

Supporting Information- File 2

for

Synthesis of a leopolic acid-inspired tetramic acid with antimicrobial activity against multidrug-resistant bacteria

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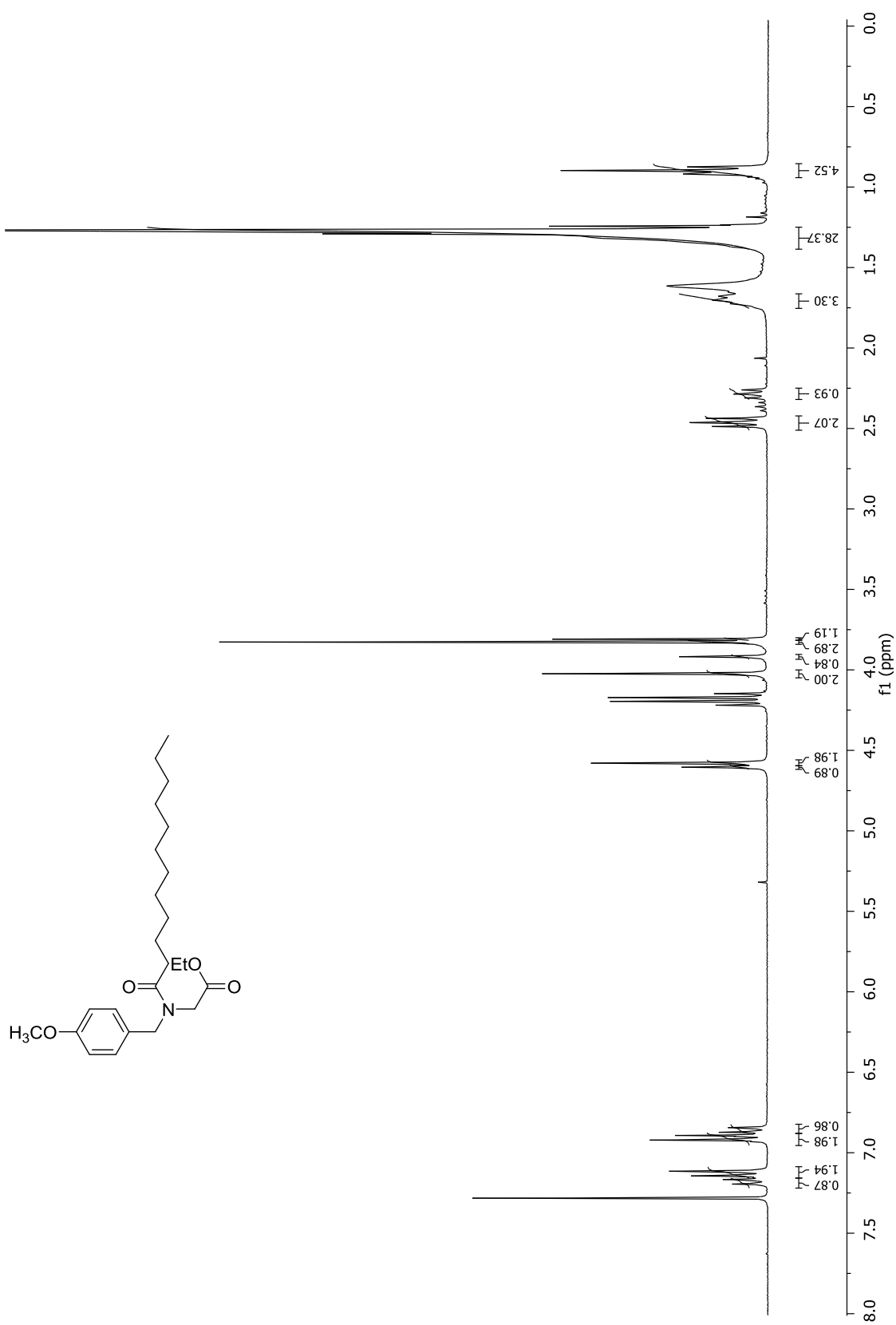
¹H NMR and ¹³C NMR spectra of the new compounds; COSY spectra of compounds **1**, **10**; HDMS spectra of compound **1**

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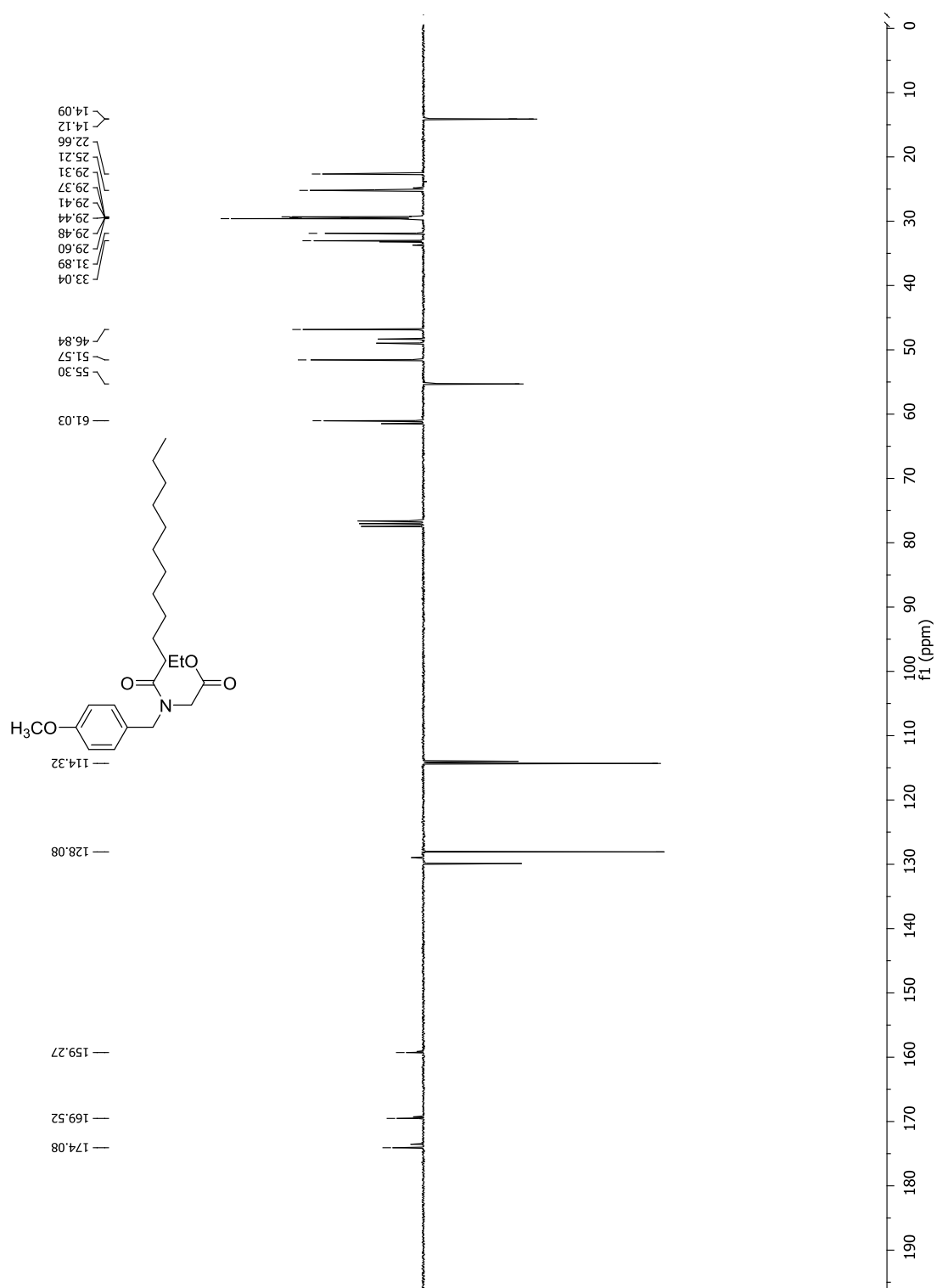
¹ H-NMR Spectrum of compound 9	S1
¹³ C-NMR Spectrum of compound 9	S2
¹ H-NMR Spectrum of compound 10	S3
¹³ C-NMR Spectrum of compound 10	S4
COSY Spectrum of compound 10	S5
¹ H-NMR Spectrum of compound 11	S6
¹ H-NMR Spectrum of compound 12	S7
¹³ C-NMR Spectrum of compound 12	S8

¹ H-NMR Spectrum of compound 13	S9
¹³ C-NMR Spectrum of compound 13	S10
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¹³ C-NMR Spectrum of compound 18	S12
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¹³ C-NMR Spectrum of compound 21	S18
¹ H-NMR Spectrum of compound 1	S19
¹³ C-NMR Spectrum of compound 1	S20
COSY Spectrum of compound 1	S21
MS Spectrum of compound 1	S22

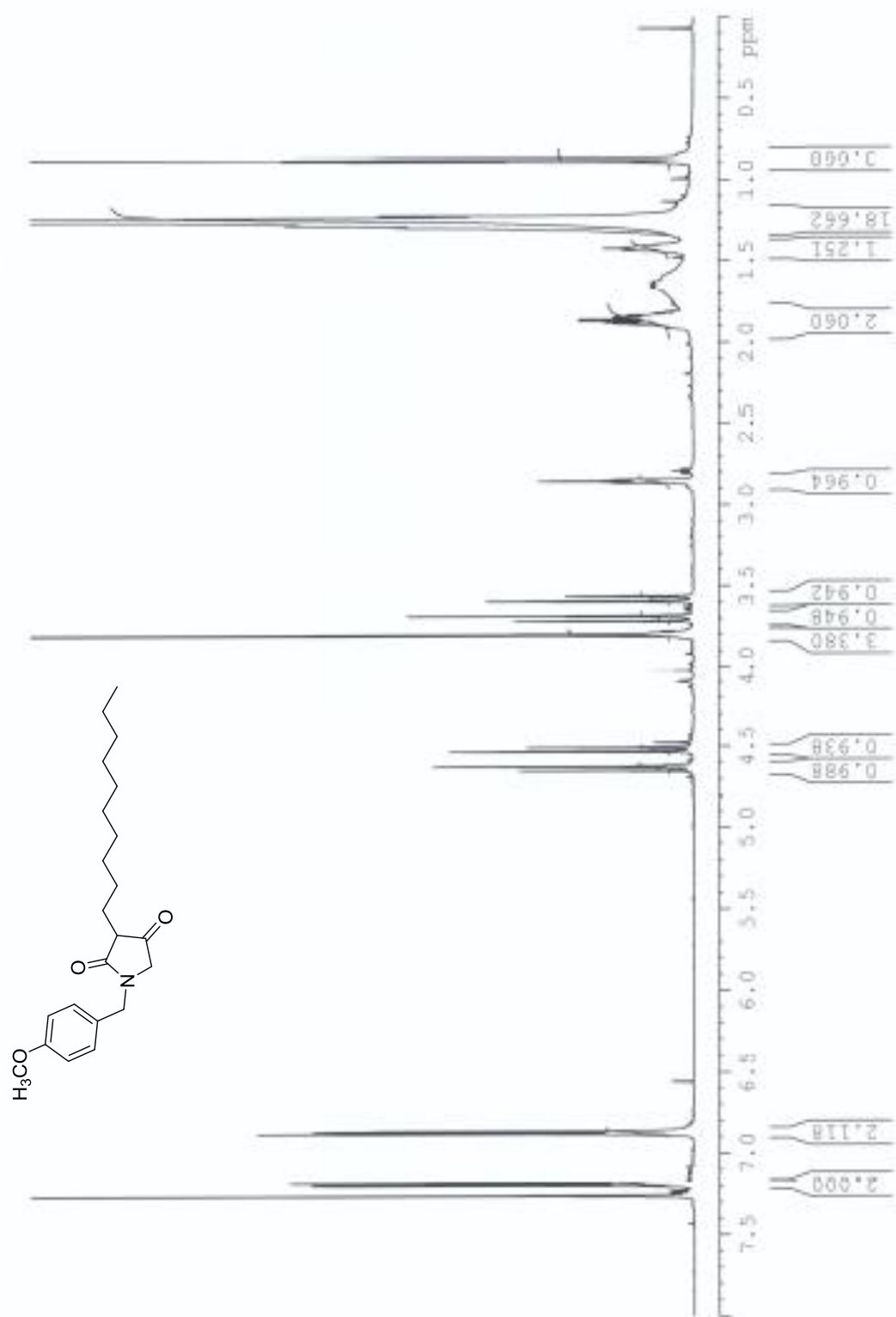
^1H -NMR (300 MHz, CDCl_3) spectrum of compound **9** (mixture of rotamers)



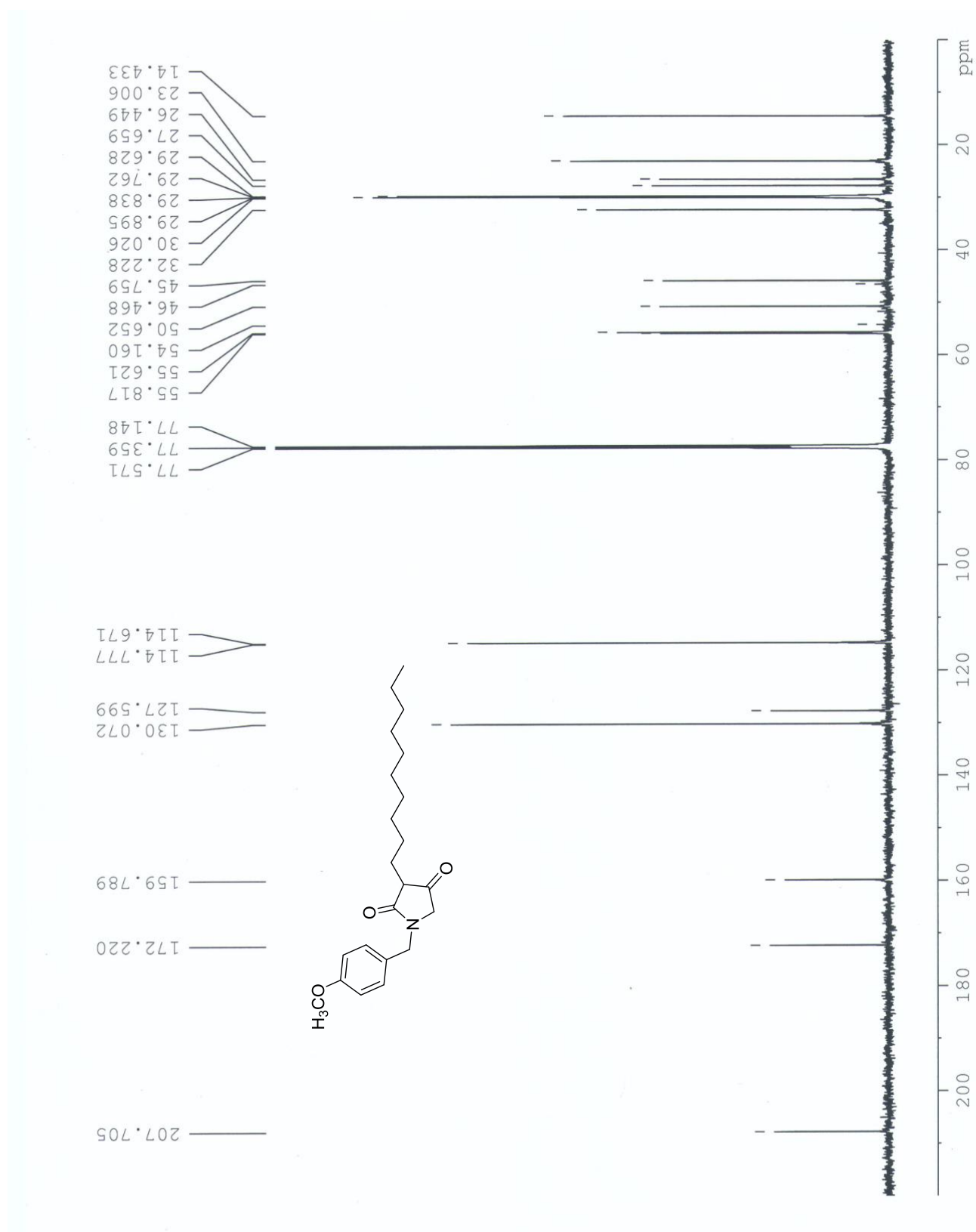
^{13}C -NMR (75 MHz, CDCl_3) spectrum of compound **9** (APT) (mixture of rotamers)



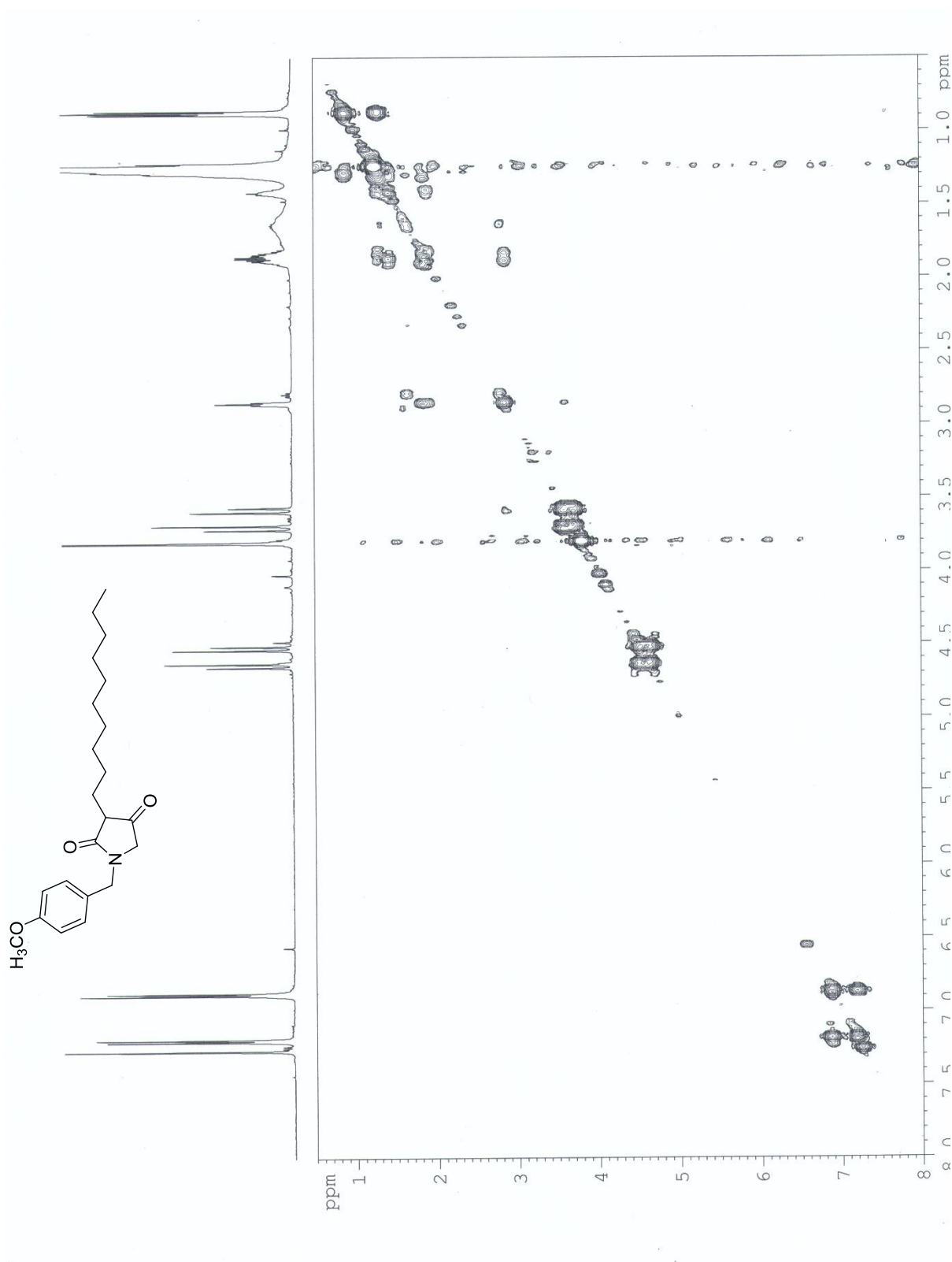
^1H -NMR (600 MHz, CDCl_3) spectrum of compound **10**



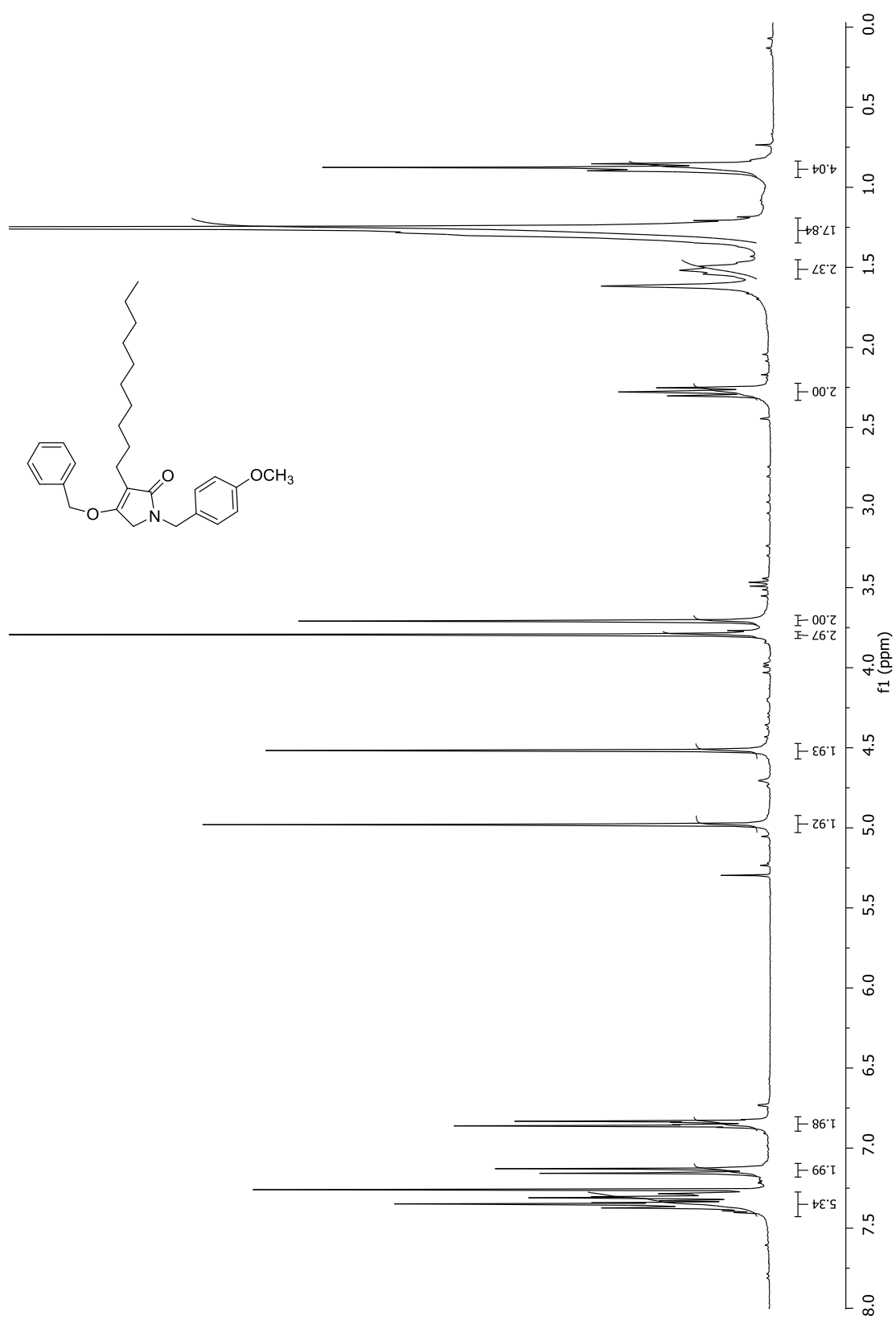
^{13}C -NMR (150 MHz, CDCl_3) spectrum of compound **10**.



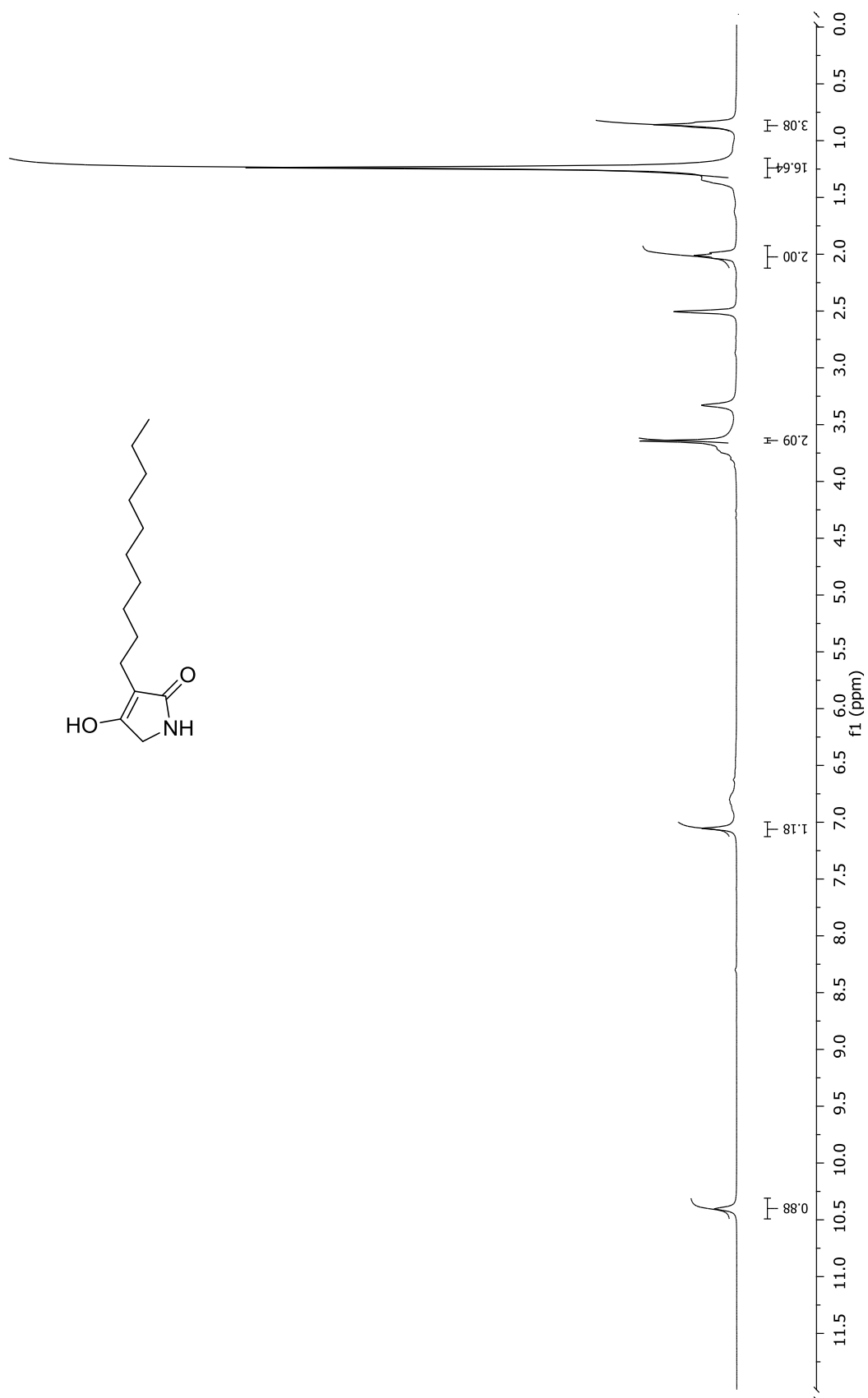
COSY (600 MHz, CDCl₃) spectrum of compound **10**.



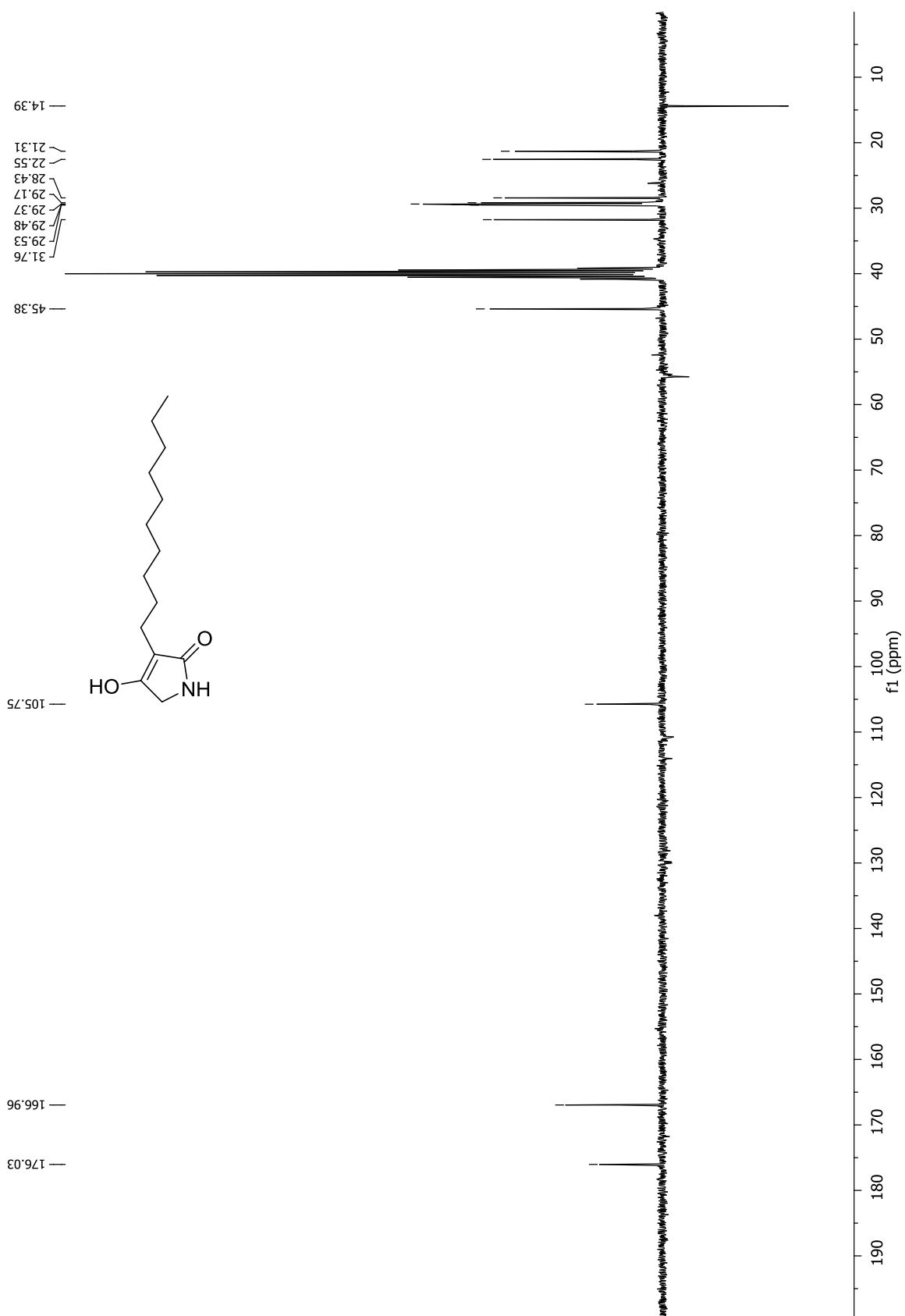
^1H -NMR (300 MHz, CDCl_3) spectrum of compound **11**.



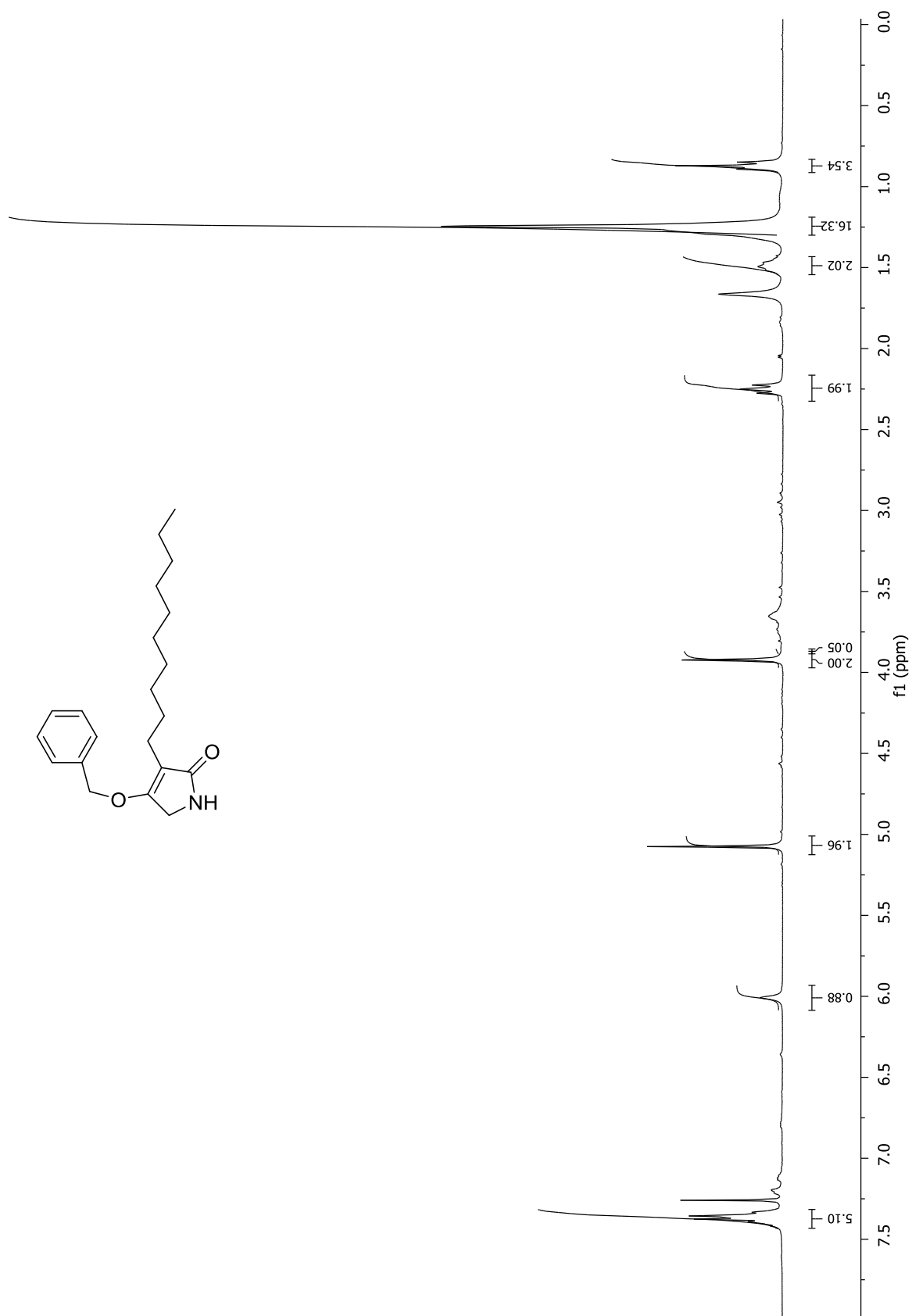
^1H -NMR (300 MHz, d_6 -DMSO) spectrum of compound **12**.



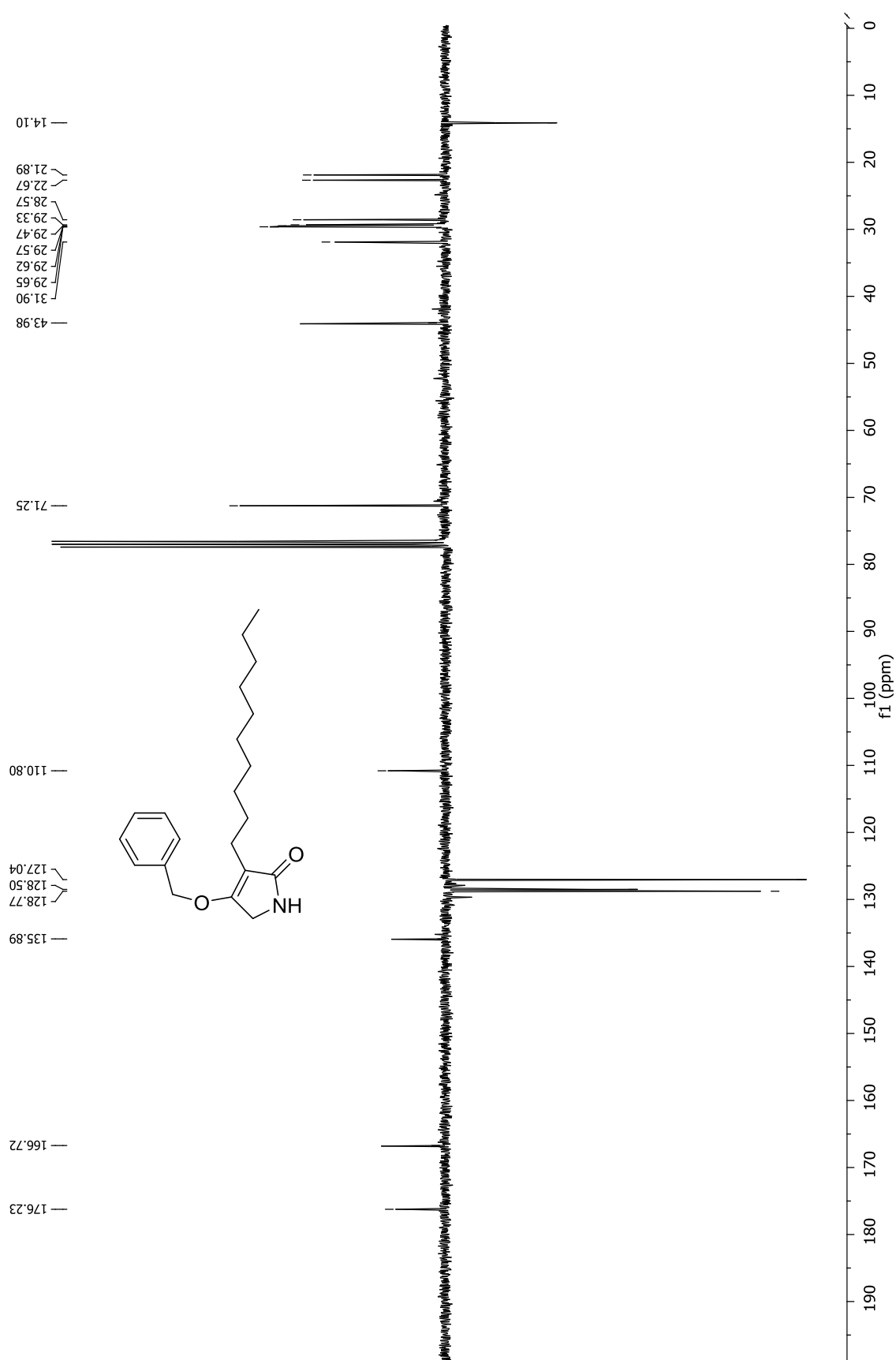
^{13}C -NMR (75 MHz, d_6 -DMSO) spectrum of compound **12** (APT)



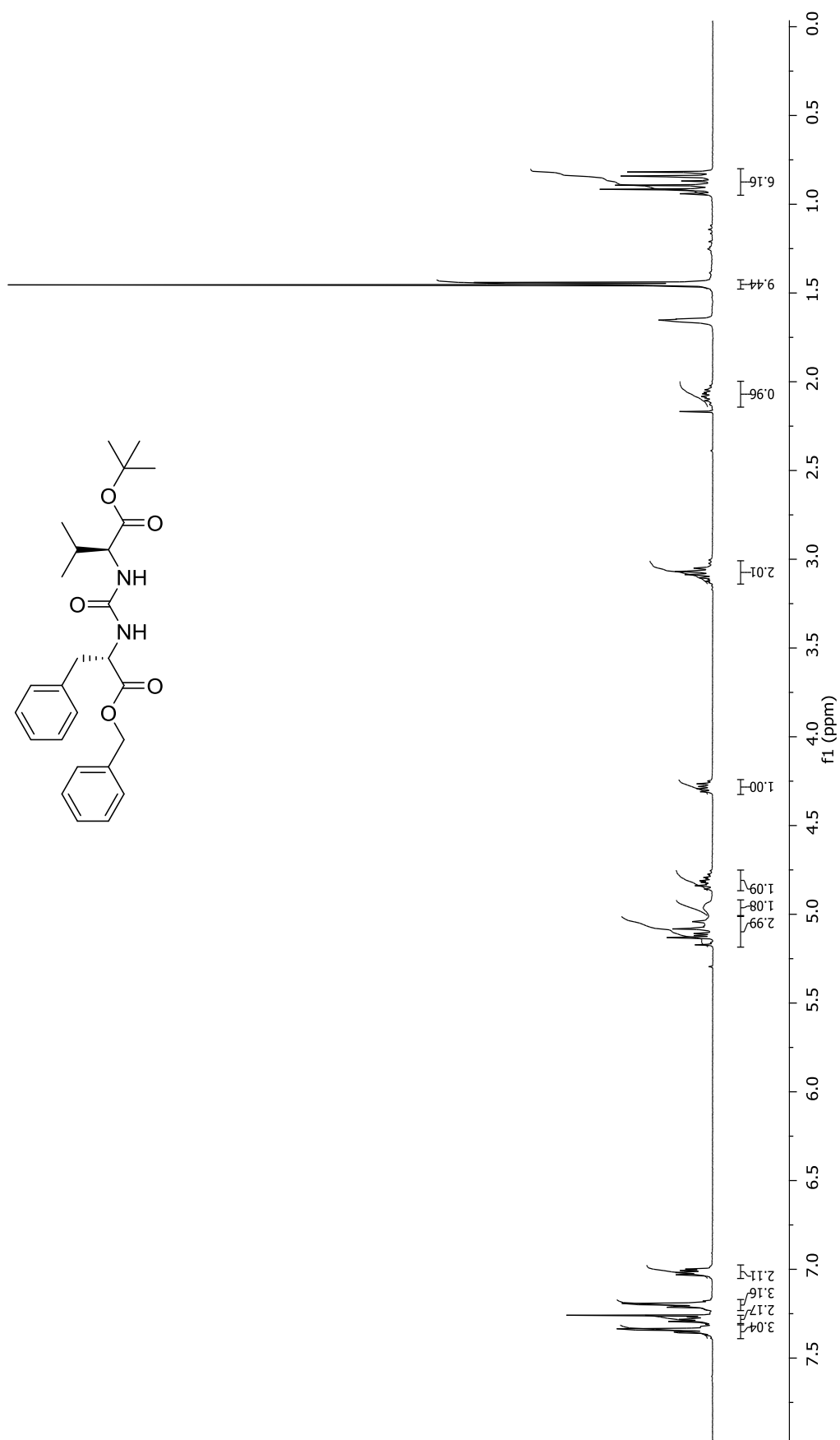
^1H -NMR (300 MHz, CDCl_3) of compound **13**.



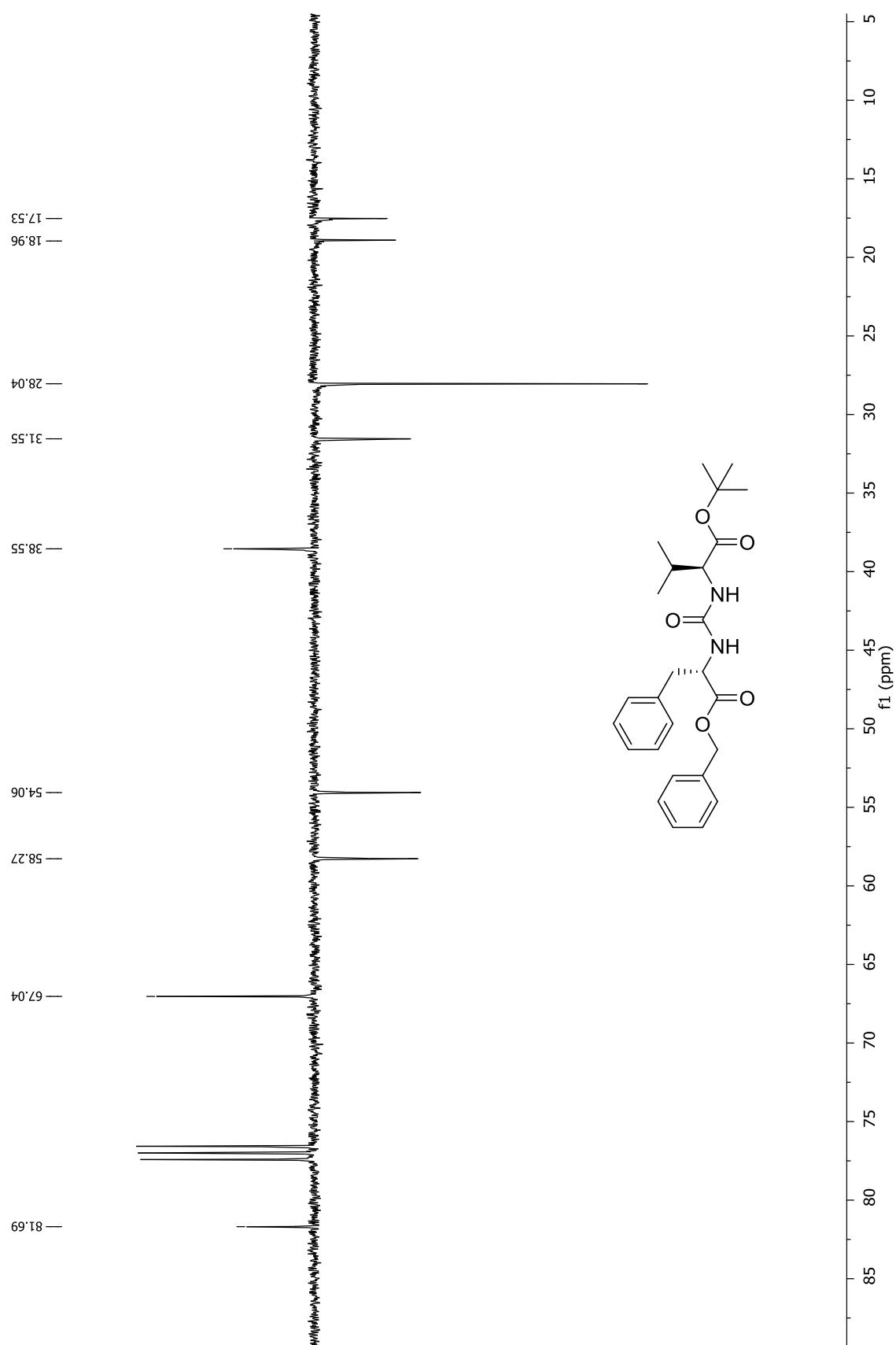
^{13}C -NMR (75 MHz, CDCl_3 , APT) spectrum of compound **13**.



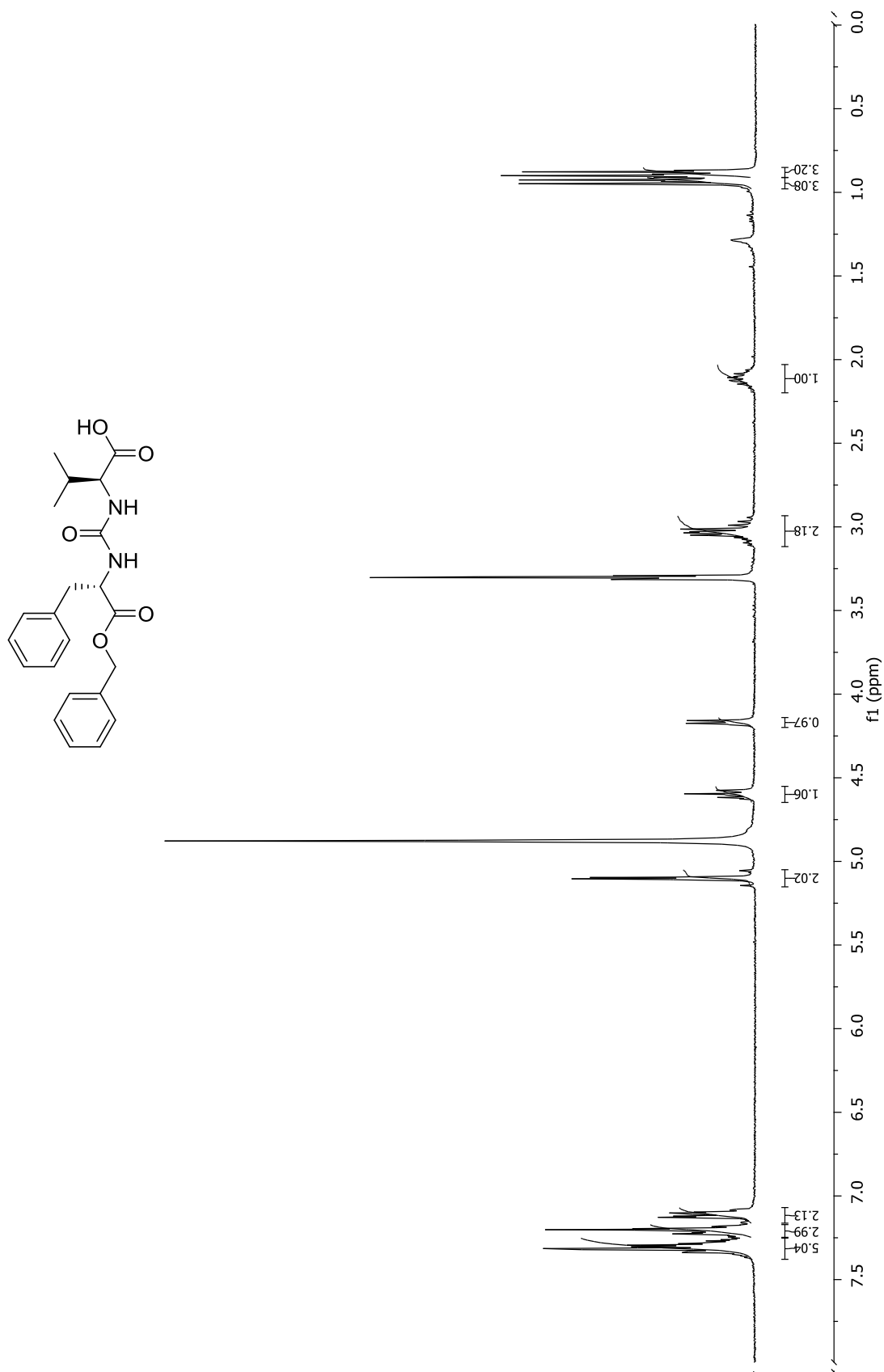
^1H -NMR (300 MHz, CDCl_3) spectrum of compound **18** (mixture of rotamers).



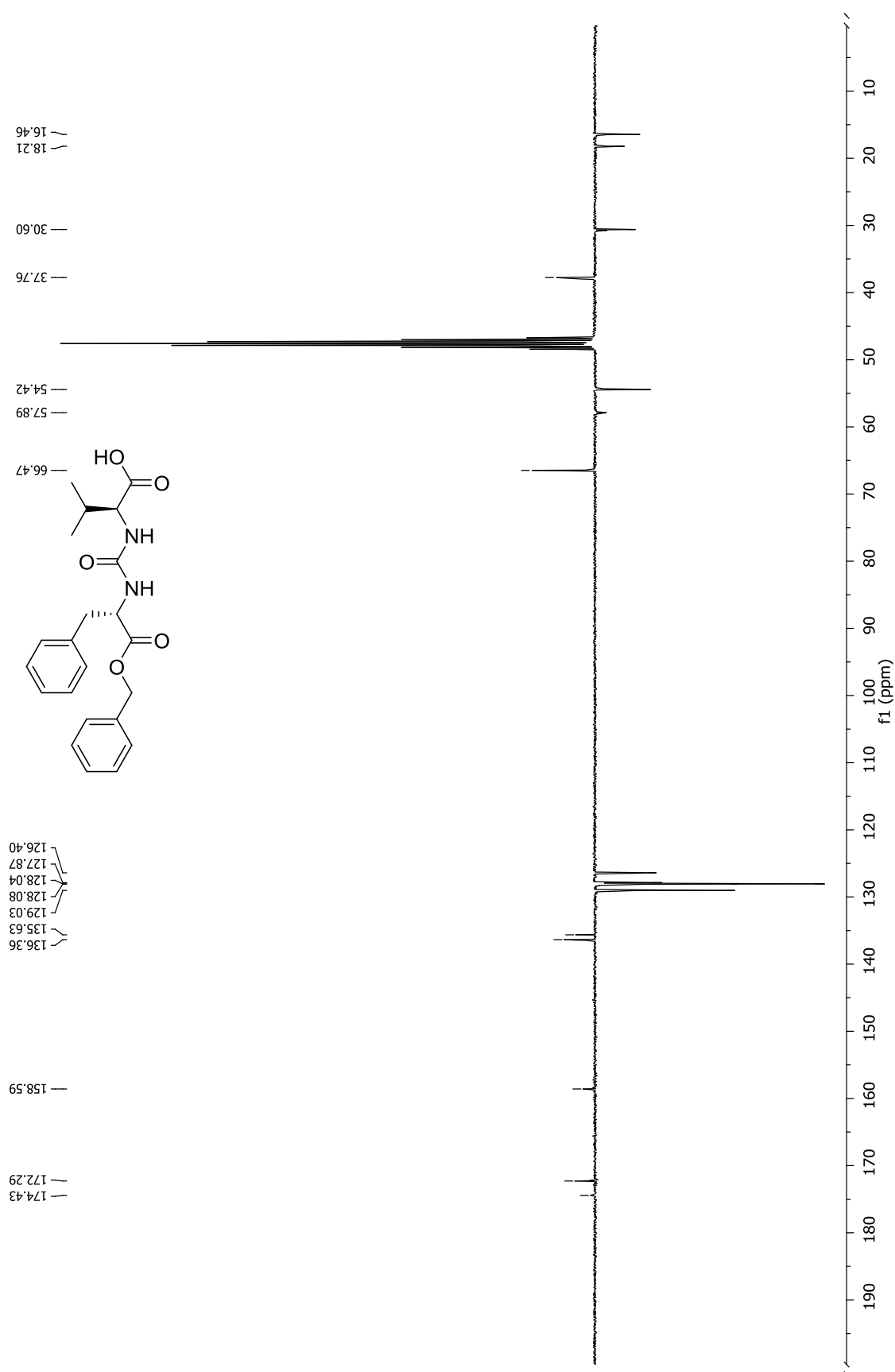
^{13}C -NMR (75 MHz, CDCl_3) APT spectrum of compound **18** (mixture of rotamers)



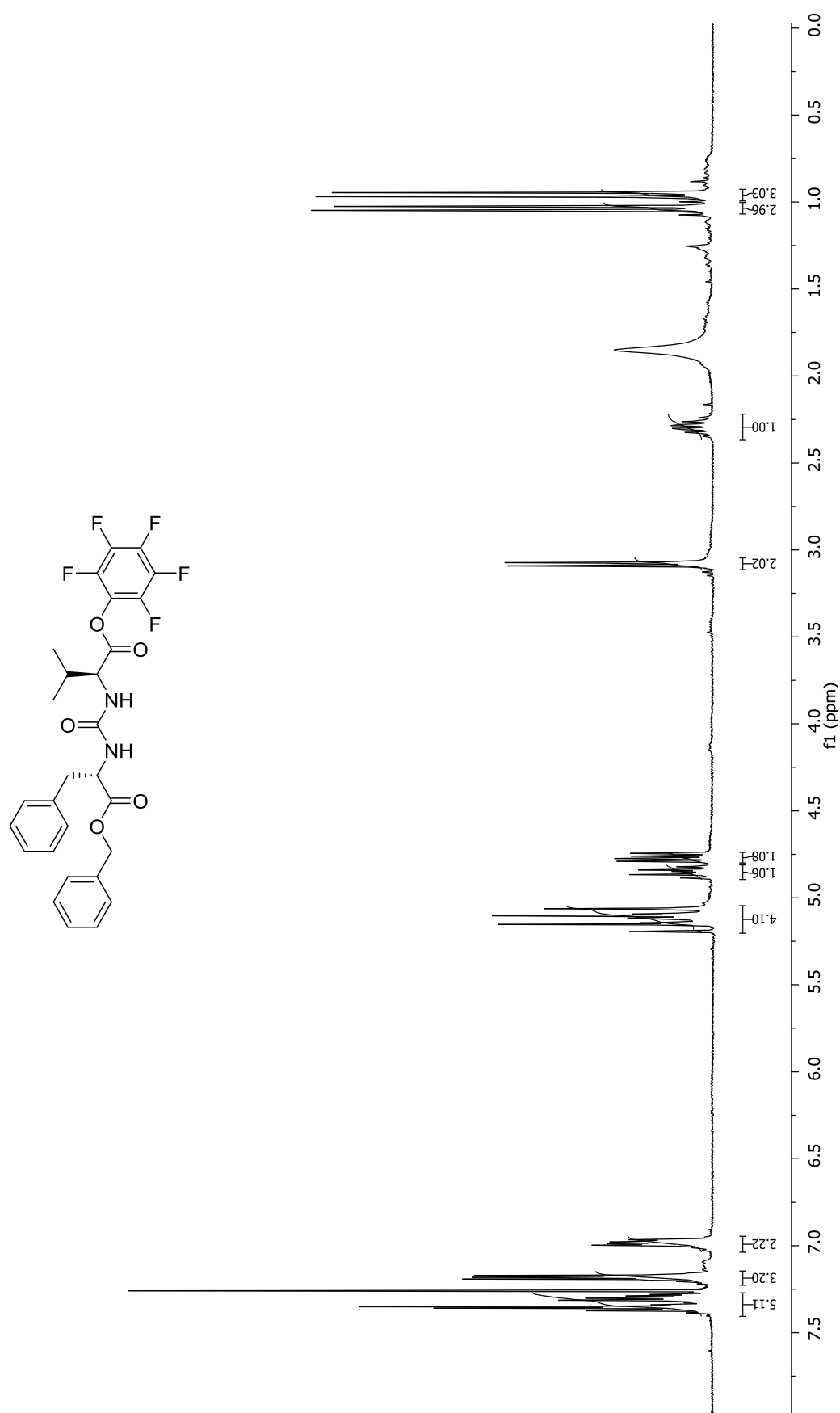
^1H -NMR (300 MHz, CD_3OD) spectrum of compound **19** (mixture of rotamers)



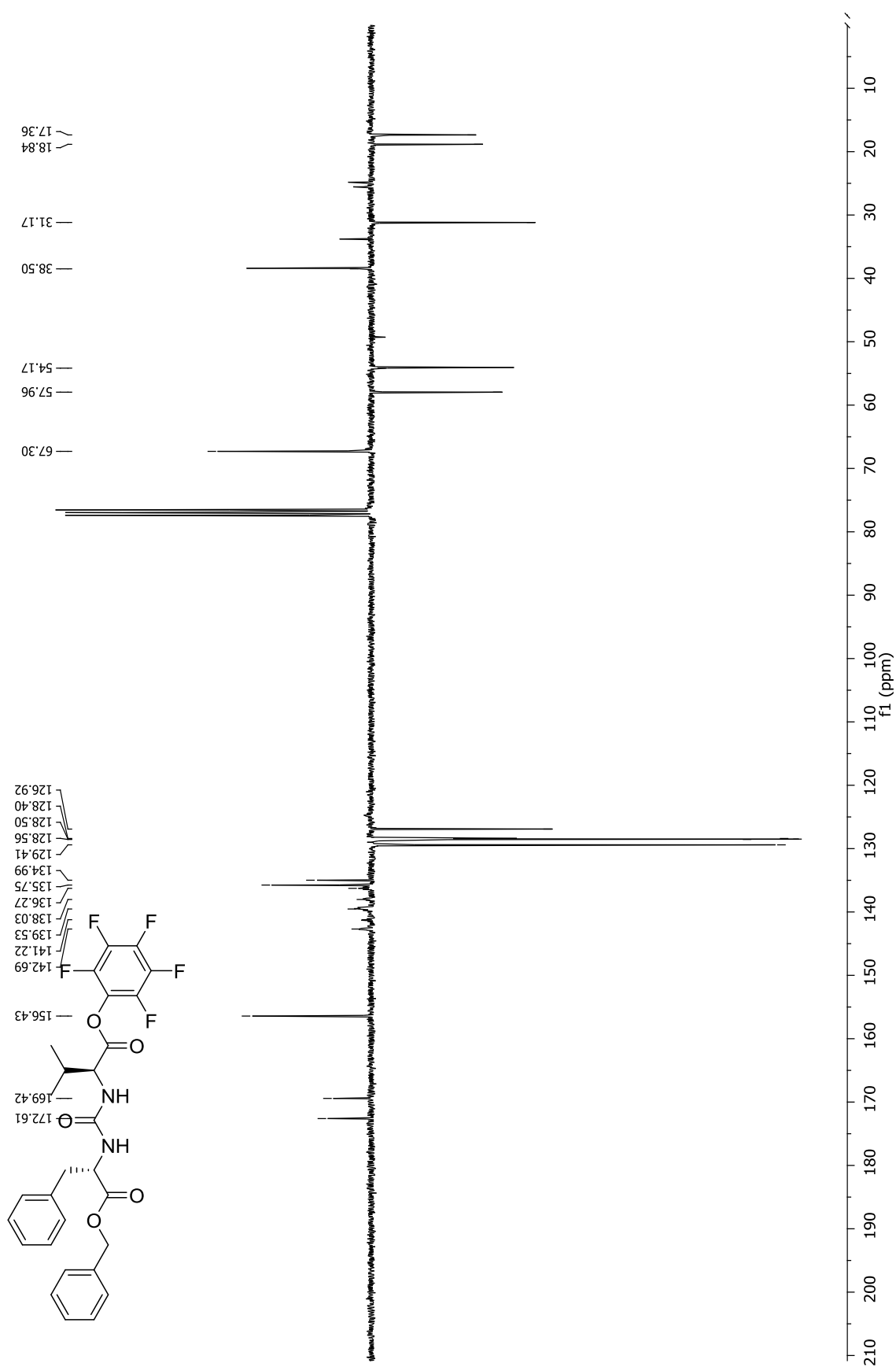
^{13}C -NMR (75 MHz, CD_3OD) spectrum of compound **19** (APT) (mixture of rotamers)



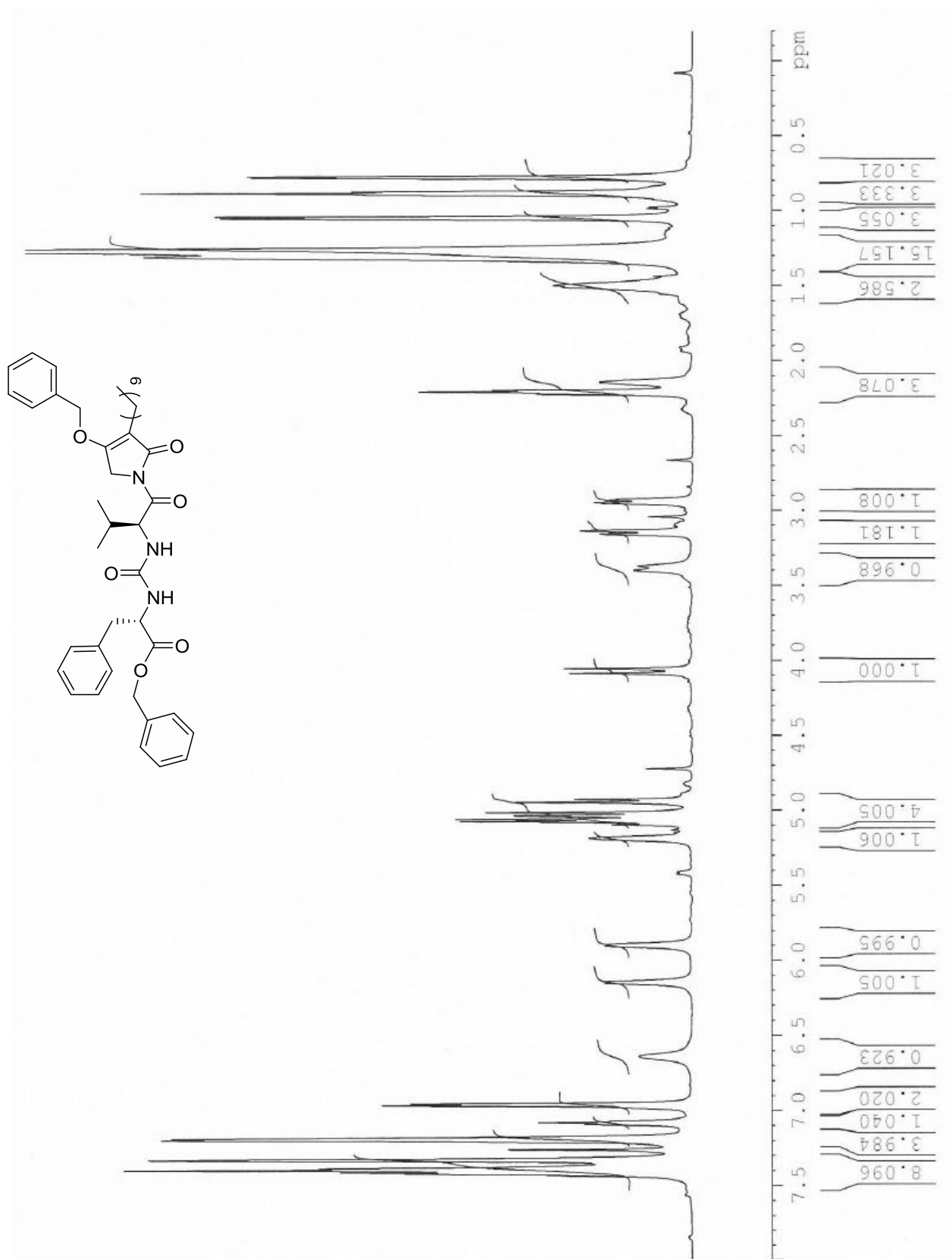
^1H -NMR (300 MHz, CDCl_3) spectrum of compound **20** (mixture of rotamers)



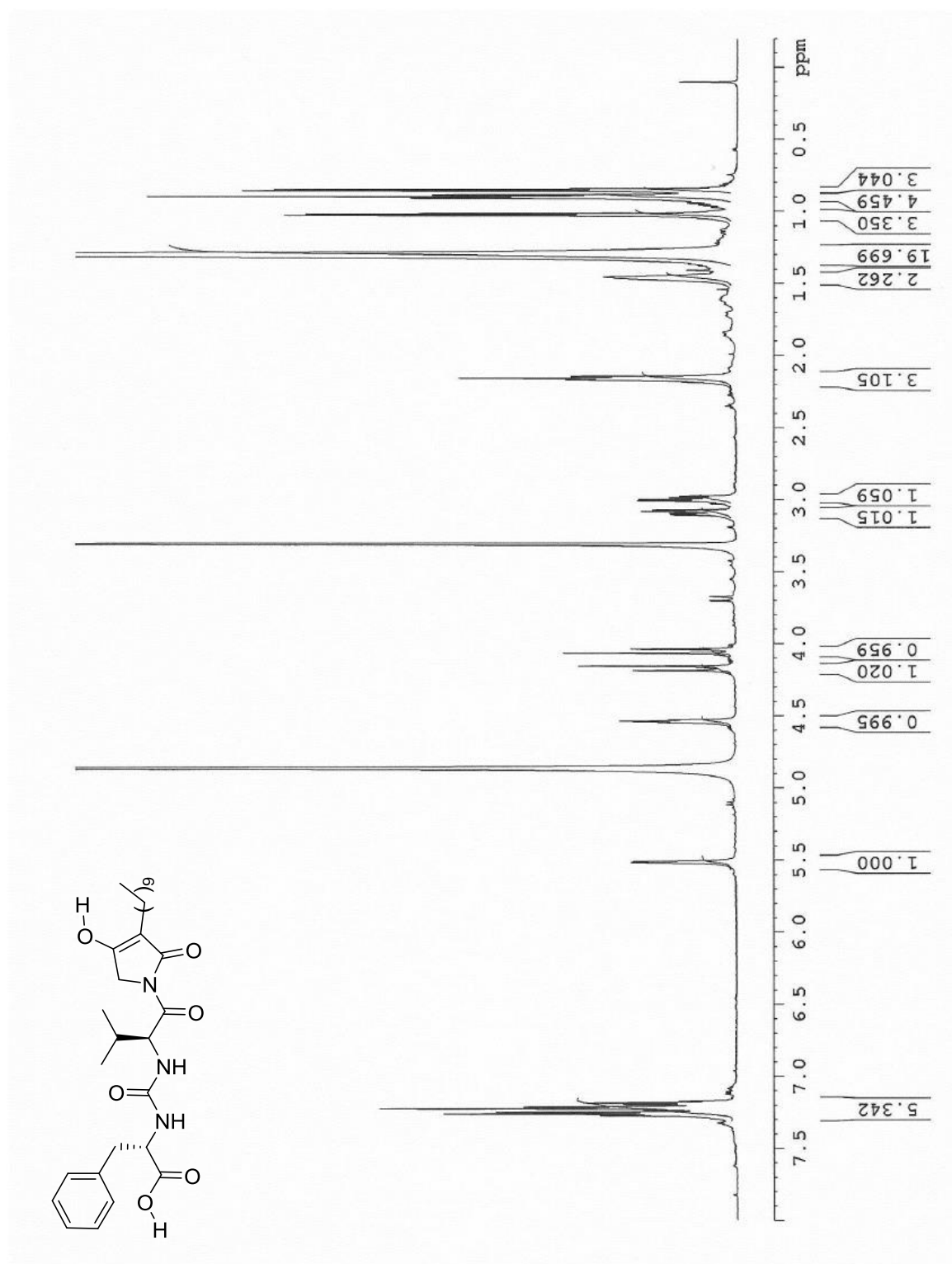
^{13}C -NMR (75 MHz, CDCl_3) spectrum of compound **20** (APT) (mixture of rotamers)



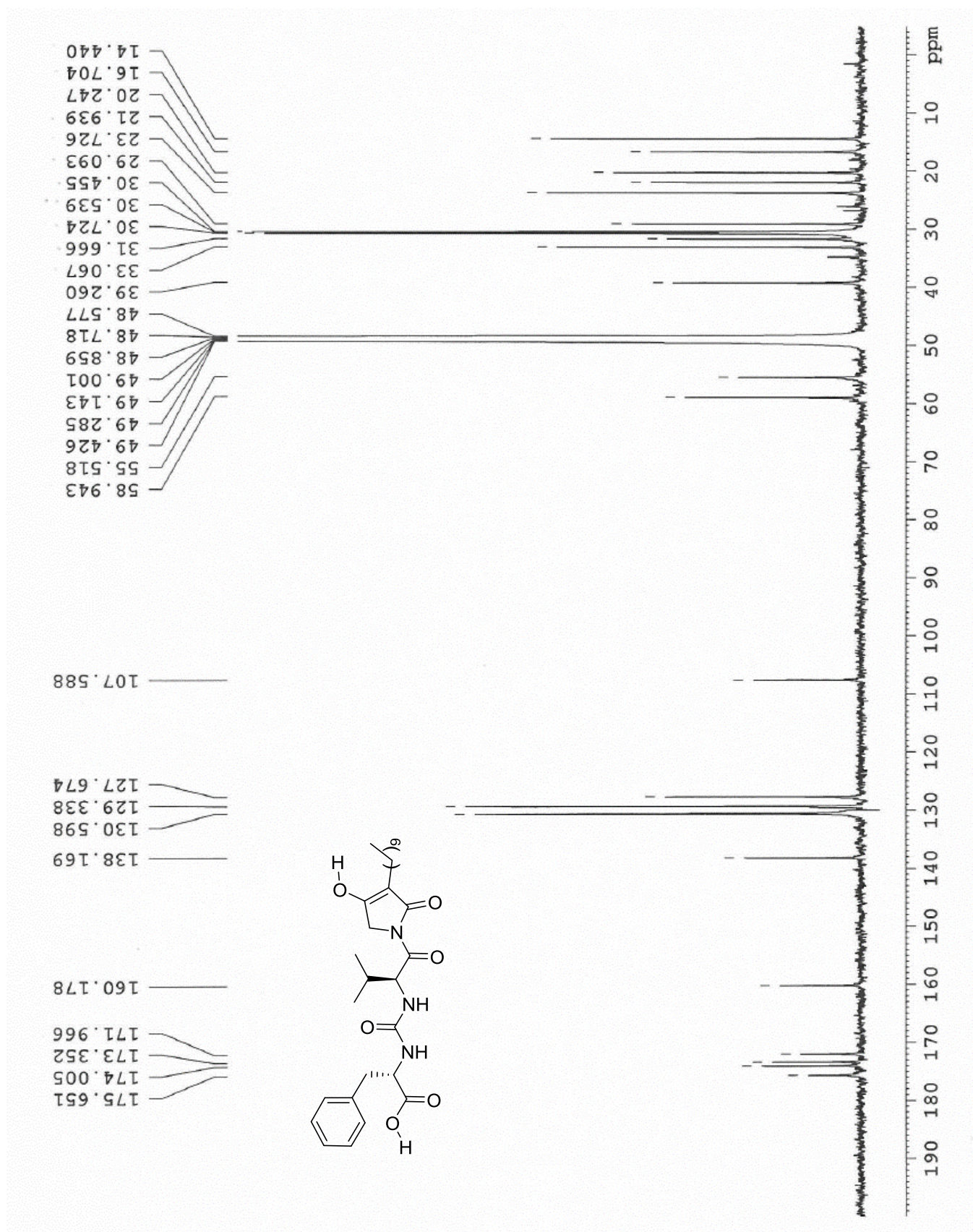
^1H -NMR (600 MHz, CDCl_3) spectrum of compound **21**



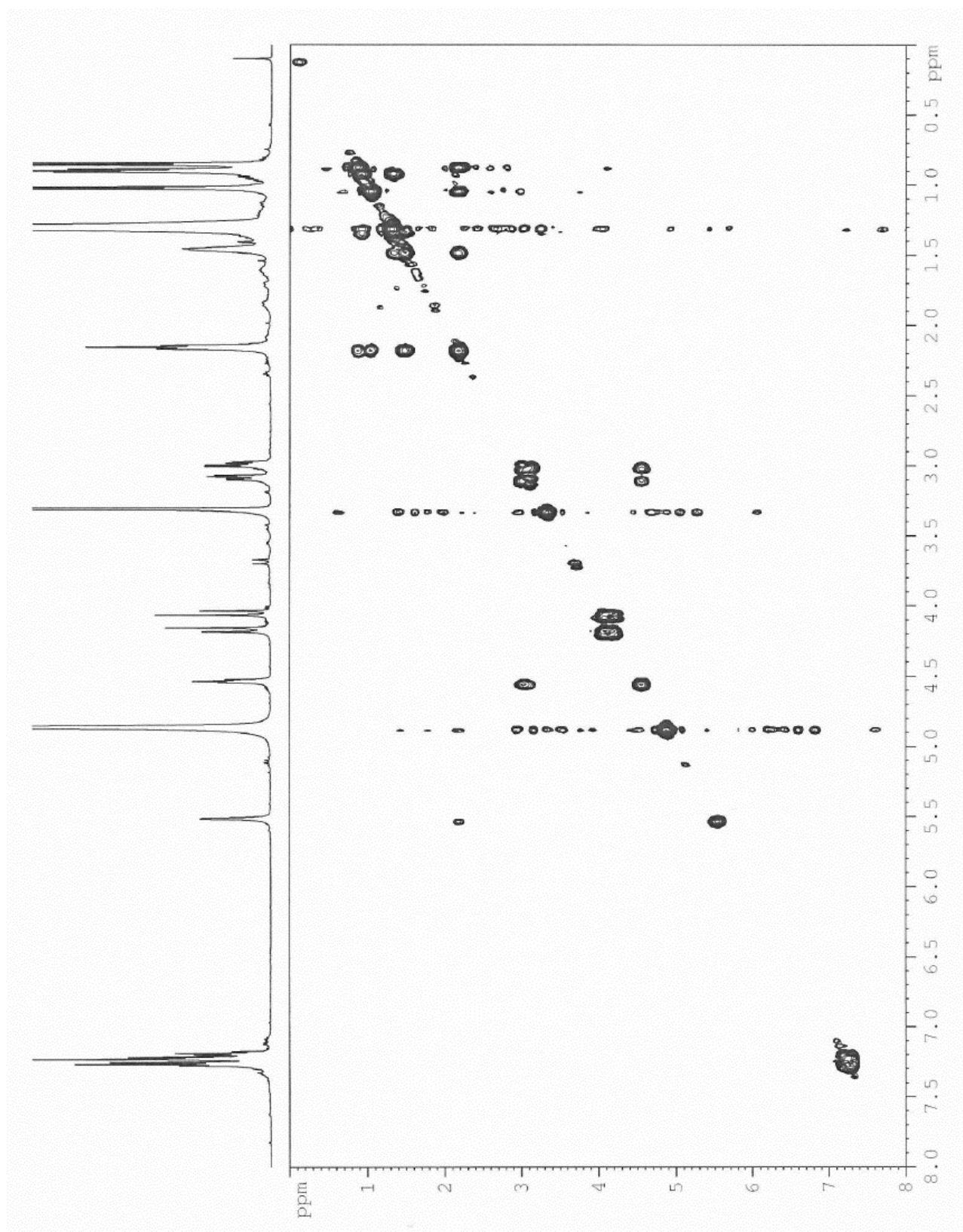
^1H -NMR (600 MHz, CD_3OD) spectrum of compound **1**



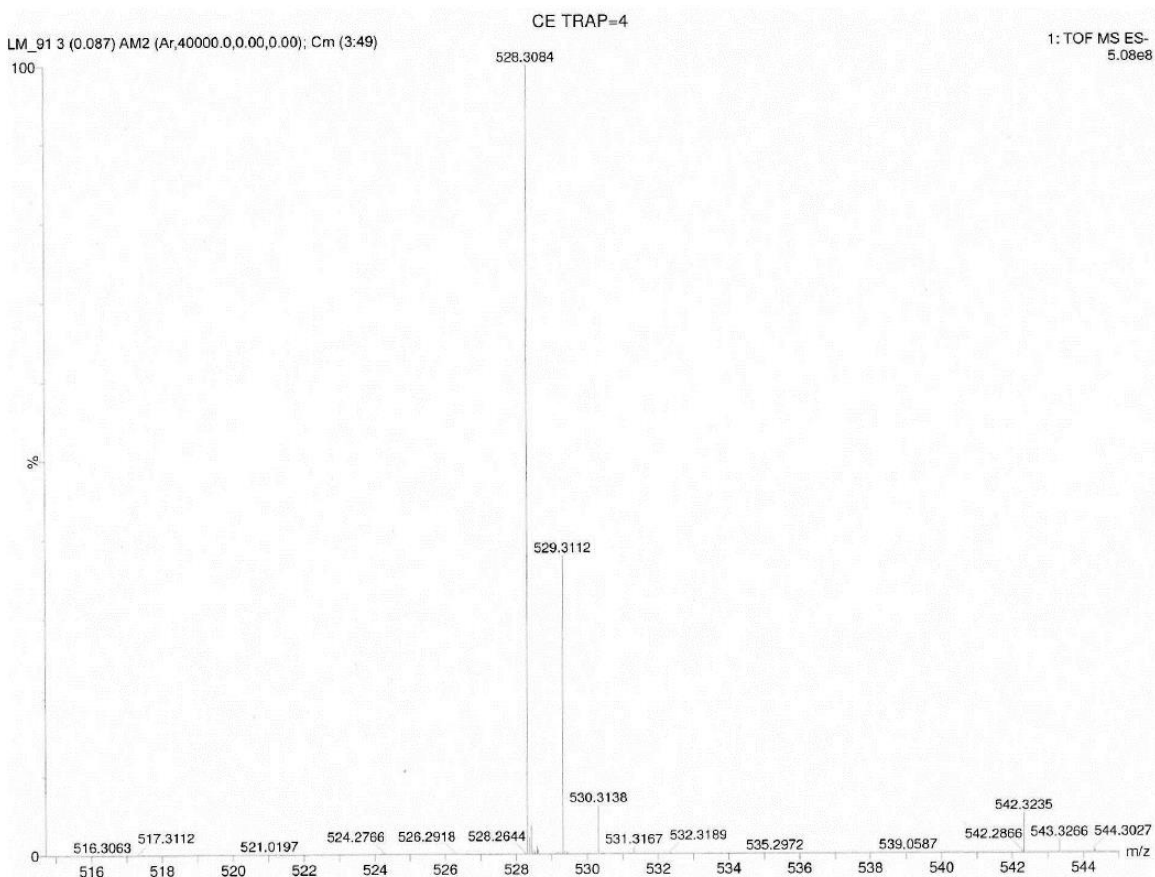
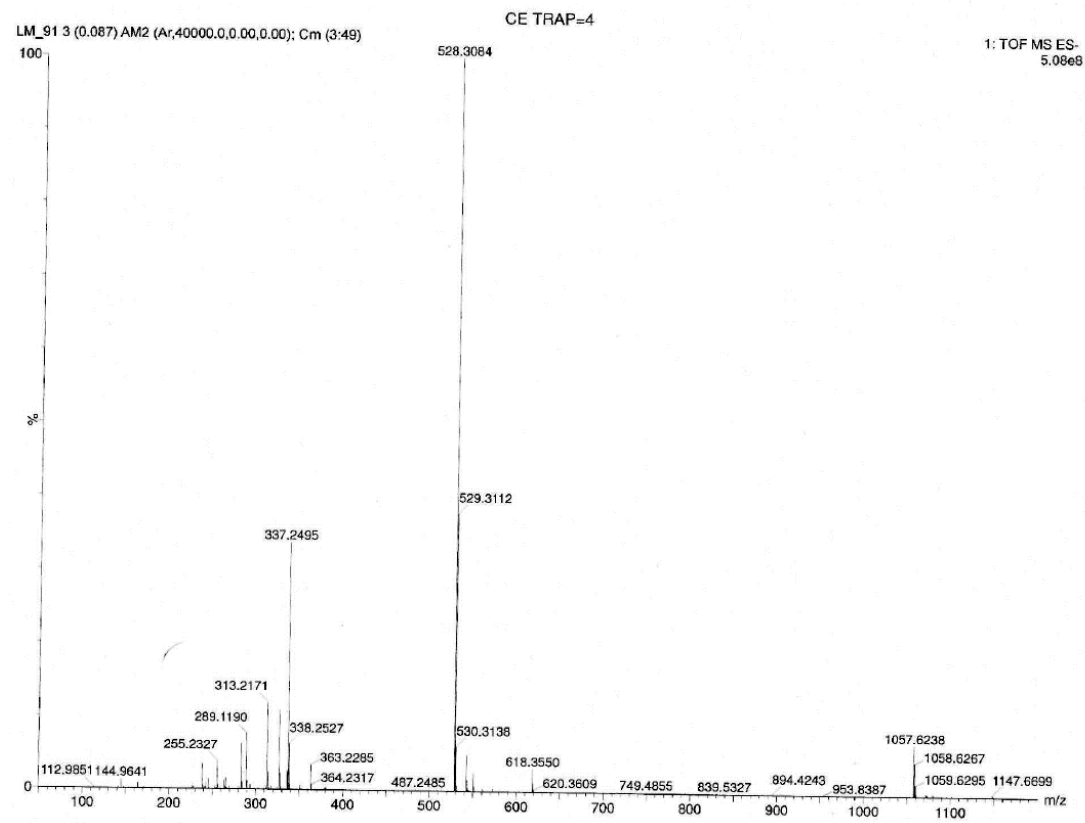
^{13}C -NMR (150 MHz, CD_3OD) spectrum of compound **1**.



COSY (600 MHz, CD₃OD) spectrum of compound **1**.



MS spectrum of compound 1.



Elemental composition report of compound 1

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 9

Monoisotopic Mass, Even Electron Ions

161 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 29-29 H: 10-100 N: 0-3 O: 0-10 Na: 0-3

CE TRAP-4

LM_913 (0.087) AMZ (Ar,40000.0,0.00,0.00): Cm (3.49)

1: TOF MS ES-



Minimum:

Maximum:

5.0 10.0

-1.5

50.0

Mass Calc. Mass mDa PPM DBE i-FIT Norm Conf(%) Formula

528.3084 528.3074 1.0 1.9 10.5 4738.3 n/a n/a C29 H42 N3 O6