

Four-step Synthesis of 3-Allyl-2-(allyloxy)-5-bromoaniline from 2-Allylphenol

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Figure S1. ^1H NMR (400 MHz, CDCl_3)

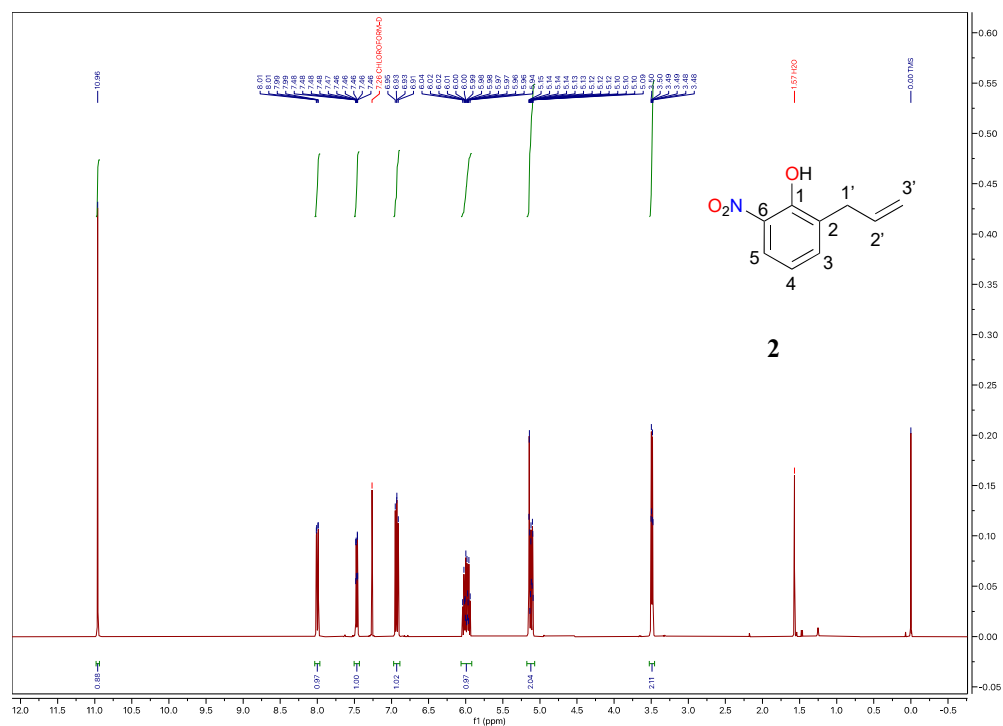


Figure S2. ^{13}C NMR (101 MHz, CDCl_3)

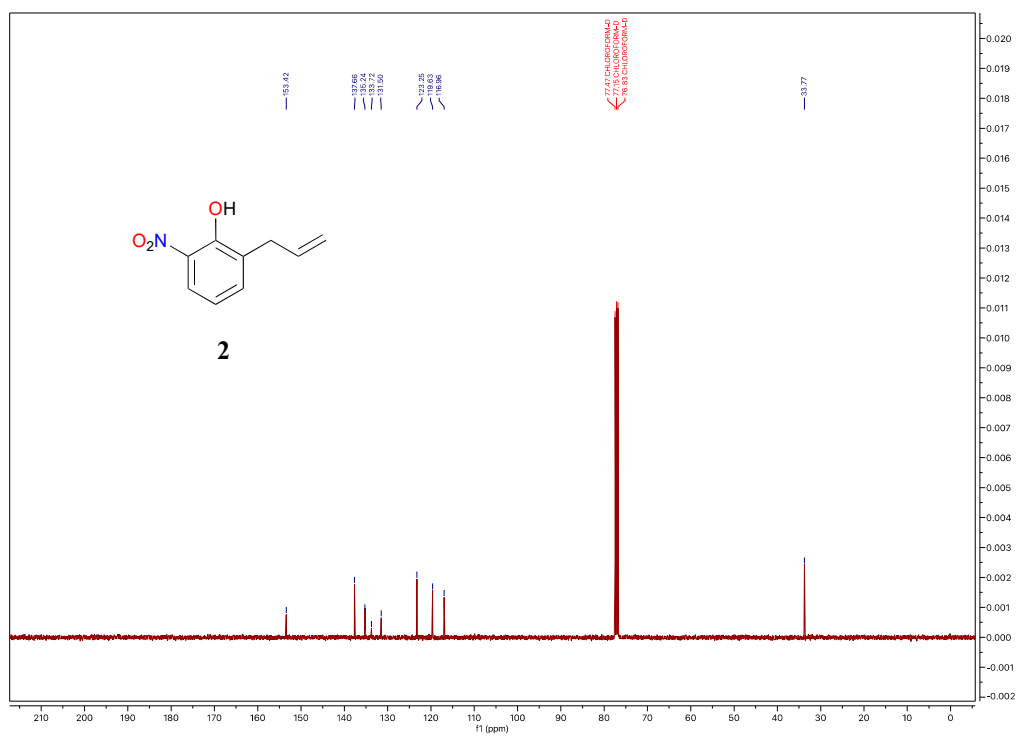
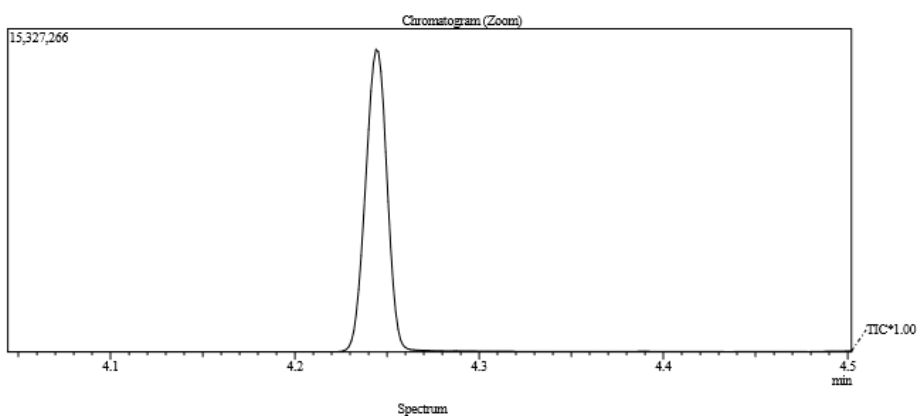
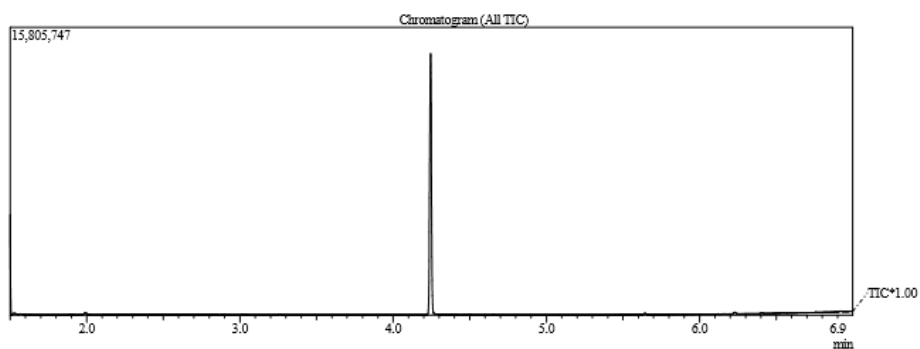


Figure S3. Mass Spectrum of Compound 2

1/17/2024 13:36:58

C:\GCMSolution\Data\1_Paul\12_001



Line#1 R.Time:4.244(Scan#2059)
MassPeaks:178
RawMode:Single 4.244(2059) BasePeak:162.10(1967439)
BGMode:None Group 1 - Event 1 Scan

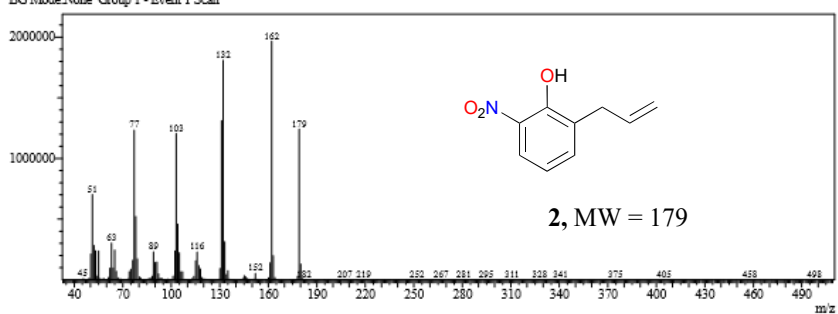
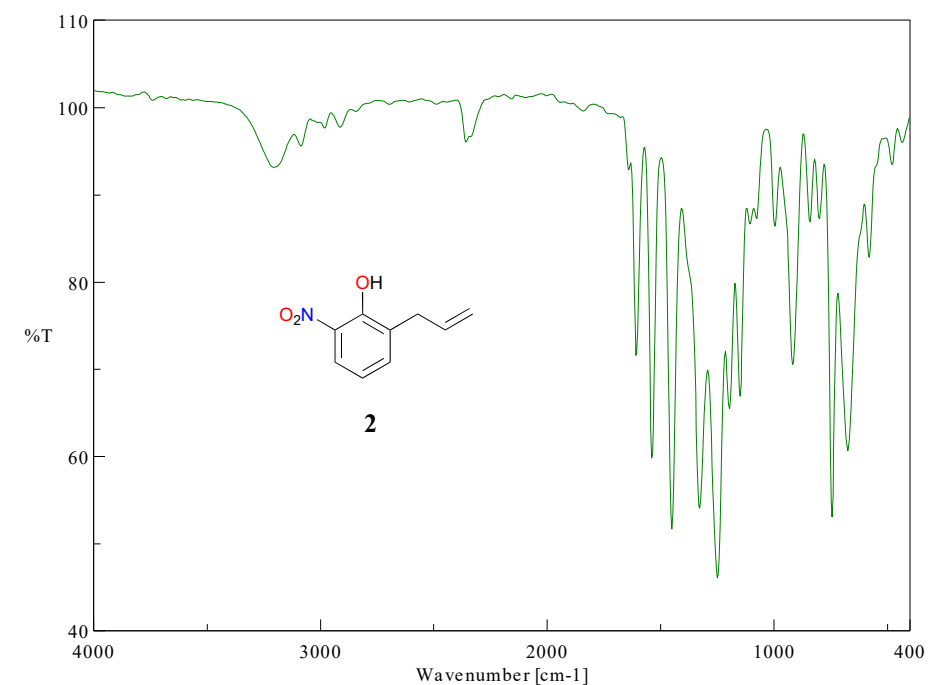


Figure S4. IR Spectrum of Compound 2



[Comments]
Sample name
Comment
User
Division
Company

Florida Gulf Coast University

— Spectrum1

[Measurement Information]

Model Name FT/IR-4700typeA
Serial Number F068961788

Accessory ATR PRO ONE
Accessory S/N C212061809
Incident angle 45 deg

Measurement Date 12/14/2023 12:24 PM

Light Source Standard
Detector TGS
Accumulation 8
Resolution 16 cm⁻¹
Zero Filling On
Apodization Cosine
Gain 1
Aperture Auto (7.1 mm)
Scanning Speed Auto (2 mm/sec)
Filter Auto (30000 Hz)

[Detailed Information]

Creation date 12/14/2023 12:24 PM

Data array type Linear data array
Horizontal axis Wavenumber [cm⁻¹]
Vertical axis %T
Start 397.264 cm⁻¹
End 4003.5 cm⁻¹
Data interval 3.85693 cm⁻¹
Data points 936

Figure S5. ^1H NMR (400 MHz, CDCl_3)

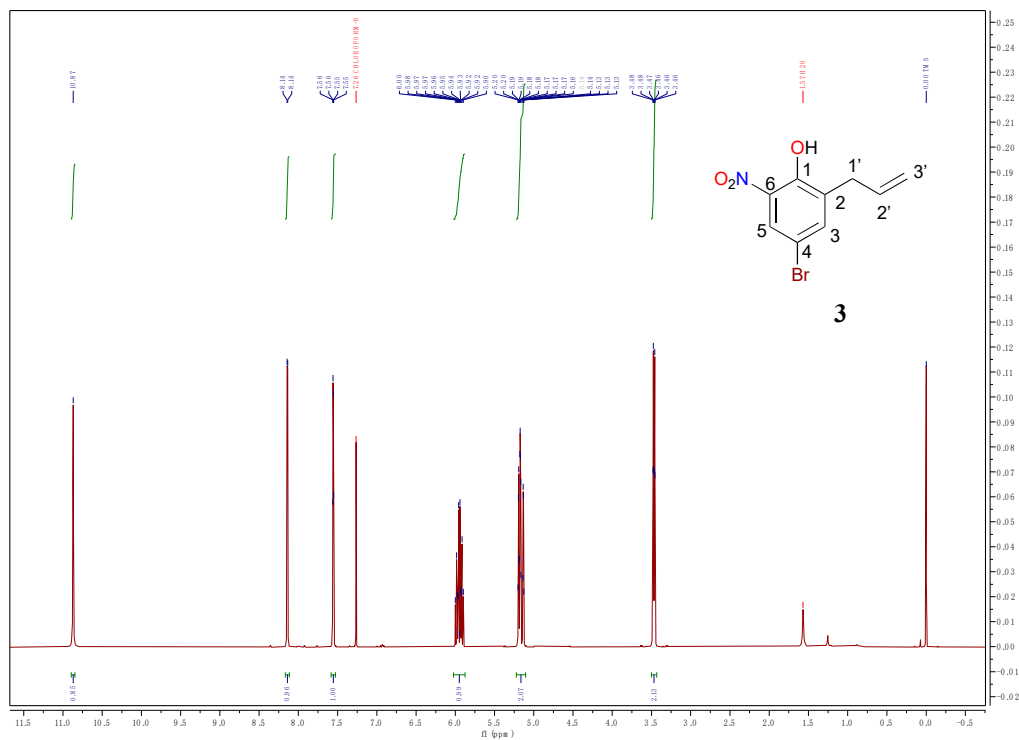


Figure S6. ^{13}C NMR (101 MHz, CDCl_3)

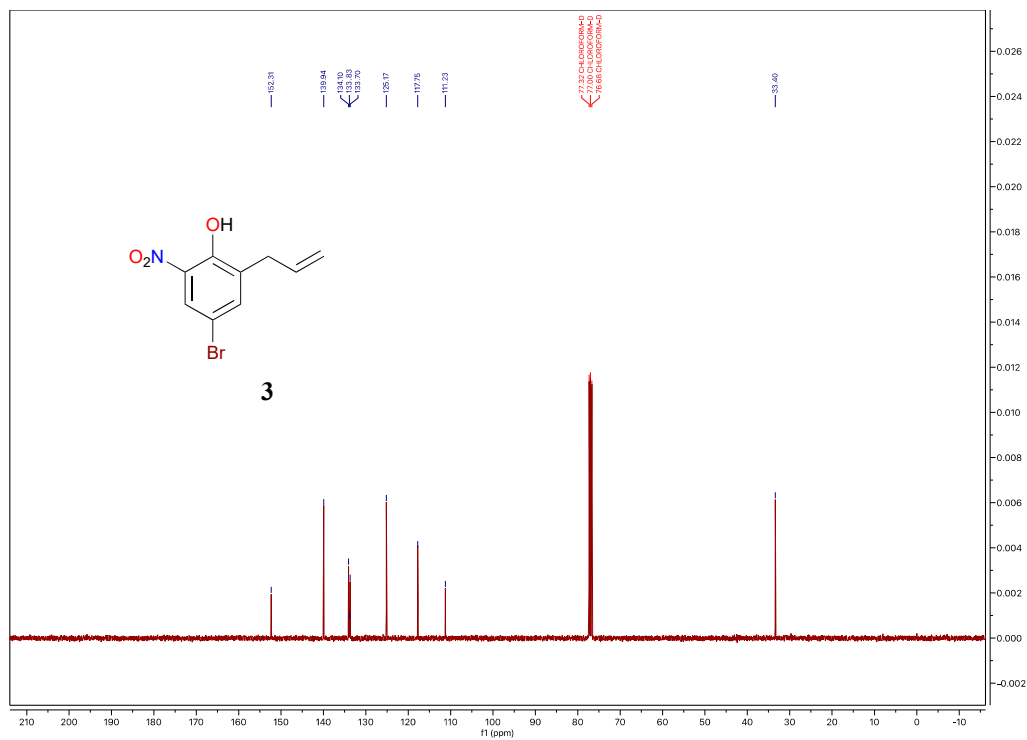
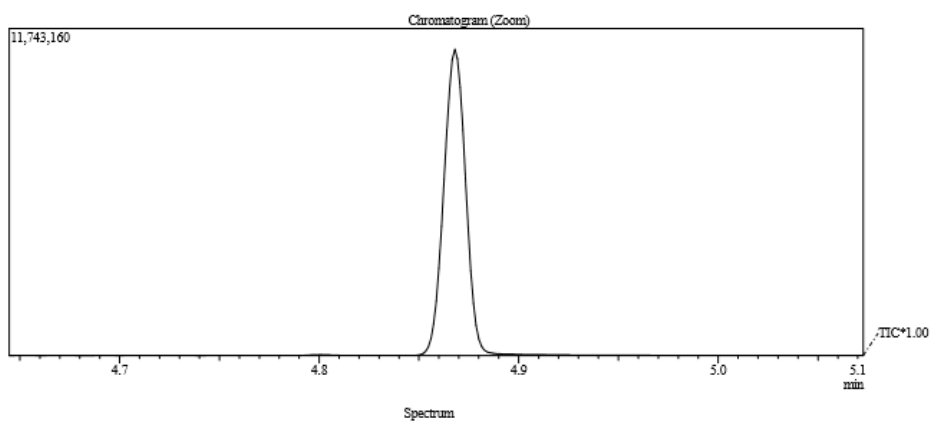
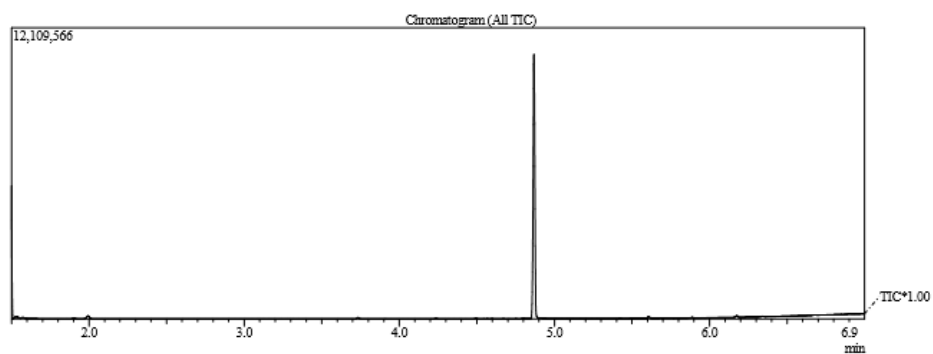


Figure S7. Mass Spectrum of Compound 3

1/17/2024 13:45:12

D:\C3.qgd



Line# 1 R.Time: 4.868 (Scan# 2527)

Mass Peaks: 232

Raw Mode: Single 4.868 (2527) Base Peak: 102.05 (930012)

BG Mode: None Group 1 - Event 1 Scan

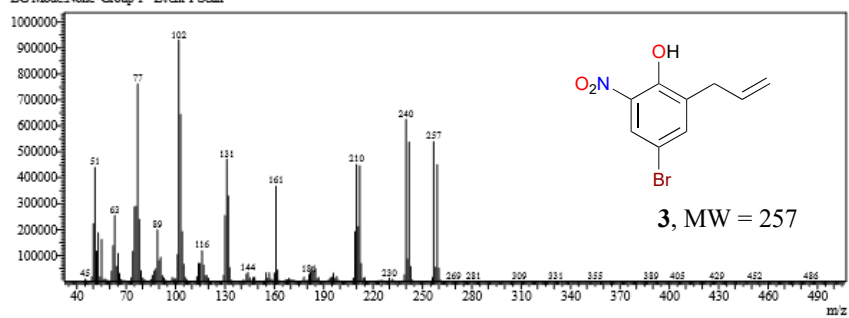
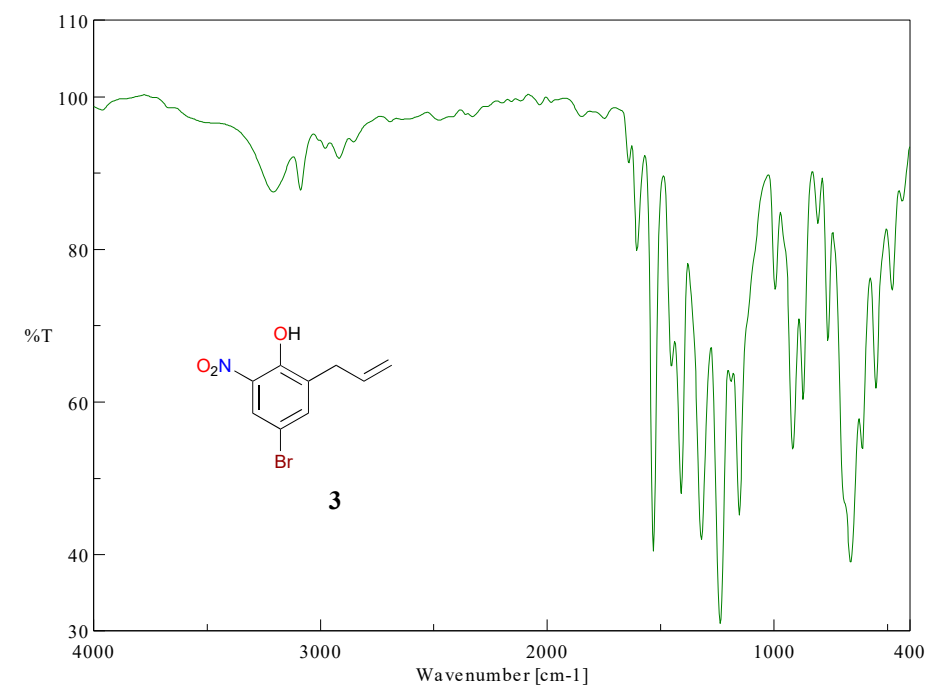


Figure S8. IR Spectrum of Compound 3



[Comments]
Sample name
Comment
User
Division
Company

Florida Gulf Coast University

— Spectrum3

[Measurement Information]

Model Name FT/IR-4700typeA
Serial Number F068961788

Accessory ATR PRO ONE
Accessory S/N C212061809
Incident angle 45 deg

Measurement Date 12/14/2023 12:36 PM

Light Source Standard
Detector TGS
Accumulation 8
Resolution 16 cm⁻¹
Zero Filling On
Apodization Cosine
Gain 1
Aperture Auto (7.1 mm)
Scanning Speed Auto (2 mm/sec)
Filter Auto (30000 Hz)

[Detailed Information]

Creation date 12/14/2023 12:36 PM

Data array type Linear data array
Horizontal axis Wavenumber [cm⁻¹]
Vertical axis %T
Start 397.264 cm⁻¹
End 4003.5 cm⁻¹
Data interval 3.85693 cm⁻¹
Data points 936

Figure S9. ^1H NMR (400 MHz, CDCl_3)

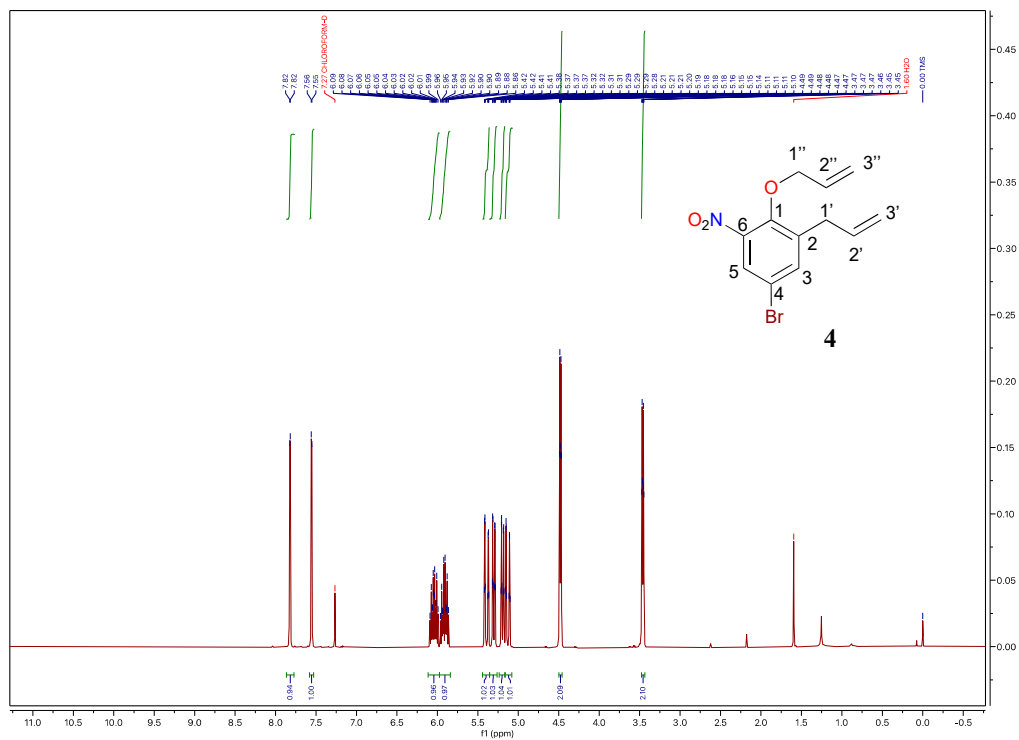


Figure S10. ^{13}C NMR (101 MHz, CDCl_3)

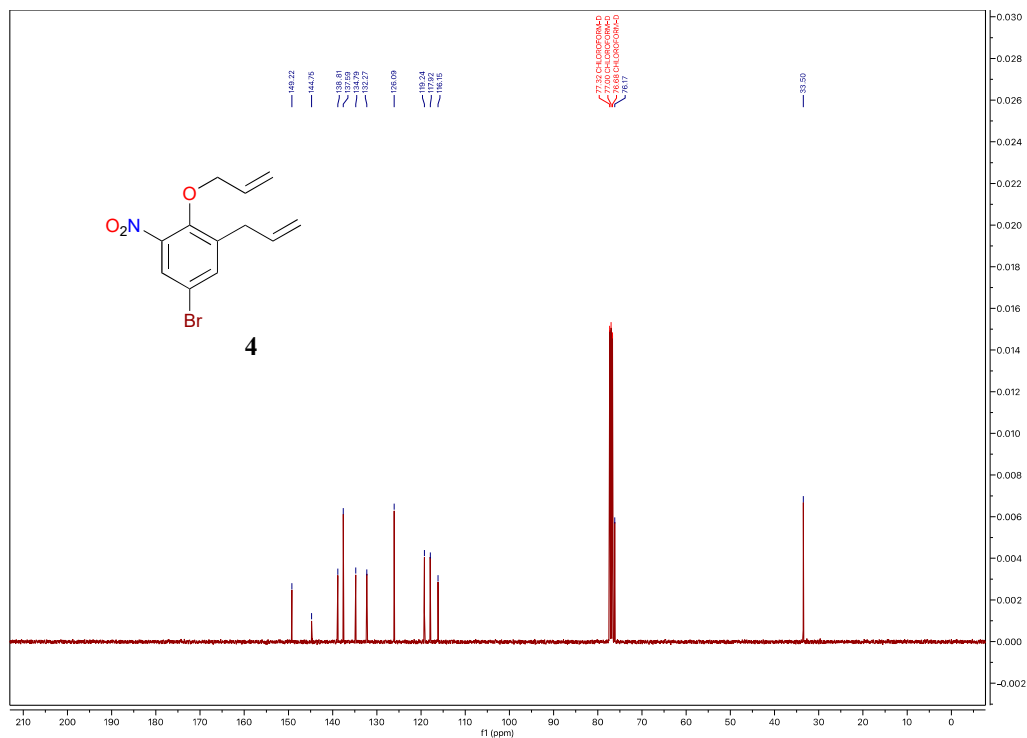
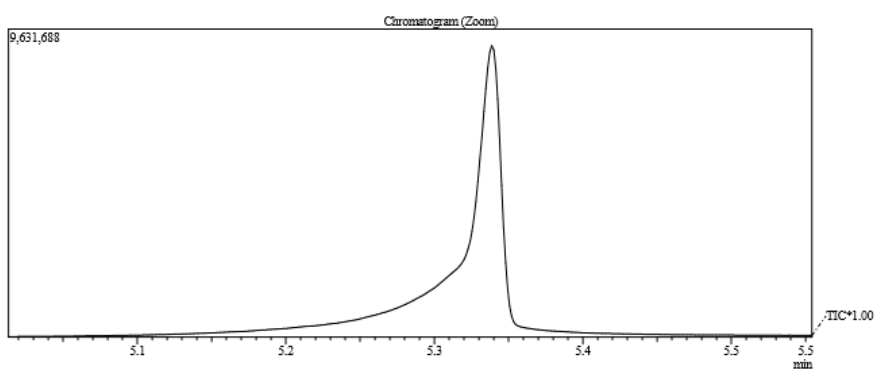
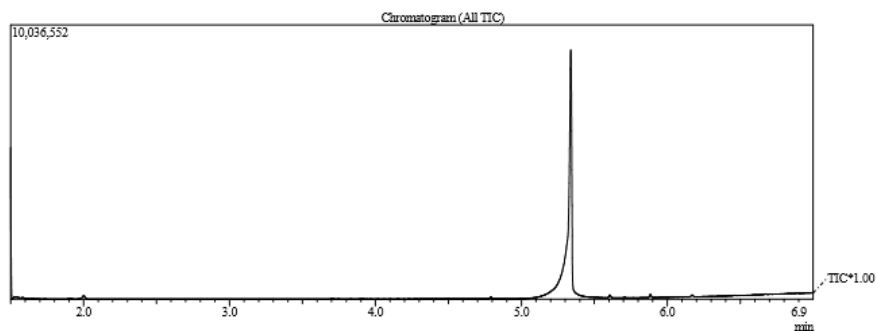


Figure S11. Mass Spectrum of Compound 4

1/17/2024 13:52:11

C:\GCMSolution\Data\Paull C4.qgd



Spectrum

Line# 1 R.Time:5.343(Scan#2883)
MassPeaks:259
RawMode:Single 5.343(2883) BasePeak:102.05(421267)
BGMode:None Group 1 - Event 1 Scan

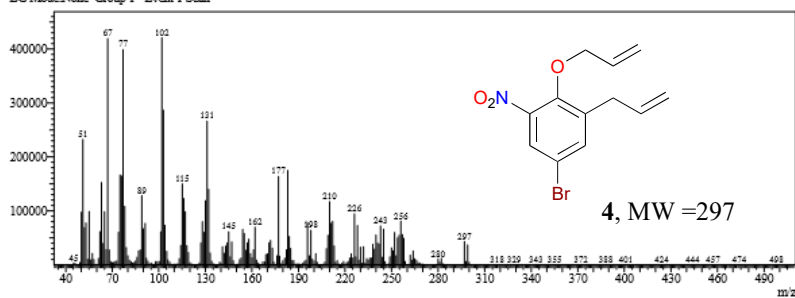
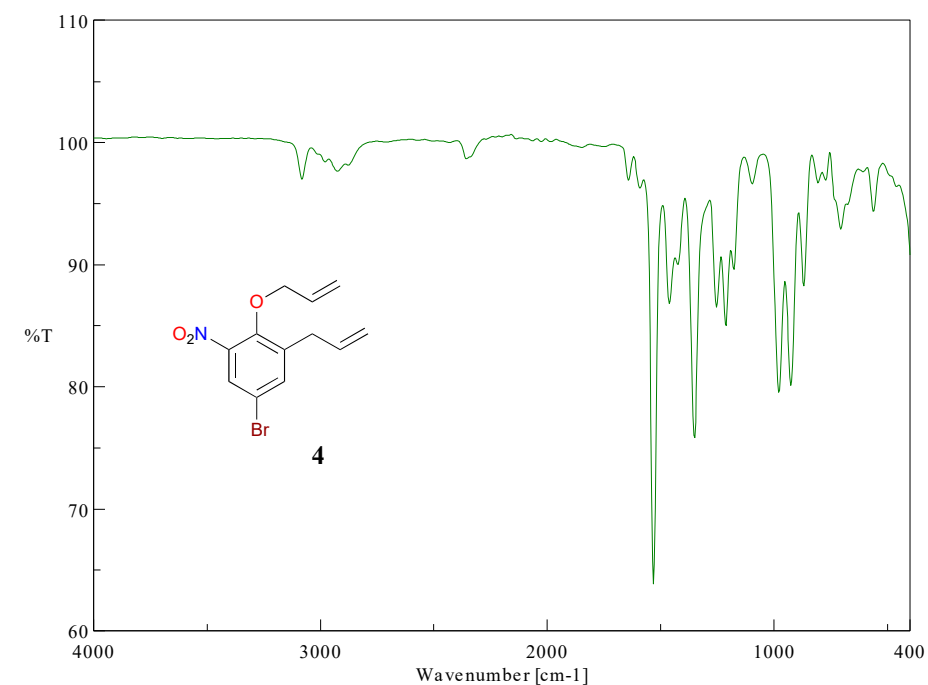


Figure S12. IR Spectrum of Compound 4



[Comments]
Sample name
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User
Division
Company

Florida Gulf Coast University

— Spectrum4

[Measurement Information]

Model Name FT/IR-4700typeA
Serial Number F068961788

Accessory ATR PRO ONE
Accessory S/N C212061809
Incident angle 45 deg

Measurement Date 12/14/2023 12:41 PM

Light Source Standard
Detector TGS
Accumulation 8
Resolution 16 cm⁻¹
Zero Filling On
Apodization Cosine
Gain 1
Aperture Auto (7.1 mm)
Scanning Speed Auto (2 mm/sec)
Filter Auto (30000 Hz)

[Detailed Information]

Creation date 12/14/2023 12:41 PM

Data array type Linear data array
Horizontal axis Wavenumber [cm⁻¹]
Vertical axis %T
Start 397.264 cm⁻¹
End 4003.5 cm⁻¹
Data interval 3.85693 cm⁻¹
Data points 936

Figure S13. ^1H NMR (400 MHz, CDCl_3)

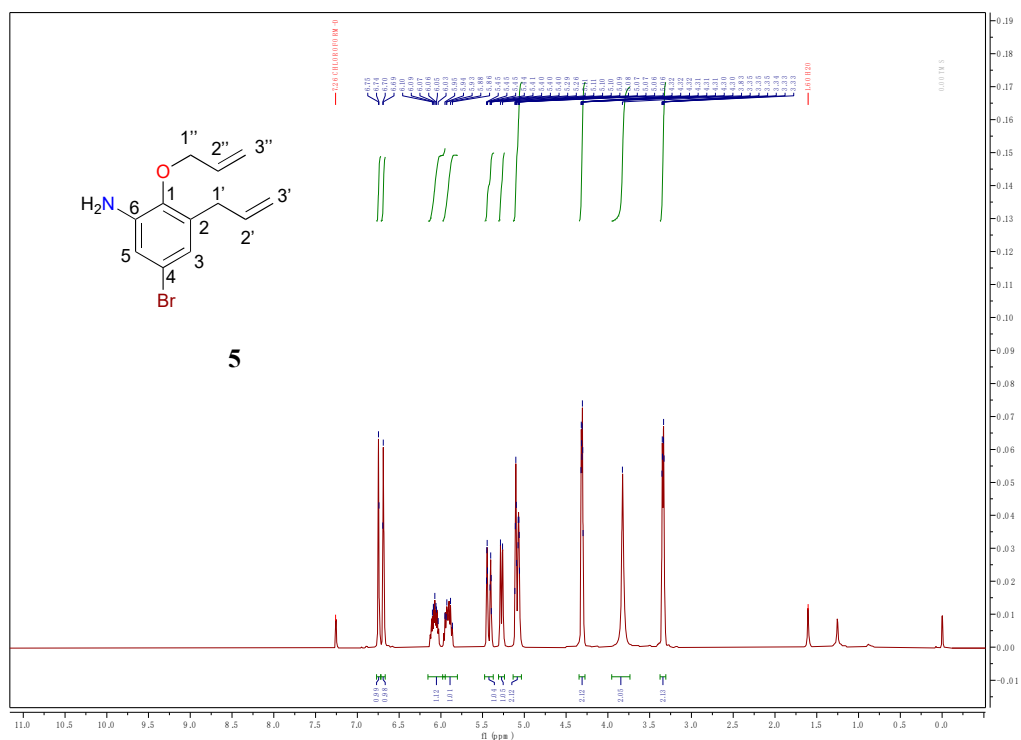


Figure S14. ^{13}C NMR (101 MHz, CDCl_3)

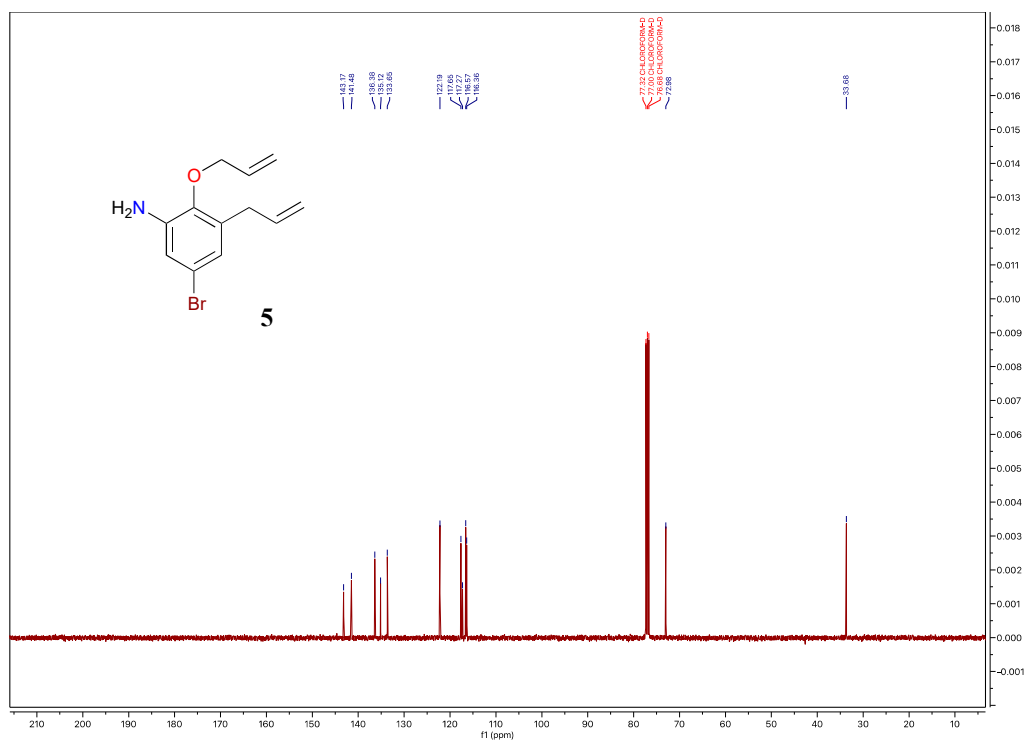
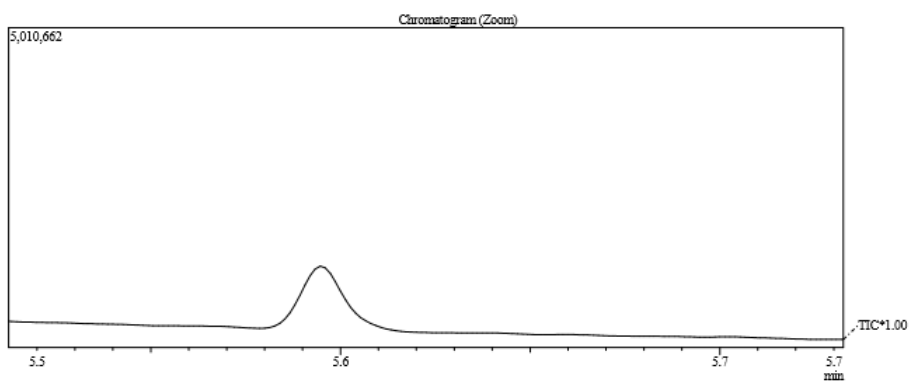
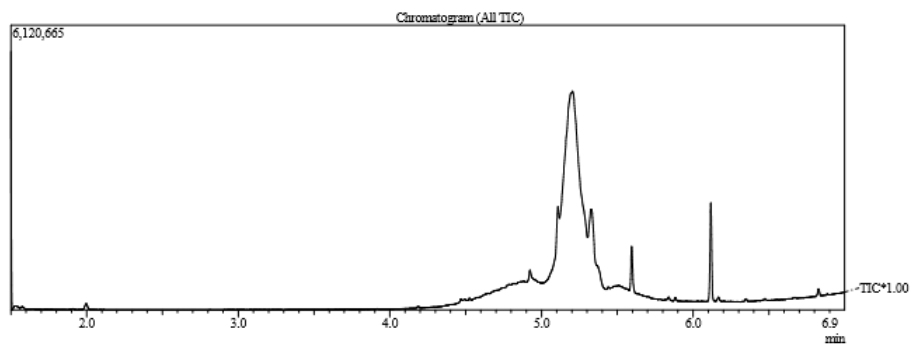


Figure S15. Mass Spectrum of Compound 5

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D:\CS.qgd



Spectrum

Line#1 R.Time:5.595(Scan#3072)

MassPeak:232

RawMode:Single 5.595(3072) BasePeak:267.00(92084)

BGMode:None Group 1 - Event 1 Scan

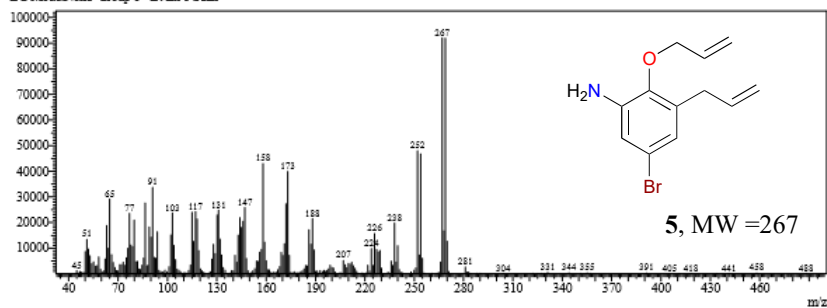
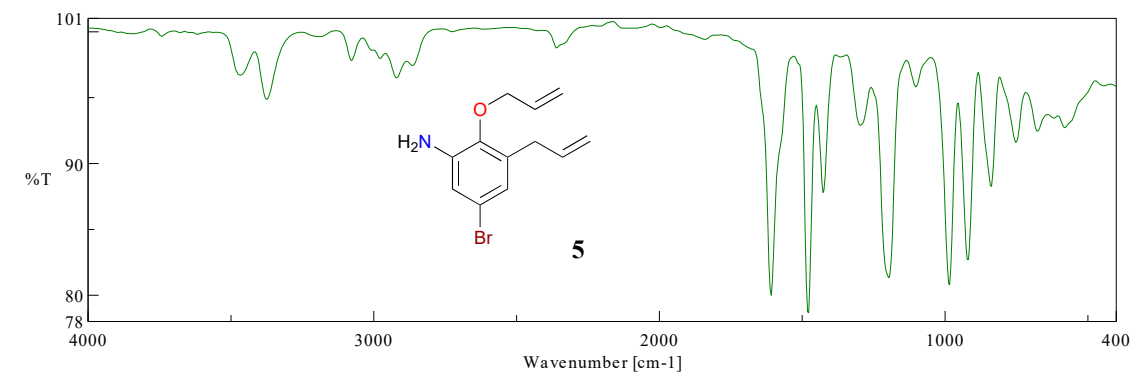
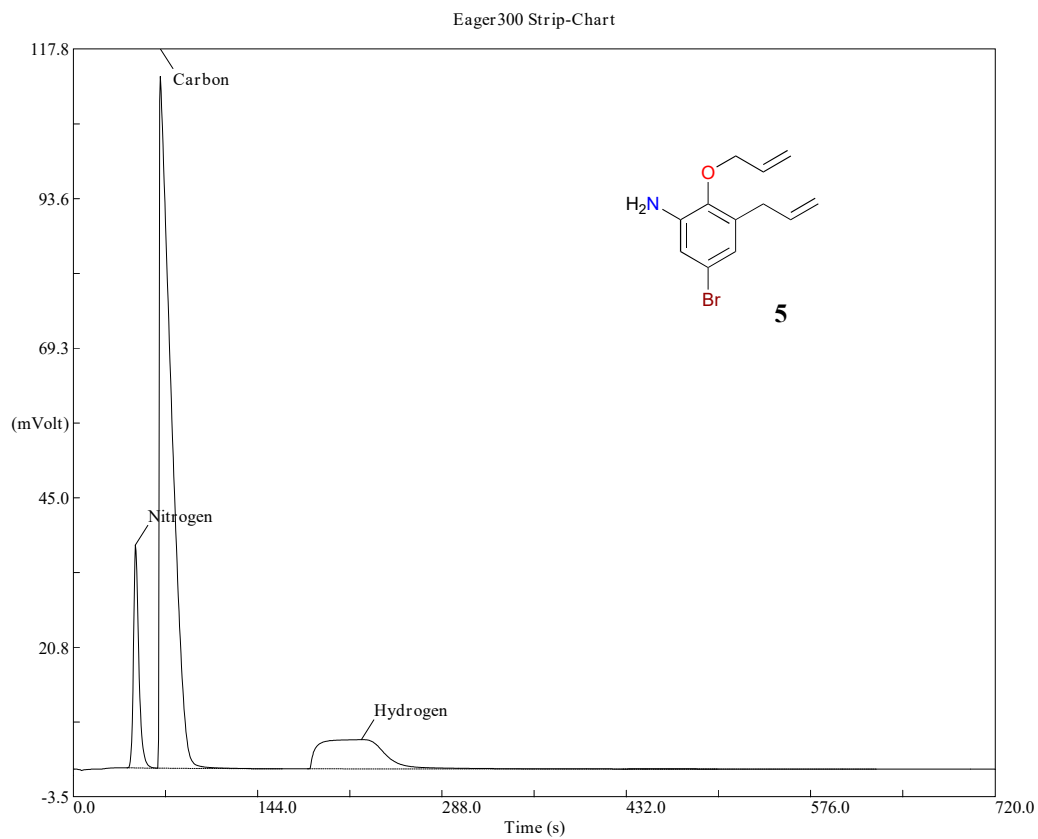


Figure S16. IR Spectrum of Compound 5



[Comments]		[Measurement Information]	
Sample name		Model Name	FT/IR-4700type A
Comment		Serial Number	F068961788
User			
Division		Accessory	ATR PRO ONE
Company	Florida Gulf Coast University	Accessory S/N	C212061809
		Incident angle	45 deg
[Detailed Information]			
Creation date	1/17/2024 2:23 PM	Measurement Date	1/17/2024 2:23 PM
Date modified	1/17/2024 2:26 PM		
Data array type	Linear data array	Light Source	Standard
Horizontal axis	Wavenumber [cm-1]	Detector	TGS
Vertical axis	%T	Accumulation	60
Start	397.264 cm-1	Resolution	16 cm-1
End	4003.5 cm-1	Zero Filling	On
Data interval	3.85693 cm-1	Apodization	Cosine
Data points	936	Gain	1
		Aperture	Auto (7.1 mm)
		Scanning Speed	Auto (2 mm/sec)
		Filter	Auto (30000 Hz)

Figure S17. Elemental Analysis Chromatogram of Compound 5



		Nitrogen	Carbon	Hydrogen	Sulphur
1	bypass	0	0	0	0
2	blank	0	0	0	0
3	Std: BBOT	6.51	72.53	6.09	0
5	Compound 5	5.18	53.71	5.24	0