

A simple case study for the introduction of the HMBC and the EI-MS techniques to second and third year undergraduate students.

Supplementary Material

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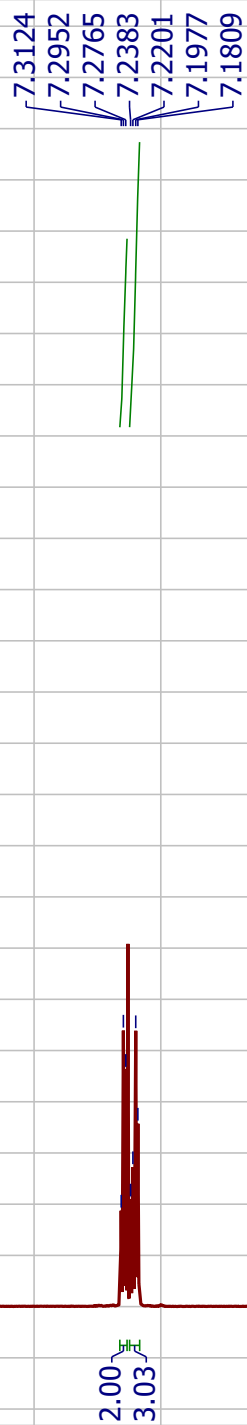
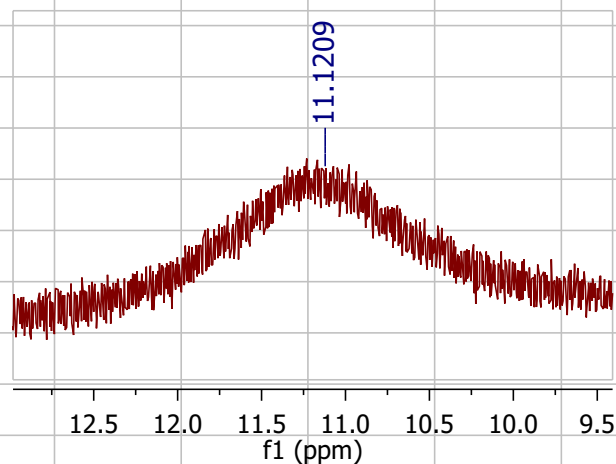
3-Phenylbutyric acid (PBA)

¹H-NMR. ¹³C-NMR, APT, COSY, HSQC, HMBC, IR, UV and Mass Spectra

α -methylhydrocinnamic acid (MHCA)

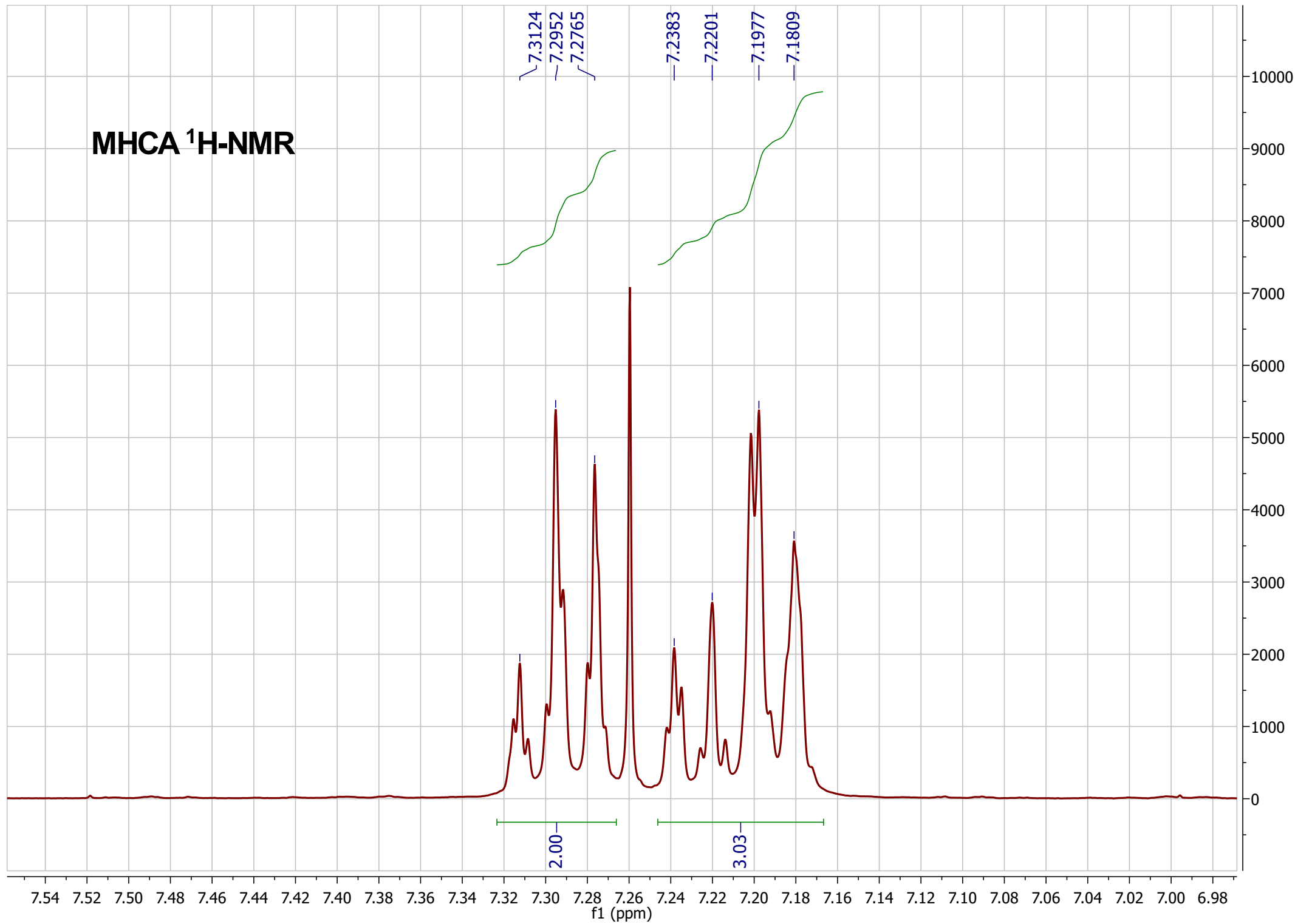
¹H-NMR. ¹³C-NMR, APT, COSY, HSQC, HMBC, IR, UV and Mass Spectra

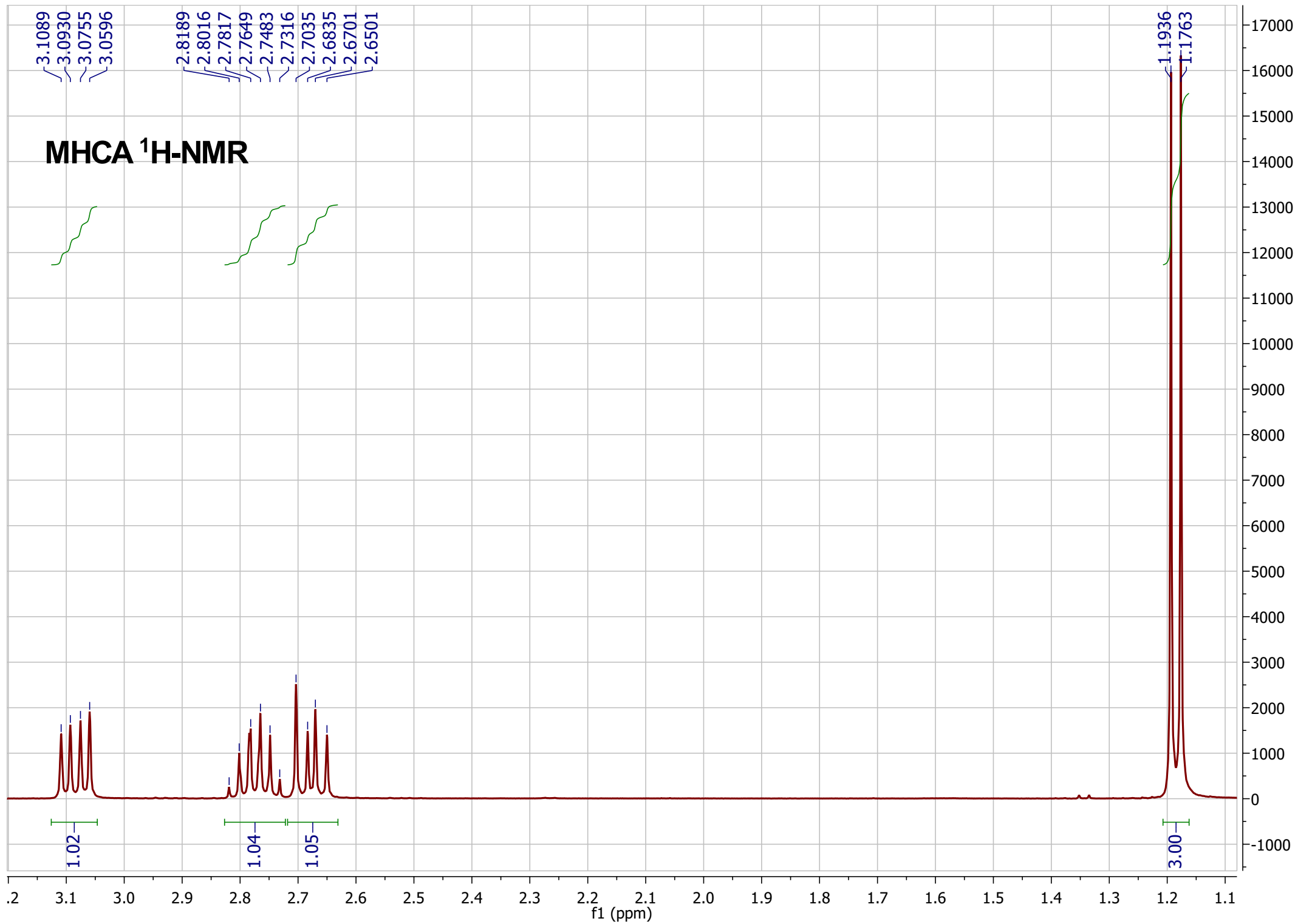
MHCA ^1H -NMR



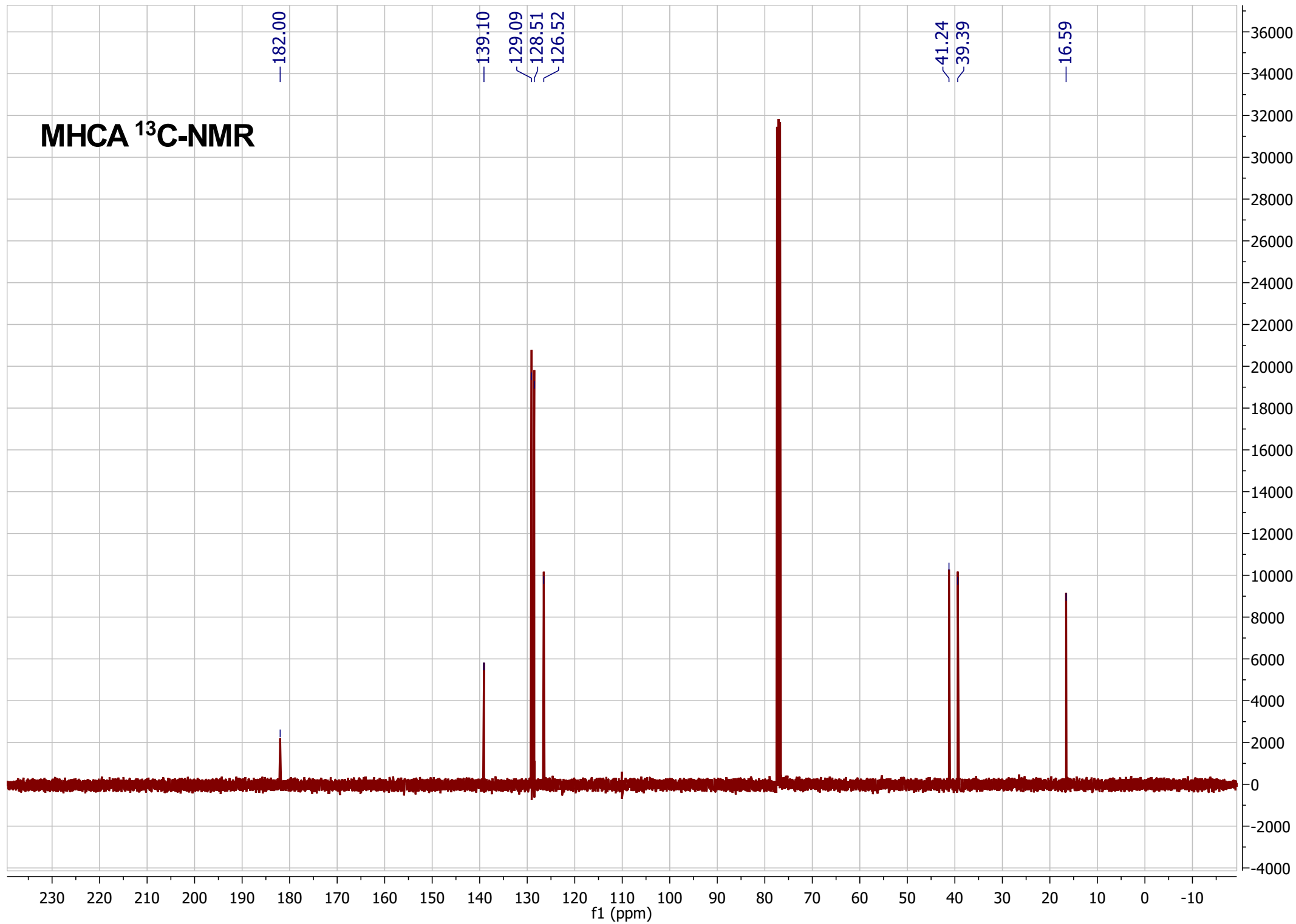
f1 (ppm)

MHCA ^1H -NMR

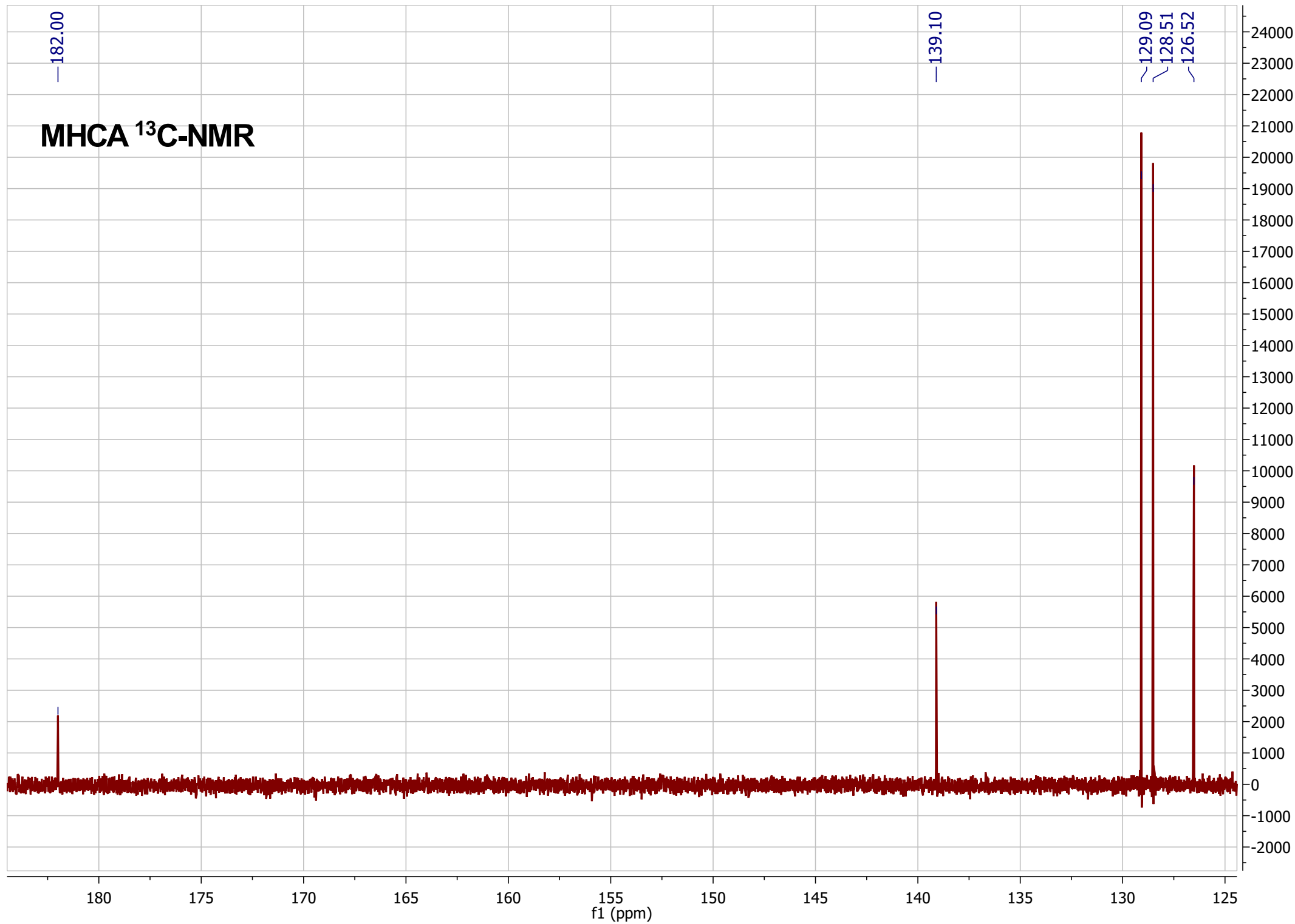




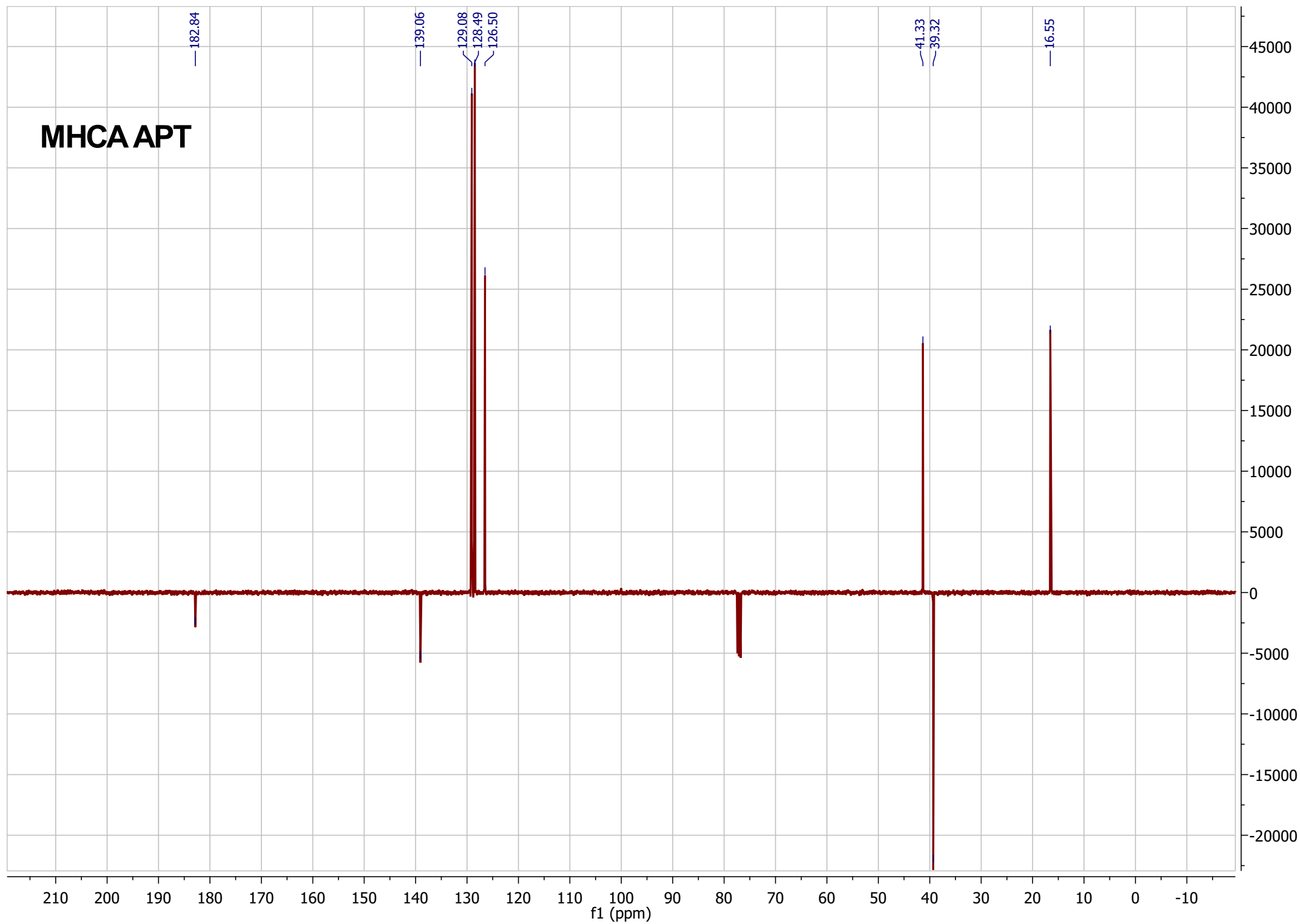
MHCA ^{13}C -NMR



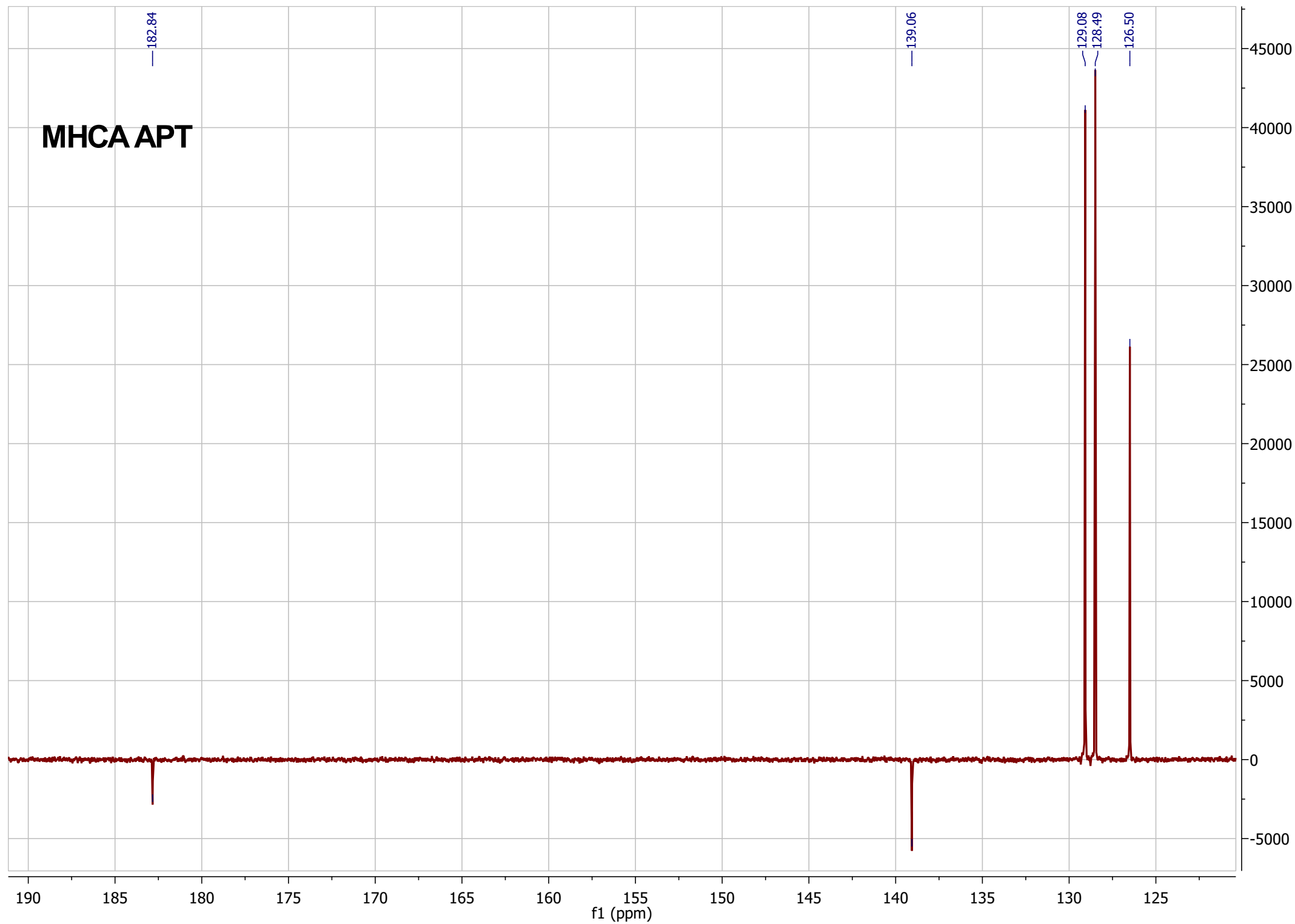
MHCA ^{13}C -NMR



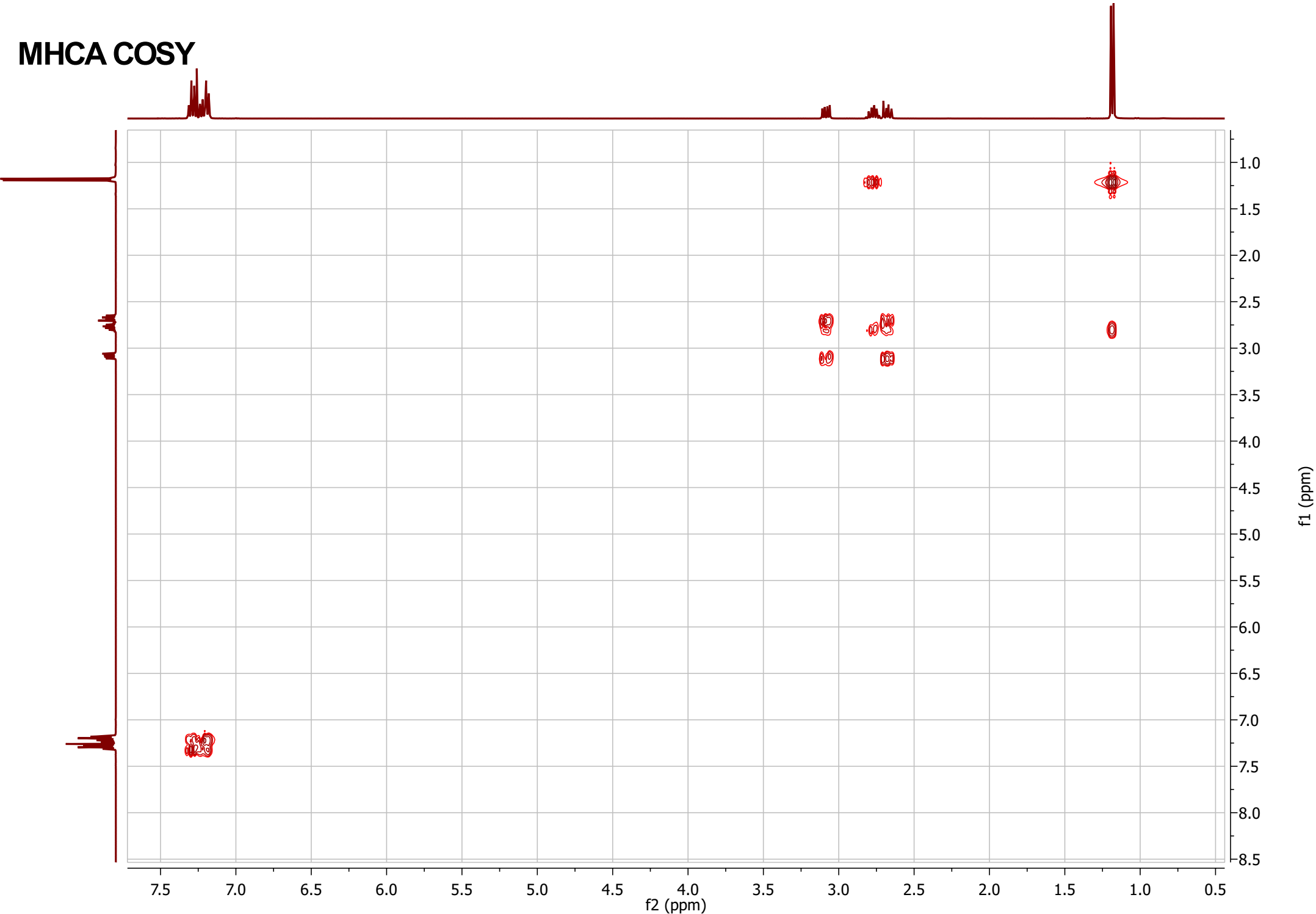
MHCA APT



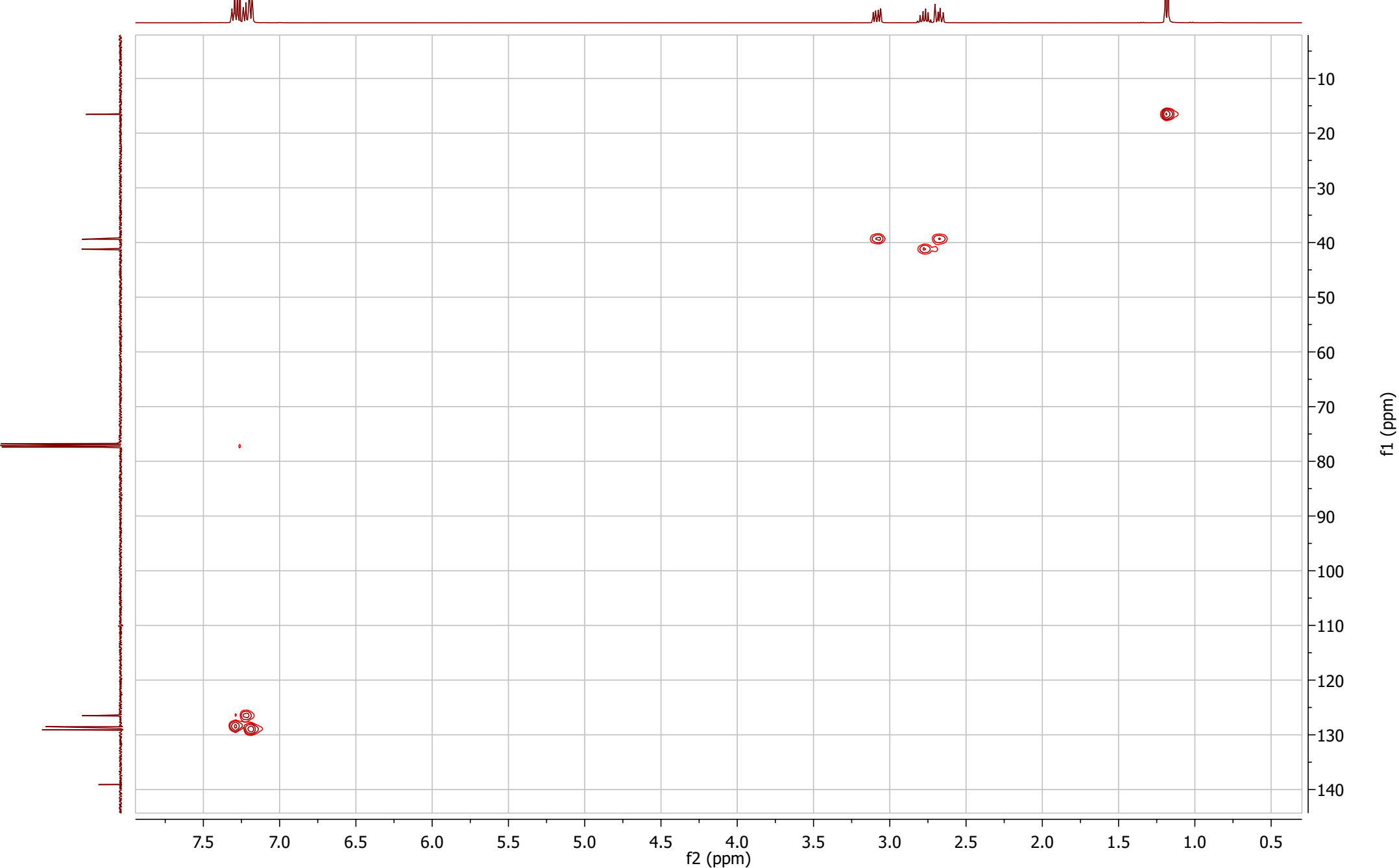
MHCA APT



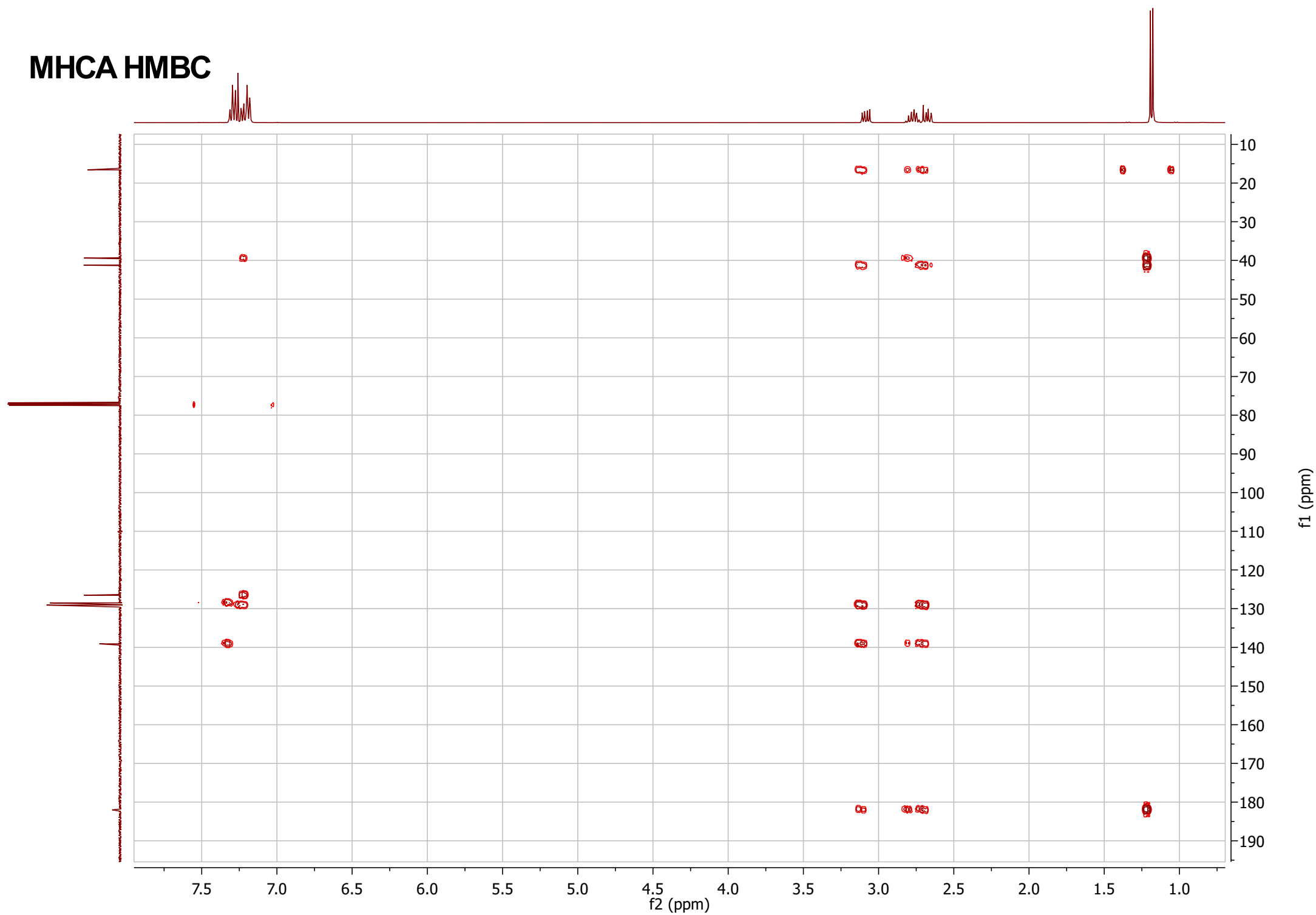
MHCA COSY



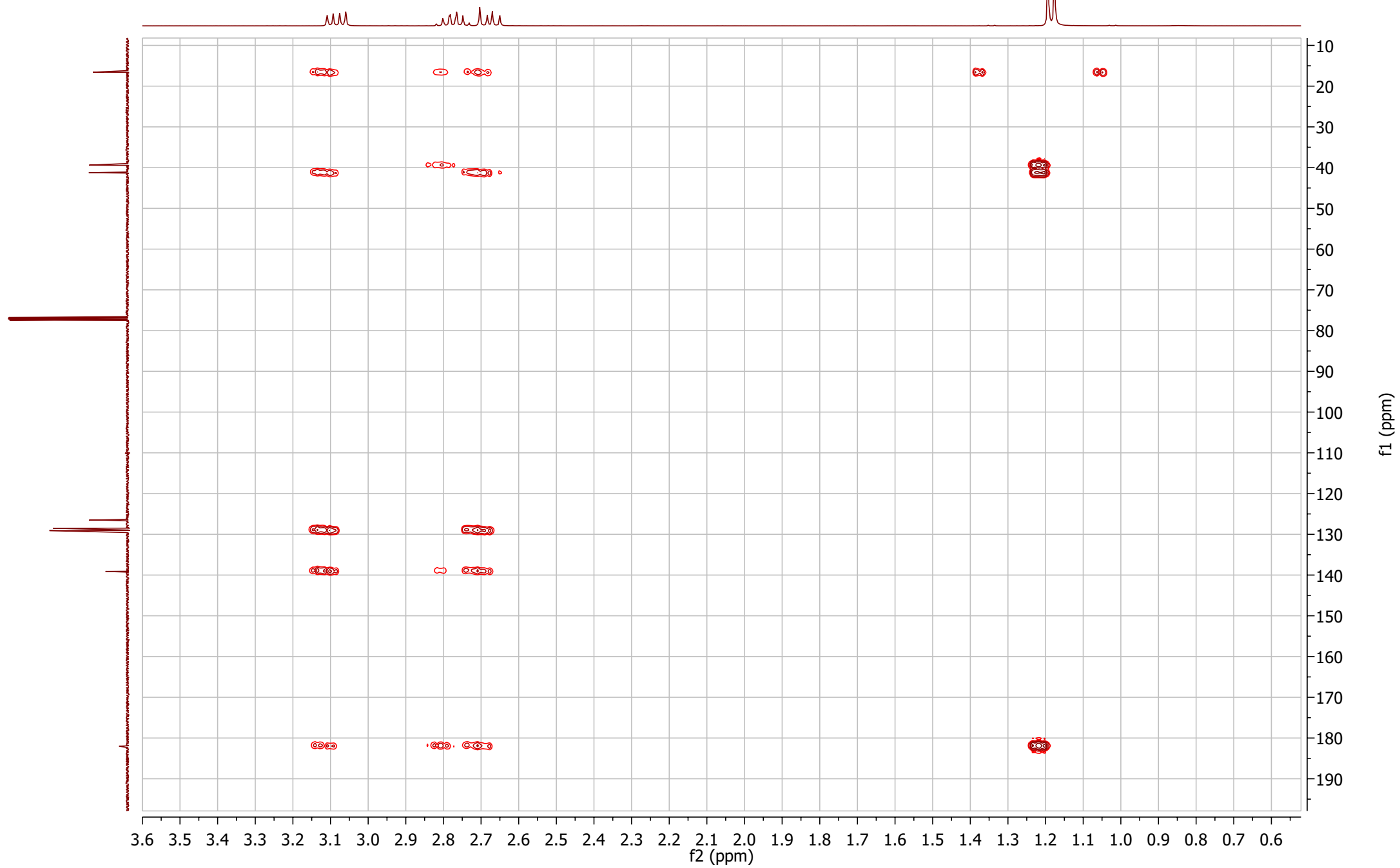
MHCA HSQC



MHCA HMBC

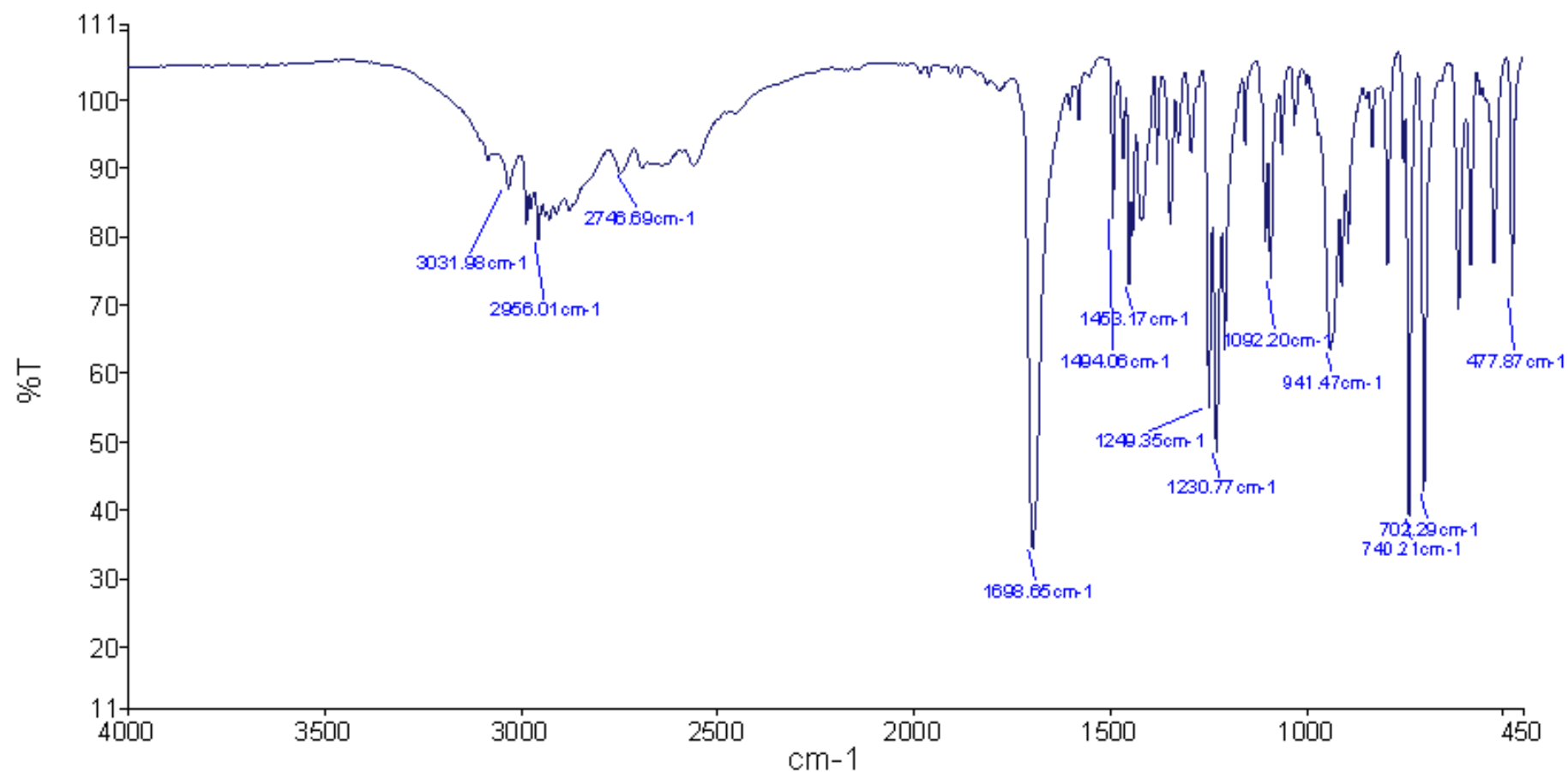


MHCA HMBC

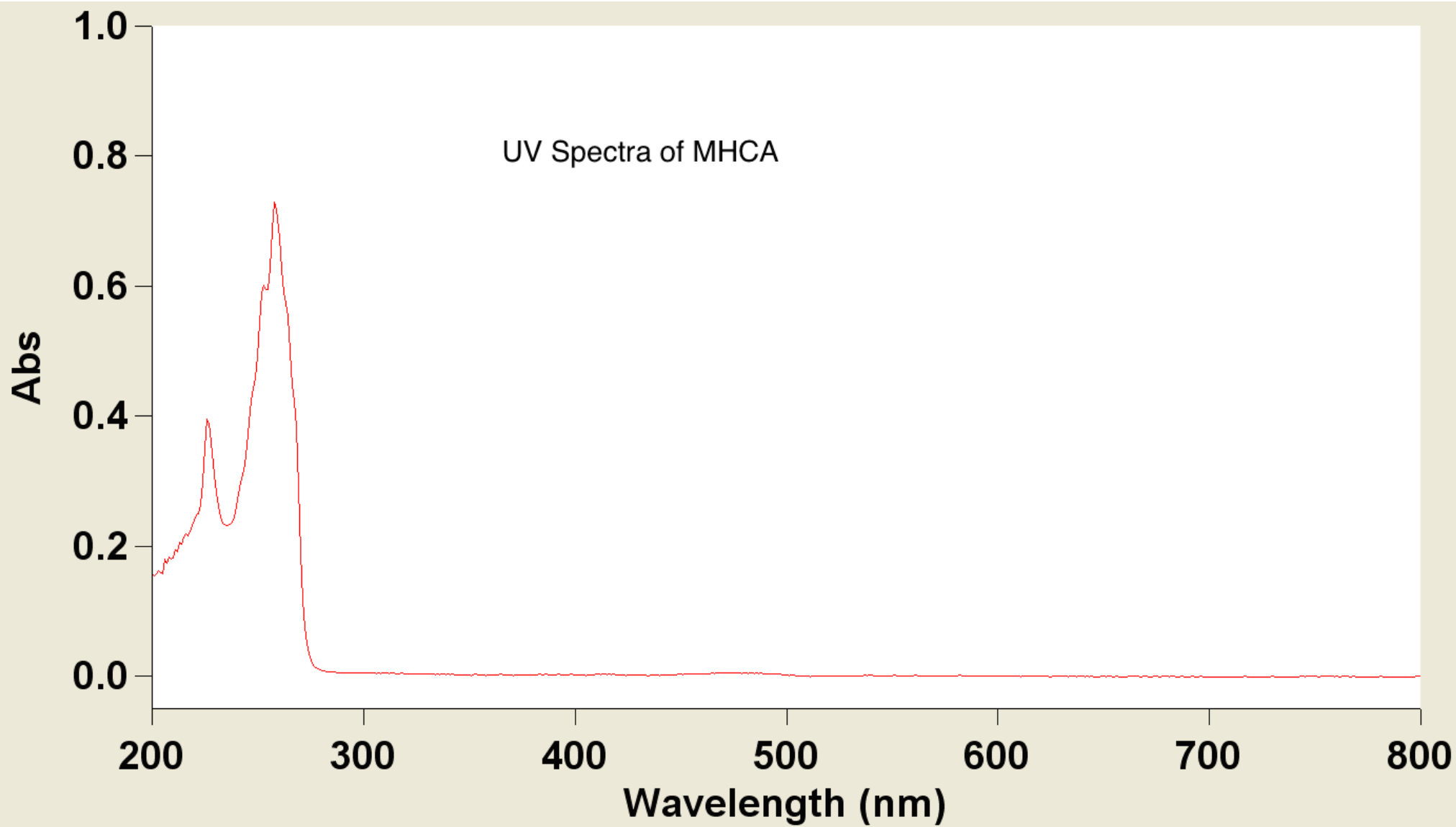


Analyst
Date

Transmission Spectra
Friday, September 18, 2015 4:04 PM

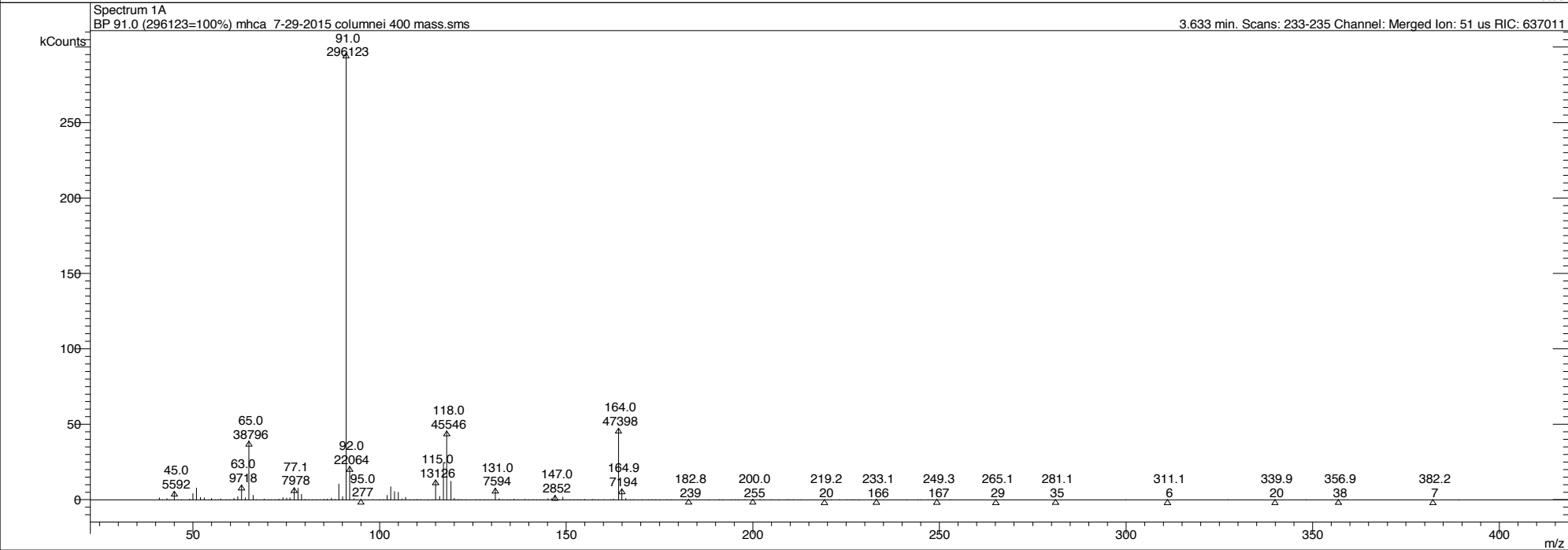
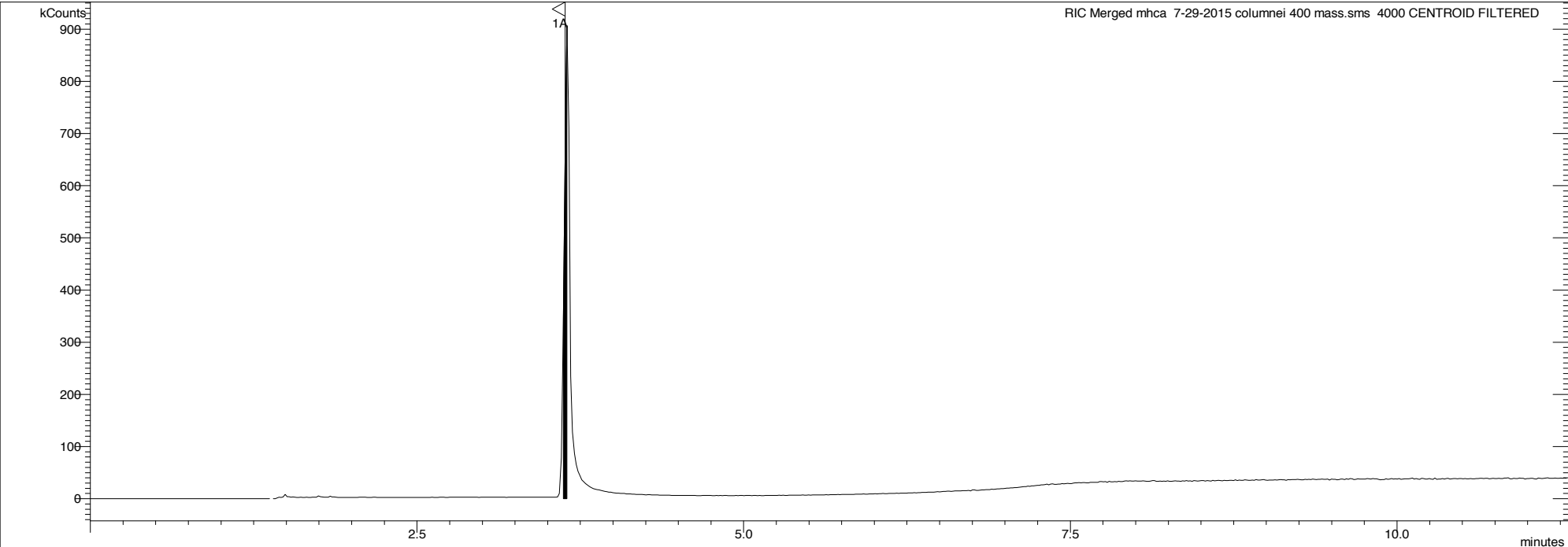


— MHCA racemic Sample 003 By Student Date Monday, June 29 2015

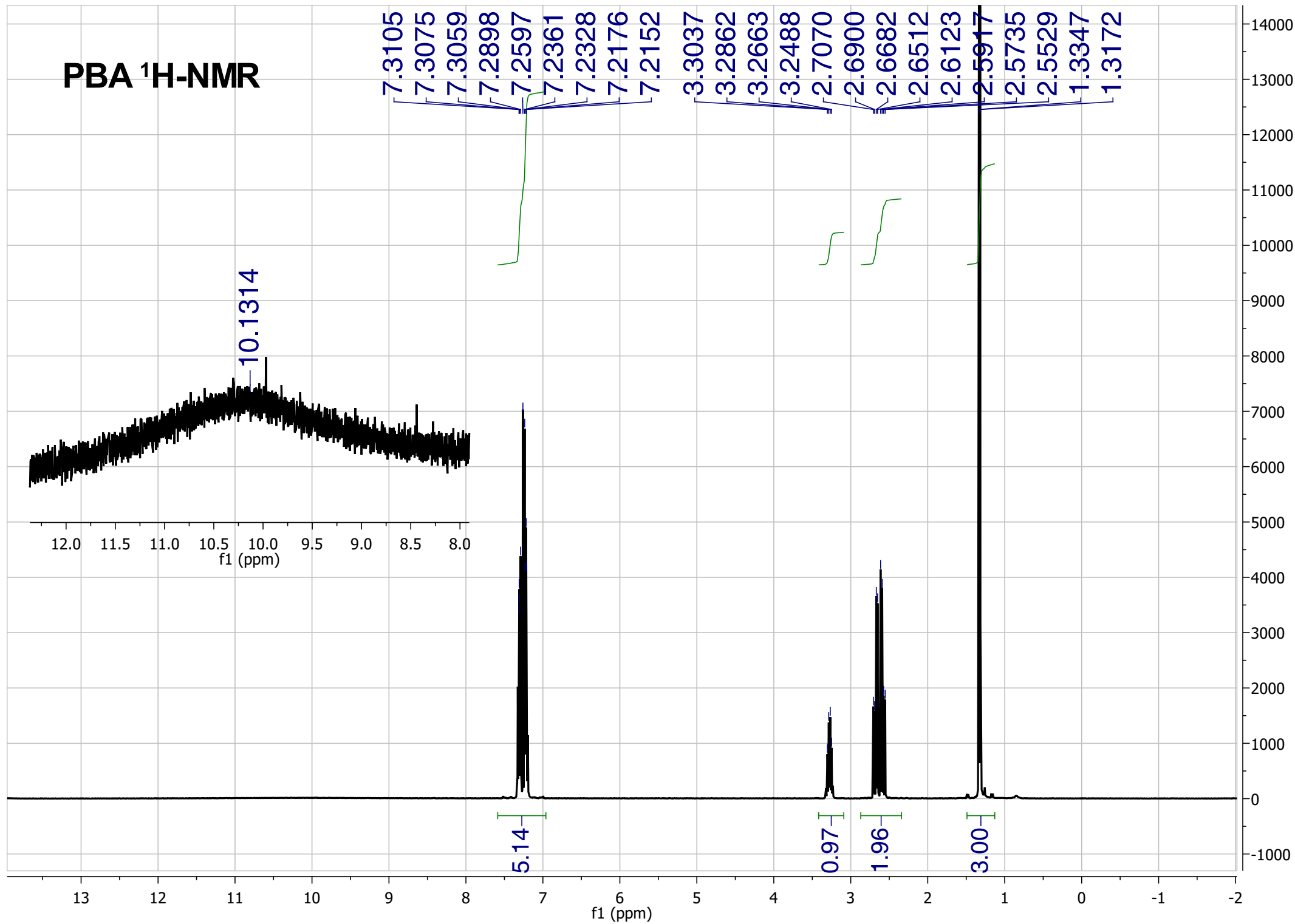


MS Data Review Active Chromatogram and Spectrum Plots - 9/18/2015 1:44 PM

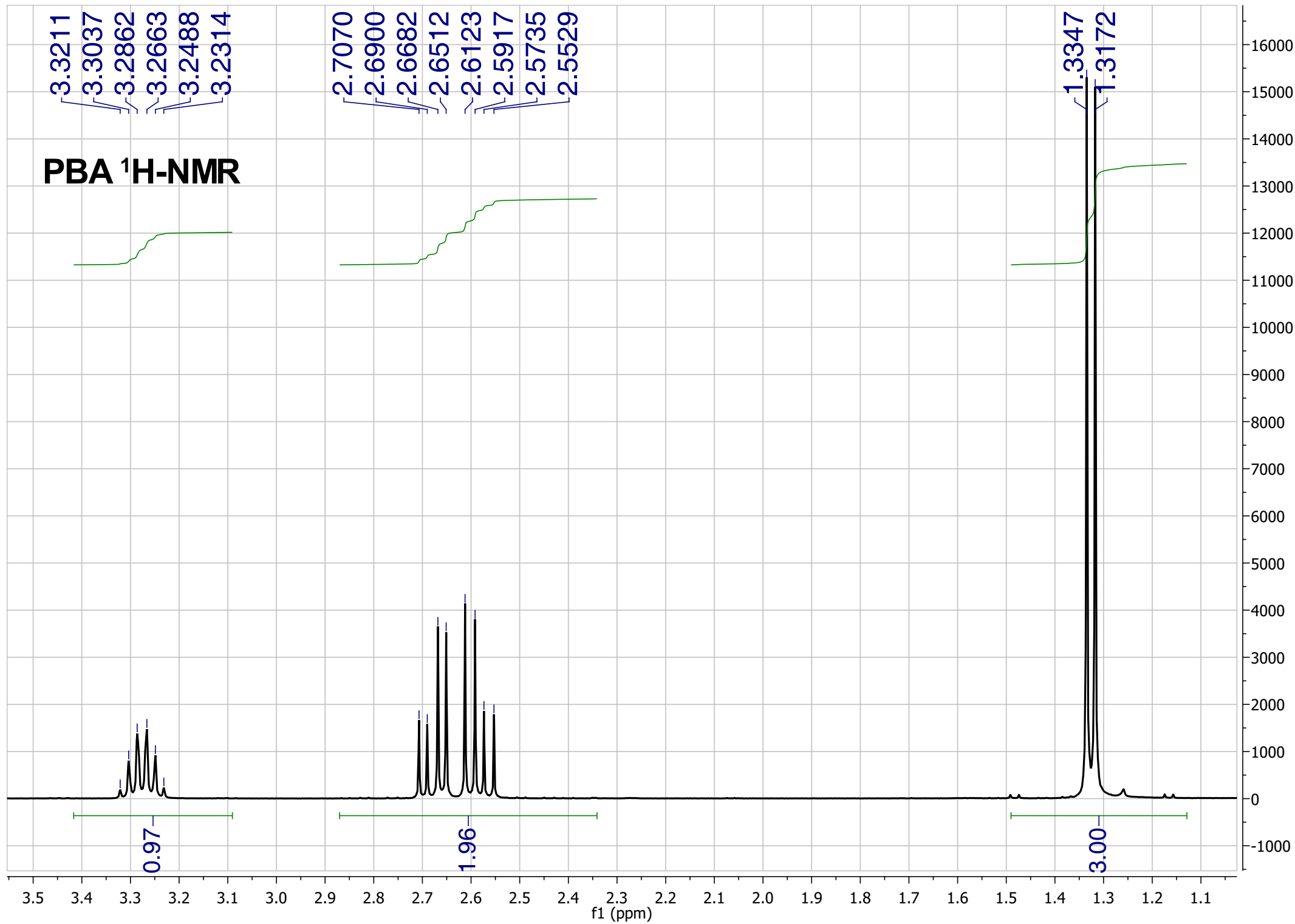
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Operator:
Date: 7/29/2015 4:20 PM



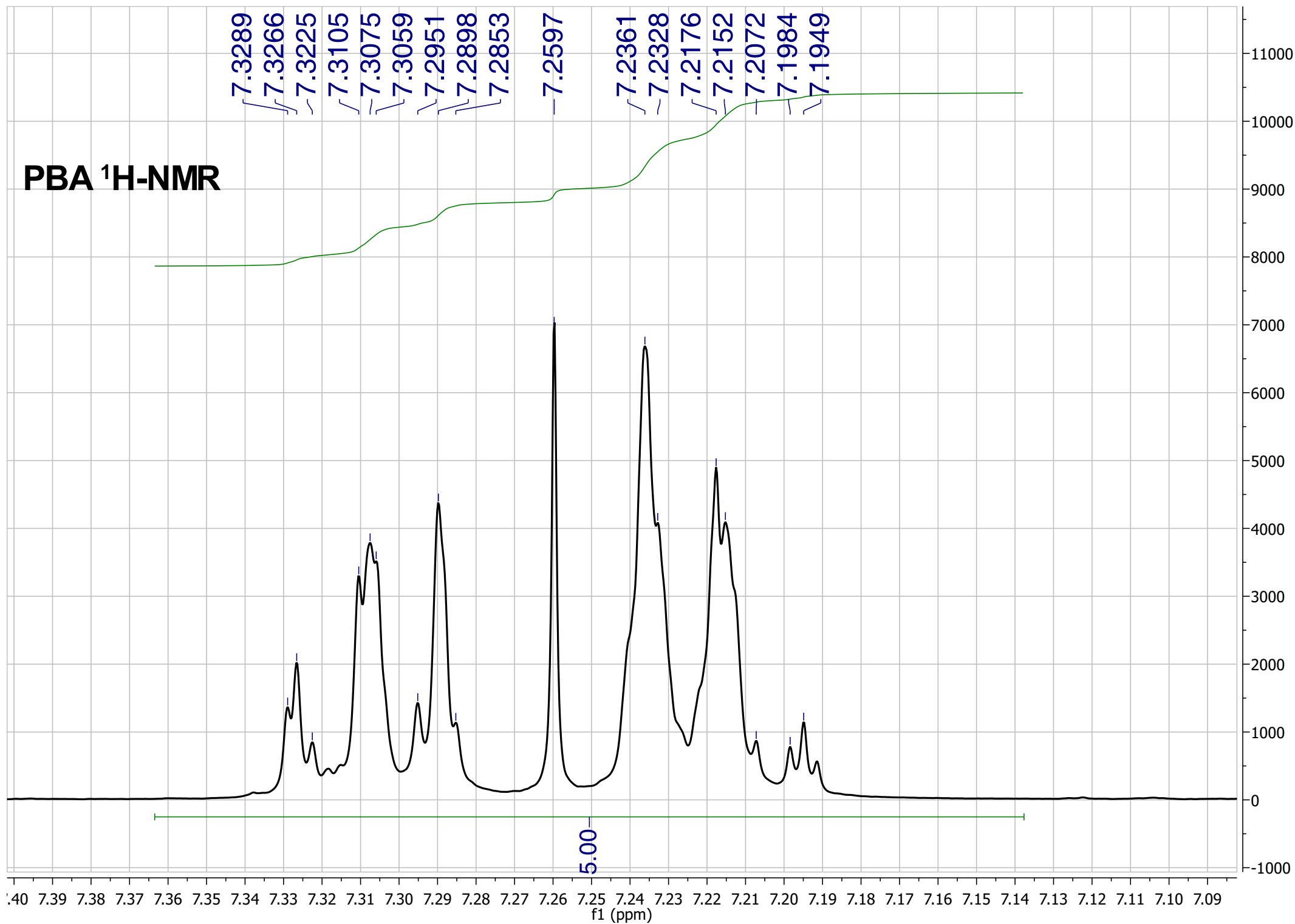
PBA ¹H-NMR



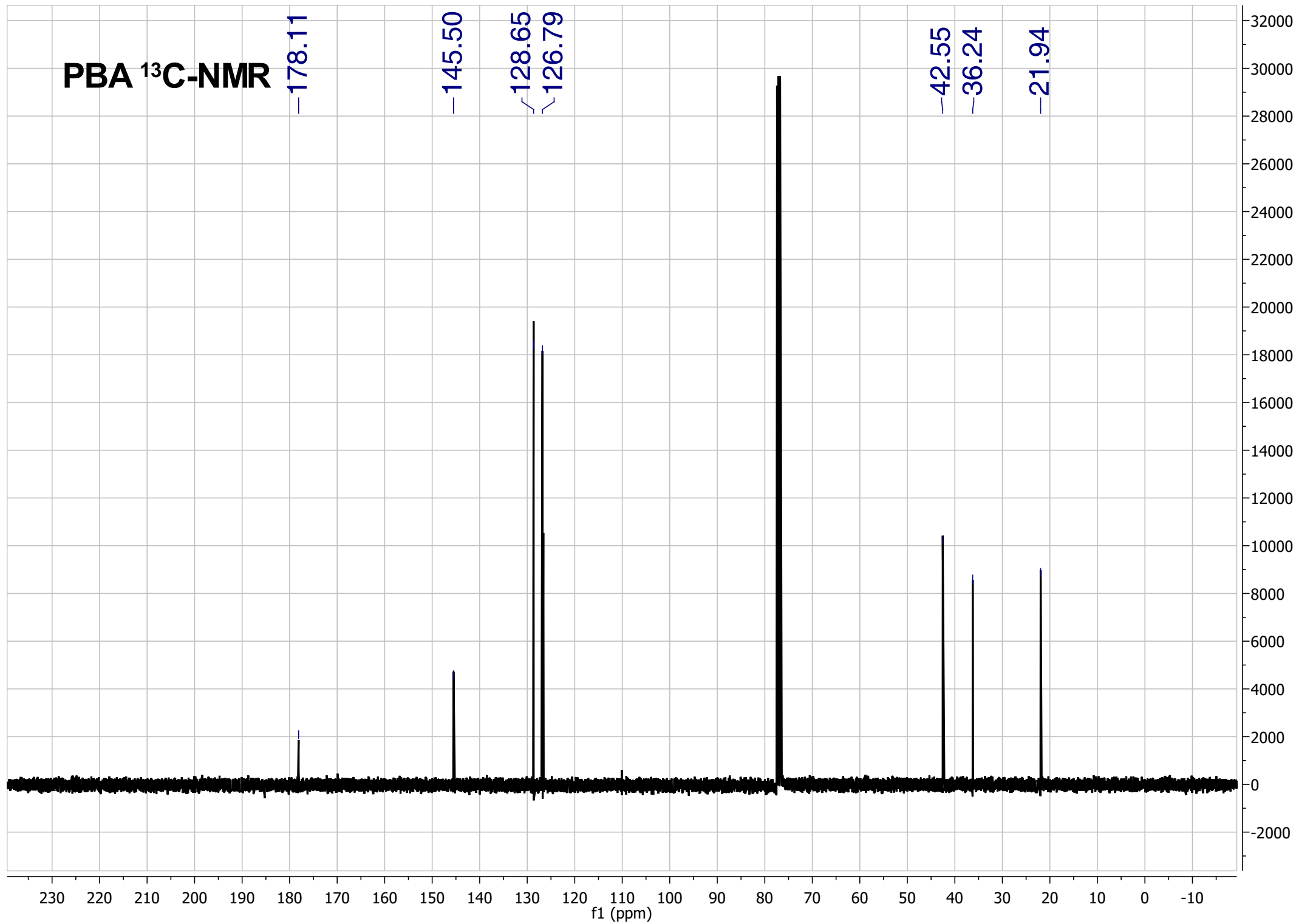
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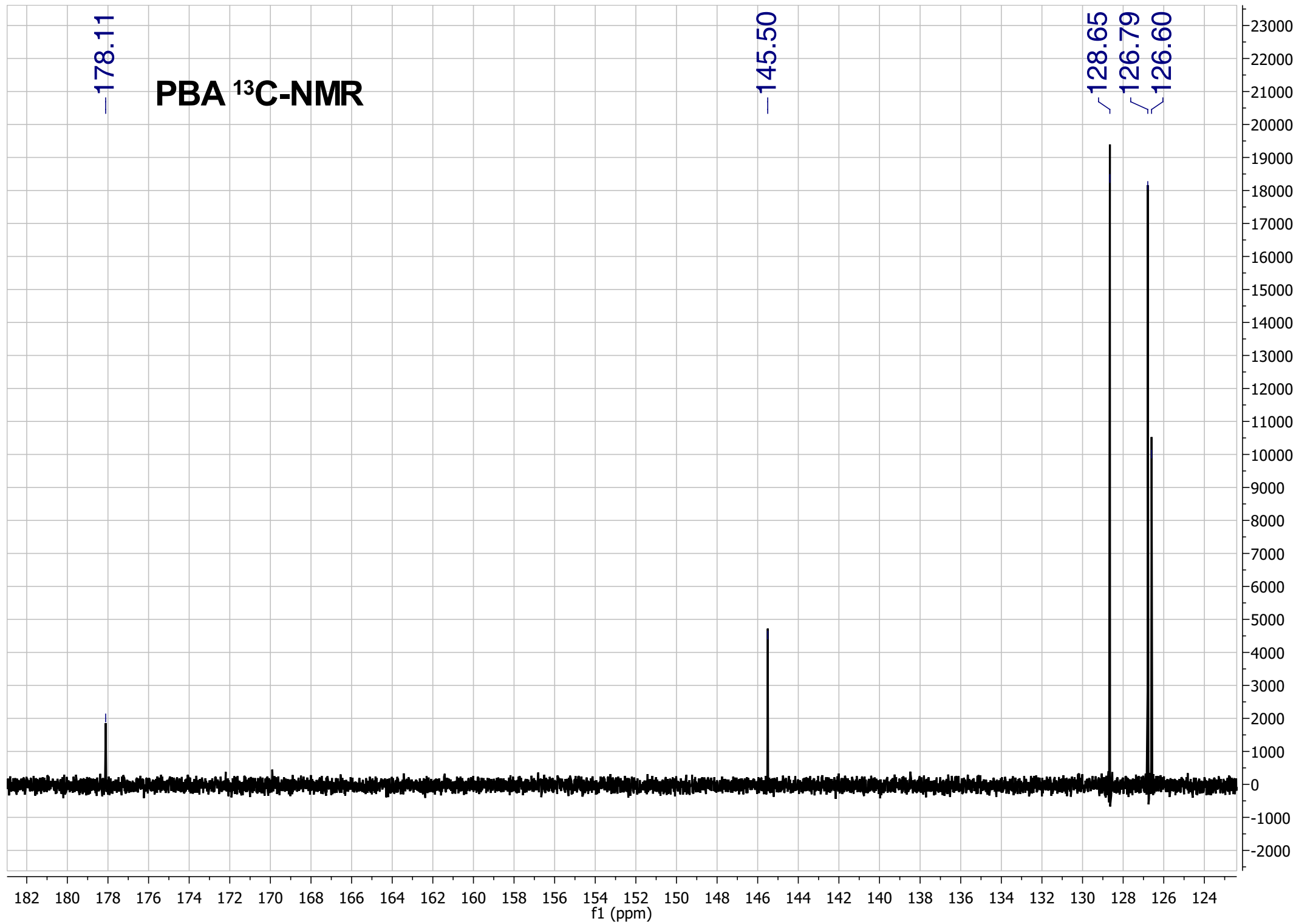
PBA ¹H-NMR



PBA ^{13}C -NMR



PBA ^{13}C -NMR



PBA APT

—179.01

—145.46

128.64

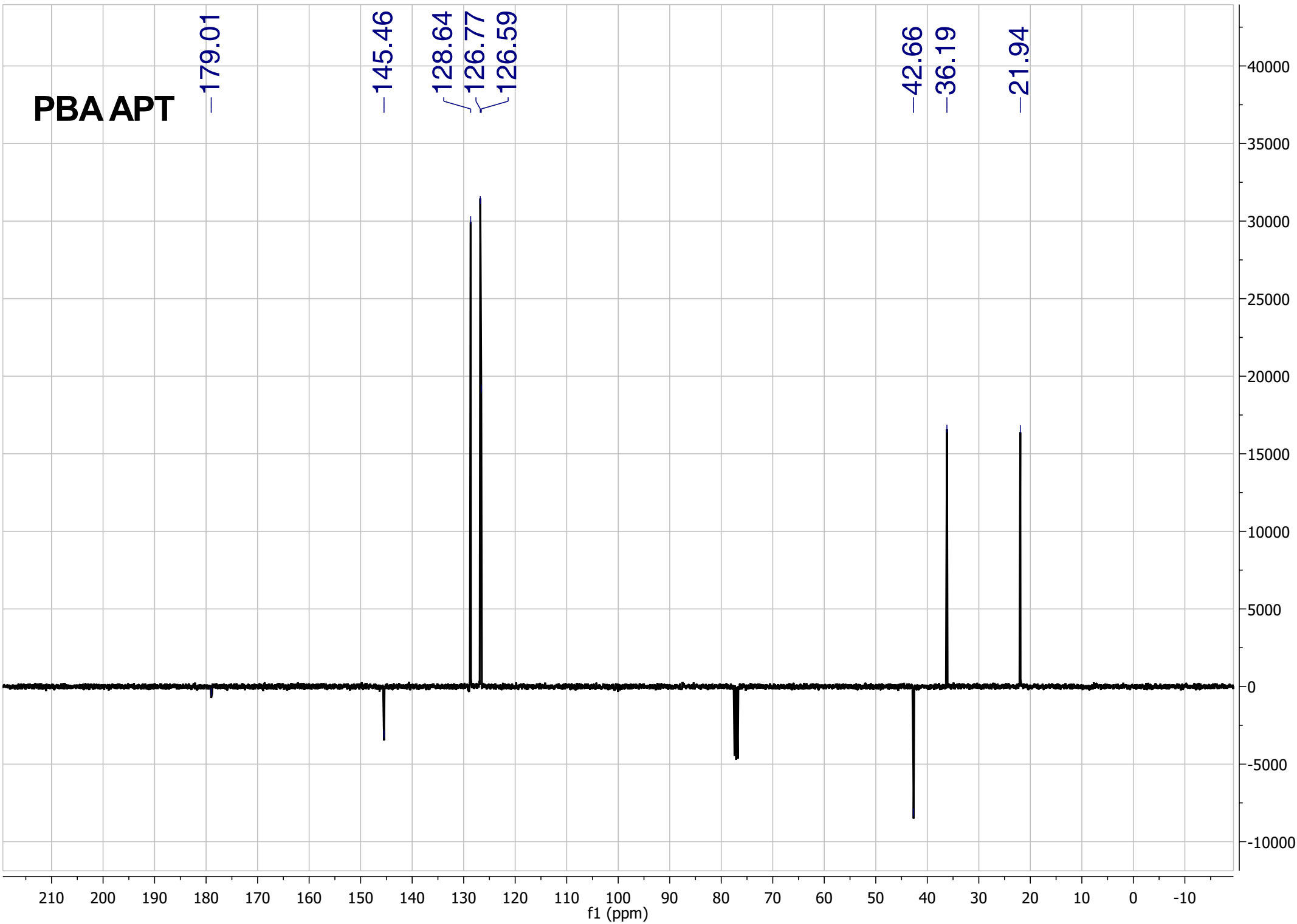
126.77

126.59

—42.66

—36.19

—21.94



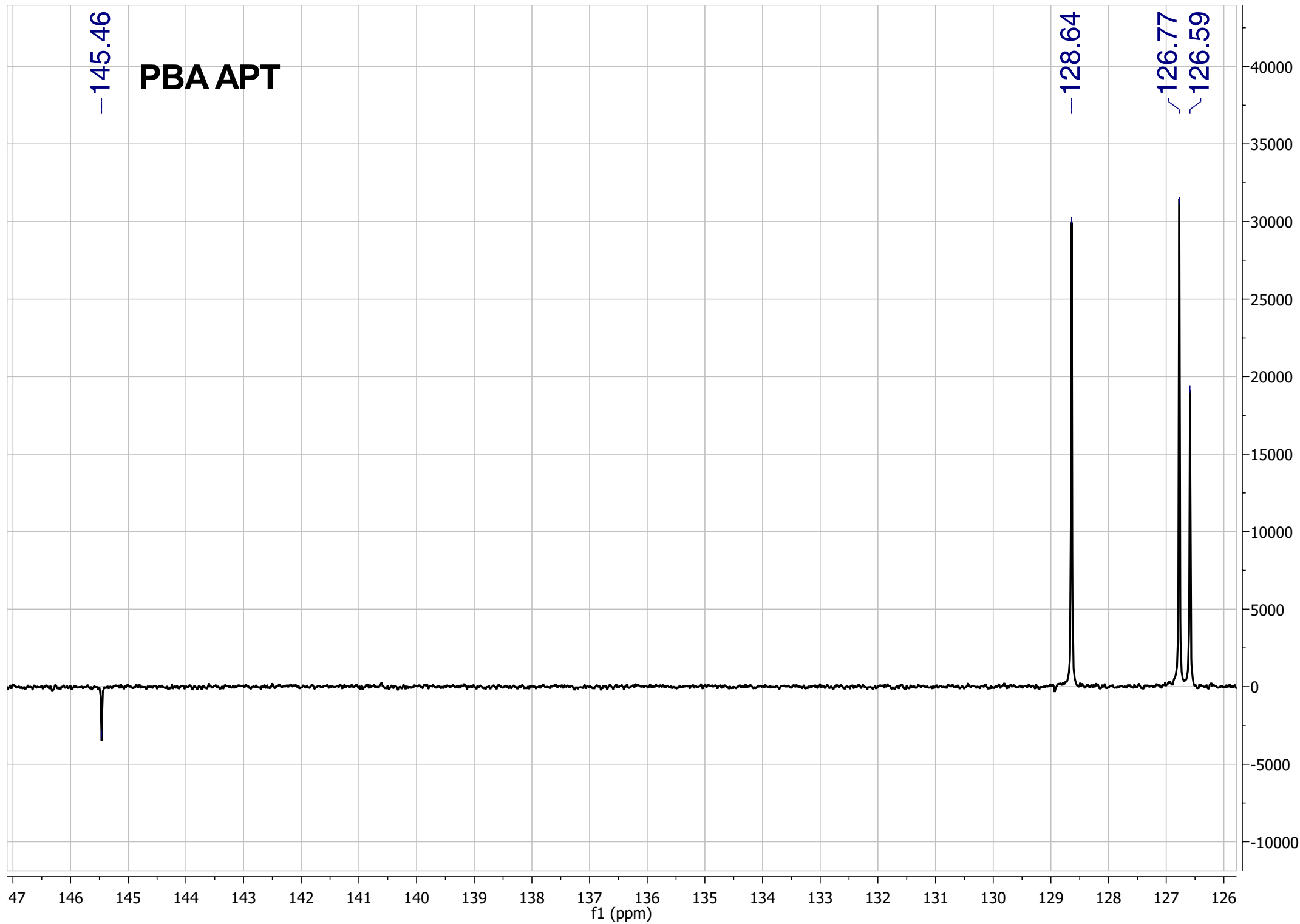
PBA APT

—145.46

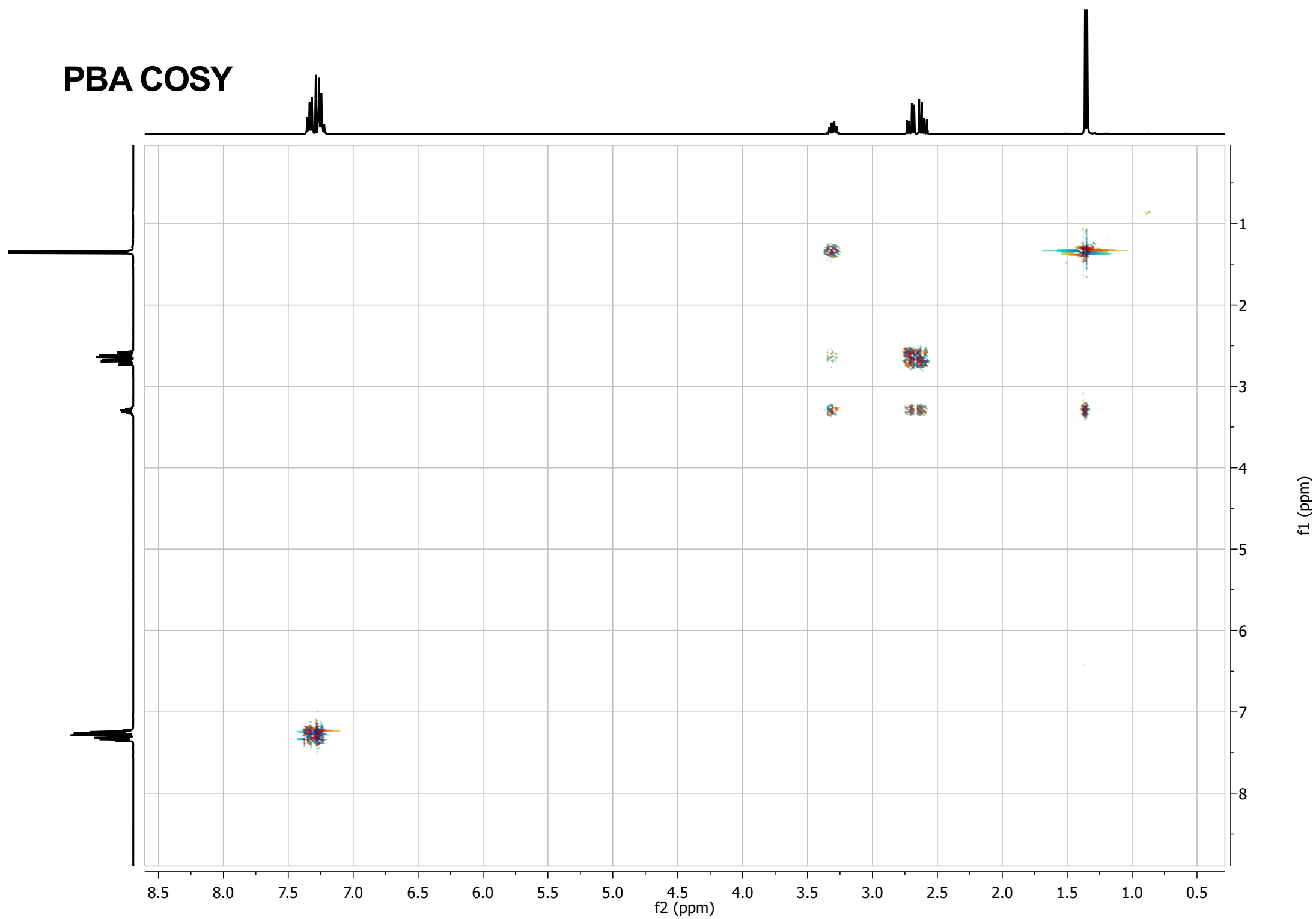
—128.64

—126.77

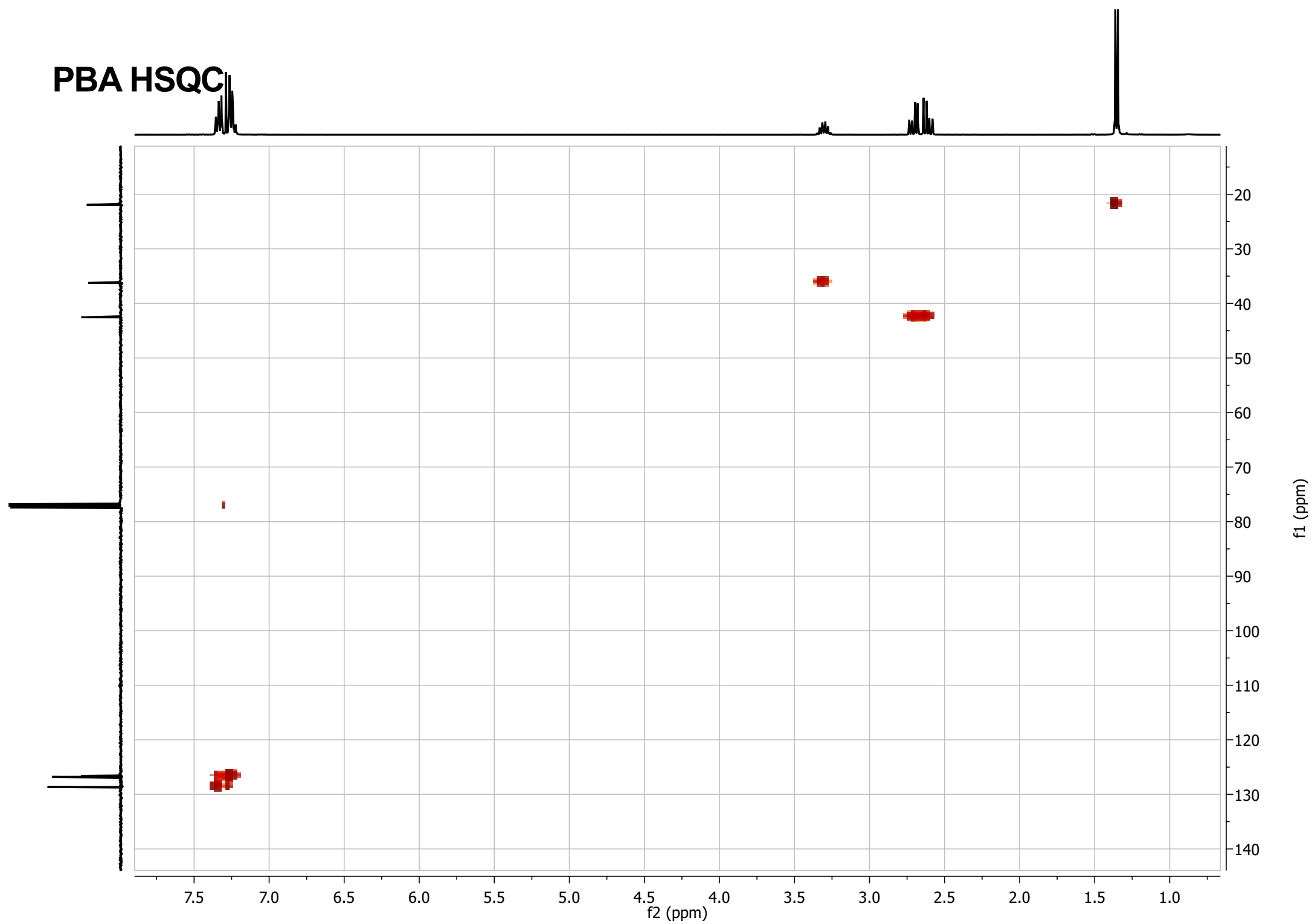
—126.59



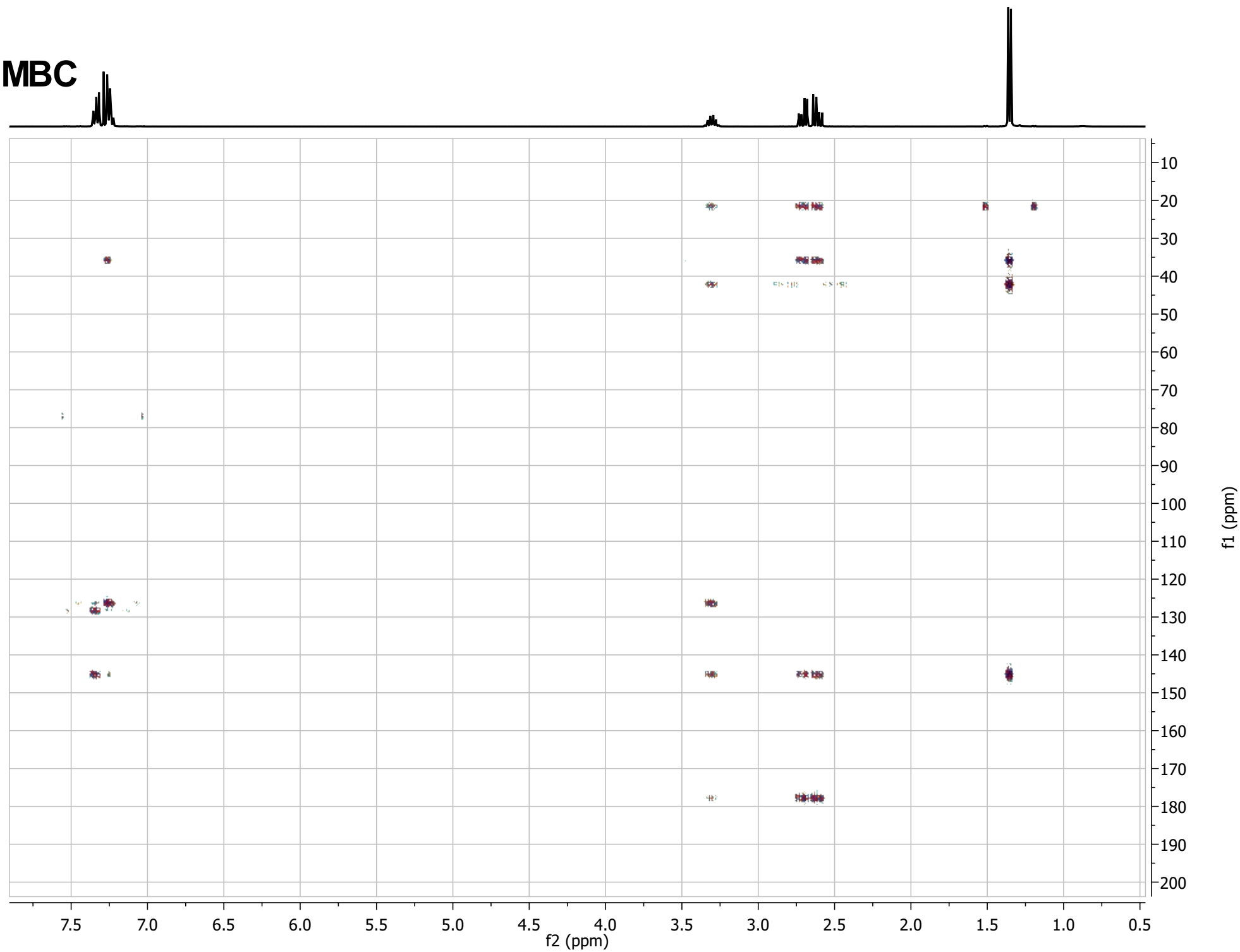
PBA COSY



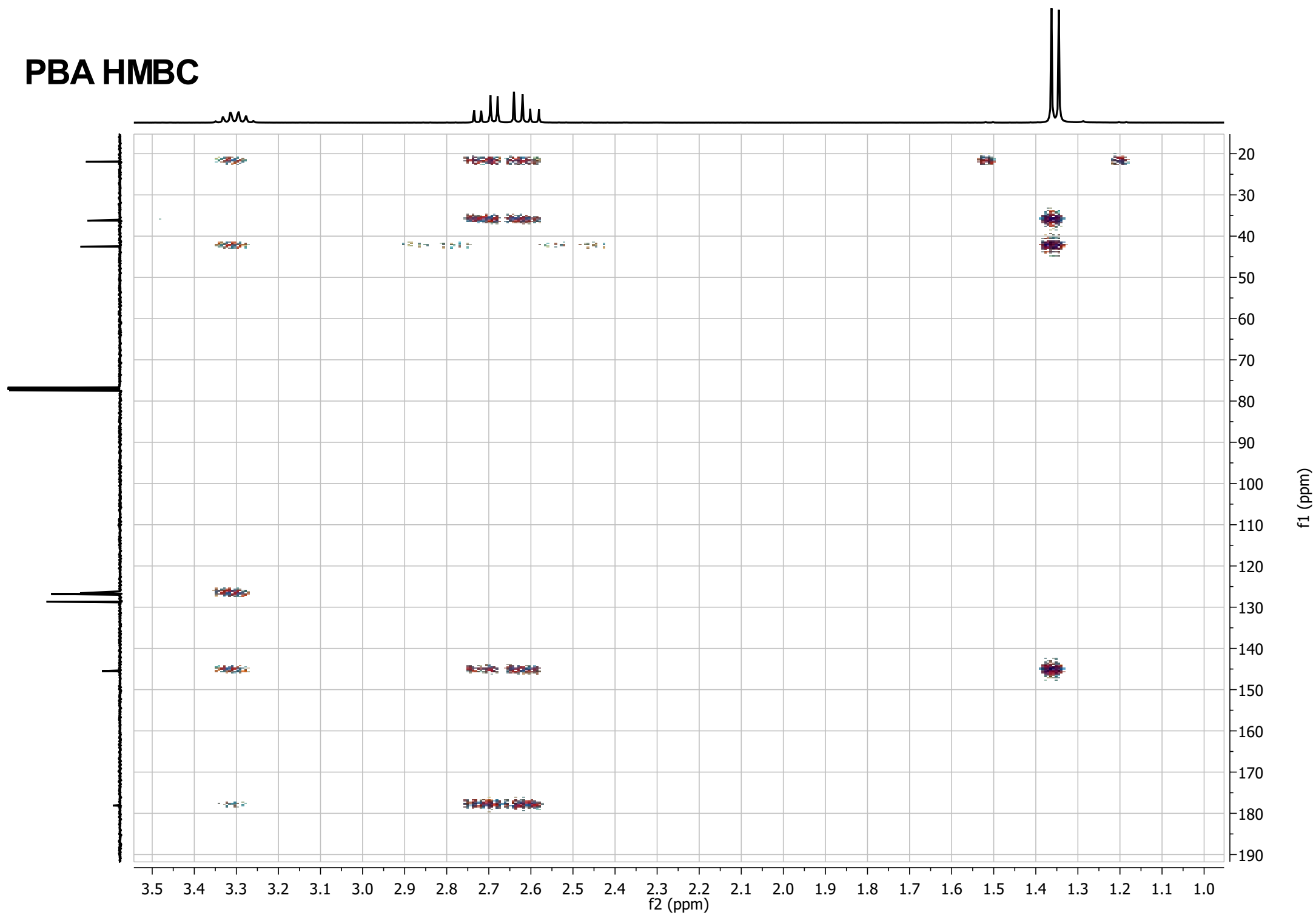
PBA HSQC



PBA HMBC

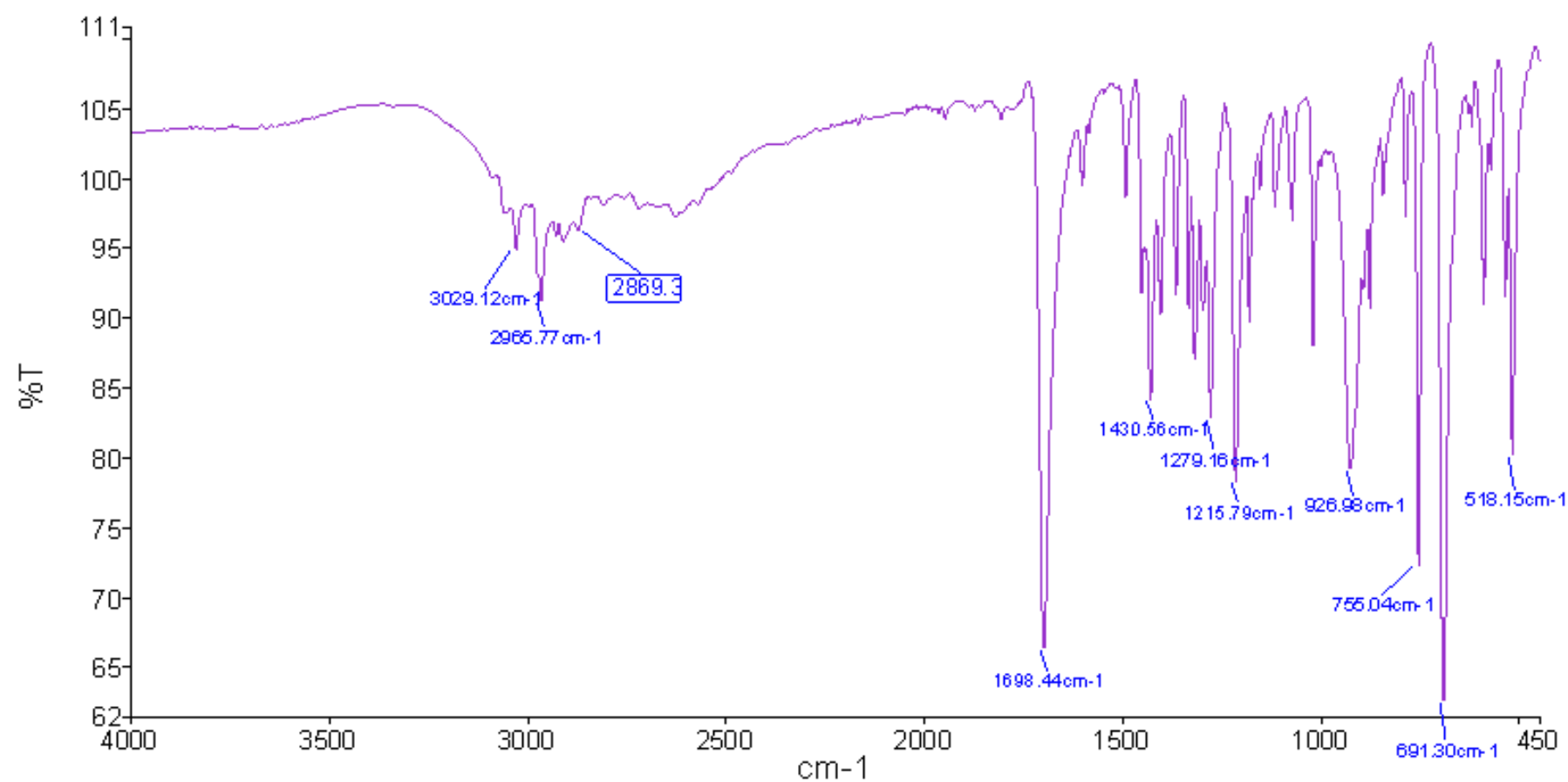


PBA HMBC

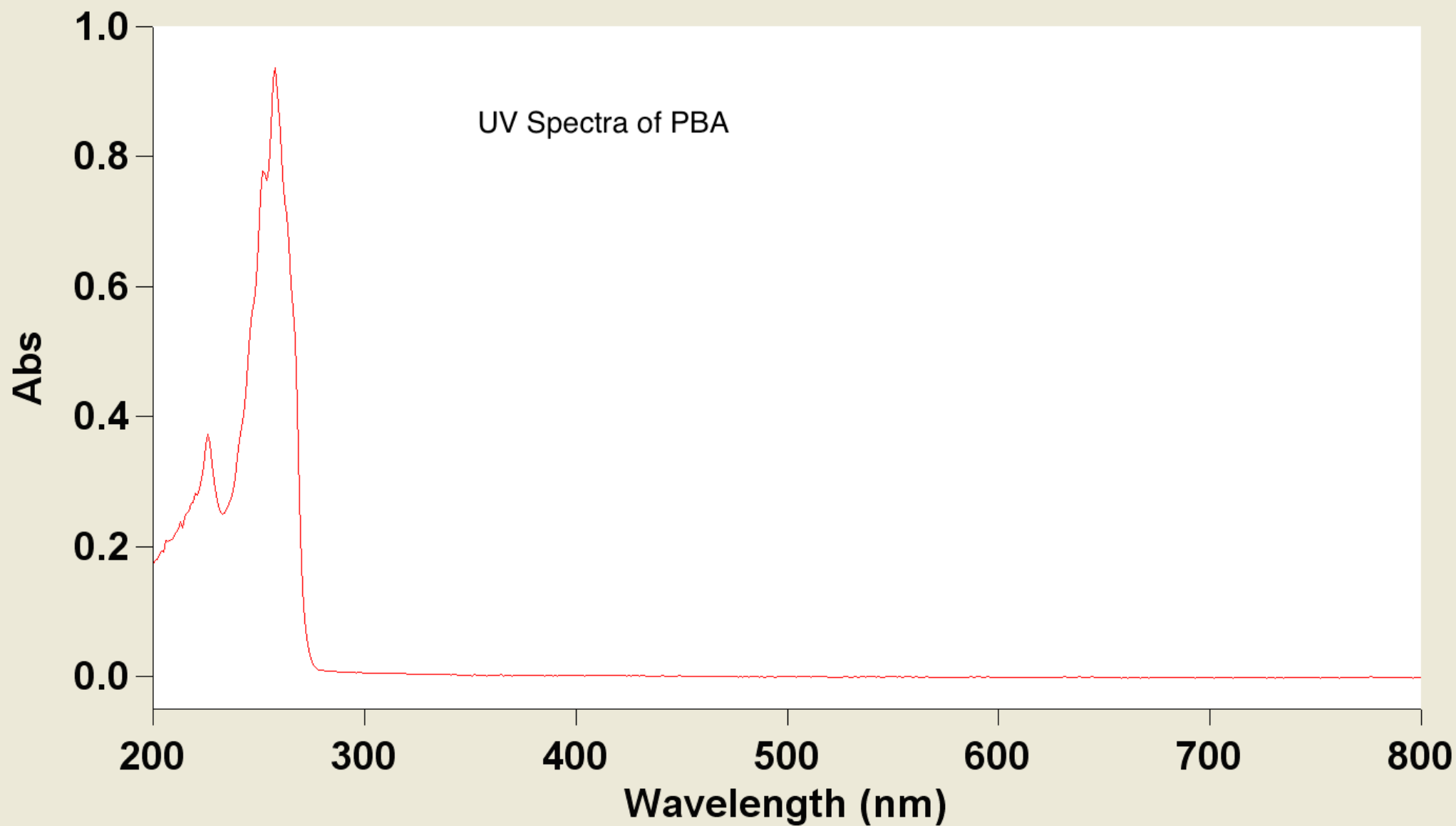


Analyst
Date

Transmission Spectra
Friday, September 18, 2015 4:00 PM



— PBA racemic Sample 004 By Student Date Monday, June 29 2015



MS Data Review Active Chromatogram and Spectrum Plots - 9/18/2015 1:46 PM

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Date: 7/29/2015 4:01 PM

