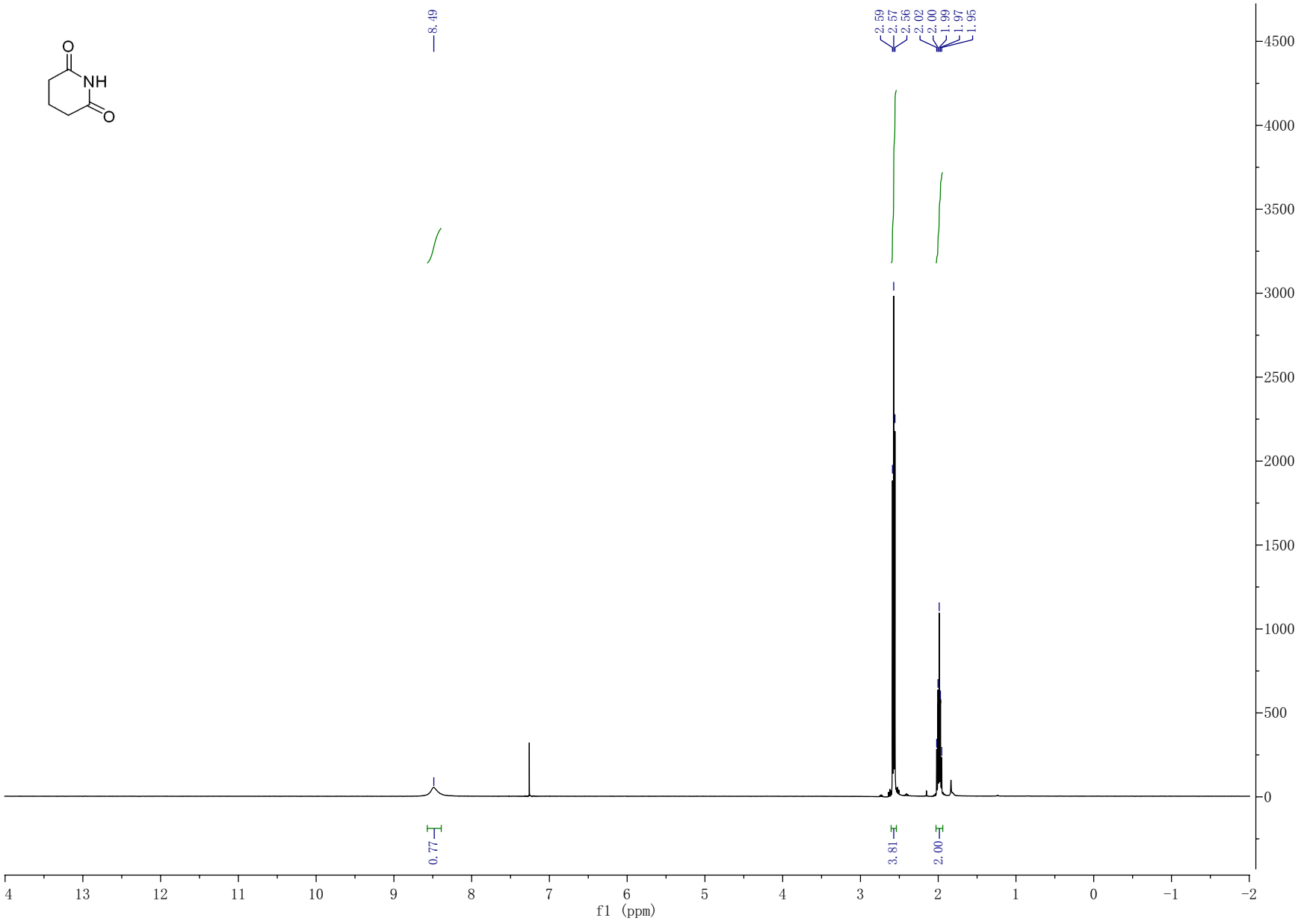
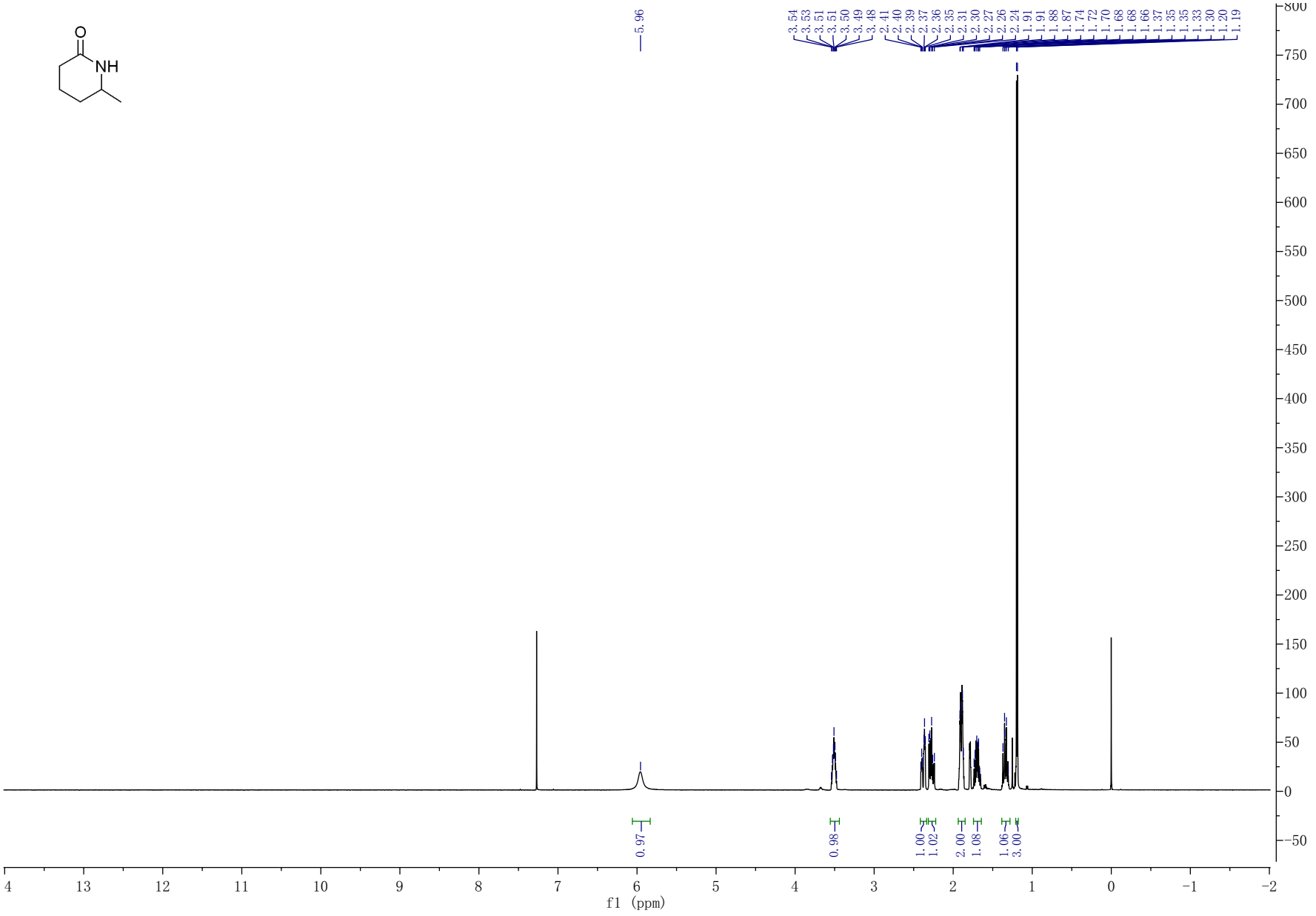
Synthesis and insecticidal activity of Fire Ant Venom Alkaloid Based 2-Methyl-6-alkyl-$\Delta^{1,6}$-piperideines

Table of Contents

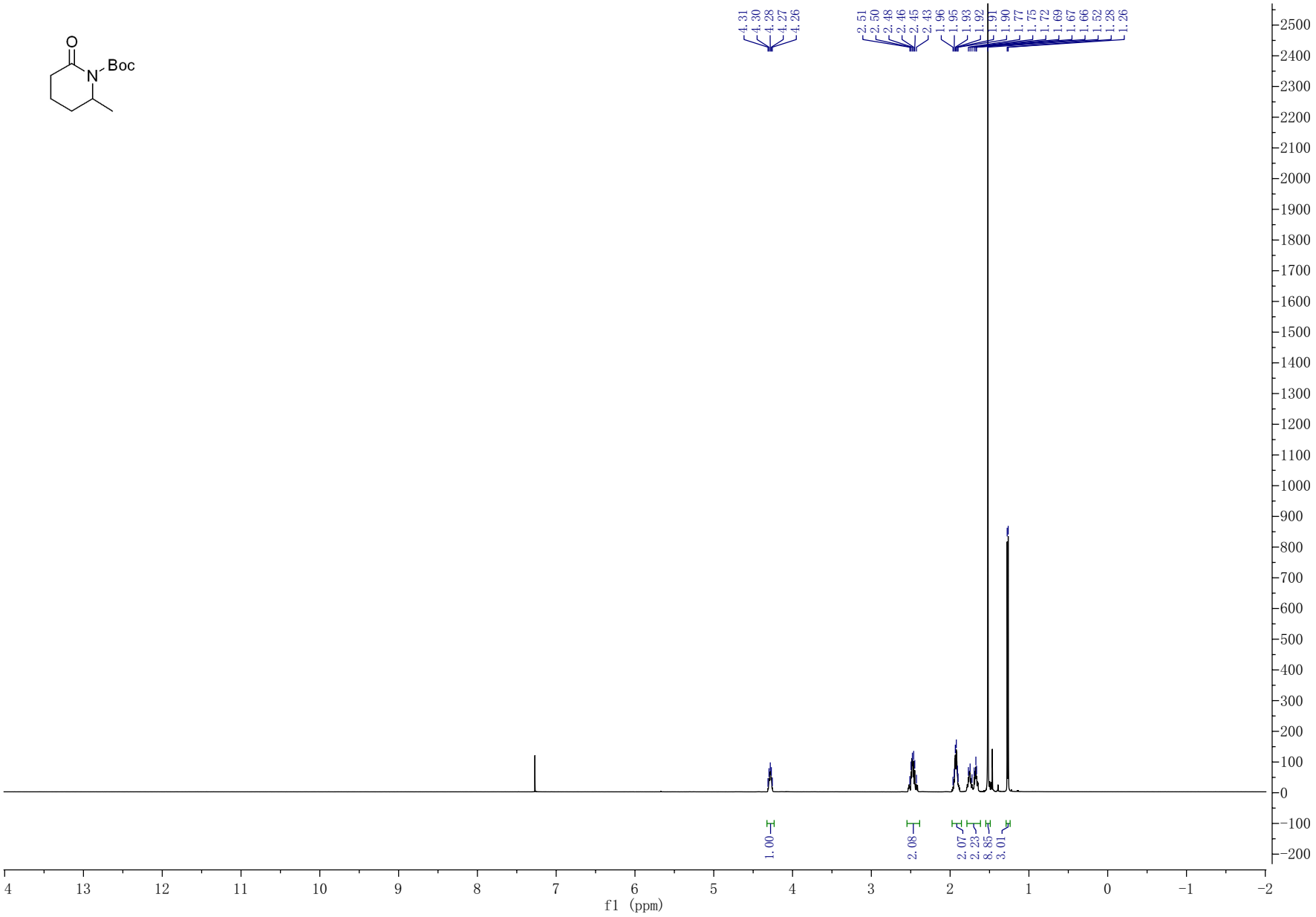
S1. ^{1}H NMR Spectrum of Compound 2



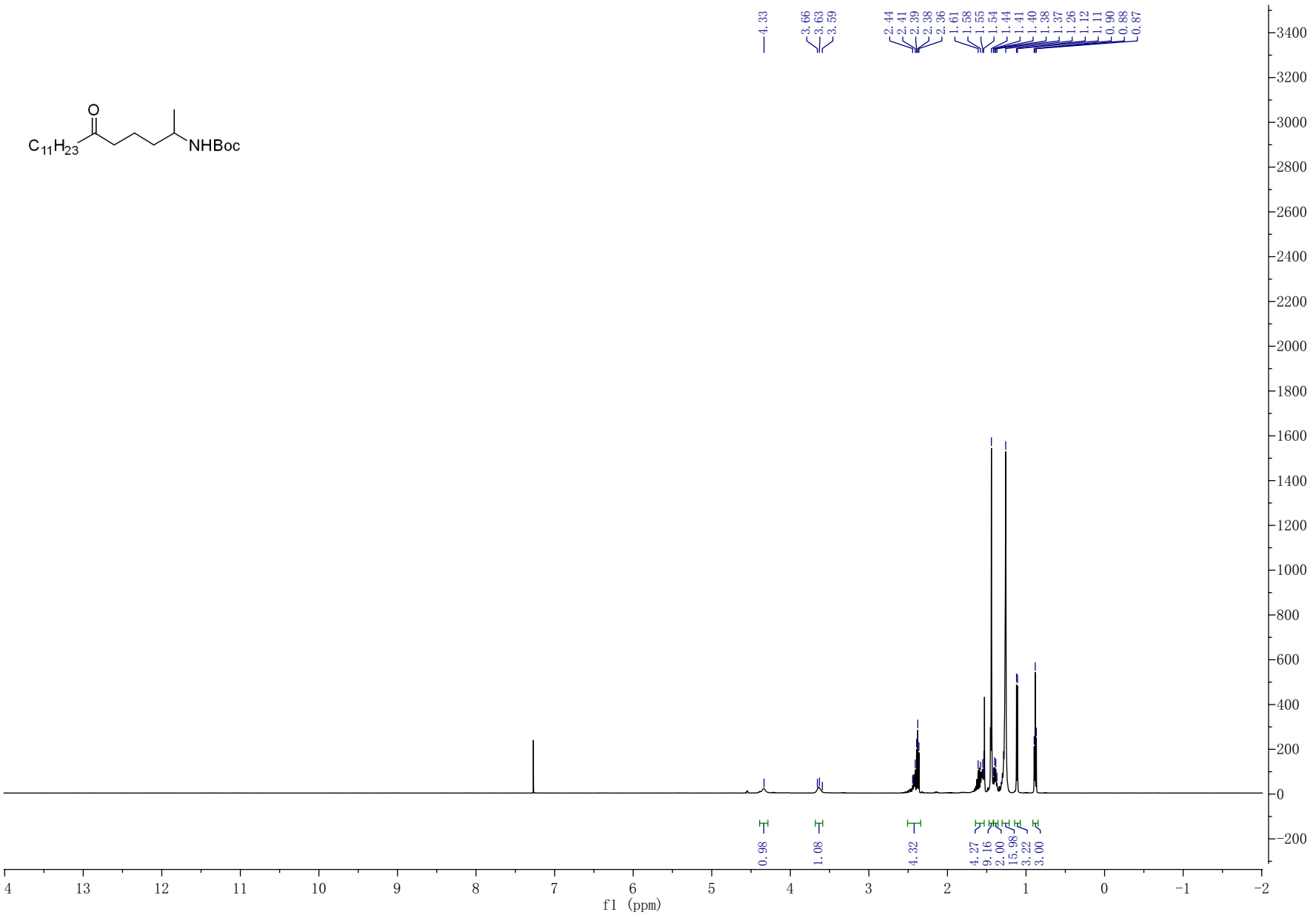
S2. ^{1}H NMR Spectrum of Compound 3



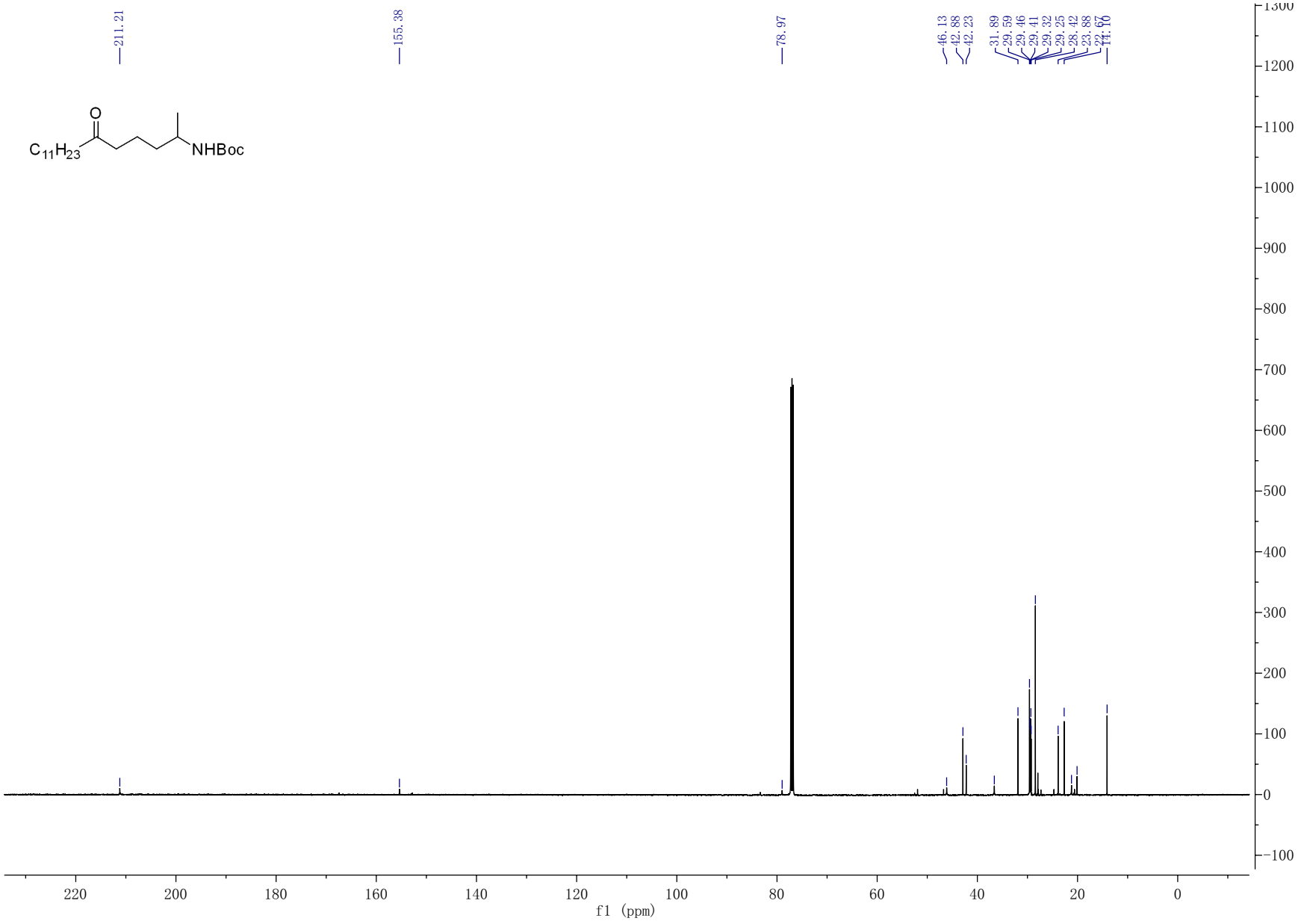
S3. ^{1}H NMR Spectrum of Compound 4



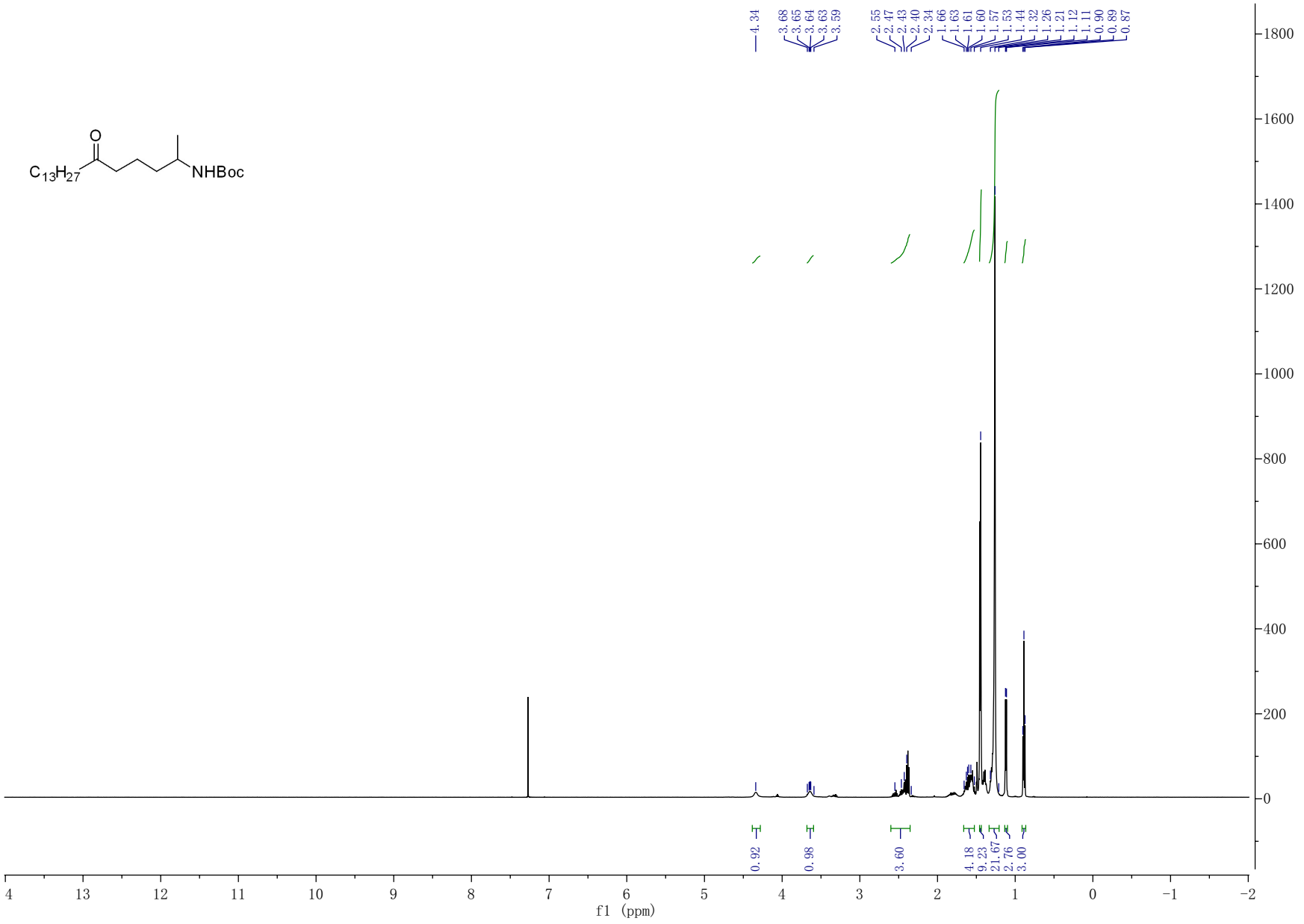
S4. ^{1}H NMR Spectrum of Compound 5a



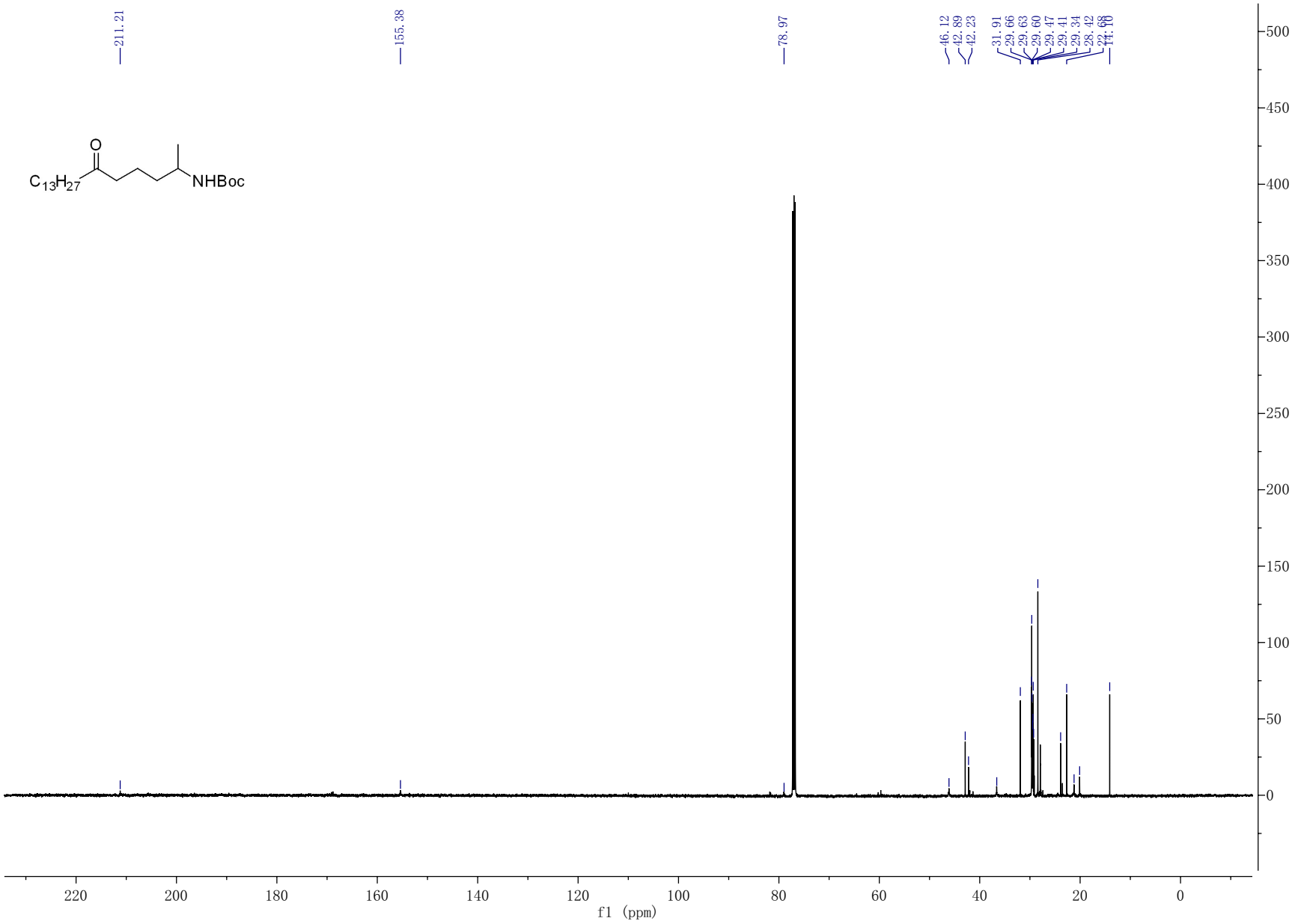
S5. ^{13}C NMR Spectrum of Compound 5a



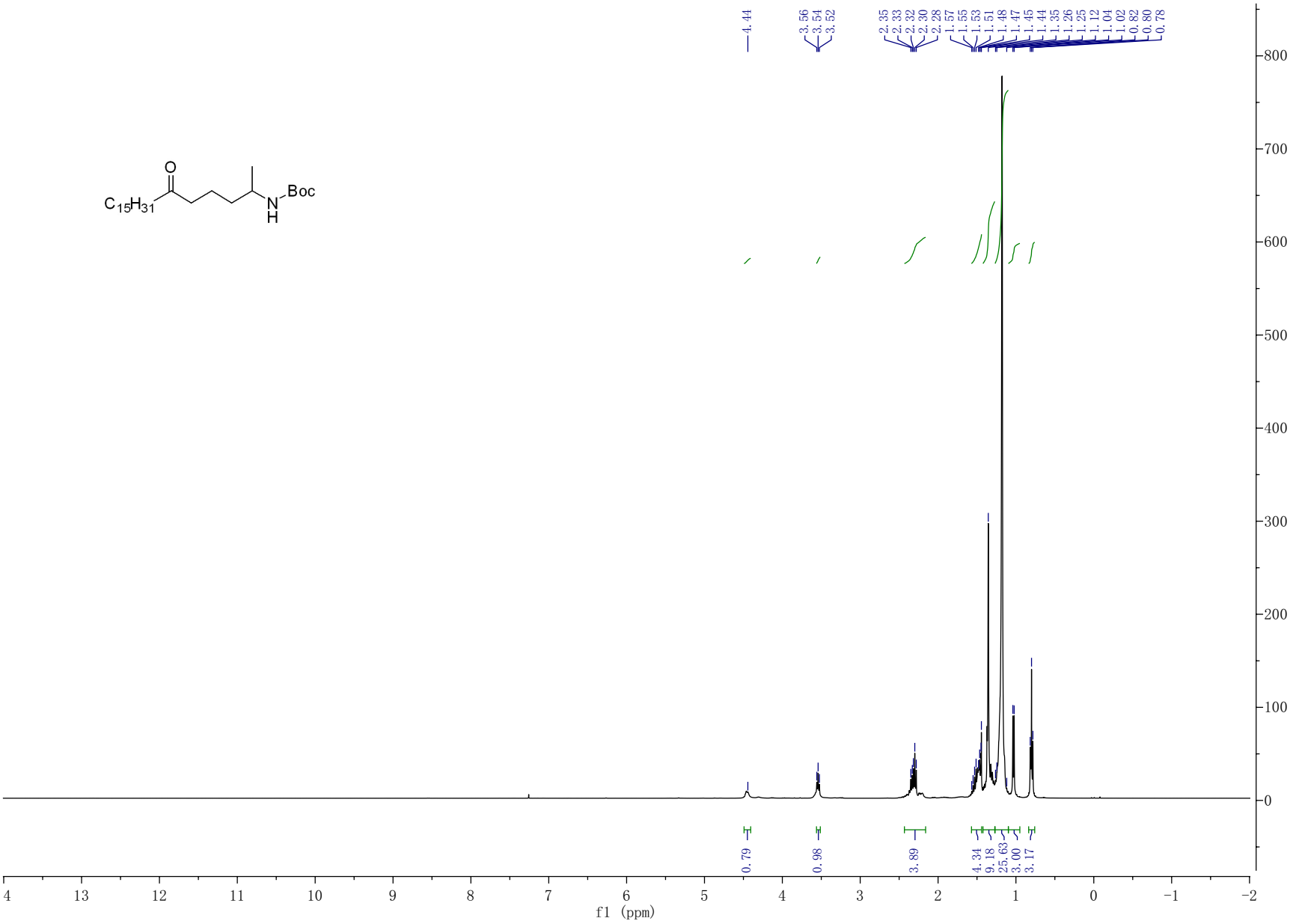
S6. ^{1}H NMR Spectrum of Compound 5b



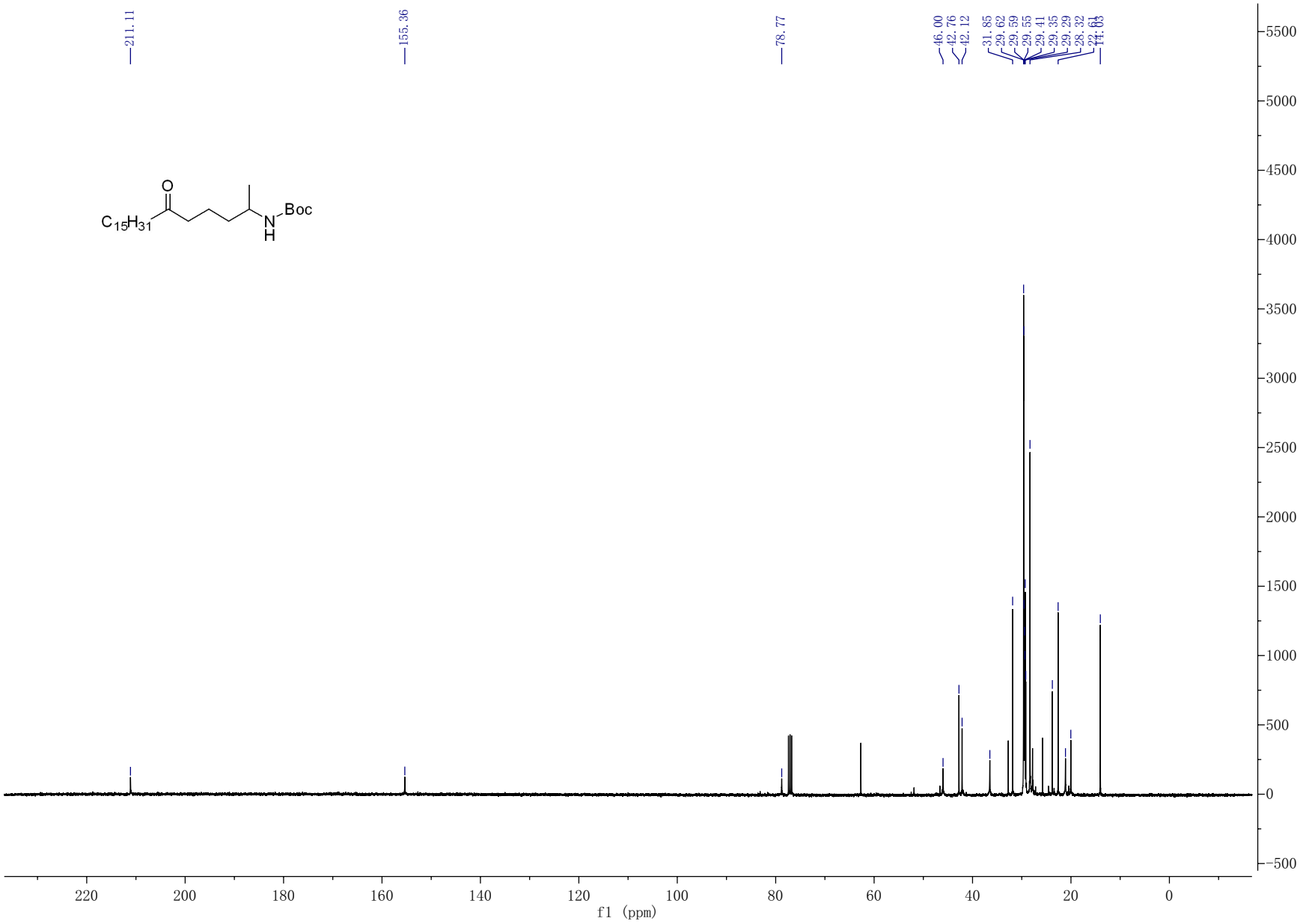
S7. ^{13}C NMR Spectrum of Compound 5b



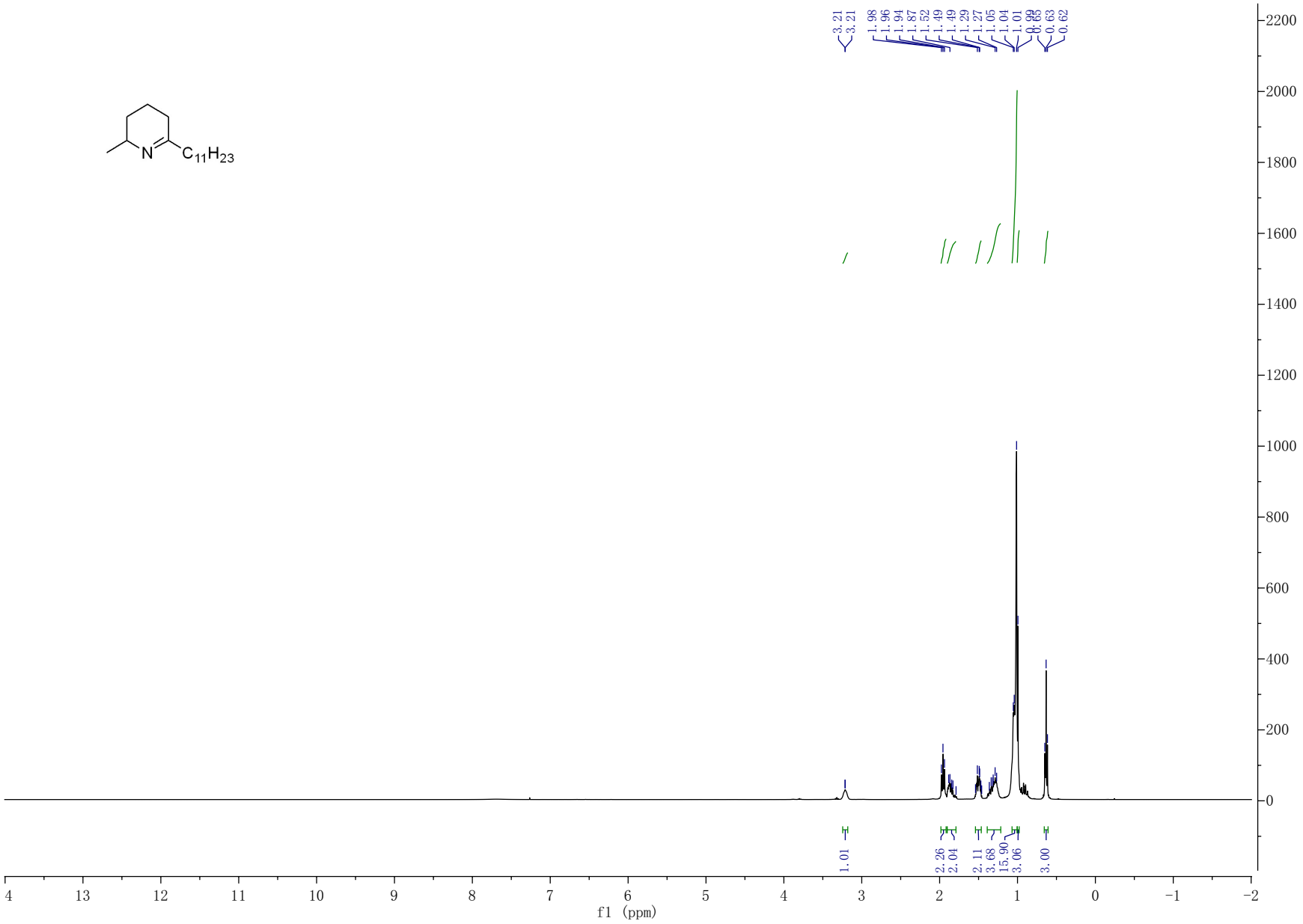
S8. ^{1}H NMR Spectrum of Compound 5c



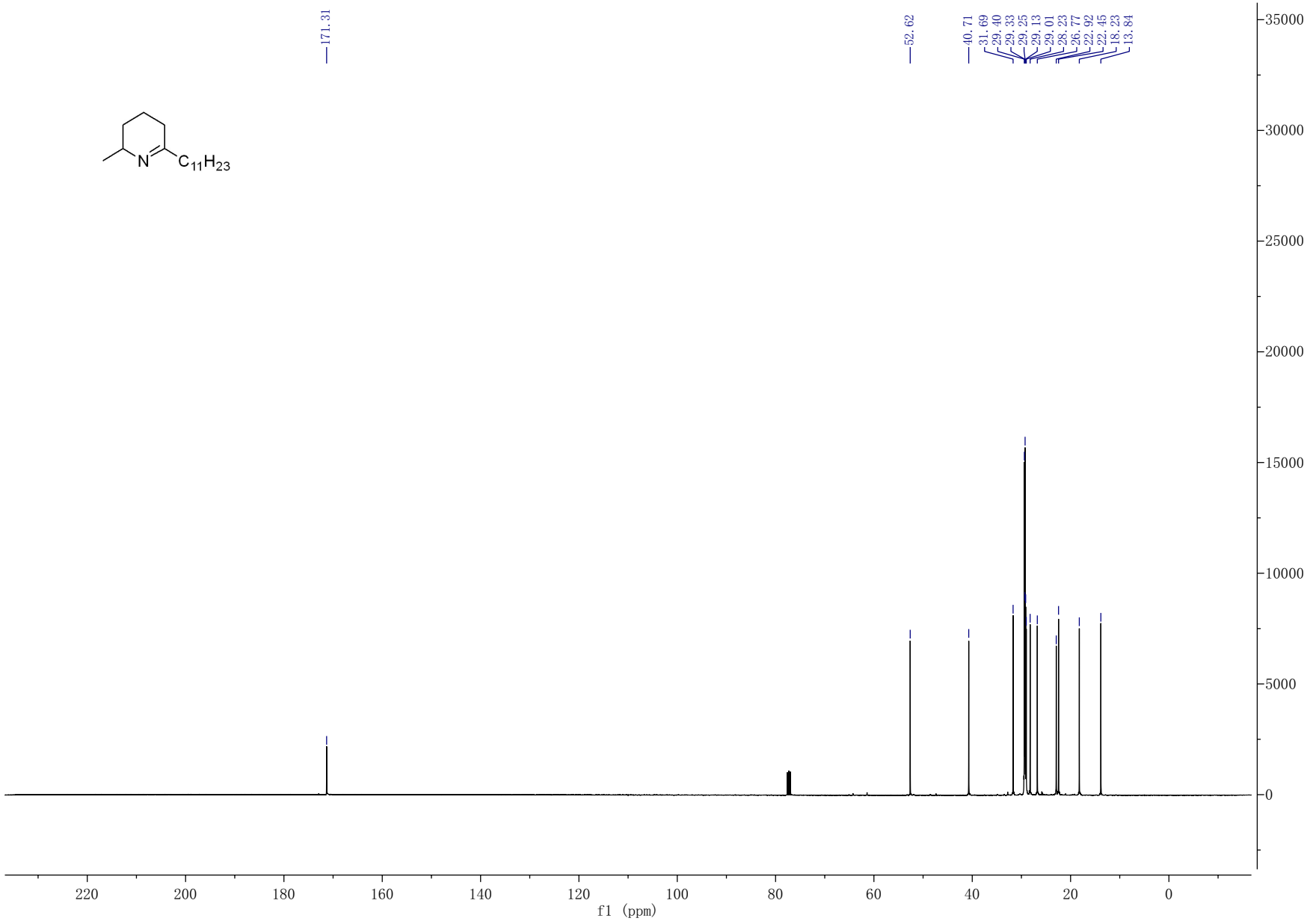
S9. ^{13}C NMR Spectrum of Compound 5c



S10. ^{1}H NMR Spectrum of Compound 6a



S11. ^{13}C NMR Spectrum of Compound6a



S12. HRMS Spectrum of Compound 6a

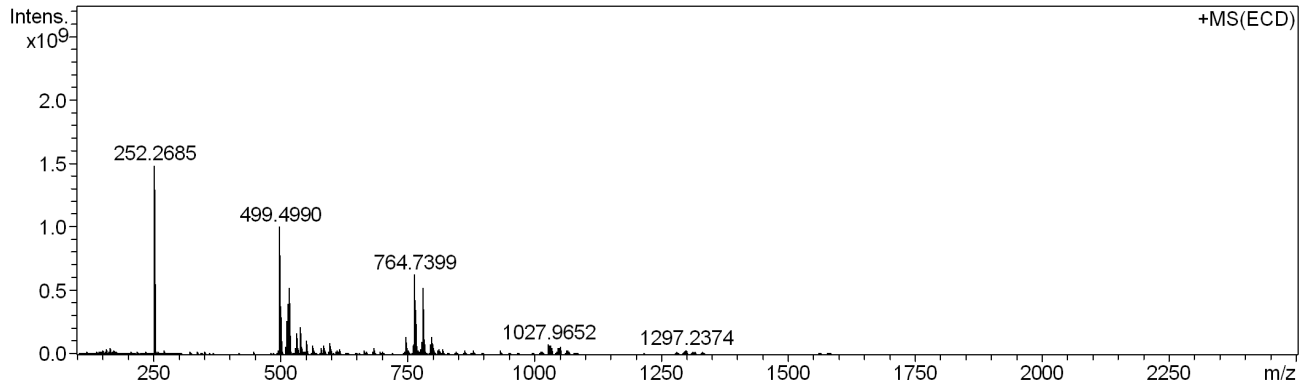
Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name	D:\Data\2020.09.25 chen li\pos-1_000001.d	Acquisition Date	9/25/2020 5:32:03 PM
Method	ESI_101506	Operator	
Sample Name	TUNMIX	Instrument	apex-Ultra
Comment			

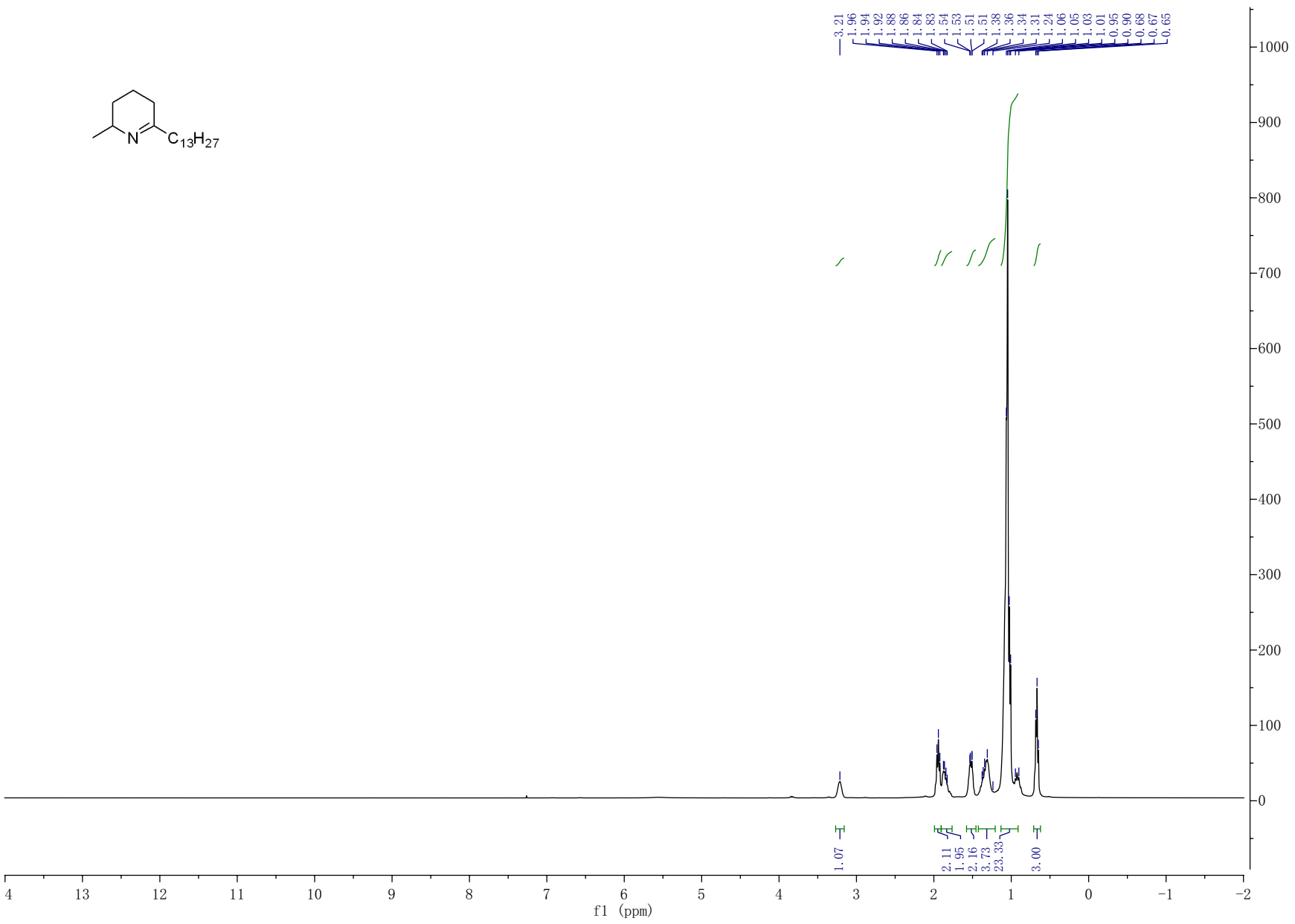
Acquisition Parameter

Polarity	Positive	Source	ESI	No. of Laser Shots	20
Averaged Scans	16	No. of Cell Fills	1	Laser Power	51.0 %
Broadband Low Mass	100.3 m/z	End Plate	4000.0 V	MALDI Plate	300.0 V
Broadband High Mass	2500.0 m/z	Capillary Entrance	4500.0 V	Imaging Spot Diameter	2000.0 µm
Acquisition Mode	Single MS	Skimmer 1	30.0 V		
Pulse Program	basic	Drying Gas Temperature	180.0 °C	Calibration Date	Fri Sep 25 08:42:02 2020
Source Accumulation	0.0 sec	Drying Gas Flow Rate	4.0 L/min	Data Acquisition Size	524288
Ion Accumulation Time	1.0 sec	Nebulizer Gas Flow Rate	1.0 L/min	Apodization	Sine-Bell Multiplication
Flight Time to Acq. Cell	0.0 sec				

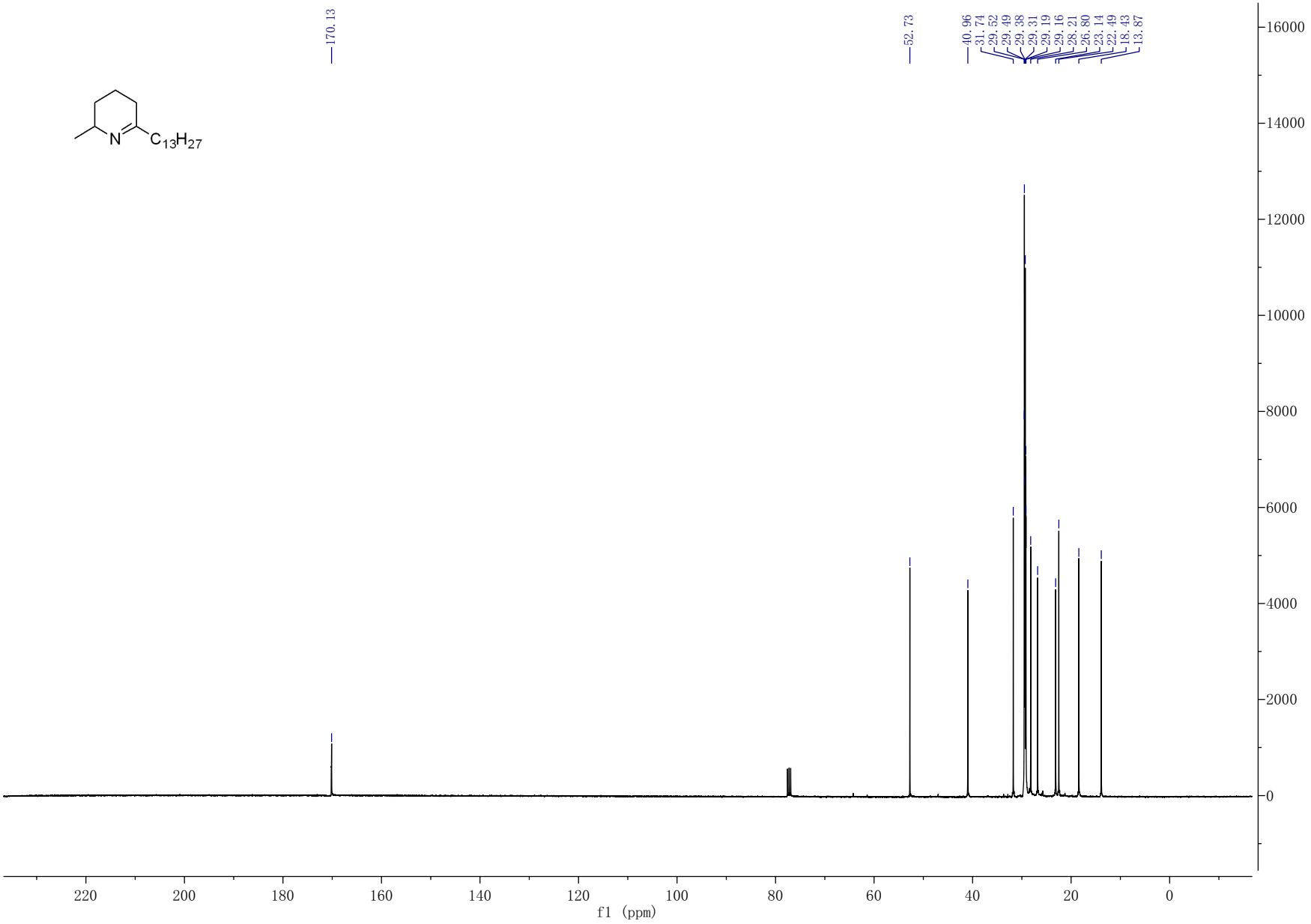


Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e^- Conf	N-Rule

S13. ^{1}H NMR Spectrum of Compound 6b



S14. ^{13}C NMR Spectrum of Compound6b



S15. HRMS Spectrum of Compound 6b

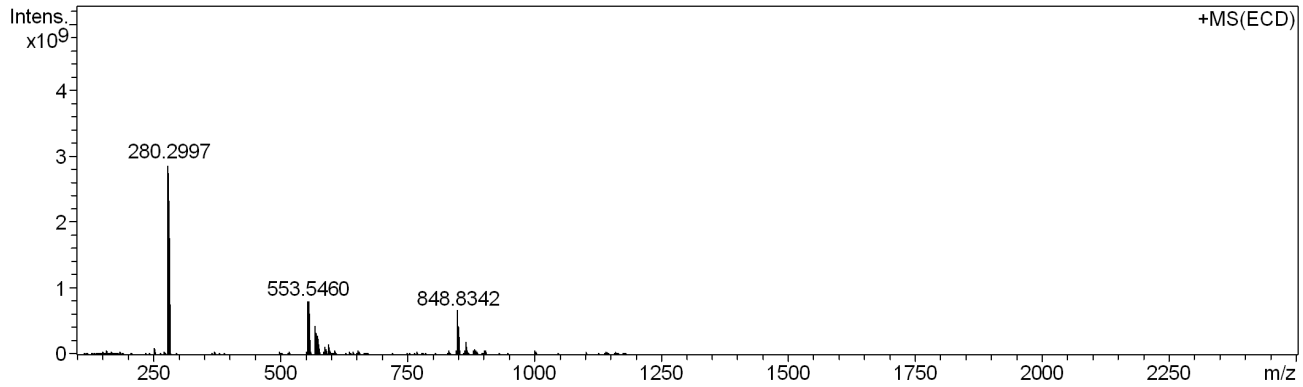
Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name	D:\Data\2020.09.25 chen li\pos-2_000001.d	Acquisition Date	9/25/2020 5:47:23 PM
Method	ESI_101506	Operator	
Sample Name	TUNMIX	Instrument	apex-Ultra
Comment			

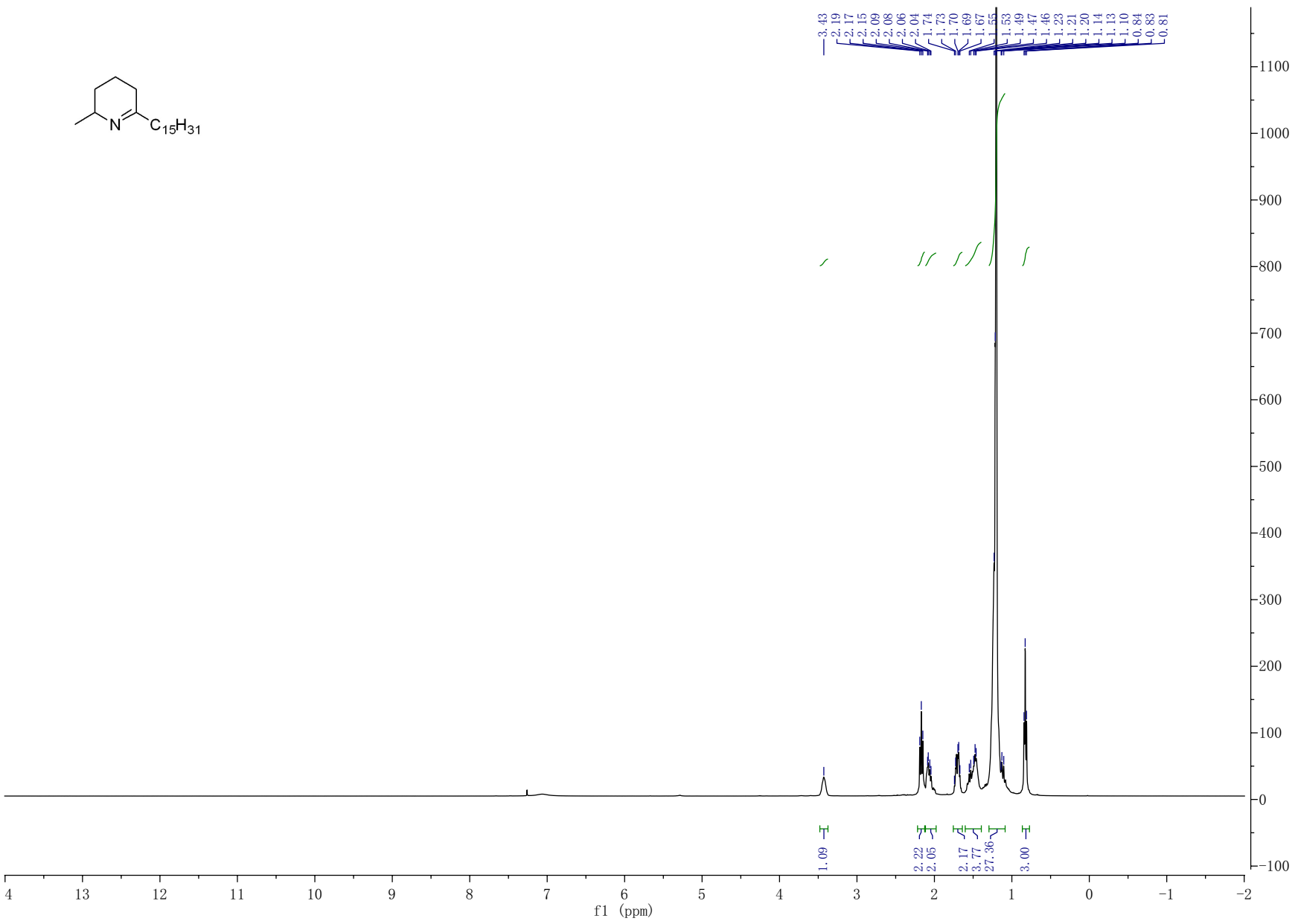
Acquisition Parameter

Polarity	Positive	Source	ESI	No. of Laser Shots	20
Averaged Scans	16	No. of Cell Fills	1	Laser Power	51.0 %
Broadband Low Mass	100.3 m/z	End Plate	4000.0 V	MALDI Plate	300.0 V
Broadband High Mass	2500.0 m/z	Capillary Entrance	4500.0 V	Imaging Spot Diameter	2000.0 µm
Acquisition Mode	Single MS	Skimmer 1	30.0 V		
Pulse Program	basic	Drying Gas Temperature	180.0 °C	Calibration Date	Fri Sep 25 08:42:02 2020
Source Accumulation	0.0 sec	Drying Gas Flow Rate	4.0 L/min	Data Acquisition Size	524288
Ion Accumulation Time	1.0 sec	Nebulizer Gas Flow Rate	1.0 L/min	Apodization	Sine-Bell Multiplication
Flight Time to Acq. Cell	0.0 sec				

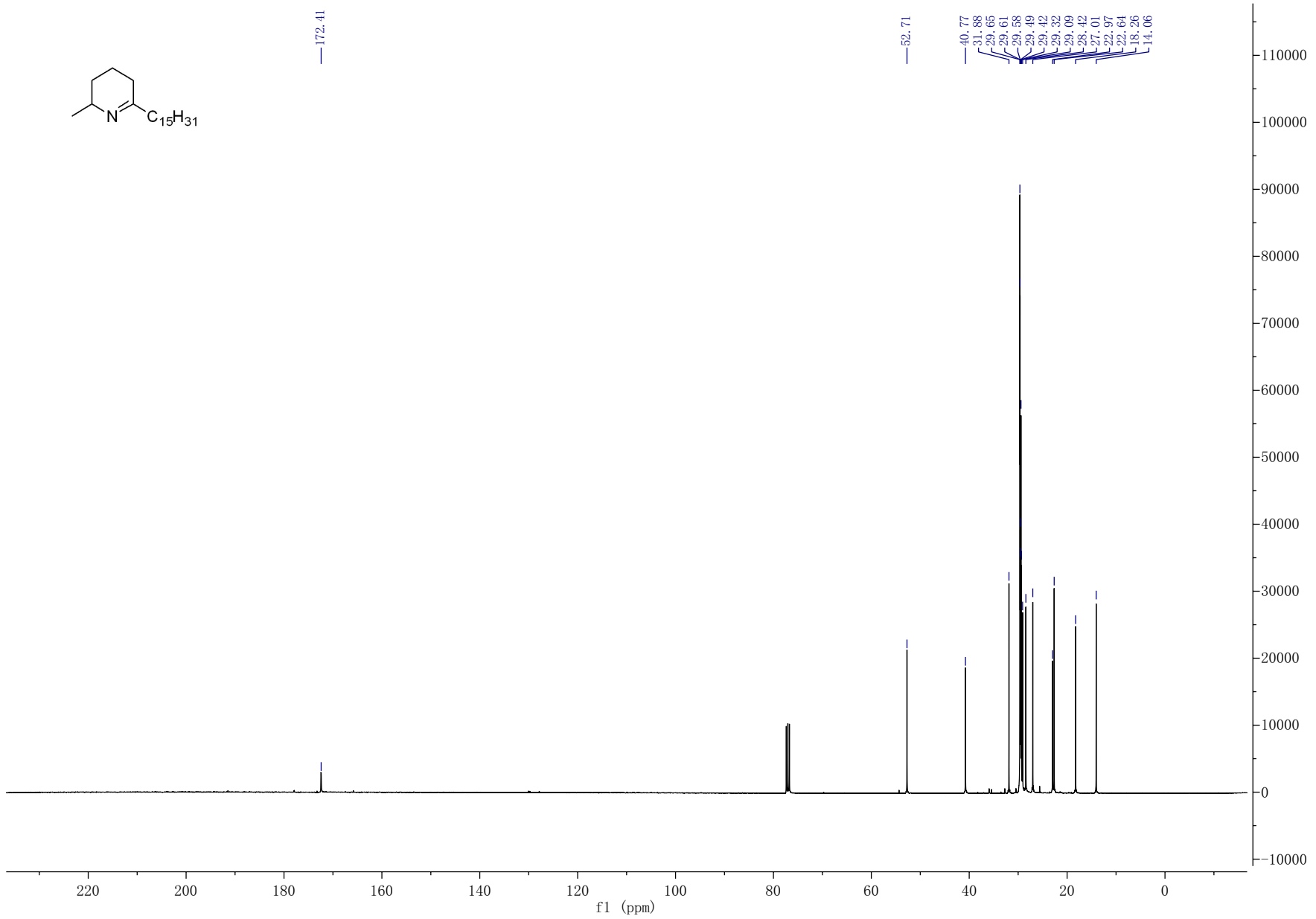


Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e^- Conf	N-Rule

S16. ^{1}H NMR Spectrum of Compound 6c



S17. ^{13}C NMR Spectrum of Compound6c



S18. HRMS Spectrum of Compound 6c

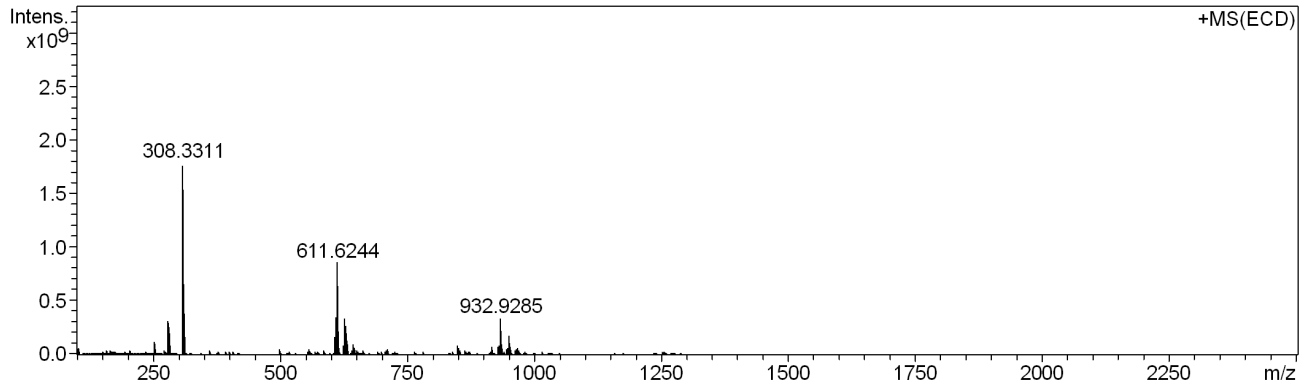
Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name	D:\Data\2020.09.25 chen li\pos-3_000001.d	Acquisition Date	9/25/2020 5:51:47 PM
Method	ESI_101506	Operator	
Sample Name	TUNMIX	Instrument	apex-Ultra
Comment			

Acquisition Parameter

Polarity	Positive	Source	ESI	No. of Laser Shots	20
Averaged Scans	16	No. of Cell Fills	1	Laser Power	51.0 %
Broadband Low Mass	100.3 m/z	End Plate	4000.0 V	MALDI Plate	300.0 V
Broadband High Mass	2500.0 m/z	Capillary Entrance	4500.0 V	Imaging Spot Diameter	2000.0 µm
Acquisition Mode	Single MS	Skimmer 1	30.0 V		
Pulse Program	basic	Drying Gas Temperature	180.0 °C	Calibration Date	Fri Sep 25 08:42:02 2020
Source Accumulation	0.0 sec	Drying Gas Flow Rate	4.0 L/min	Data Acquisition Size	524288
Ion Accumulation Time	1.0 sec	Nebulizer Gas Flow Rate	1.0 L/min	Apodization	Sine-Bell Multiplication
Flight Time to Acq. Cell	0.0 sec				



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e^- Conf	N-Rule