

Supporting Information

Applications of Convertible Isonitriles in the Ligation and Macrocyclization of Multicomponent Reaction-Derived Peptides and Depsipeptides

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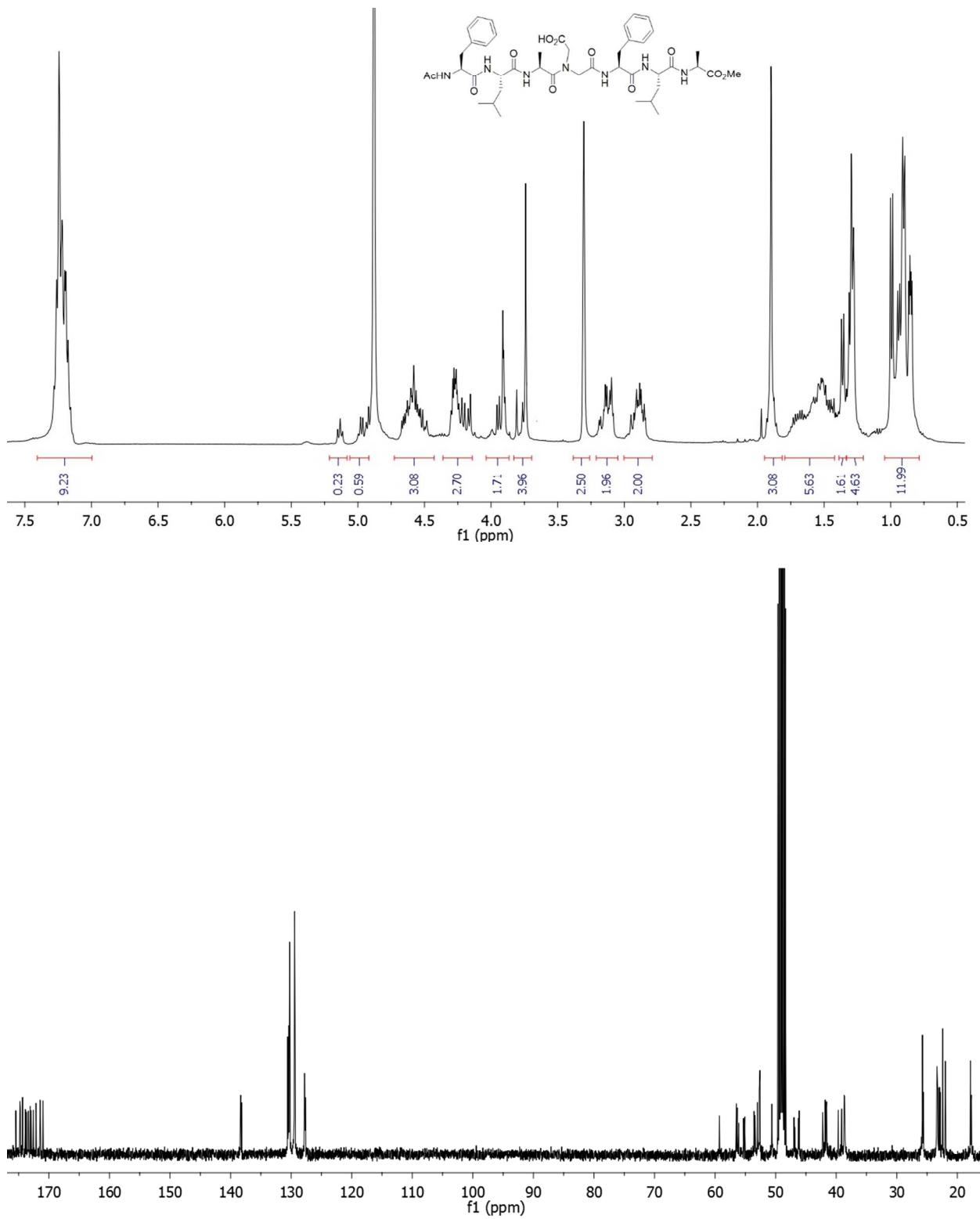


Figure 1. 400 MHz NMR spectra of peptide **8** in CD₃OD.

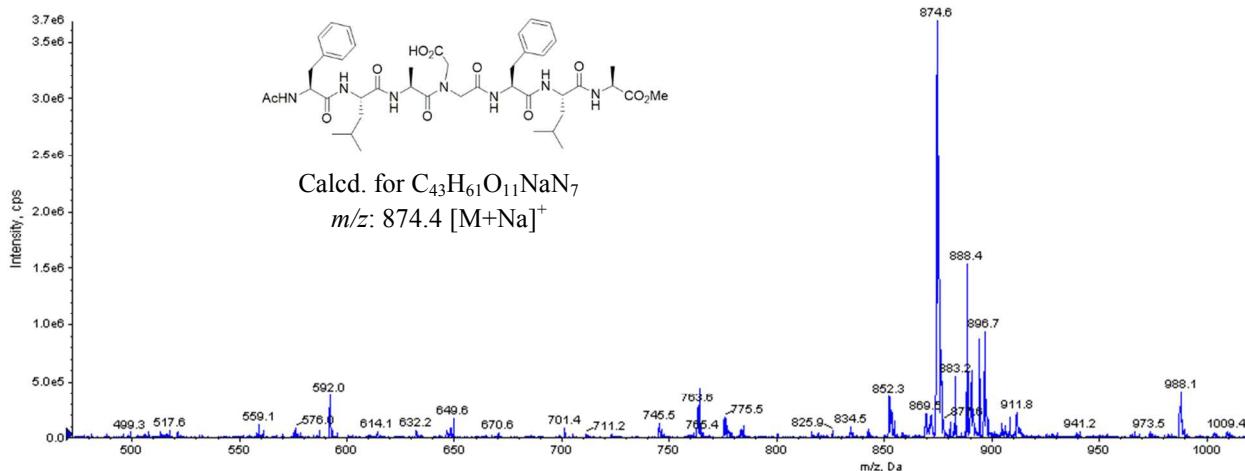


Figure 2. ESI-MS analysis of peptide 8.

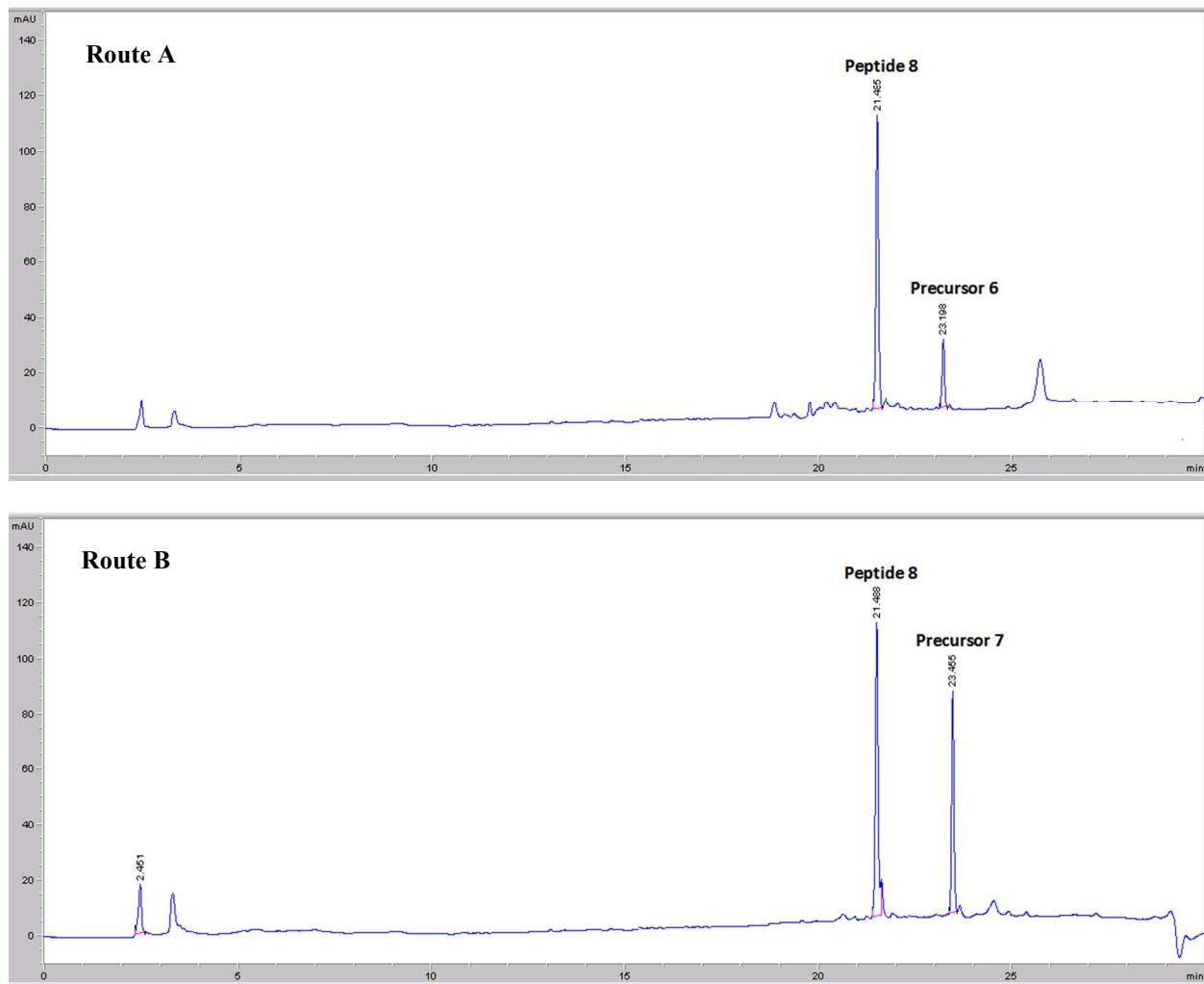


Figure 3. HPLC chromatogram of crude peptide 8 as obtained by routes A and B.

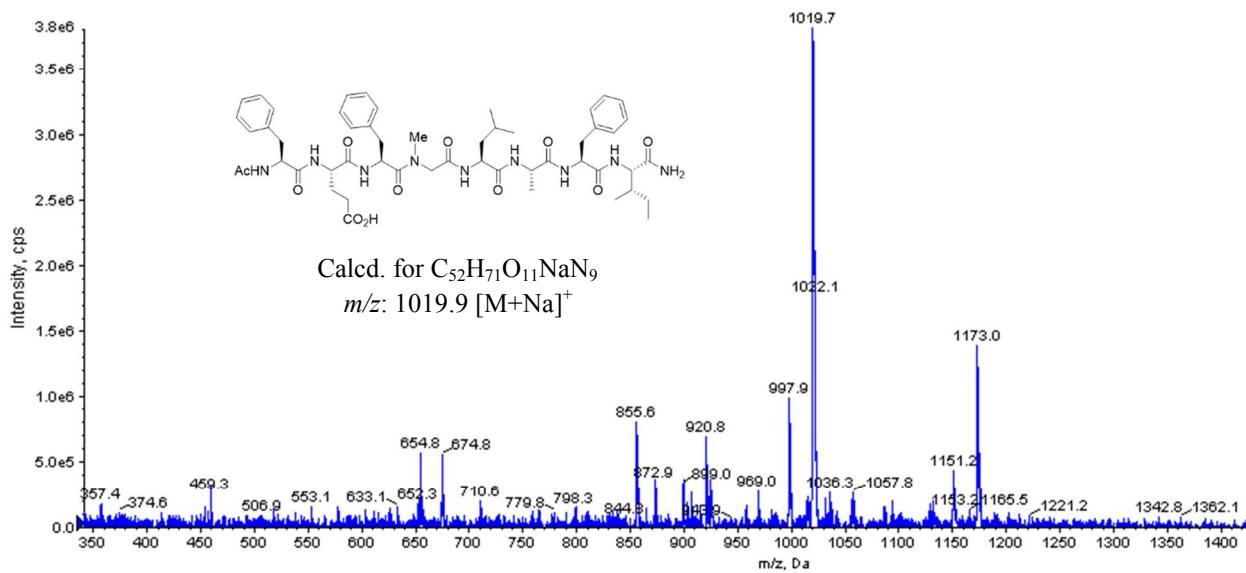


Figure 4. ESI-MS analysis of peptide 12.

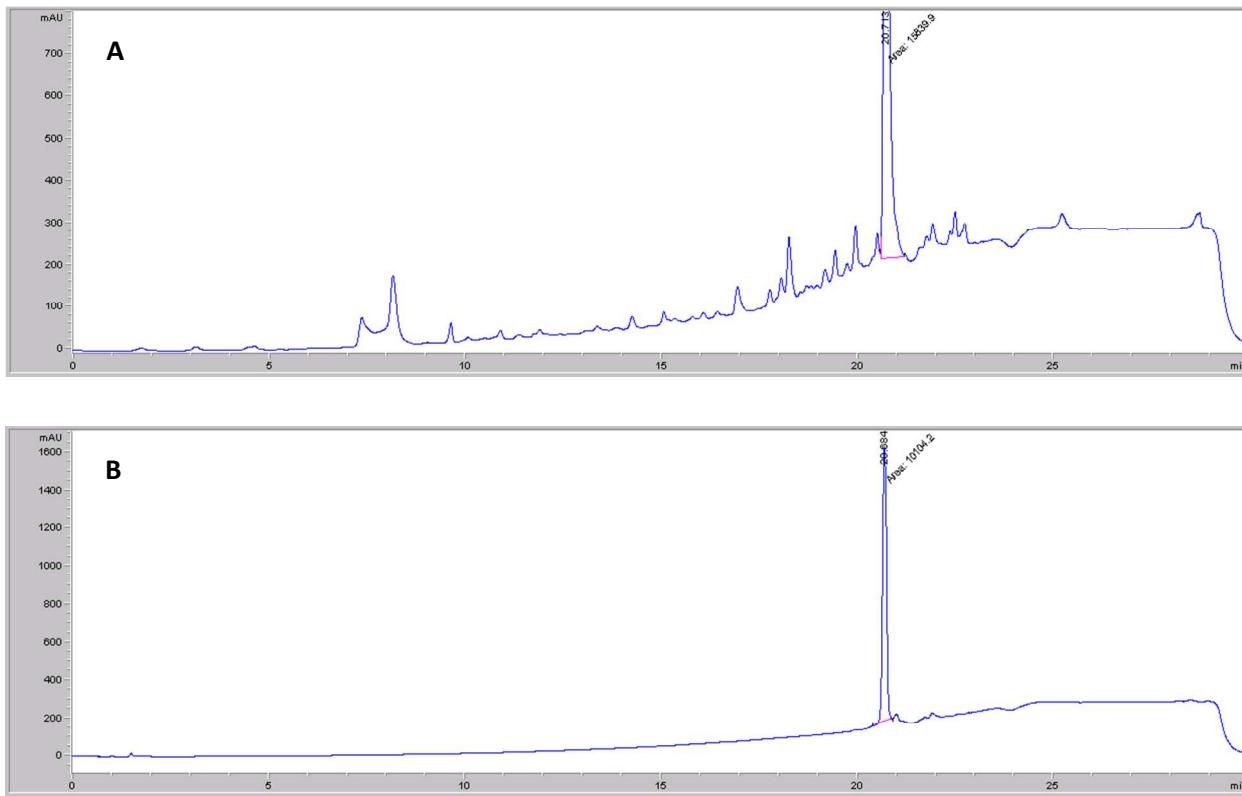
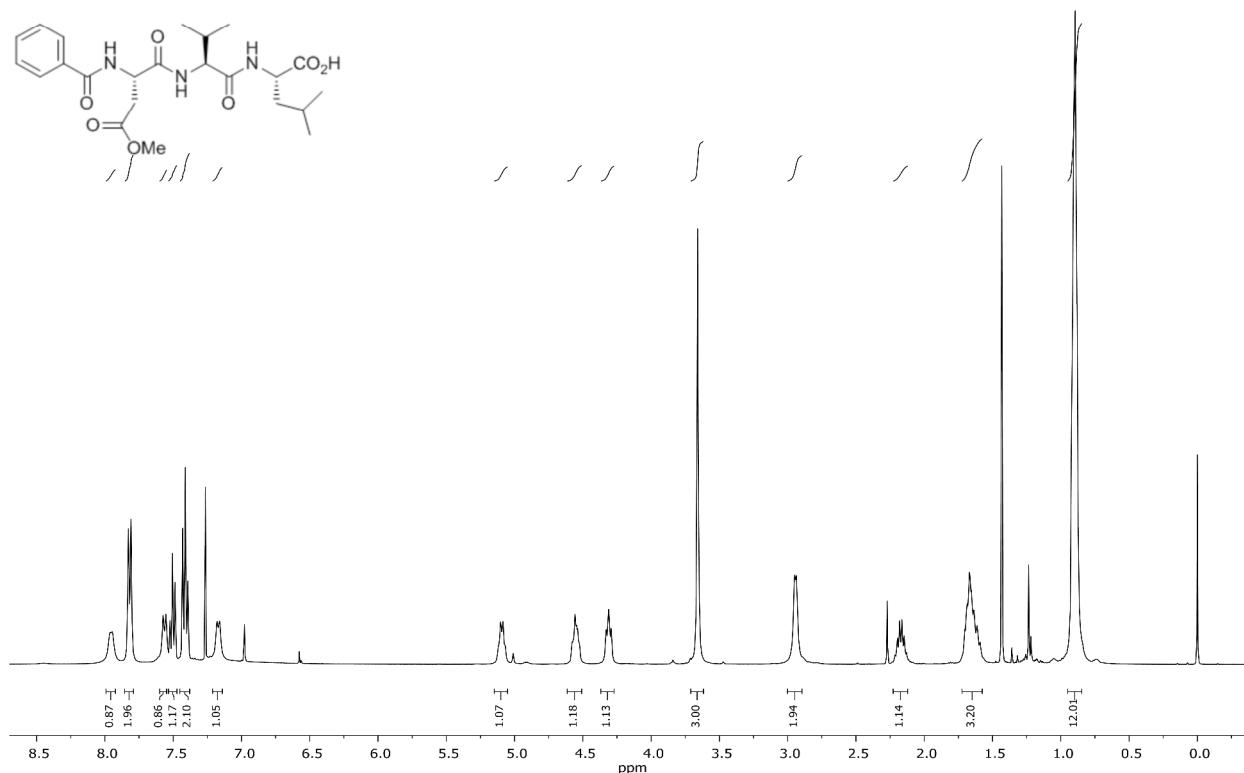


Figure 5. HPLC chromatograms of crude (A) and pure (B) peptide 12.

CMM194_PROTON_01
CMM194/CDCl₃/1H
Chavez 20160114_09



CMM194_CARBON_02
CMM194/CDCl₃/13C
Chavez 20160114_09

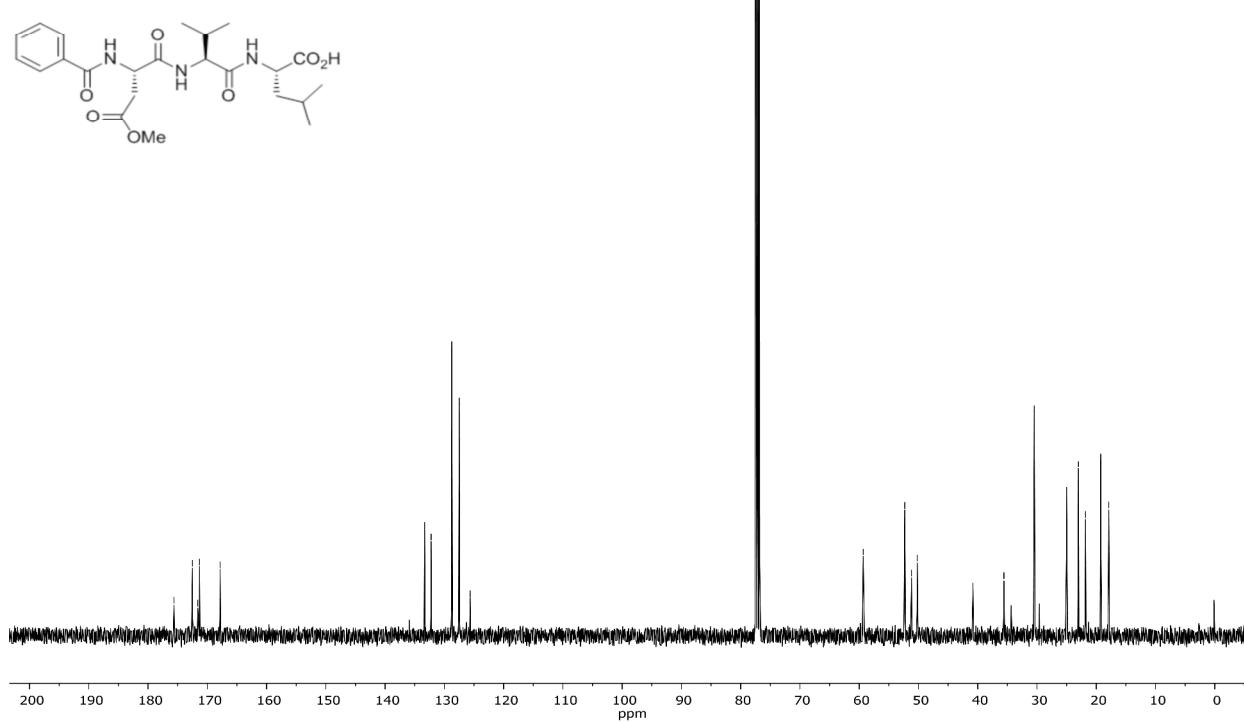


Figure 6. 400 MHz NMR spectra of peptide 13 in CDCl₃.

CMM194_neg #12 RT: 0.05 AV: 1 NL: 2.51E6
T: FTMS - p ESI Full ms [50.00-2000.00]

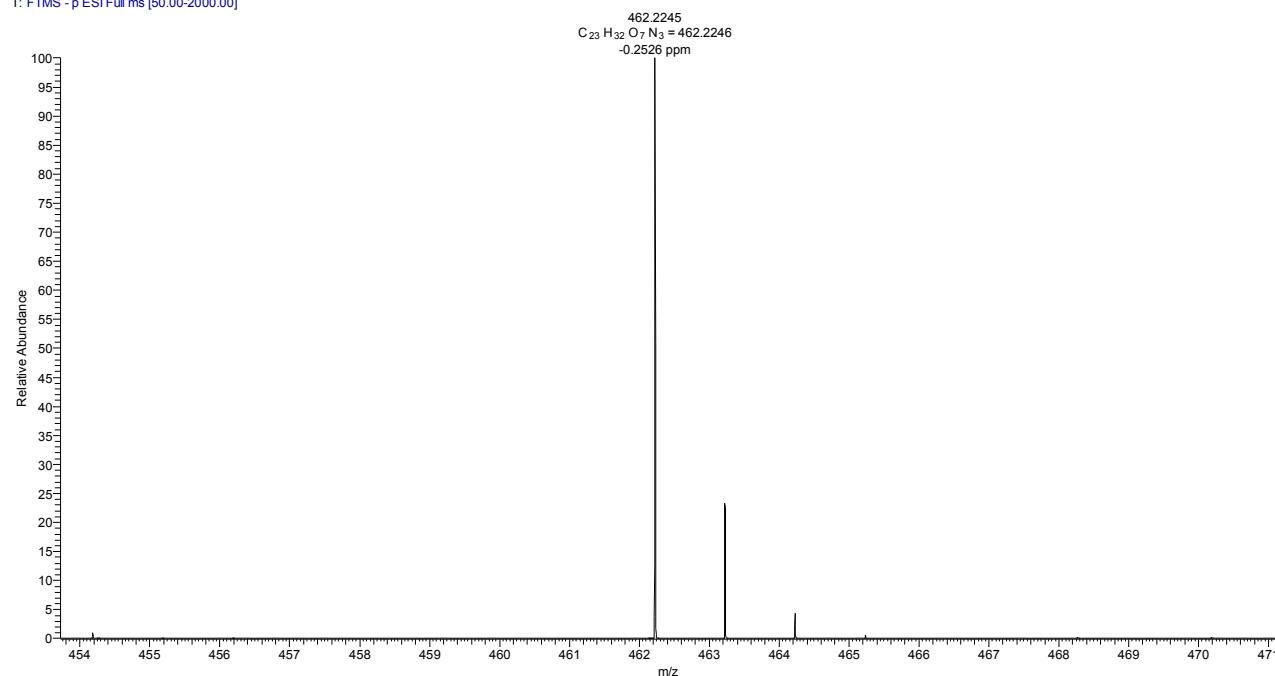


Figure 7. ESI-MS analysis of peptide **13**.

CMM210_neg #3-38 RT: 0.04-0.75 AV: 36 NL: 5.26E6
T: FTMS - p ESI Full ms [50.00-2000.00]

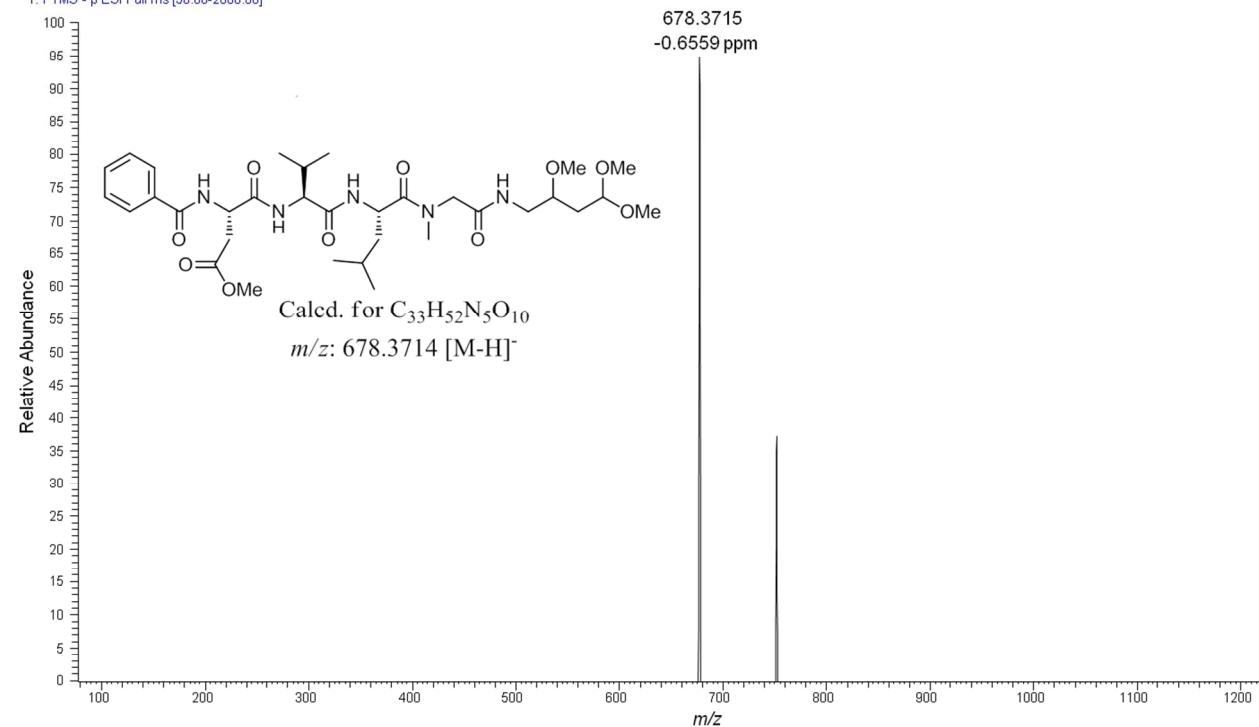


Figure 8. ESI-MS analysis of peptide **14**.

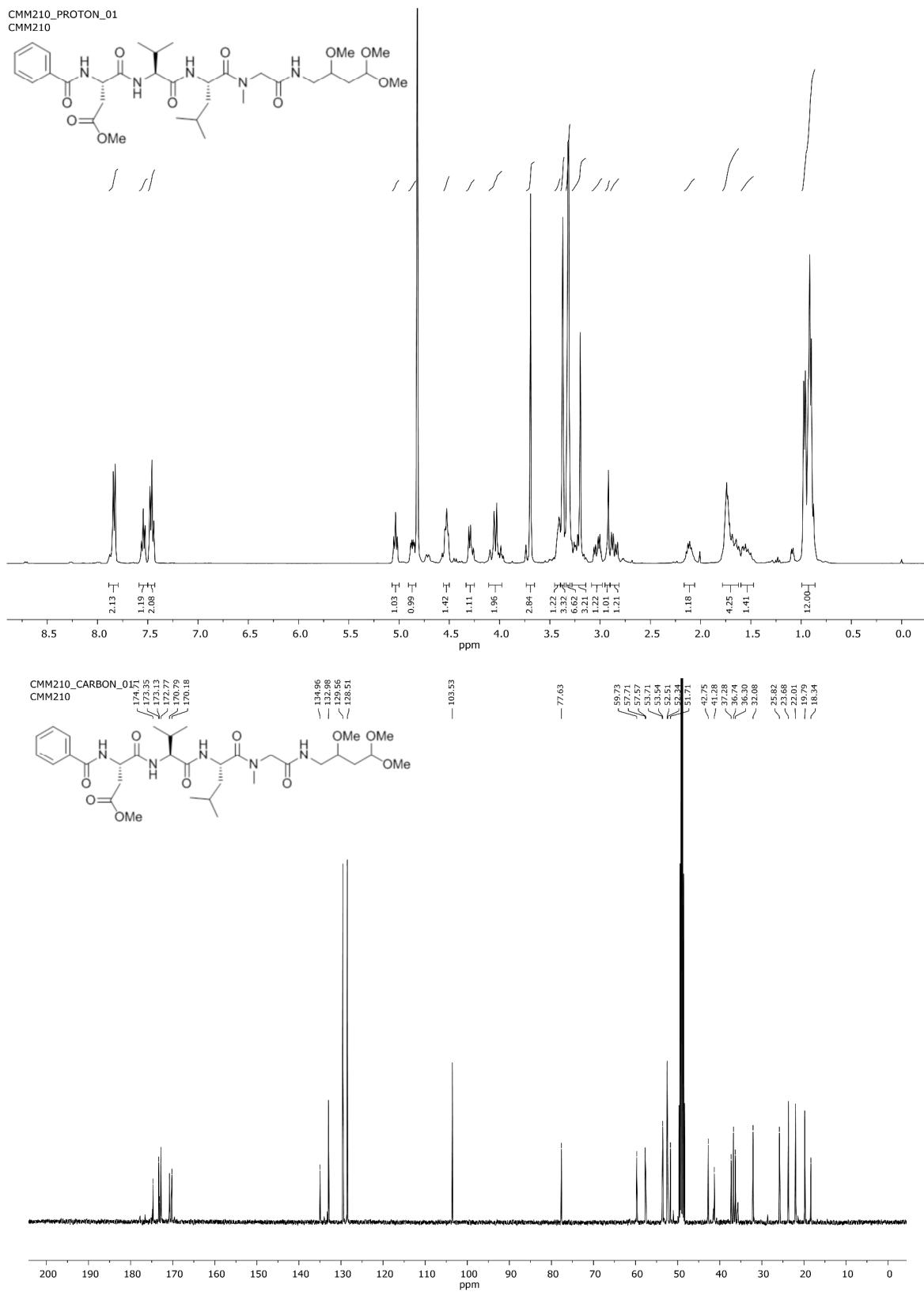


Figure 9. 400 MHz NMR spectra of peptide **14** in CD₃OD.

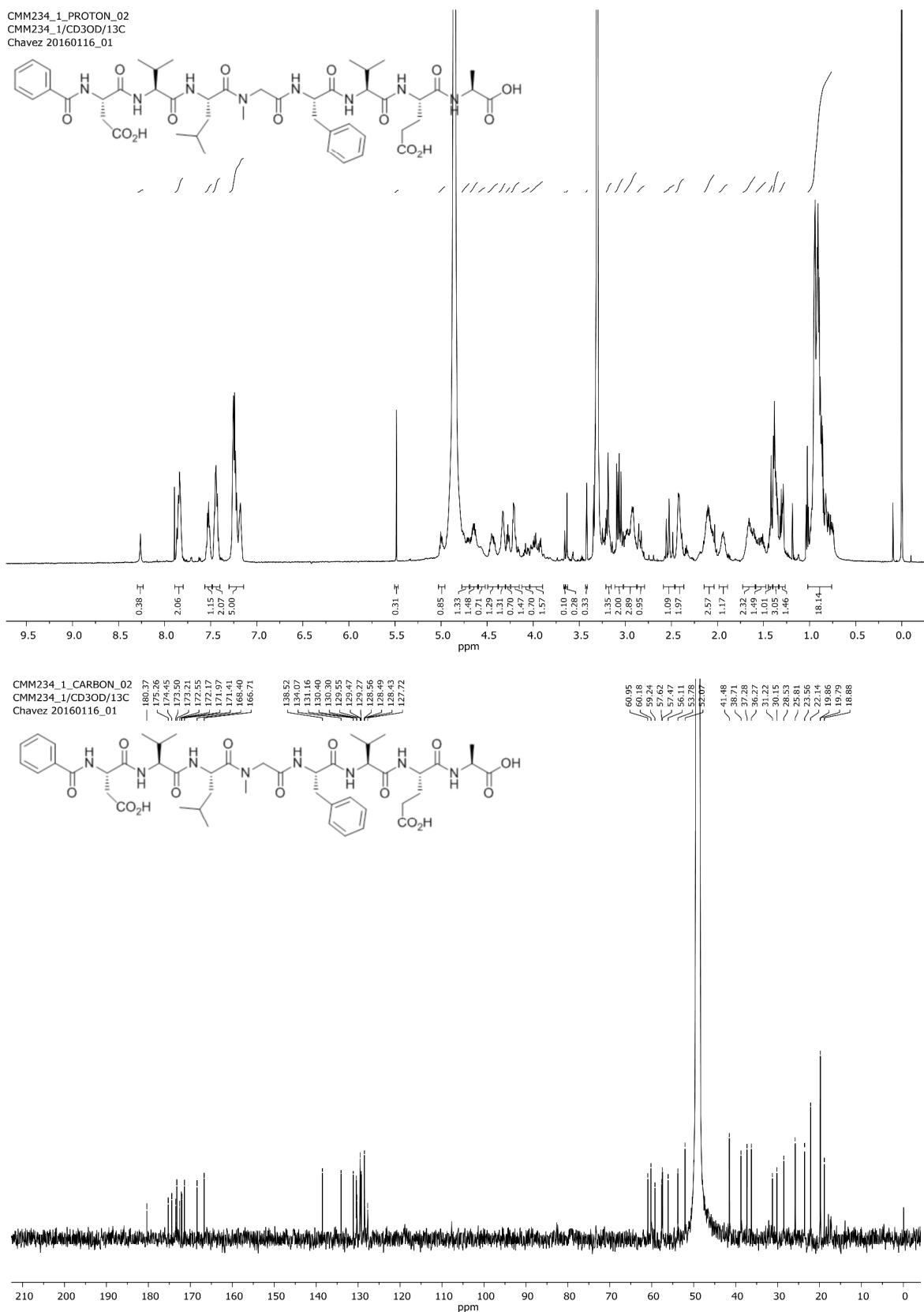


Figure 10. 600 MHz NMR spectra of peptide **16** in CD₃OD.

CMM234_2_nMS2_965 #4233 RT: 13.28 AV: 1 NL: 1.61E7
F: FTMS - p ESI Full ms [250.00-1500.00]

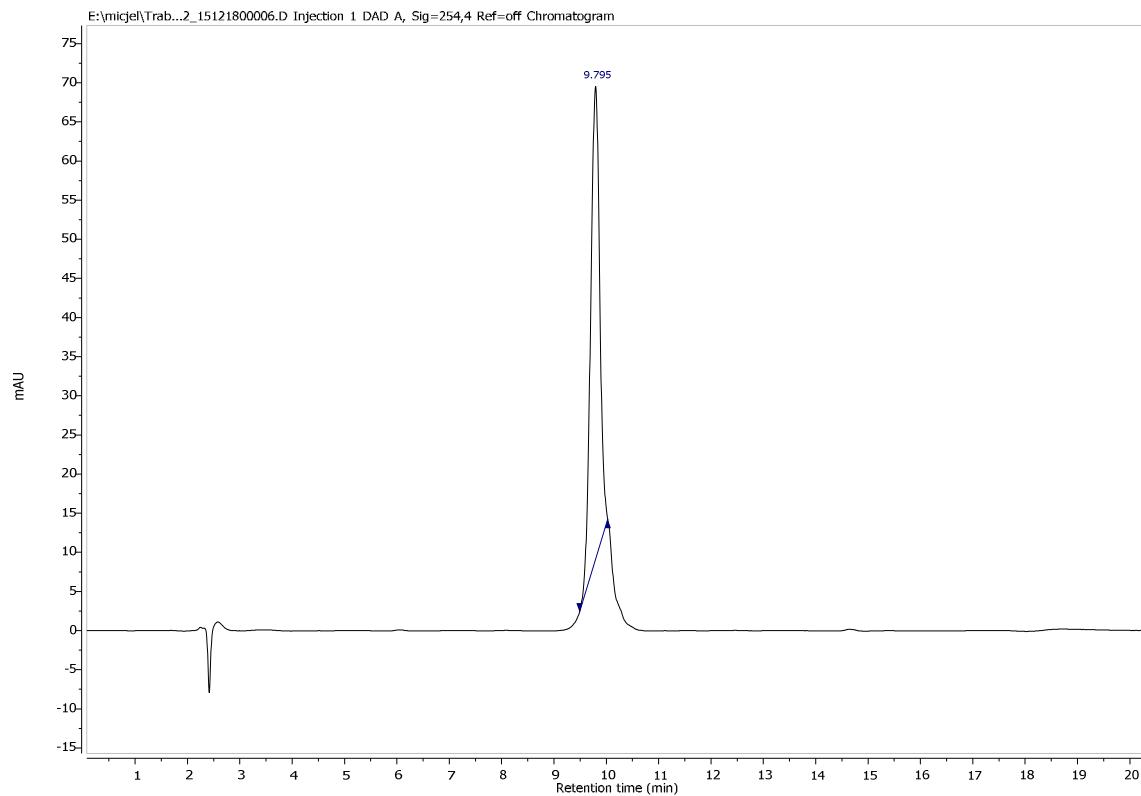
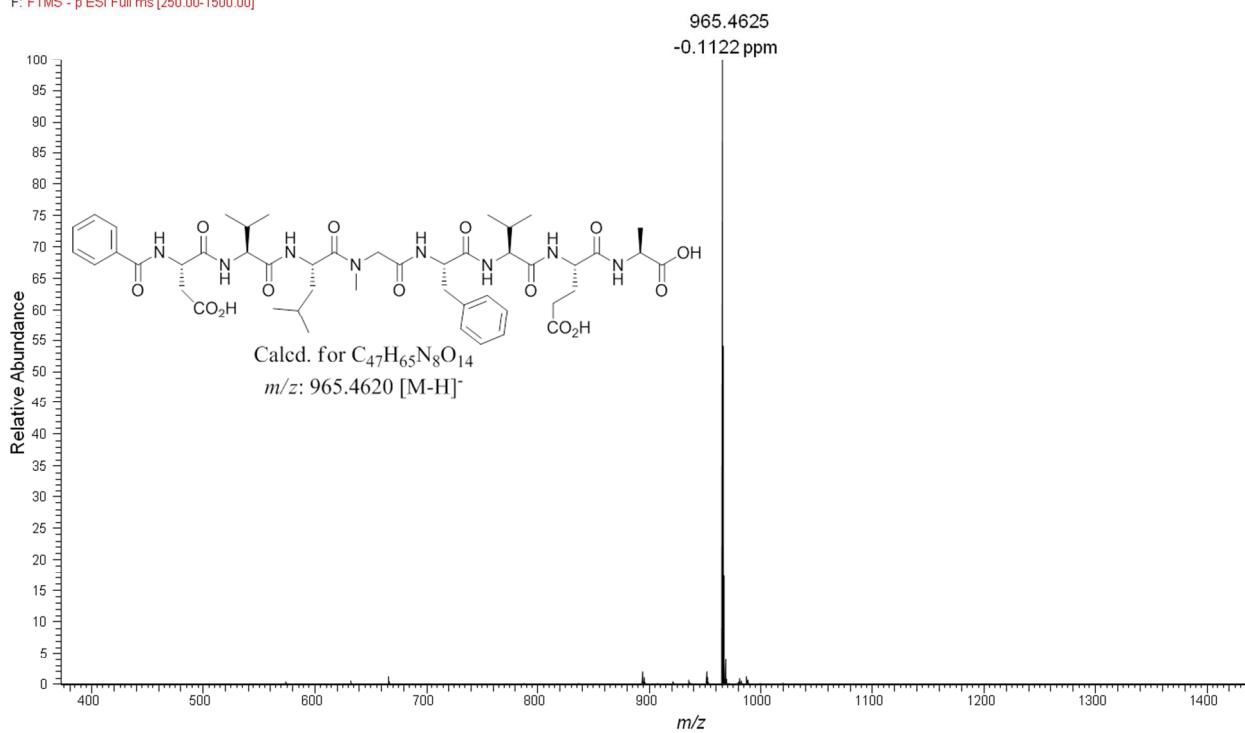


Figure 11. ESI-MS and HPLC chromatogram of pure peptide **16**.

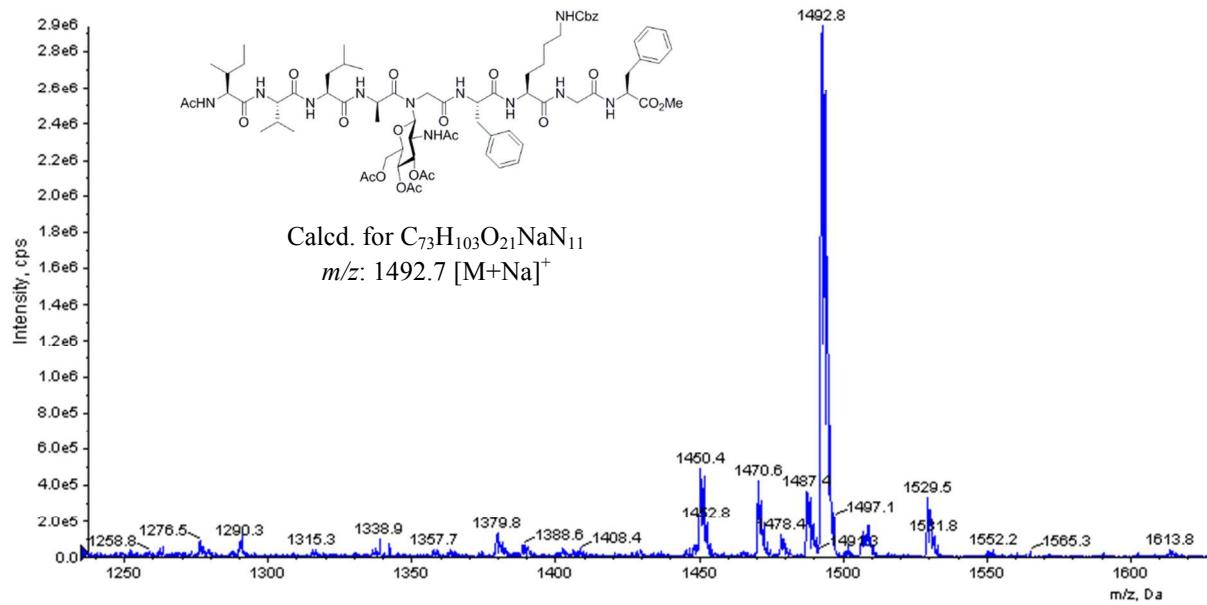


Figure 12. ESI-MS analysis of peptide 21.

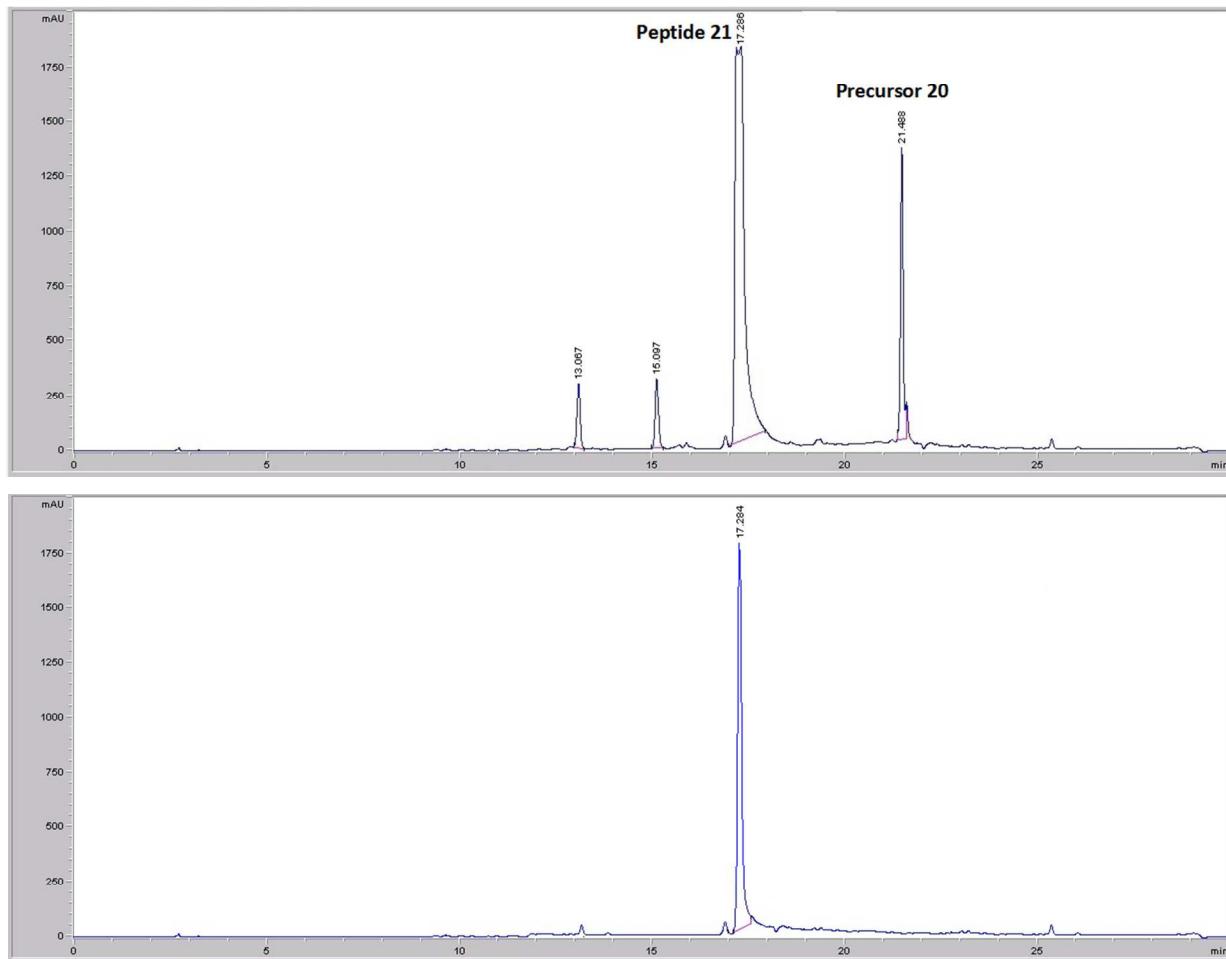
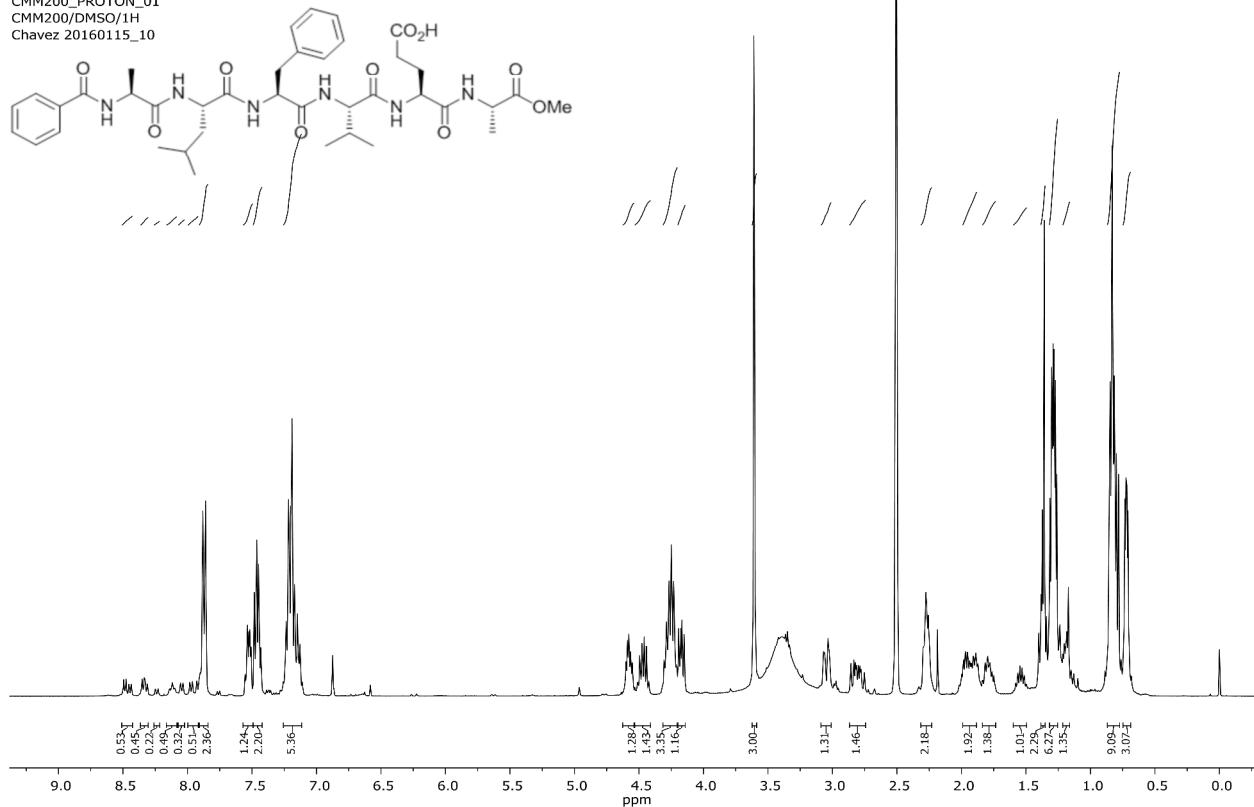


Figure 13. HPLC chromatograms of crude (A) and pure (B) peptide 21.

CMM200_PROTON_01
CMM200/DMSO/1H
Chavez 20160115_10



CMM200_CARBON_028
CMM200/DMSO/13C
Chavez 20160115_10

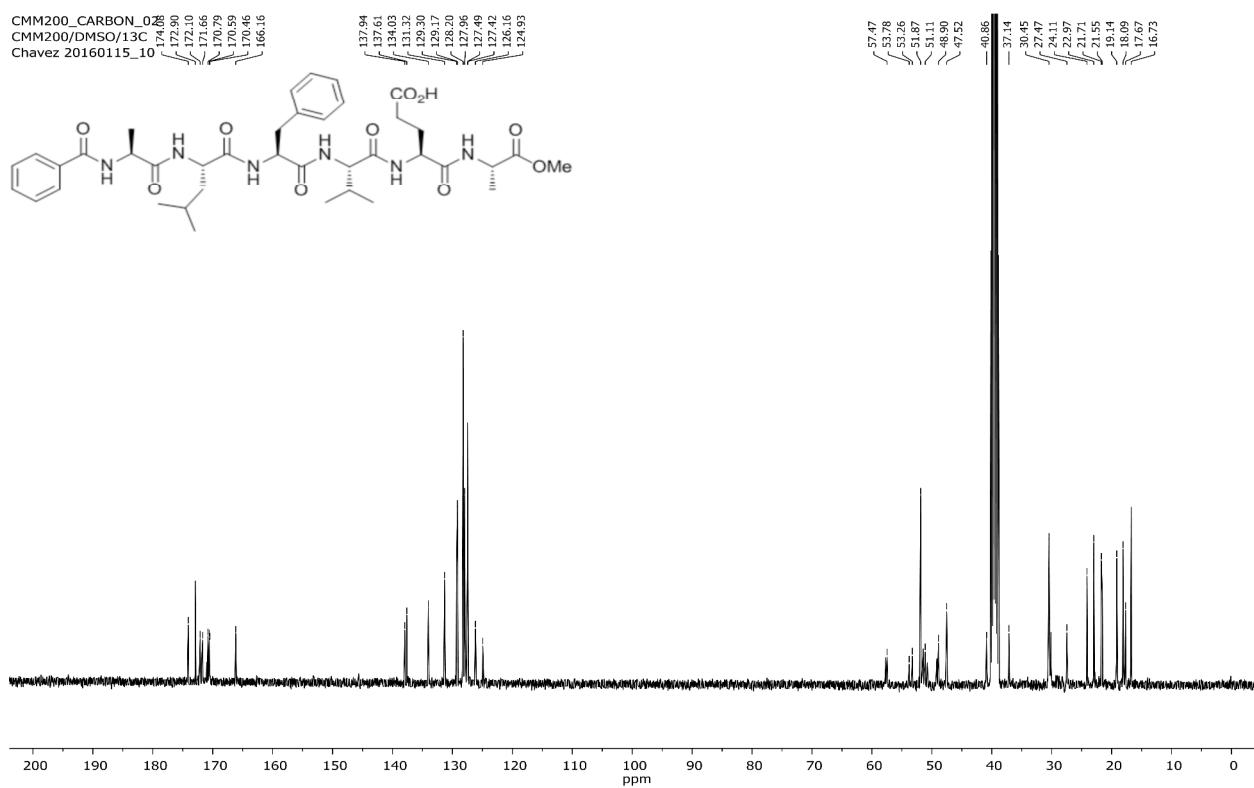


Figure 14. 400 MHz NMR spectra of peptide **22** in DMSO-d₆.

CMM200_neg #173 RT: 0.71 AV: 1 NL: 5.66E4
T: FTMS - p ESI Full ms [50.00-2000.00]

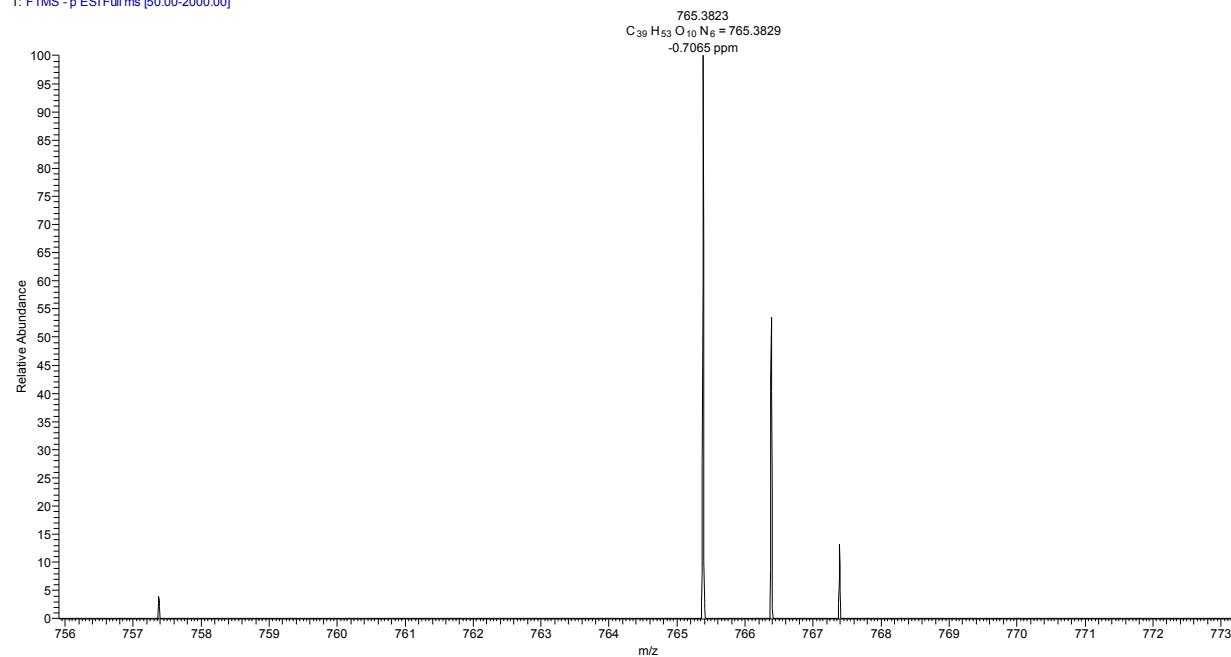


Figure 15. ESI-MS analysis of peptide **22**.

CMM211_neg#34 RT: 0.67 AV: 1 NL: 1.31E5
T: FTMS - p ESI Full ms [50.00-2000.00]

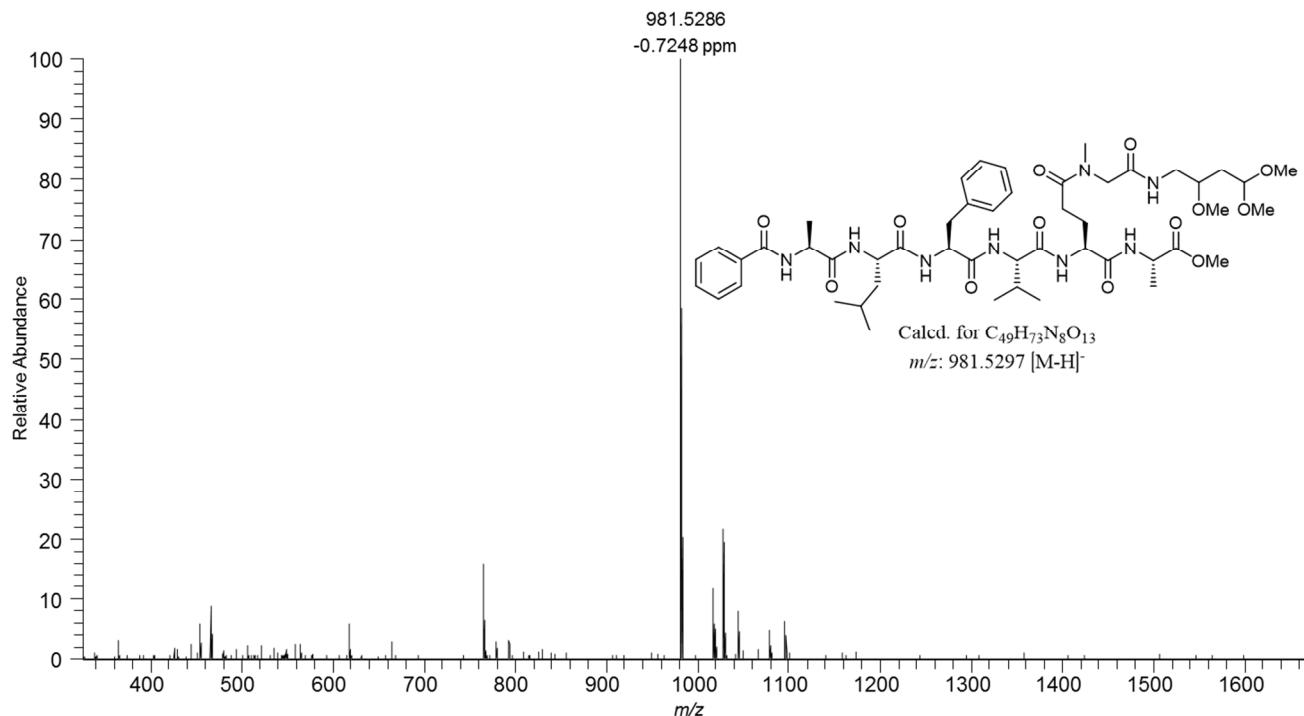


Figure 16. ESI-MS analysis of peptide **23**.

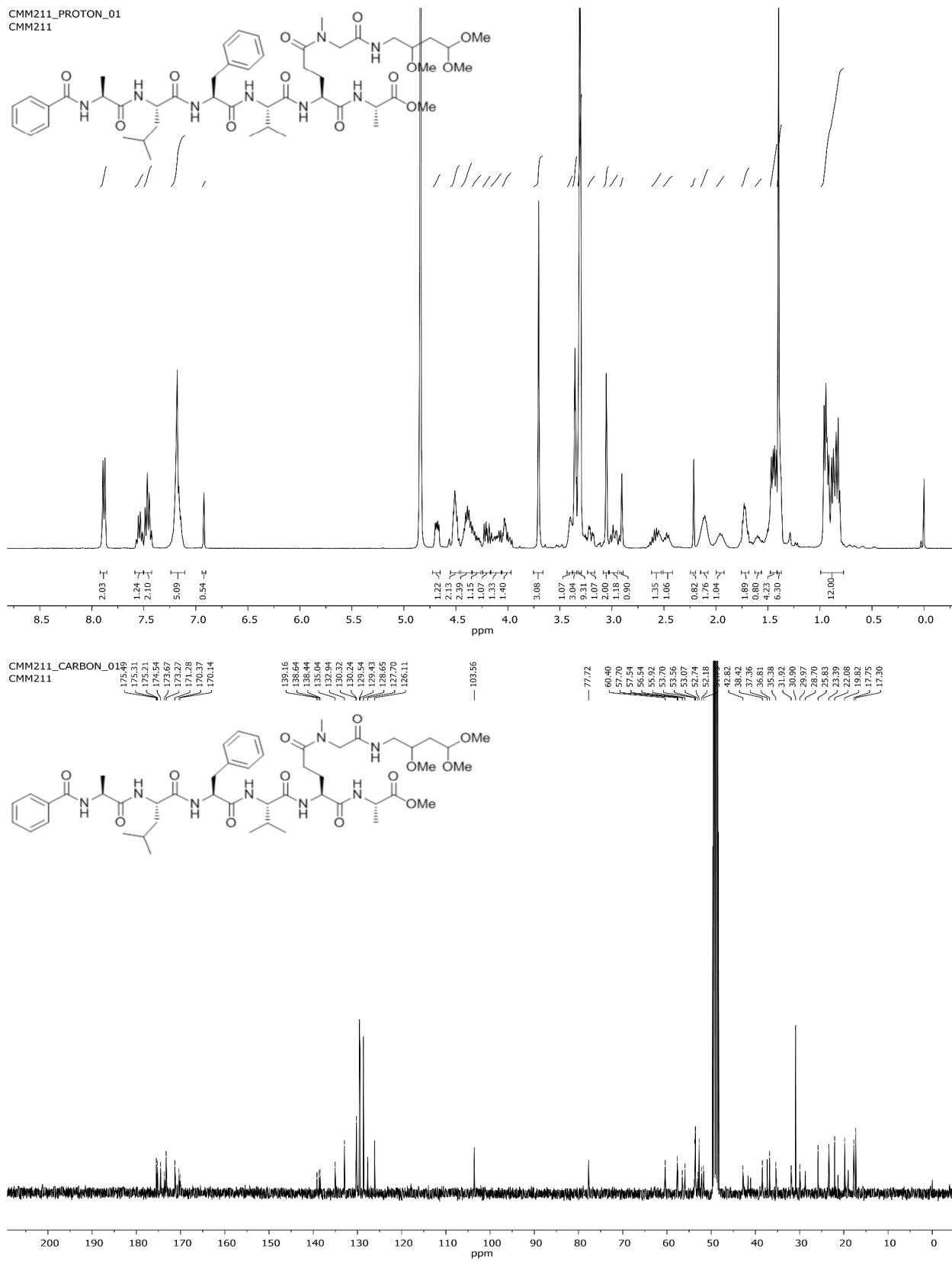
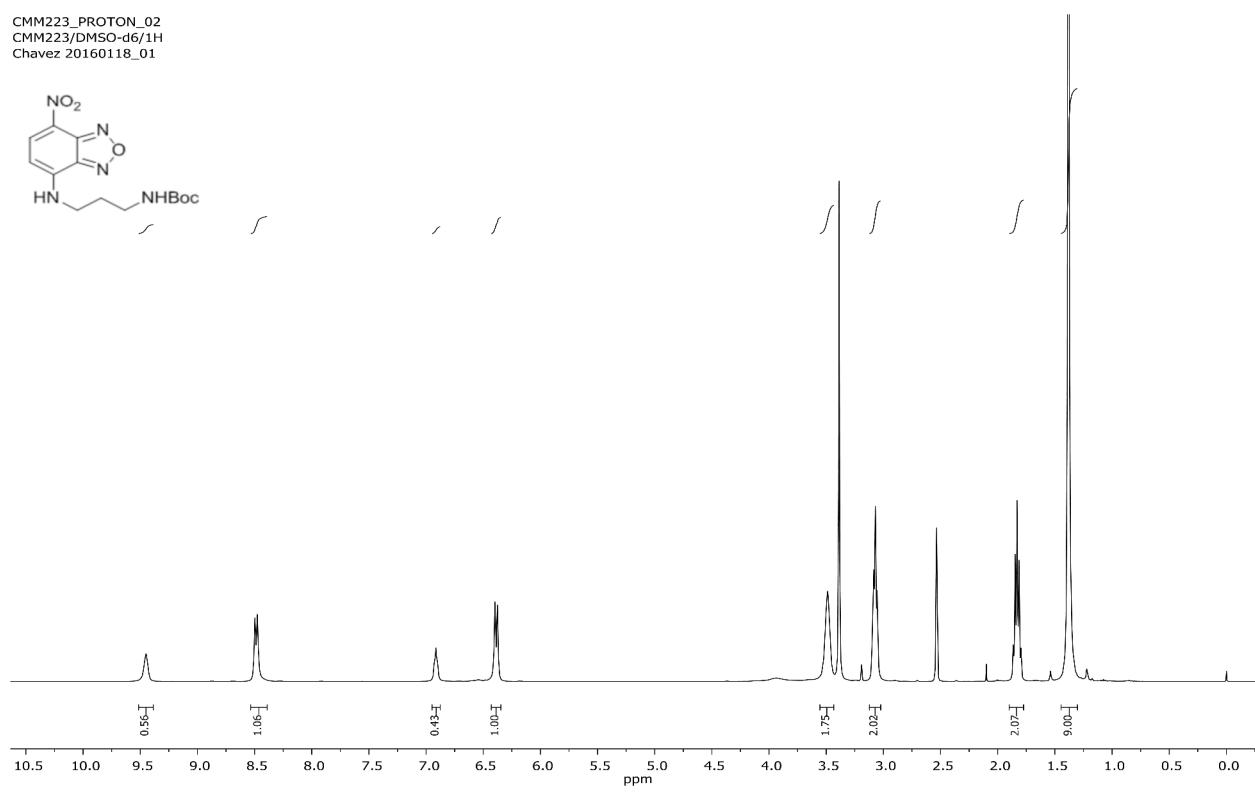


Figure 17. 400 MHz NMR spectra of peptide **23** in CD₃OD.

CMM223_PROTON_02
CMM223/DMSO-d6/1H
Chavez 20160118_01



CMM223_CARBON_03
CMM223/DMSO-d6/13C
Chavez 20160118_01

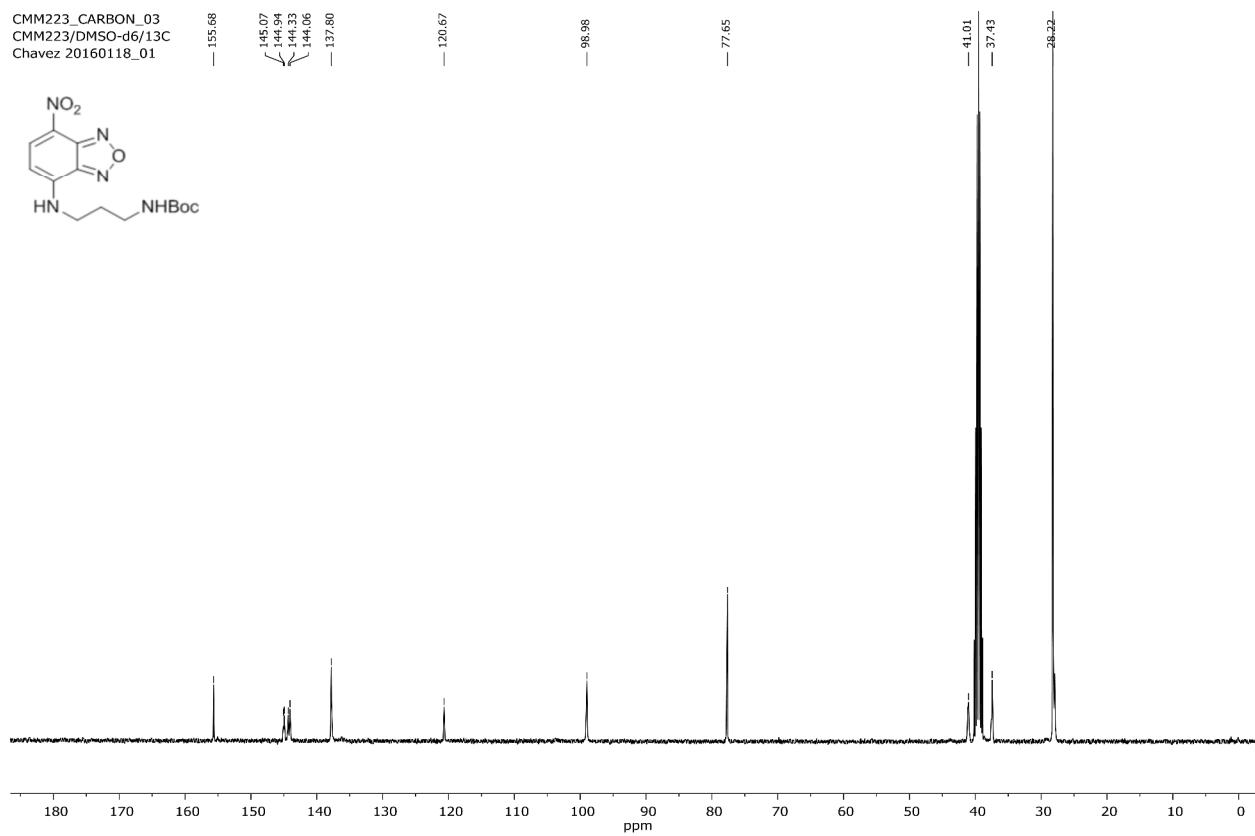
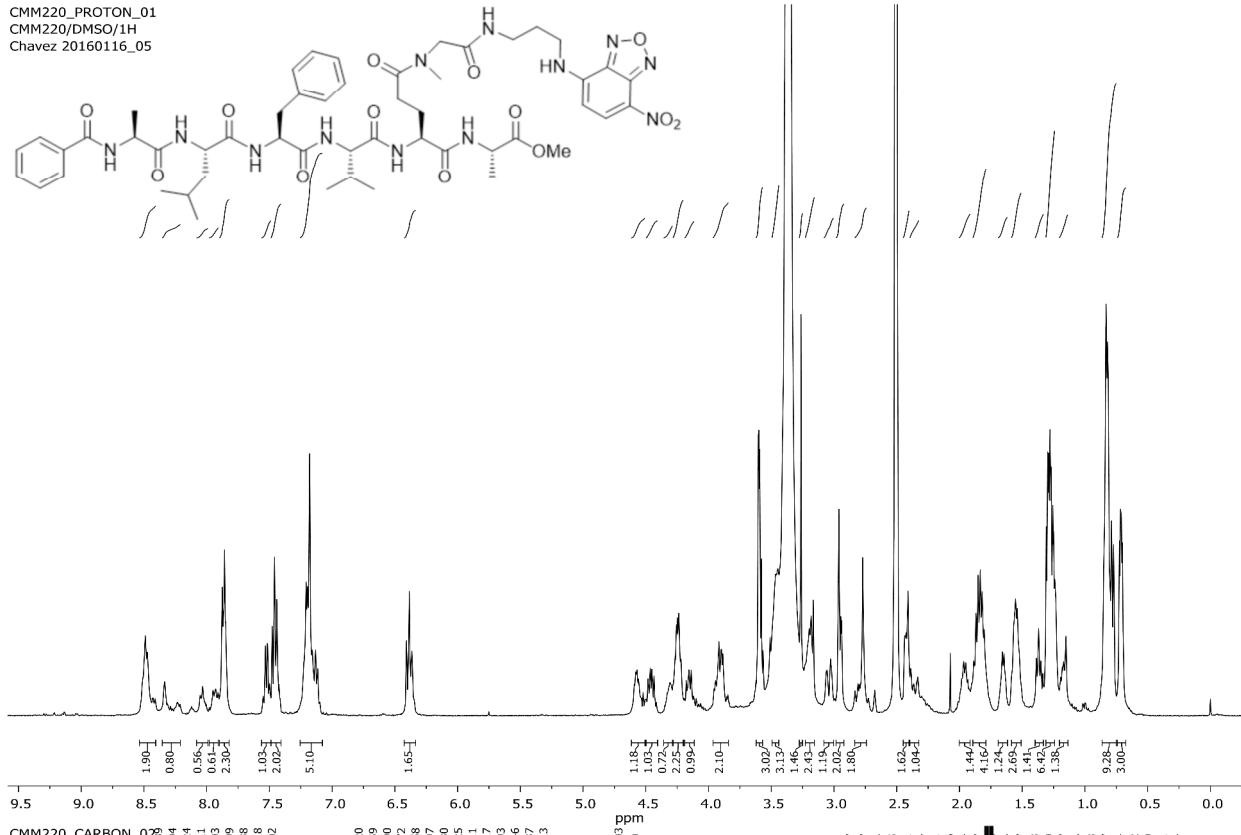


Figure 18. 400 MHz NMR spectra of amine **25** in DMSO-d₆.

CMM220_PROTON_01
CMM220/DMSO/1H
Chavez 20160116_05



CMM220_CARBON_028
CMM220/DMSO/13C
Chavez 20160116_05

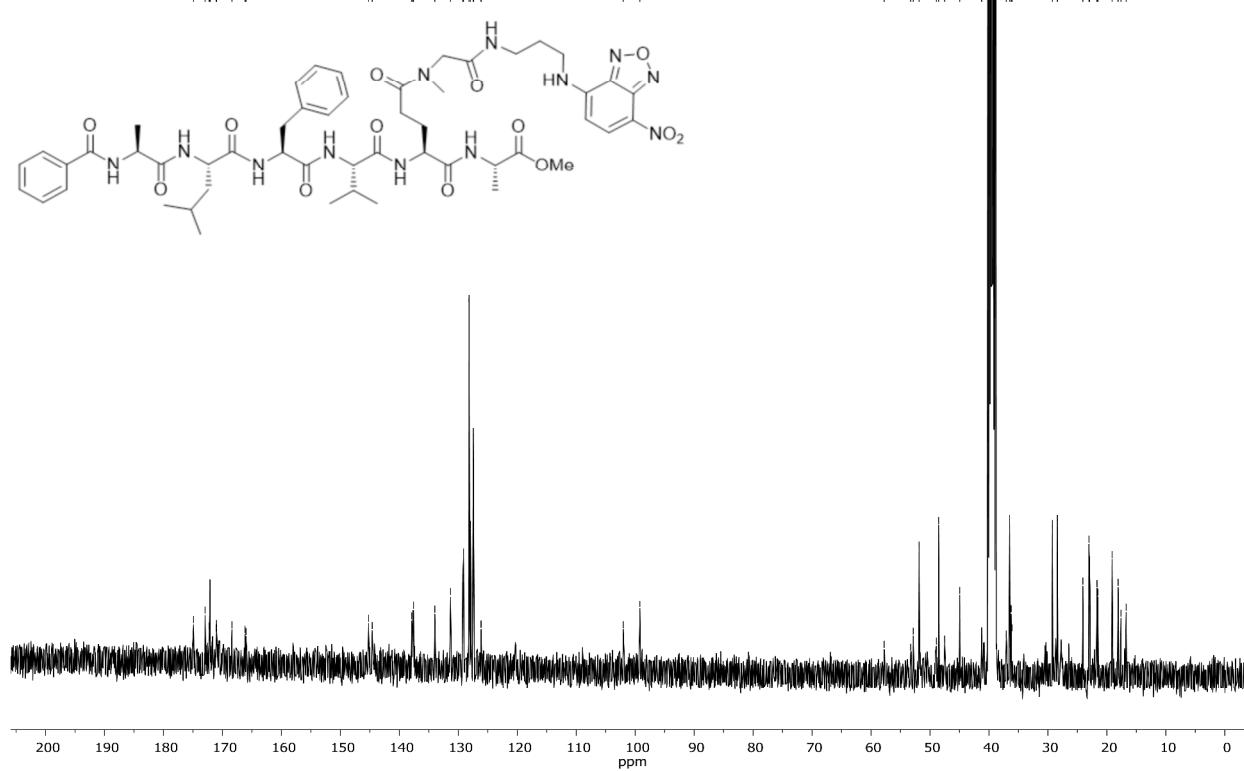


Figure 19. 400 MHz NMR spectra of peptide **26** in DMSO-d₆.

CMM220_nMS2_1055#4871 RT: 15.25 AV: 1 NL: 2.02E7
F: FTMS - p ESI Full ms [250.00-2000.00]

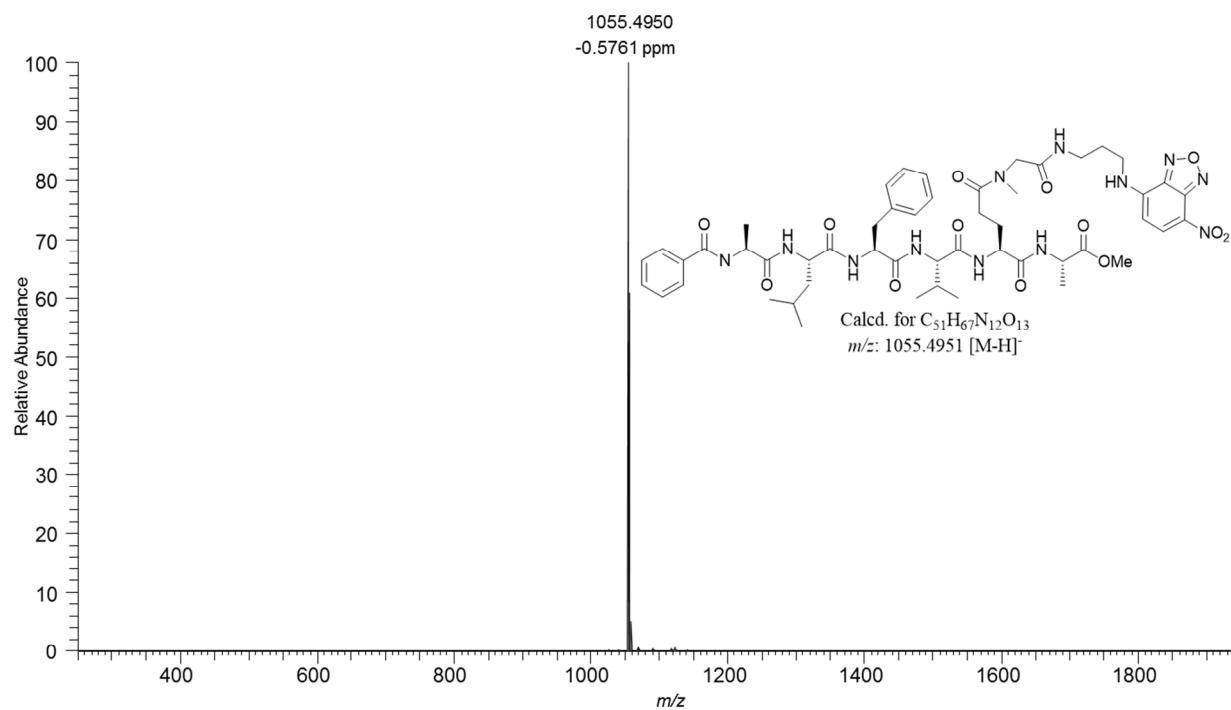


Figure 20. ESI-MS analysis of peptide **26**.

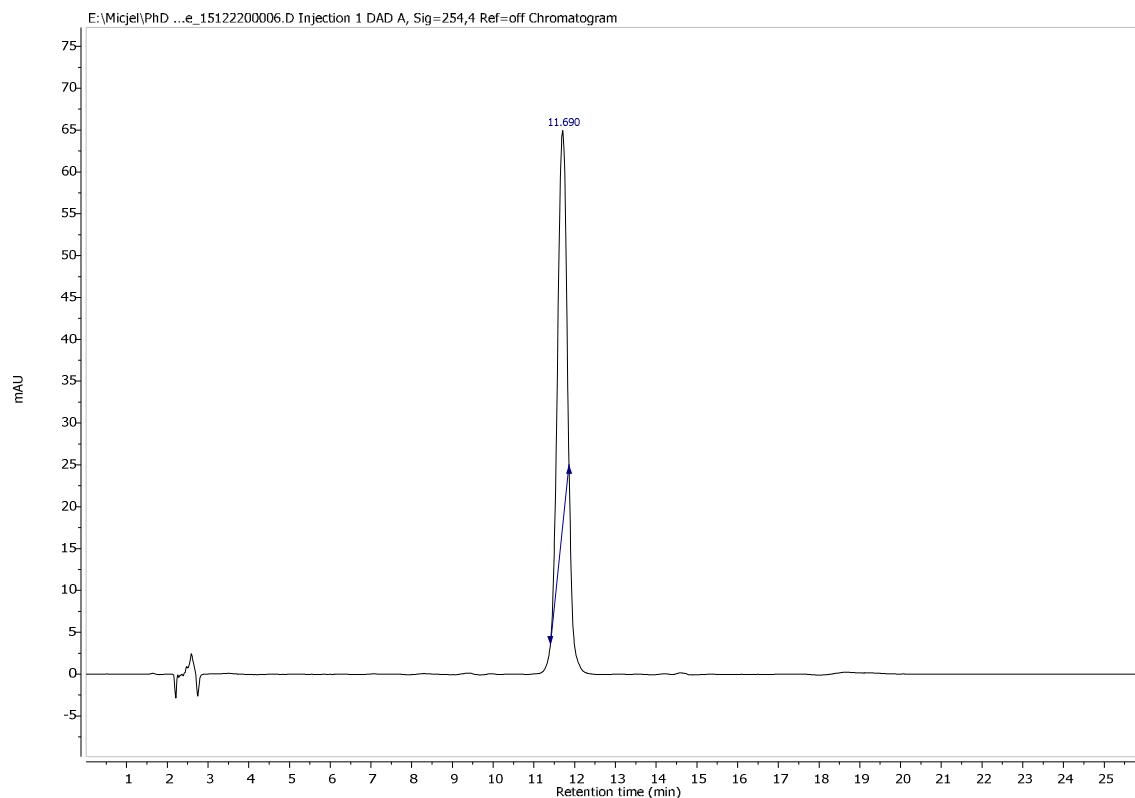


Figure 21. HPLC chromatogram of pure peptide **26**.

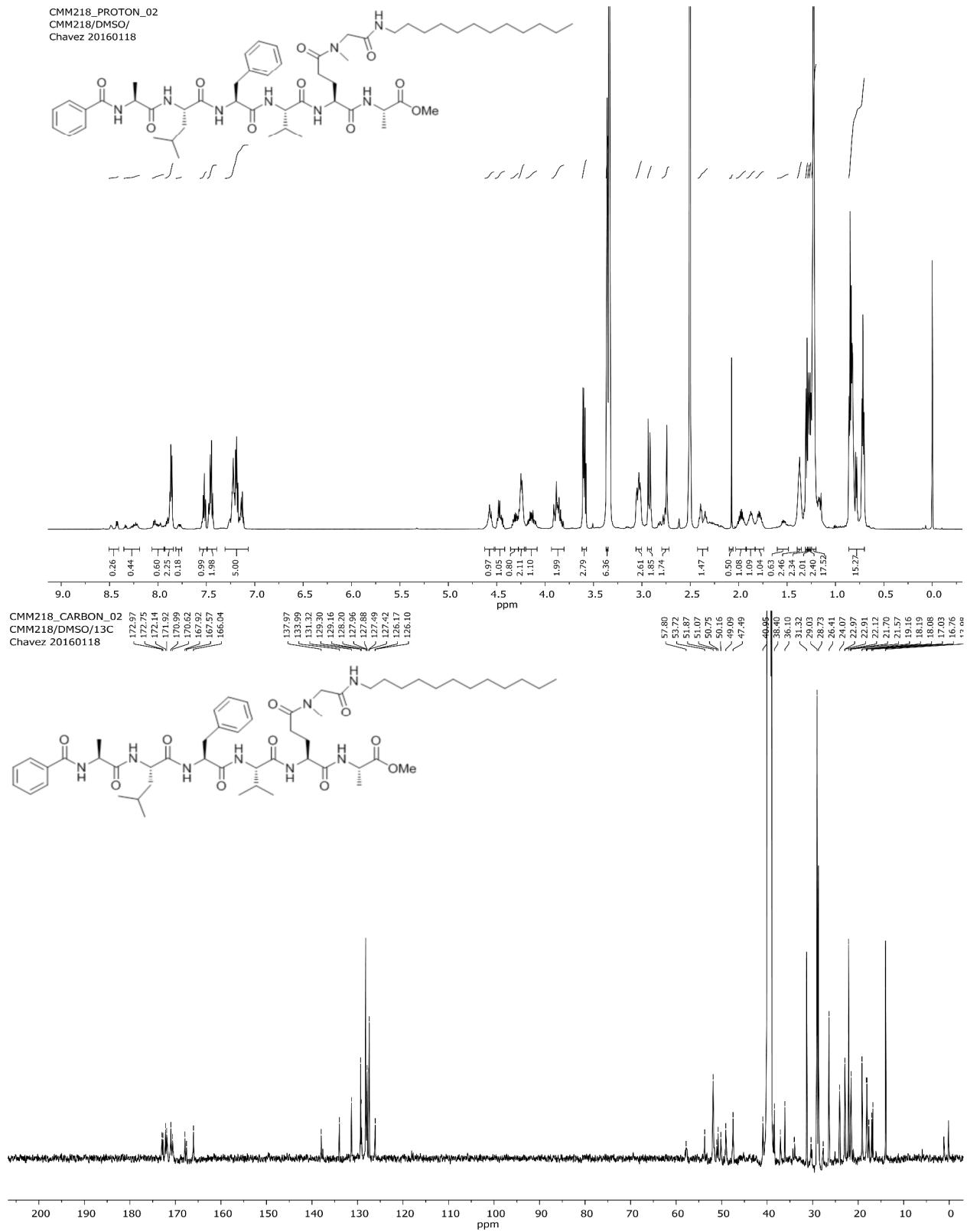


Figure 22. 400 MHz NMR spectra of peptide **27** in DMSO-d₆.

CMM218_nMS2_1003#6263 RT: 19.55 AV: 1 NL: 3.24E6
F: FTMS - p ESI Full ms [250.00-2000.00]

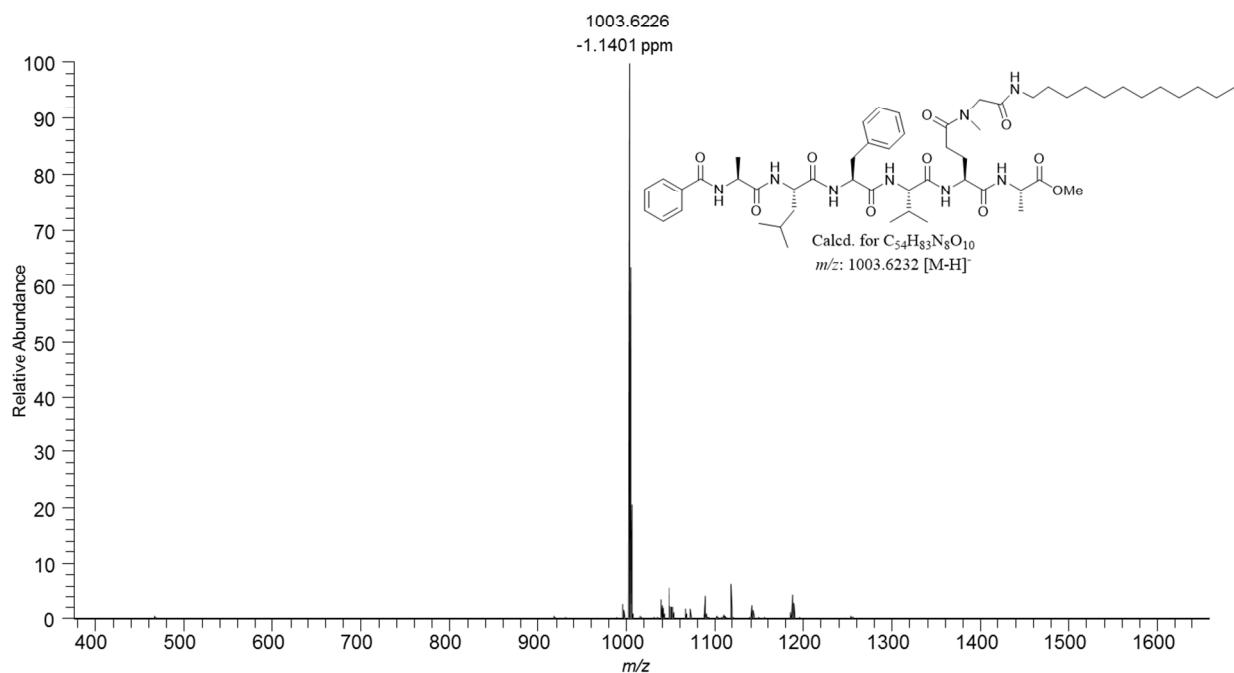


Figure 23. ESI-MS analysis of peptide 27.

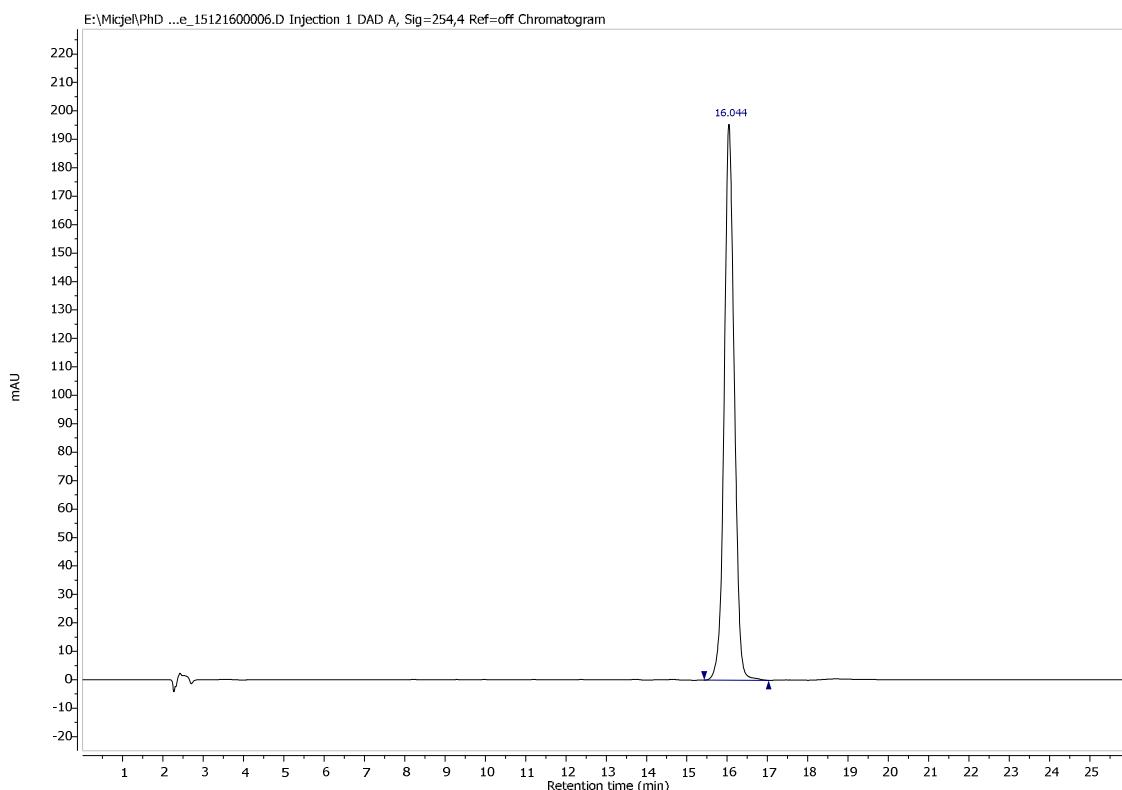


Figure 24. HPLC chromatogram of pure peptide 27.

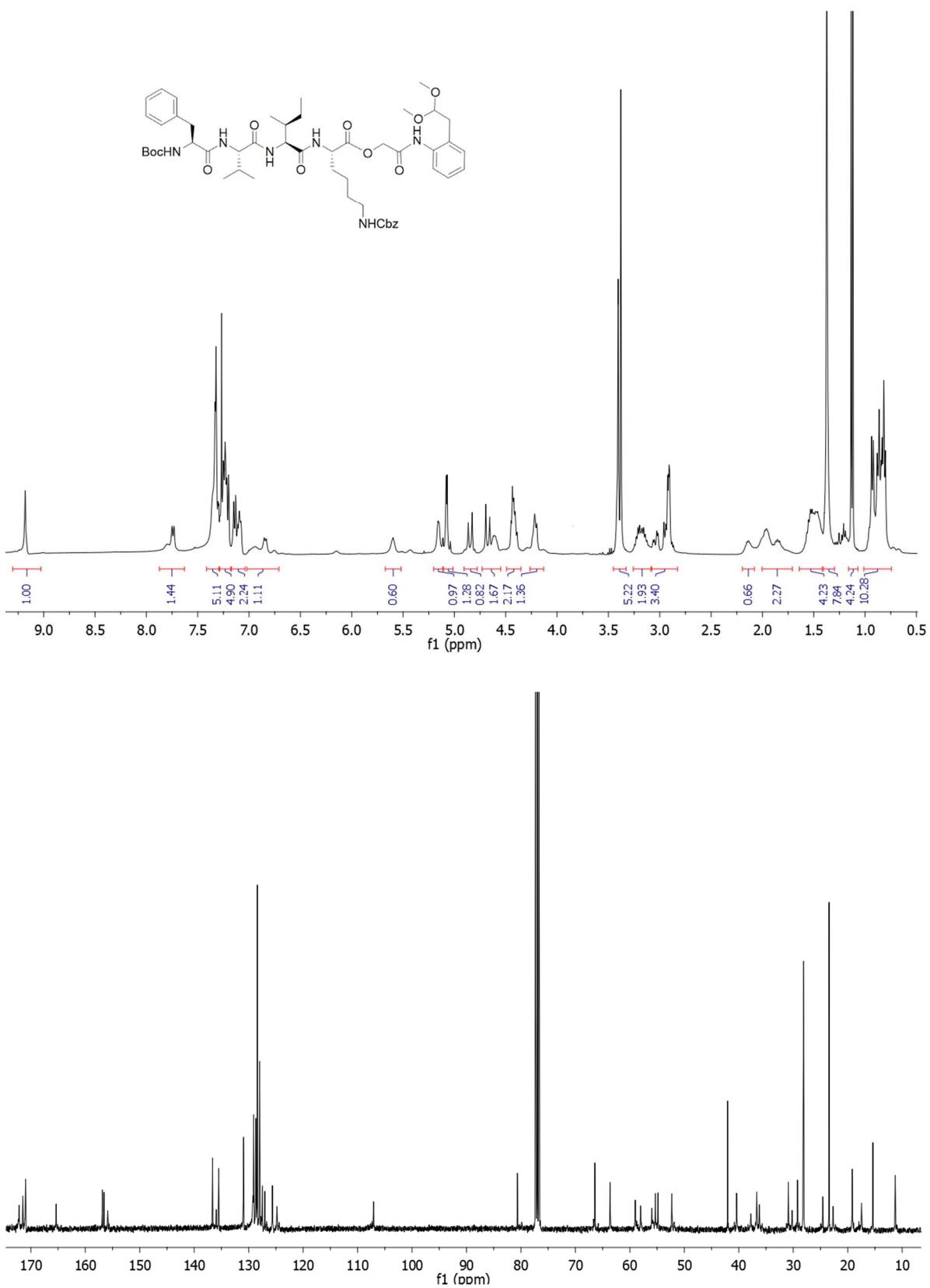


Figure 25. 400 MHz NMR spectra of Paserini-derived peptide **29** in CDCl₃.

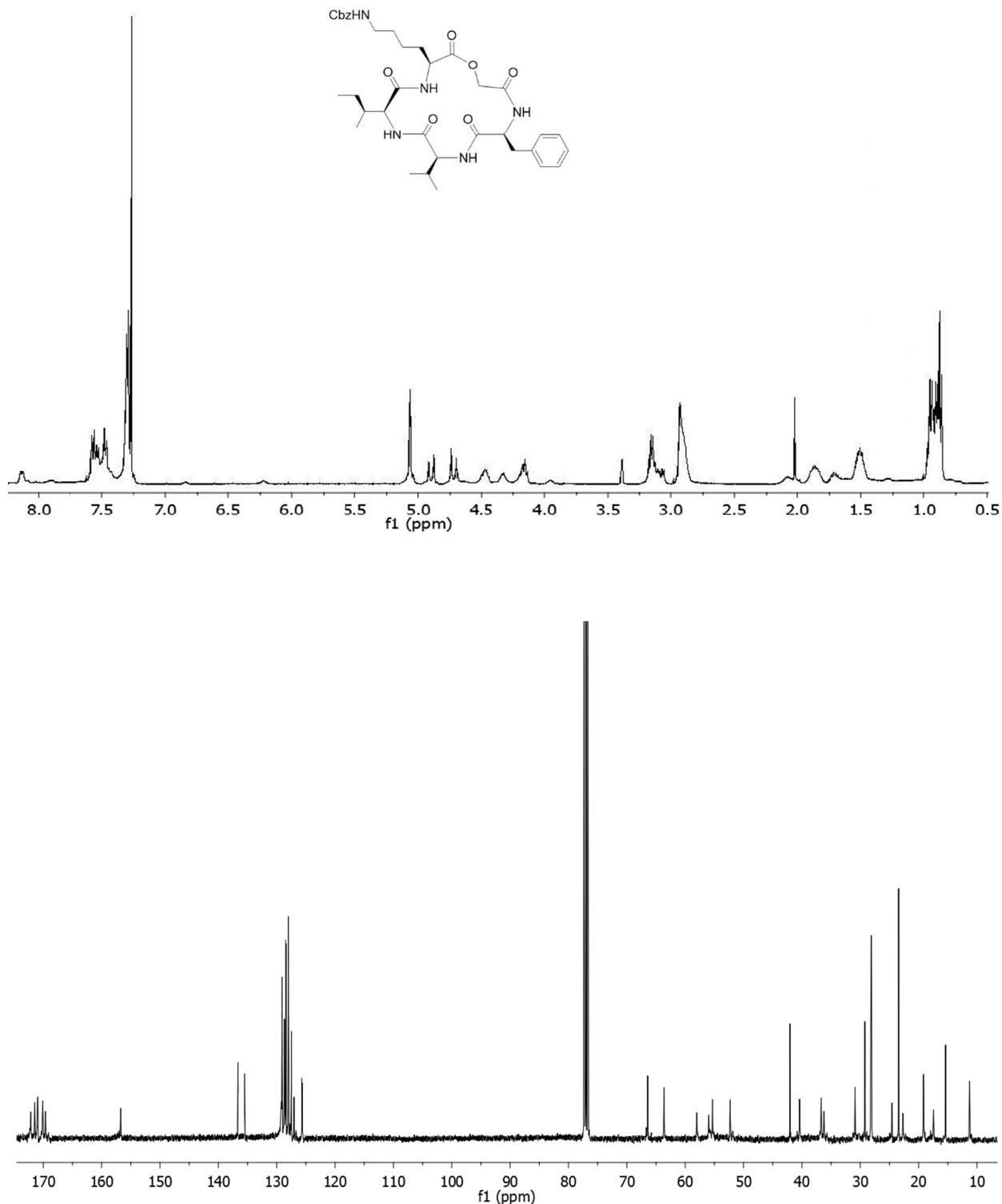


Figure 26. 400 MHz NMR spectra of cyclodepsipeptide **30** in CDCl_3 .

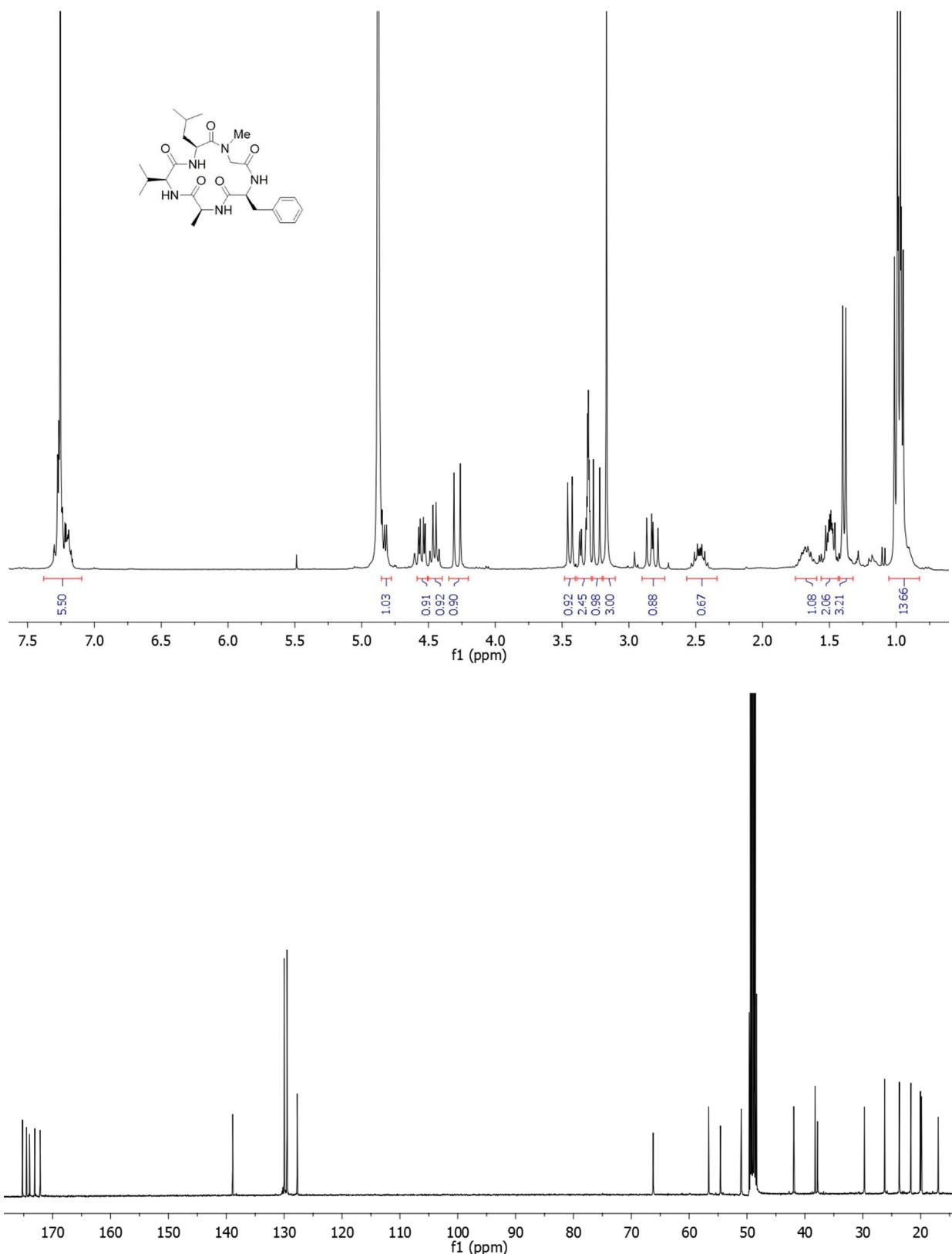


Figure 27. 400 MHz NMR spectra of cyclopeptide **33** in CD_3OD .

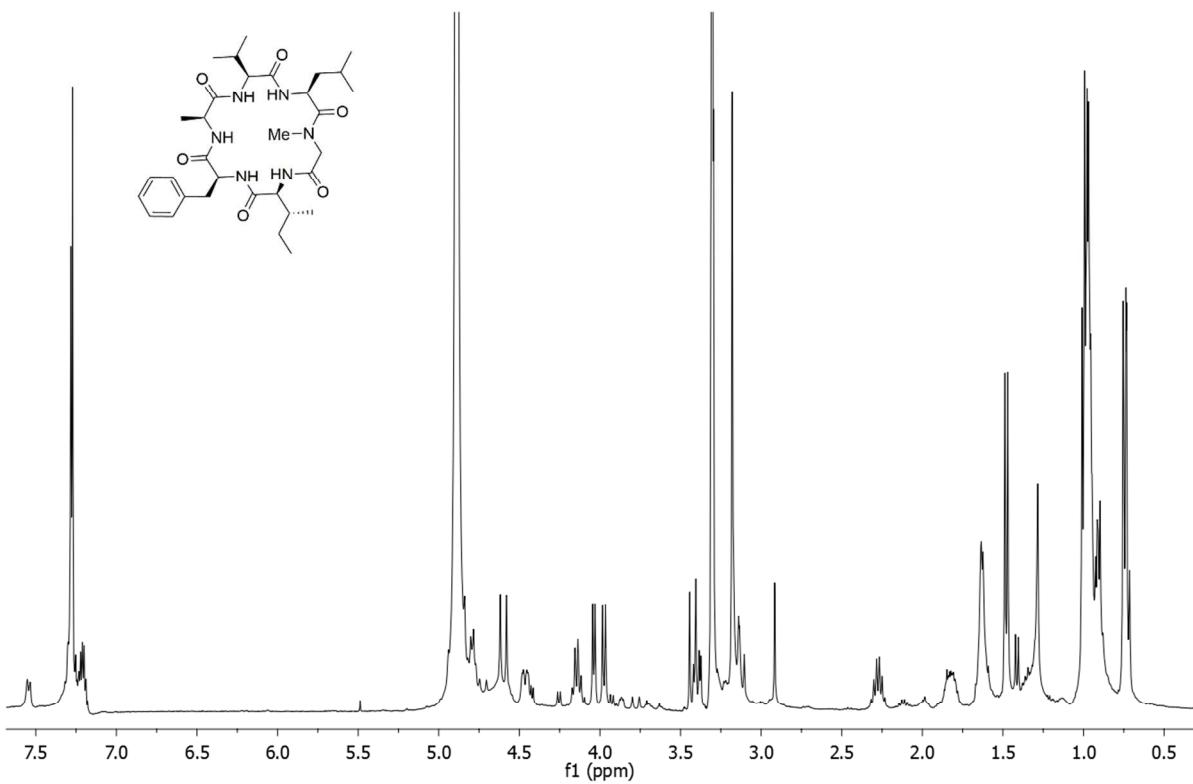


Figure 28. 400 MHz ^1H NMR spectrum of cyclohexapeptide **36** in DMSO-d_6 .

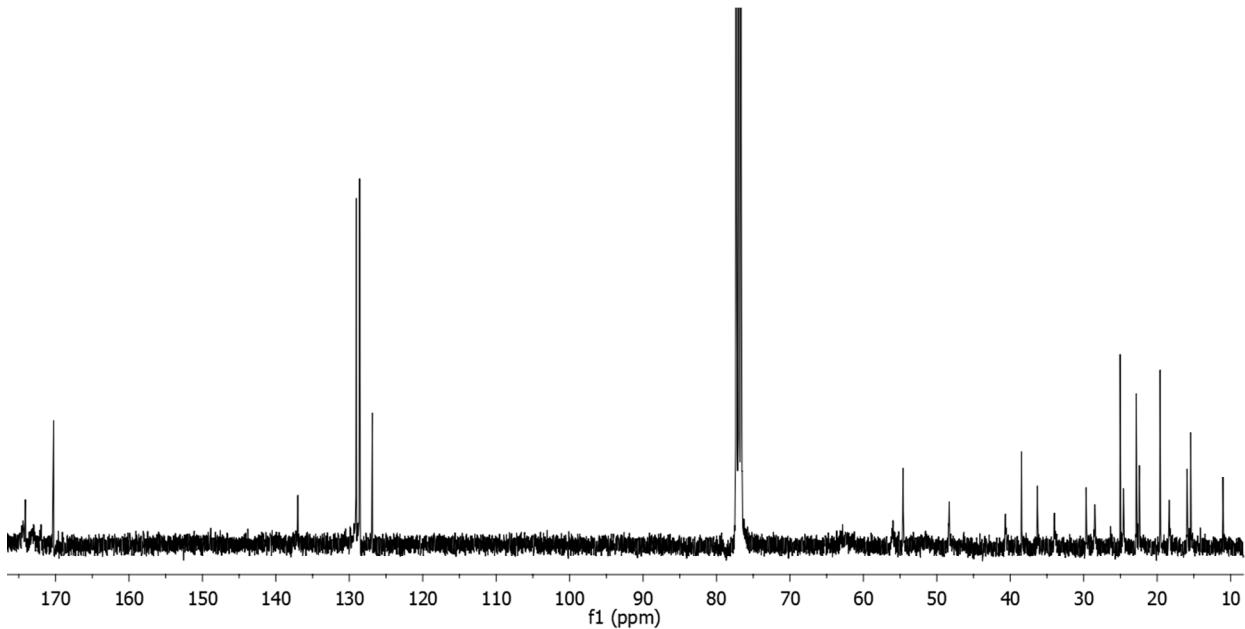


Figure 29. ^{13}C NMR spectrum of cyclohexapeptide **36** in CDCl_3 .

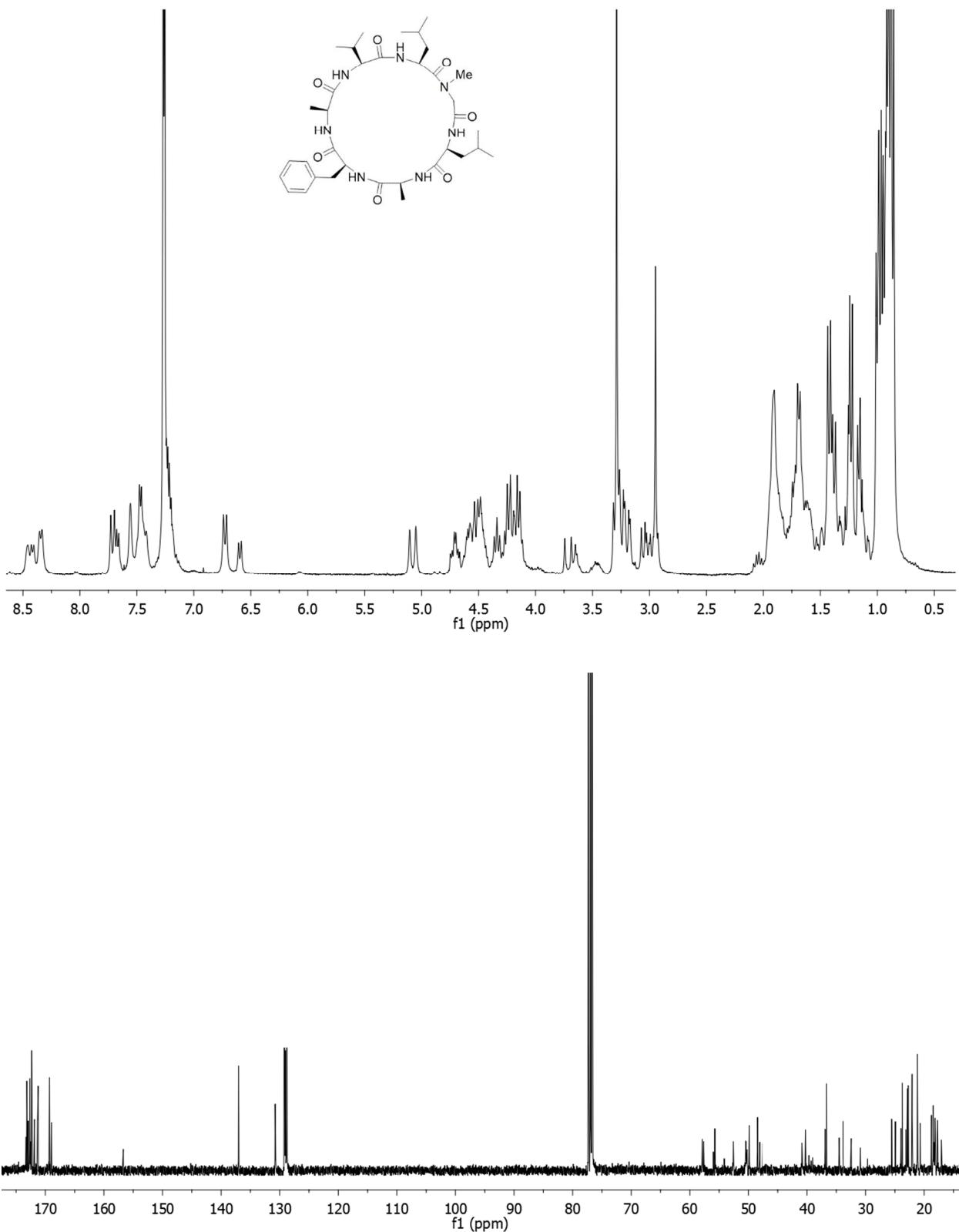
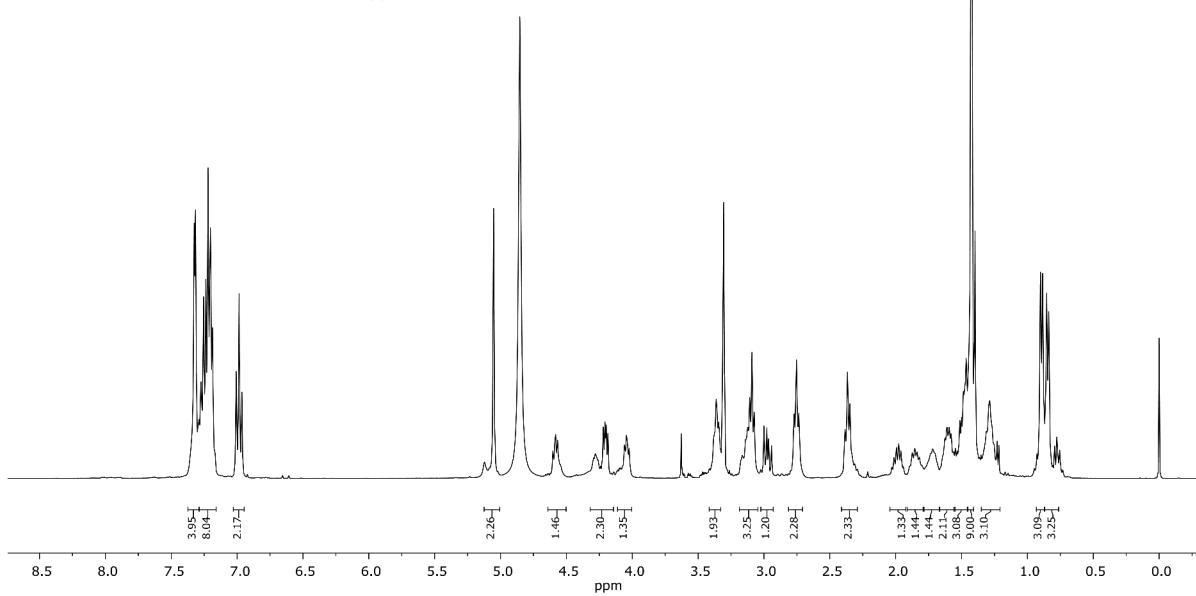
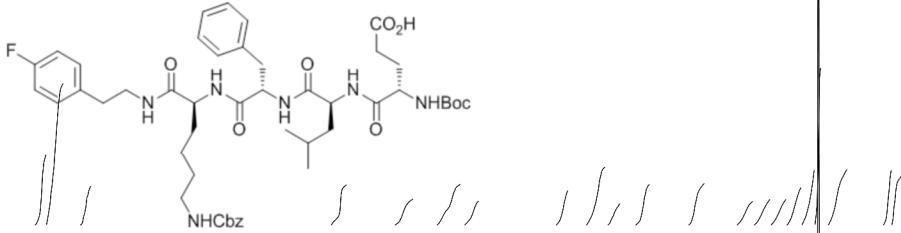


Figure 30. 400 MHz NMR spectra of cycloheptapeptide **39** in CDCl_3 .

CMM233_PROTON_01
CMM233/CD3OD/1H
Chavez 20160115_06



CMM233_CARBON_02
CMM233/CD3OD/13C
Chavez 20160115_06

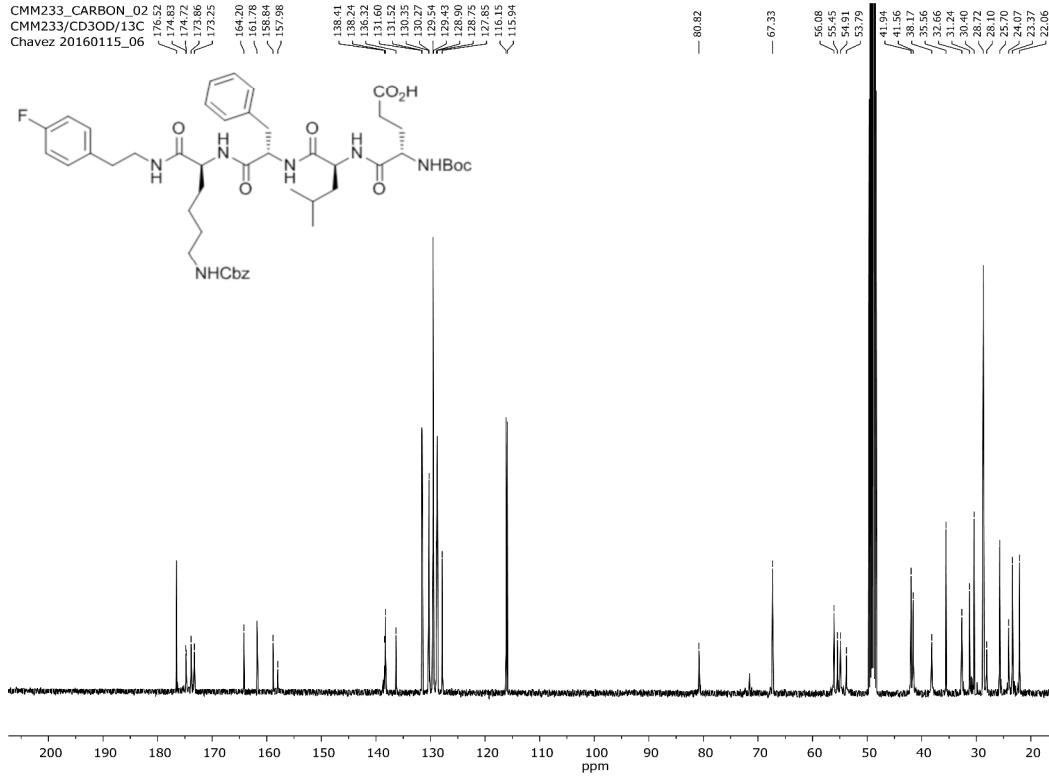
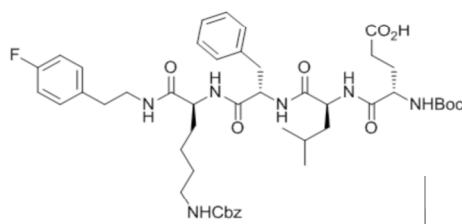


Figure 31. 400 MHz NMR spectra of peptide **40** in CD₃OD.

CMM233_neg #37 RT: 0.73 AV: 1 NL: 1.52E5
T: FTMS - p ESI Full ms [50.00-2000.00]

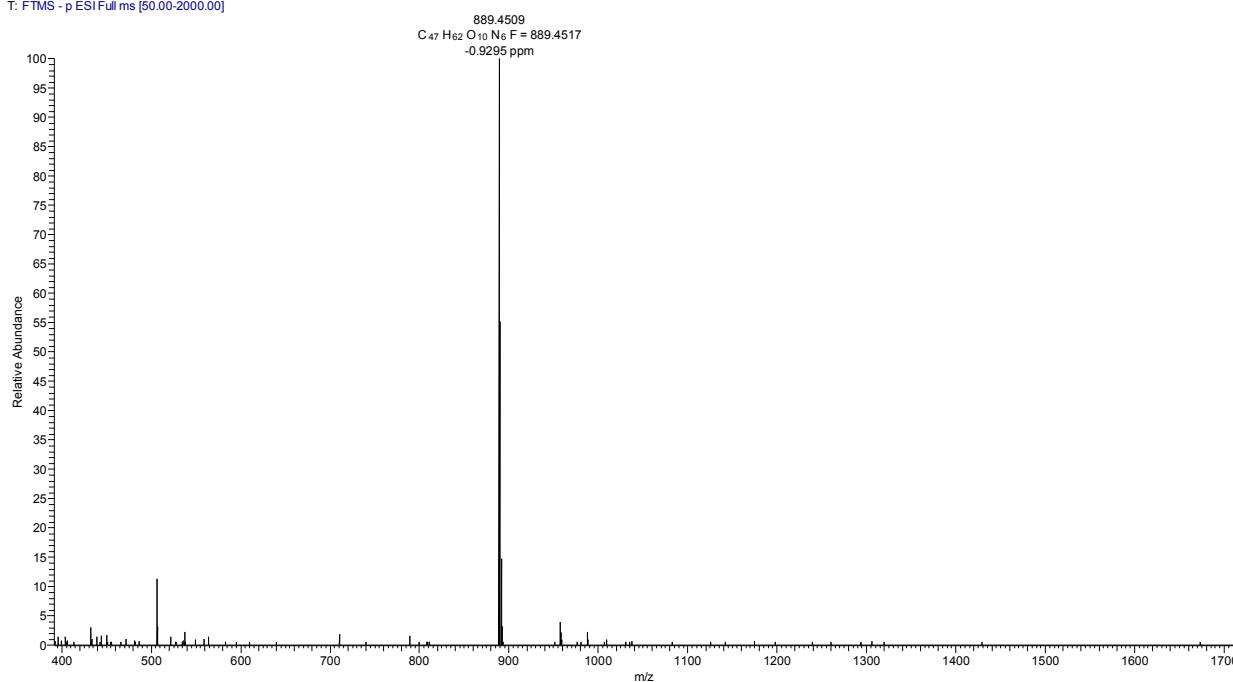


Figure 32. ESI-MS analysis of peptide 40.

CMM236_neg #2 RT: 0.02 AV: 1 NL: 2.62E5
T: FTMS - p ESI Full ms [50.00-2000.00]

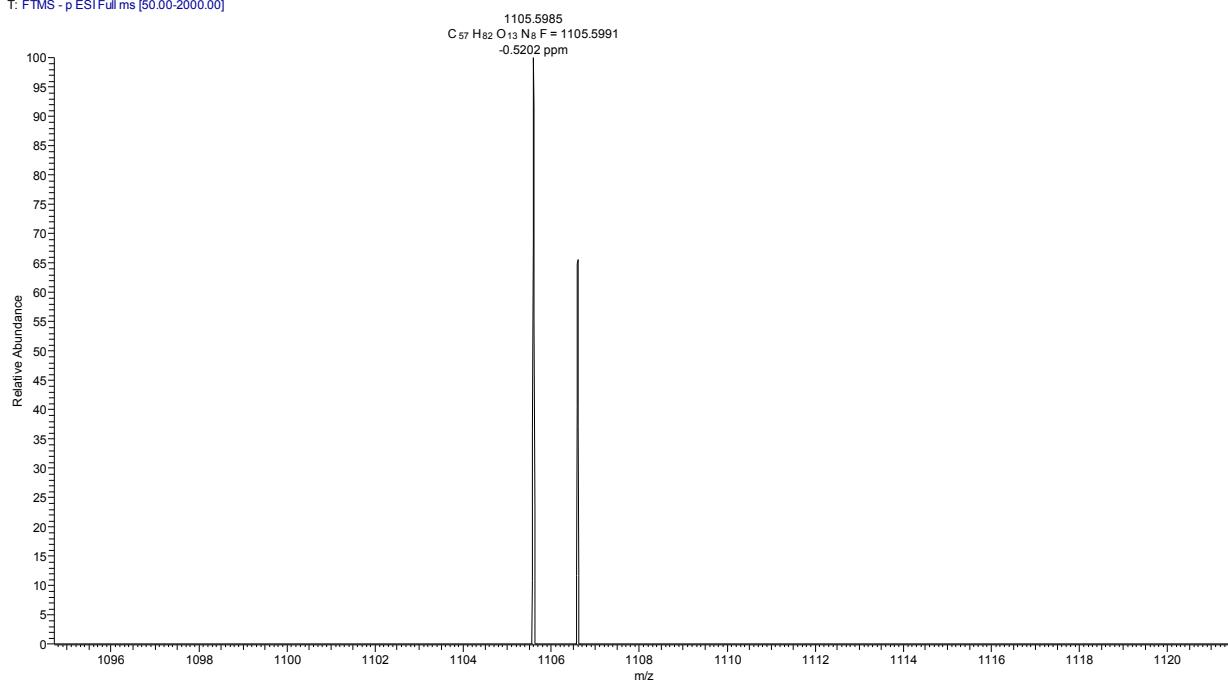


Figure 33. ESI-MS analysis of peptide 41.

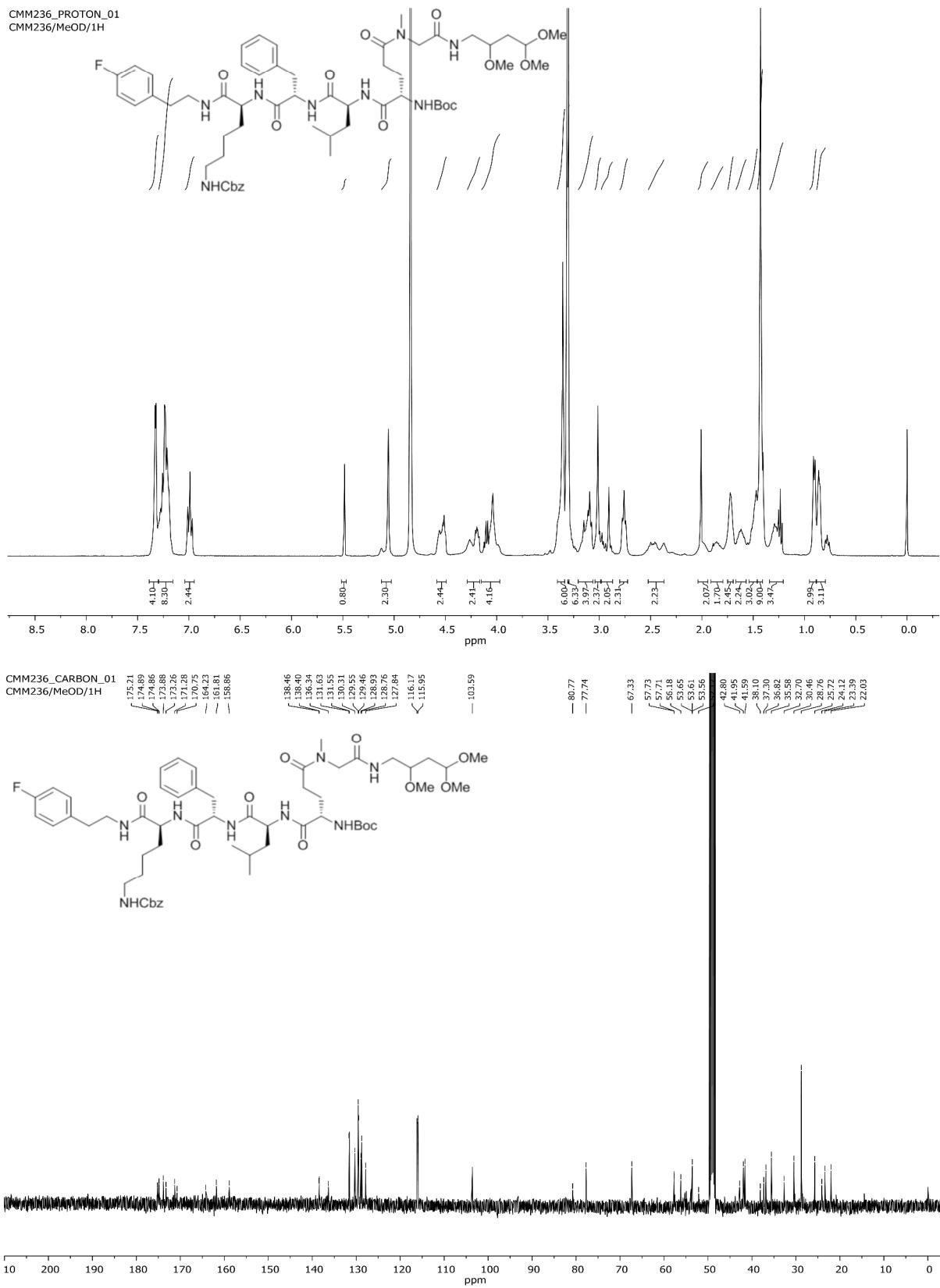
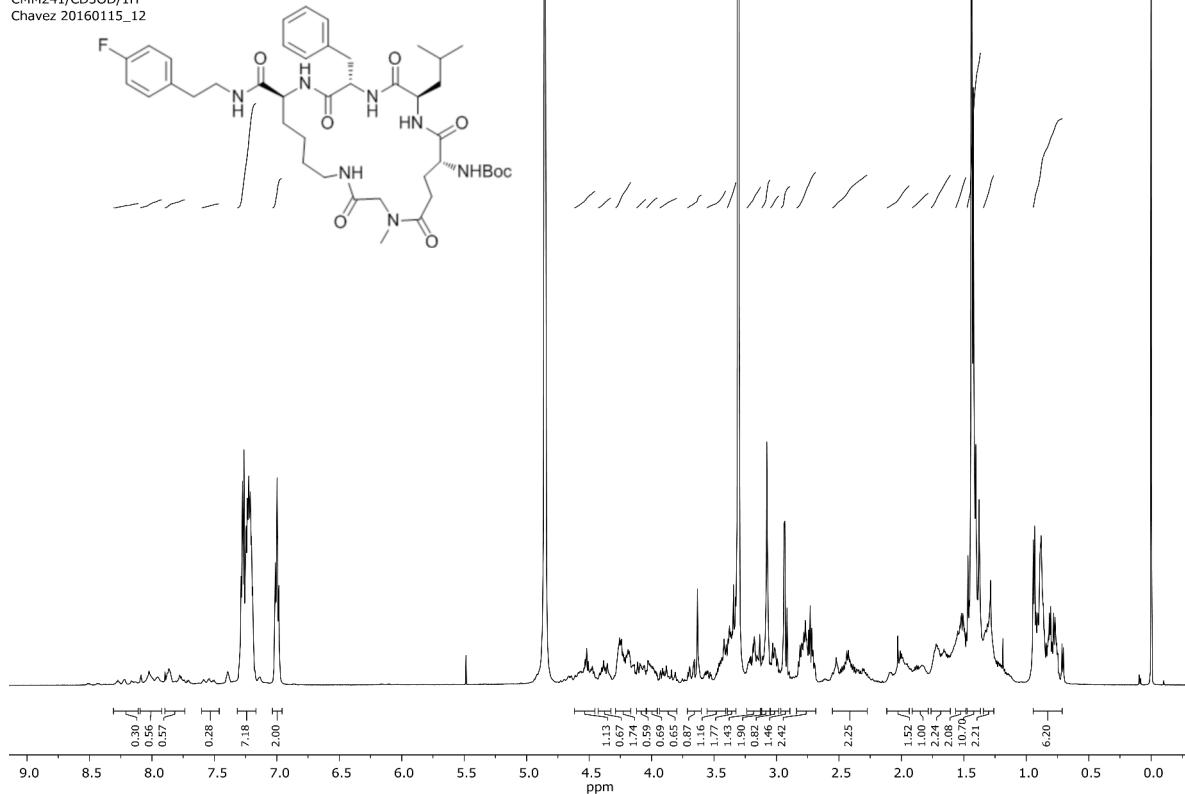


Figure 34. 400 MHz NMR spectra of peptide **41** in CD₃OD.

CMM241_PROTON_02
CMM241/CD3OD/1H
Chavez 20160115_12



CMM241_CARBON_03
CMM241/CD3OD/13C
Chavez 20160115_12

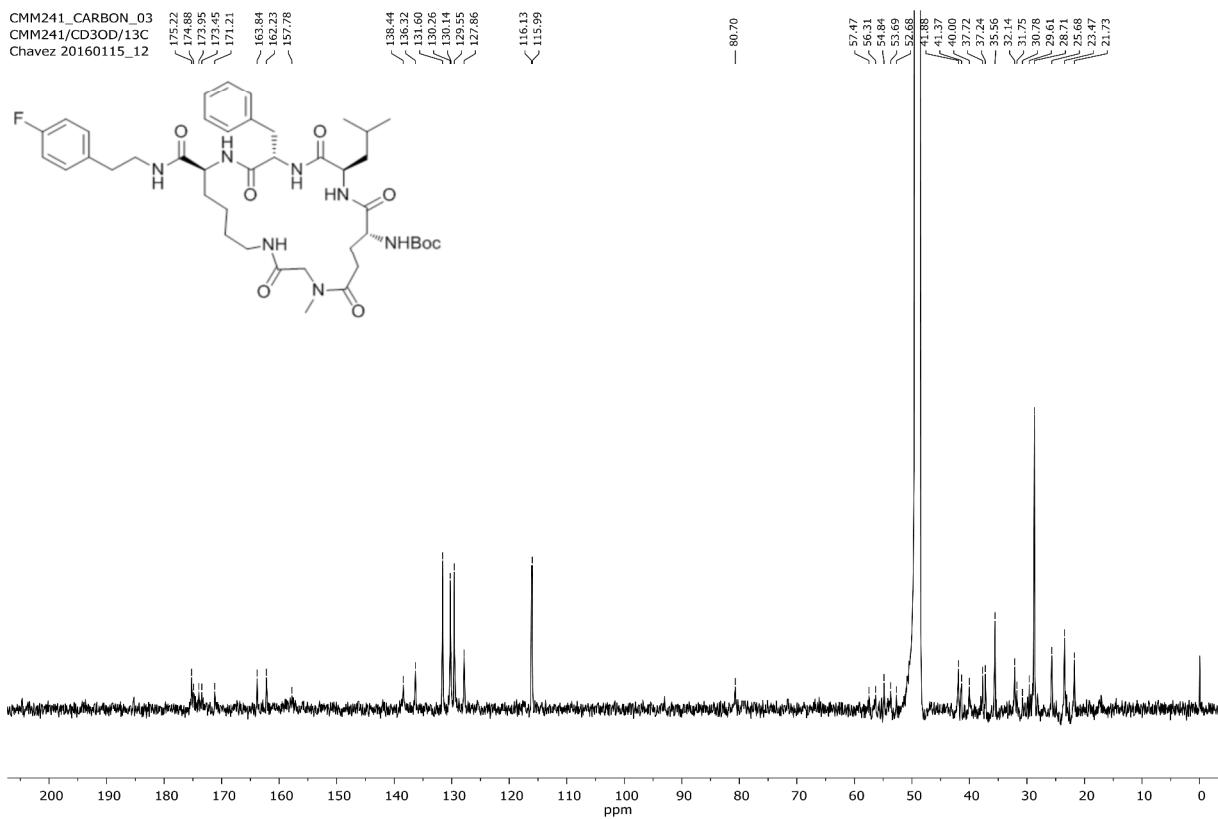


Figure 35. 400 MHz NMR spectra of peptide **42** in CD₃OD.

CMM241_nMS2_808 #4901 RT: 15.38 AV: 1 NL: 1.35E7
F: FTMS - p ESI Full ms [250.00-1500.00]

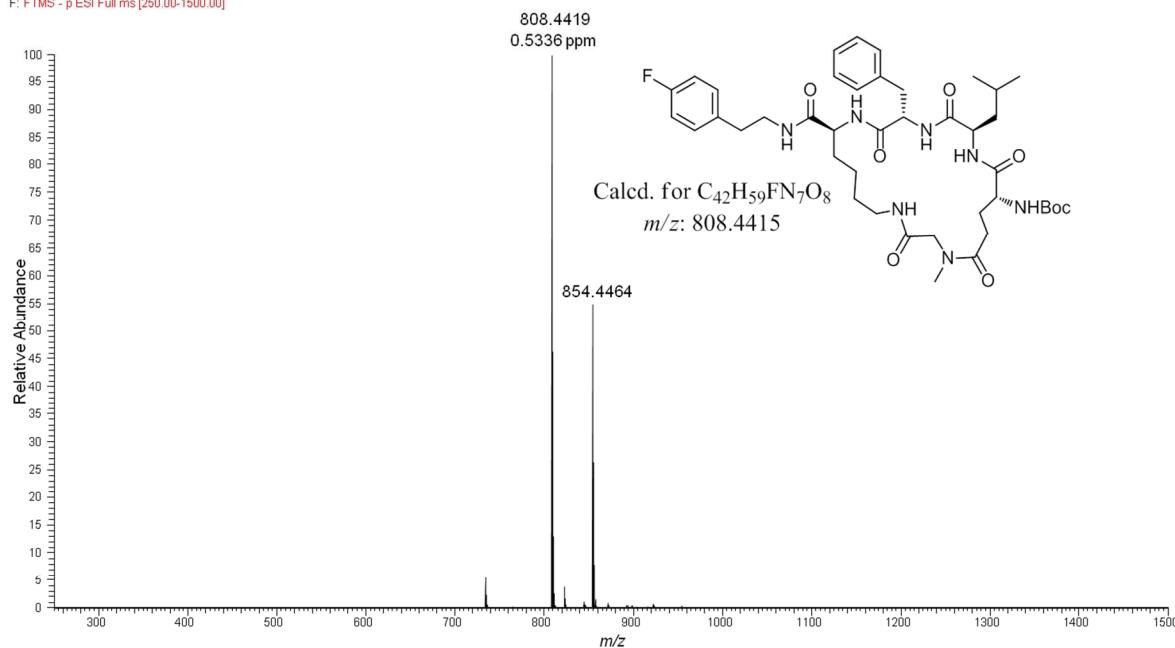


Figure 36. ESI-MS analysis of peptide **42**.

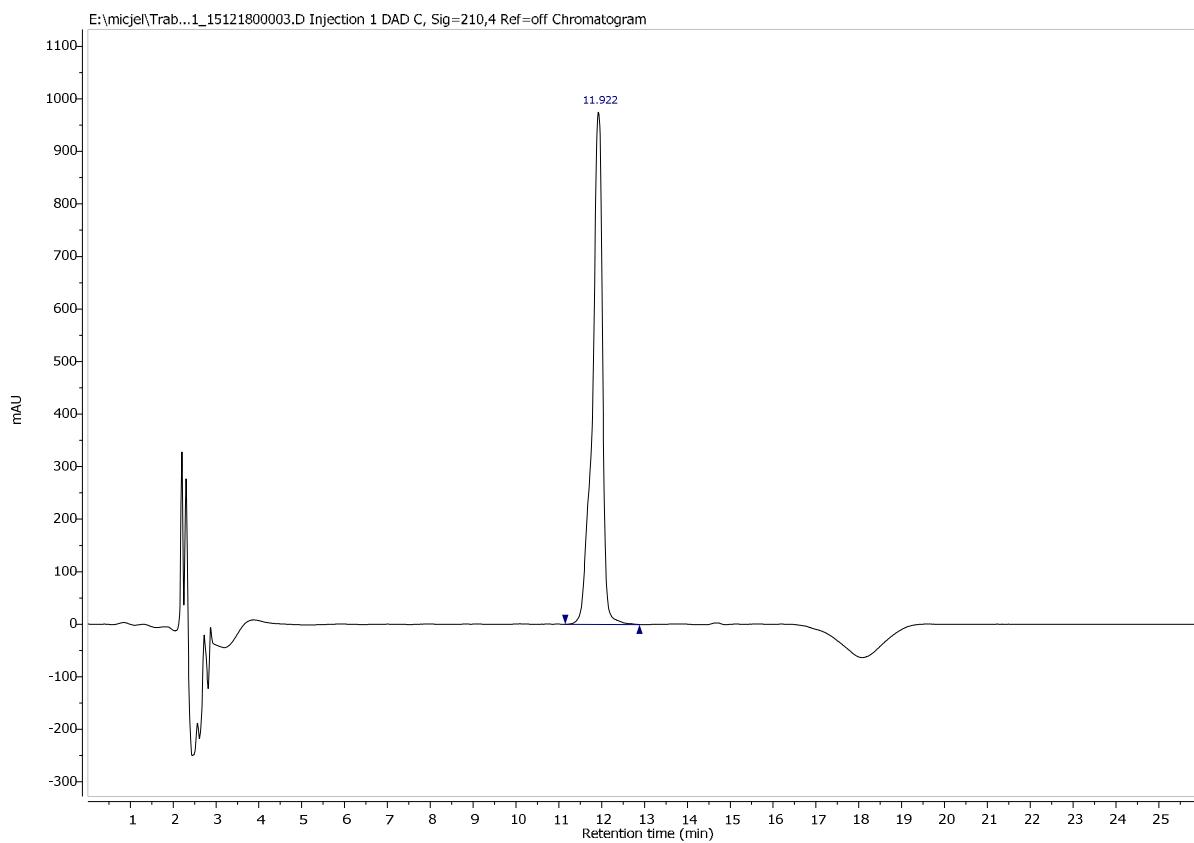


Figure 37. HPLC chromatogram of pure peptide **42**.