

## Supporting Information

### **A Stereoselective Entry to Enantiopure (S)-2-Amino-2-methyl-5-arylpent-4-ynoic Acids and Evaluation of Their Inhibitory Activity Against Bacterial Collagenase G**

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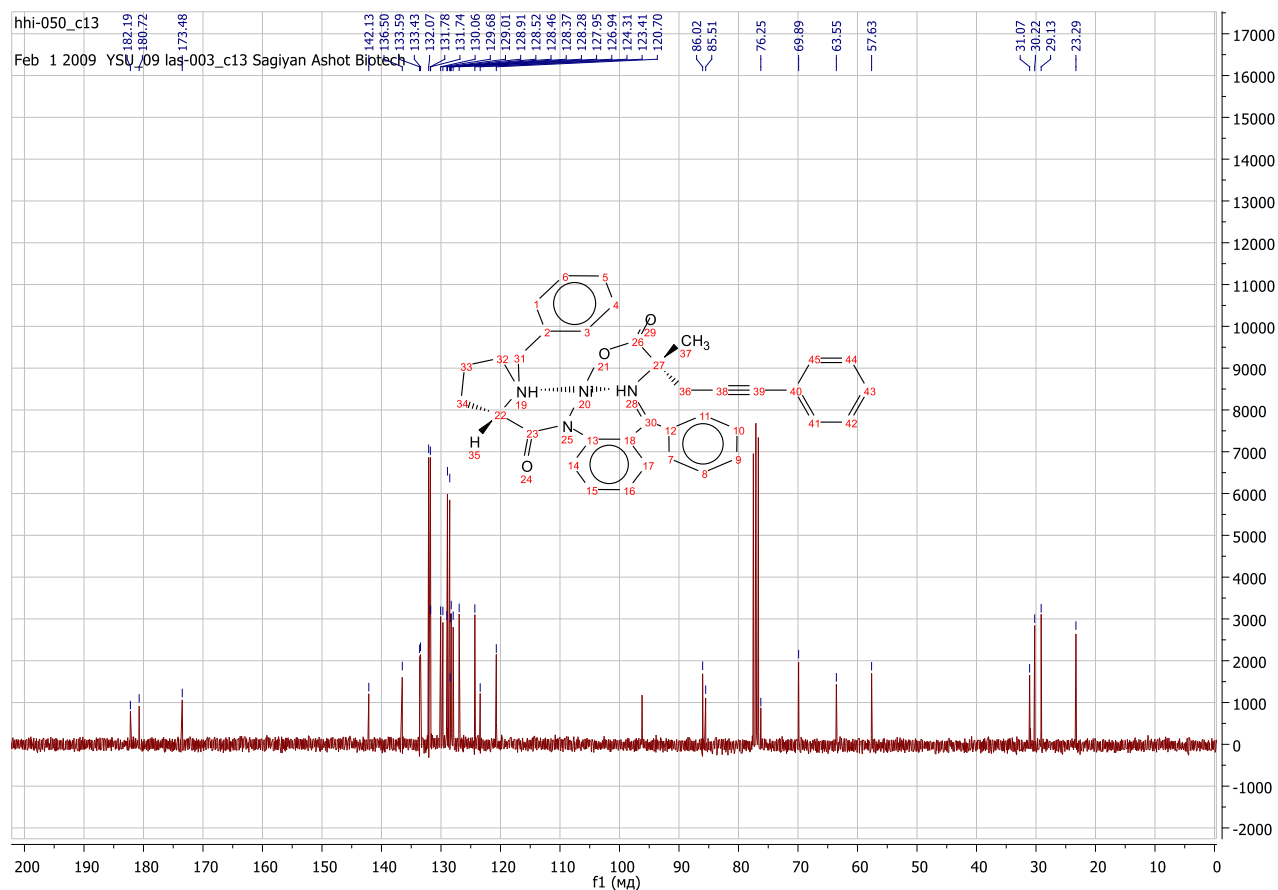
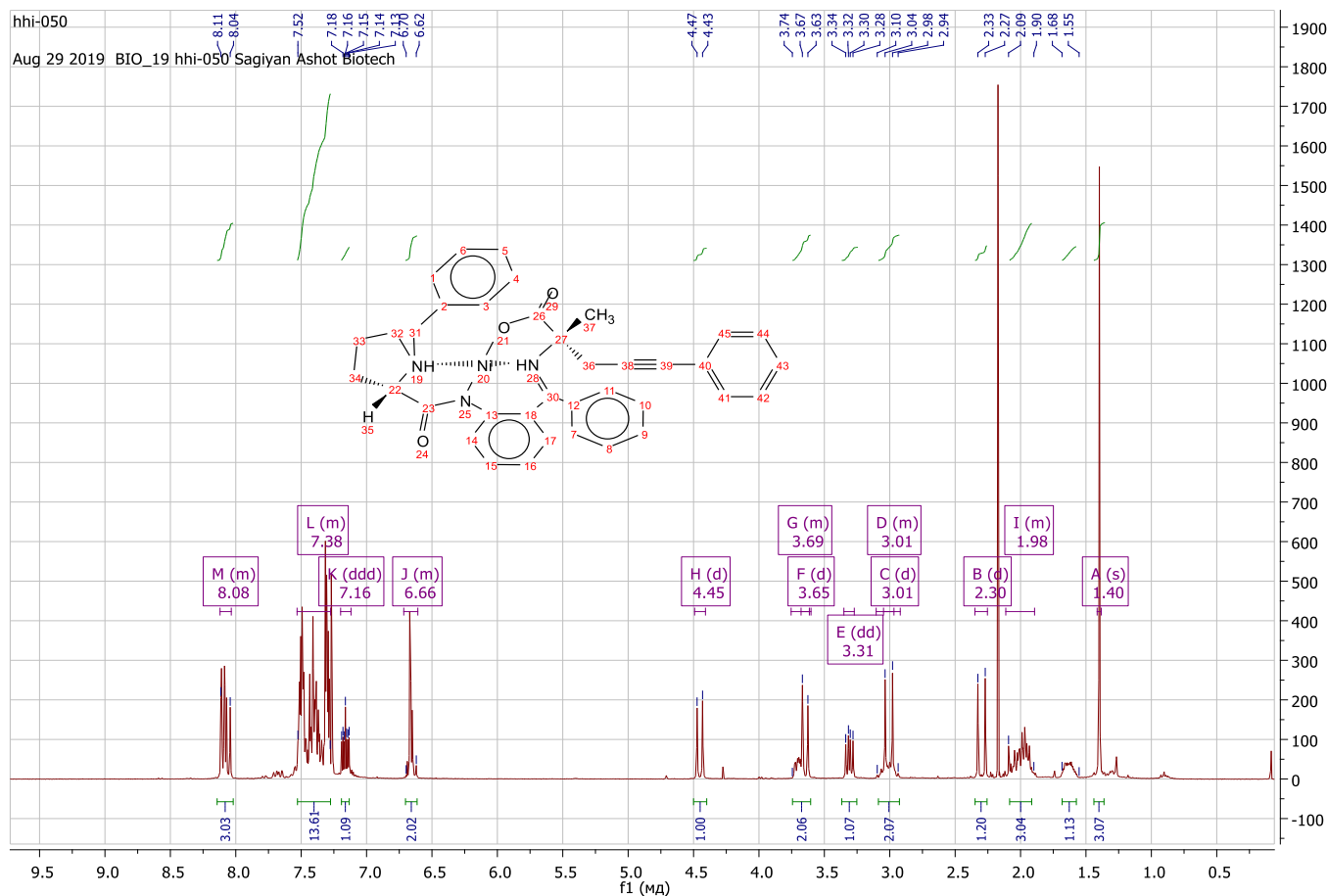
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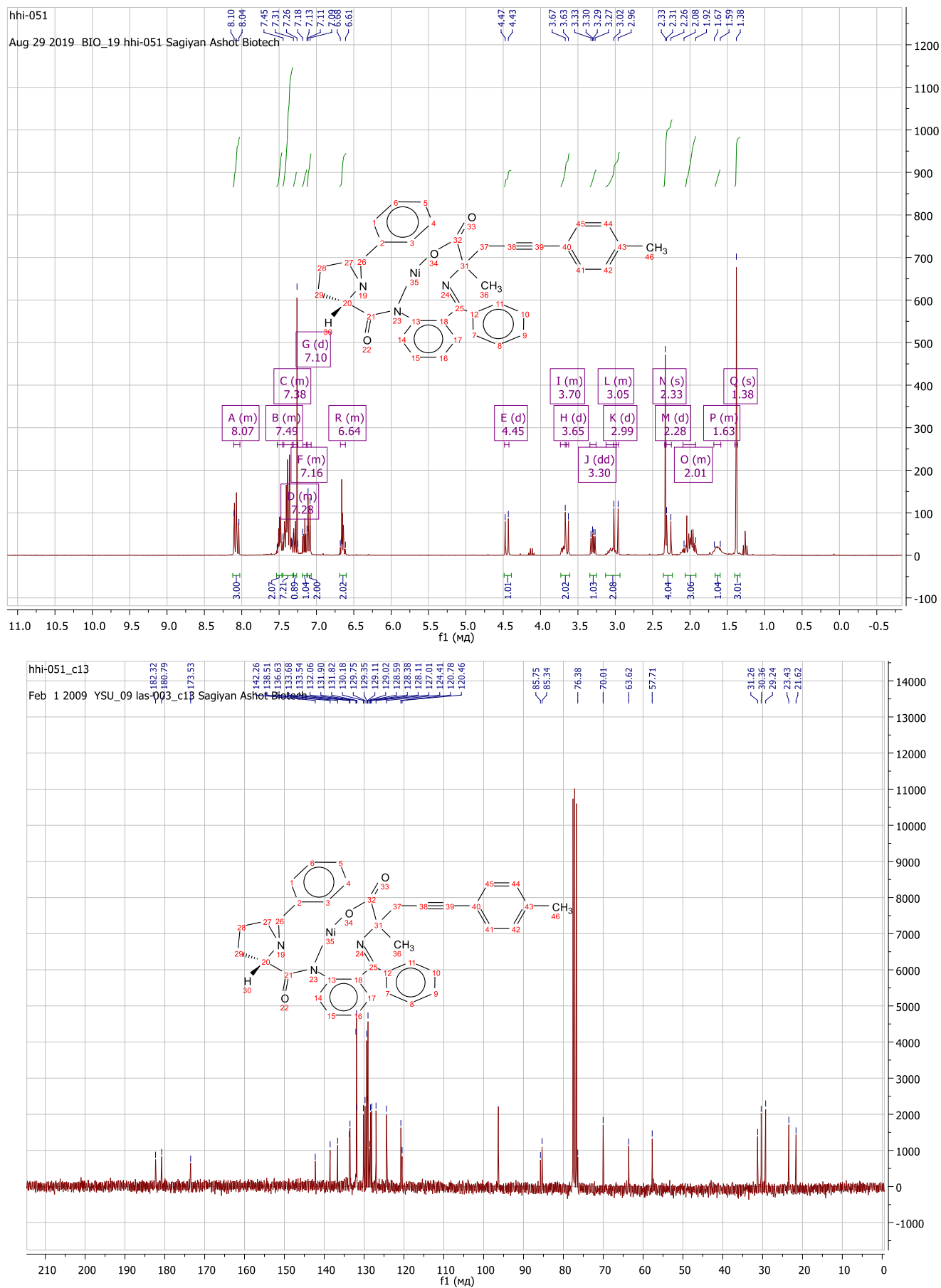
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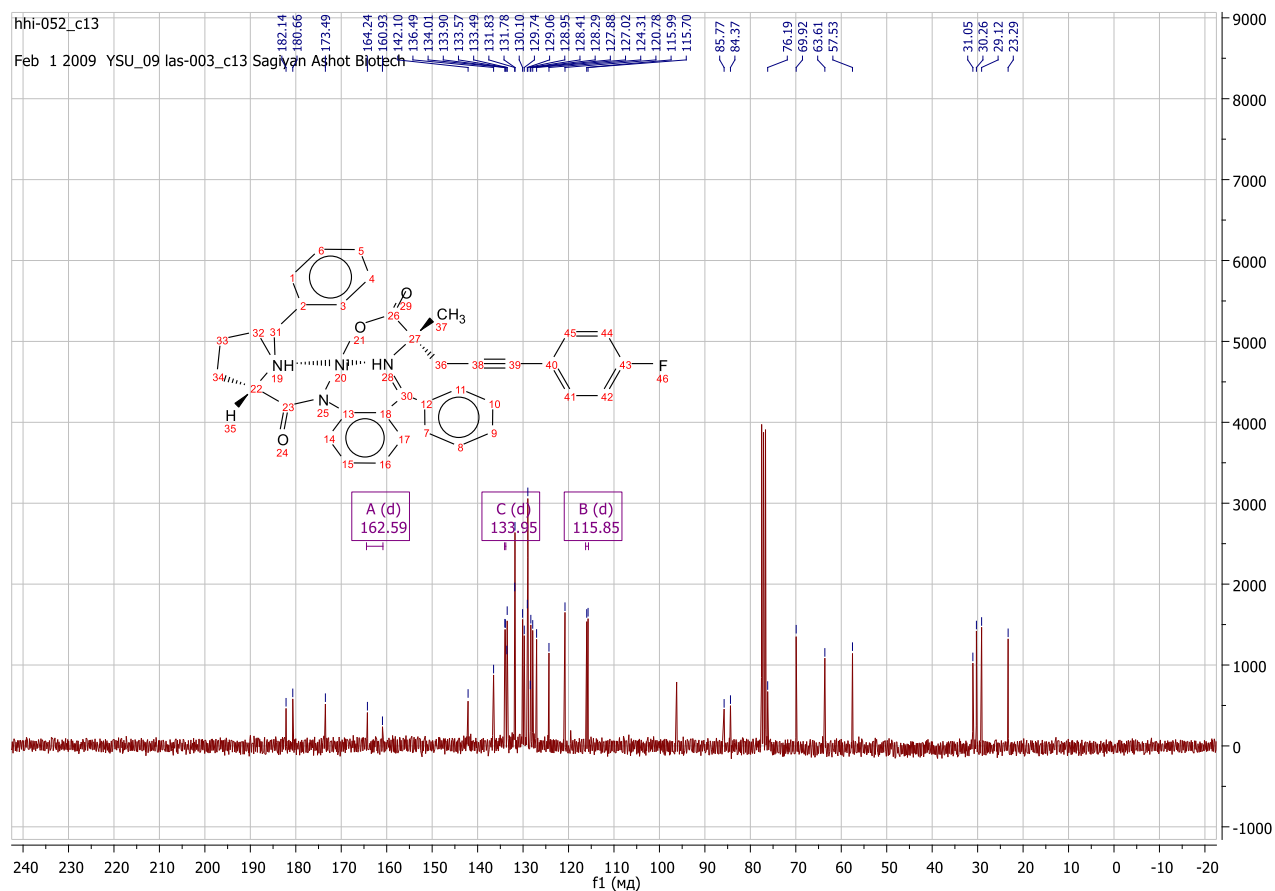
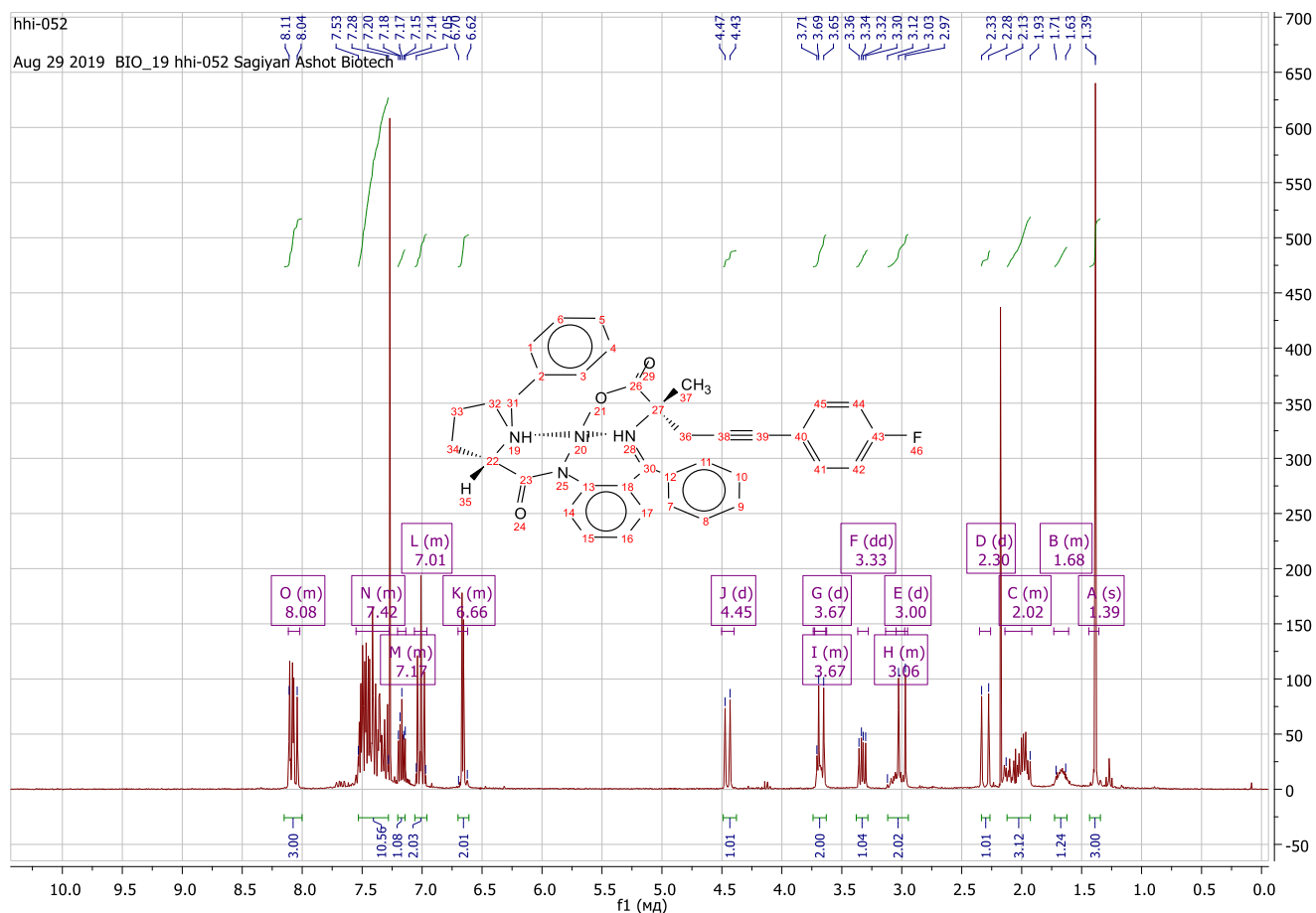
\* Correspondence: larionov@ineos.ac.ru (V.A.L.); zmardiyani89@gmail.com (Z.Z.M.)



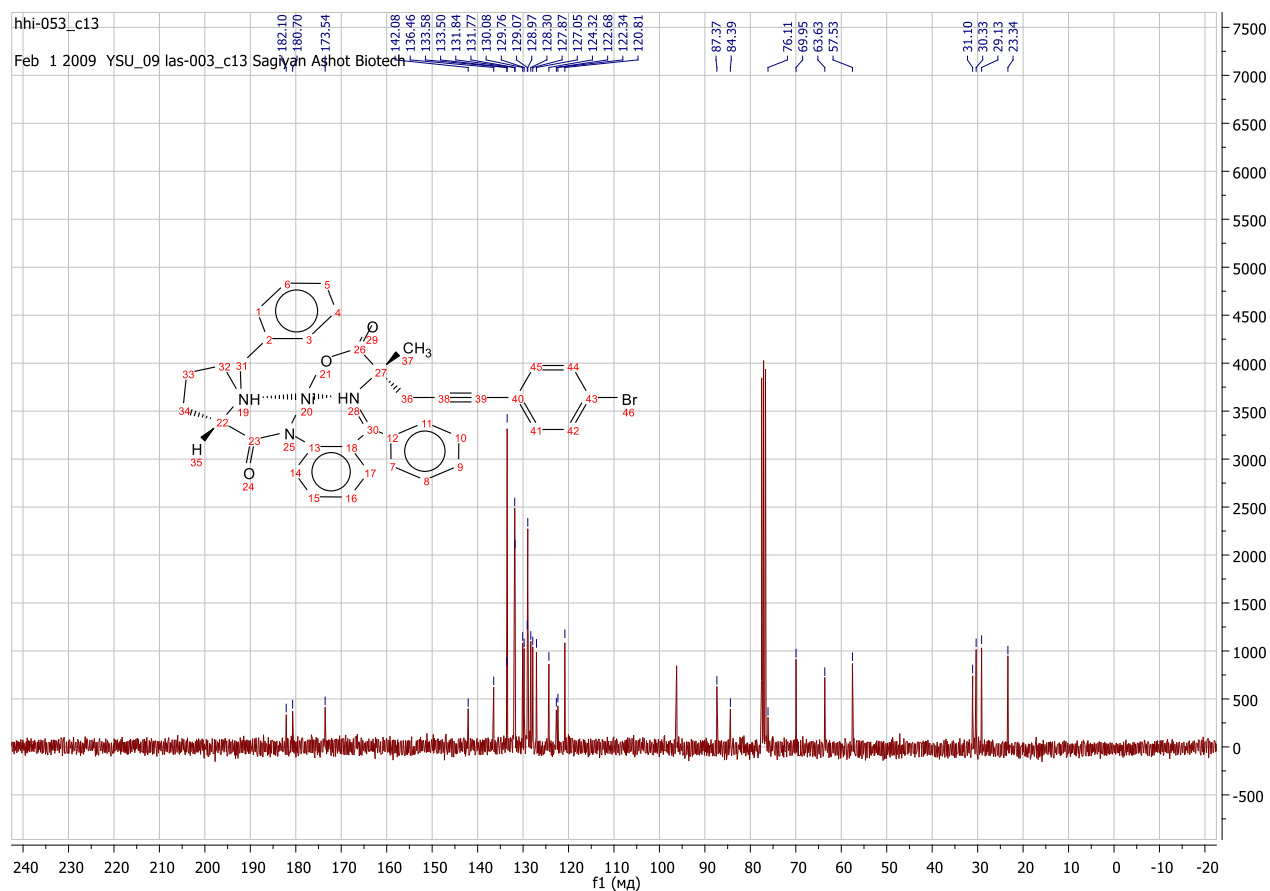
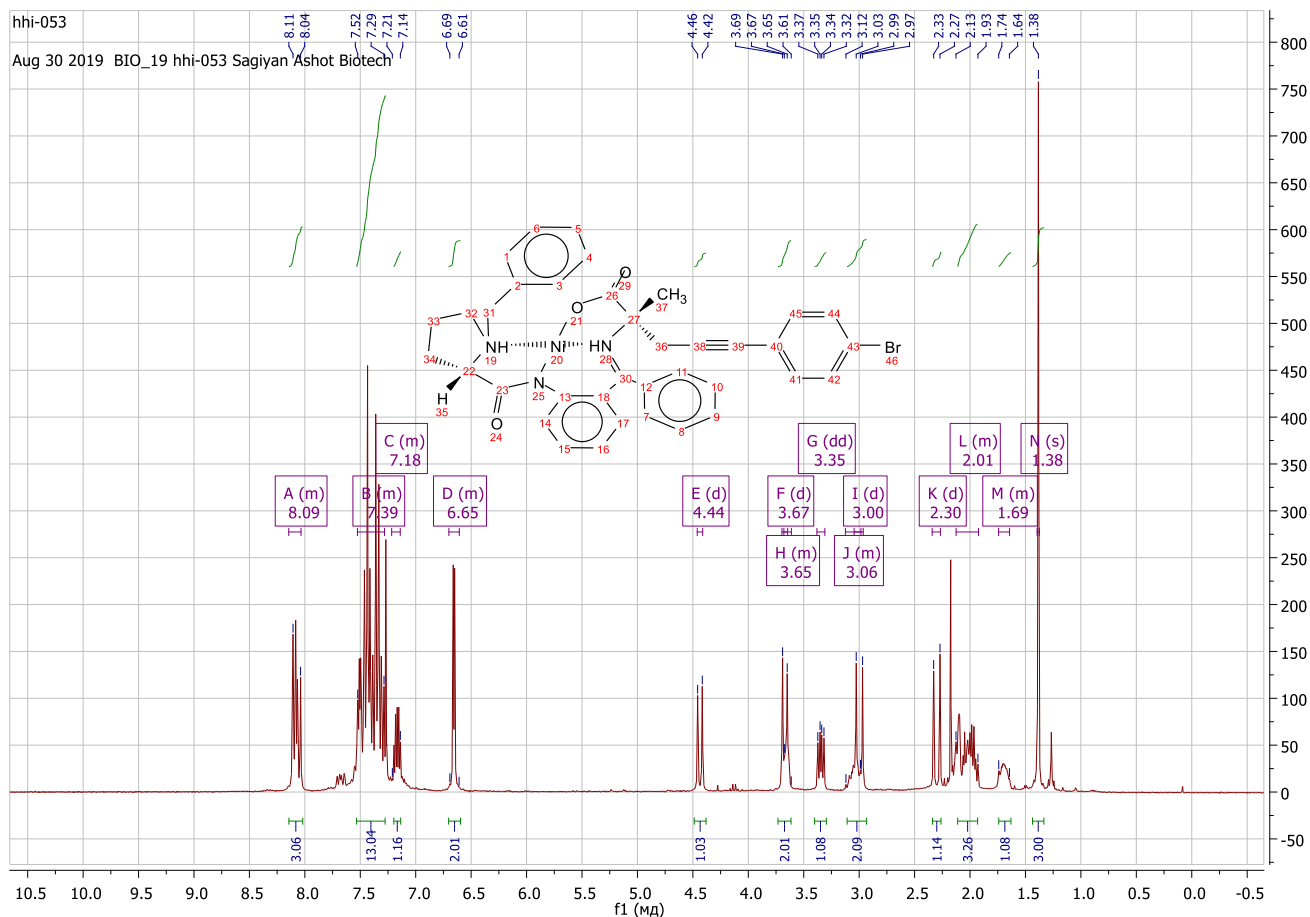
**Figure S1.** <sup>1</sup>H (300 MHz) and <sup>13</sup>C (75 MHz) NMR spectra of the Ni(II) complex **2a** (in CDCl<sub>3</sub>)



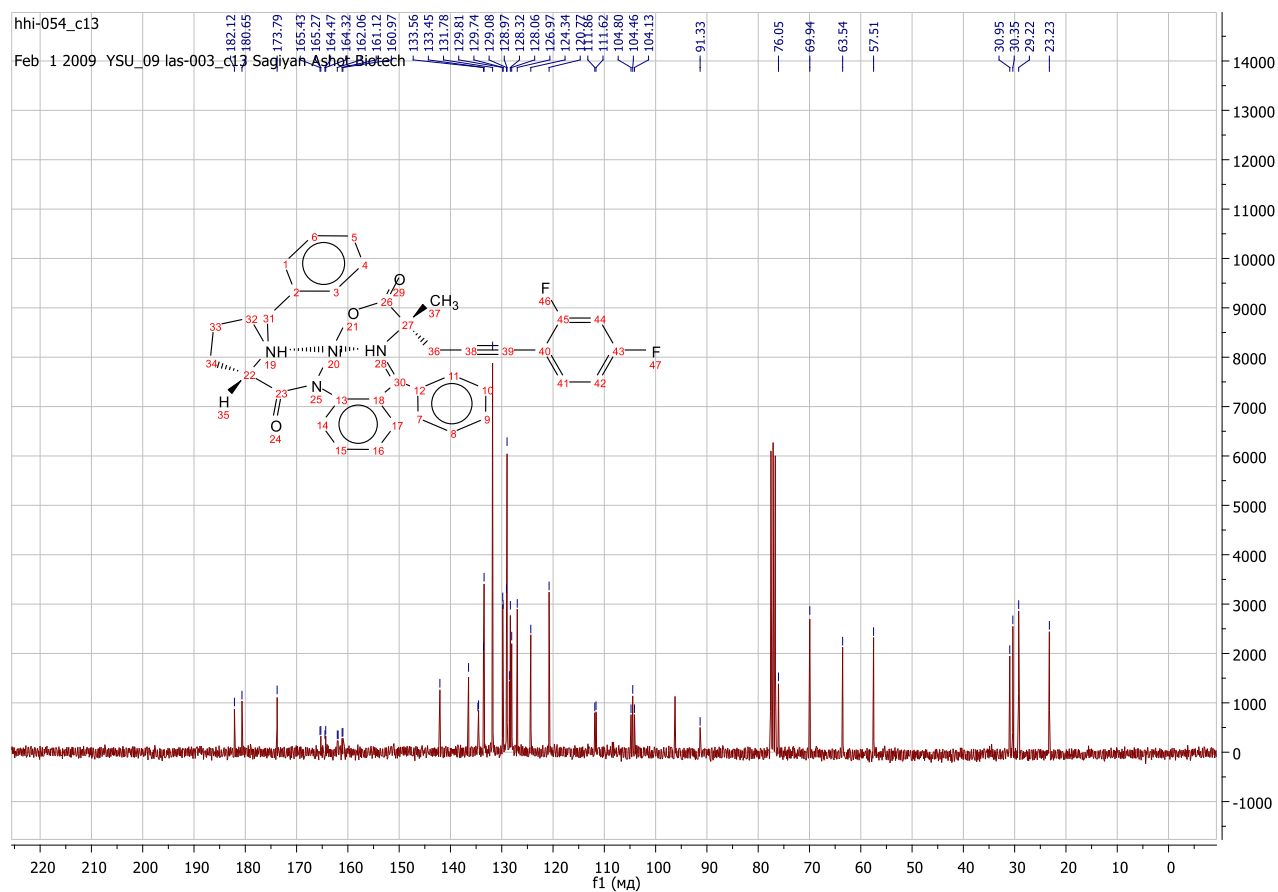
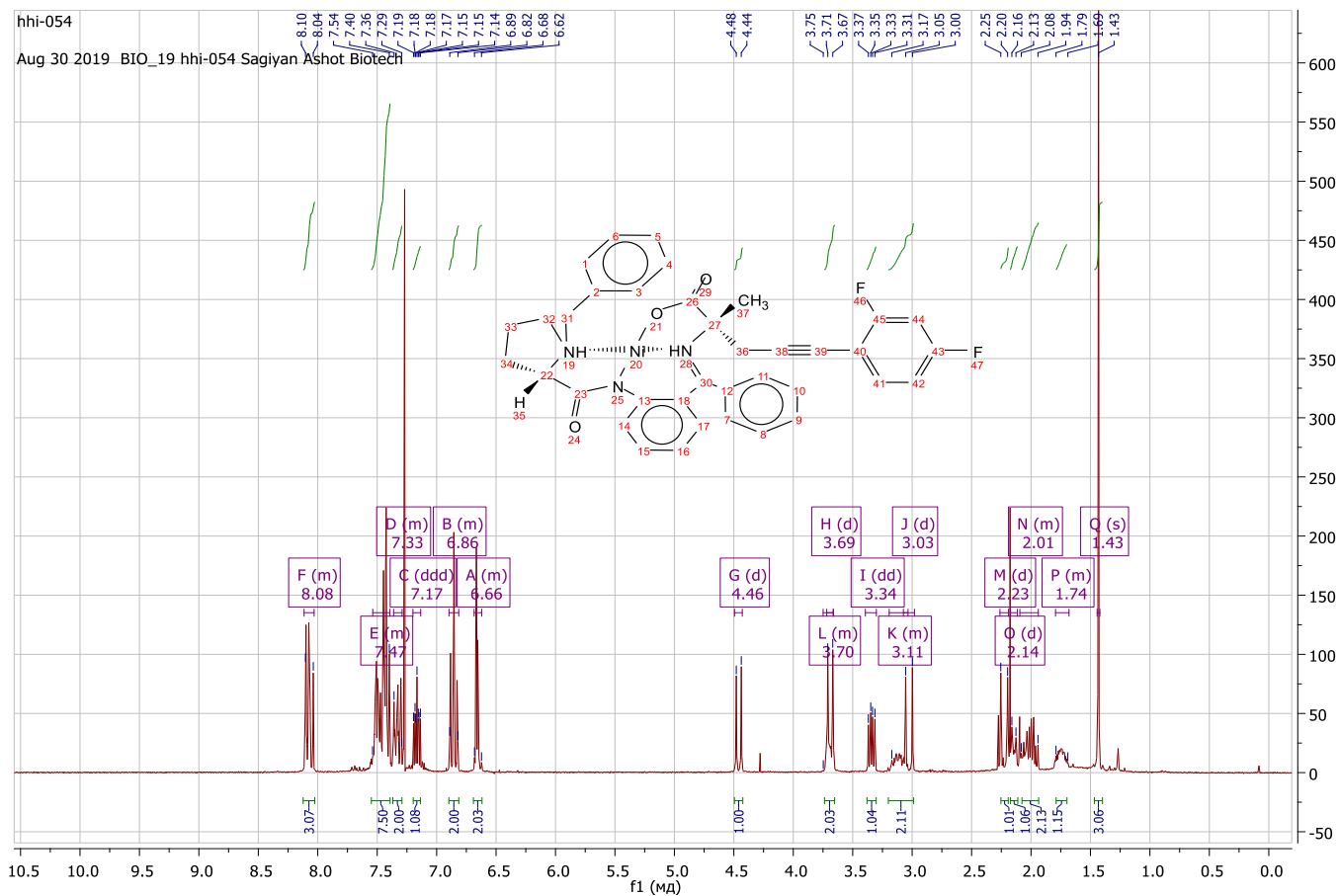
**Figure S2.** <sup>1</sup>H (300 MHz) and <sup>13</sup>C (75 MHz) NMR spectra of the Ni(II) complex **2b** (in CDCl<sub>3</sub>)



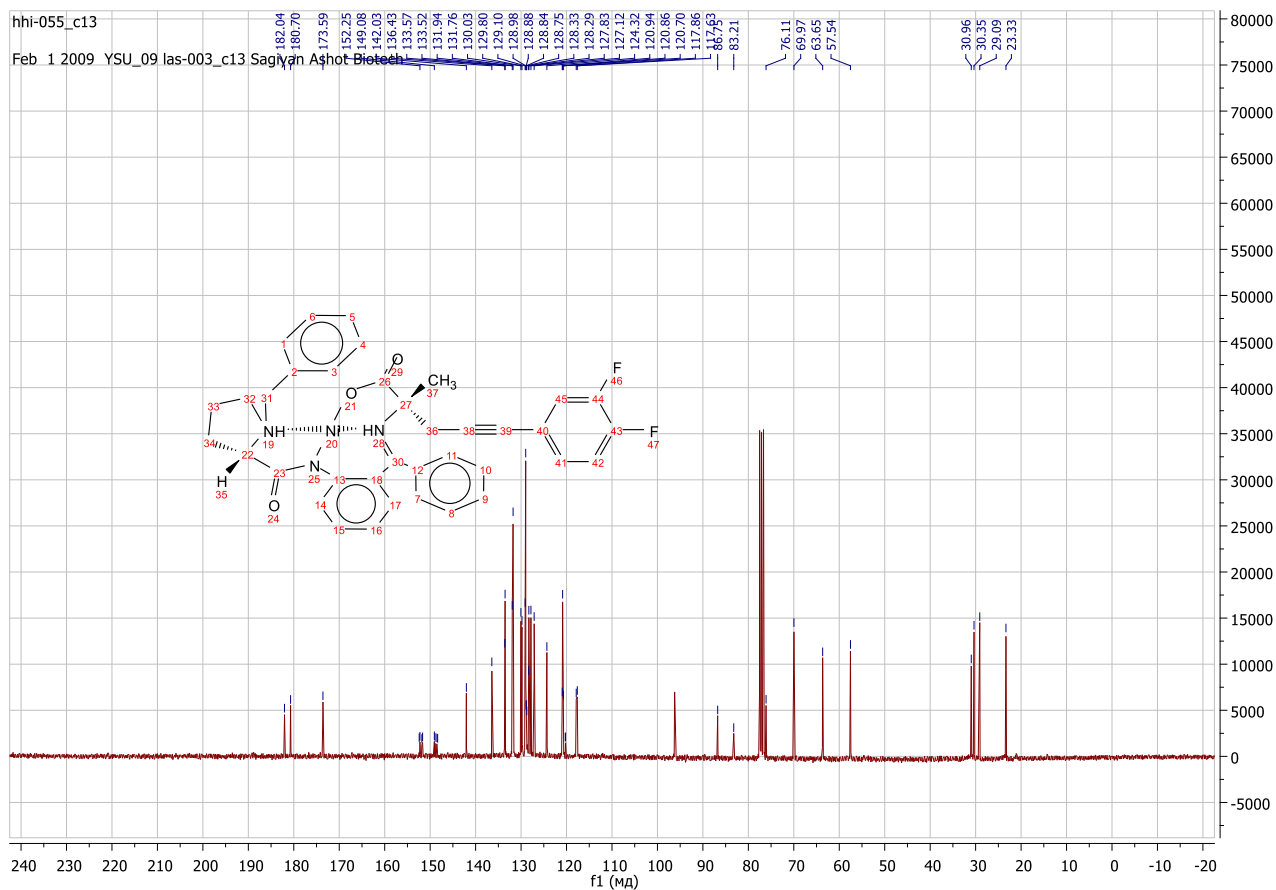
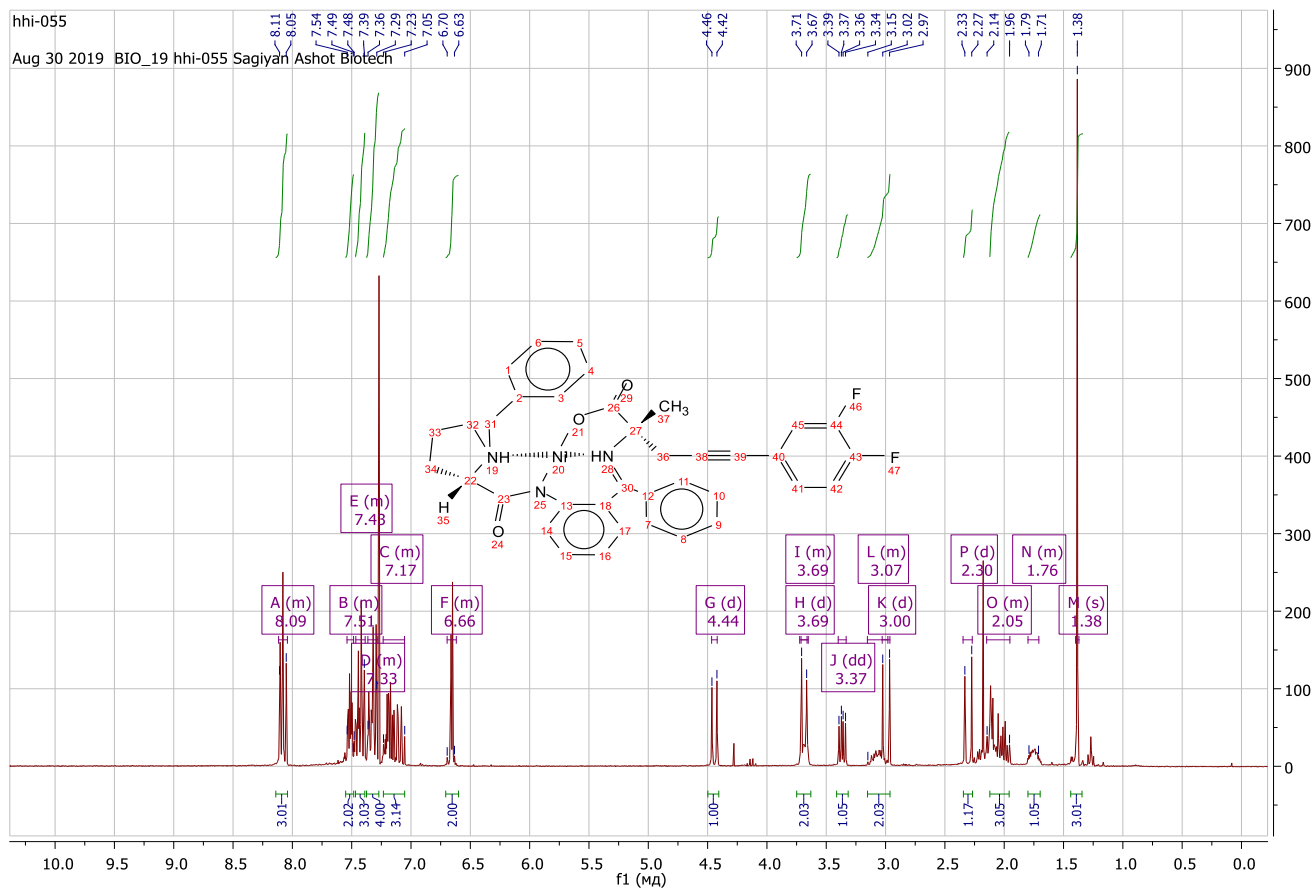
**Figure S3.** <sup>1</sup>H (300 MHz) and <sup>13</sup>C (75 MHz) NMR spectra of the Ni(II) complex **2c** (in CDCl<sub>3</sub>)



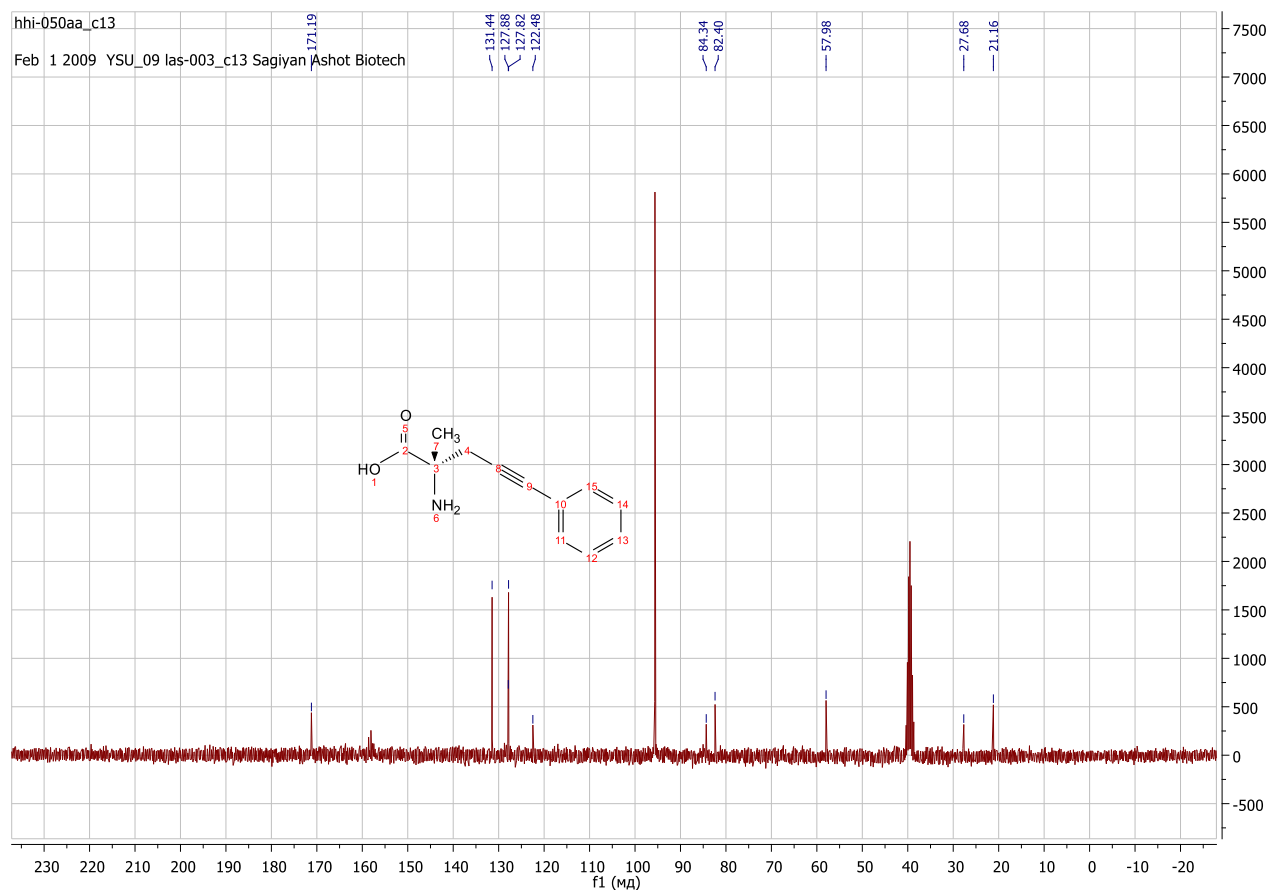
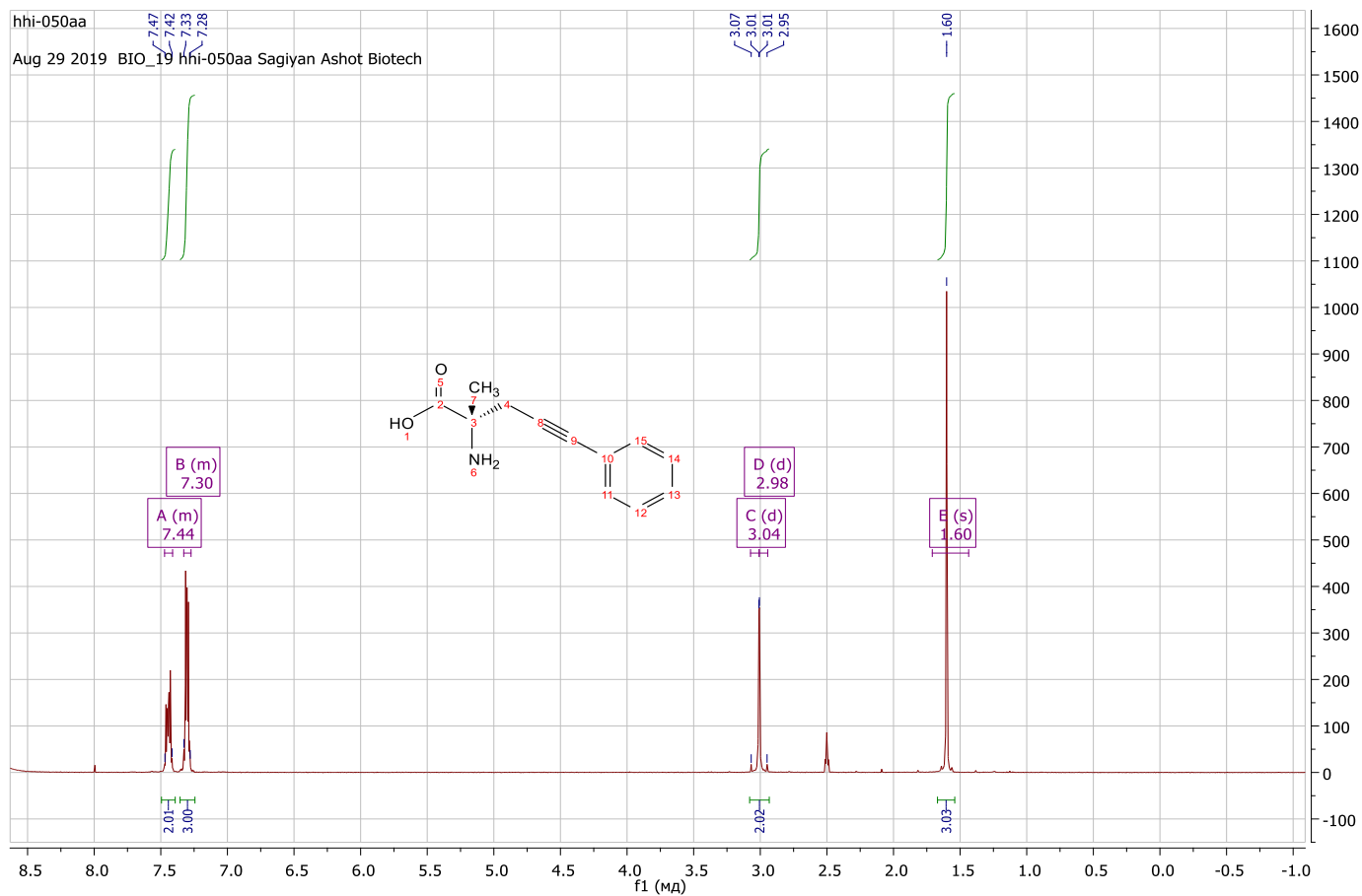
**Figure S4.** <sup>1</sup>H (300 MHz) and <sup>13</sup>C (75 MHz) NMR spectra of the Ni(II) complex **2d** (in CDCl<sub>3</sub>)



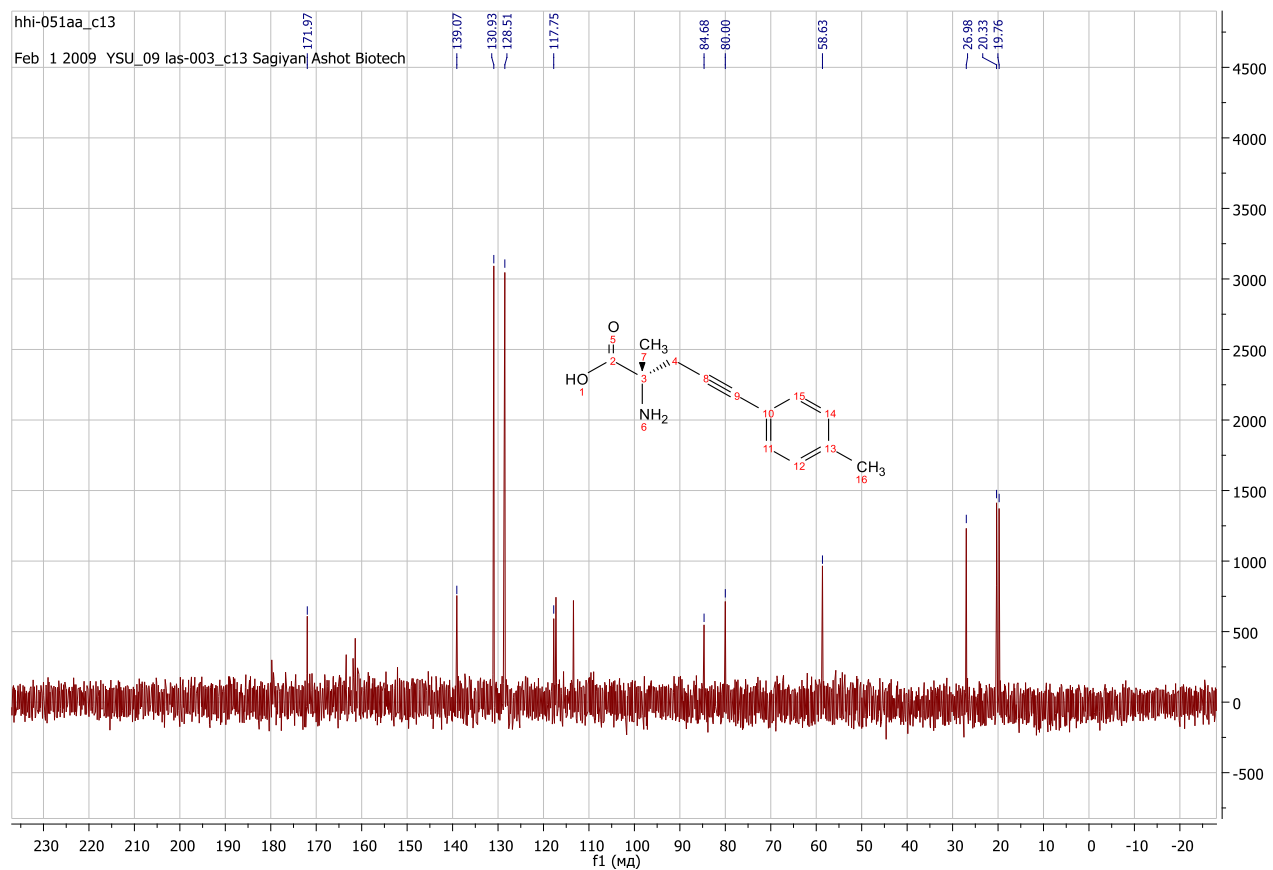
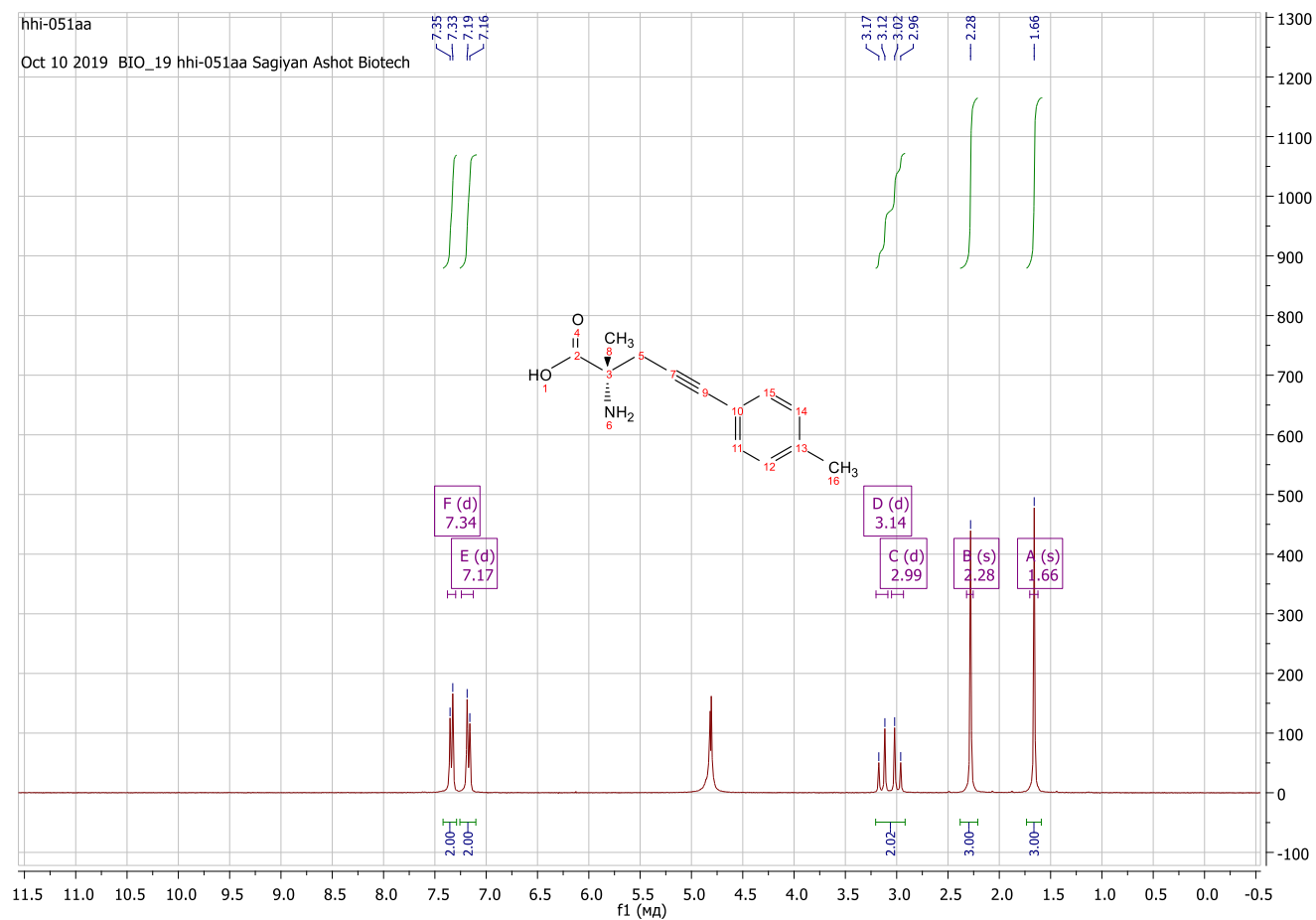
**Figure S5.** <sup>1</sup>H (300 MHz) and <sup>13</sup>C (75 MHz) NMR spectra of the Ni(II) complex **2e** (in CDCl<sub>3</sub>)



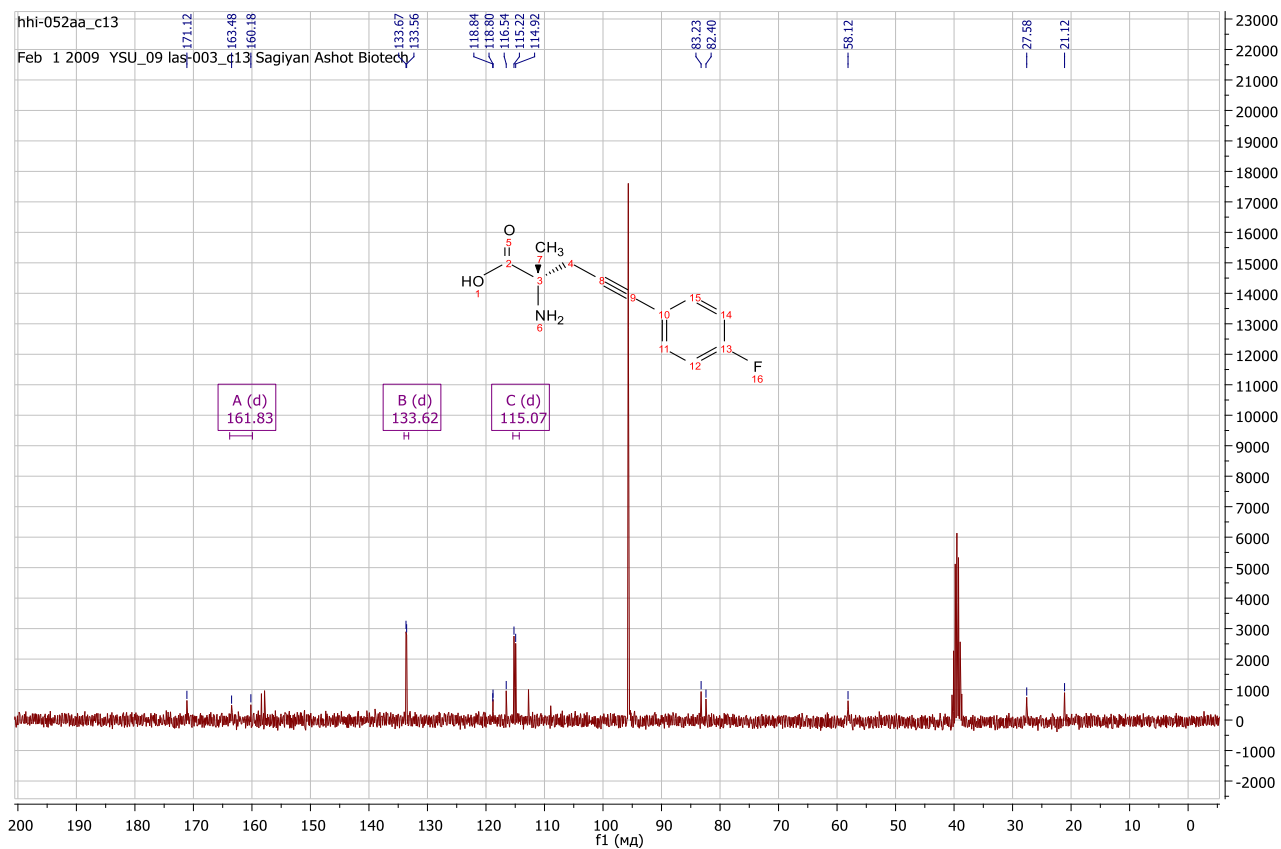
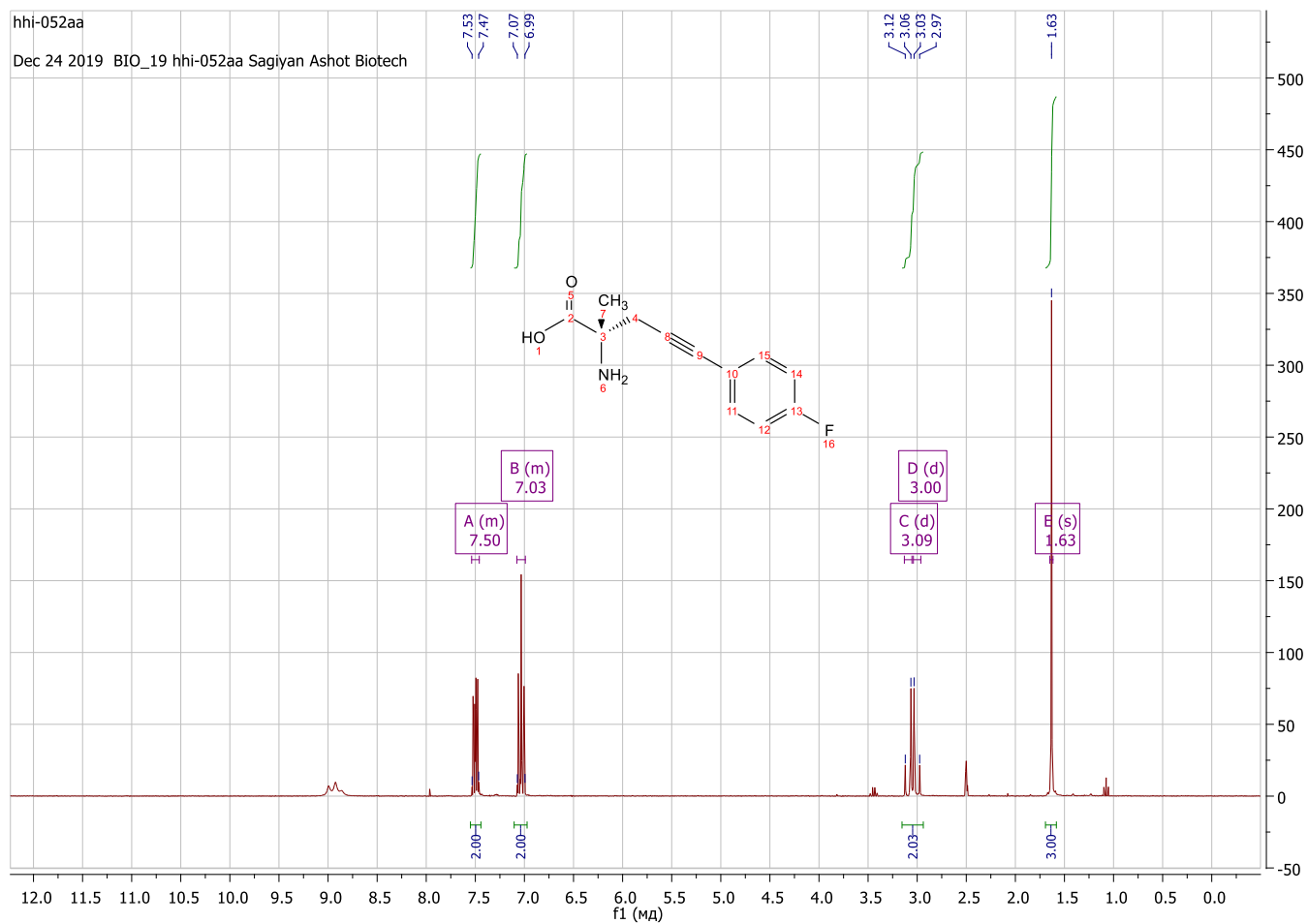
**Figure S6.**  $^1\text{H}$  (300 MHz) and  $^{13}\text{C}$  (75 MHz) NMR spectra of the Ni(II) complex **2f** (in  $\text{CDCl}_3$ )



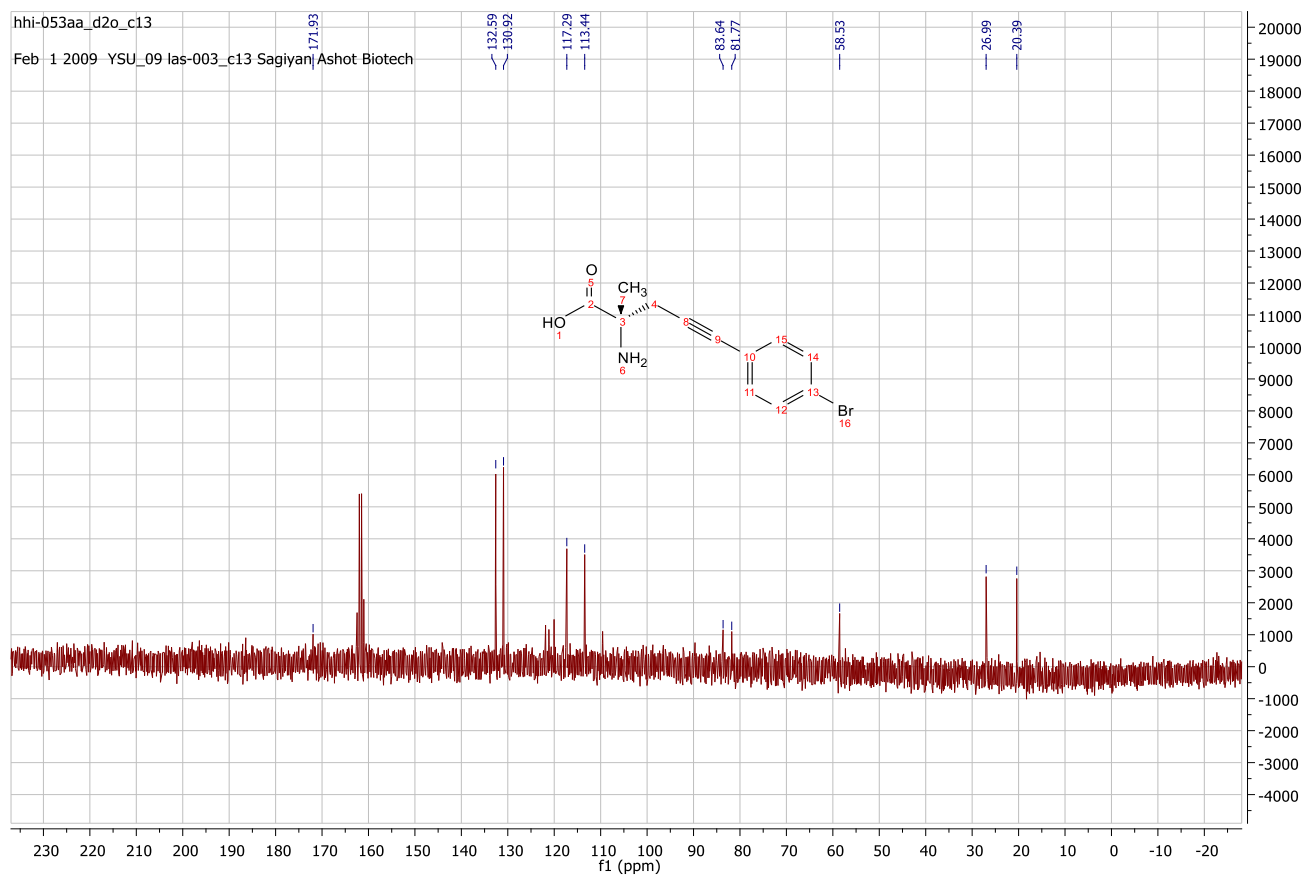
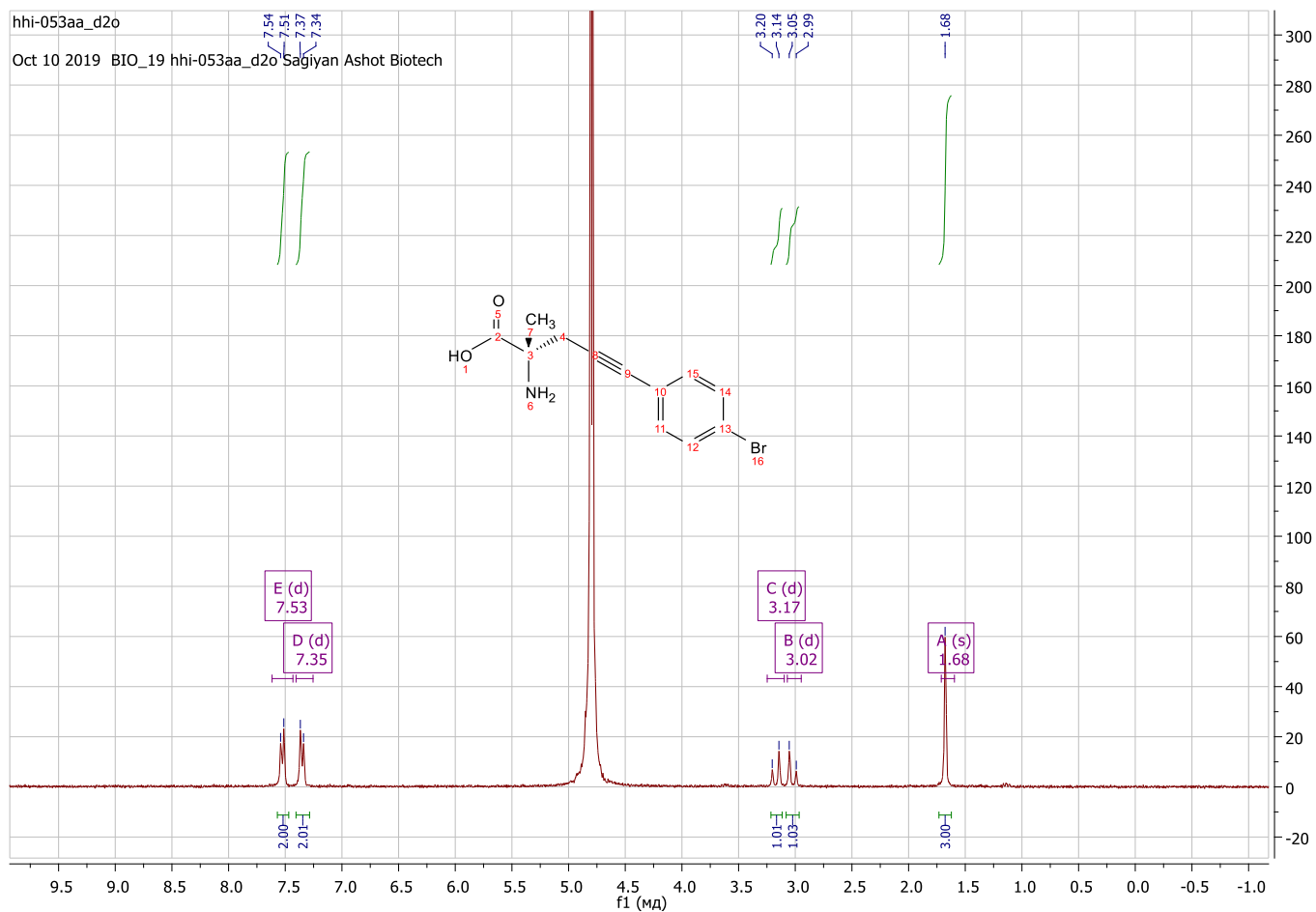
**Figure S7.** <sup>1</sup>H (300 MHz) and <sup>13</sup>C (75 MHz) NMR spectra of AA **3a** (in DMSO-d<sub>6</sub>+CCl<sub>4</sub>+CF<sub>3</sub>COOD)



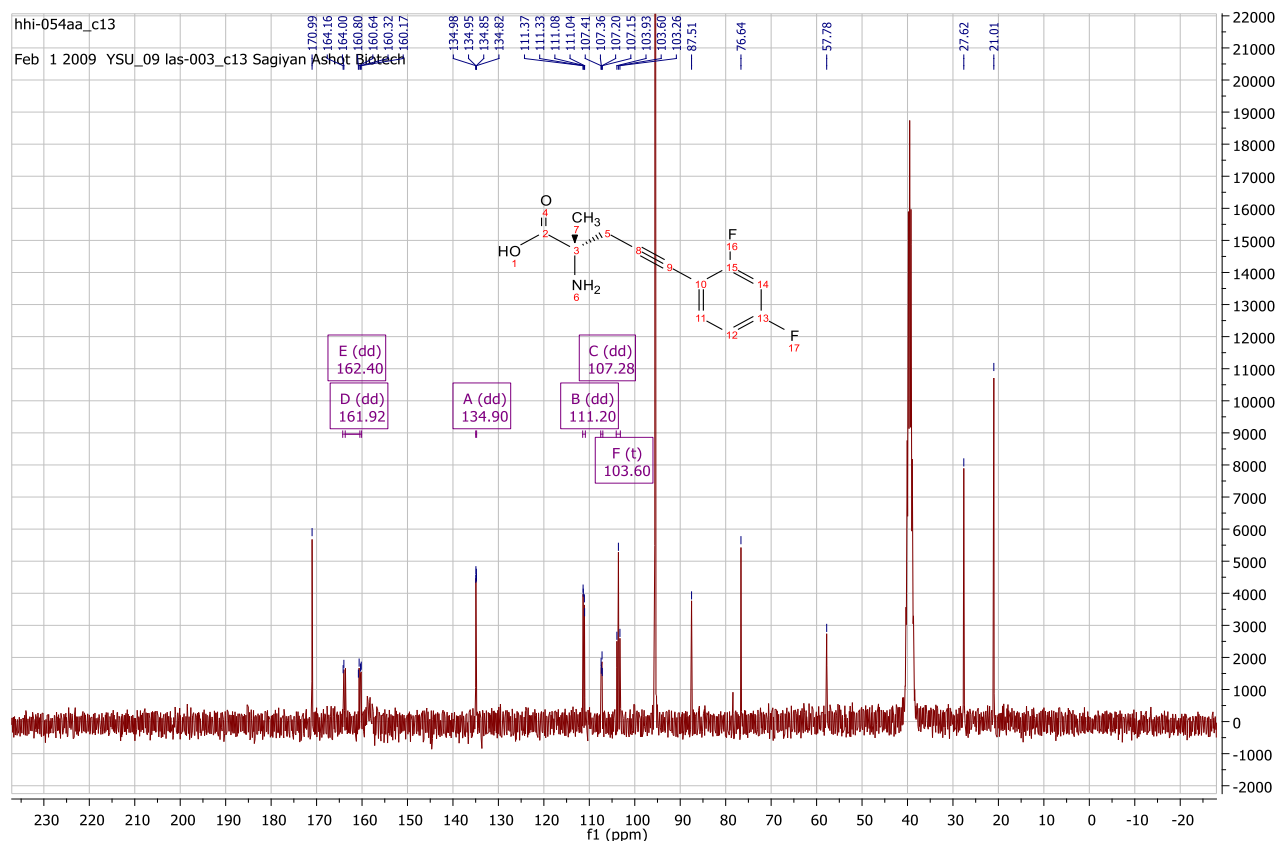
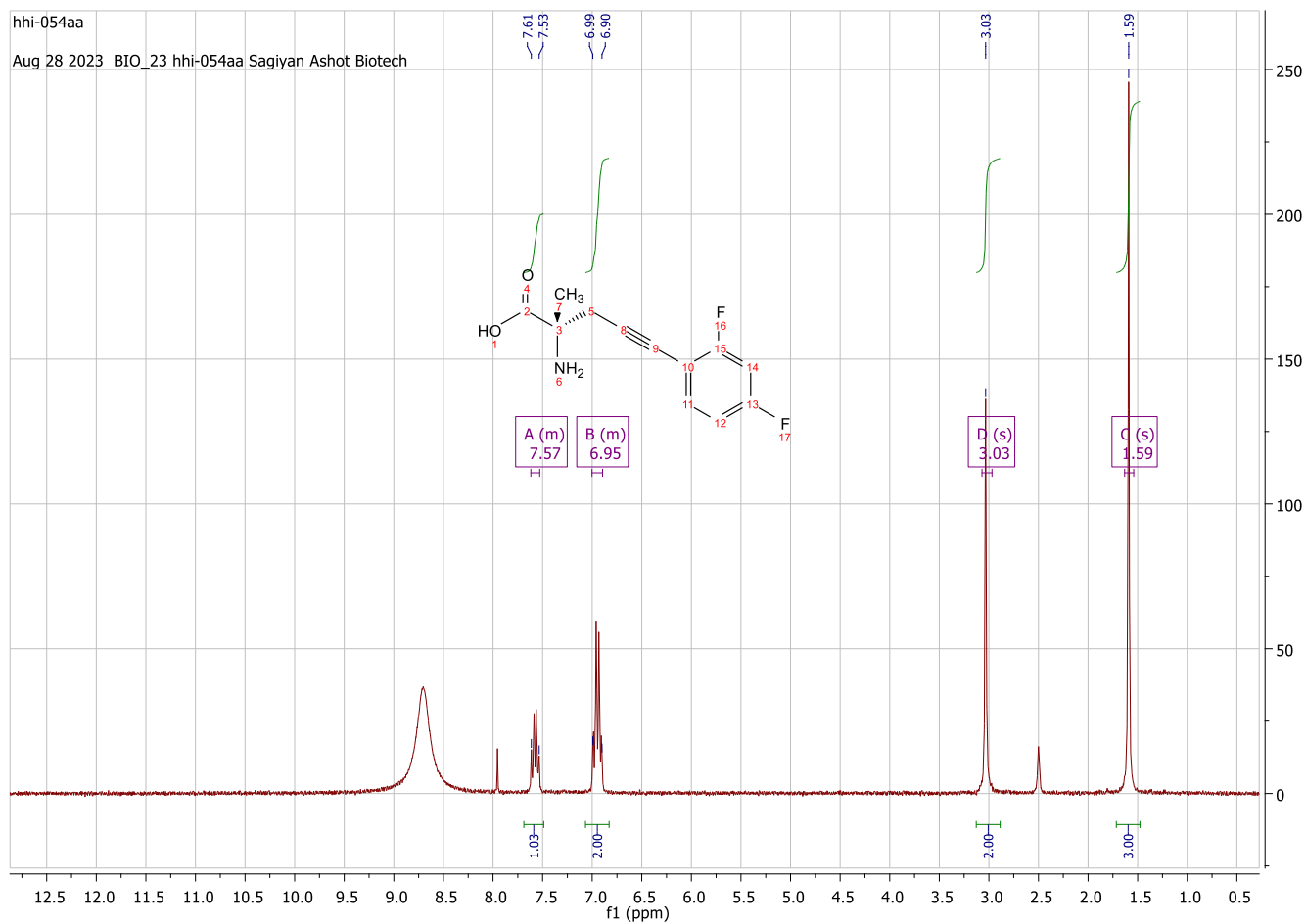
**Figure S8.** <sup>1</sup>H (300 MHz) and <sup>13</sup>C (75 MHz) NMR spectra of AA **3b** (in D<sub>2</sub>O+CF<sub>3</sub>COOD)



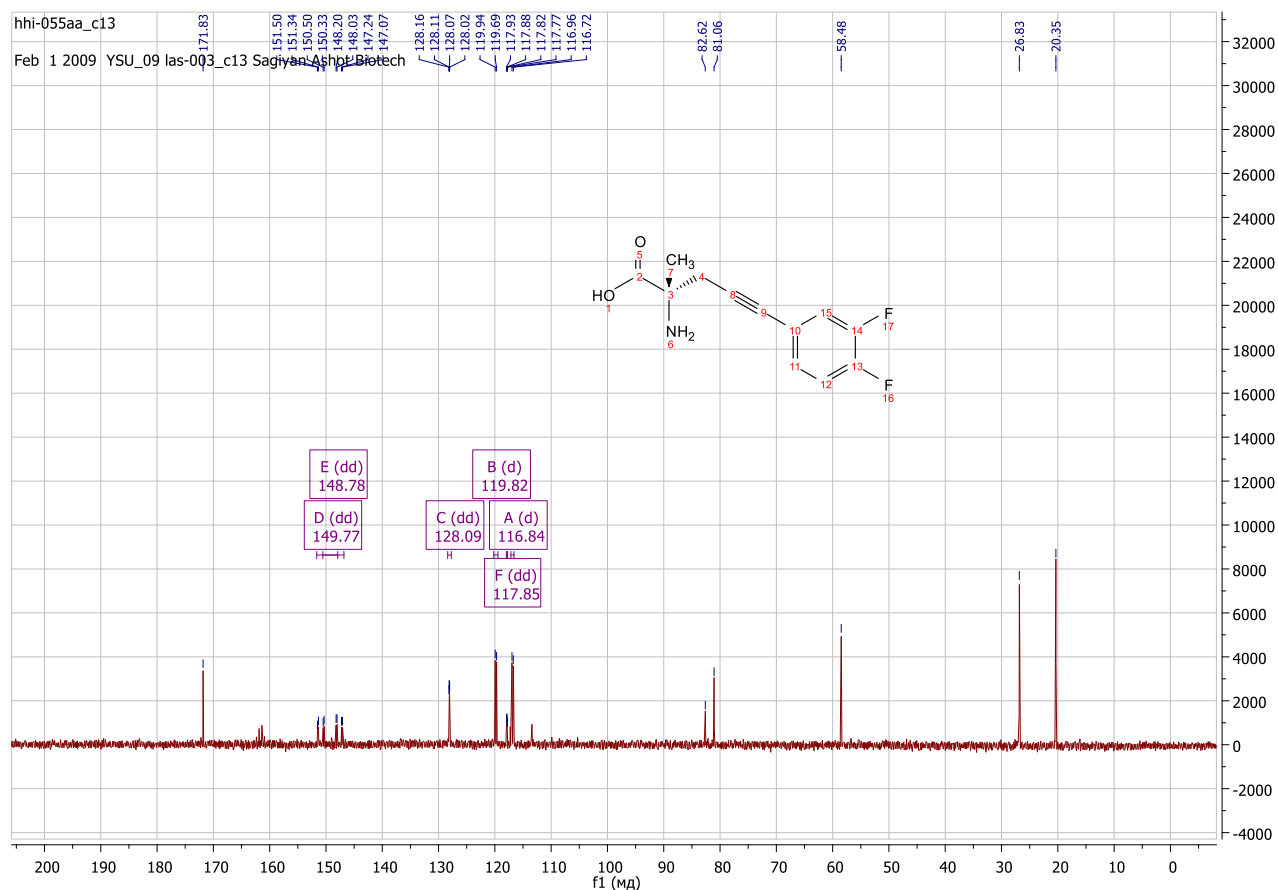
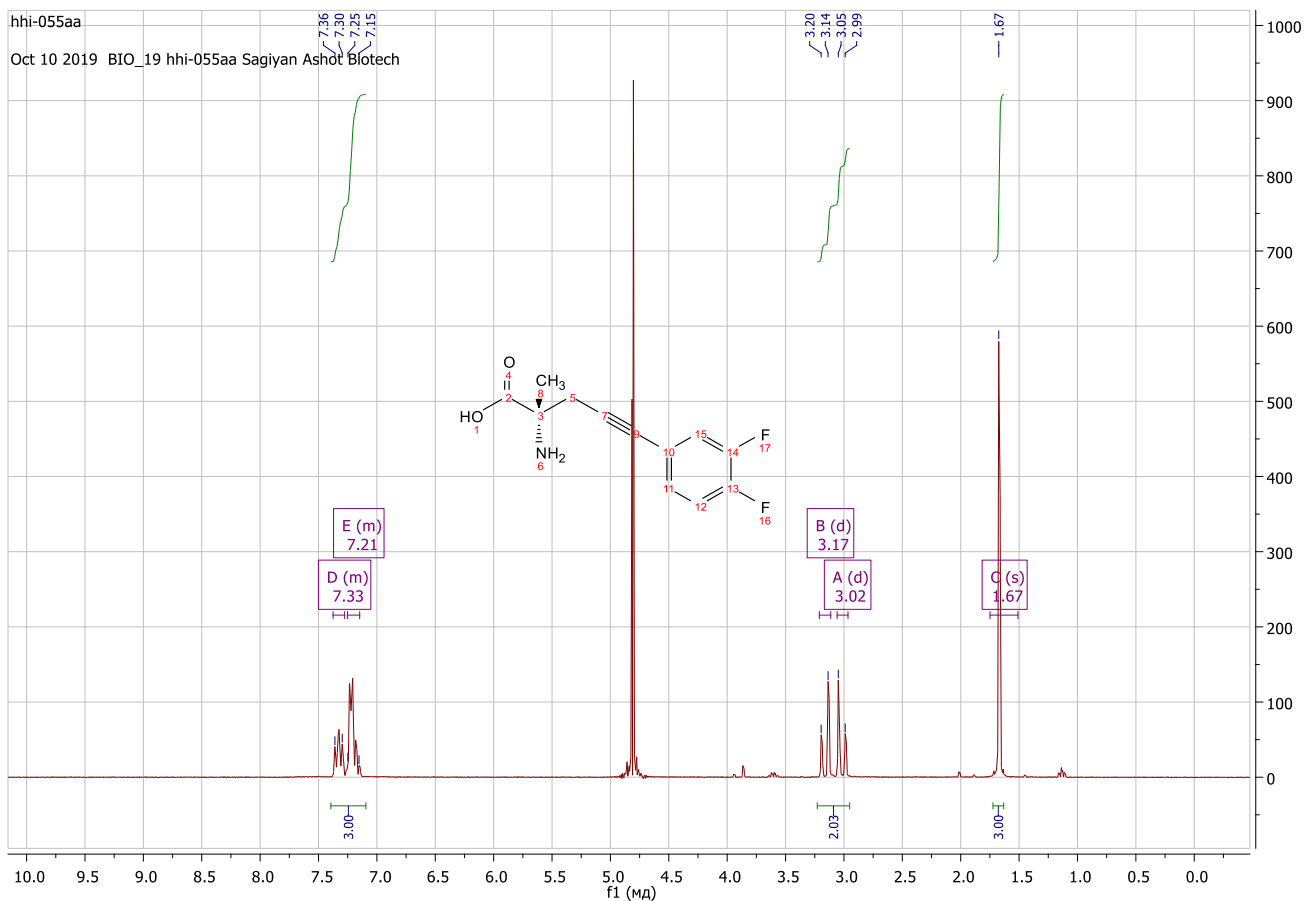
**Figure S9.** <sup>1</sup>H (300 MHz) and <sup>13</sup>C (75 MHz) NMR spectra of AA 3c (in DMSO-d<sub>6</sub>+CF<sub>3</sub>COOD)



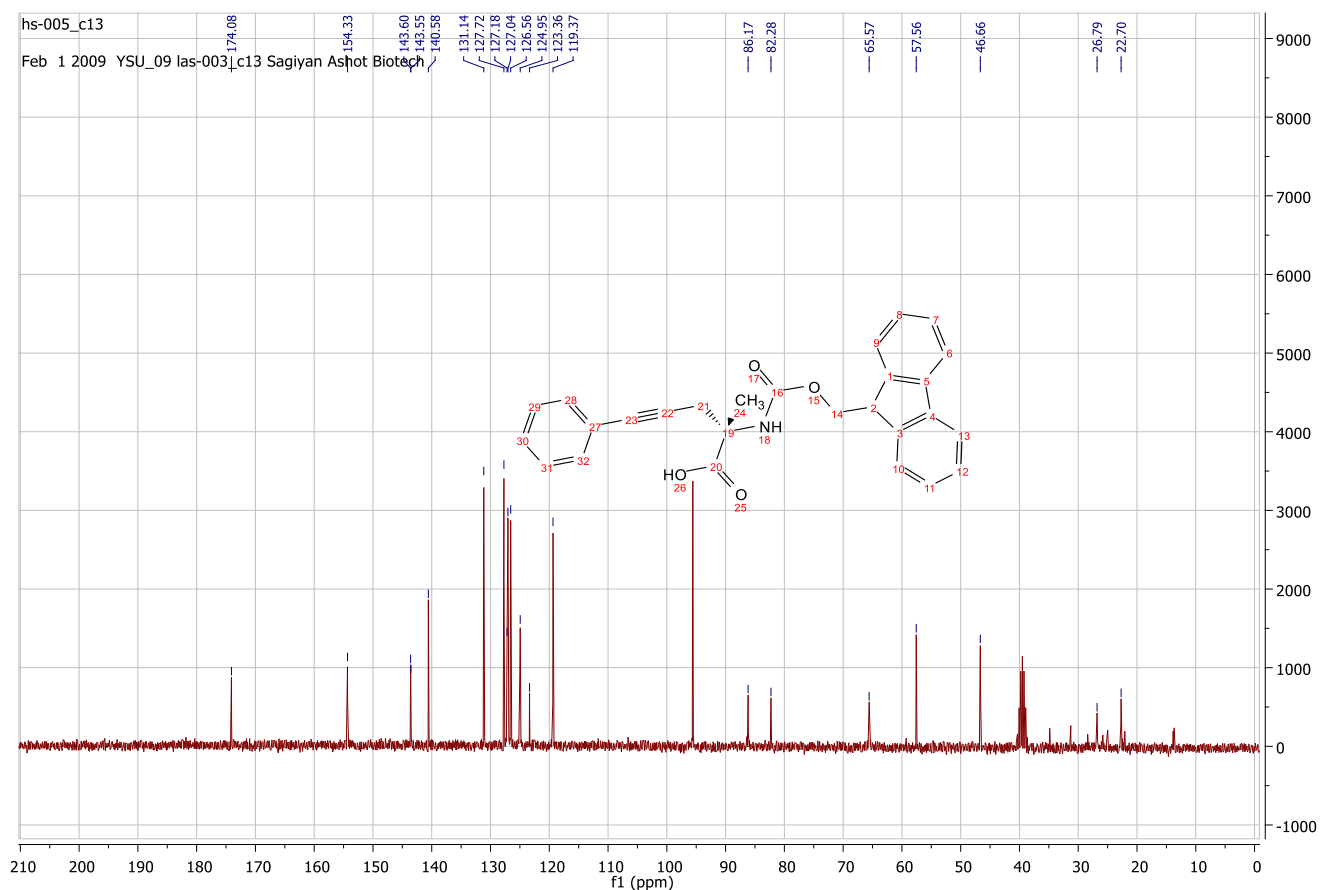
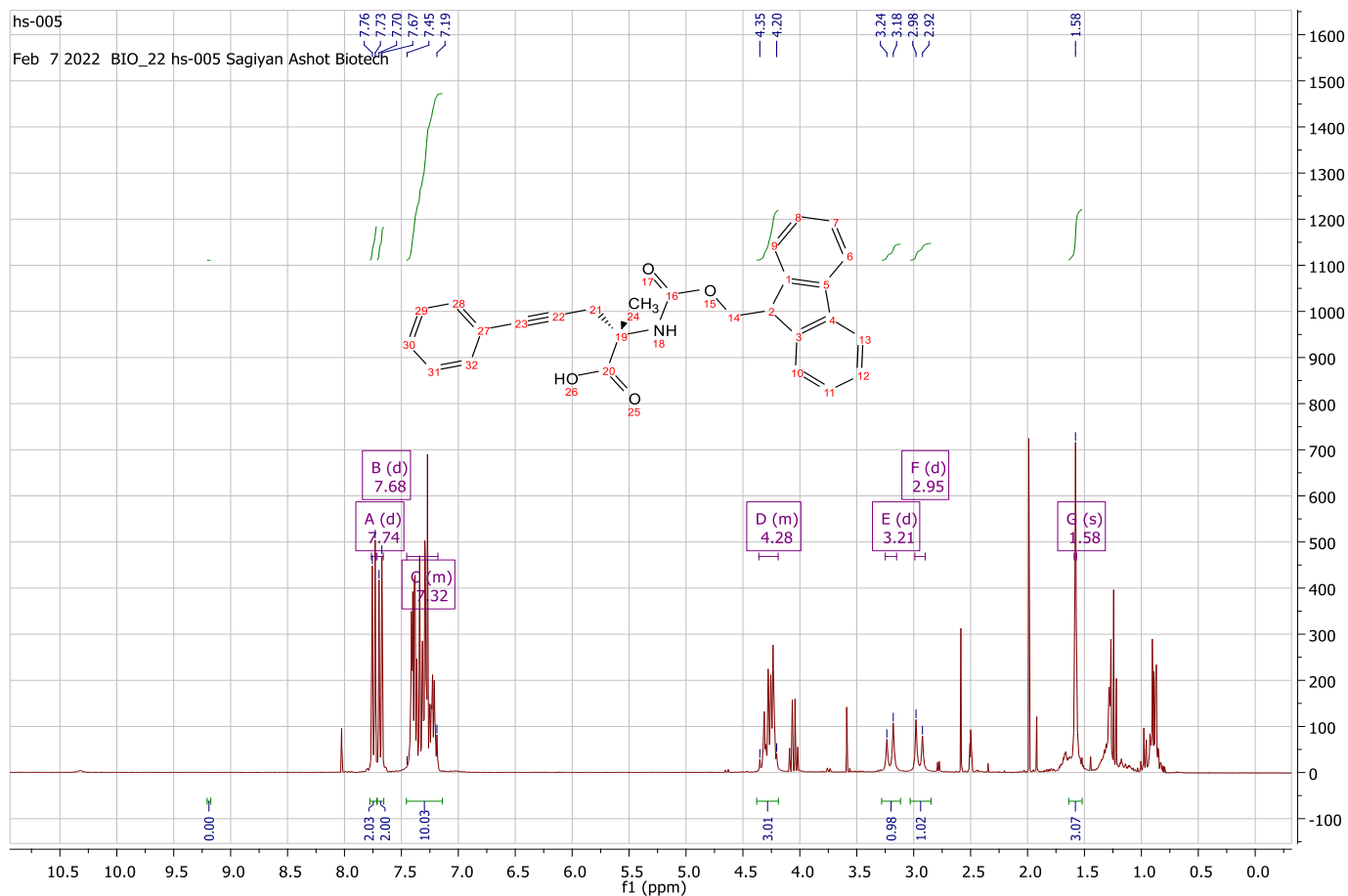
**Figure S10.** <sup>1</sup>H (300 MHz) and <sup>13</sup>C (75 MHz) NMR spectra of AA **3d** (in D<sub>2</sub>O+CF<sub>3</sub>COOD)



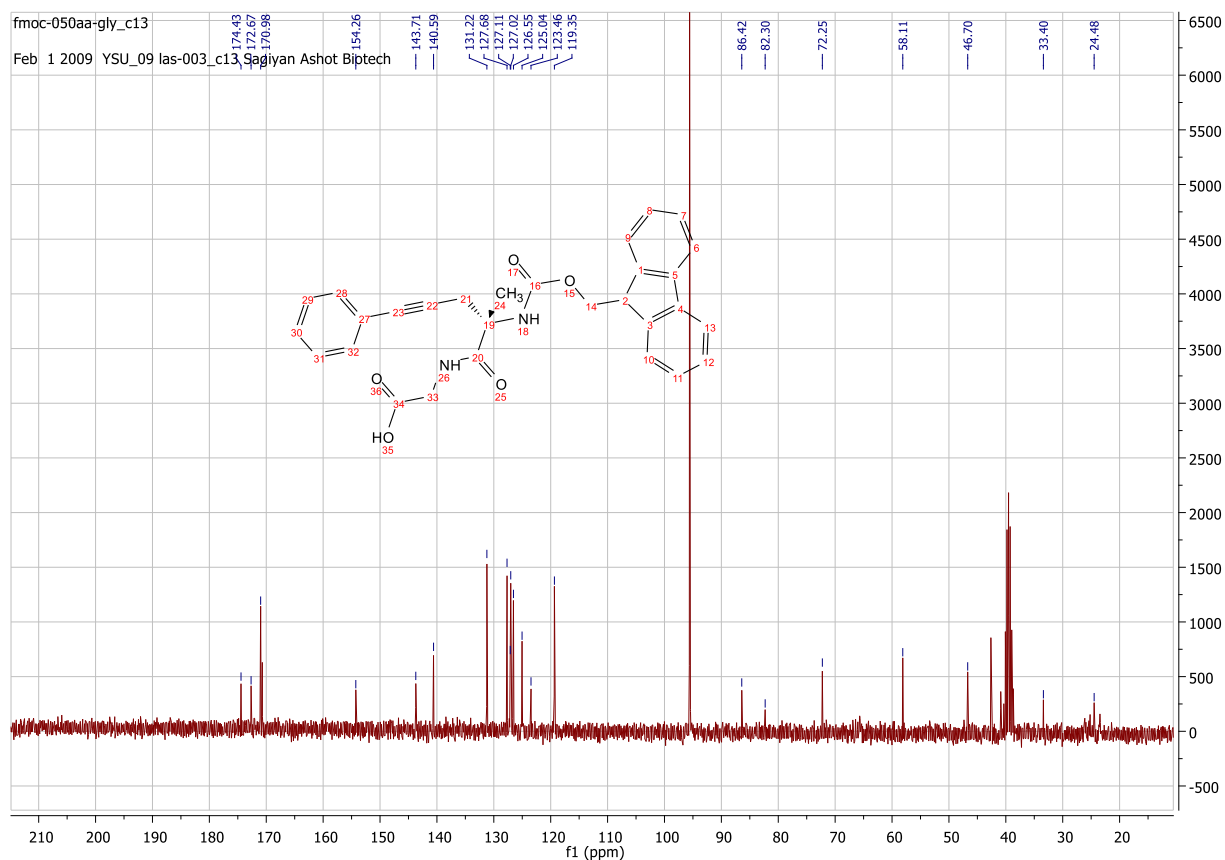
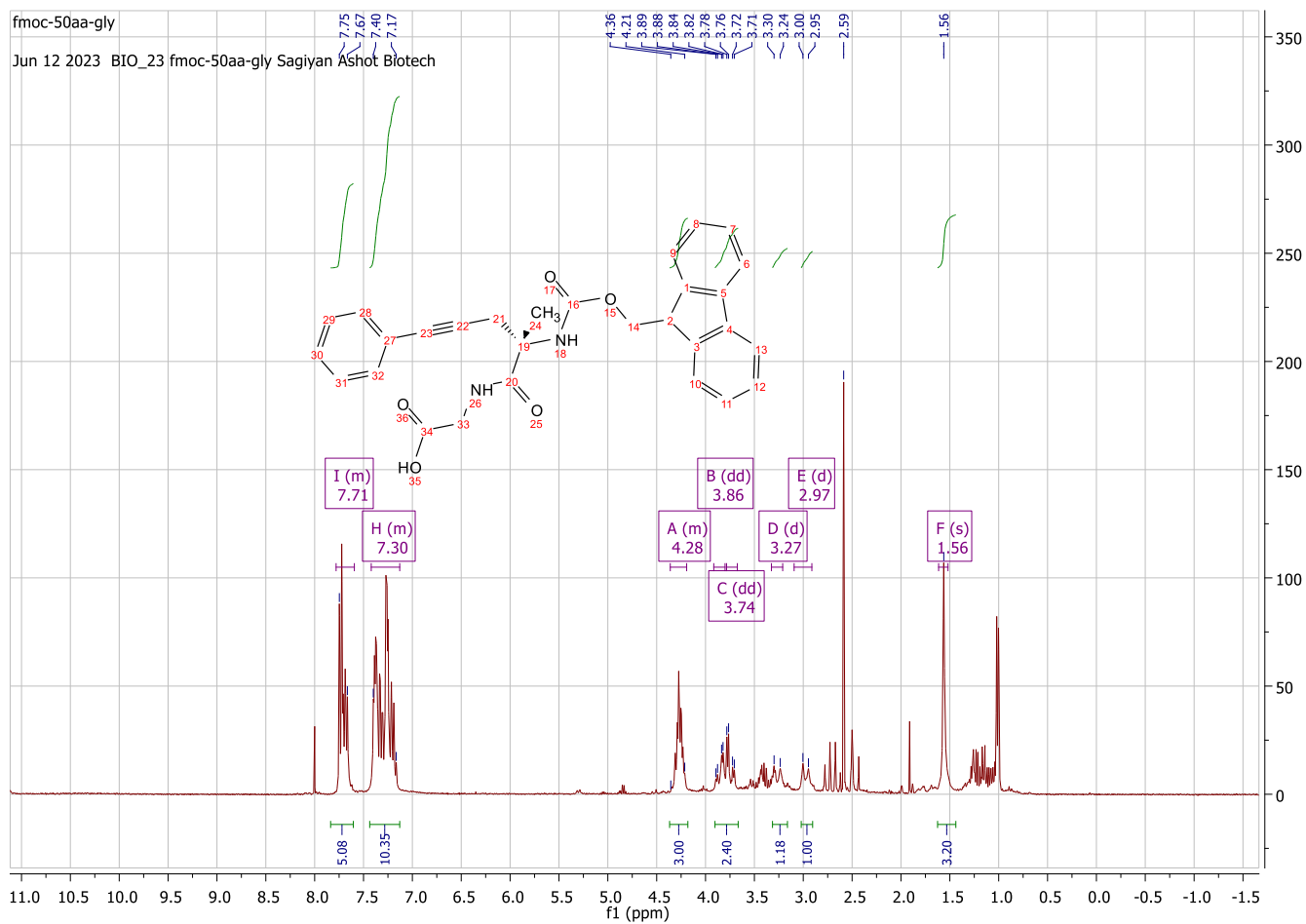
**Figure S11.** <sup>1</sup>H (300 MHz) and <sup>13</sup>C (75 MHz) NMR spectra of AA **3e** (in DMSO-d<sub>6</sub>+CF<sub>3</sub>COOD)



**Figure S12.**  $^1H$  (300 MHz) and  $^{13}C$  (75 MHz) NMR spectra of AA 3f (in  $D_2O+CF_3COOD$ )

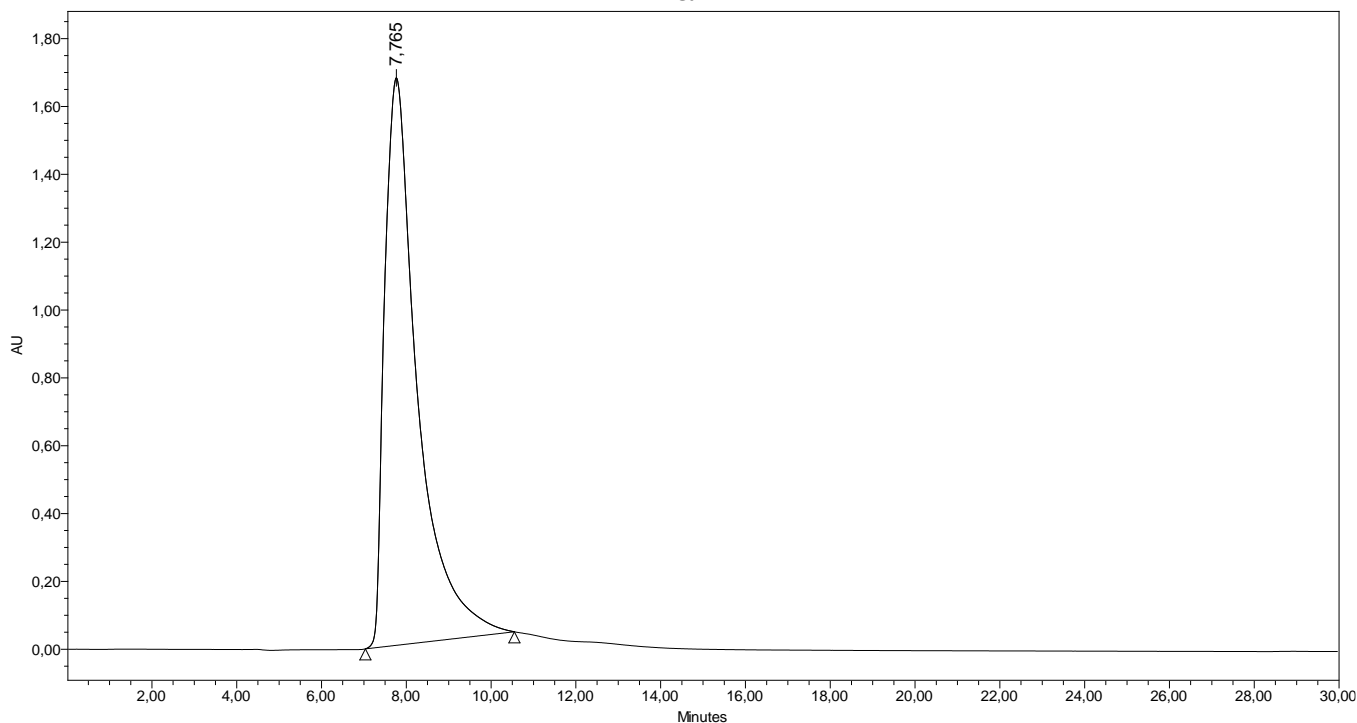


**Figure S13.**  $^1\text{H}$  (300 MHz) and  $^{13}\text{C}$  (75 MHz) NMR spectra of Fmoc-AA **4** (in DMSO- $d_6$ )



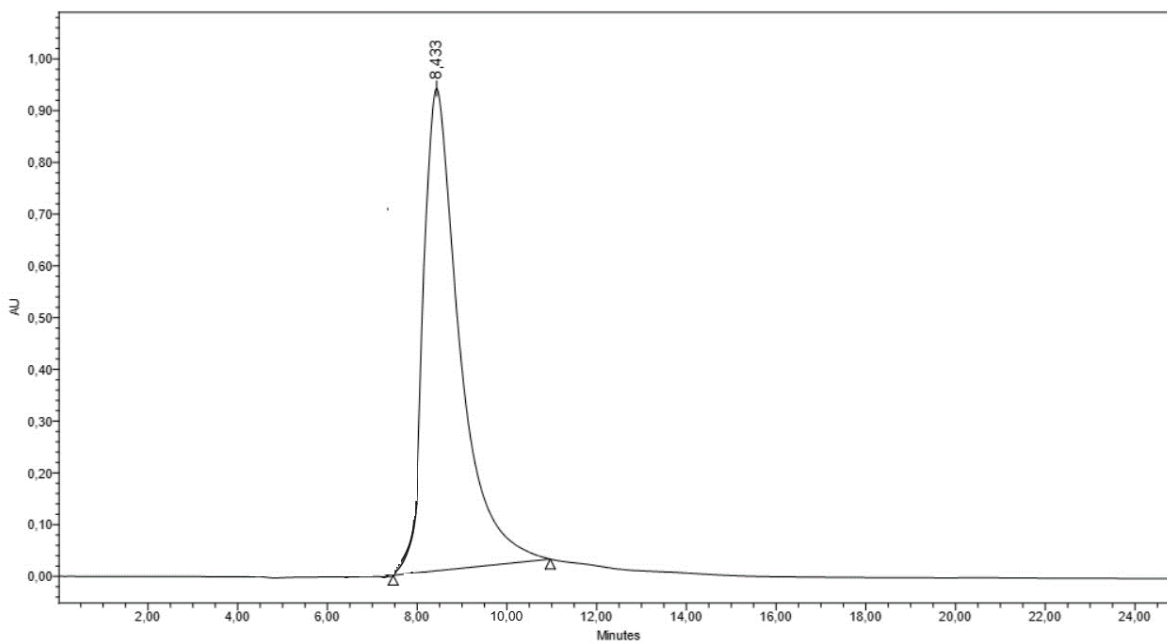
**Figure S14.** <sup>1</sup>H (300 MHz) and <sup>13</sup>C (75 MHz) NMR spectra of dipeptide **6** (in DMSO-d<sub>6</sub>)

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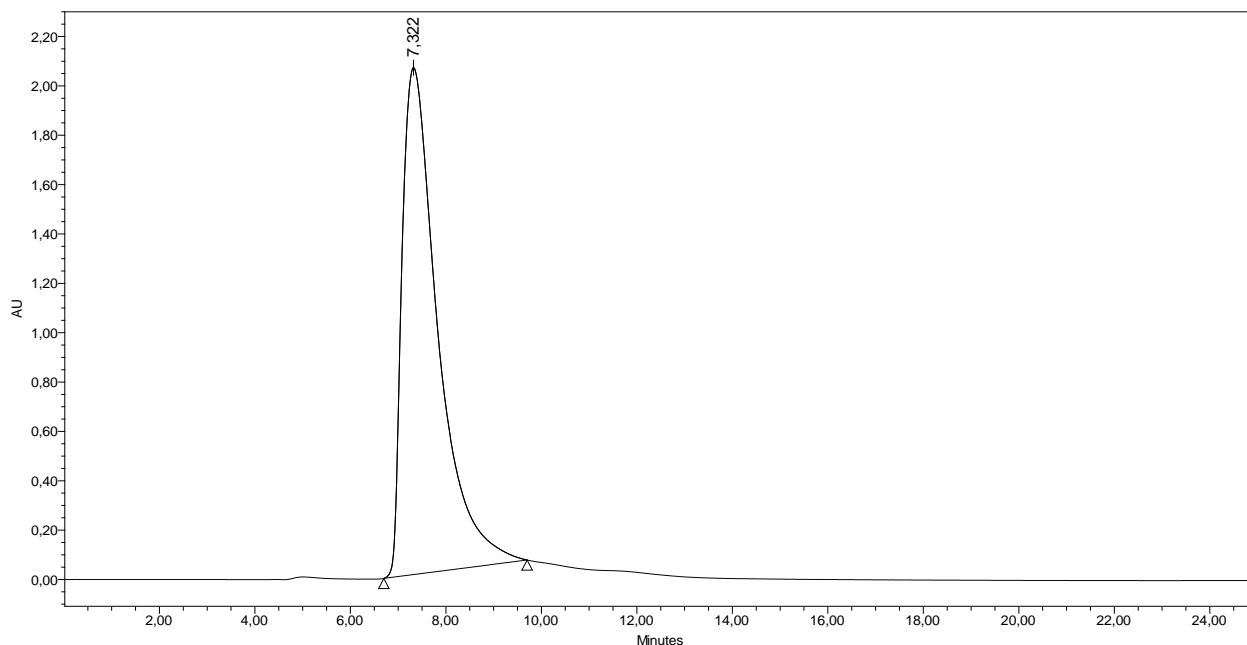
Nº	Name	Retention Time	Area	% Area	Height
1	( <i>S</i> )-2-amino-2-methyl-5-phenylpent-4-ynoic acid <b>3a</b>	7,765	90184069	100,00	1673077

**Figure S15.** HPLC trace of the enantiopure AA (*S*)-**3a**



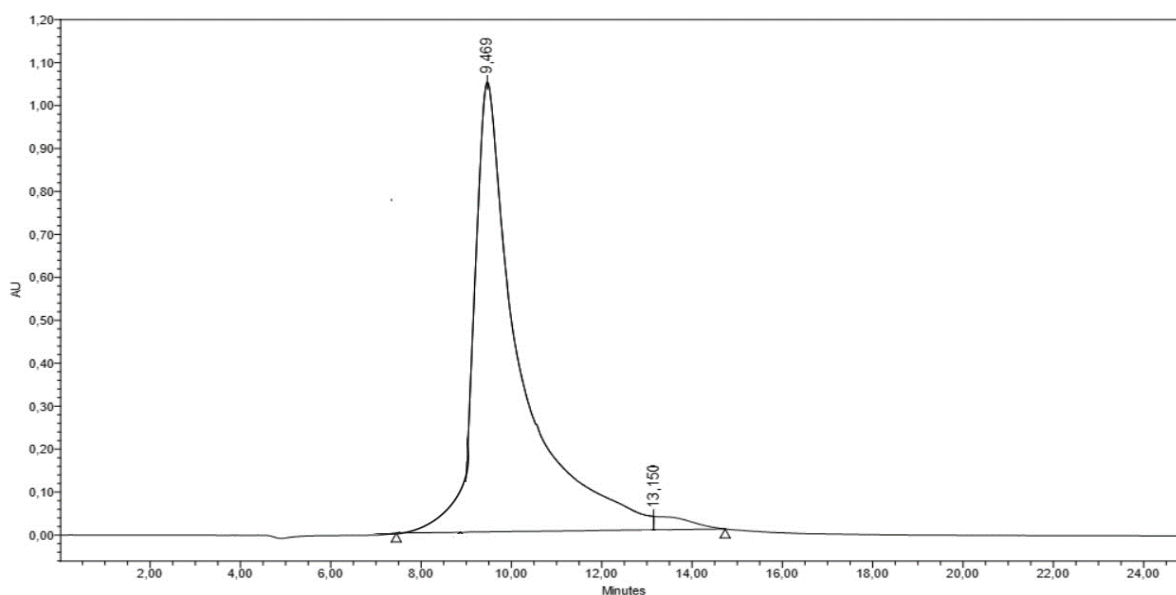
	Name	Retention Time	Area	% Area	Height
1	( <i>S</i> )-2-amino-2-methyl-5-(p-tolyl)pent-4-ynoic acid <b>3b</b>	8,433	51935377	100	931938

**Figure S16.** HPLC trace of the enantiopure AA (*S*)-**3b**



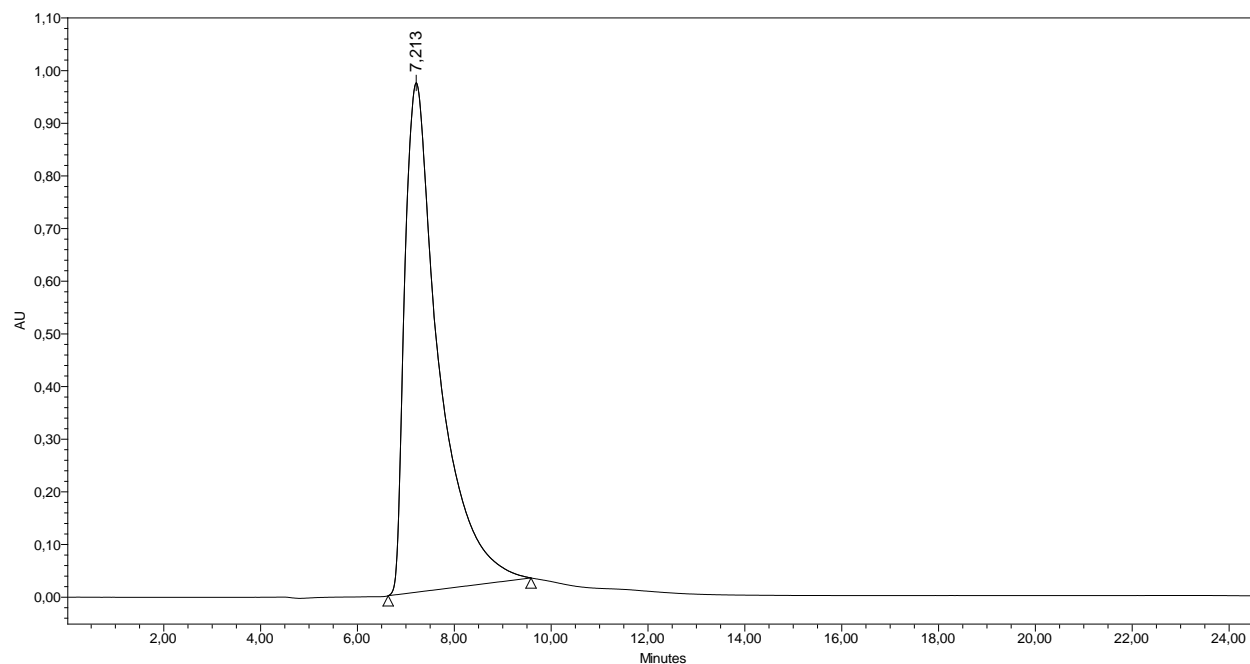
Nº	Name	Retention Time	Area	% Area	Height
1	( <i>S</i> )-2-amino-5-(4-fluorophenyl)-2-methylpent-4-ynoic acid <b>3c</b>	7,322	107229329	100,00	2054392

**Figure S17.** HPLC trace of the enantiopure AA (*S*)-**3c**



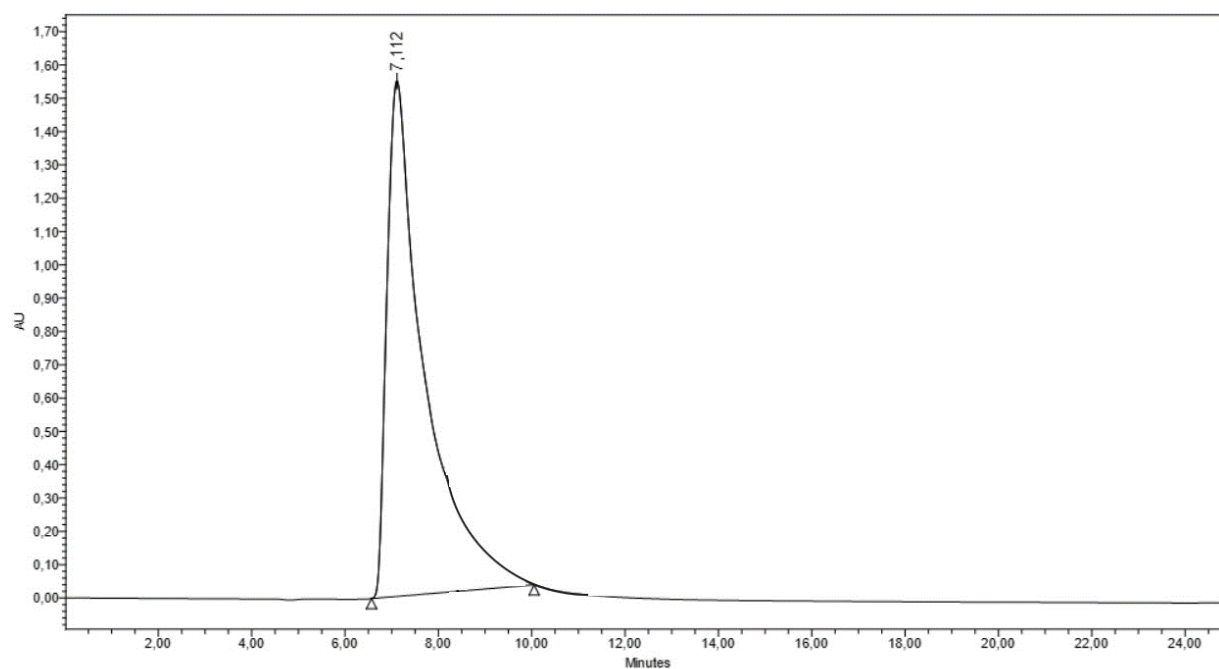
Nº	Name	Retention Time	Area	% Area	Height
1	( <i>S</i> )-2-amino-5-(4-bromophenyl)-2-methylpent-4-ynoic acid <b>3d</b>	9,469	71480284	98,97	1047045
2	( <i>R</i> )-2-amino-5-(4-bromophenyl)-2-methylpent-4-ynoic acid <b>3d</b>	13,150	1669131	1,03	31136

**Figure S18.** HPLC trace of the enantiopure AA (*S*)-**3d**



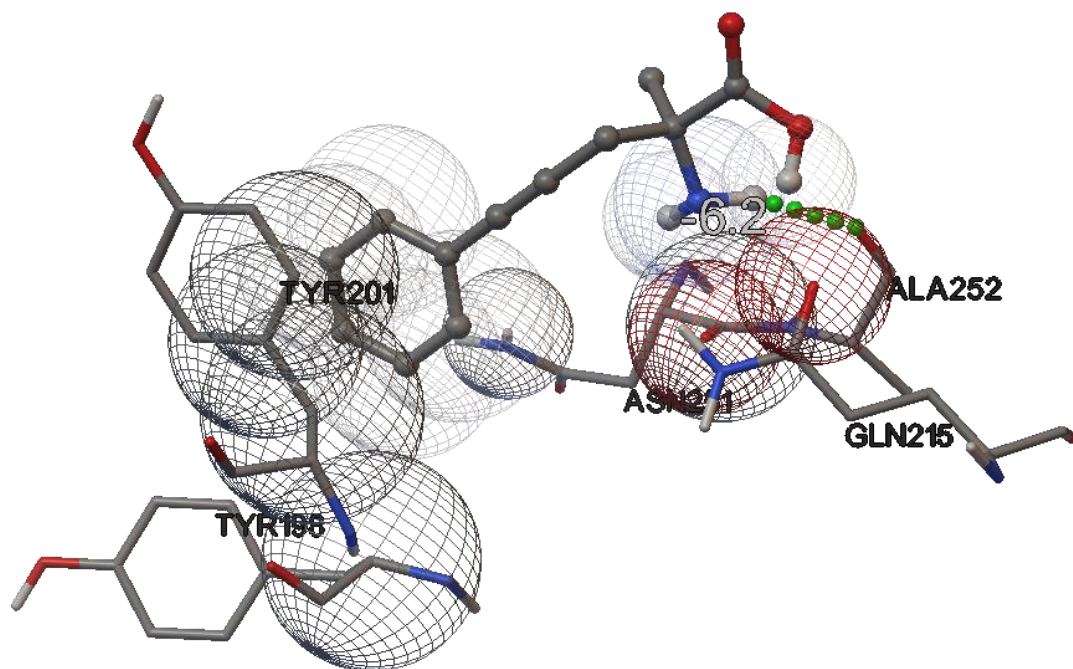
No	Name	Retention Time	Area	% Area	Height
1	(S)-2-amino-5-(2,4-difluorophenyl)-2-methylpent-4-ynoic acid <b>3e</b>	7,213	47368874	100,00	967682

**Figure S19.** HPLC trace of the enantiopure AA (*S*)-**3e**

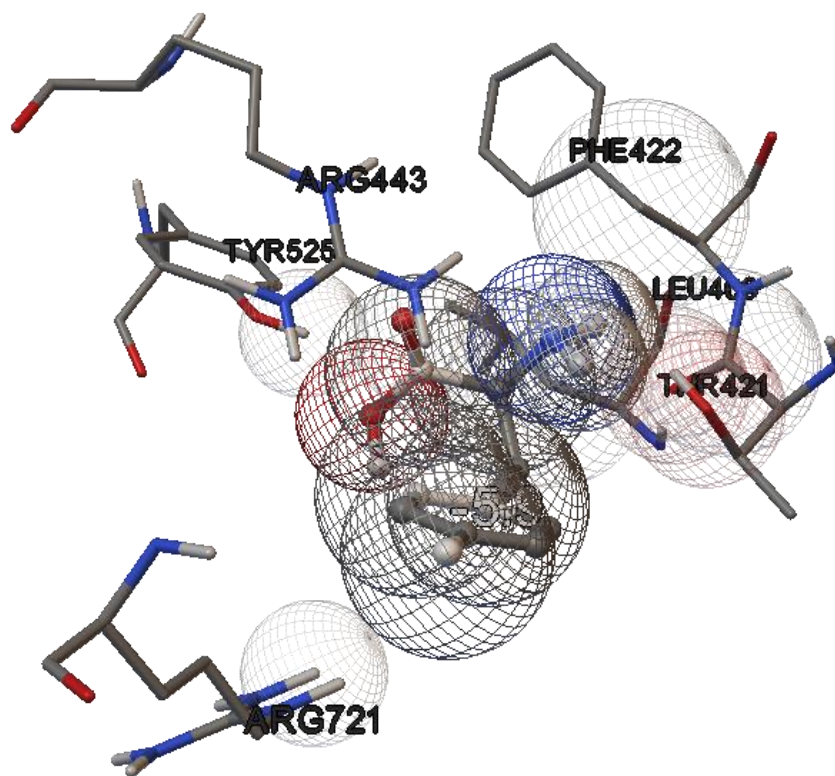


No	Name	Retention Time	Area	% Area	Height
1	(S)-2-amino-5-(3,4-difluorophenyl)-2-methylpent-4-ynoic acid <b>3f</b>	7,112	78091517	100	1547612

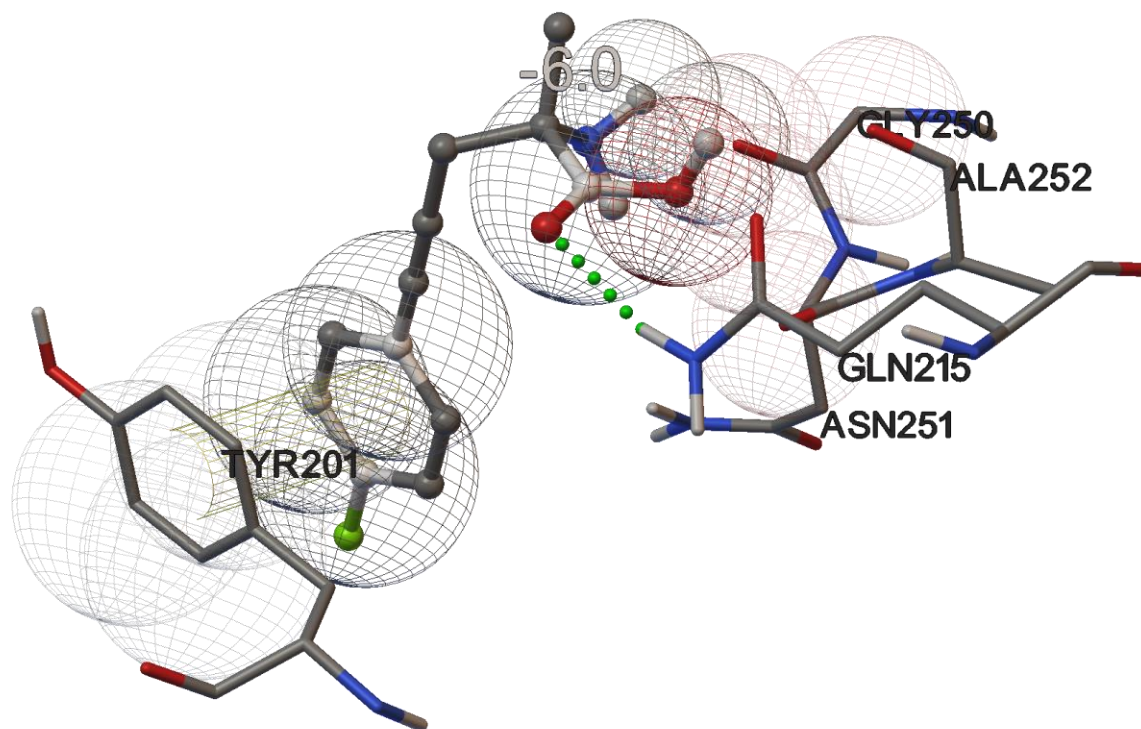
**Figure S20.** HPLC trace of the enantiopure AA (*S*)-**3f**



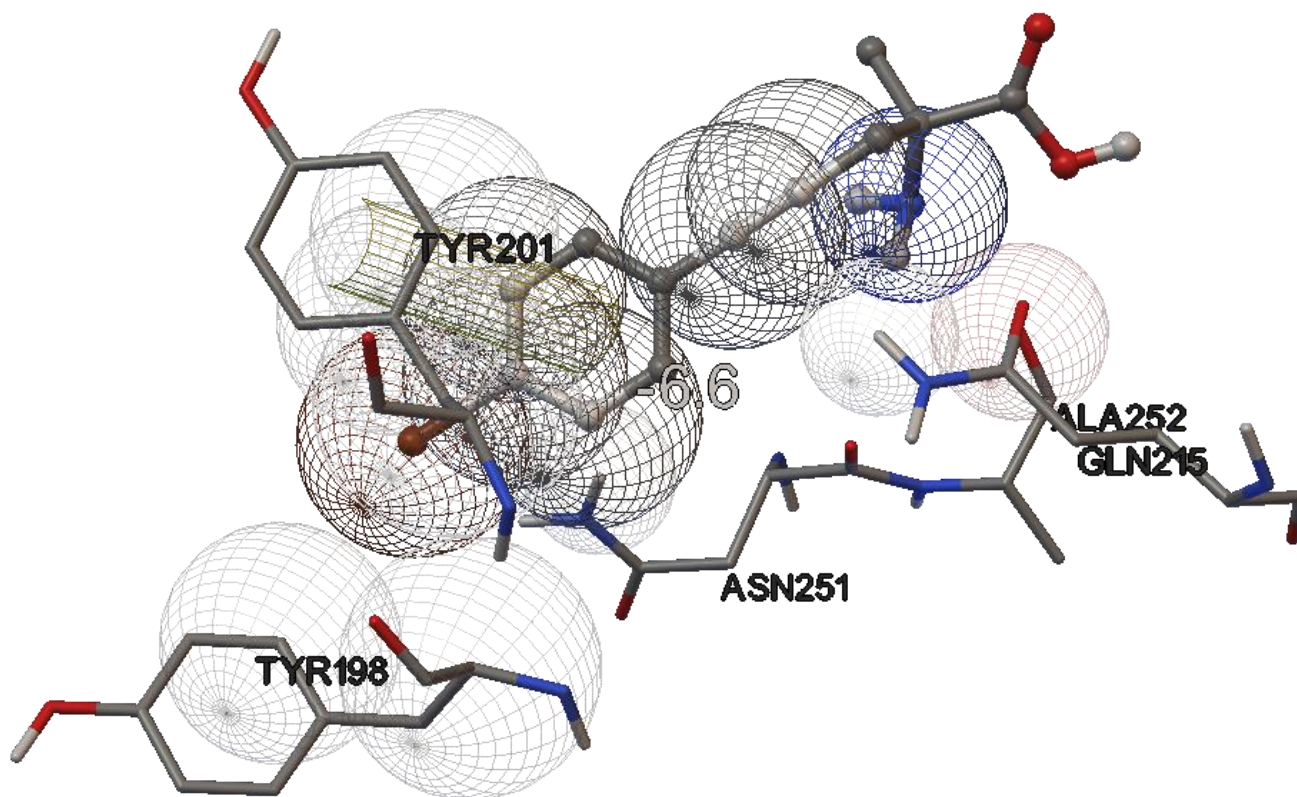
**Figure S21.** Molecular docking of the enantiopure AA (*S*)-3a



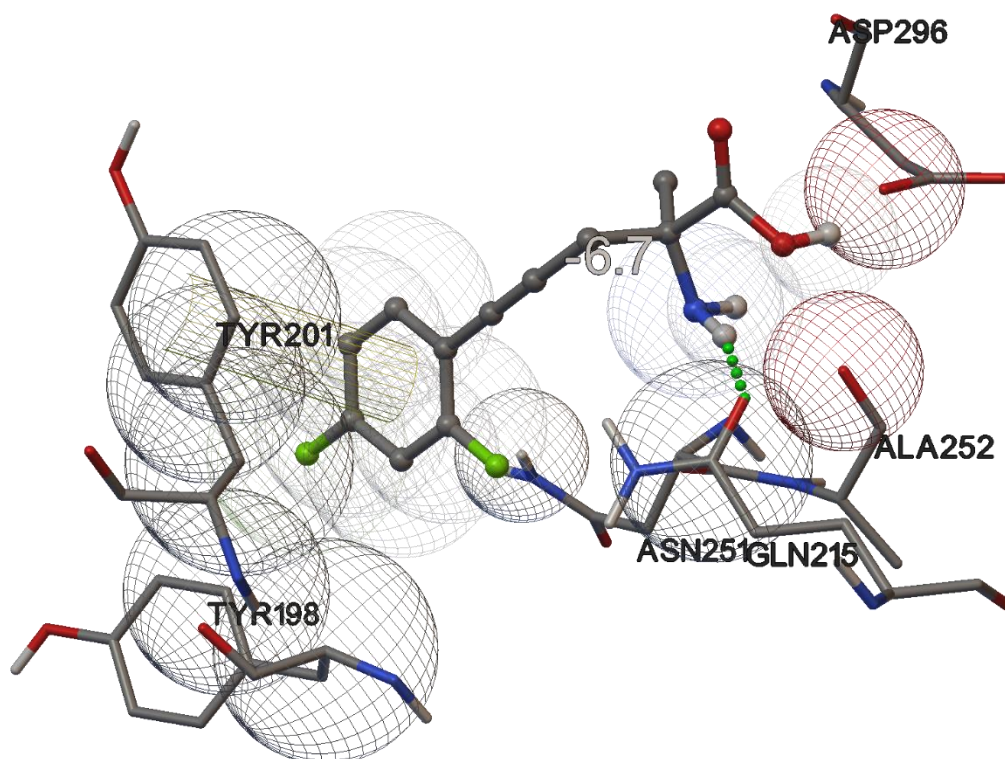
**Figure S22.** Molecular docking of the enantiopure AA (*S*)-3b



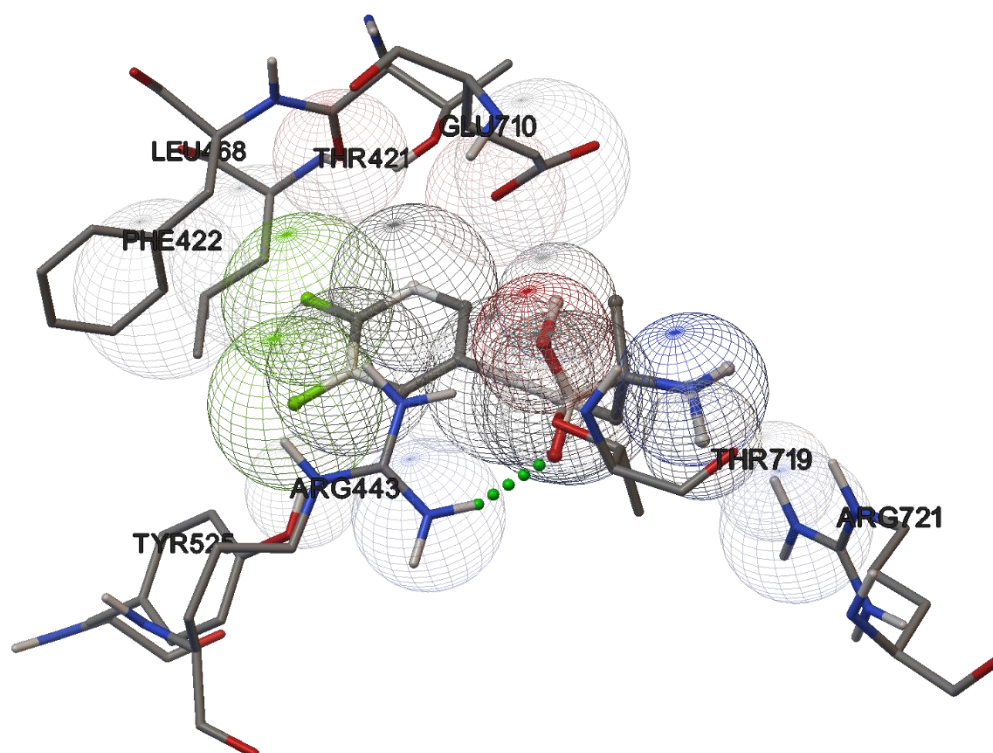
**Figure S23.** Molecular docking of the enantiopure AA (*S*)-3c



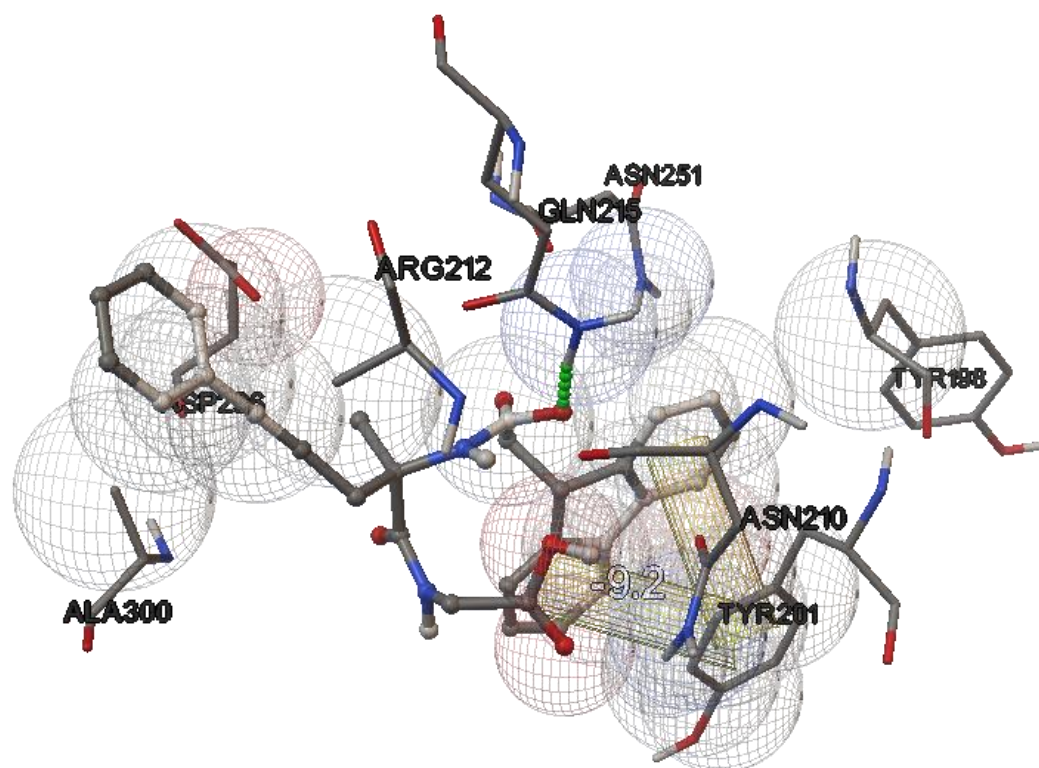
**Figure S24.** Molecular docking of the enantiopure AA (*S*)-3d



**Figure S25.** Molecular docking of the enantiopure AA (*S*)-3e



**Figure S26.** Molecular docking of the enantiopure AA (*S*)-3f



**Figure S27.** Molecular docking of the dipeptide 6