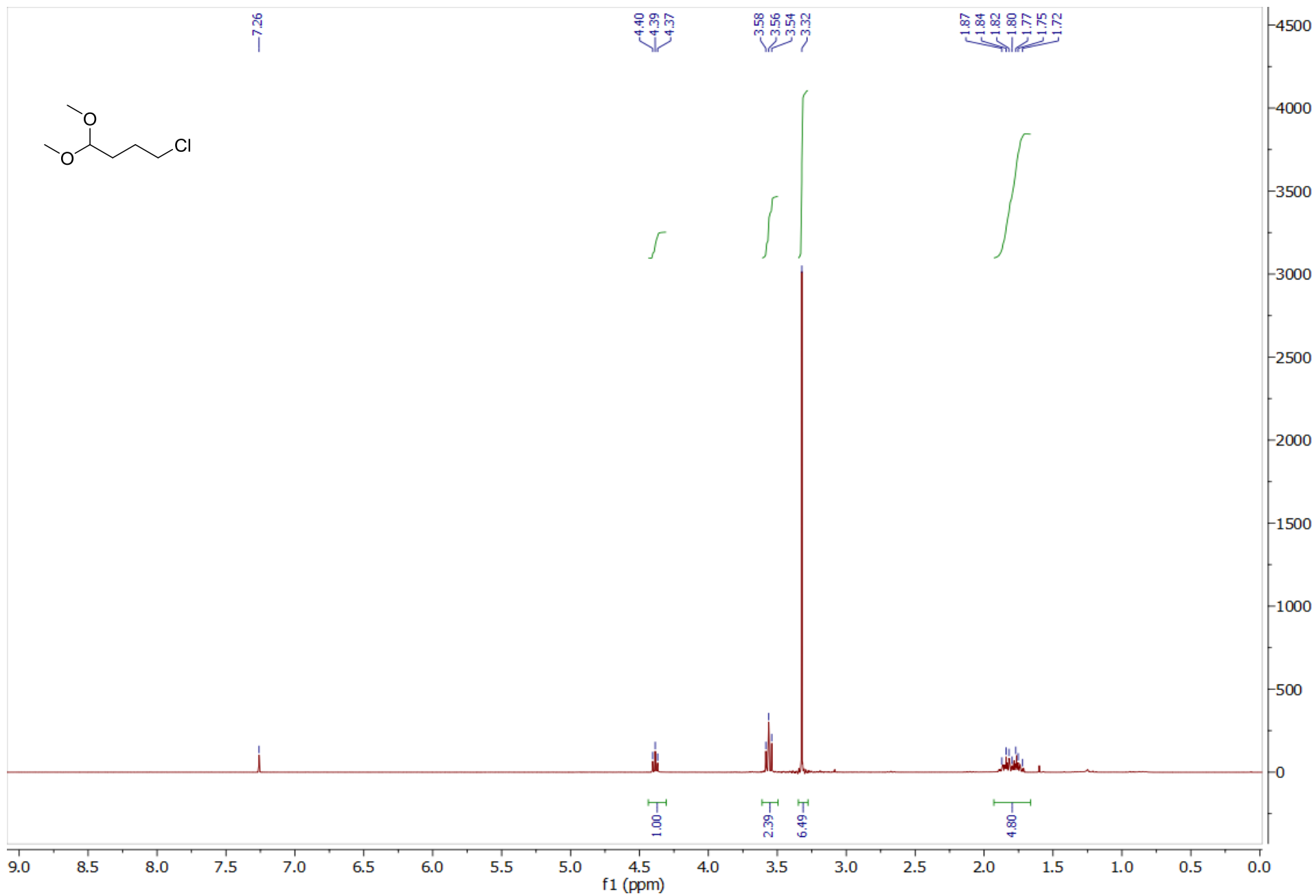
$^1\text{H}$  NMR of 4-(carboxymethoxy)phenylhydrazinium chloride (**7b**) (300 MHz,  $\text{DMSO-d}_6$ )



$^{13}\text{C}$  NMR of 4-(carboxymethoxy)phenylhydrazinium chloride (**7b**) (75 MHz, DMSO- $\text{d}_6$ )

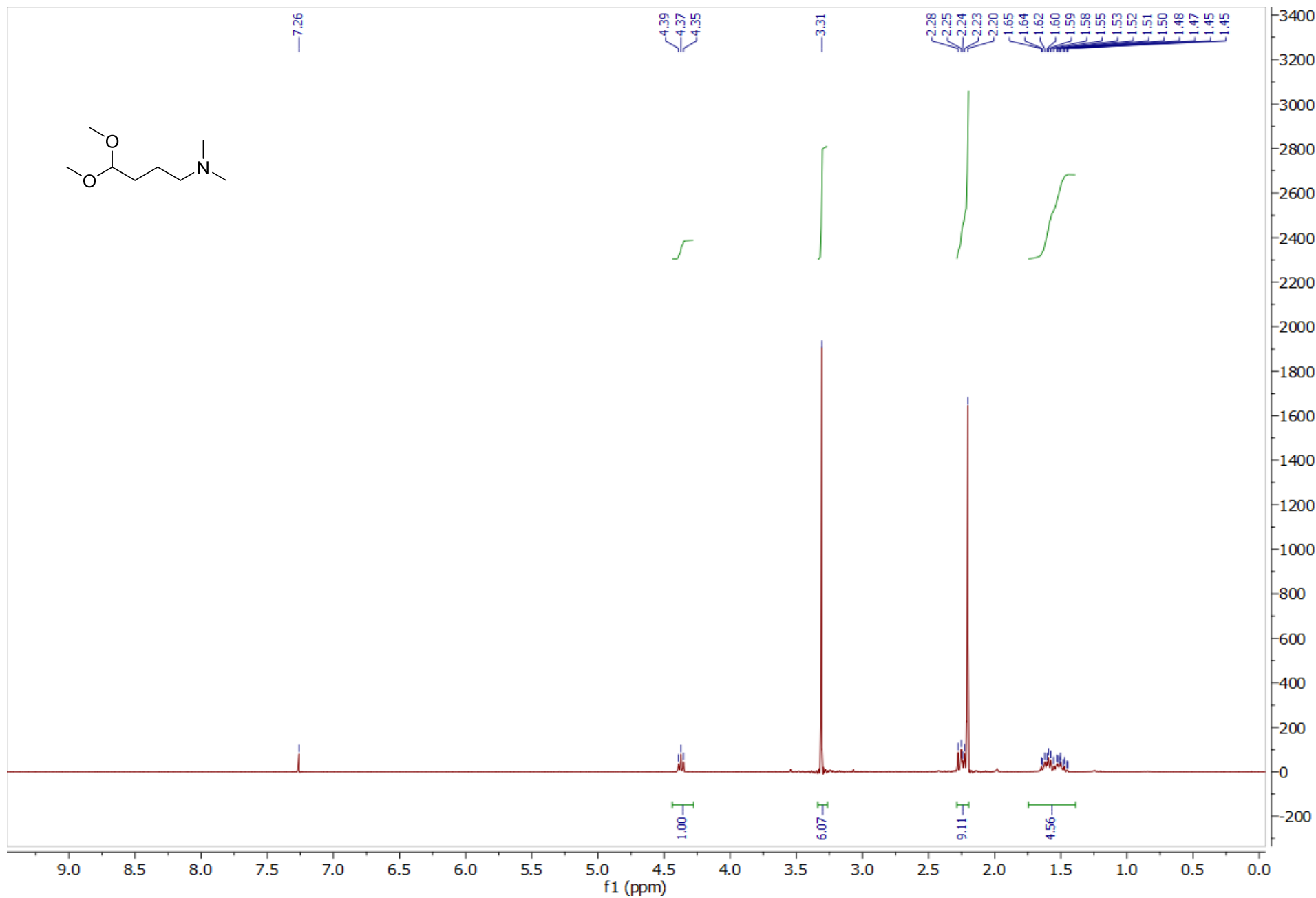


$^1\text{H}$  NMR of 4-chloro-1,1-dimethoxybutane (**12**) (300 MHz,  $\text{CDCl}_3$ )

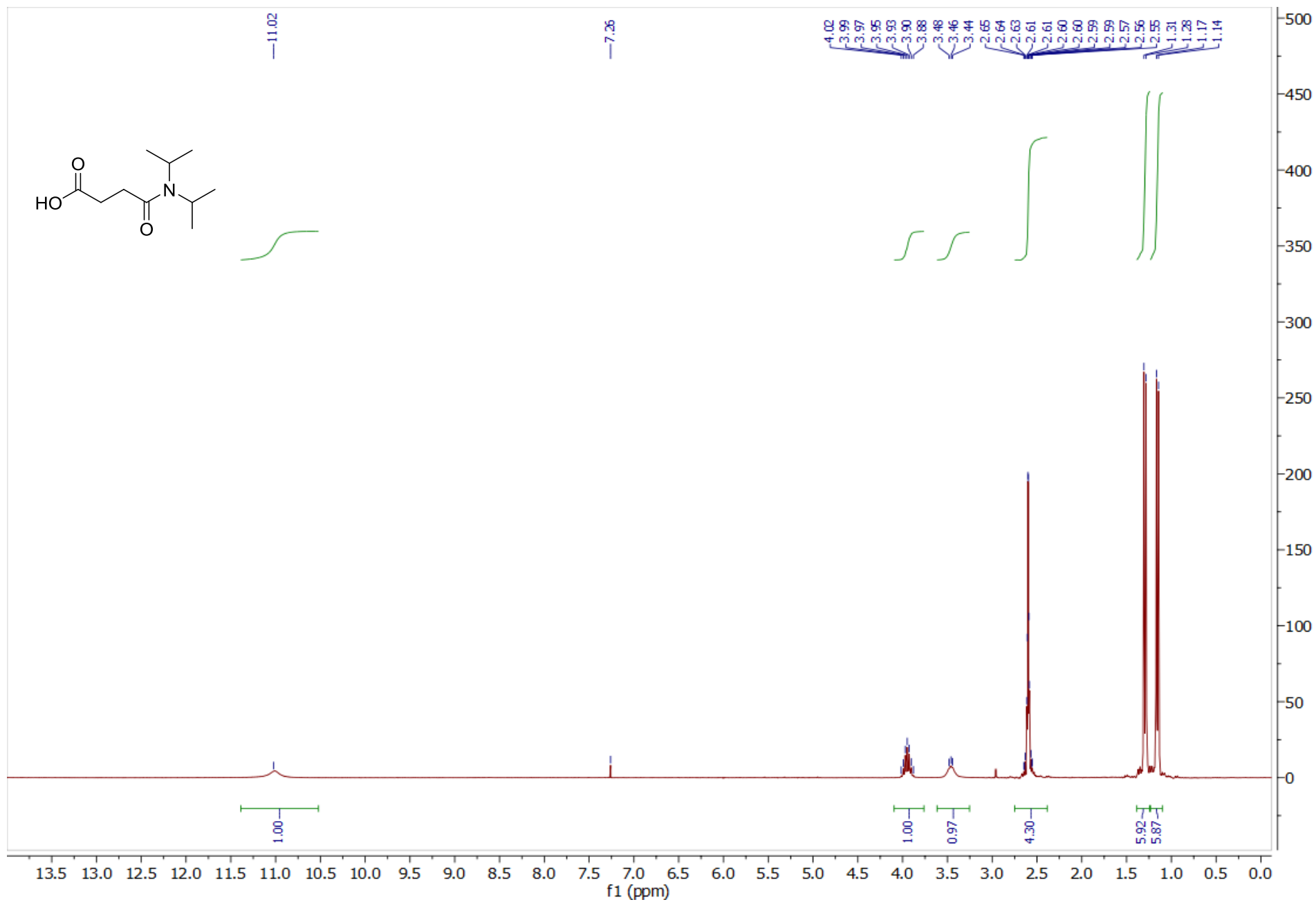




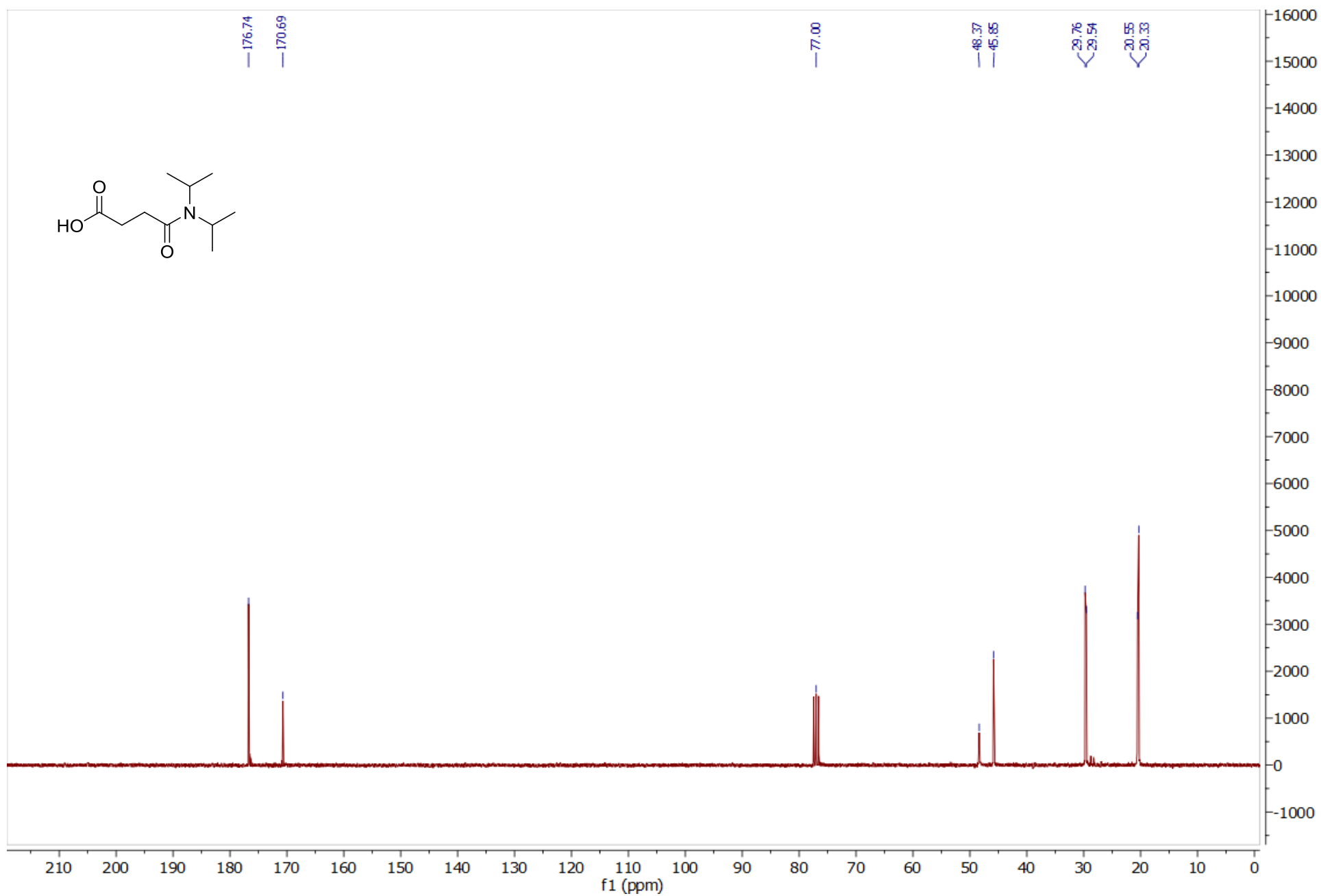
$^1\text{H}$  NMR of 4-(*N,N*-dimethylamino)-1,1-dimethoxybutane (**9**) (300 MHz,  $\text{CDCl}_3$ )



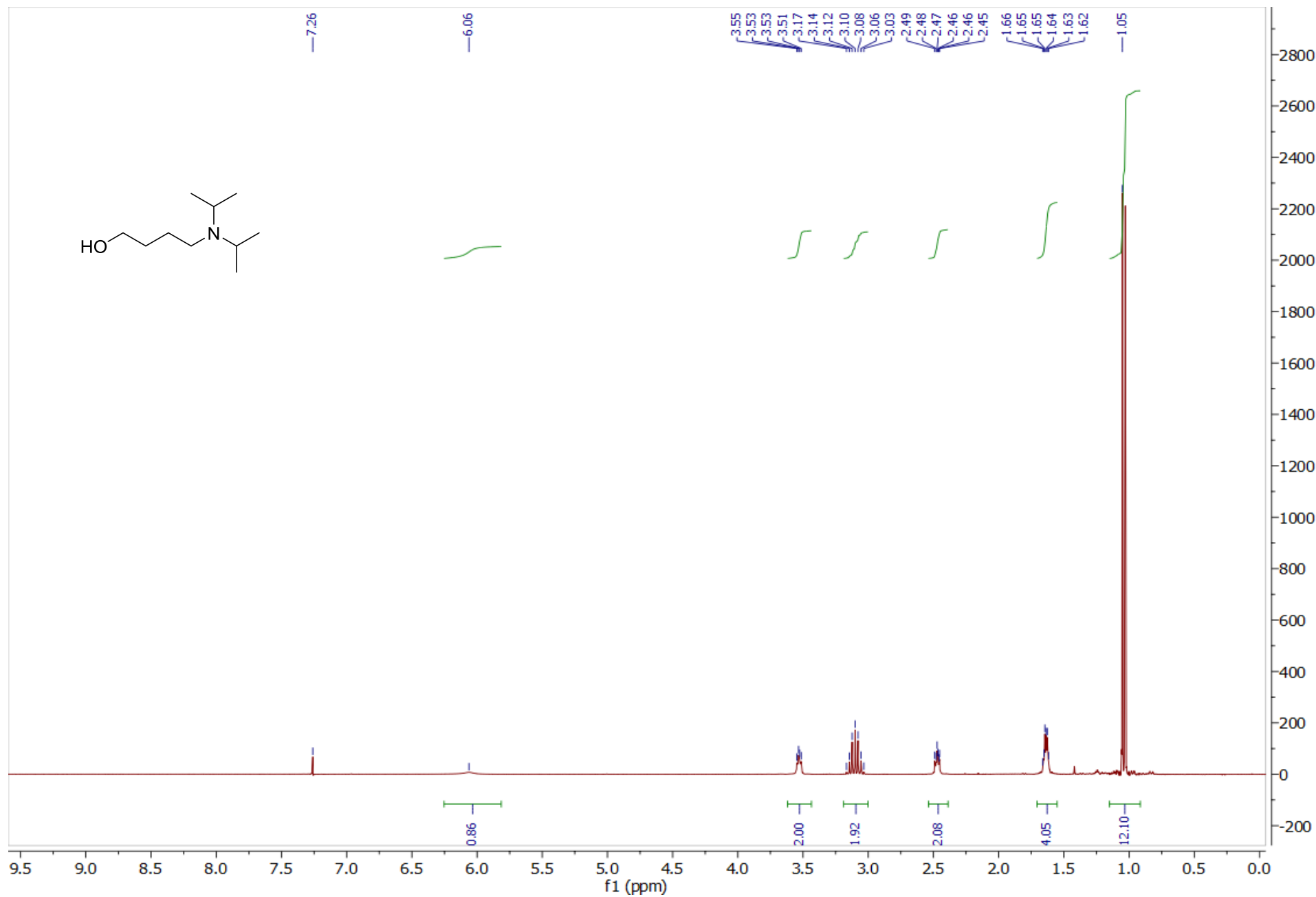
$^1\text{H}$  NMR of 4-(*N,N*-diisopropylamino)-4-oxobutanoic acid (**14**) (300 MHz,  $\text{CDCl}_3$ )



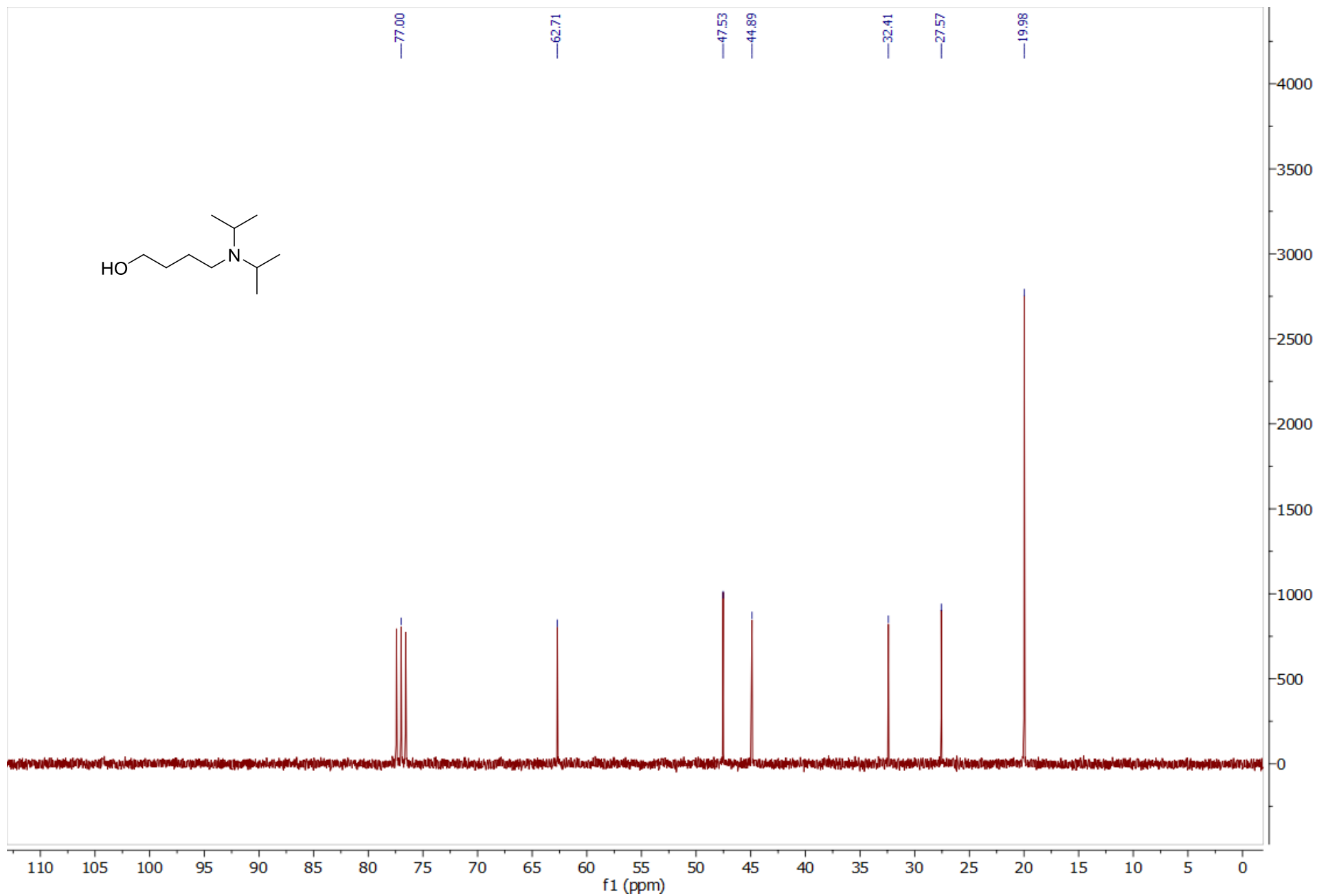
<sup>13</sup>C NMR of 4-(*N,N*-diisopropylamino)-4-oxobutanoic acid (**14**) (75 MHz, CDCl<sub>3</sub>)



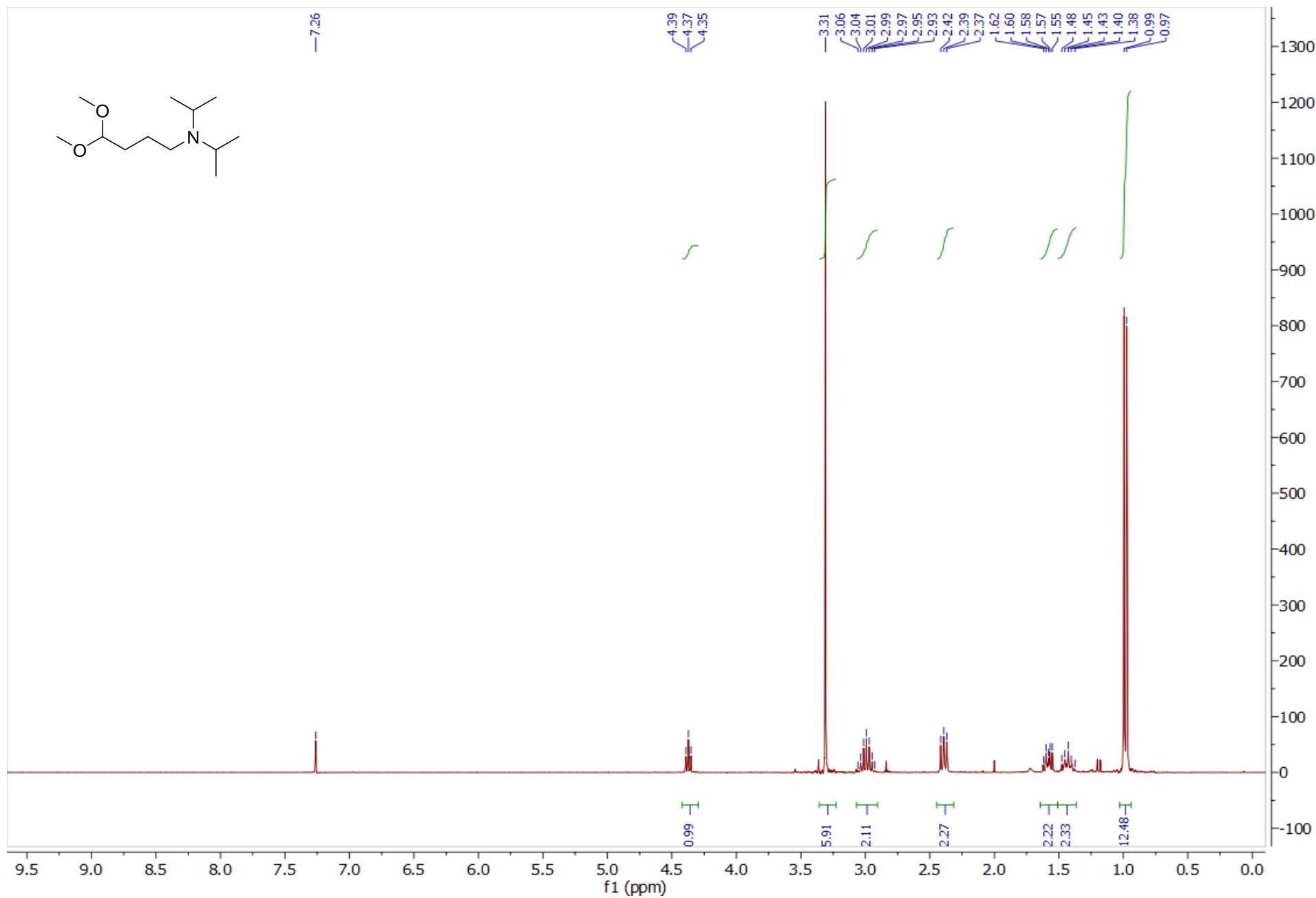
$^1\text{H}$  NMR of 4-(*N,N*-diisopropylamino)butan-1-ol (**15**) (300 MHz,  $\text{CDCl}_3$ )



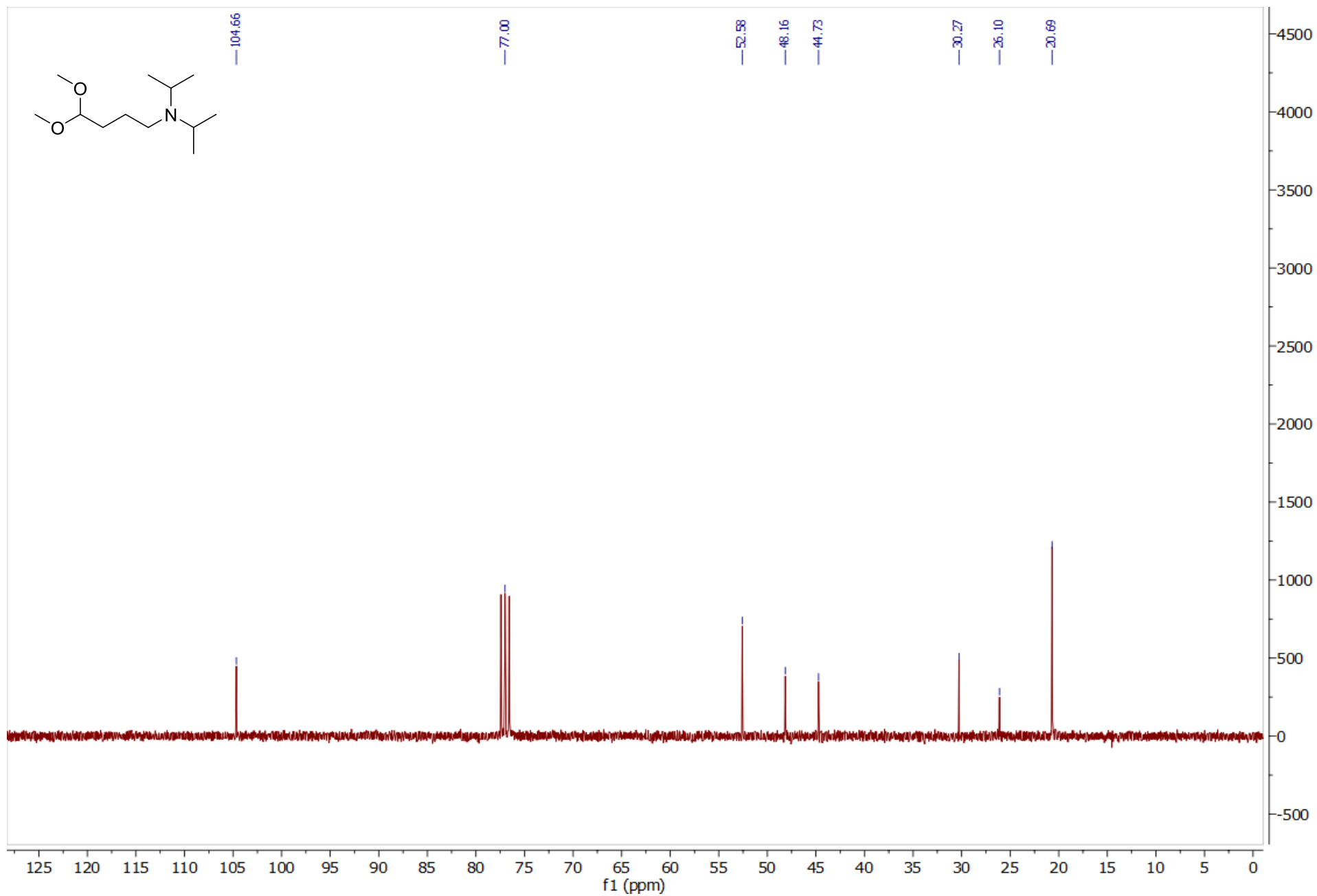
$^{13}\text{C}$  NMR of 4-(*N,N*-diisopropylamino)butan-1-ol (**15**) (75 MHz,  $\text{CDCl}_3$ )



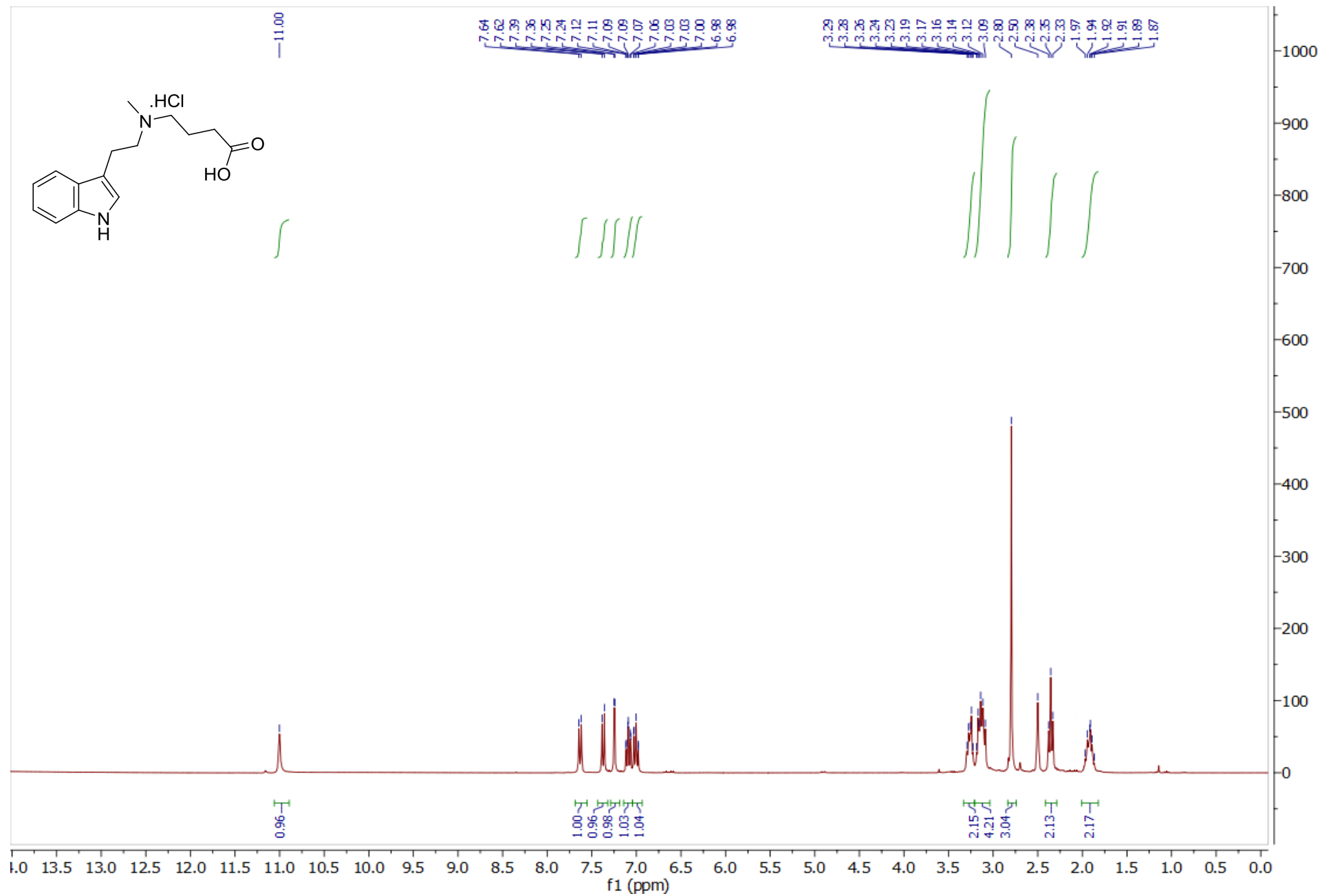
$^1\text{H}$  NMR of 4-(*N,N*-diisopropylamino)-1,1-dimethoxybutane (**10**) (300 MHz,  $\text{CDCl}_3$ )



$^{13}\text{C}$  NMR of 4-(*N,N*-diisopropylamino)-1,1-dimethoxybutane (**10**) (75 MHz,  $\text{CDCl}_3$ )

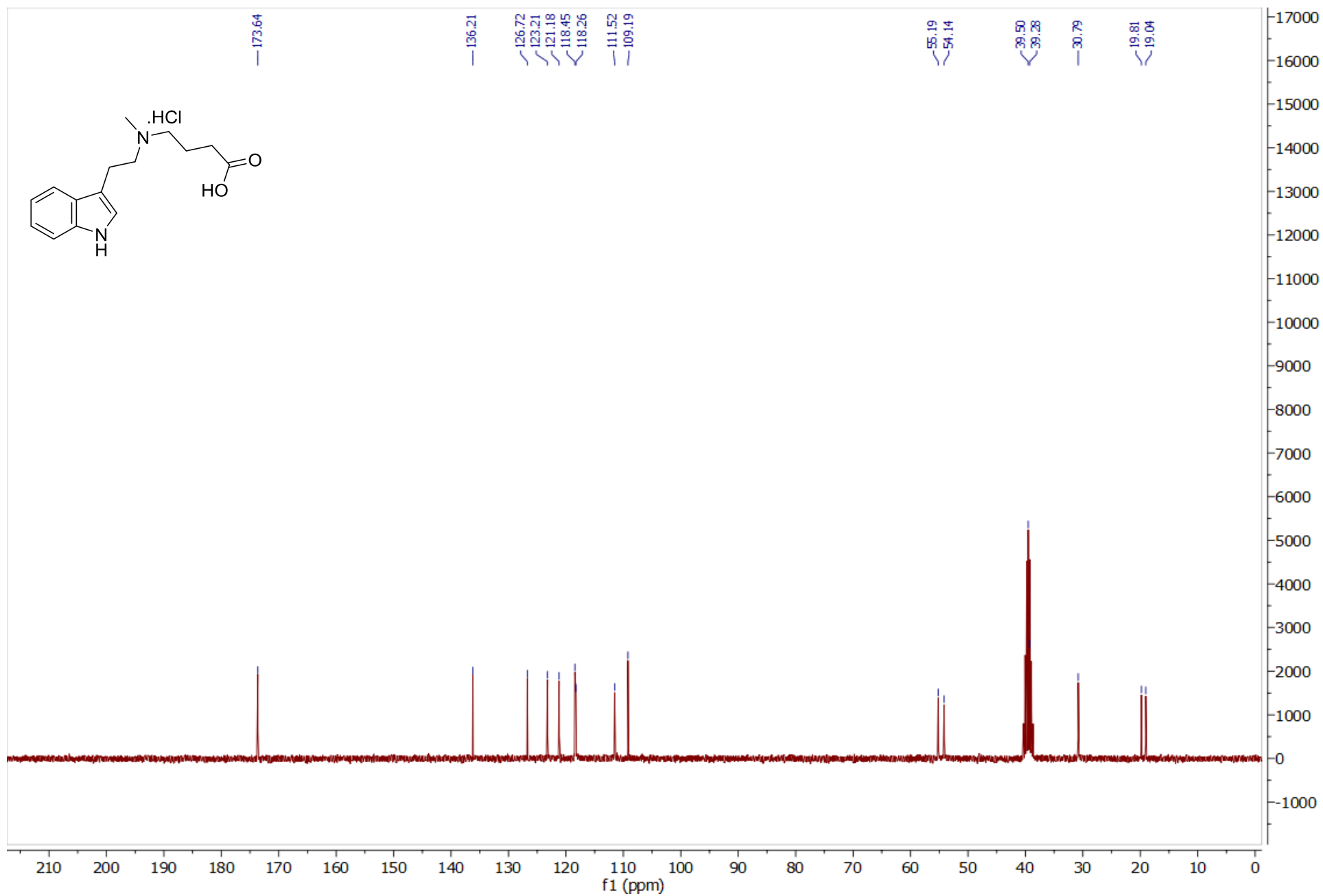


$^1\text{H}$  NMR of 4-[N-[2-(1*H*-indol-3-yl)ethyl]-N-methyl]aminobutanoic acid hydrochloride (**1a**, **hapten I**) (300 MHz, DMSO- $d_6$ )

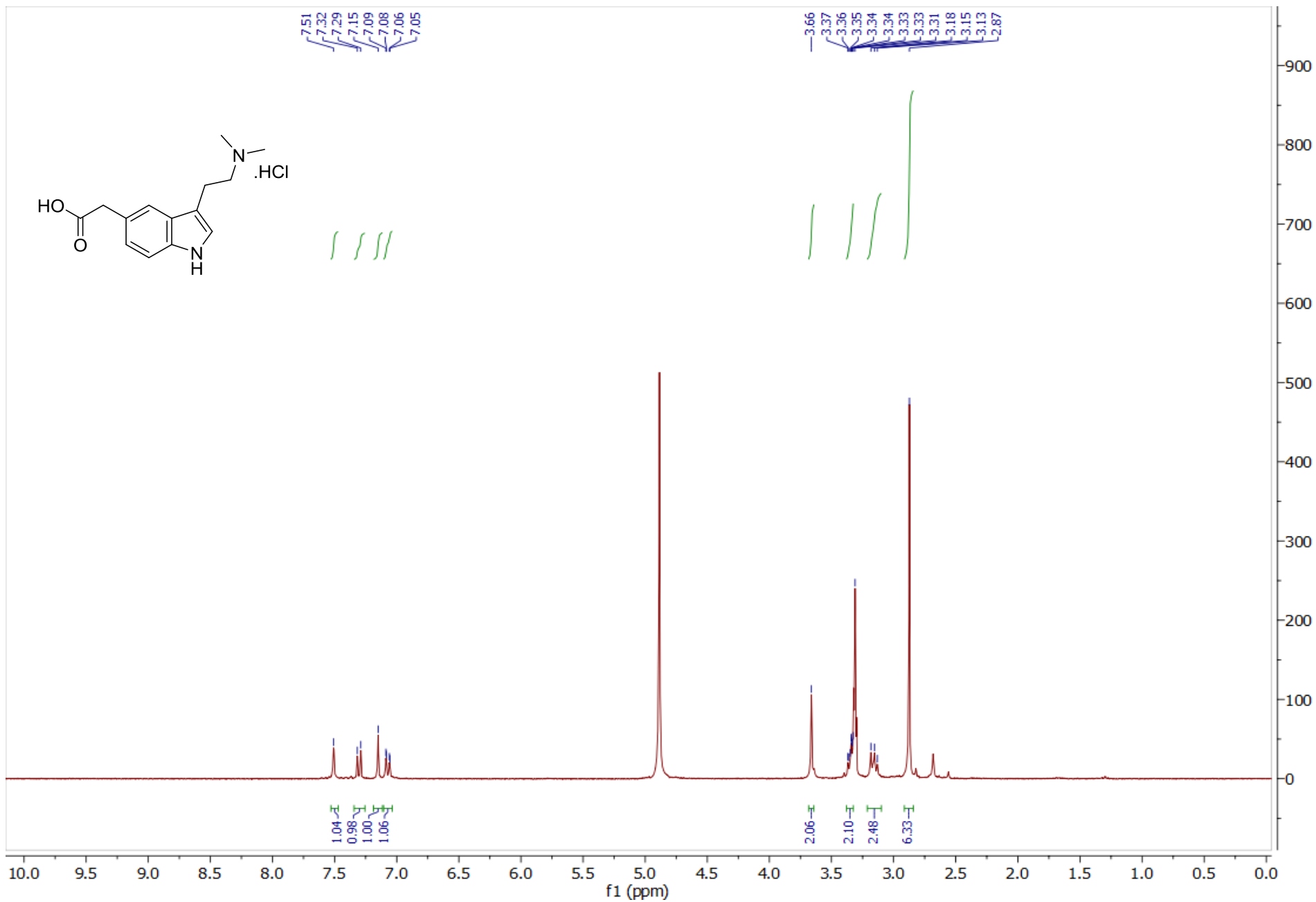




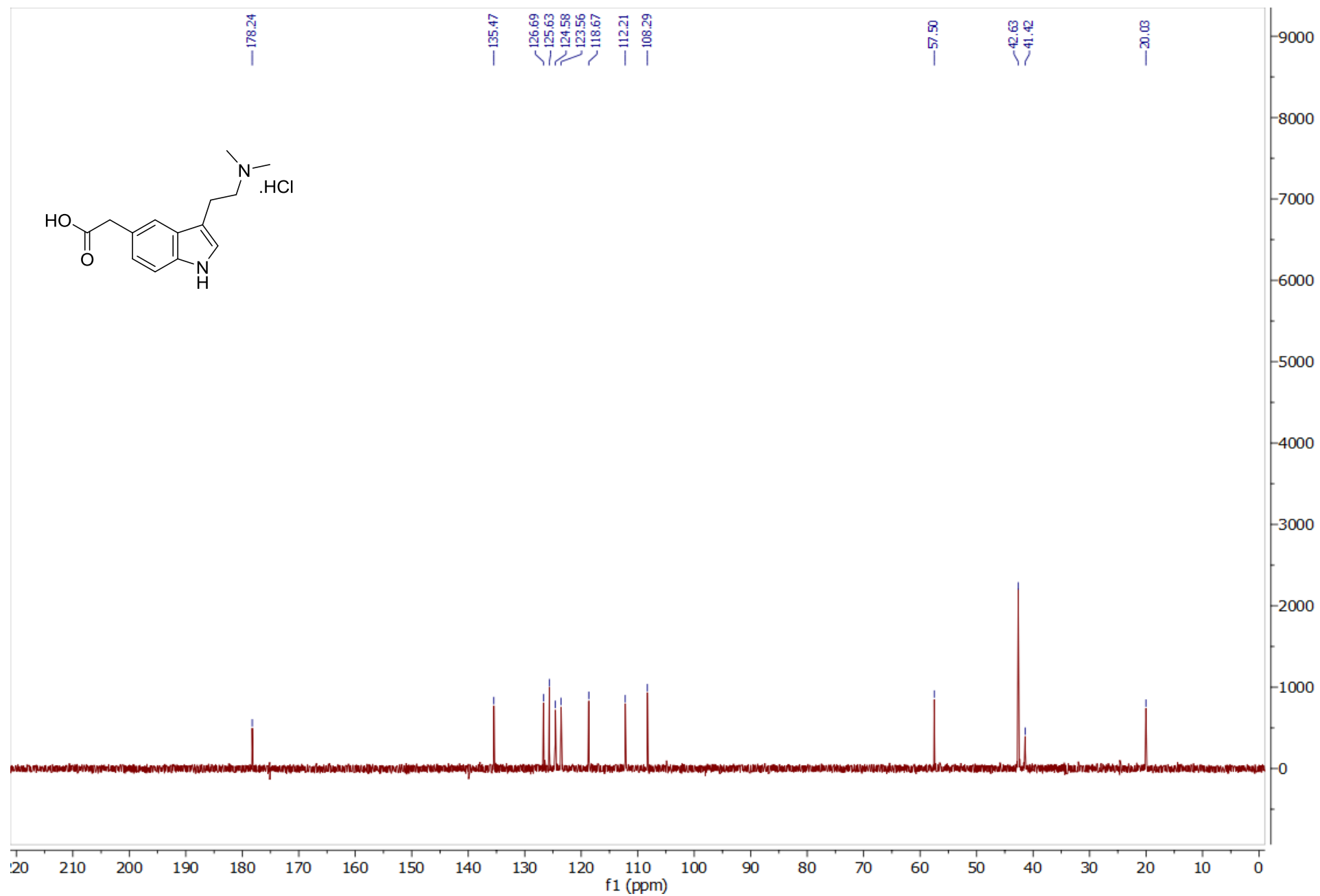
$^{13}\text{C}$  NMR of 4-[*N*-[2-(*1H*-indol-3-yl)ethyl]-*N*-methyl]aminobutanoic acid hydrochloride (**1a**, **haptin I**) (75 MHz, DMSO- $\text{d}_6$ )



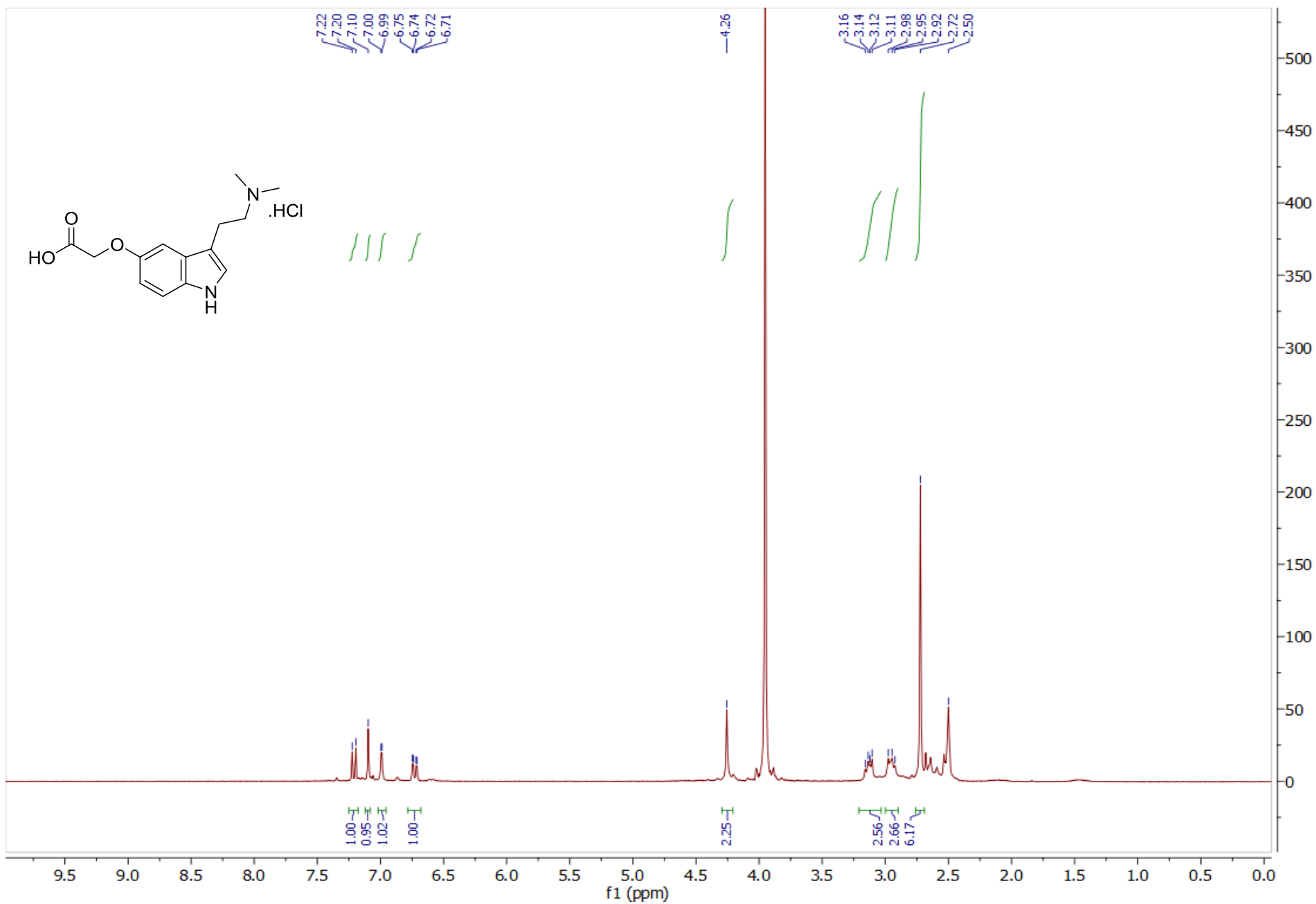
<sup>1</sup>H NMR of 2-[3-[2-(*N,N*-dimethylamino)ethyl]-1*H*-indol-5-yl]acetic acid hydrochloride (**1b**, **hapten II**) (300 MHz, CD<sub>3</sub>OD)



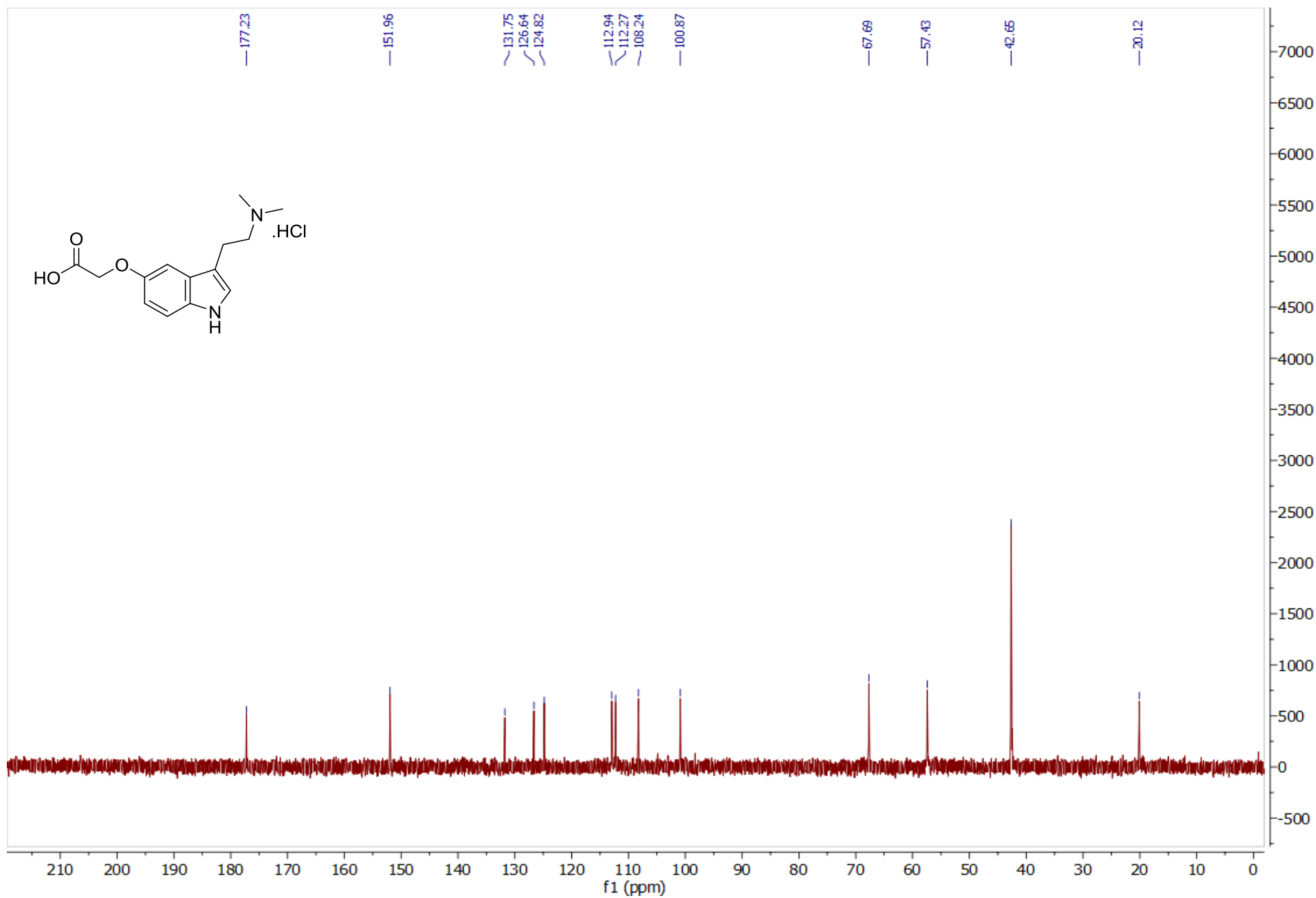
$^{13}\text{C}$  NMR of 2-[3-[2-(*N,N*-dimethylamino)ethyl]-*1H*-indol-5-yl]acetic acid hydrochloride (**1b**, **hapten II**) (75 MHz,  $\text{D}_2\text{O}$ )



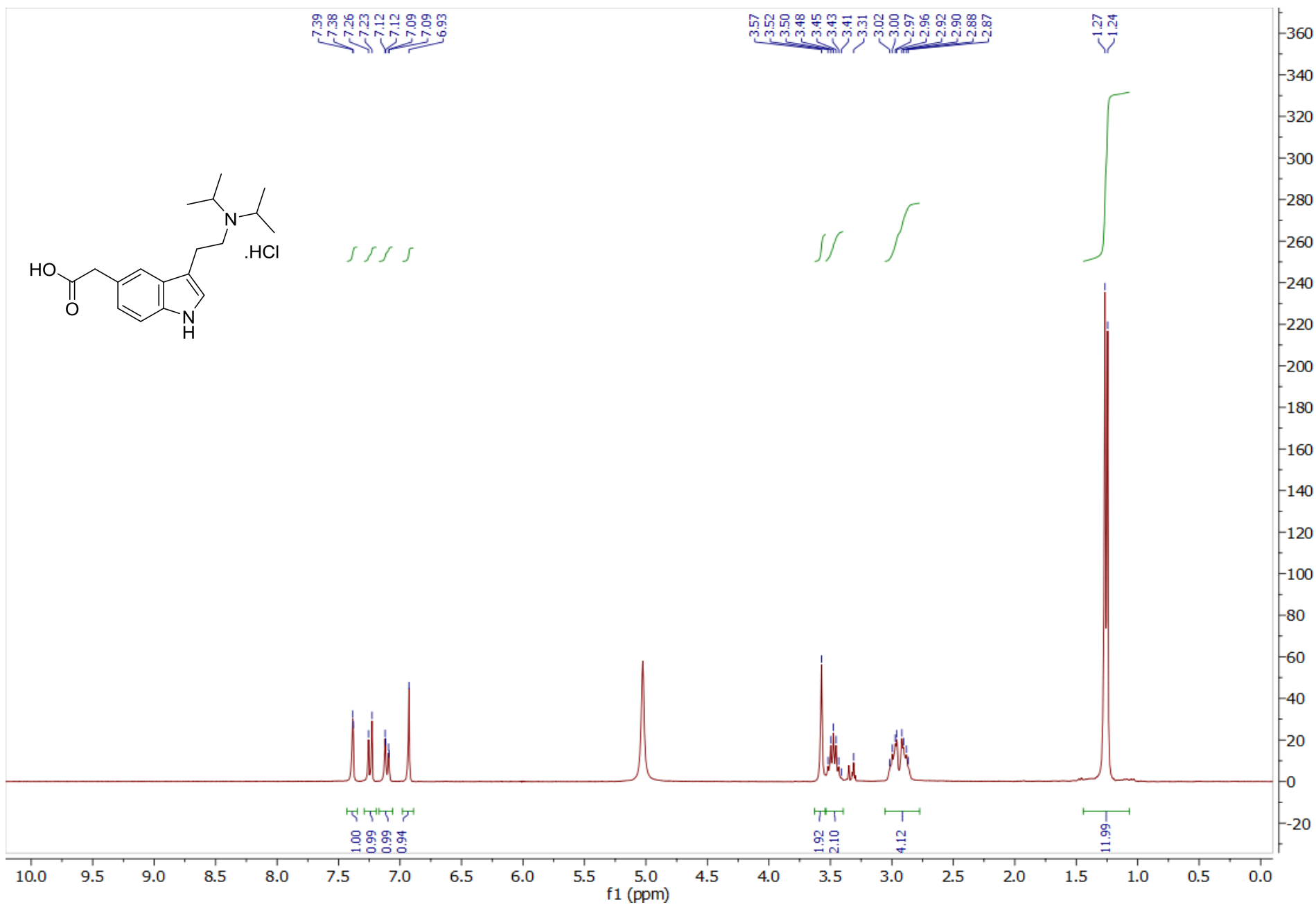
$^1\text{H}$  NMR of 2-[3-[2-(*N,N*-dimethylamino)ethyl]-1*H*-indol-5-yloxy]acetic acid hydrochloride (**1c**, **haptent III**) (300 MHz,  $\text{D}_2\text{O}$  +  $\text{DMSO-d}_6$ )



$^{13}\text{C}$  NMR of 2-[3-[2-(*N,N*-dimethylamino)ethyl]-*1H*-indol-5-yloxy]acetic acid hydrochloride (**1c**, **hapten III**) (75 MHz,  $\text{D}_2\text{O}$ )



$^1\text{H}$  NMR of -[3-[2-(*N,N*-diisopropylamino)ethyl]-1*H*-indol-5-yl]acetic acid hydrochloride (**1d**, **hapten IV**) (300 MHz,  $\text{CD}_3\text{OD}$ )



$^{13}\text{C}$  APT NMR of -[3-[2-(*N,N*-diisopropylamino)ethyl]-*1H*-indol-5-yl]acetic acid hydrochloride (**1d**, **hapten IV**) (75 MHz,  $\text{CD}_3\text{OD}$ )

