

Supporting Information

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Synthesis of ^{13}C labeled β -cyano-L-alanine

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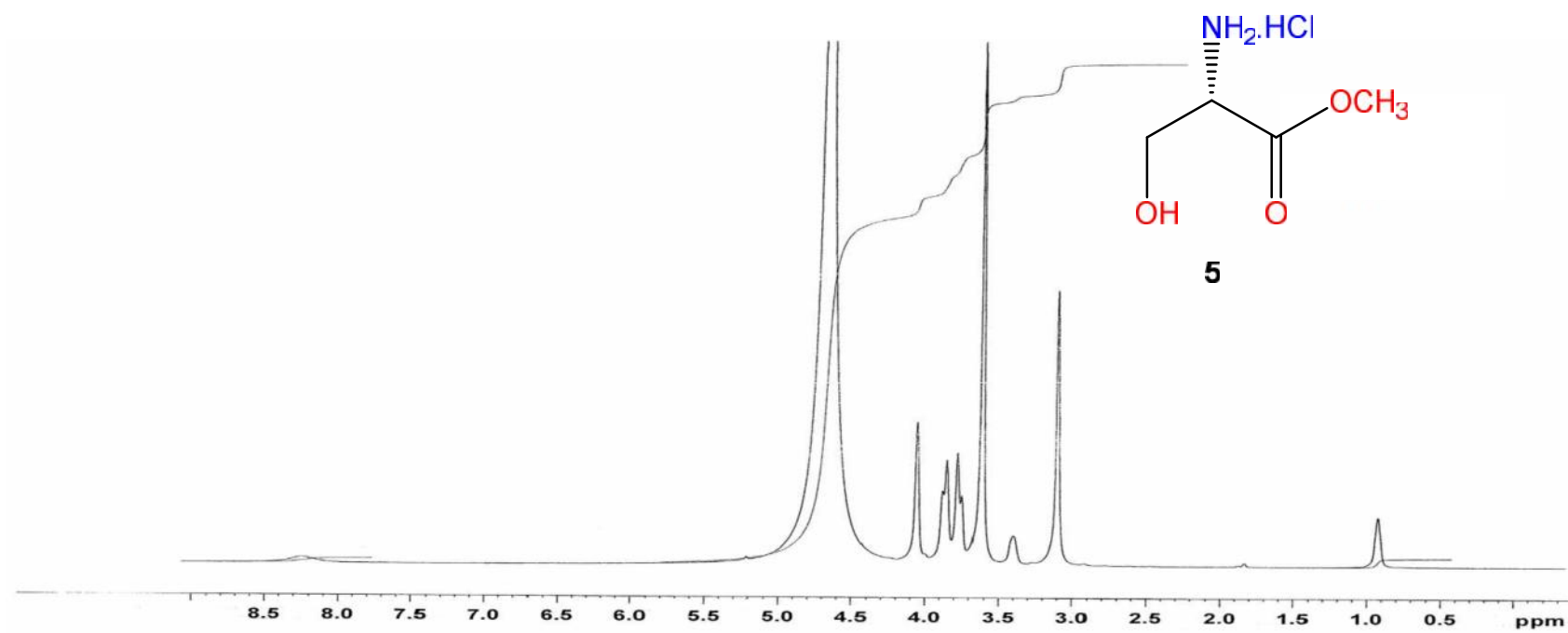
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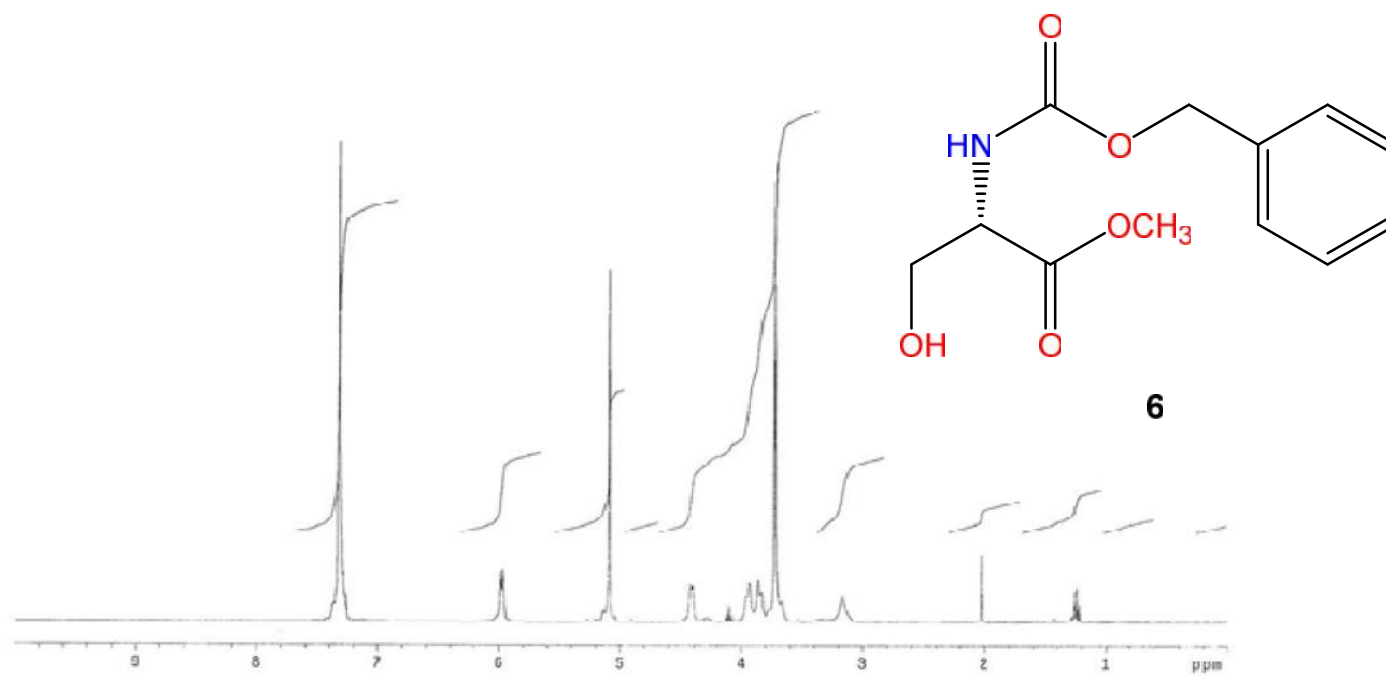
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HRMS Spectrum of ^{13}C labelled compounds 2	19

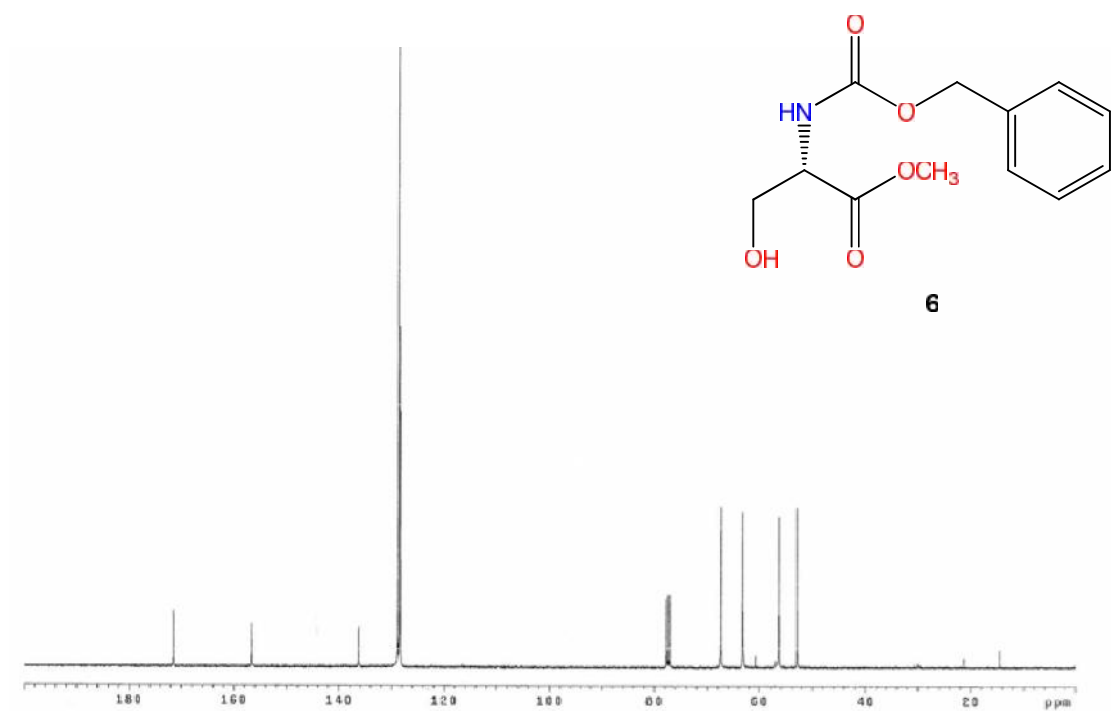
* Corresponding author: E-Mail: hsecen@atauni.edu.tr

All reagents were of commercial quality and were used as received:

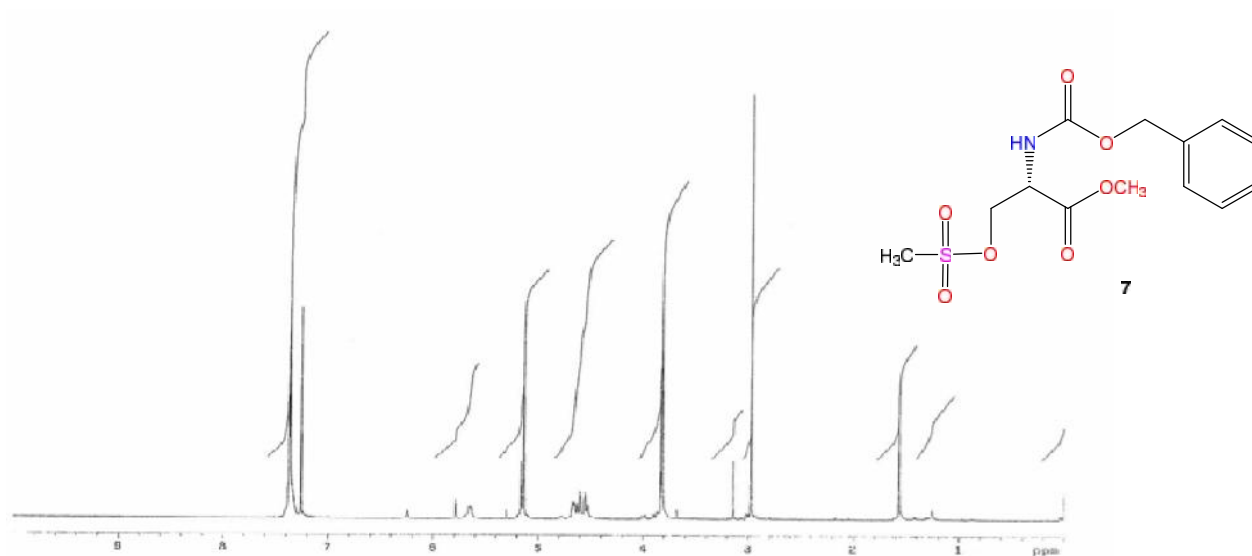
AcCl: Acetyl chloride, $\geq 98\%$, Merck, (822252.1000); PhCH₂O(CO)Cl: benzyl chloroformate, 95%, Aldrich, (119938); NaHCO₃: sodium bicarbonate, $\geq 99.7\%$, Sigma-Aldrich, (31437); CH₃SO₂Cl: methanesulfonyl chloride, $>99.5\%$, Aldrich, (471259); NE₃: triethylamine, $\geq 99.5\%$, Fluka, (90340); NaCN: sodium cyanide, $\geq 95.0\%$, Merck, (1.06437.1000); DMF: N,N-dimethylformamide, anhydrous, 99.8%, Sigma-Aldrich, (227056); KOH: potassium hydroxide, Sigma-Aldrich, (06005); HCl: hydrochloric acid, $\geq 37\%$, Sigma-Aldrich, (30721); Pd-C: palladium on carbon, Aldrich, (205699).

 $^1\text{H-N}$

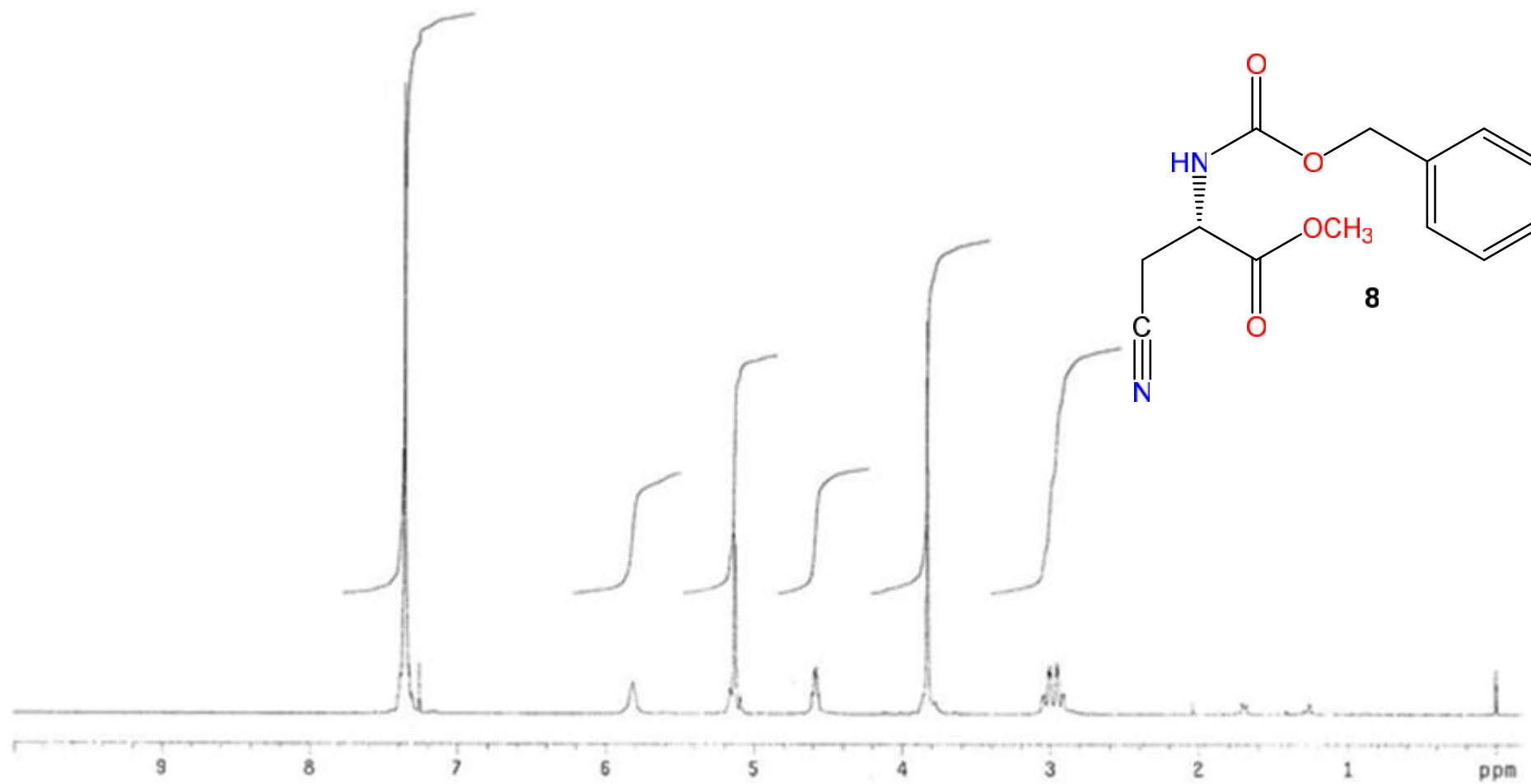




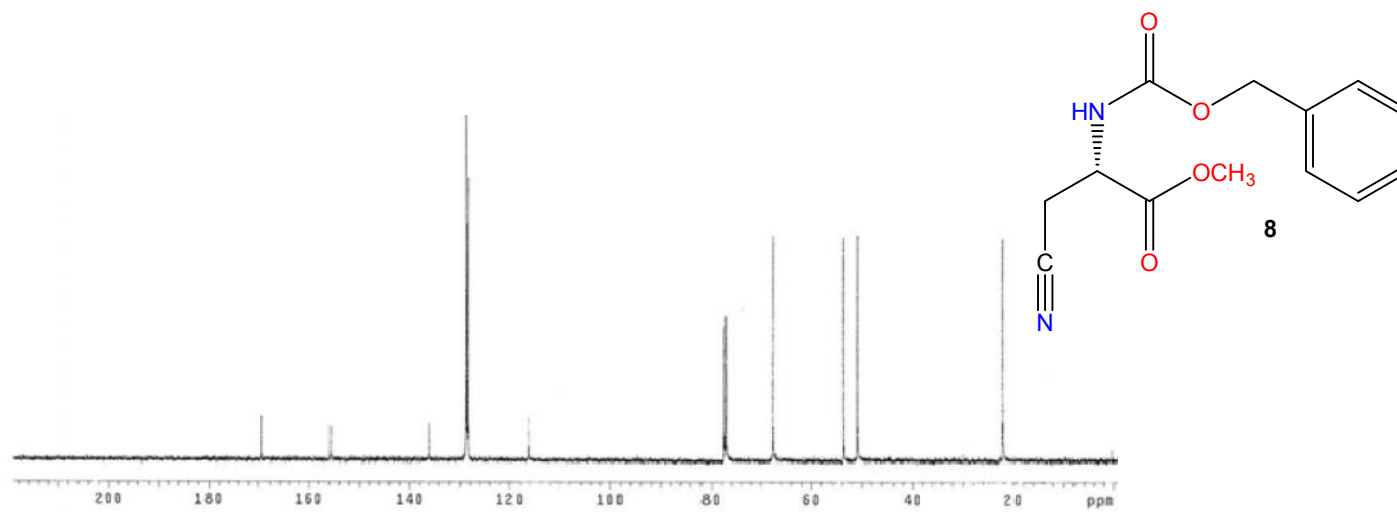
¹³C-NMR Spectrum of compound **6** (100 MHz, CDCl₃)



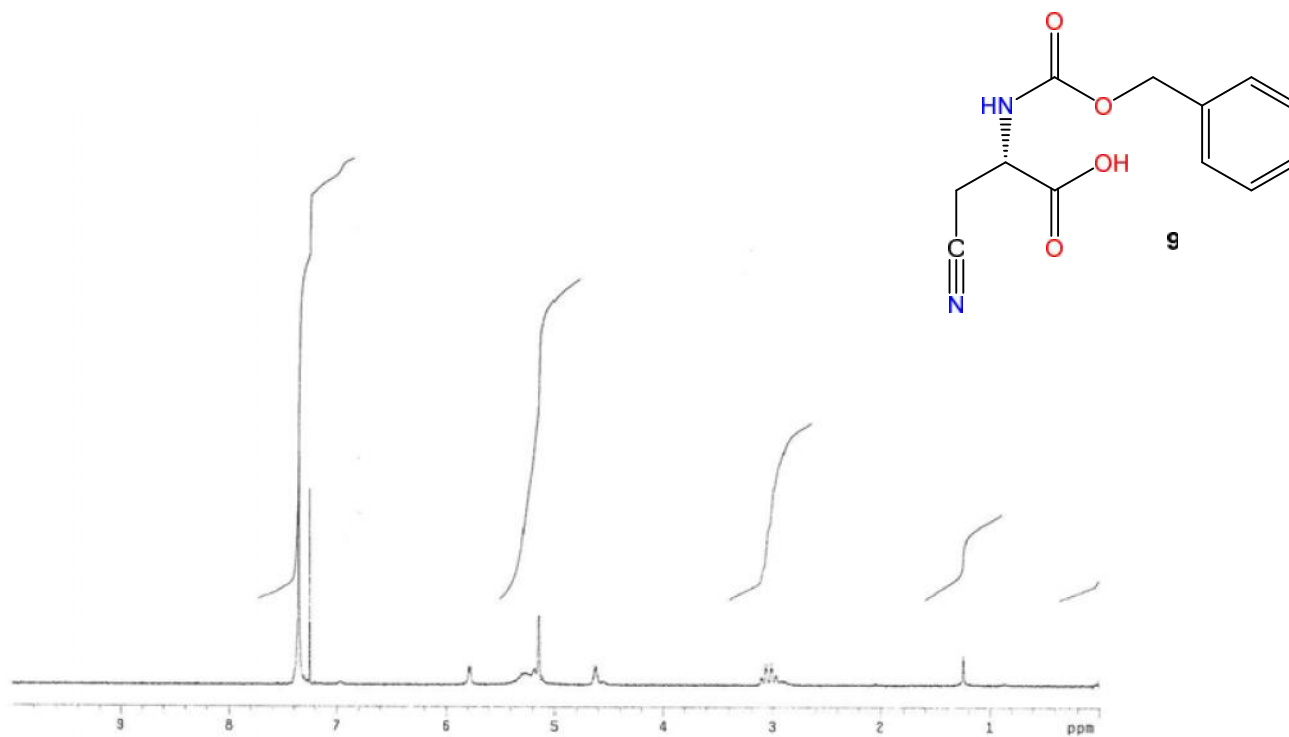
¹H-NMR Spectrum of compound 7 (400 MHz, CDCl₃).



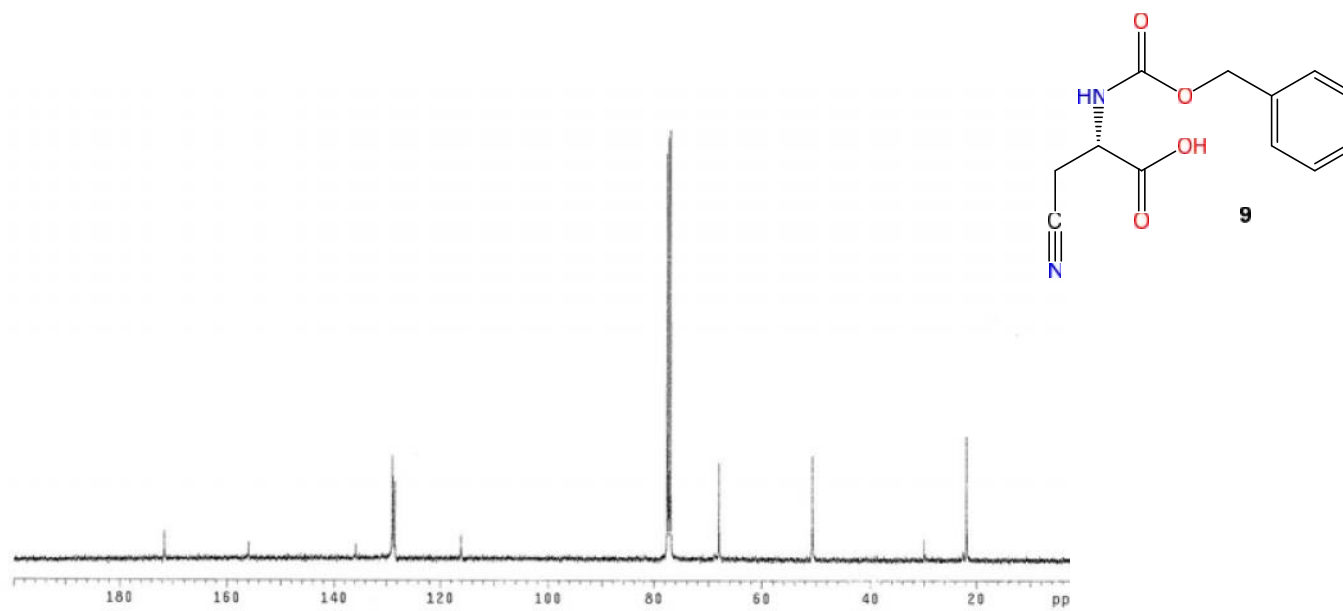
¹H-NMR Spectrum of compound **8** (400 MHz, CDCl₃).



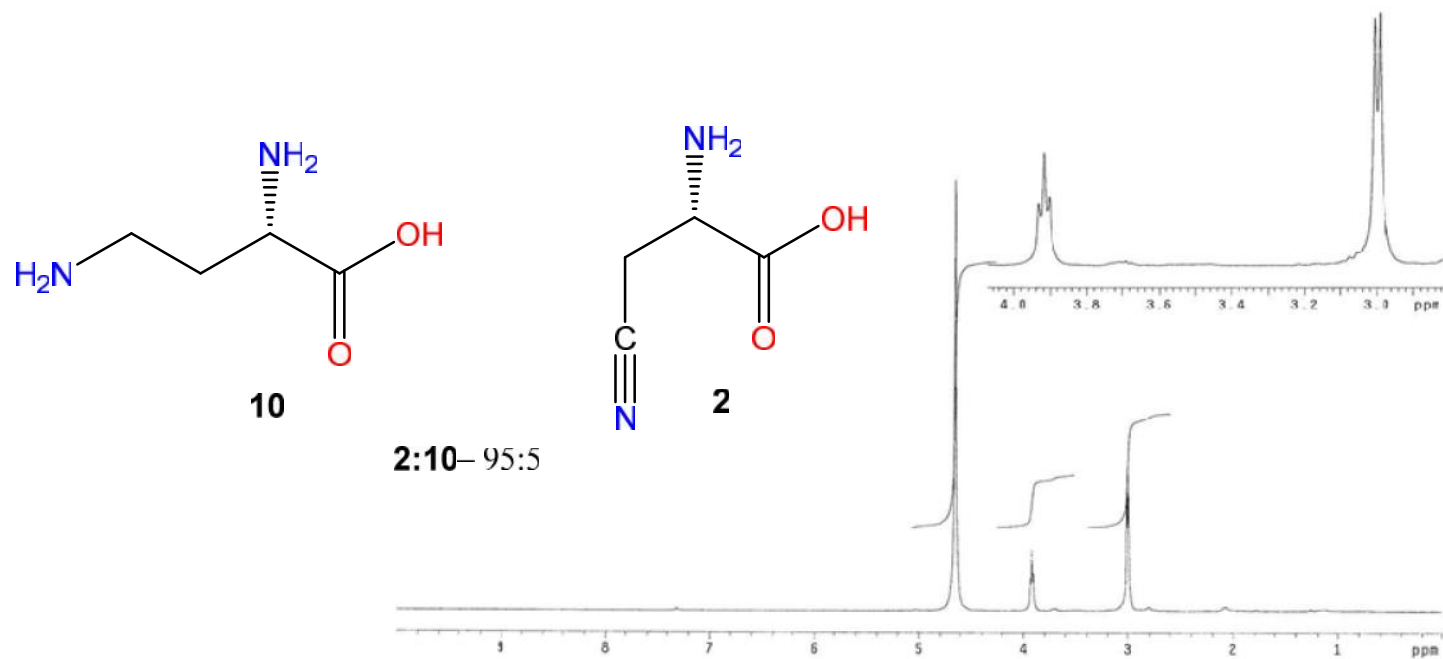
^{13}C -NMR Spectrum of compound **8** (100 MHz, CDCl_3).



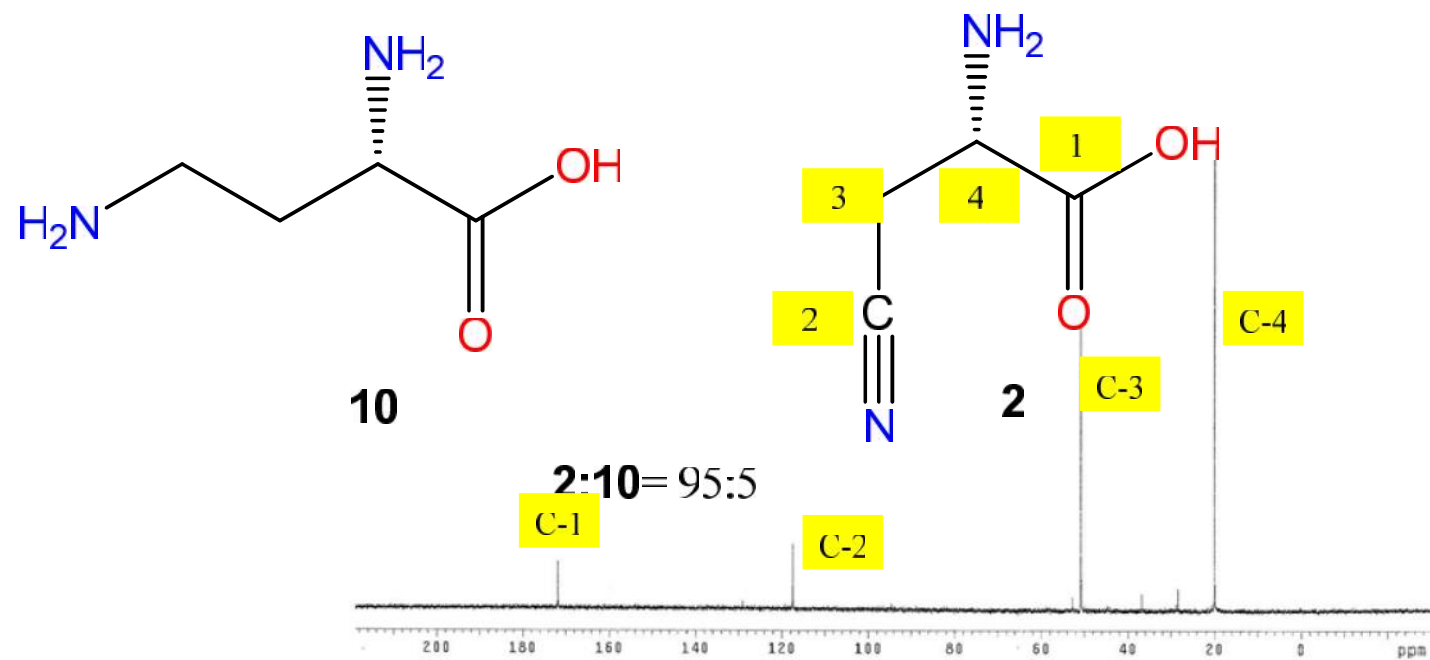
¹H-NMR Spectrum of compound **9** (400 MHz, CDCl₃).



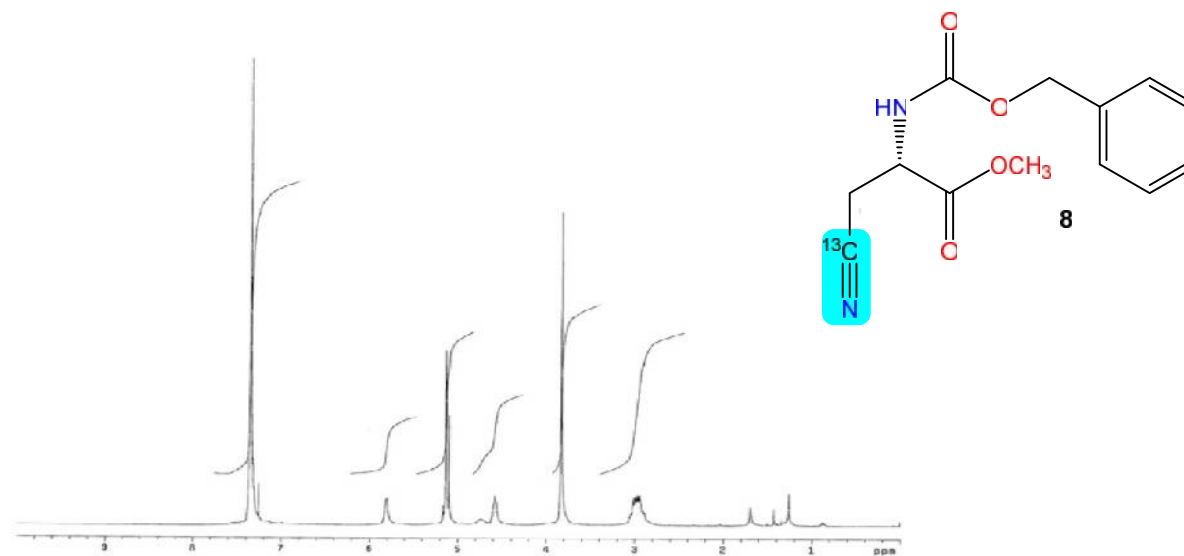
^{13}C -NMR Spectrum of compound **9** (100 MHz, CDCl_3).



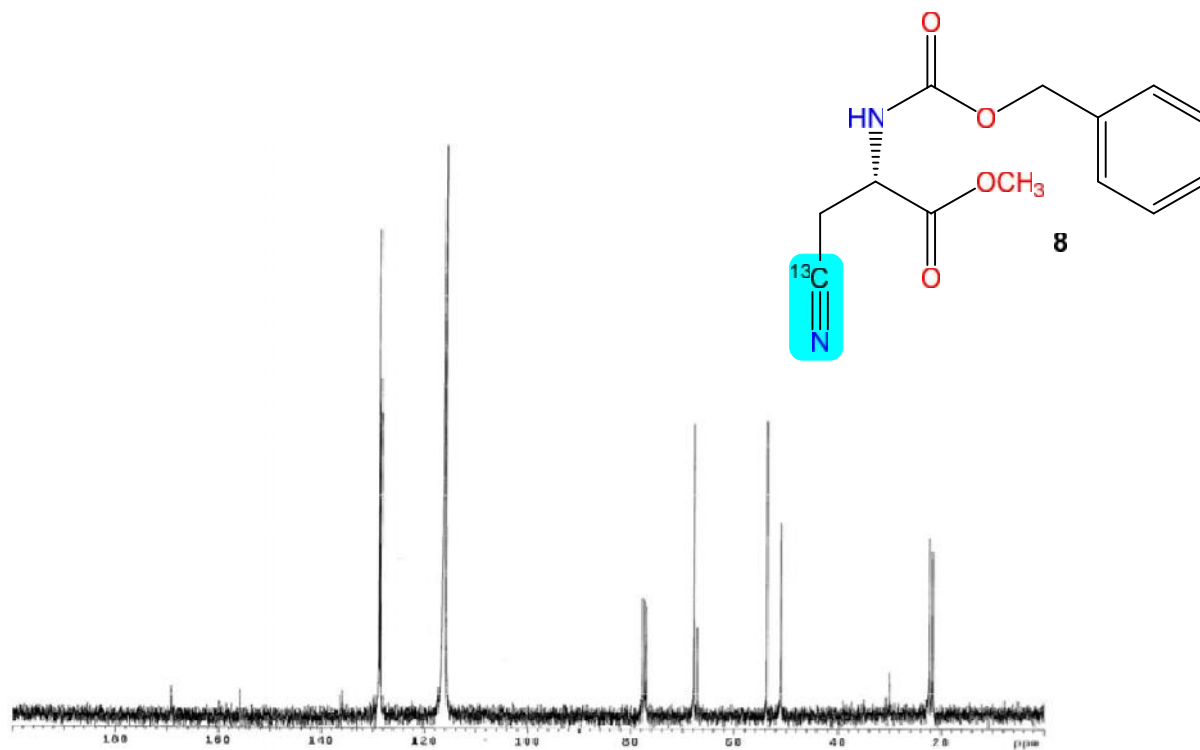
$^1\text{H-NMR}$ Spectrum of the mixture of compounds **2** and **10** (400 MHz, D_2O)



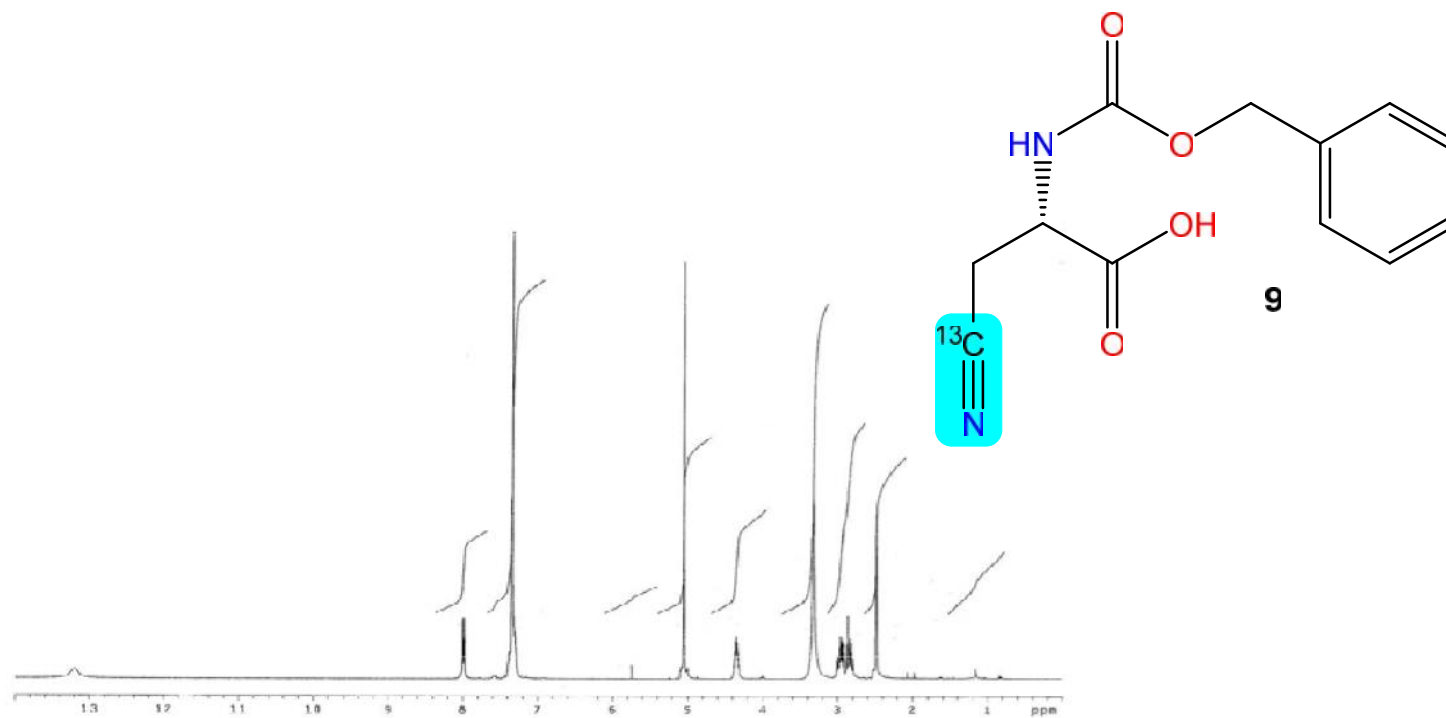
^{13}C -NMR Spectrum of the mixture of compounds **2** and **10** (100 MHz, D_2O)



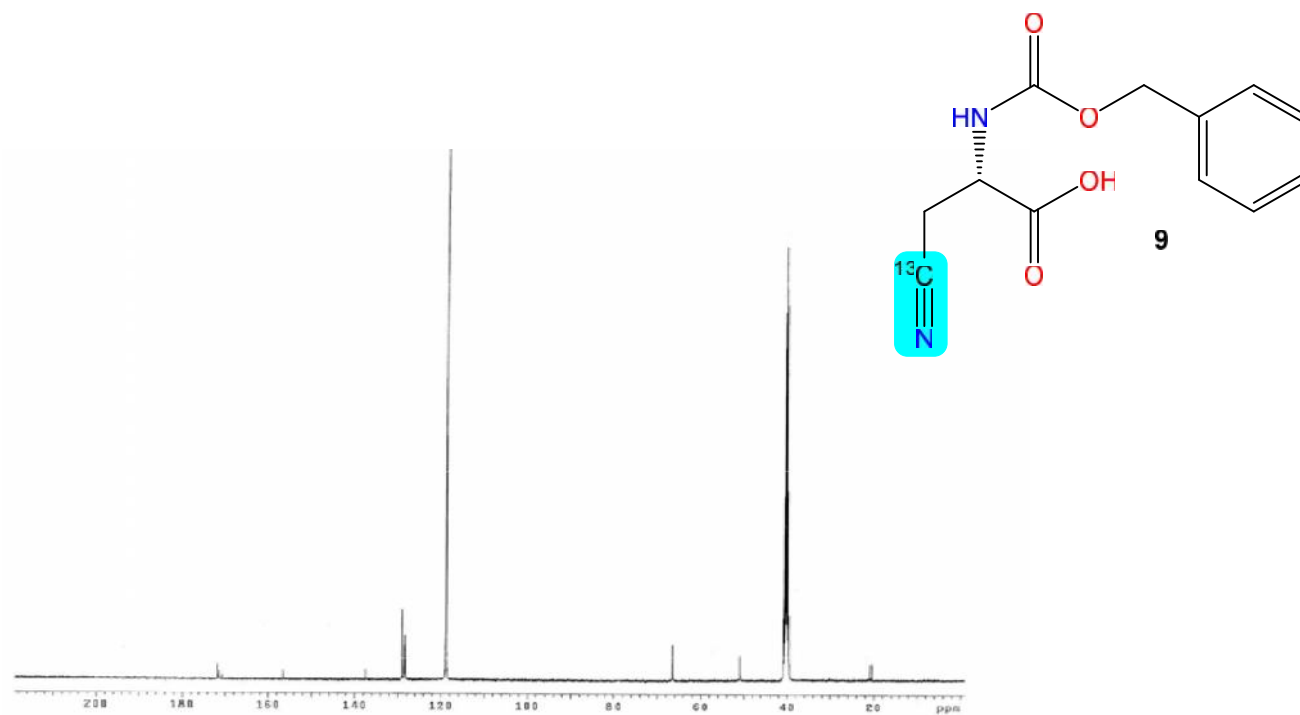
$^1\text{H-NMR}$ Spectrum of ^{13}C labelled compound **8** (400 MHz, CDCl_3).



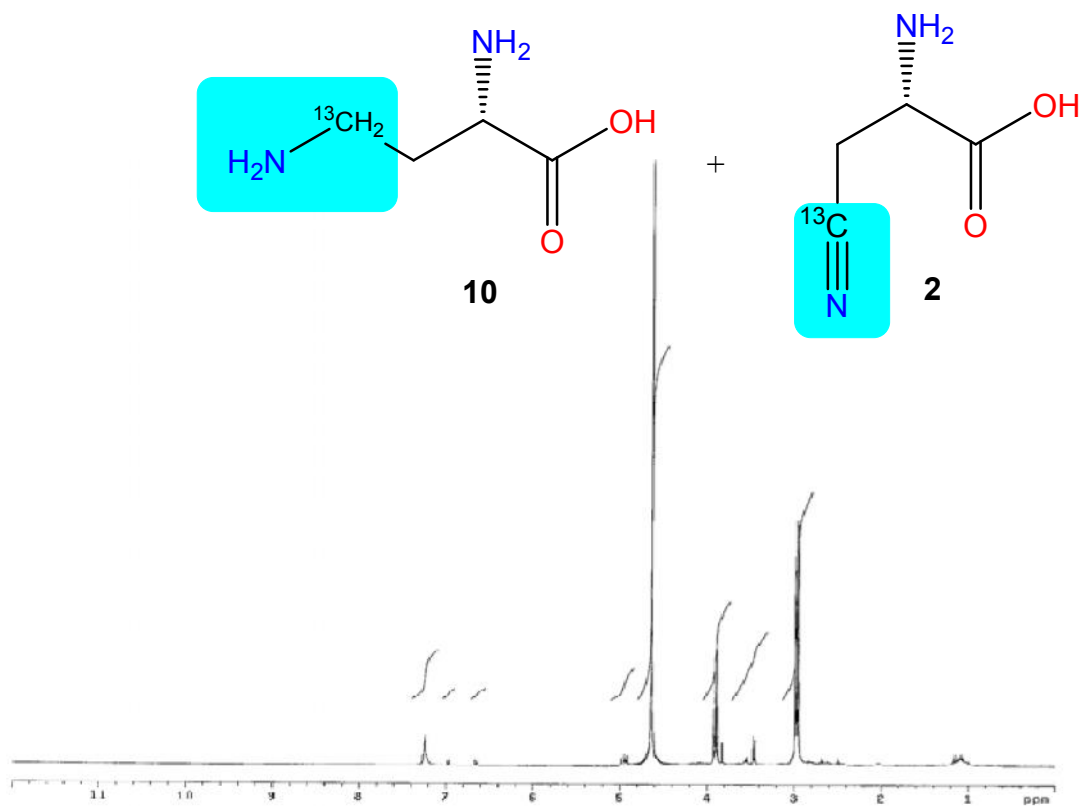
^{13}C -NMR Spectrum of ^{13}C labelled compound **8** (100 MHz, CDCl_3).



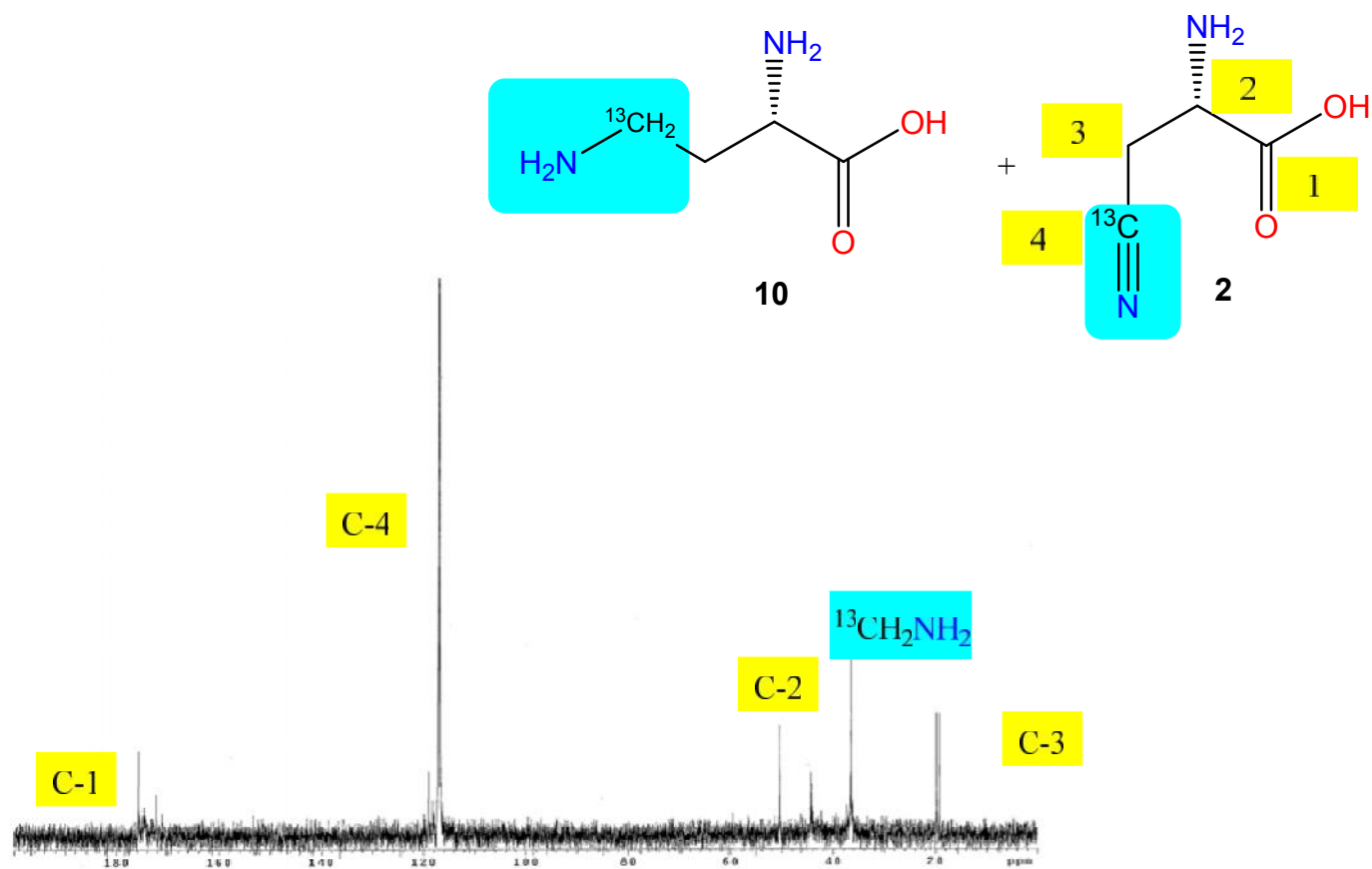
^1H -NMR Spectrum of ^{13}C labelled compound **9** (400 MHz, DMSO-d_6).



^{13}C -NMR Spectrum of ^{13}C labelled compound **9** (100 MHz, DMSO- d_6).

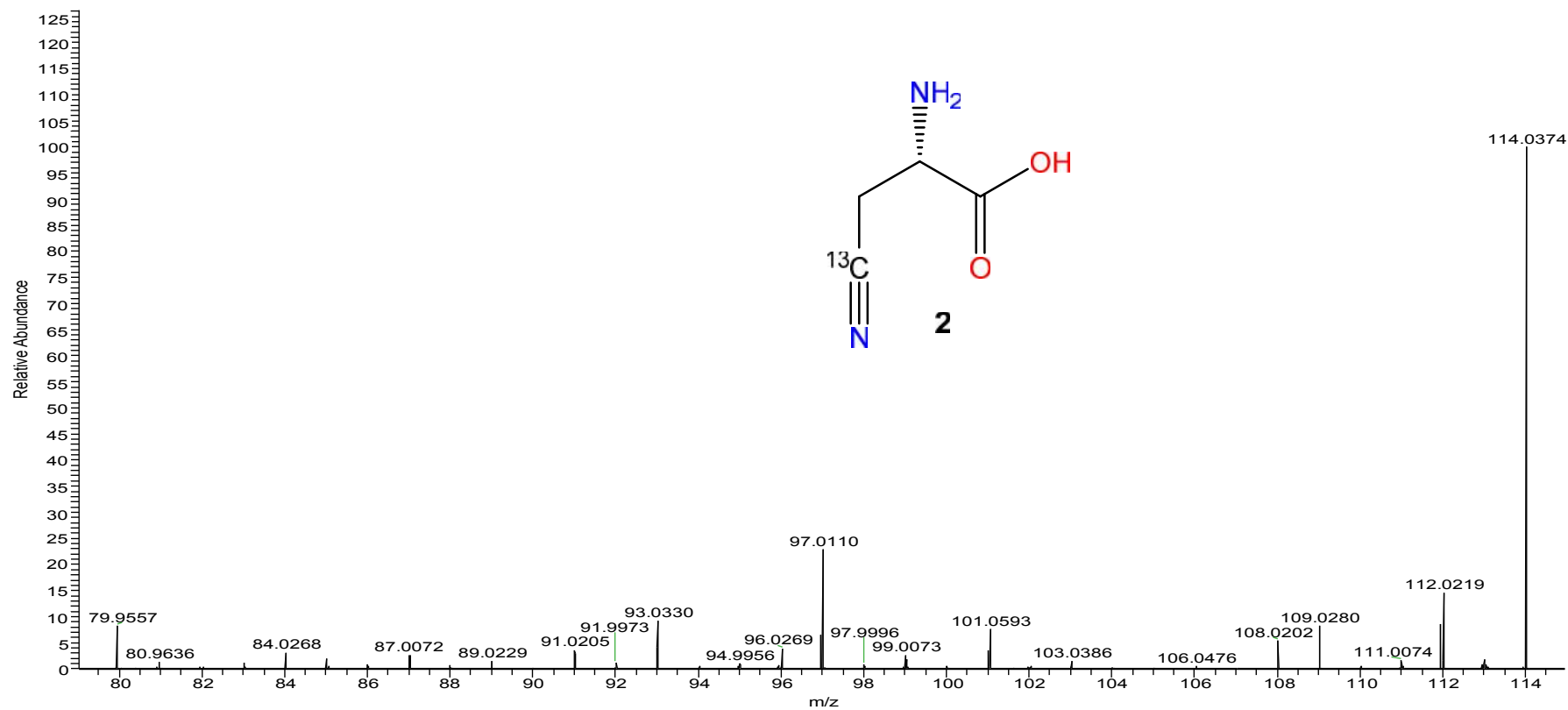


^1H -NMR Spectrum of the mixture of ^{13}C labelled compounds **2** and **10** (400 MHz, D_2O)



^{13}C -NMR Spectrum of the mixture of ^{13}C labelled compounds **2** and **10** (100 MHz, D_2O)

bca_13_#197 RT: 0.46 AV: 1 NL: 1.42E7
T: FTMS - p ESI Full ms [75.00-200.00]



m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
114.0379		-4.72	3.5	C3 [13]C H5 O2 N2

HRMS of ^{13}C labelled compound 2.

HRMS Spectrum of ^{13}C labelled compounds 2

