

## Supporting Information

### Synthesis and physical chemical properties of 2-amino-4-(trifluoromethoxy)butanoic acid – CF<sub>3</sub>O-containing analogue of natural lipophilic amino acids.

*Ivan S. Kondratov,<sup>\*a,b</sup> Ivan G. Logvinenko,<sup>a,b</sup> Nataliya. A. Tolmachova,<sup>a,b</sup> Roman N. Morev,<sup>a</sup> Maria A. Kliachyna,<sup>a</sup> Florian Clausen,<sup>c</sup> Constantin G. Daniliuc<sup>c</sup> and Günter Haufe<sup>\*c,d</sup>*

<sup>a</sup> *Enamine Ltd, Chervonotkatska St 78, Kyiv, 02094, Ukraine.*

<sup>b</sup> *Institute of Bioorganic Chemistry and Petrochemistry, National Academy of Sciences of Ukraine, Murmanska Str. 1, Kyiv, 02660, Ukraine*

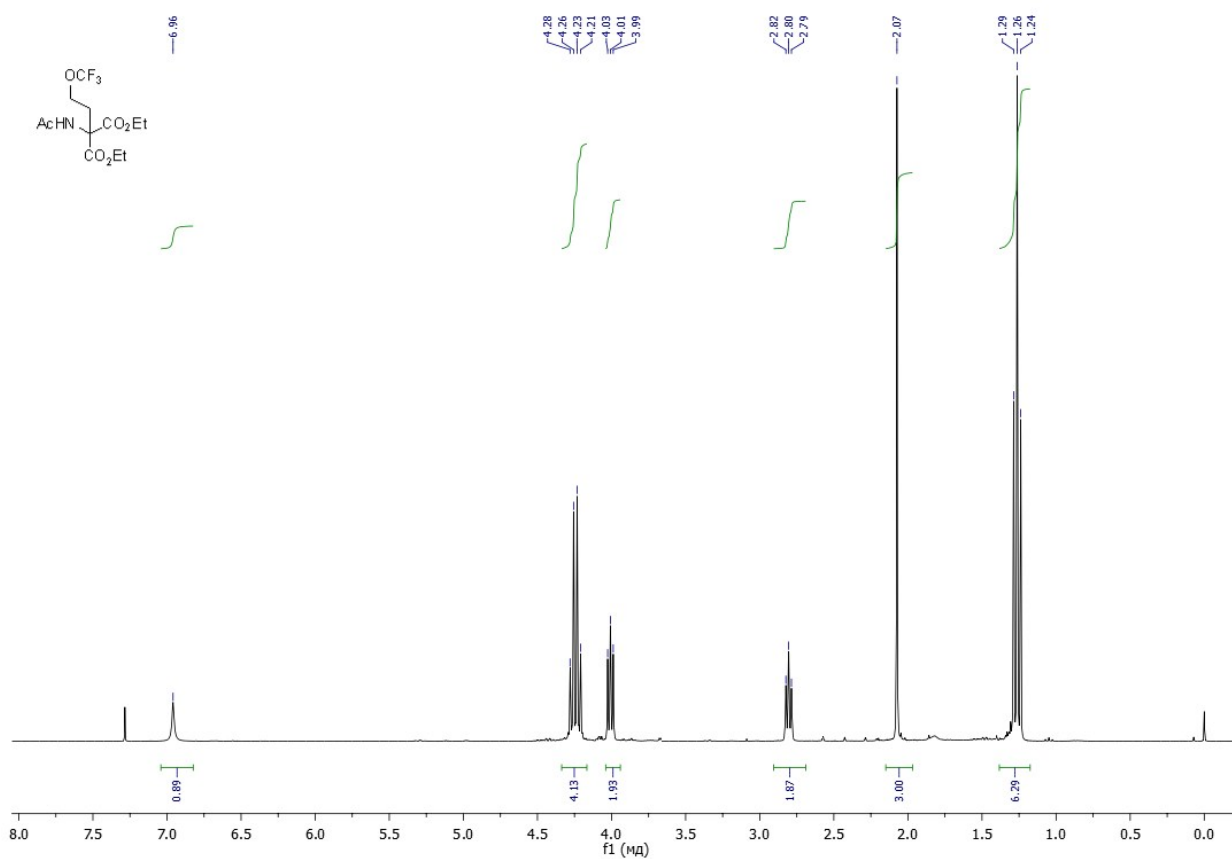
<sup>c</sup> *Organisch-Chemisches Institut, Universität Münster, Corrensstraße 40, Münster 48149, Germany.*

<sup>d</sup> *Cells-in-Motion Cluster of Excellence, Universität Münster, Waldeyerstraße 15, 48149 Münster, Germany.*

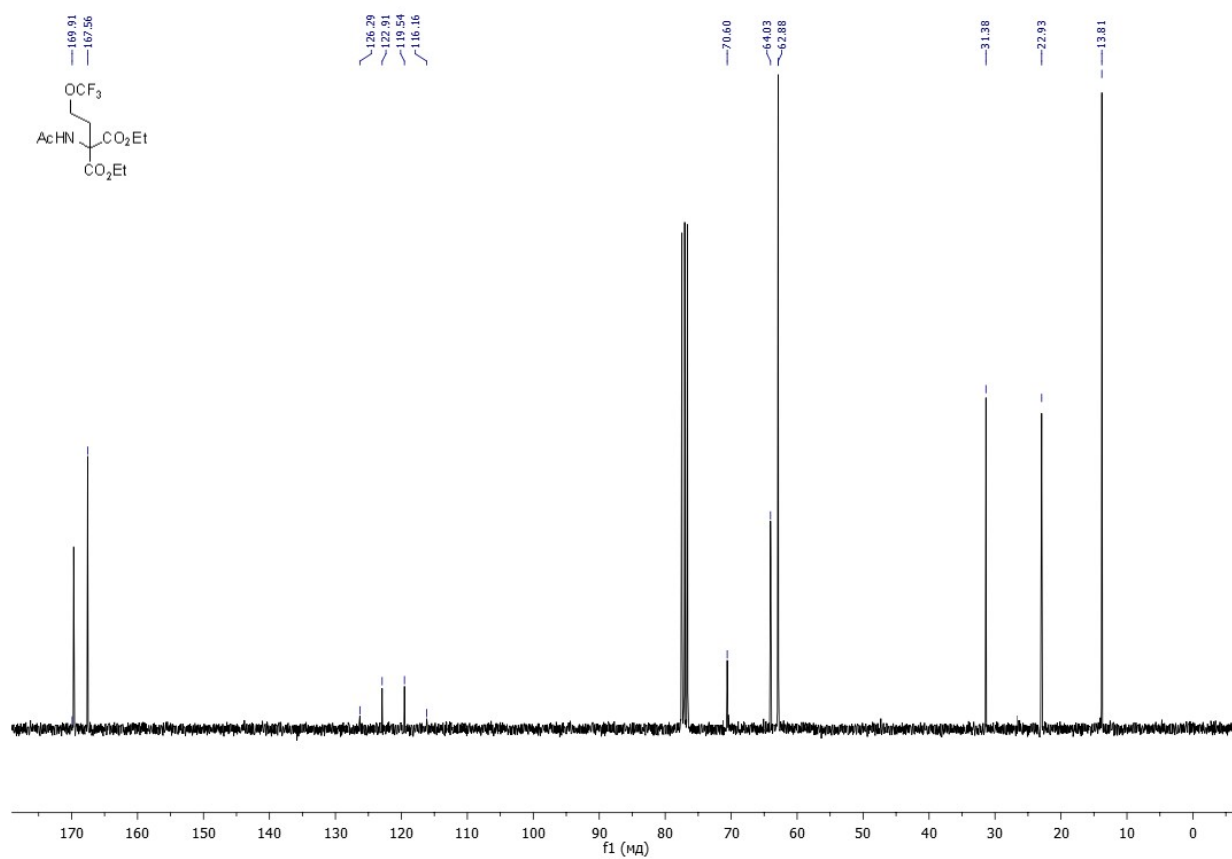
#### Contents

Copies of NMR spectra of new compounds

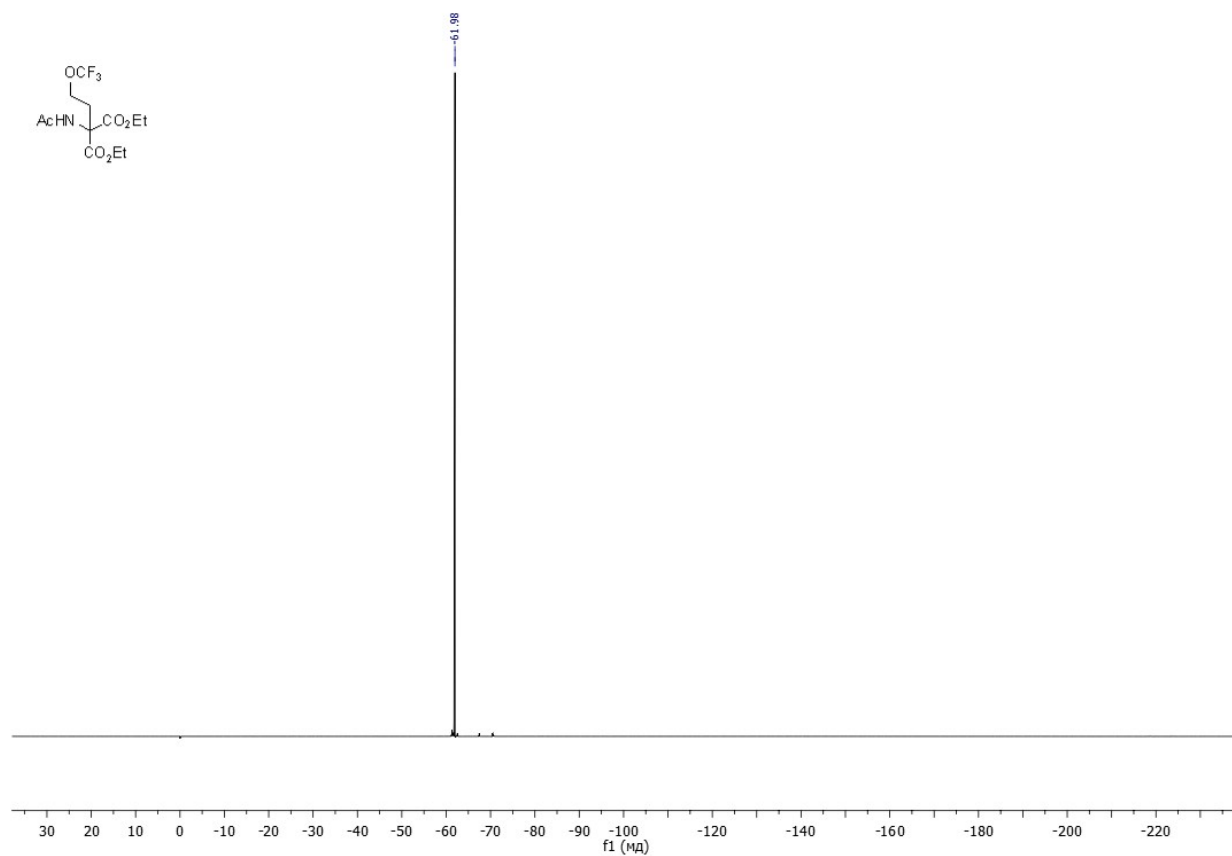
### Compound 9 ( $^1\text{H}$ NMR, $\text{CDCl}_3$ ):



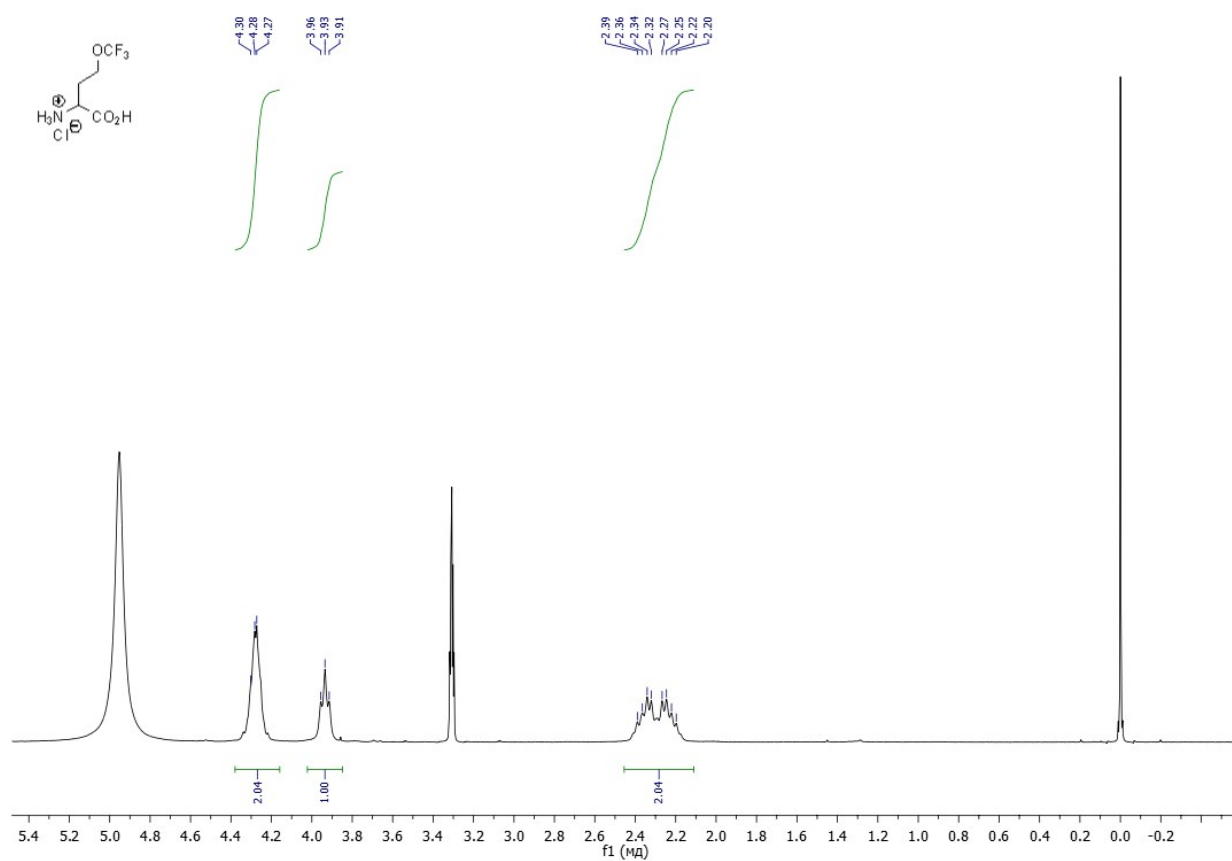
### Compound 9 ( $^{13}\text{C}$ NMR, $\text{CDCl}_3$ ):



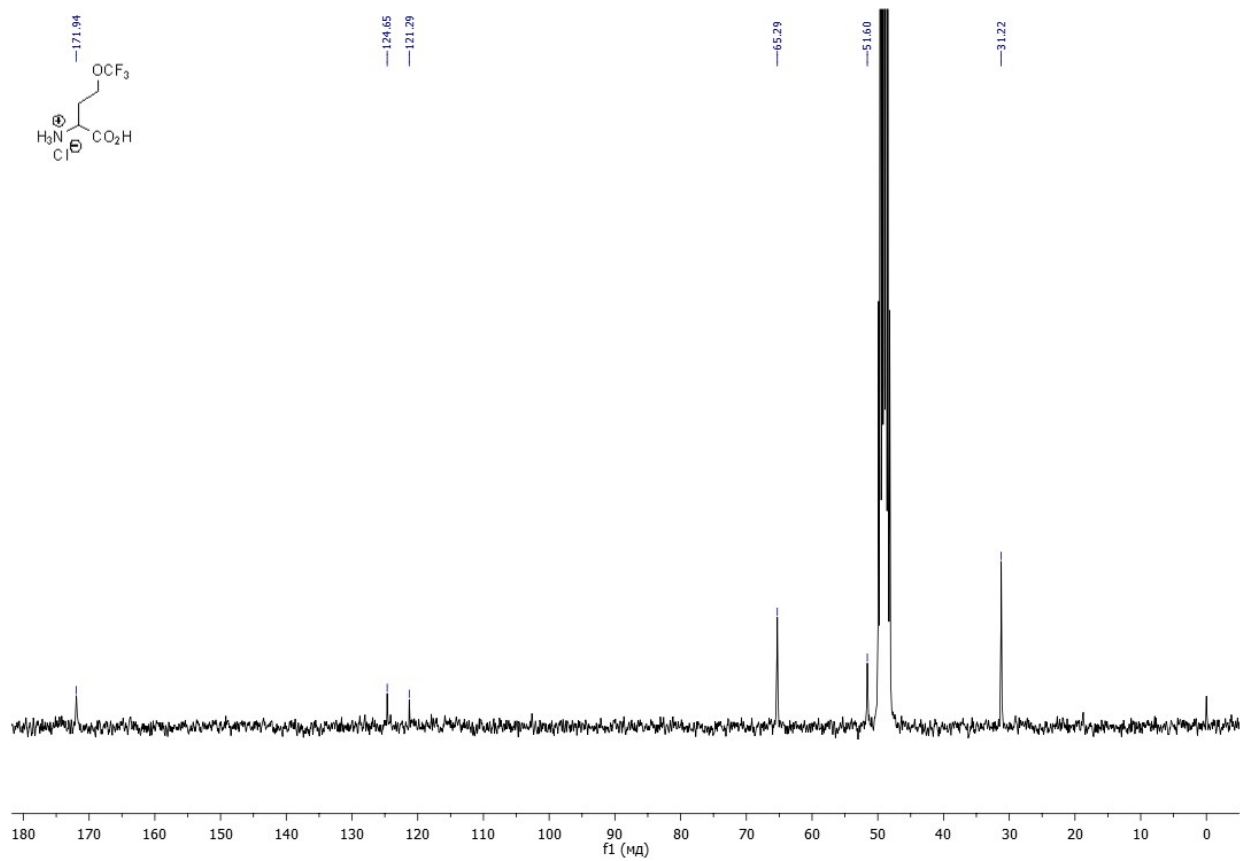
**Compound 9 ( $^{19}\text{F}$  NMR,  $\text{CDCl}_3$ ):**



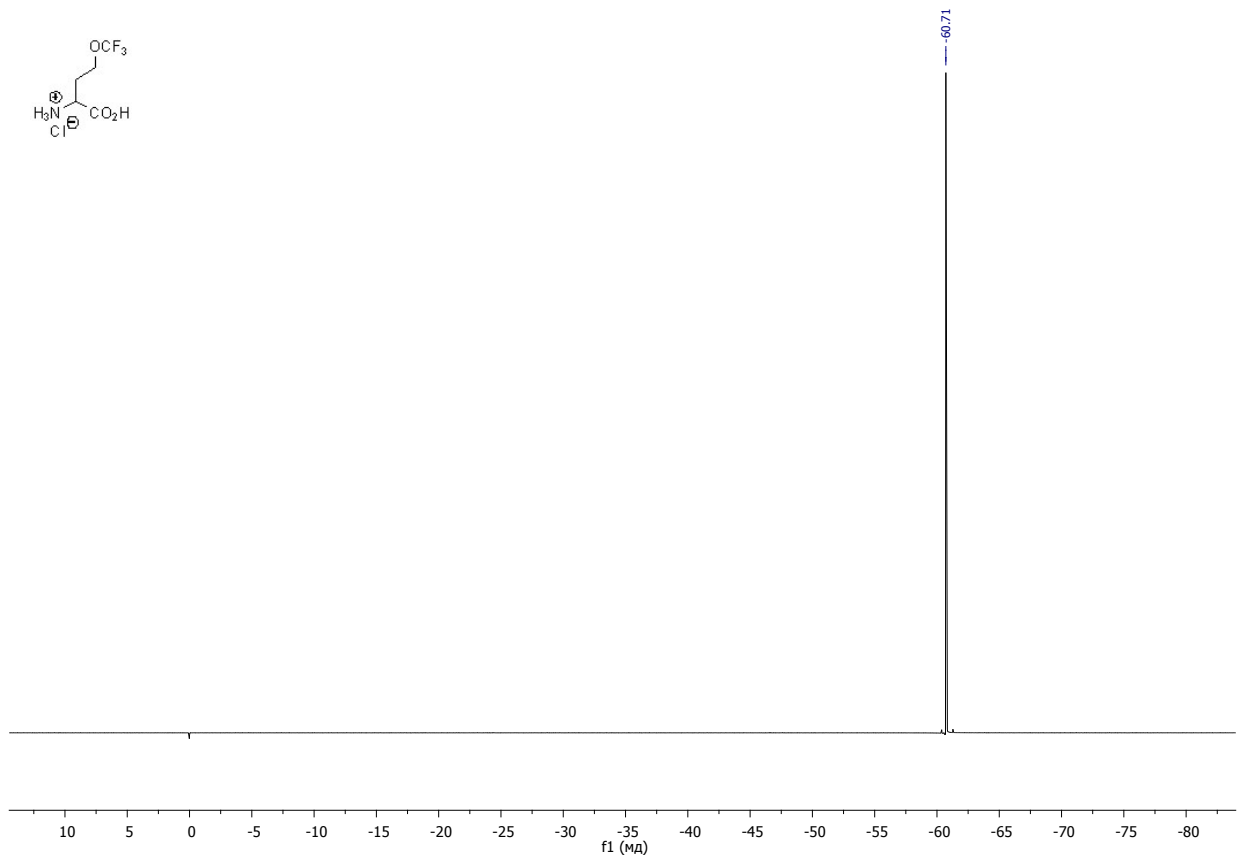
**Compound 3 ( $^1\text{H}$  NMR,  $\text{CD}_3\text{OD}$ ):**



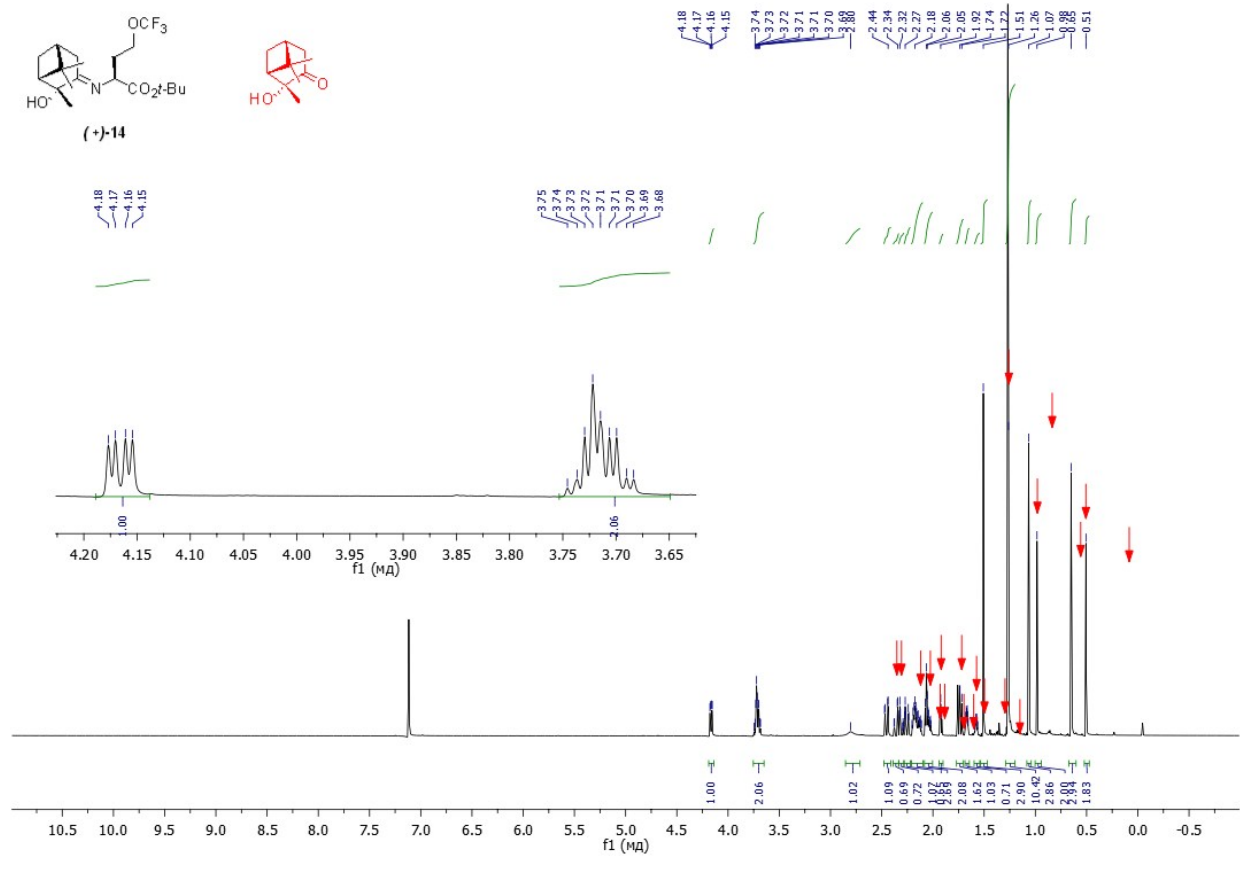
**Compound 3 (<sup>13</sup>C NMR, CD<sub>3</sub>OD):**



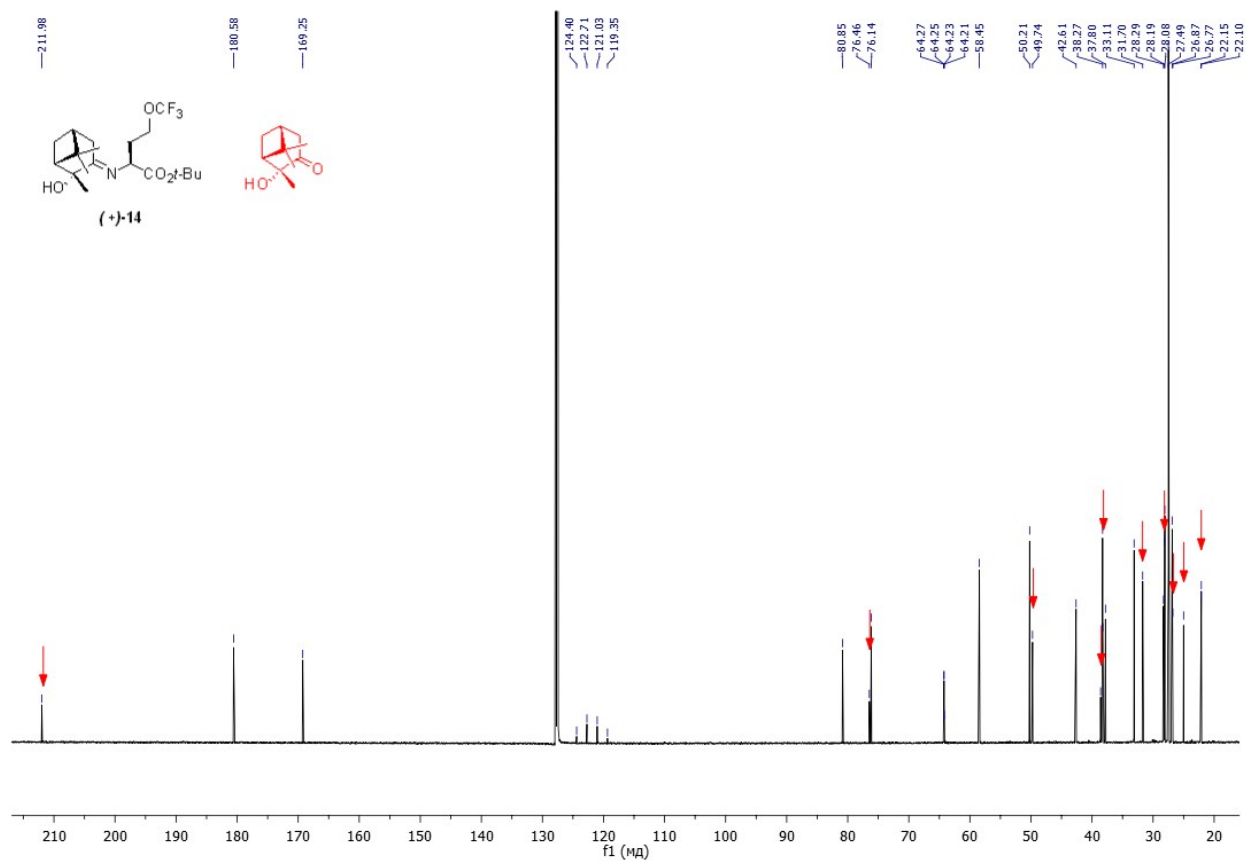
**Compound 3 (<sup>19</sup>F NMR, CD<sub>3</sub>OD):**



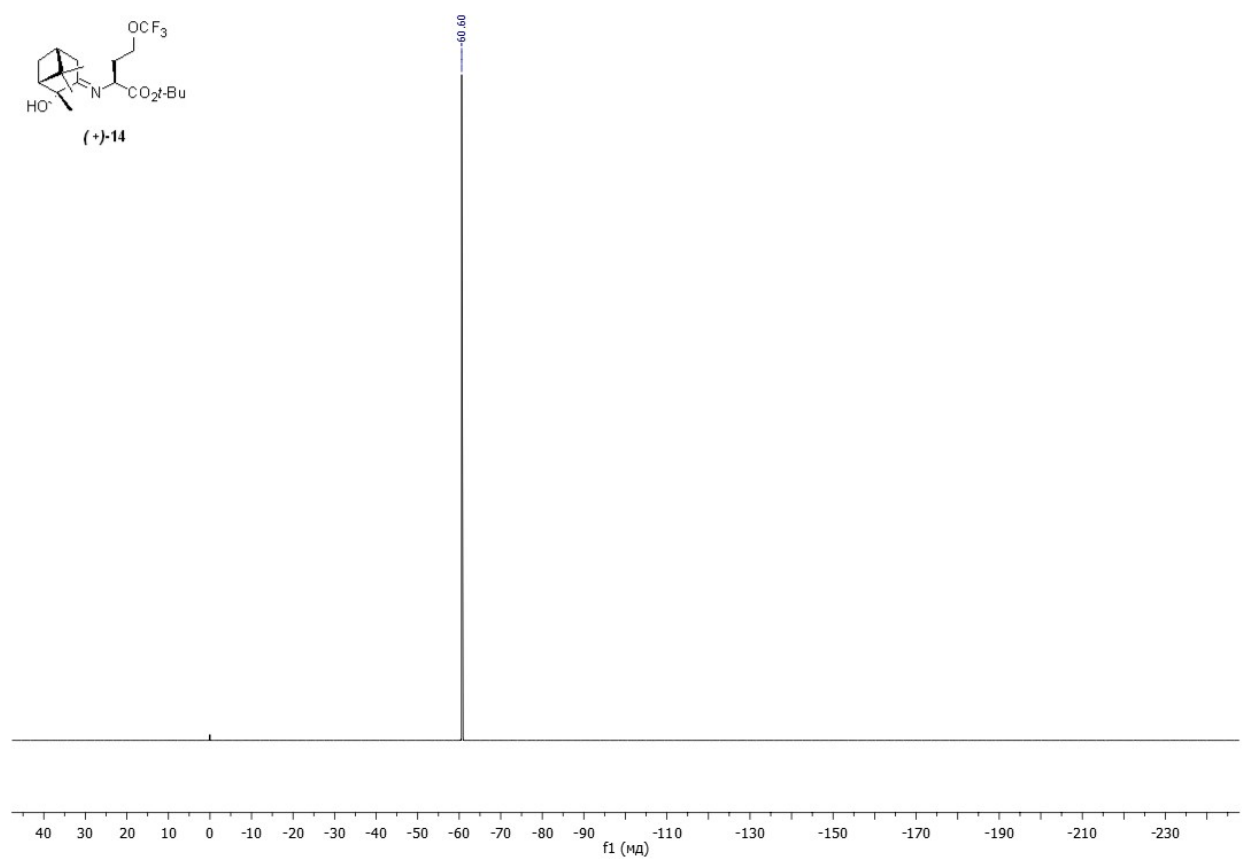
Compound (+)-14 ( $^1\text{H NMR}$ , CDCl<sub>3</sub>; red arrows indicate the signals of compound (+)-12):



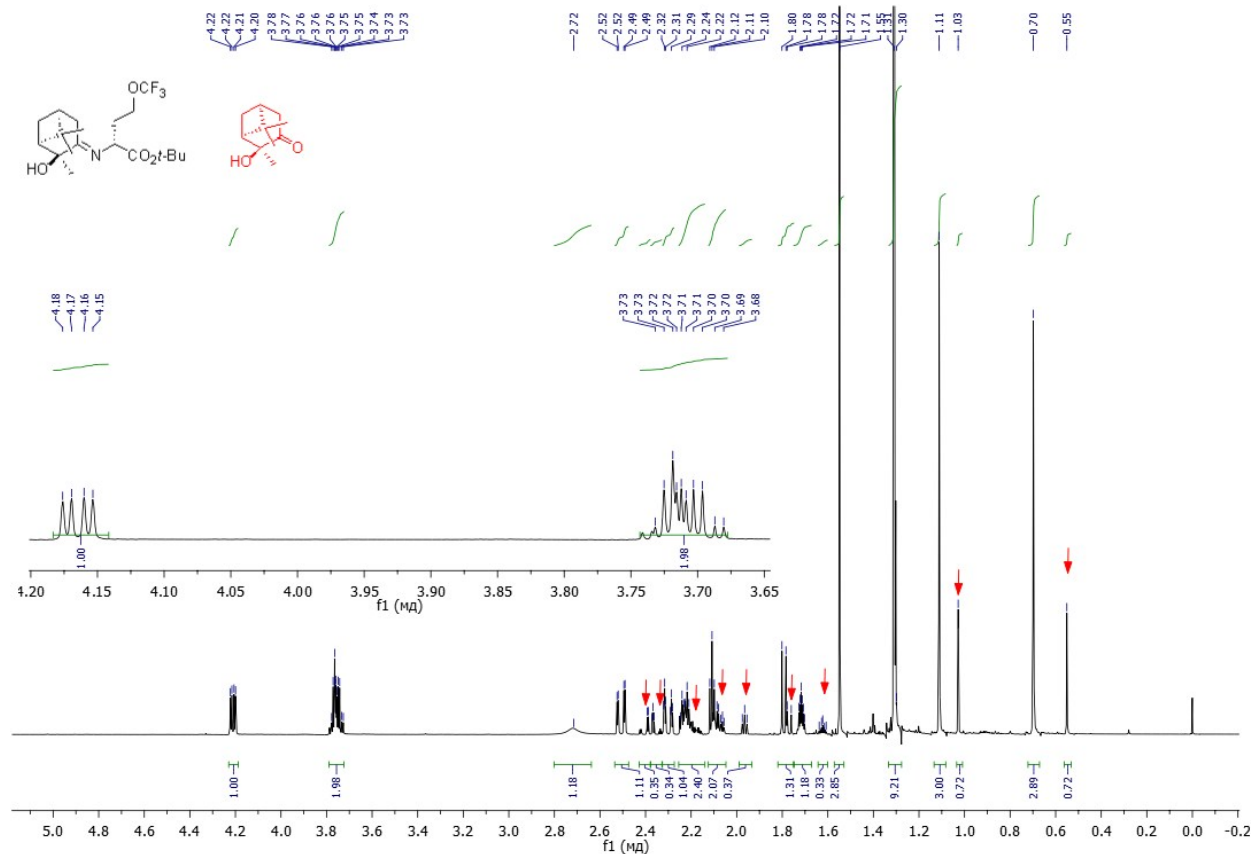
Compound (+)-14 ( $^{13}\text{C}$  NMR,  $\text{CDCl}_3$ ; red arrows indicate the signals of compound (+)-12):



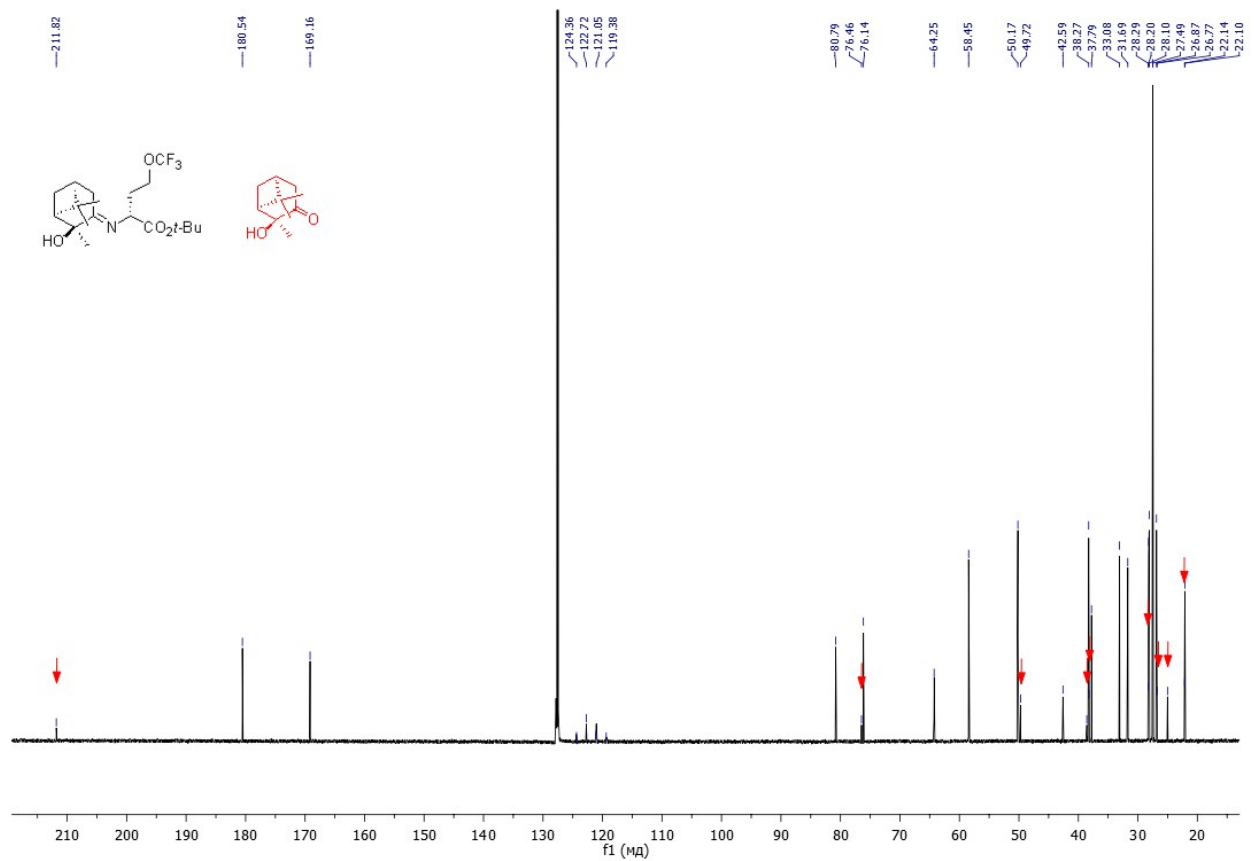
Compound (+)-14 ( $^{19}\text{F}$  NMR,  $\text{CDCl}_3$ )



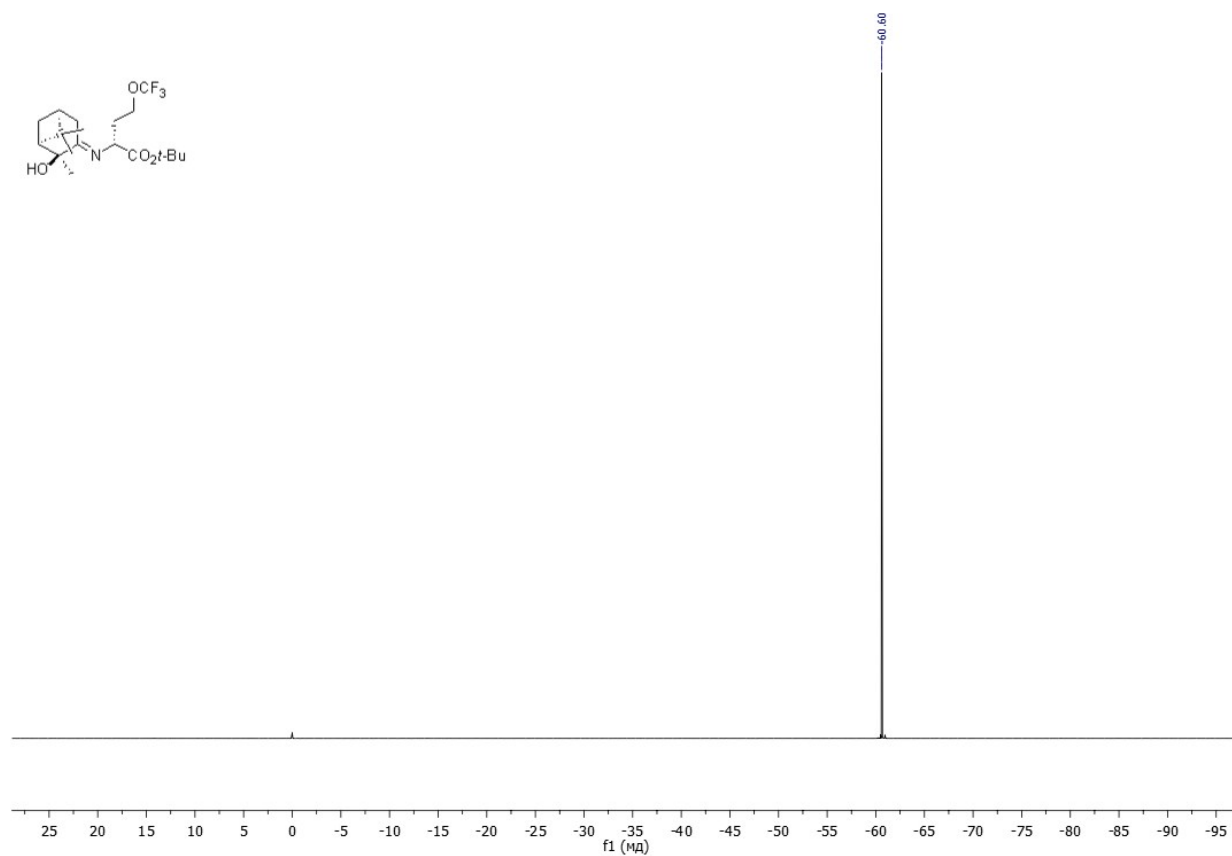
**Compound (-)-14 (<sup>1</sup>H NMR, CDCl<sub>3</sub>; red arrows indicate the signals of compound (-)-12):**



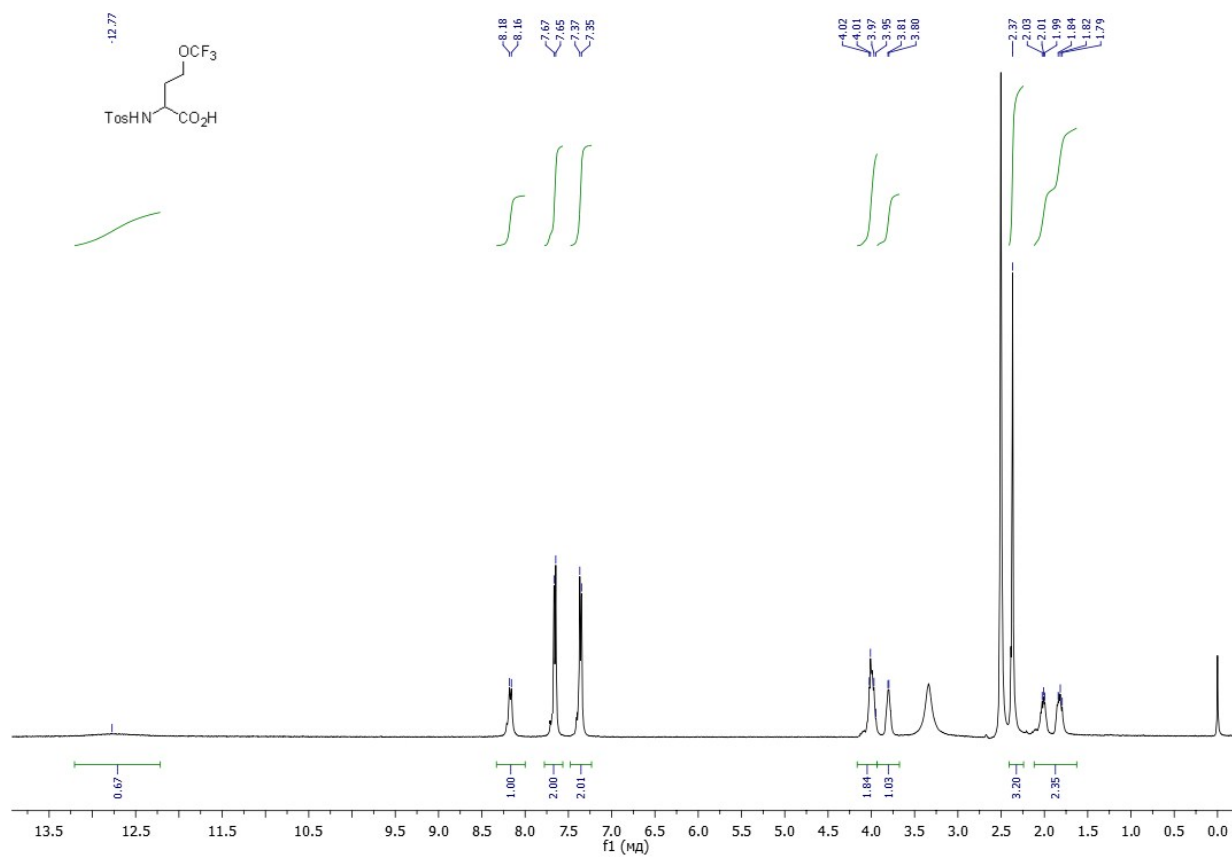
**Compound (-)-14 (<sup>13</sup>C NMR, CDCl<sub>3</sub>; red arrows indicate the signals of compound (-)-12):**



Compound (-)-14 ( $^{19}\text{F}$  NMR,  $\text{CDCl}_3$ ; red arrows indicate the signals of compound (-)-12):

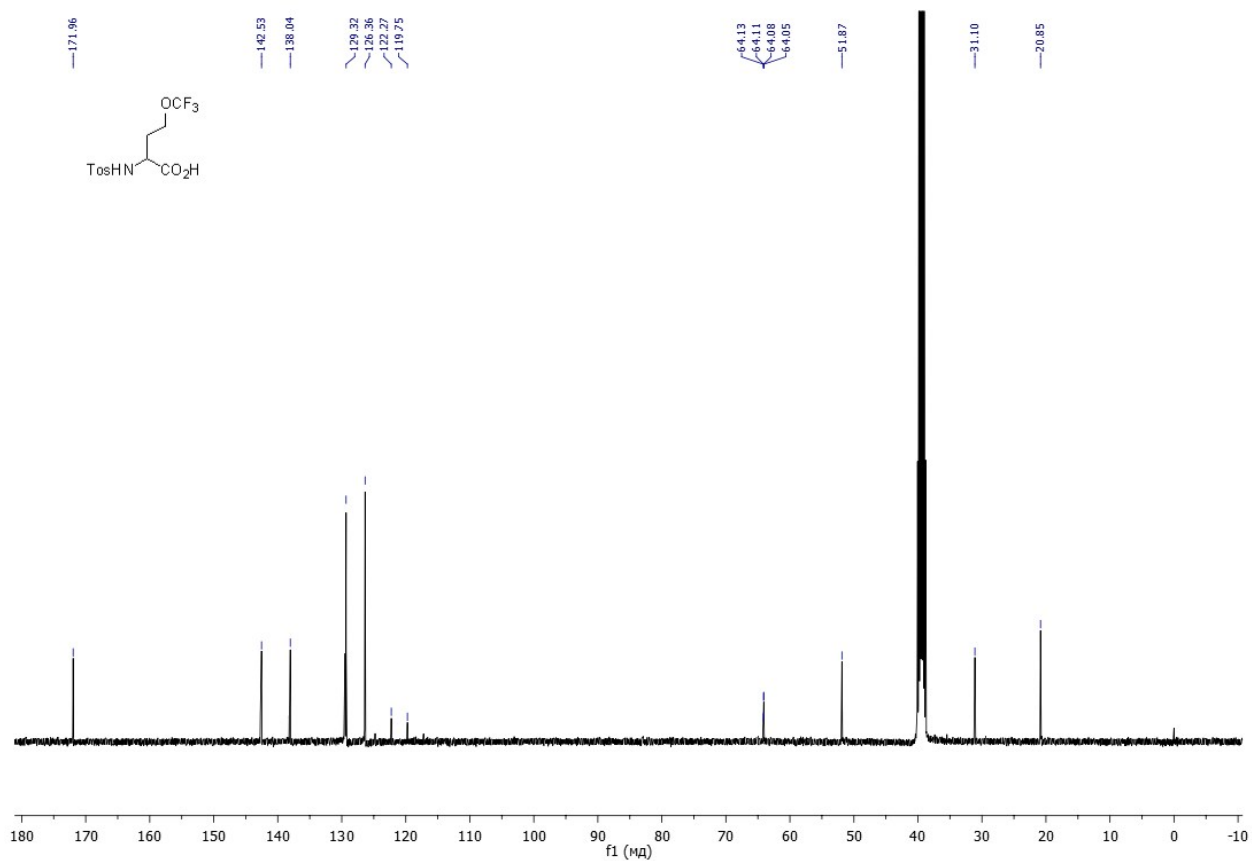


Compound 15 ( $^1\text{H}$  NMR,  $\text{DMSO-d}_6$ ):

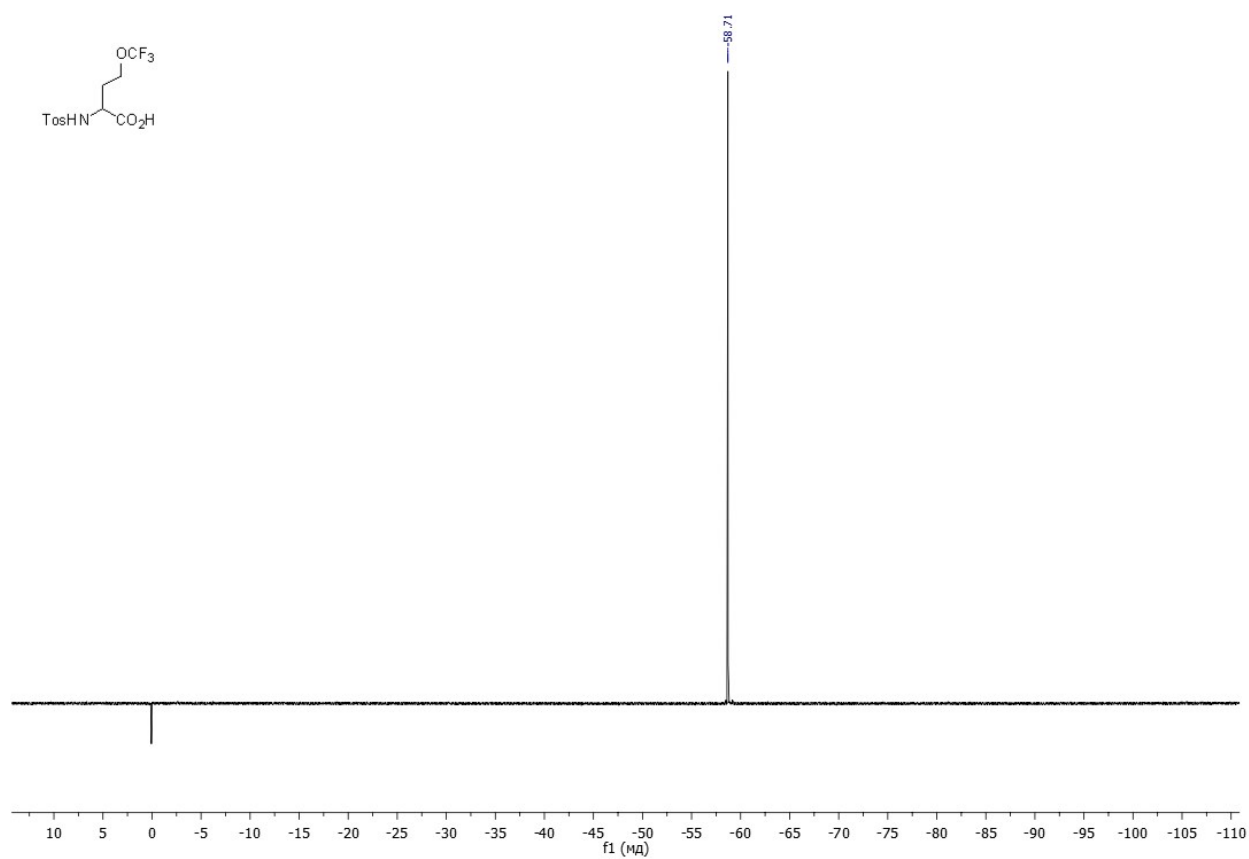




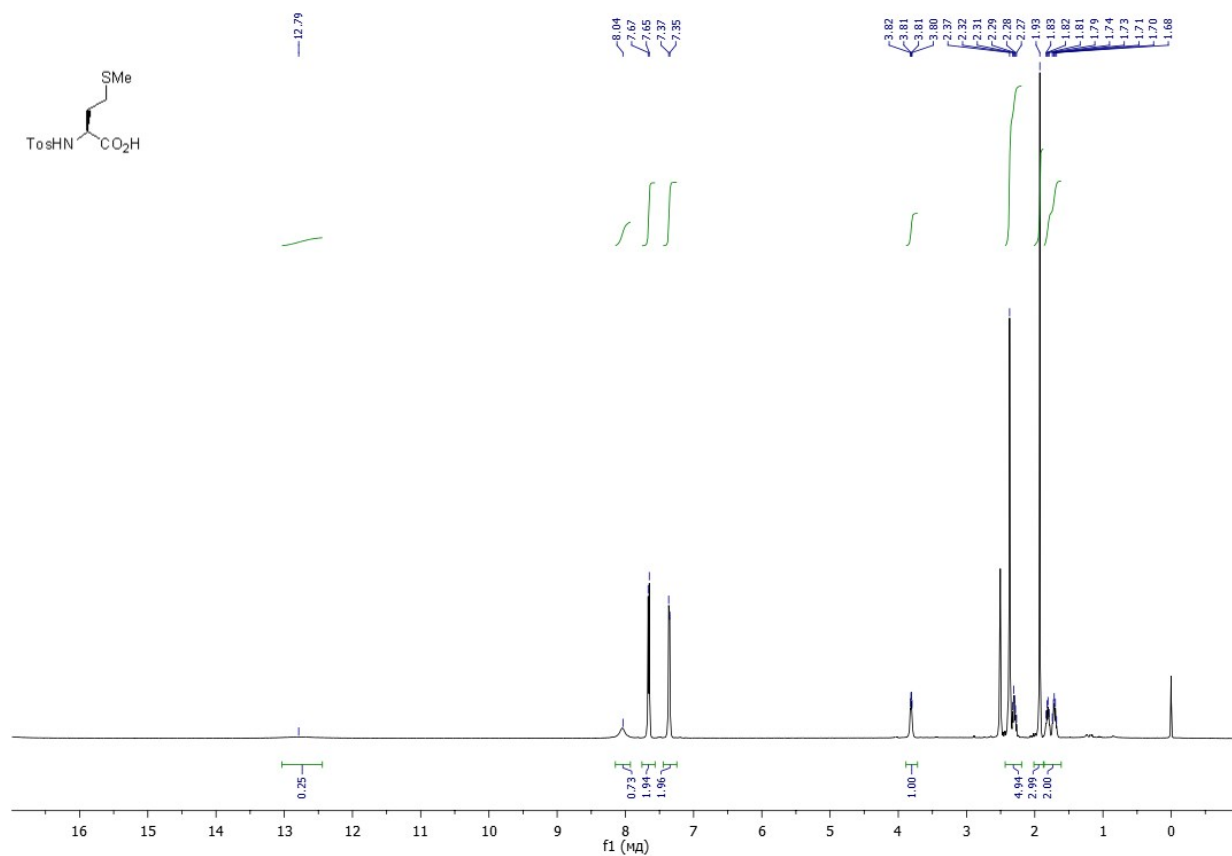
**Compound 15 ( $^{13}\text{C}$  NMR,  $\text{DMSO-d}_6$ ):**



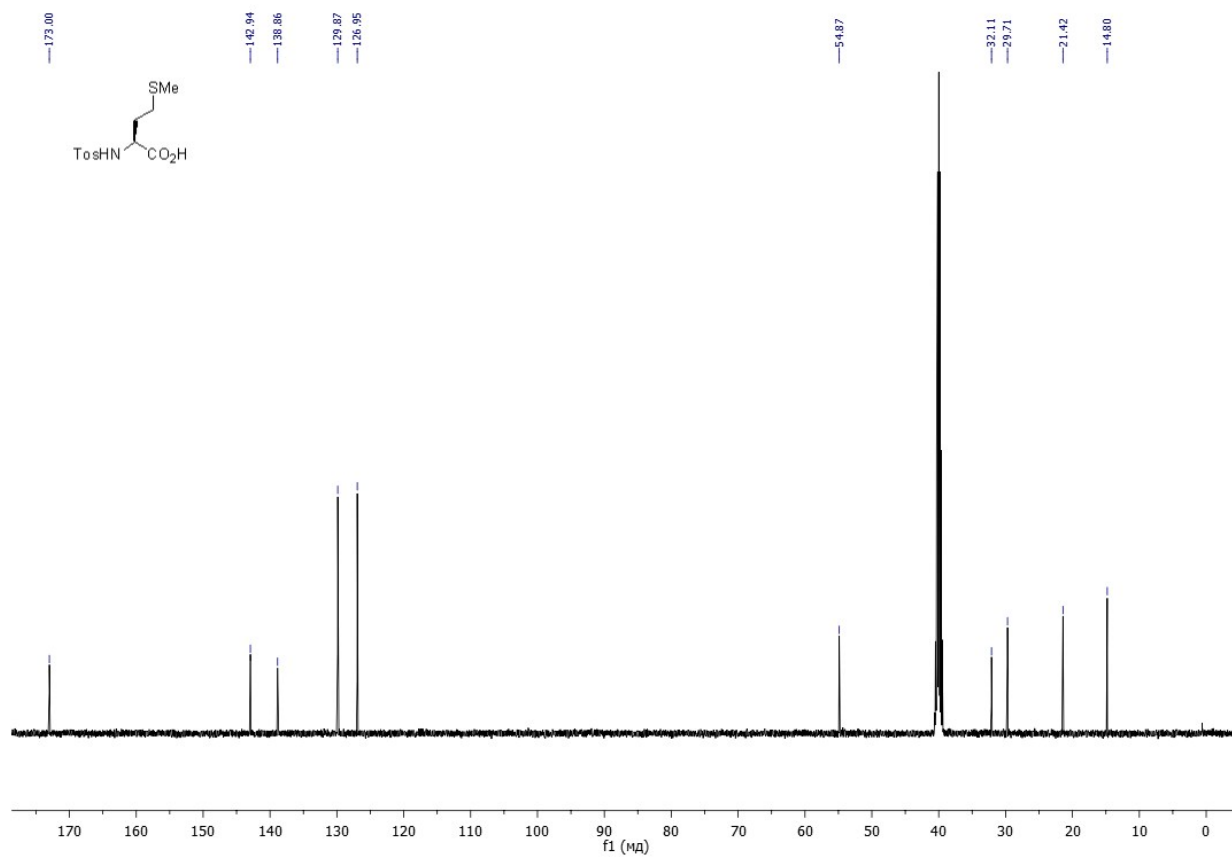
**Compound 15 ( $^{19}\text{F}$  NMR,  $\text{DMSO-d}_6$ ):**



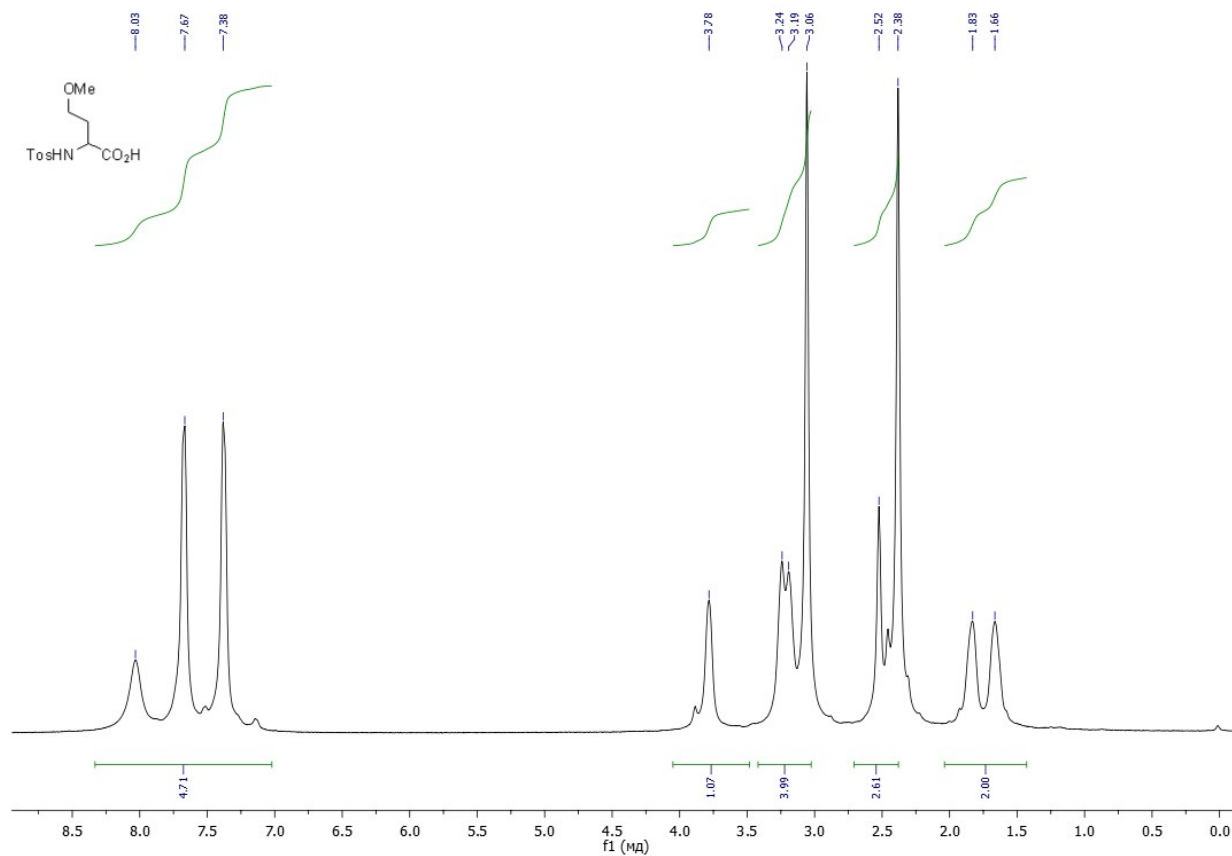
Compound 17a (<sup>1</sup>H NMR, DMSO-d<sub>6</sub>):



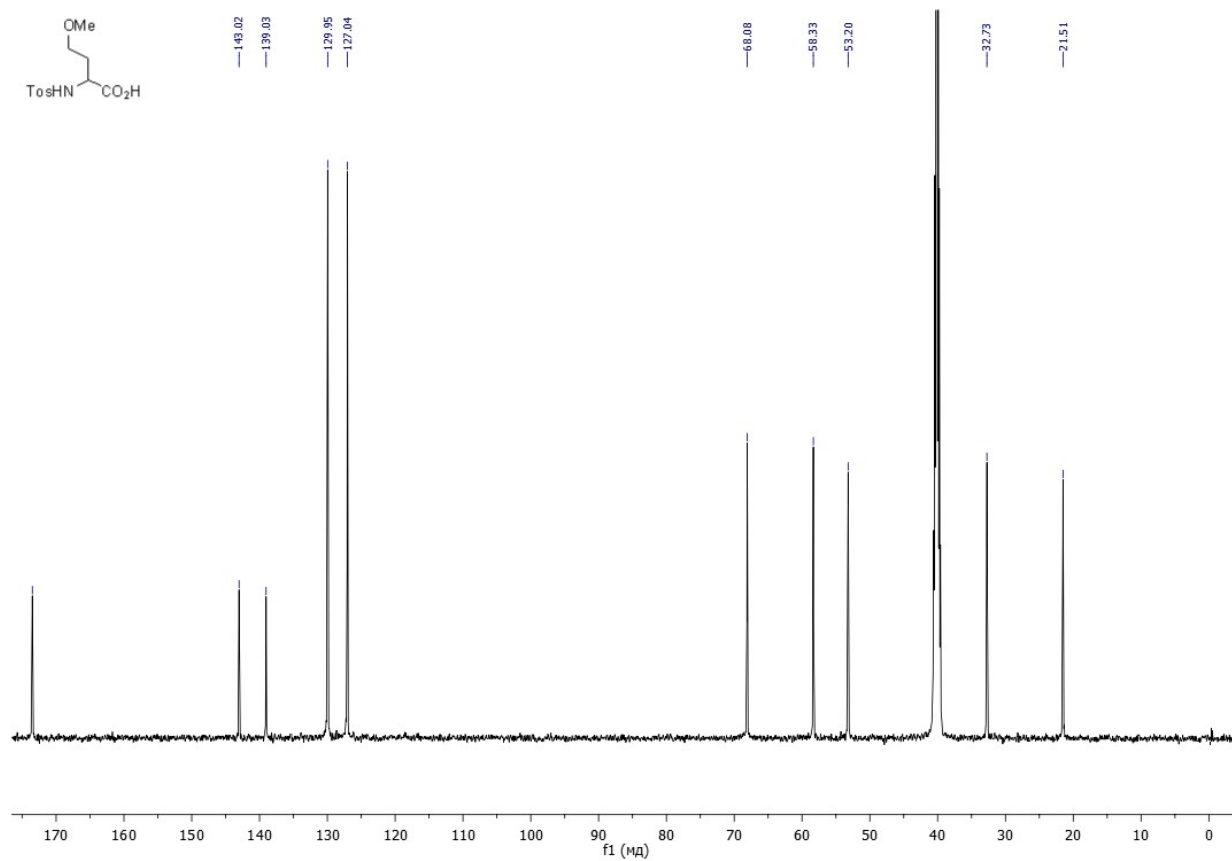
Compound 17a (<sup>13</sup>C NMR, DMSO-d<sub>6</sub>):



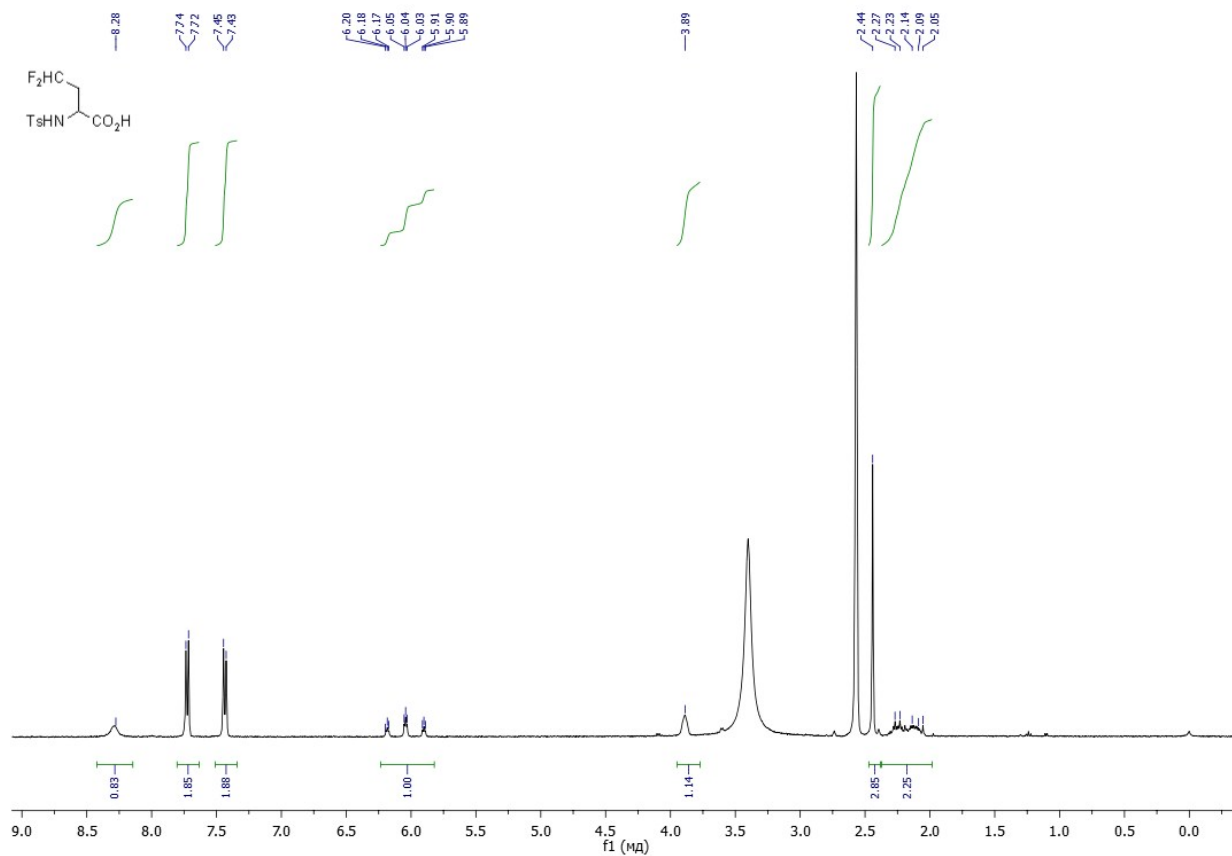
**Compound 17d (<sup>1</sup>H NMR, DMSO-d<sub>6</sub>):**



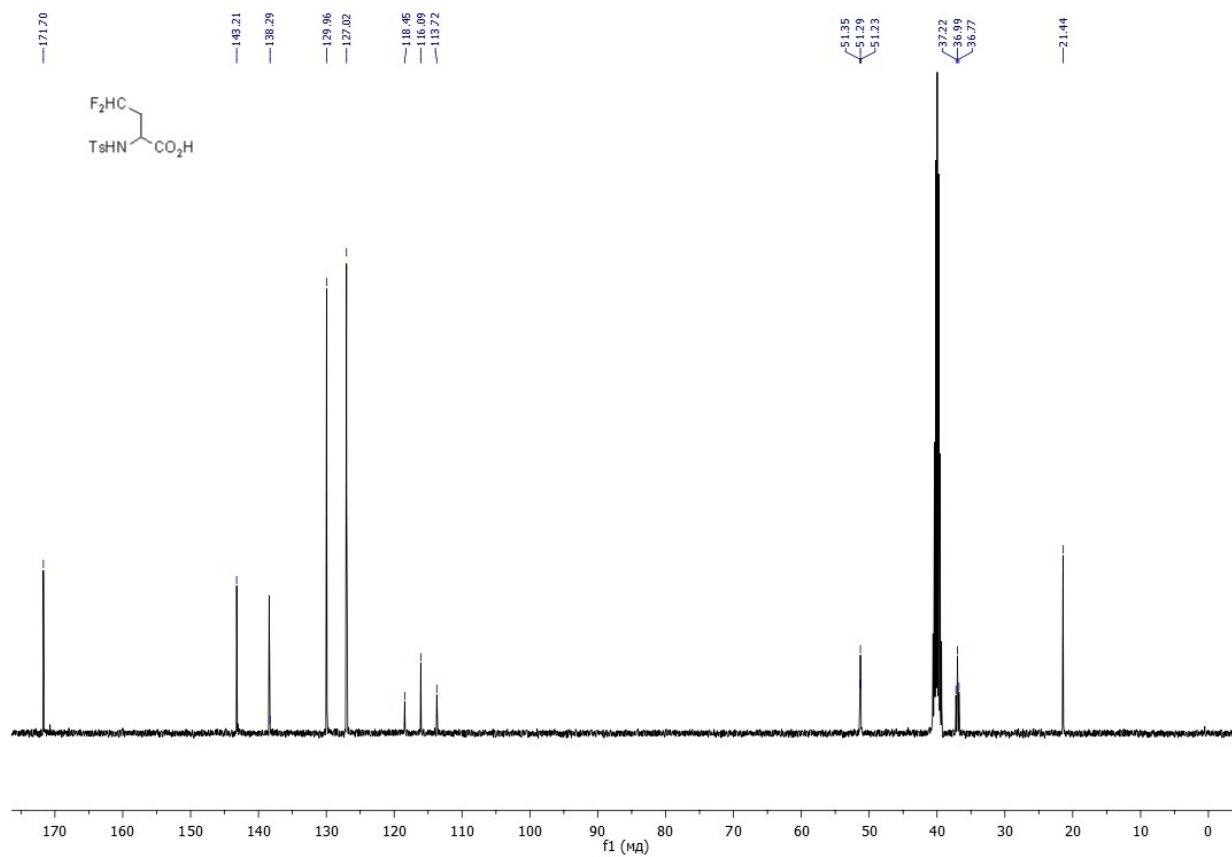
**Compound 17d (<sup>13</sup>C NMR, DMSO-d<sub>6</sub>):**



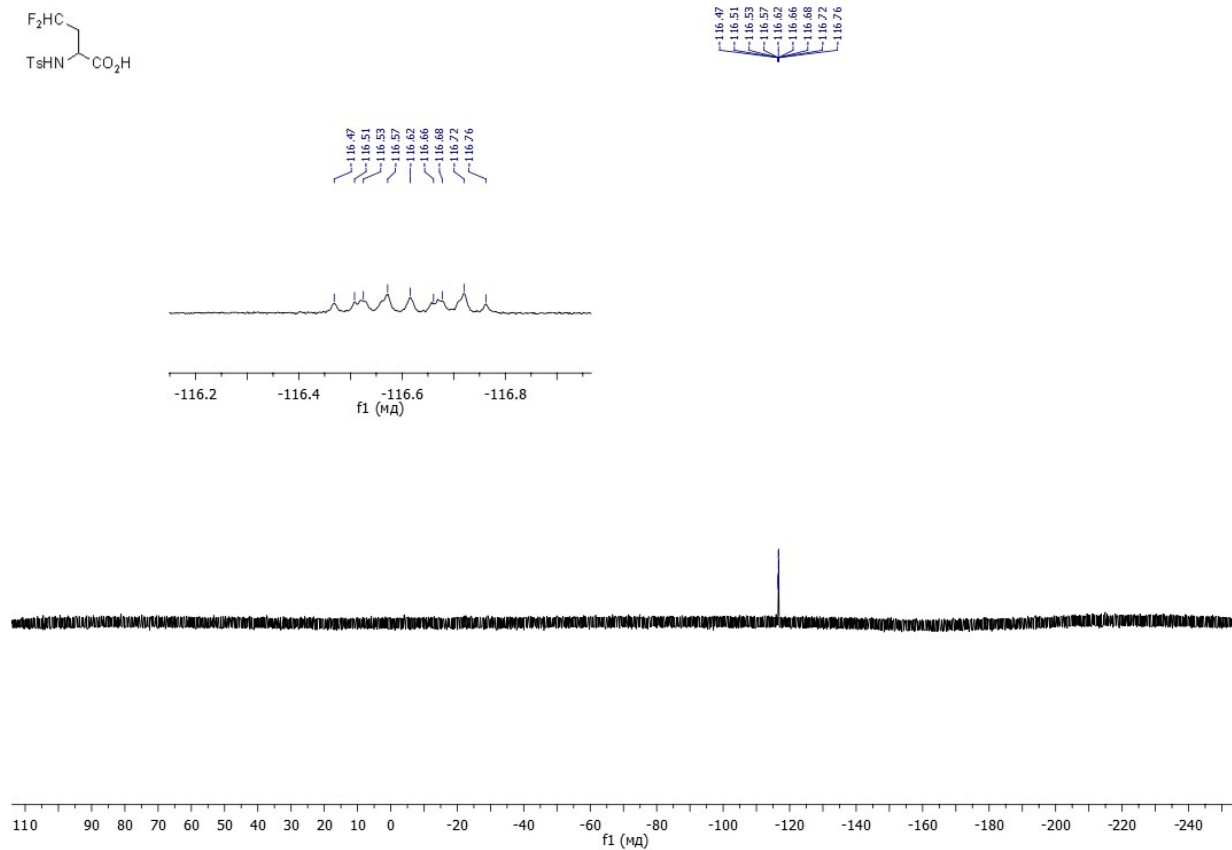
Compound 17e (<sup>1</sup>H NMR, DMSO-d<sub>6</sub>):



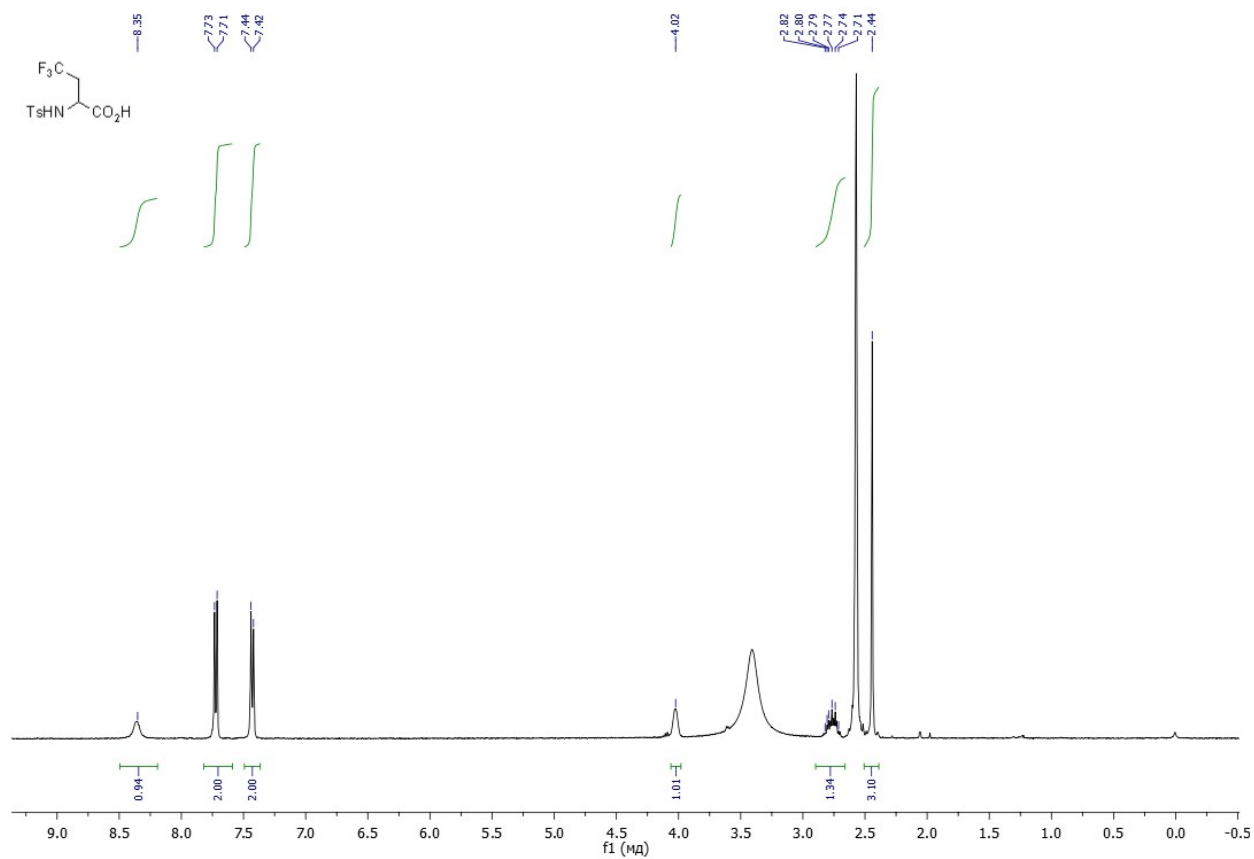
Compound 17e (<sup>13</sup>C NMR, DMSO-d<sub>6</sub>):



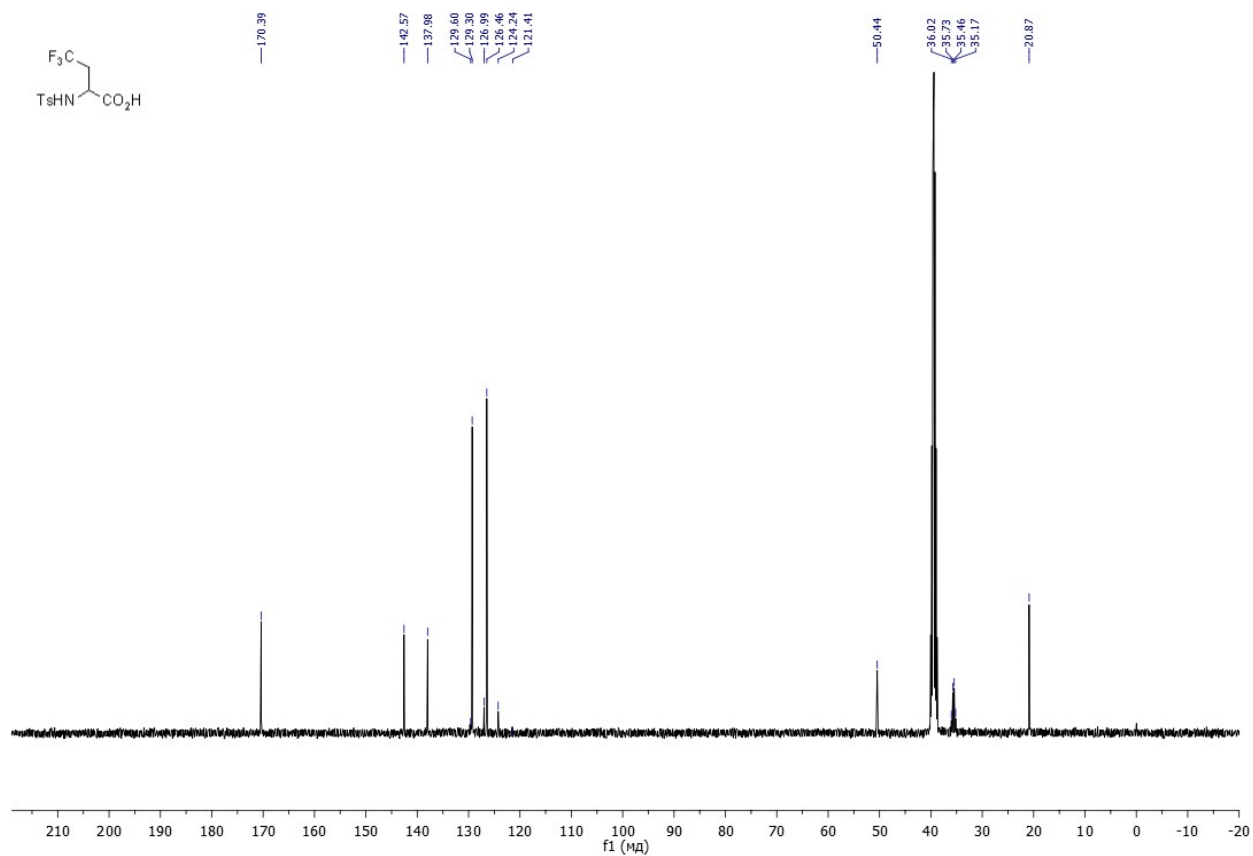
**Compound 17e (<sup>19</sup>F NMR, DMSO-d<sub>6</sub>):**



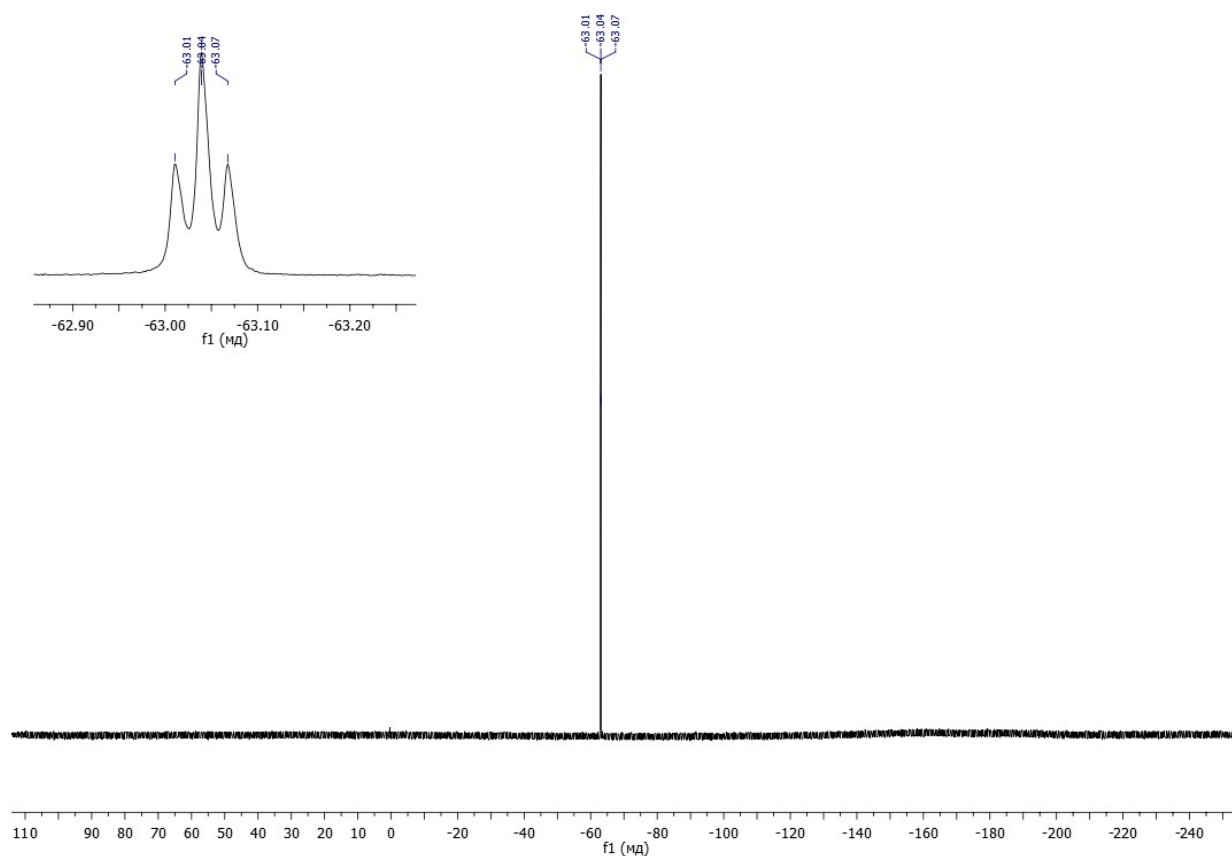
**Compound 17f (<sup>1</sup>H NMR, DMSO-d<sub>6</sub>):**



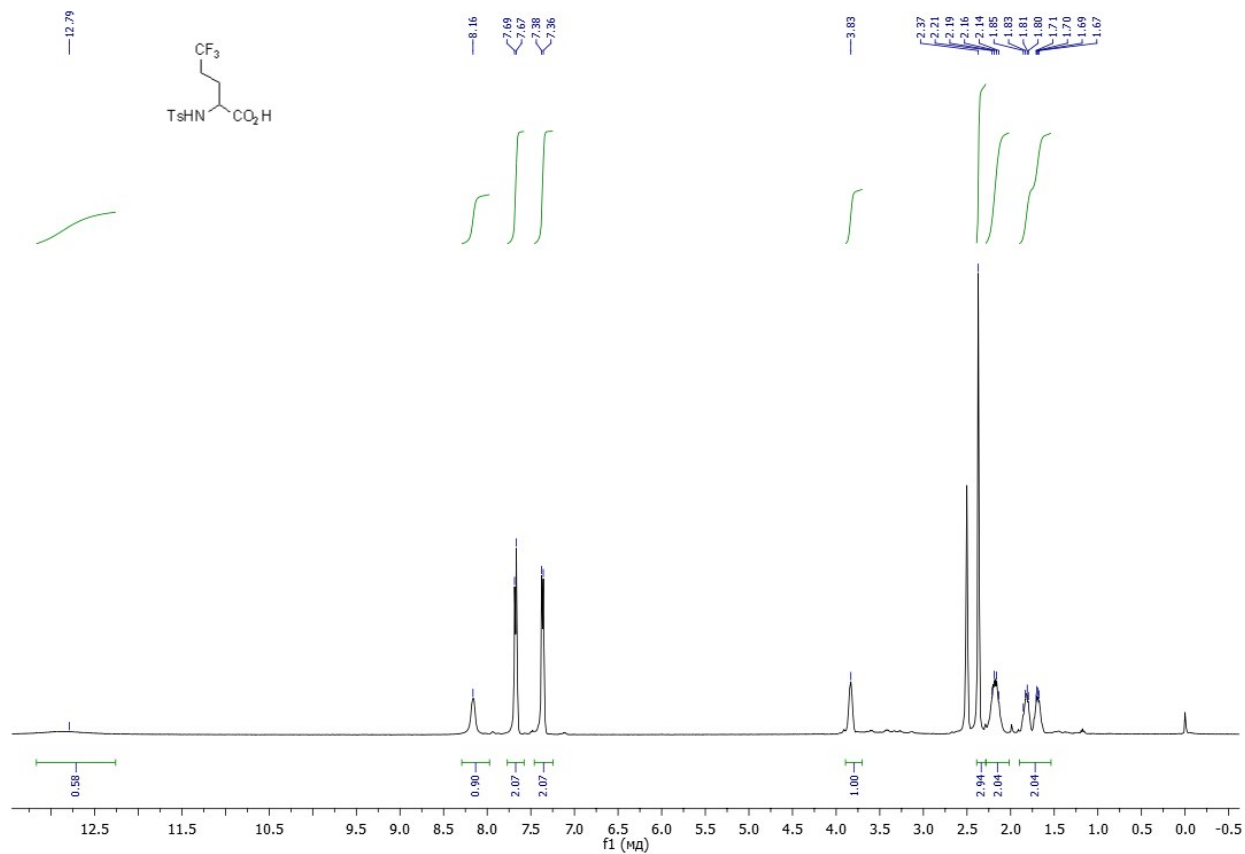
Compound 17f (<sup>13</sup>C NMR, DMSO-d<sub>6</sub>):



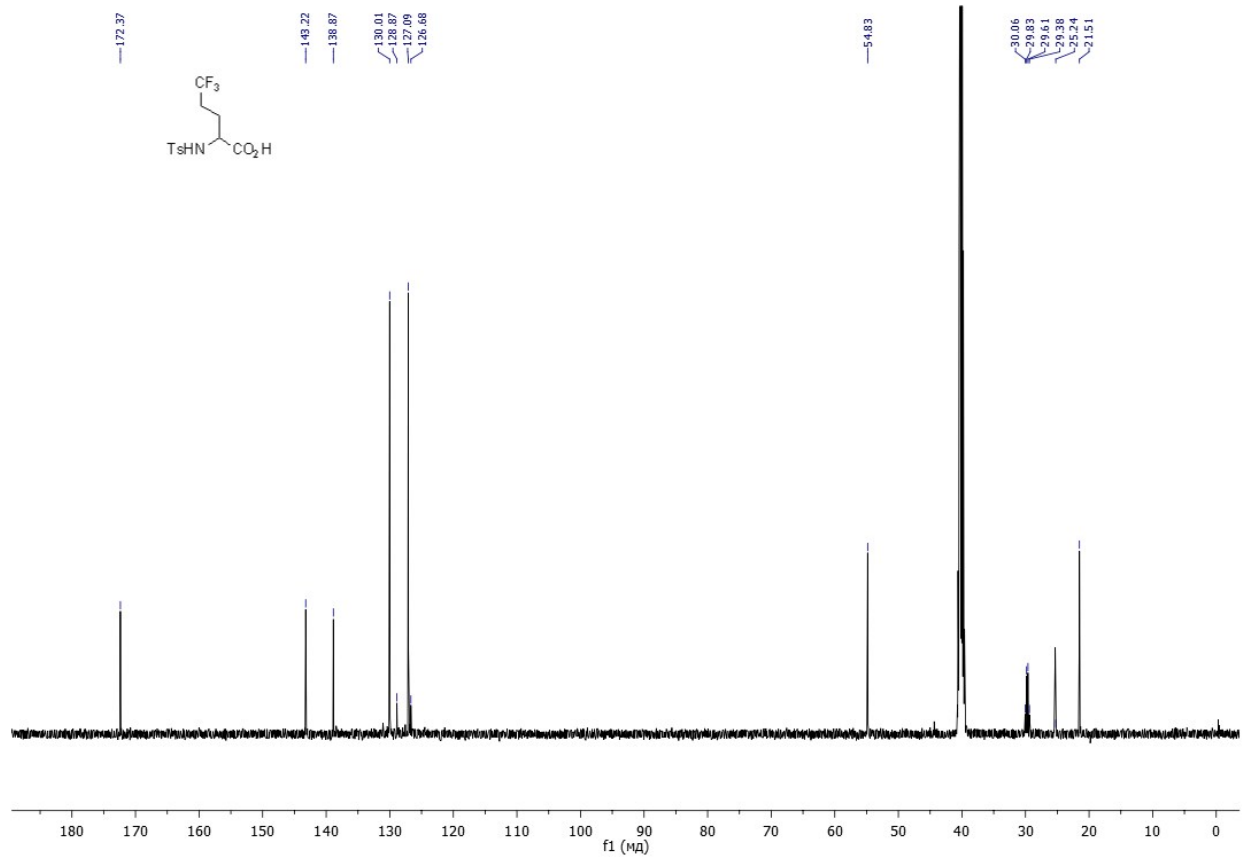
Compound 17f (<sup>19</sup>F NMR, DMSO-d<sub>6</sub>):



Compound 17g ( $^1\text{H}$  NMR,  $\text{DMSO-d}_6$ ):



Compound 17g ( $^{13}\text{C}$  NMR,  $\text{DMSO-d}_6$ ):



Compound 17g ( $^{19}\text{F}$  NMR,  $\text{DMSO-d}_6$ ):

