

Supporting Information

Cross Coupling of Benzylammonium Salts with Boronic Acids Using a Well-Defined *N*-Heterocyclic Carbene Palladium(II) Precatalyst

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Characterization Data of the Catalysis Products 3aa-3am and 3ba-3bi

Complex (3aa)^[1, 2, 4]: ¹H NMR (400 MHz, CDCl₃): δ 7.18 (t, *J* = 7.5 Hz, 2H, ArH), 7.09 (t, *J* = 7.8 Hz, 3H, ArH), 7.01 (d, *J* = 8.5 Hz, 2H, ArH), 6.73(d, *J* = 8.5 Hz, 2H, ArH), 3.83(s, 2H, CH₂), 3.67(s, 3H, OMe). ¹³C NMR (100 MHz, CDCl₃): δ 158.0, 141.6, 133.3, 129.9, 128.9, 128.5, 126.0, 113.9, 55.3, 41.1.

Complex (3ab)^[2, 4]: ¹H NMR (400 MHz, CDCl₃): δ 7.30-7.26 (m, 2H, ArH), 7.22-7.18 (m, 4H, ArH), 6.79-6.73 (m, 3H, ArH), 3.96 (s, 2H, CH₂), 3.76 (s, 3H, OMe). ¹³C NMR (100 MHz, CDCl₃): δ 159.7, 142.7, 140.9, 129.4, 128.9, 128.5, 126.1, 121.4, 114.8, 111.3, 55.2, 42.0.

Complex (3ac)^[2, 4]: ¹H NMR (400 MHz, CDCl₃): δ 7.26-7.13 (m, 6H, ArH), 7.04 (d, *J* = 6.4 Hz, 1H, ArH), 6.85 (t, *J* = 7.3 Hz, 2H, ArH), 3.95 (s, 2H, CH₂), 3.79 (s, 3H, OMe). ¹³C NMR (100 MHz, CDCl₃): δ 157.4, 141.0, 130.3, 129.7, 129.0, 128.3, 127.4, 125.8, 120.5, 110.4, 55.4, 35.9.

Complex (3ad): ¹H NMR (400 MHz, CDCl₃): δ 7.28-7.25 (m, 2H, ArH), 7.20-7.16 (m, 3H, ArH), 6.34 (d, *J* = 2.2 Hz, 2H, ArH), 6.30 (t, *J* = 2.2 Hz, 1H, ArH), 3.90 (s, 2H, CH₂), 3.72 (s, 6H, OMe). ¹³C NMR (100 MHz, CDCl₃): δ 160.9, 143.5, 140.8, 128.9, 128.5, 126.2, 107.2, 98.0, 55.3, 42.2. GC-MS (EI) calcd for C₁₅H₁₆O₂: 228.1, found: 228.2.

Complex (3ae)^[2-4]: ¹H NMR (400 MHz, CDCl₃): δ 7.28-7.24 (m, 2H, ArH), 7.20-7.16 (m, 3H, ArH), 7.10-7.05 (m, 4H, ArH), 3.93 (s, 2H, CH₂), 2.30 (s, 3H, CH₃). ¹³C NMR (100 MHz, CDCl₃): δ 141.5, 138.1, 135.6, 129.2, 128.9, 128.8, 128.5, 126.0, 41.6, 21.1.

Complex (3af)^[3]: ¹H NMR (400 MHz, CDCl₃): δ 7.30-7.26 (m, 2H, ArH), 7.22-7.15 (m, 4H, ArH), 7.01-6.98 (m, 3H, ArH), 3.94 (s, 2H, CH₂), 2.30 (s, 3H, CH₃). ¹³C NMR (100 MHz, CDCl₃): δ 141.3, 141.1, 138.1, 129.7, 128.9, 128.5, 128.4, 126.8, 126.0, 125.9, 41.9, 21.4.

Complex (3ag)^[1, 3, 4]: ¹H NMR (400 MHz, CDCl₃): δ 7.28-7.23 (m, 3H, ArH), 7.20-7.09 (m, 6H, ArH), 3.98 (s, 2H, CH₂), 2.24 (s, 3H, CH₃). ¹³C NMR (100 MHz, CDCl₃): δ 140.4, 138.9, 136.7, 130.3, 130.0, 128.8, 128.4, 126.5, 126.0, 125.9, 39.5, 19.7.

Complex (3ah)^[4]: ¹H NMR (400 MHz, CDCl₃): δ 7.28-7.25 (m 1H, ArH), 7.19-7.16 (m, 4H, ArH), 6.81 (d, *J* = 9.1 Hz, 3H, ArH), 3.89 (s, 2H, CH₂), 2.26 (s, 6H, CH₃). ¹³C NMR

(100 MHz, CDCl₃): δ 141.4, 141.0, 138.0, 129.0, 128.5, 127.8, 126.8, 126.0, 41.9, 21.3.

Complex (3ai)^[2-4]: ¹H NMR (400 MHz, CDCl₃): δ 7.30-7.27 (m, 2H, ArH), 7.23-7.20 (m, 1H, ArH), 7.17-7.11 (m, 4H, ArH), 6.99-6.93 (m, 2H, ArH), 3.94 (s, 2H, CH₂). ¹³C NMR (100 MHz, CDCl₃): δ 162.7, 160.2, 141.0, 136.8 (d, $J = 3.0$ Hz), 130.3 (d, $J = 7.9$ Hz), 128.7 (d, $J = 29.2$ Hz), 126.2, 115.3 (d, $J = 21.0$ Hz), 41.1.

Complex (3aj)^[2-4]: ¹H NMR (400 MHz, CDCl₃): δ 7.73-7.67 (m, 1H, ArH), 7.52 (d, $J = 8.1$ Hz, 2H, ArH), 7.31-7.27 (m, 3H, ArH), 7.24-7.20 (m, 1H, ArH), 7.17-7.16 (m, 2H, ArH), 4.02 (s, 2H, CH₂). ¹³C NMR (100 MHz, CDCl₃): δ 145.3, 140.0, 129.2, 129.0, 128.7, 127.0 (q, $J = 263.2$ Hz), 126.5, 126.0 (q, $J = 3.7$ Hz), 125.4 (q, $J = 3.7$ Hz), 41.7.

Complex (3ak)^[3-4]: ¹H NMR (400 MHz, CDCl₃): δ 7.99-7.96 (m, 1H, ArH), 7.85-7.83 (m, 1H, ArH), 7.74 (d, $J = 8.2$ Hz, 1H, ArH), 7.44-7.38 (m, 3H, ArH), 7.28-7.23 (m, 3H, ArH), 7.19-7.15 (m, 3H, ArH), 4.43 (s, 2H, CH₂). ¹³C NMR (100 MHz, CDCl₃): δ 141.0, 138.6, 133.6, 132.1, 129.0, 128.5, 128.1, 127.7, 127.6, 127.5, 127.1, 126.2, 126.0, 125.4, 42.1.

Complex (3al)^[1-2]: ¹H NMR (400 MHz, CDCl₃): δ 7.80-7.34 (m, 3H, ArH), 7.62 (s, 1H, ArH), 7.46-7.39 (m, 2H, ArH), 7.32-7.27 (m, 3H, ArH), 7.23-7.18 (m, 3H, ArH), 4.13 (s, 2H, CH₂). ¹³C NMR (100 MHz, CDCl₃): δ 141.0, 138.6, 133.6, 132.1, 129.1, 128.5, 128.1, 127.7, 127.6, 127.5, 127.1, 126.1, 126.0, 125.4, 42.1.

Complex (3am): ¹H NMR (400 MHz, CDCl₃): δ 7.36-7.29 (m, 2H, ArH), 7.24-7.18 (m, 4H, ArH), 6.91-6.89 (m, 2H, ArH), 3.97 (s, 2H, CH₂). ¹³C NMR (100 MHz, CDCl₃): δ 141.5, 140.6, 128.8, 128.5, 126.2, 125.6, 121.3, 119.8, 36.6. GC-MS (EI) calcd for C₁₁H₁₀S: 174.1, found: 174.1.

Complex (3ba)^[1]: ¹H NMR (400 MHz, CDCl₃): δ 7.10-7.04 (m, 6H, ArH), 6.83-6.79 (m, 2H, ArH), 3.87 (s, 2H, CH₂), 3.76 (s, 3H, OMe), 2.30 (s, 3H, CH₃). ¹³C NMR (100 MHz, CDCl₃): δ 157.9, 138.6, 135.5, 133.6, 129.8, 129.2, 128.7, 113.9, 55.3, 40.6, 21.0.

Complex (3bb): ¹H NMR (400 MHz, CDCl₃): δ 7.16 (t, $J = 7.8$ Hz, ArH), 7.10 (d, $J = 8.6$ Hz, 2H, ArH), 6.98 (t, $J = 8.8$ Hz, 3H, ArH), 6.84-6.80 (m, 2H, ArH), 3.87 (s, 2H, CH₂), 3.76 (s, 3H, OMe), 2.30 (s, 3H, CH₃). ¹³C NMR (100 MHz, CDCl₃): δ 158.0, 141.5, 138.0, 133.4, 129.9, 129.6, 128.4, 126.8, 125.9, 113.9, 55.3, 41.0, 21.5. GC-MS (EI) calcd for C₁₅H₁₆O: 212.1, found: 212.1.

Complex (3bc)^[1]: ¹H NMR (400 MHz, CDCl₃): δ 7.15-7.12 (m, 3H, ArH), 7.09-7.06 (m,

1H, ArH), 7.05-7.01 (m, 2H, ArH), 6.82-6.79 (m, 2H, ArH), 3.91 (s, 2H, CH₂), 3.76 (s, 3H, OMe), 2.23 (s, 3H, CH₃). ¹³C NMR (100 MHz, CDCl₃): δ 156.8, 138.3, 135.5, 131.4, 129.2, 128.7, 128.6, 125.3, 124.9, 112.7, 54.2, 37.5, 18.6.

Complex (3bd): ¹H NMR (400 MHz, CDCl₃): δ 7.31-7.28 (m, 2H, ArH), 7.12-7.09 (m, 4H, ArH), 6.84-6.81 (m, 2H, ArH), 3.89 (s, 2H, CH₂), 3.77 (s, 3H, OMe), 1.29 (s, 9H, CH₃). ¹³C NMR (100 MHz, CDCl₃): δ 157.9, 148.8, 138.6, 133.5, 129.9, 128.4, 125.4, 113.9, 55.3, 40.5, 34.4, 31.4. GC-MS (EI) calcd for C₁₈H₂₂O: 254.2, found: 254.2.

Complex (3be): ¹H NMR (400 MHz, CDCl₃): δ 7.13-7.06 (m, 4H, ArH), 6.95 (t, *J* = 8.7 Hz, 2H, ArH), 6.83 (d, *J* = 8.6 Hz, 2H, ArH), 3.88 (s, 2H, CH₂), 3.77 (s, 3H, OMe). ¹³C NMR (100 MHz, CDCl₃): δ 161.4 (d, *J* = 242.2 Hz), 158.1, 137.3 (d, *J* = 30.8 Hz), 133.1, 130.2 (d, *J* = 78.9 Hz), 129.8, 115.2 (d, *J* = 210.8 Hz), 114.0, 55.3, 40.2. GC-MS (EI) calcd for C₁₄H₁₃FO: 216.1, found: 216.1.

Complex (3bf): ¹H NMR (400 MHz, CDCl₃): δ 8.13 (d, *J* = 8.8 Hz, 2H, ArH), 7.32 (d, *J* = 8.8 Hz, 2H, ArH), 7.09 (d, *J* = 8.7 Hz, 2H, ArH), 6.86 (d, *J* = 8.7 Hz, 2H, ArH), 4.02 (s, 2H, CH₂), 3.79 (s, 3H, OMe). ¹³C NMR (100 MHz, CDCl₃): δ 158.4, 149.4, 146.5, 131.3, 130.0, 129.5, 123.8, 114.2, 55.3, 40.9. GC-MS (EI) calcd for C₁₄H₁₃NO₃: 243.1, found: 243.1.

Complex (3bg): ¹H NMR (400 MHz, CDCl₃): δ 8.00-7.98 (m, 1H, ArH), 7.85-7.83 (m, 1H, ArH), 7.74 (d, *J* = 8.2 Hz, 1H, ArH), 7.45-7.38 (m, 3H, ArH), 7.26 (d, *J* = 6.9 Hz, 1H, ArH), 7.10 (d, *J* = 8.7 Hz, 2H, ArH), 6.82-6.78 (m, 2H, ArH), 4.38 (s, 2H, CH₂), 3.75 (s, 3H, OMe). ¹³C NMR (100 MHz, CDCl₃): δ 157.9, 137.1, 134.0, 132.7, 132.1, 129.7, 128.7, 127.2, 127.1, 126.0, 125.6, 125.5, 124.3, 113.9, 55.3, 38.2. GC-MS (EI) calcd for C₁₈H₁₆O: 248.1, found: 248.2.

Complex (3bh)^[1]: ¹H NMR (400 MHz, CDCl₃): δ 7.79-7.73 (m, 3H, ArH), 7.60 (s, 1H, ArH), 7.45-7.38 (m, 2H, ArH), 7.30-7.28 (m, 1H, ArH), 7.13 (d, *J* = 8.7 Hz, 2H, ArH), 6.85-6.81 (m, 2H, ArH), 4.07 (s, 2H, CH₂), 3.76 (s, 3H, OMe). ¹³C NMR (100 MHz, CDCl₃): δ 158.1, 139.1, 133.7, 133.1, 132.1, 130.0, 128.1, 127.7, 127.6, 127.5, 127.0, 126.0, 125.3, 114.0, 55.3, 41.3.

Complex (3bi)^[1, 2, 4]: ¹H NMR (400 MHz, CDCl₃): δ 7.29-7.25 (m, 2H, ArH), 7.20-7.16 (m, 3H, ArH), 7.09 (d, *J* = 8.6 Hz, 2H, ArH), 6.84-6.80 (m, 2H, ArH), 3.92 (s, 2H, CH₂), 3.76 (s, 3H, OMe). ¹³C NMR (100 MHz, CDCl₃): δ 158.0, 141.6, 133.3, 129.9, 128.9, 128.5,

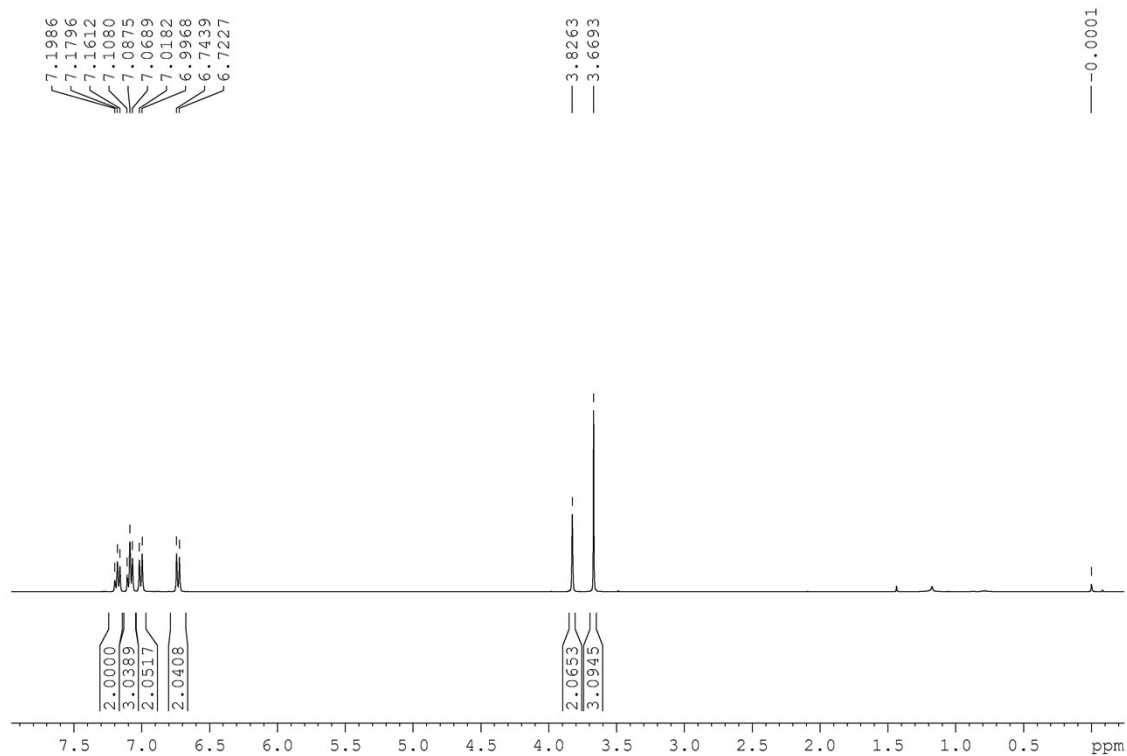
126.0, 113.9, 55.3, 41.1.

References

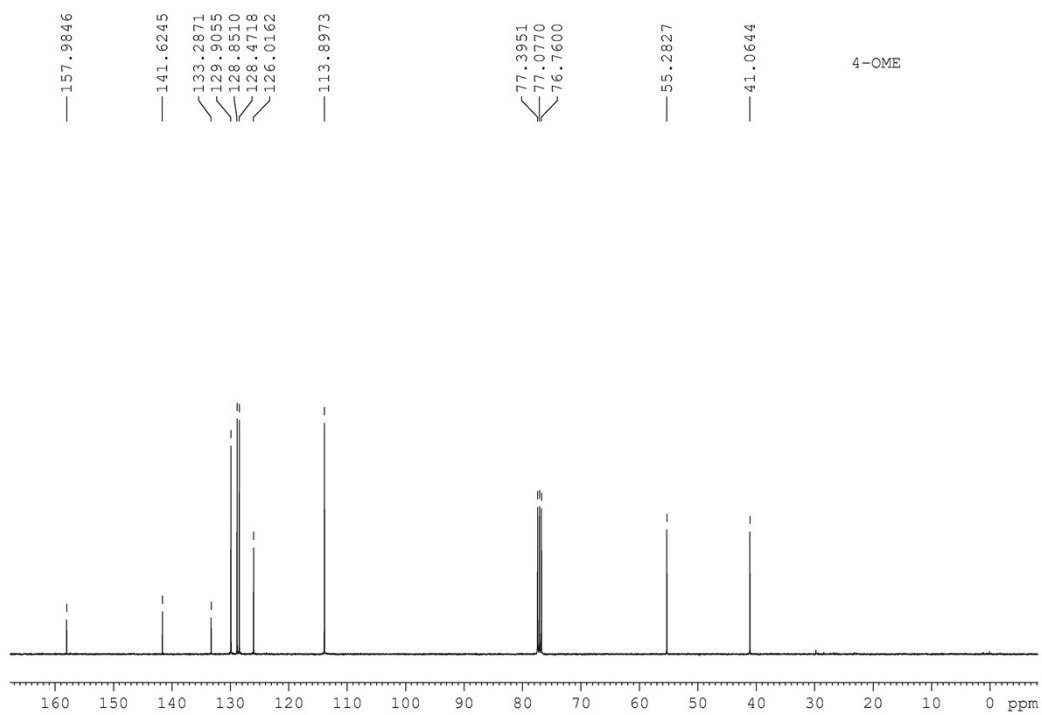
- [1]. P. L. Türtcher , H. J. Davis , R. J. Phipps, *Synthesis*, **2018**, *50*, 793.
- [2]. P. Maity, D. M. Shacklady-McAtee, G. P. A. Yap, E. R. Sirianni, M. P. Watson, *J. Am. Chem. Soc.*, **2013**, *135*, 280.
- [3]. T. Wang, K. Xu, T. Meng, A. Zhang, H. Wang, S. Shen, L. Liu, *Chin. J. Org. Chem.*, **2017**, *37*, 1794.
- [4]. X. -X. Wang, B. -B. Xu, W. -T. Song, K. -X. Sun, J. -M. Lu, *Org. Biomol. Chem.*, **2015**, *13*, 4925.

Copies of the ^1H NMR and ^{13}C NMR Spectra of Complexes 3aa-3am

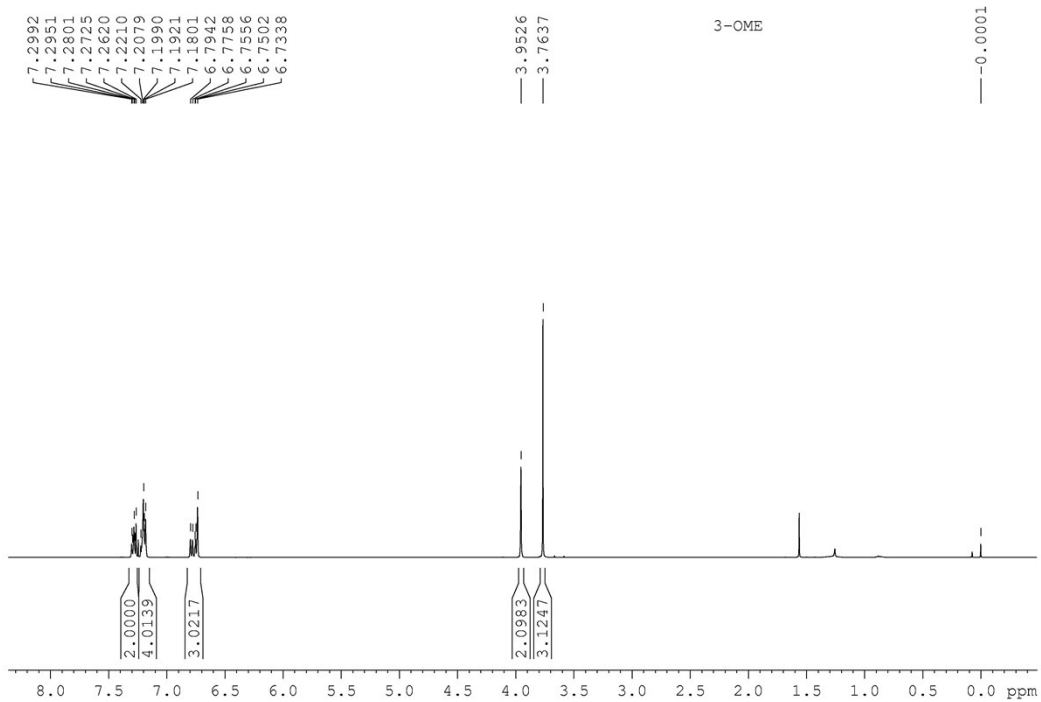
^1H NMR(3aa)



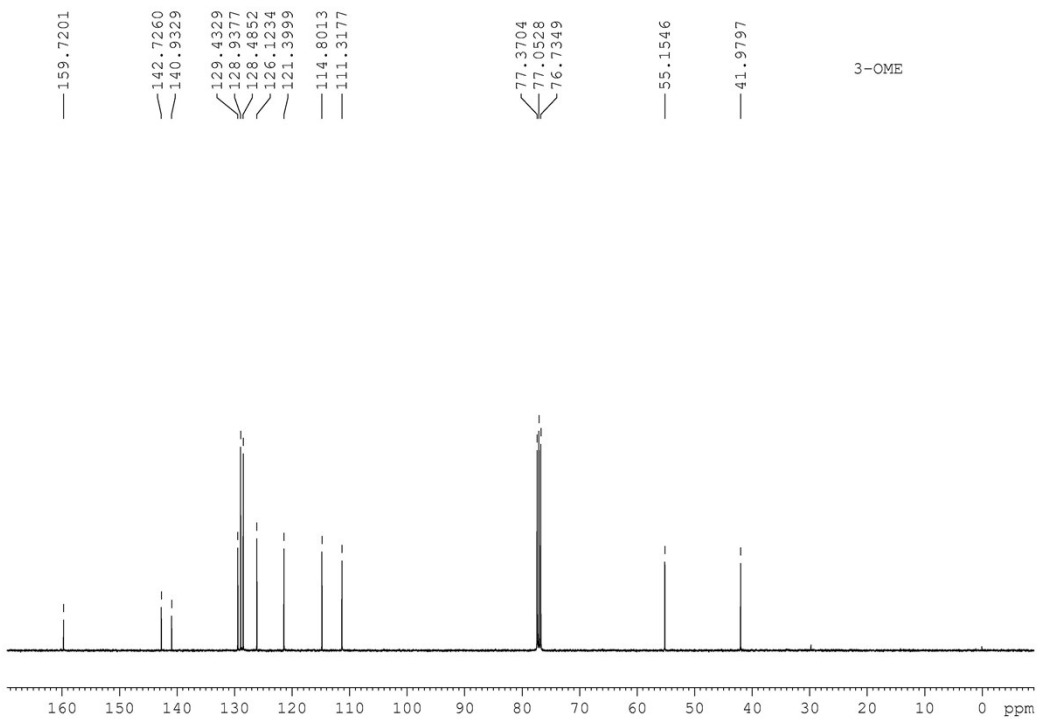
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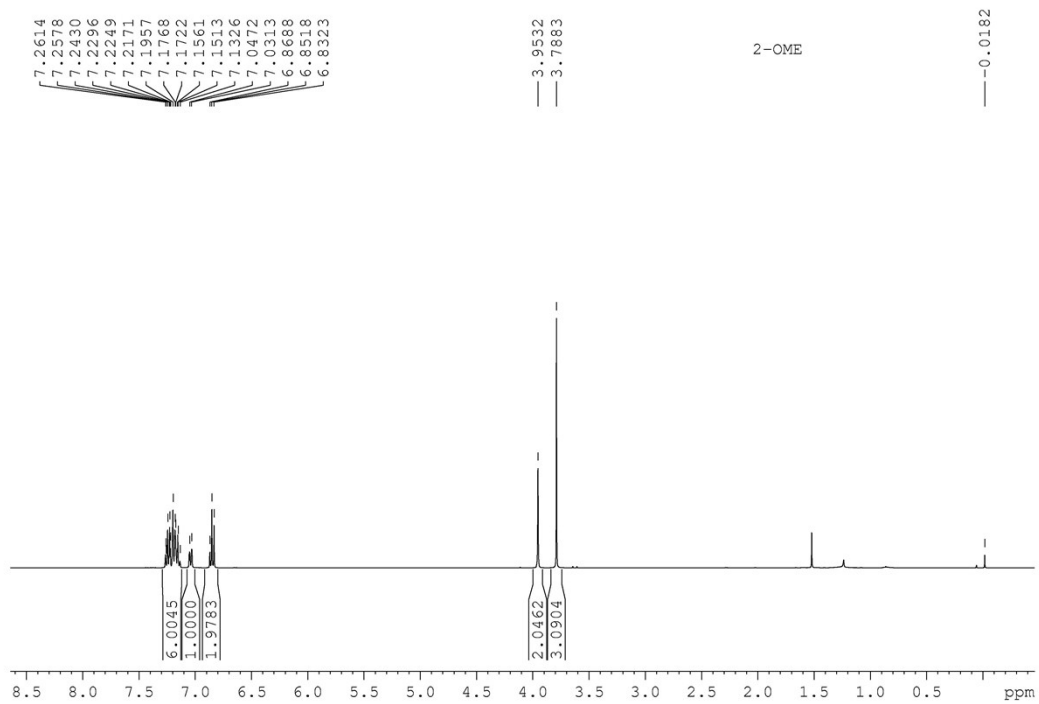
¹H NMR(3ab)



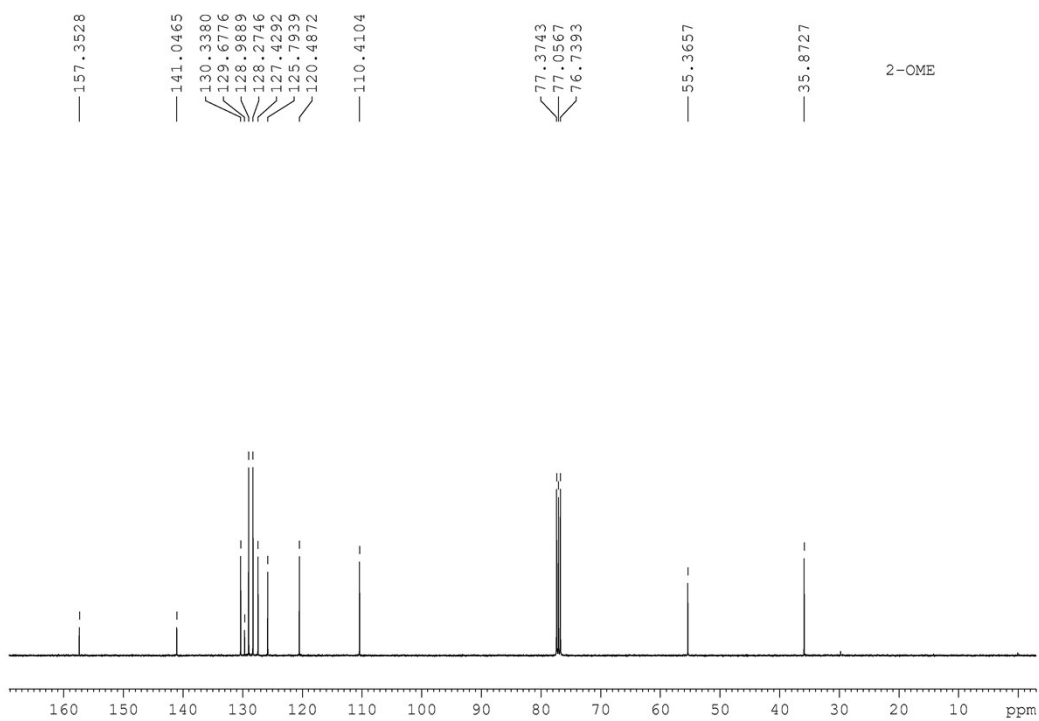
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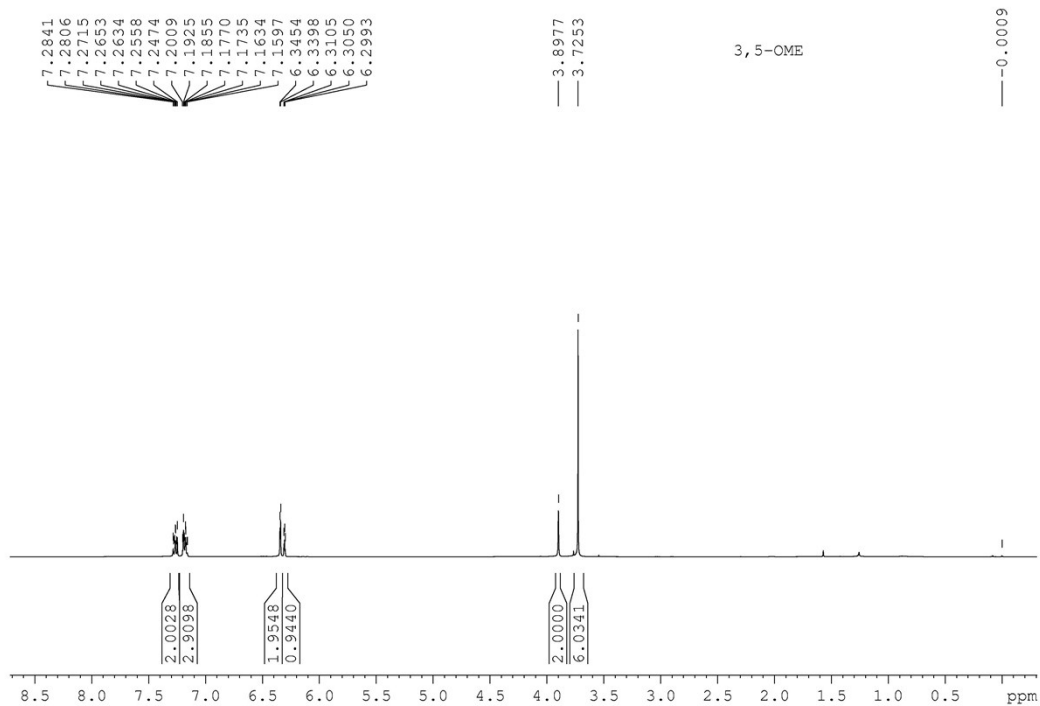
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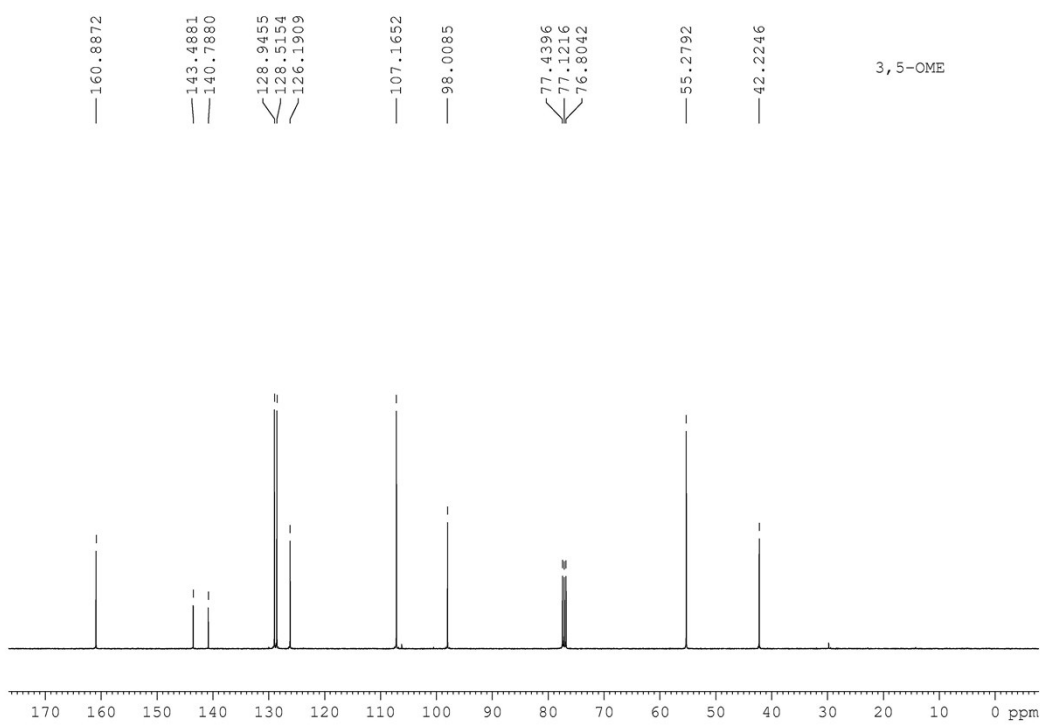
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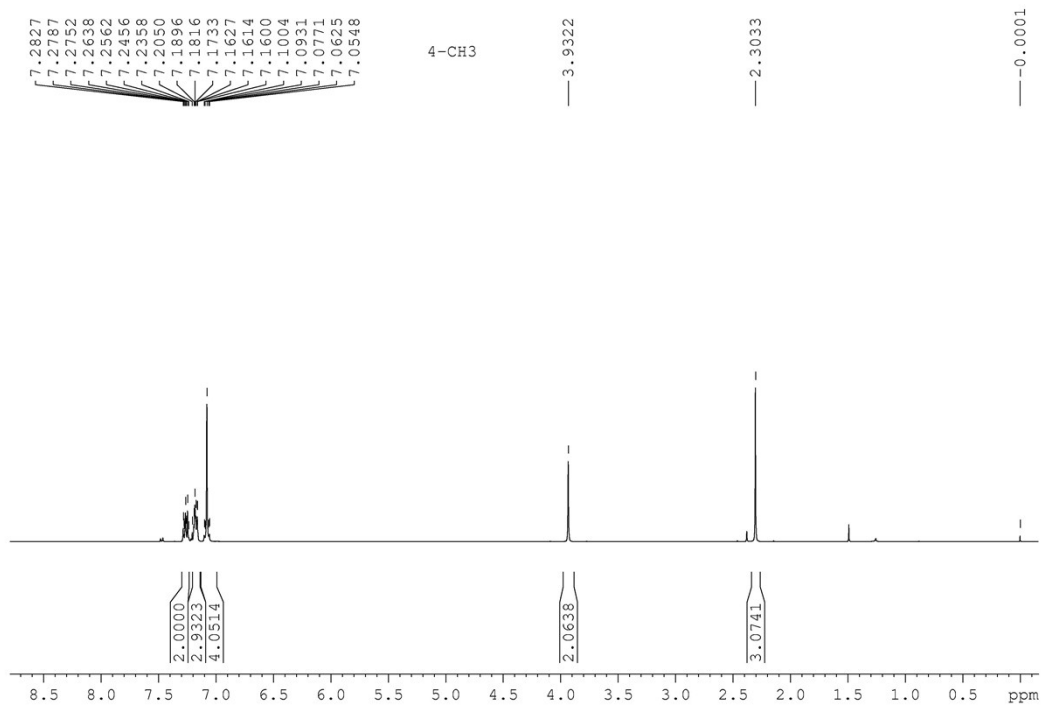
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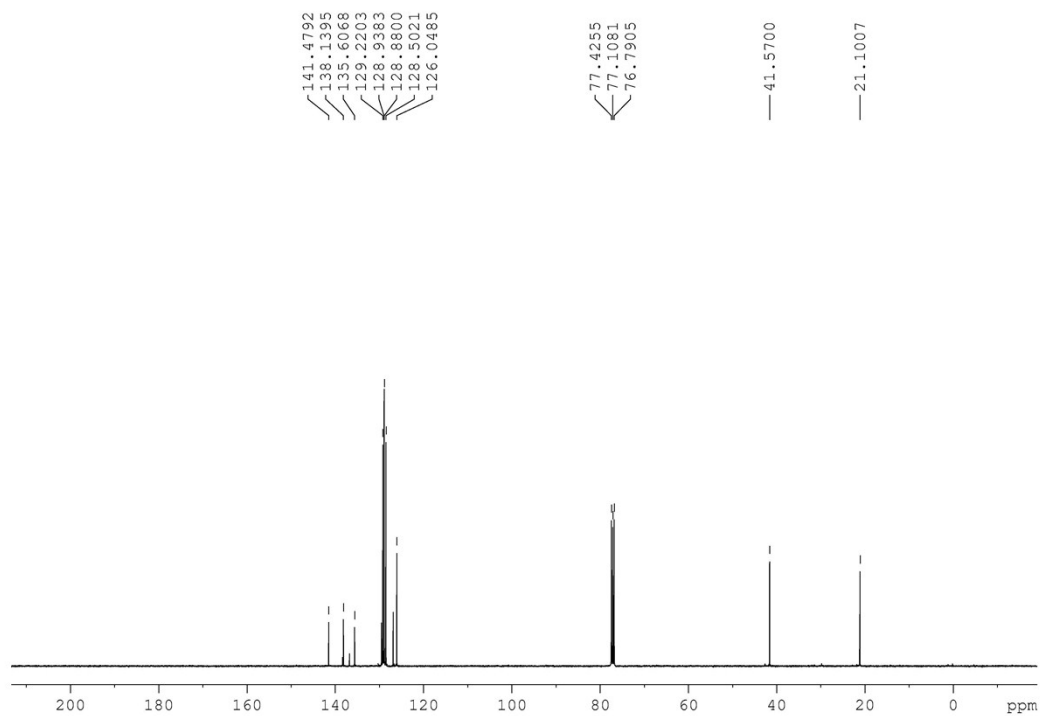
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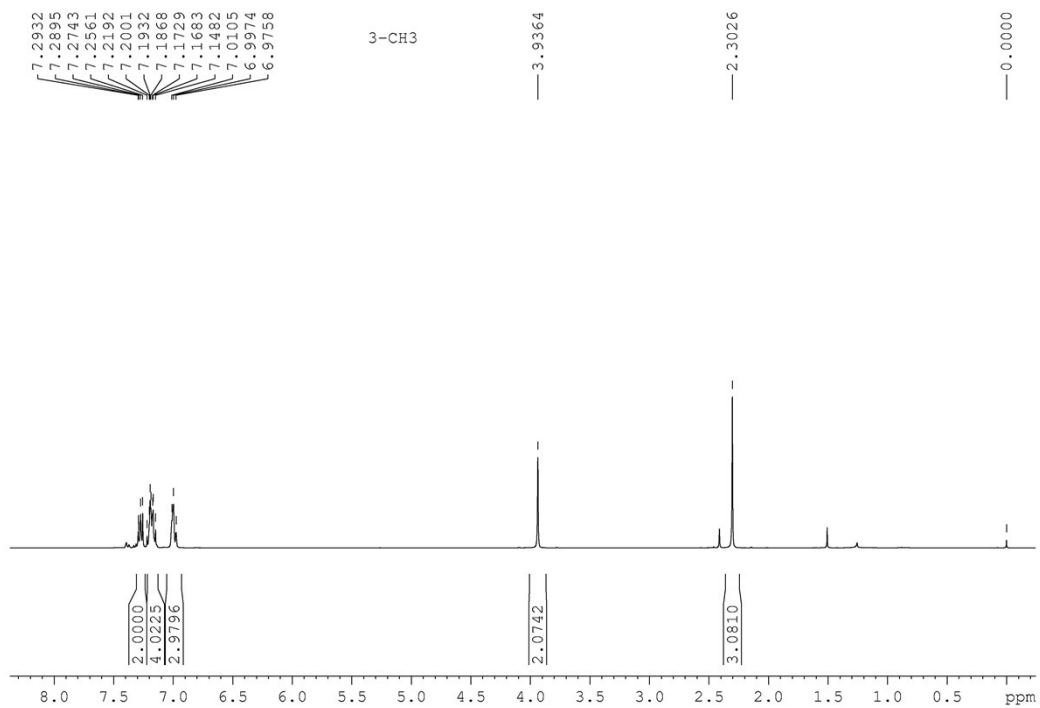
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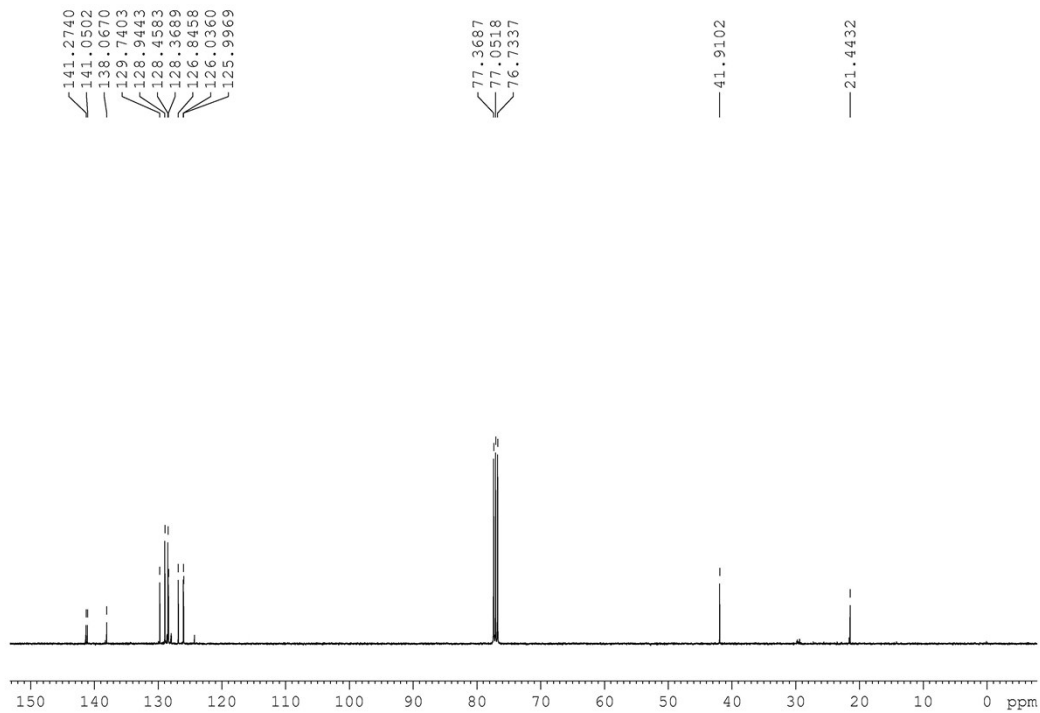
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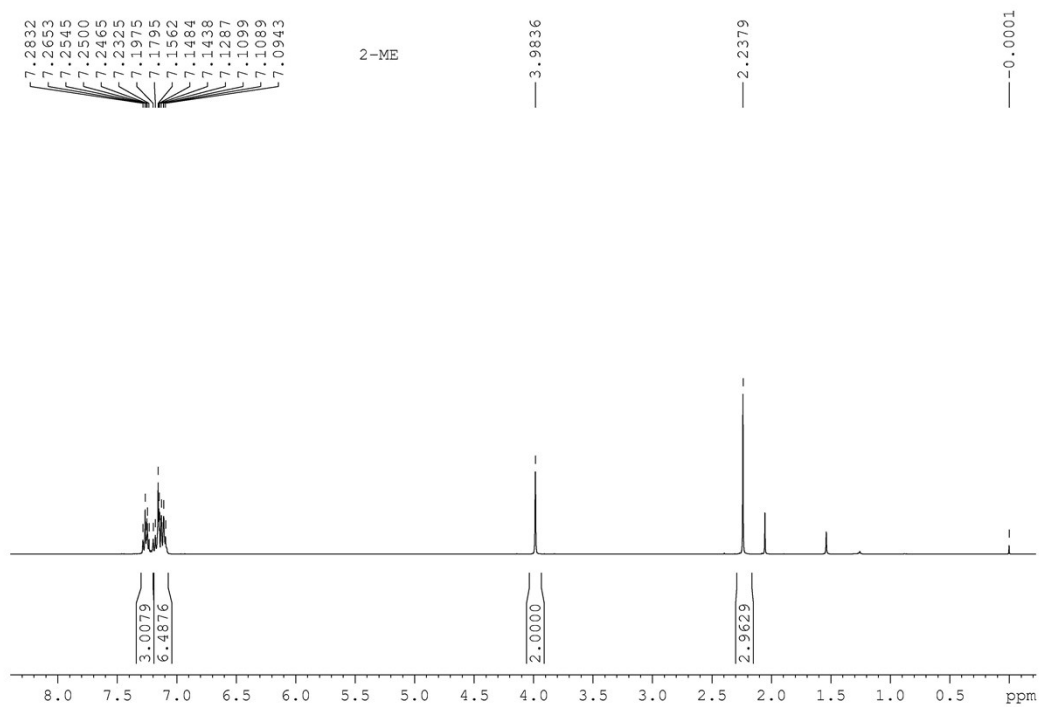
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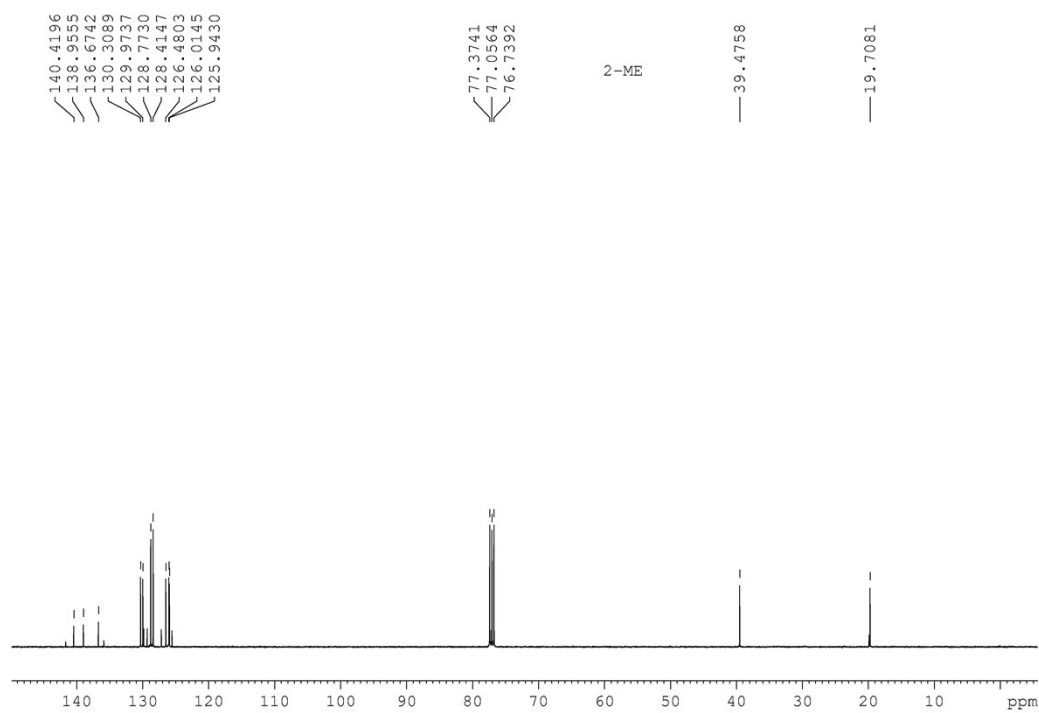
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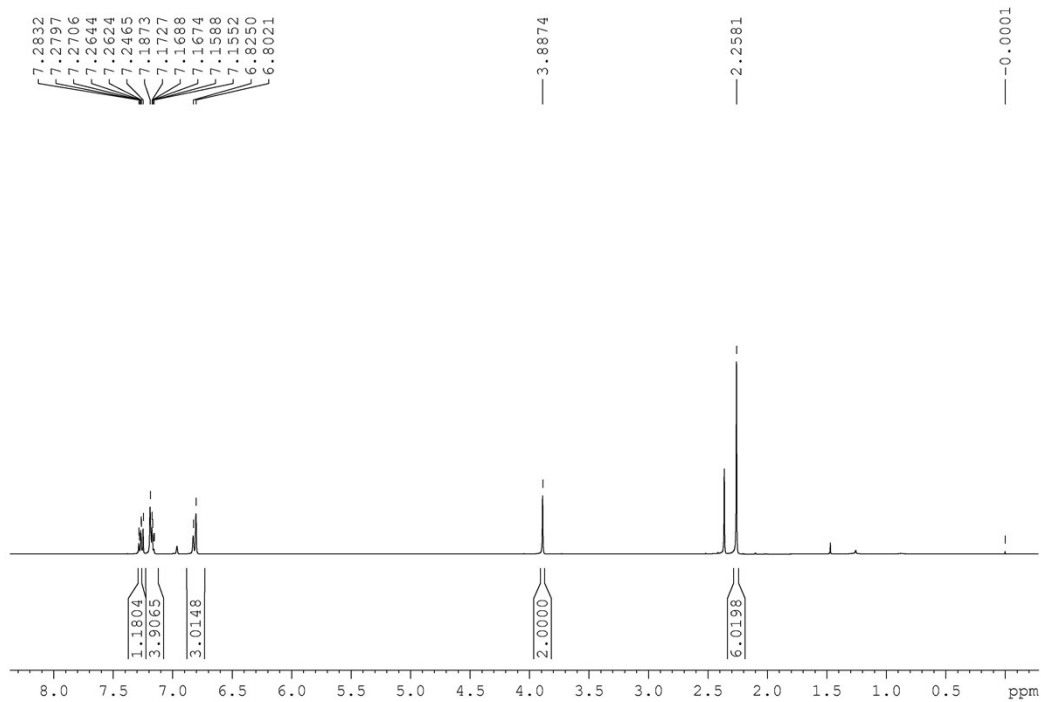
¹H NMR(3ag)



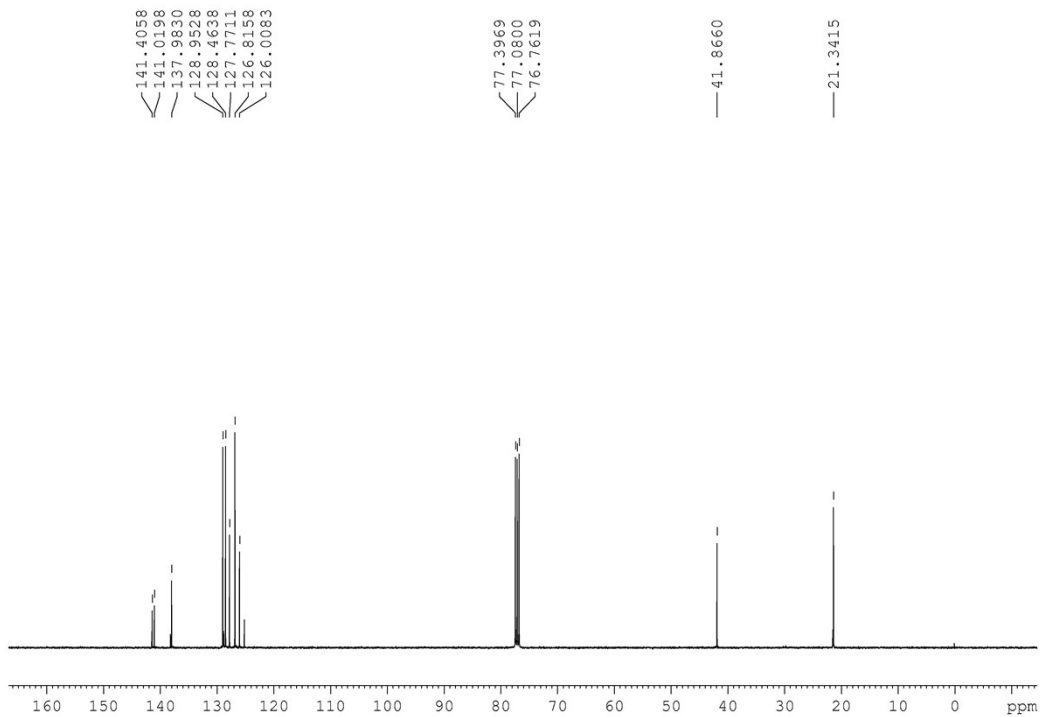
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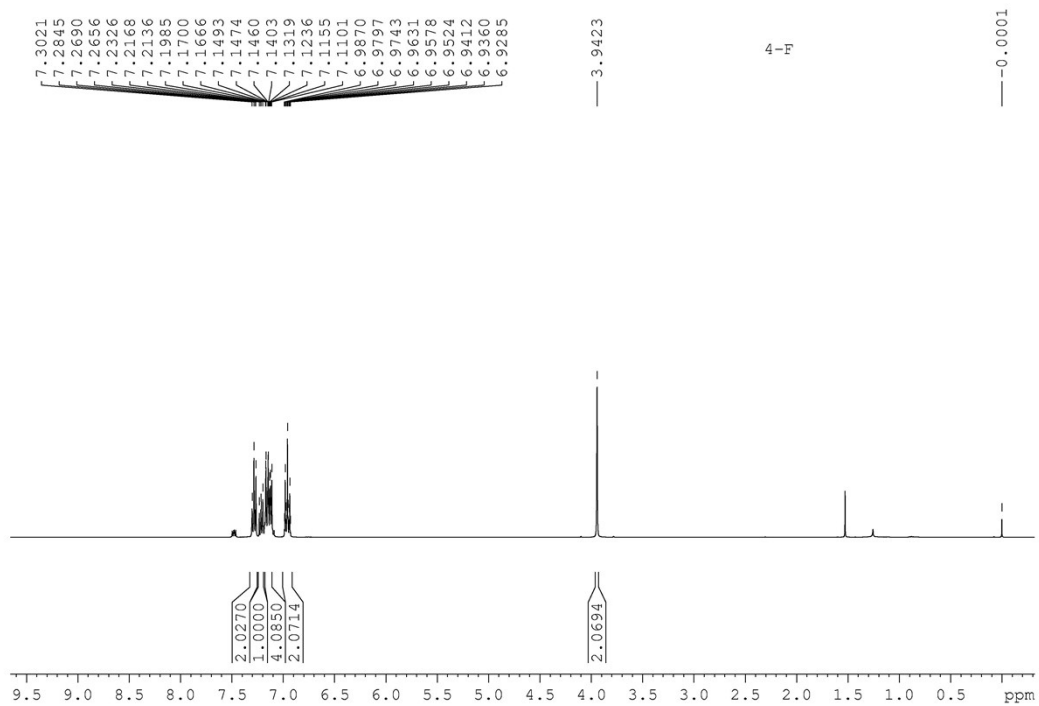
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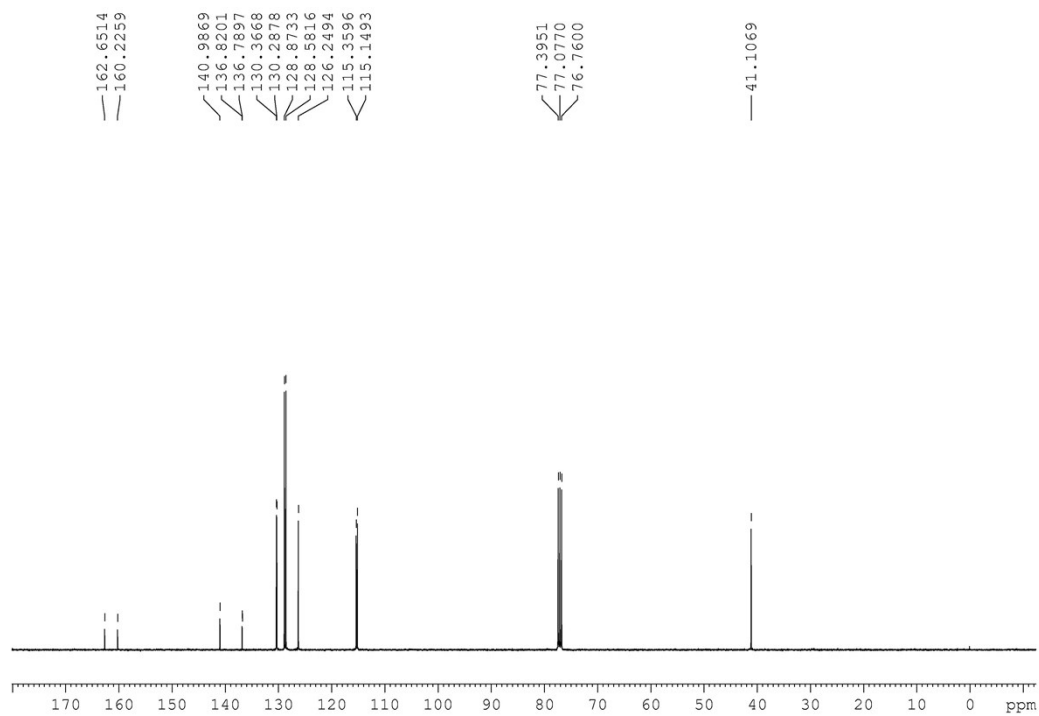
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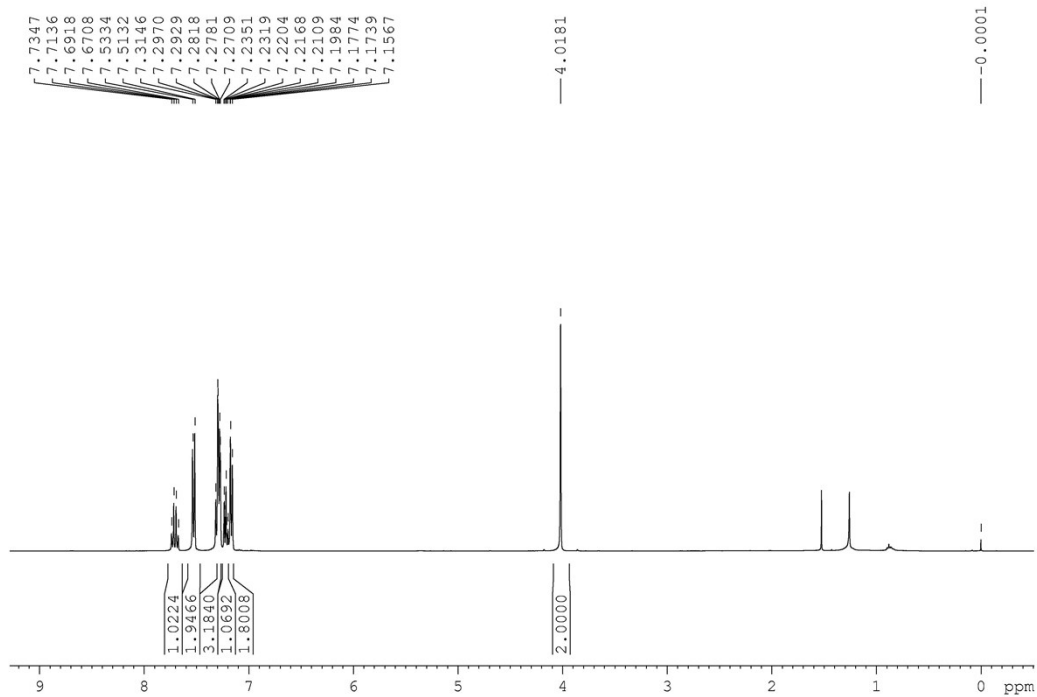
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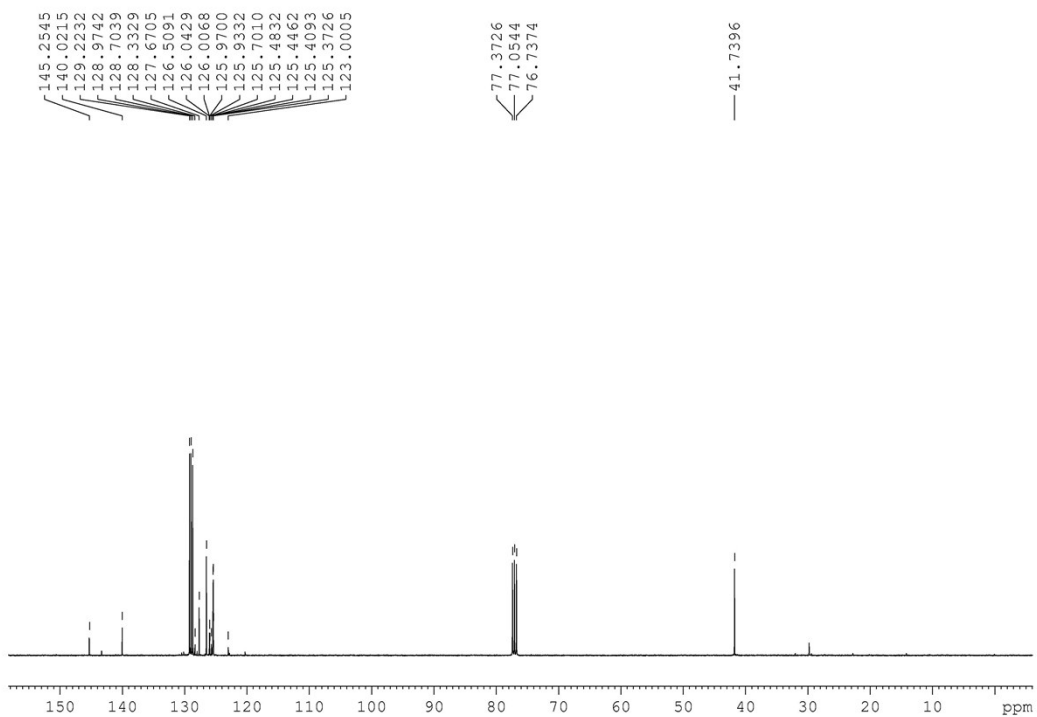
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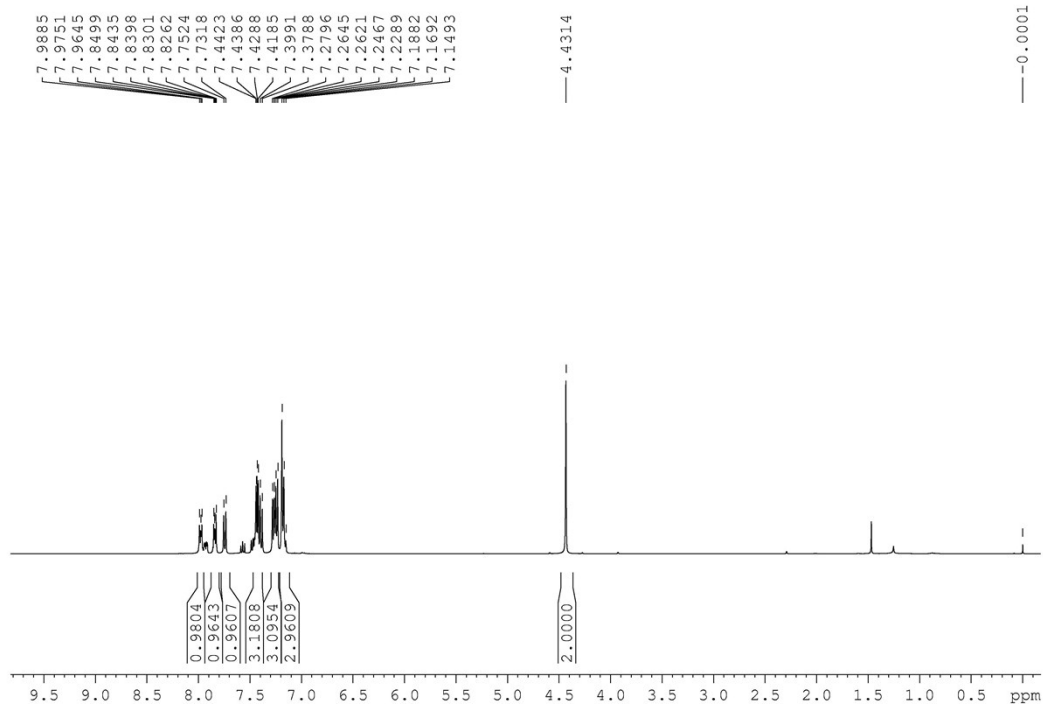
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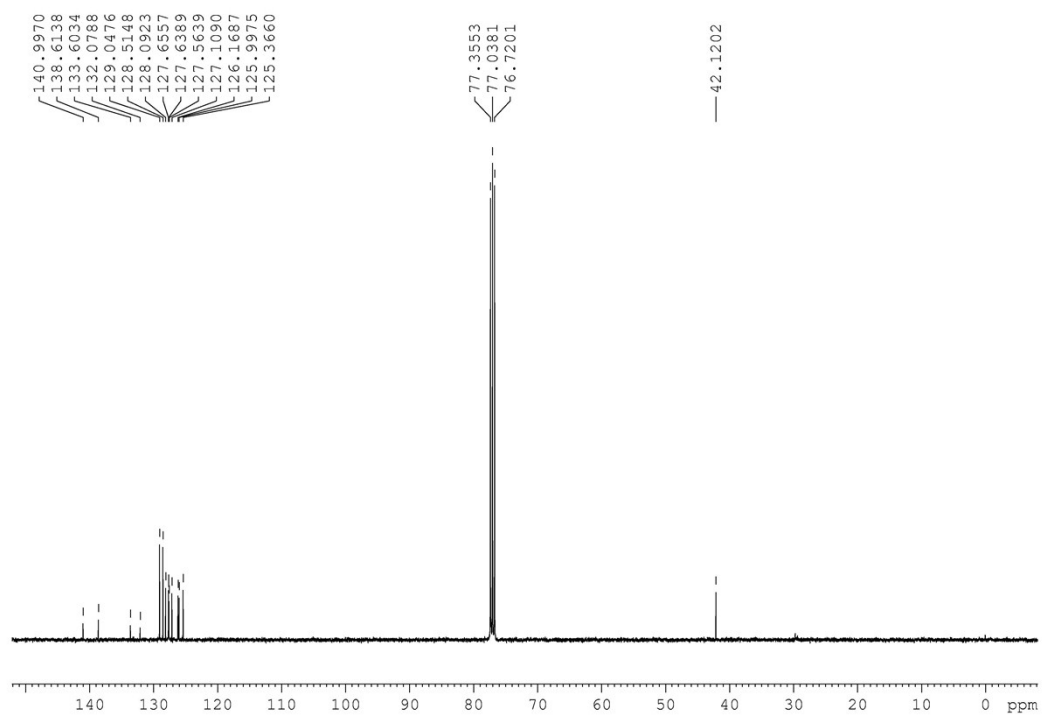
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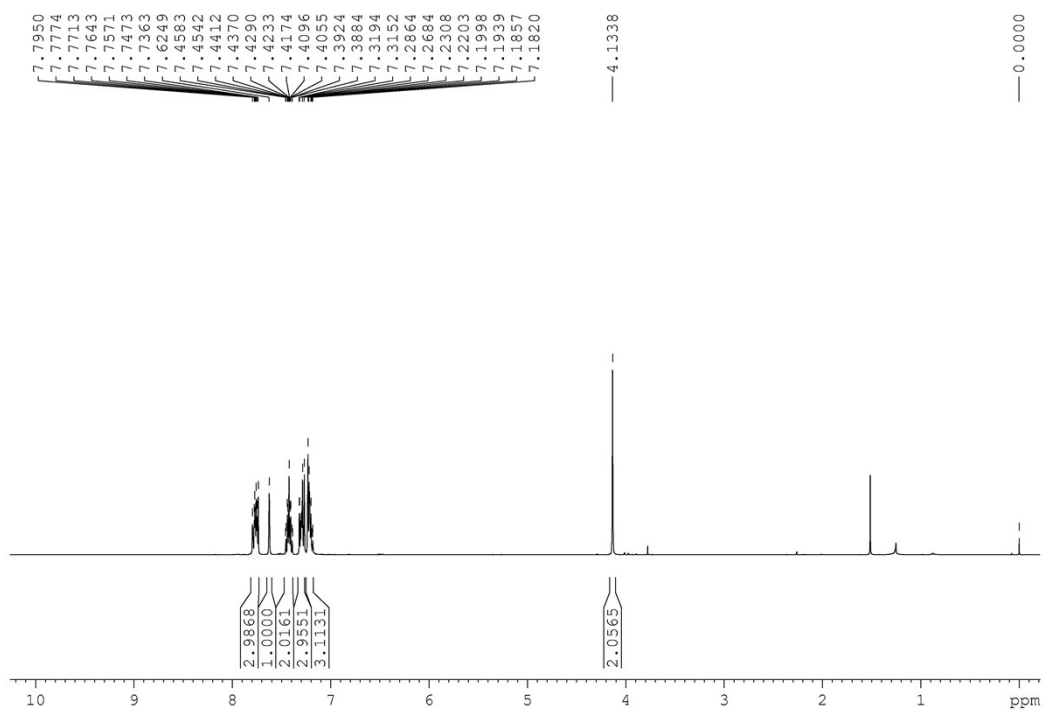
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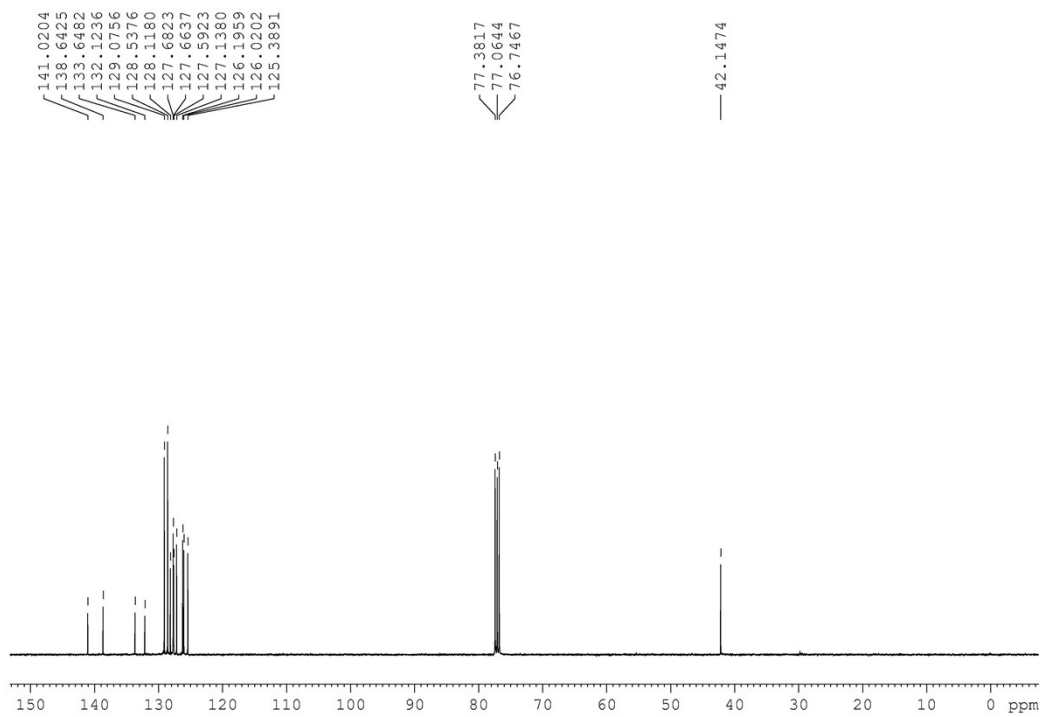
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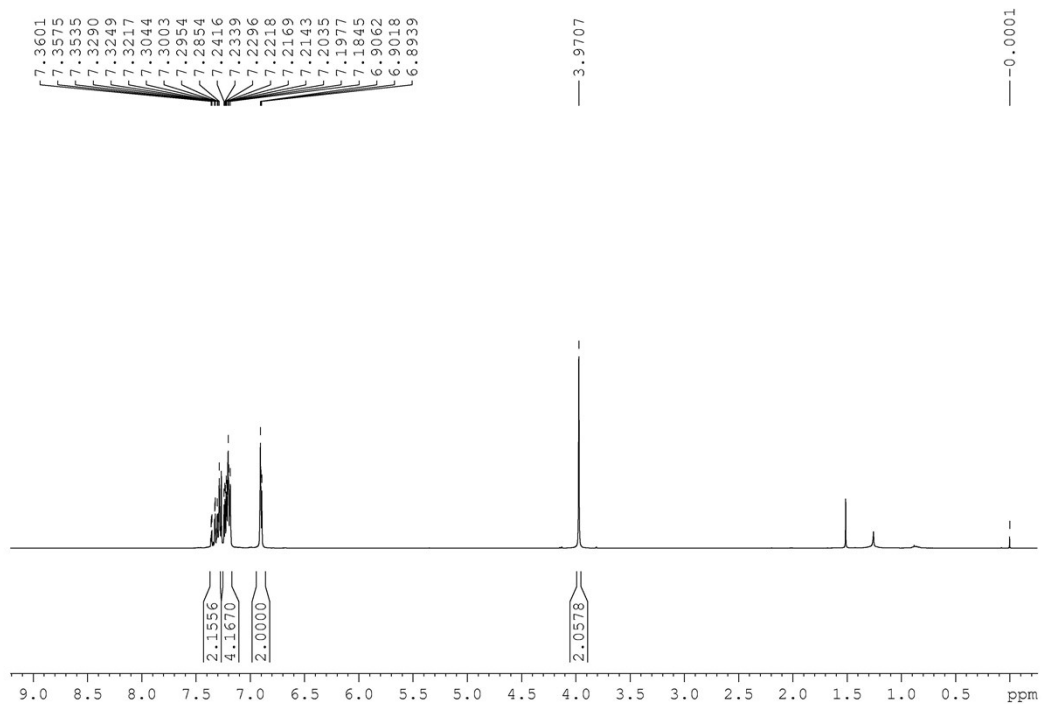
¹H NMR(3al)



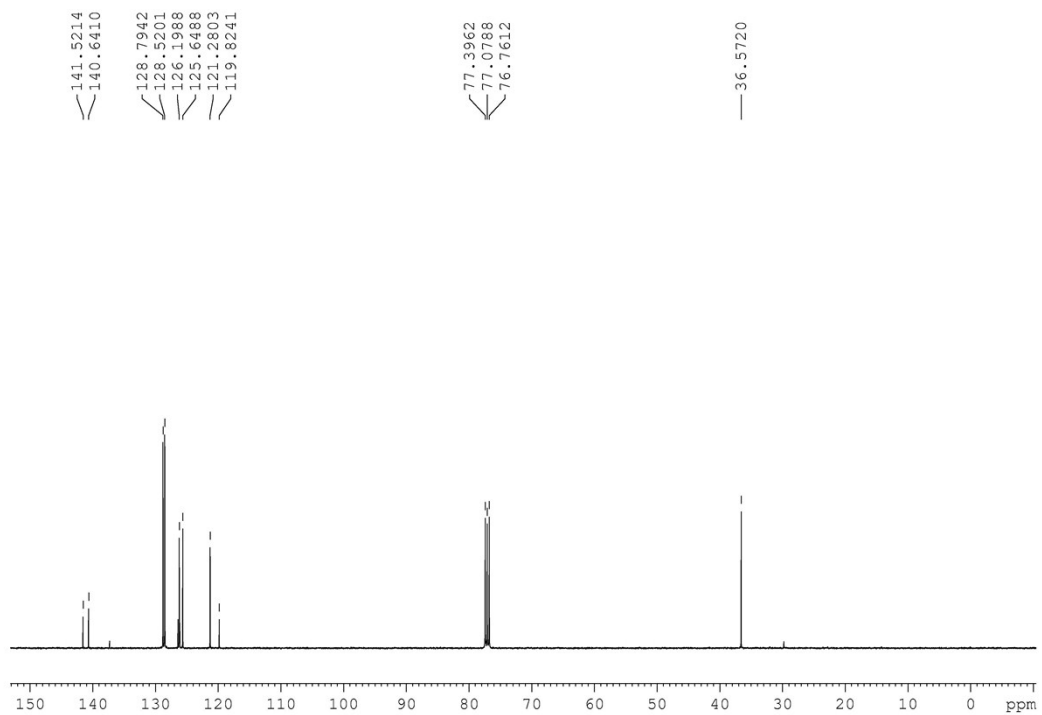
¹³C NMR(3al)



^1H NMR(3am)

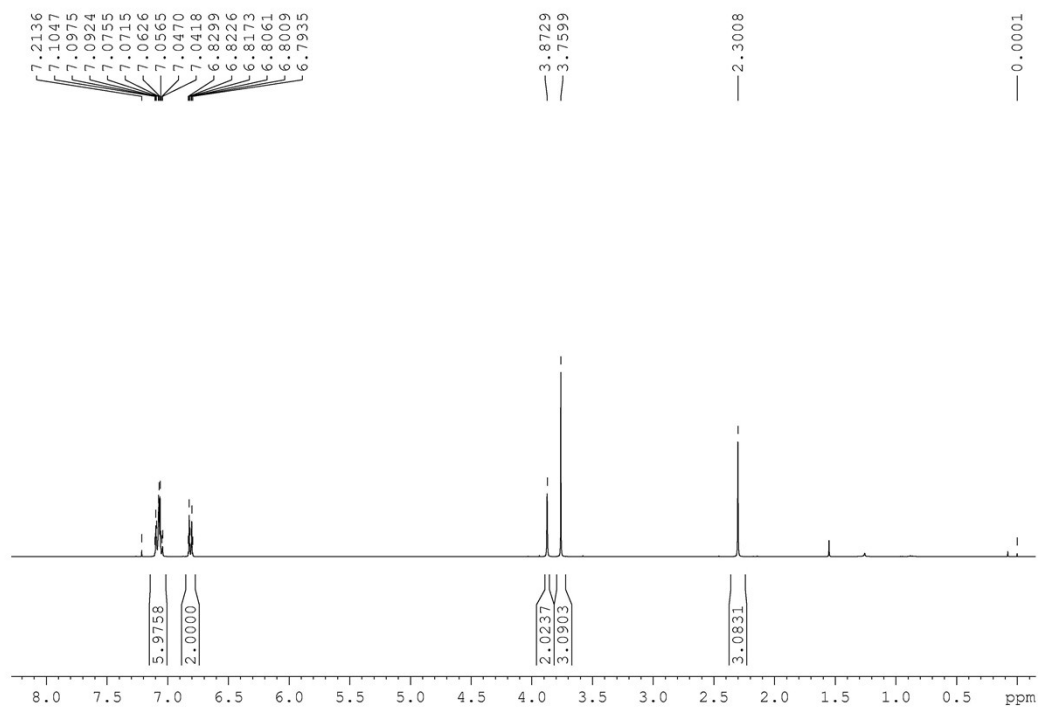


^{13}C NMR(3am)

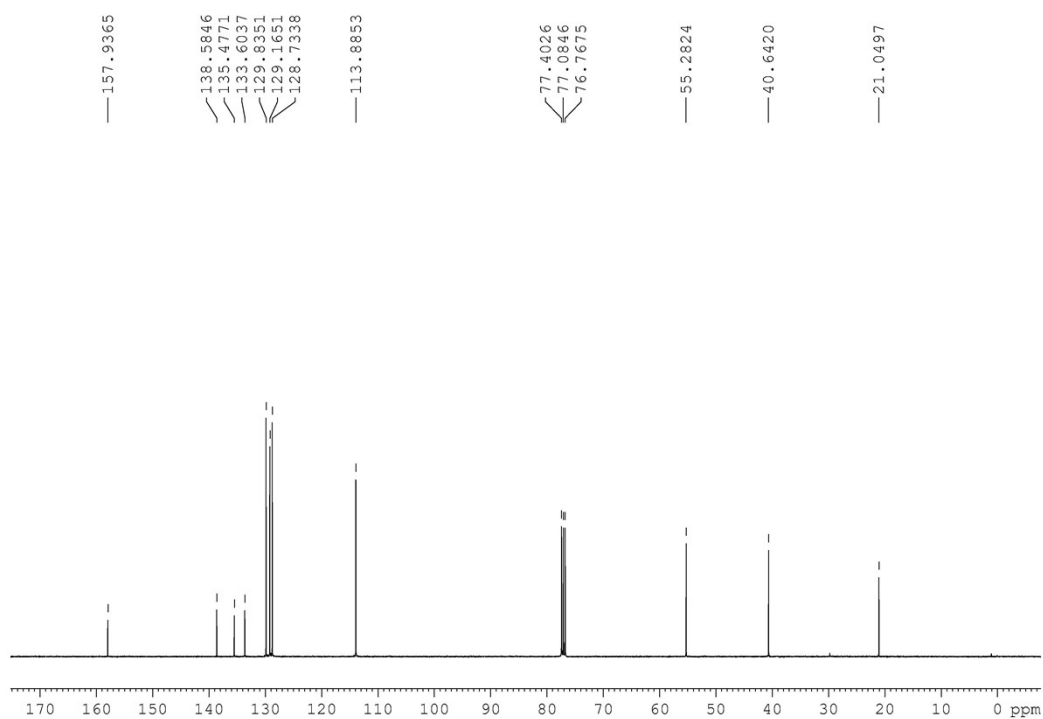


Copies of the ^1H NMR and ^{13}C NMR Spectra of Complexes 3ba-3bi

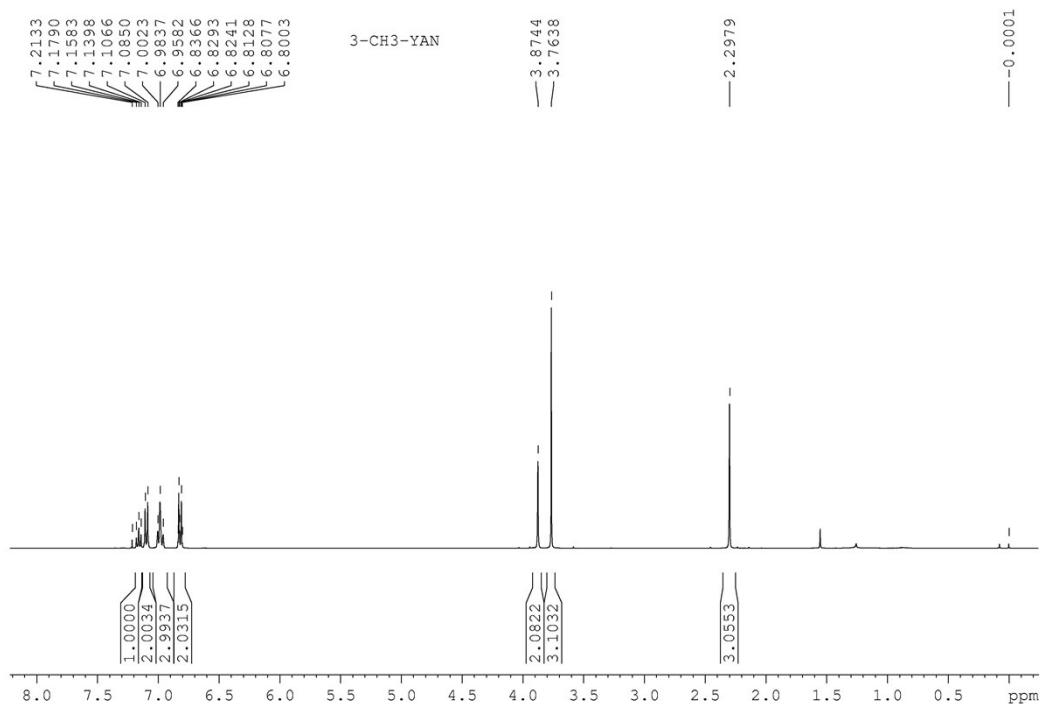
^1H NMR(3ba)



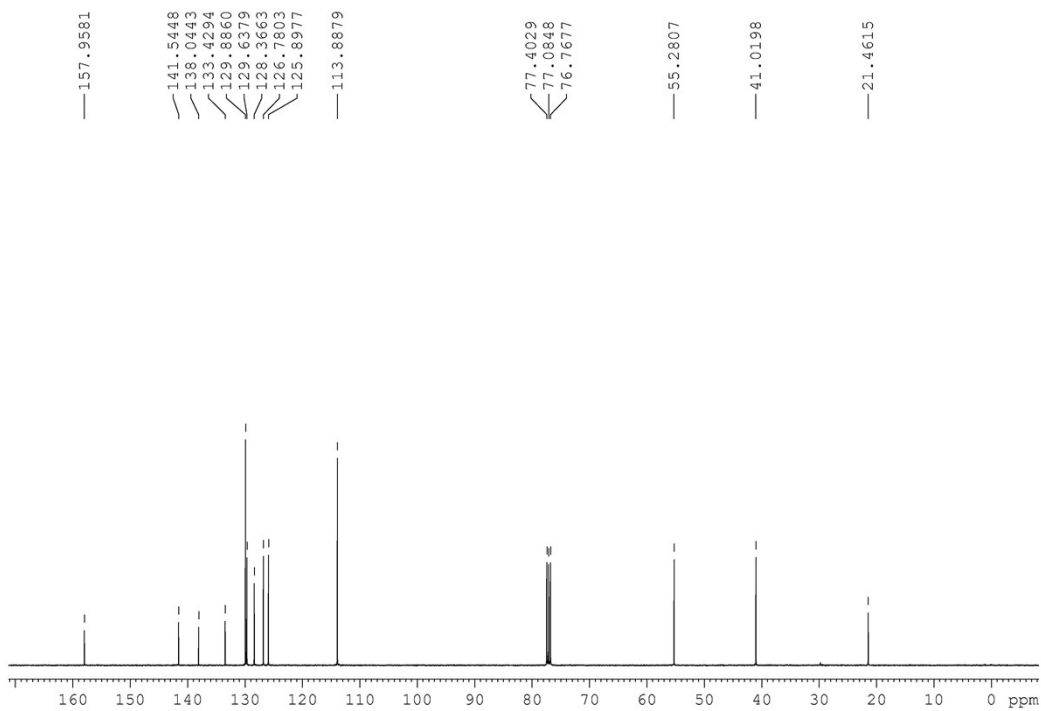
^{13}C NMR(3ba)



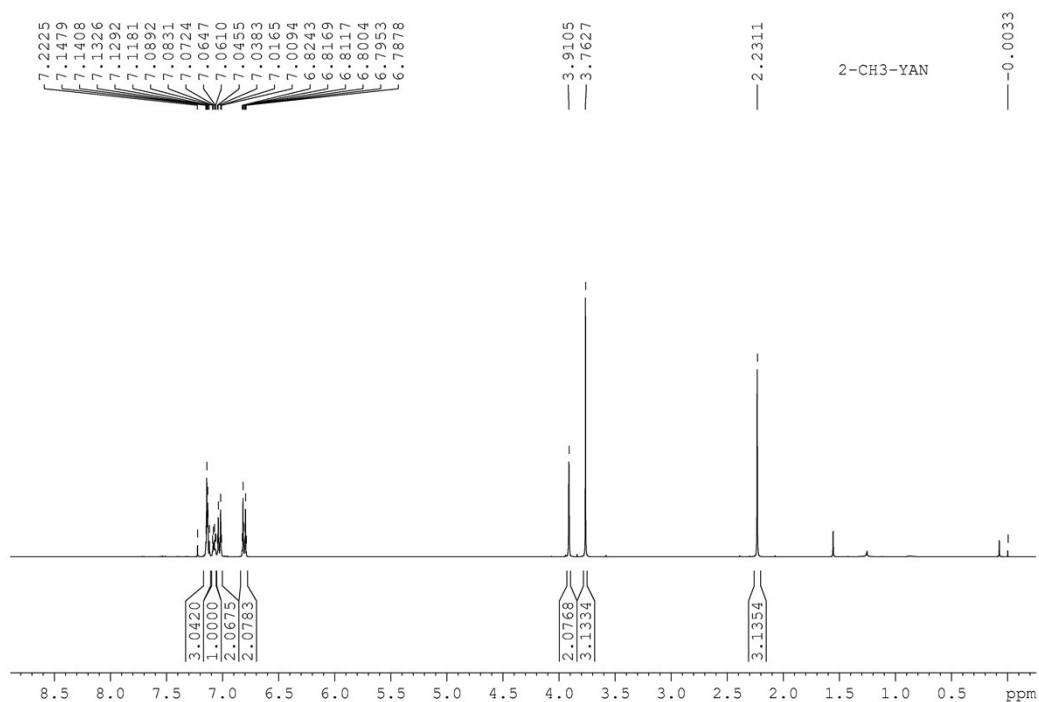
¹H NMR(3bb)



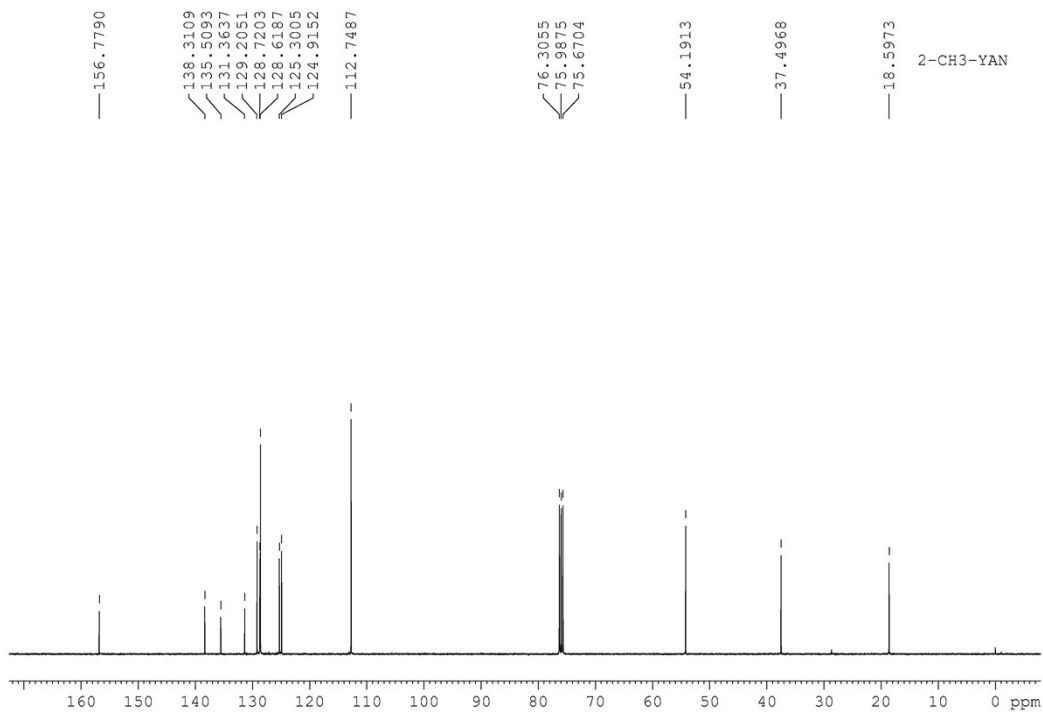
¹³C NMR(3bb)



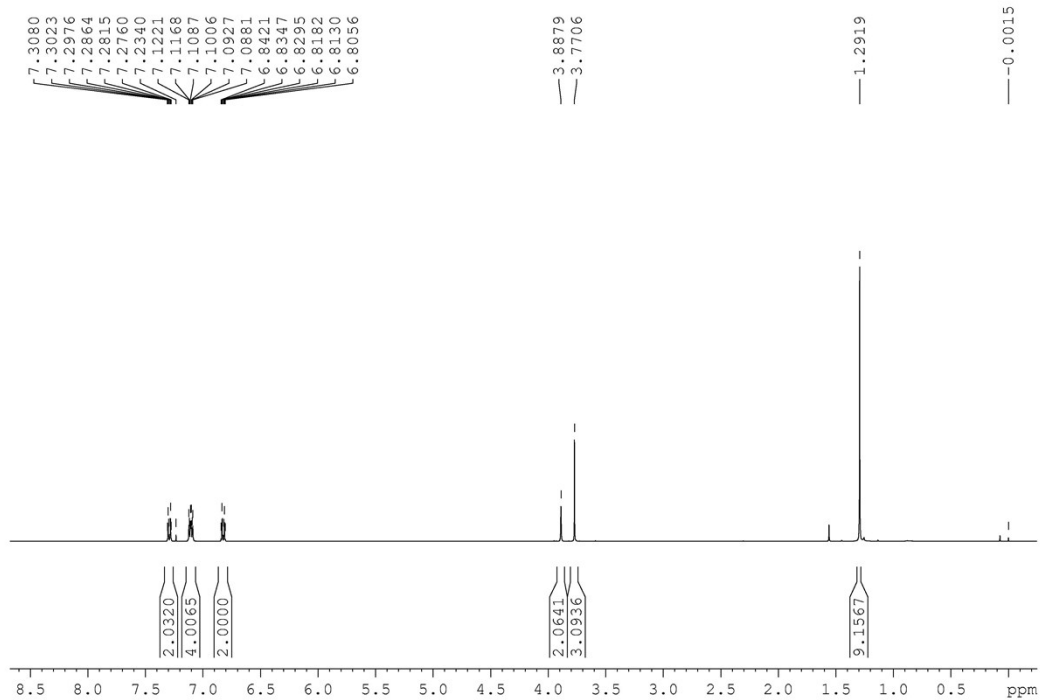
¹H NMR(3bc)



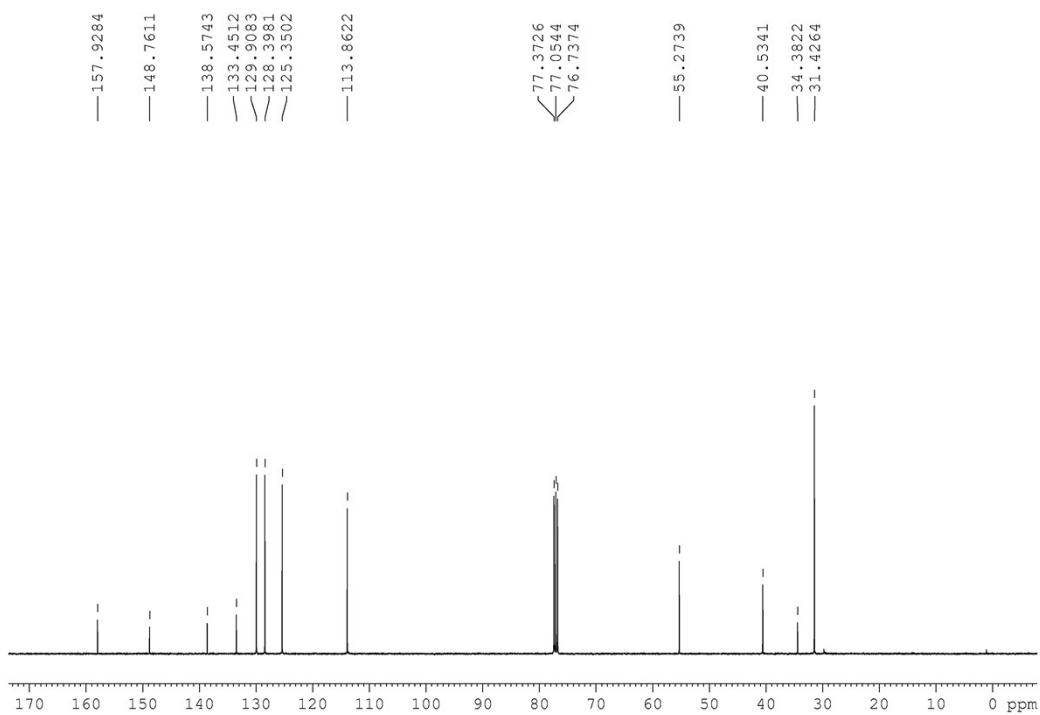
¹³C NMR(3bc)



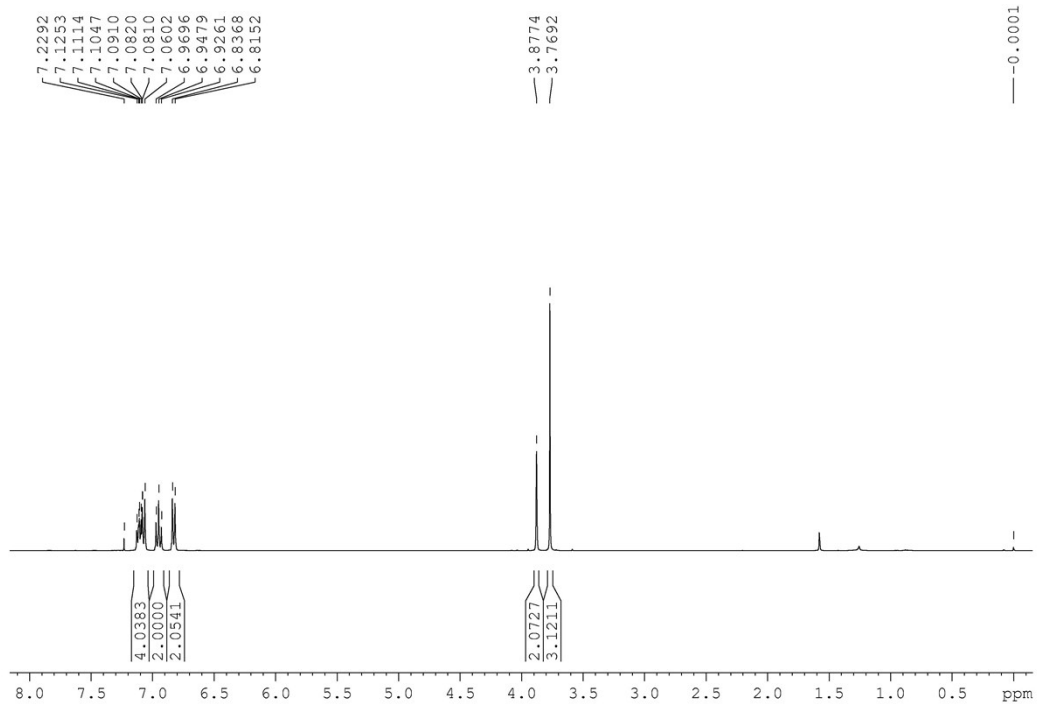
¹H NMR(3bd)



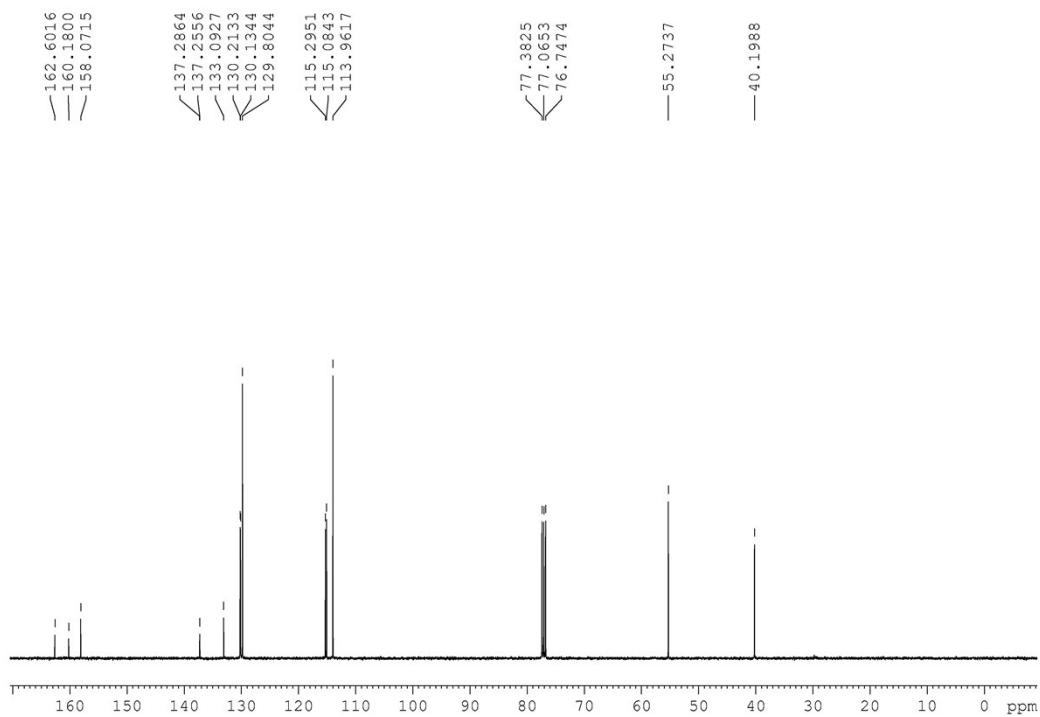
¹³C NMR(3bd)



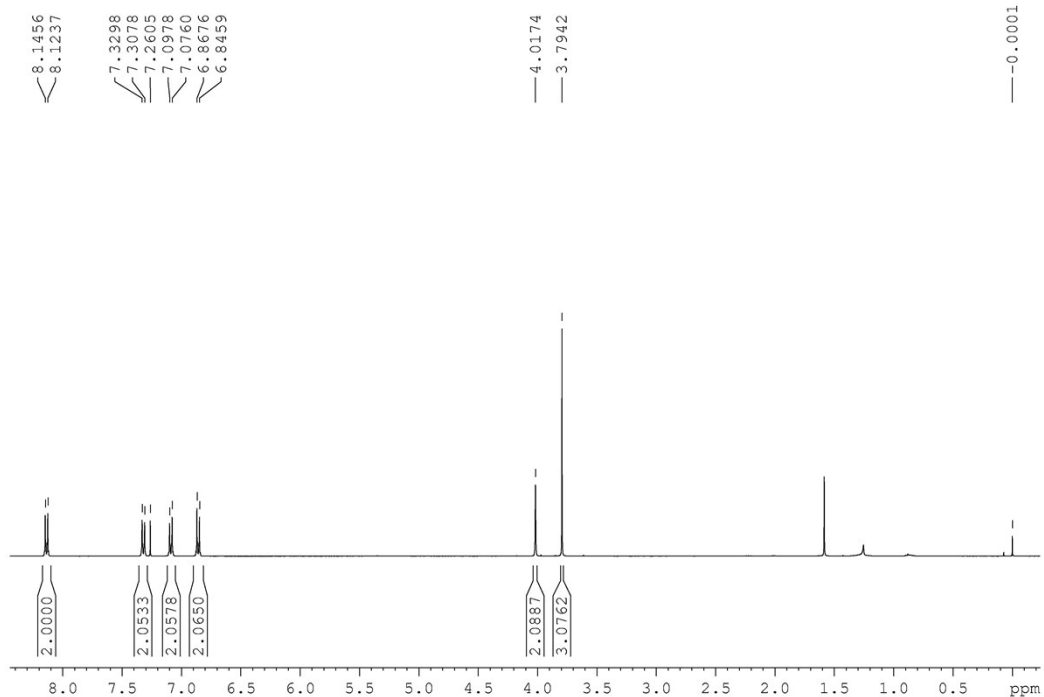
^1H NMR(3be)



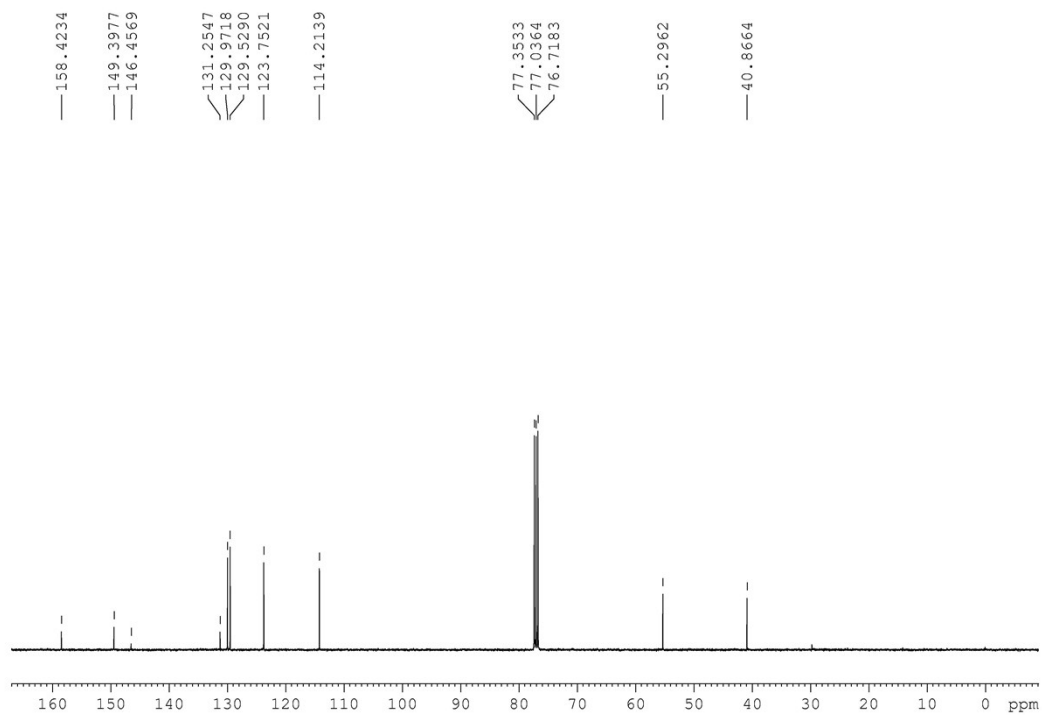
^{13}C NMR(3be)



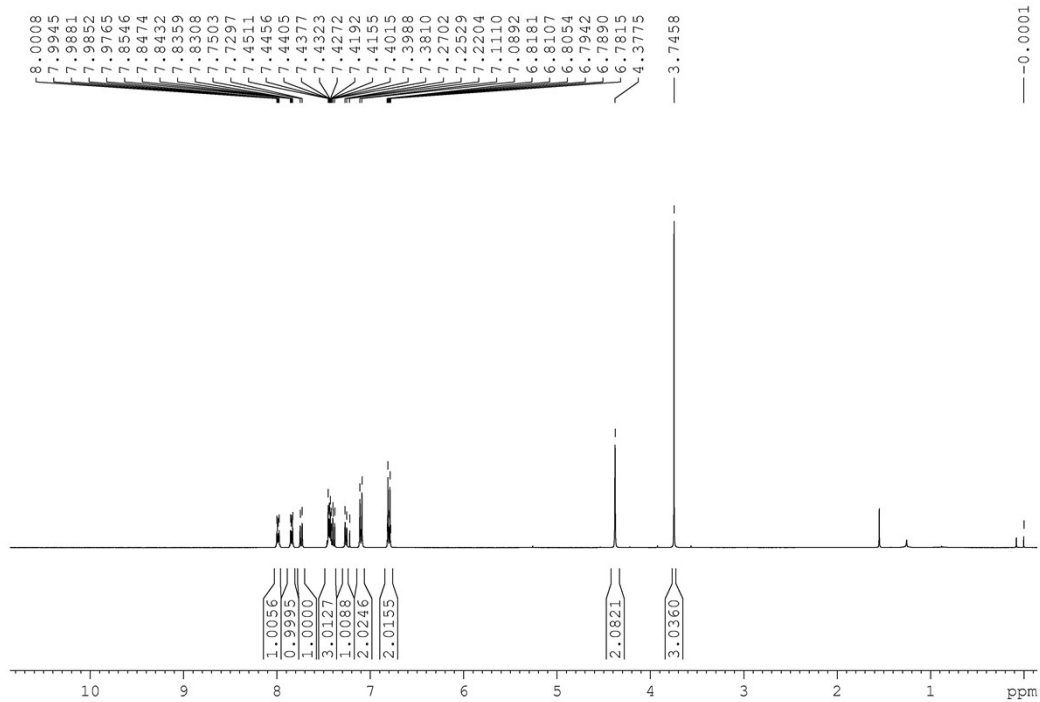
¹H NMR(3bf)



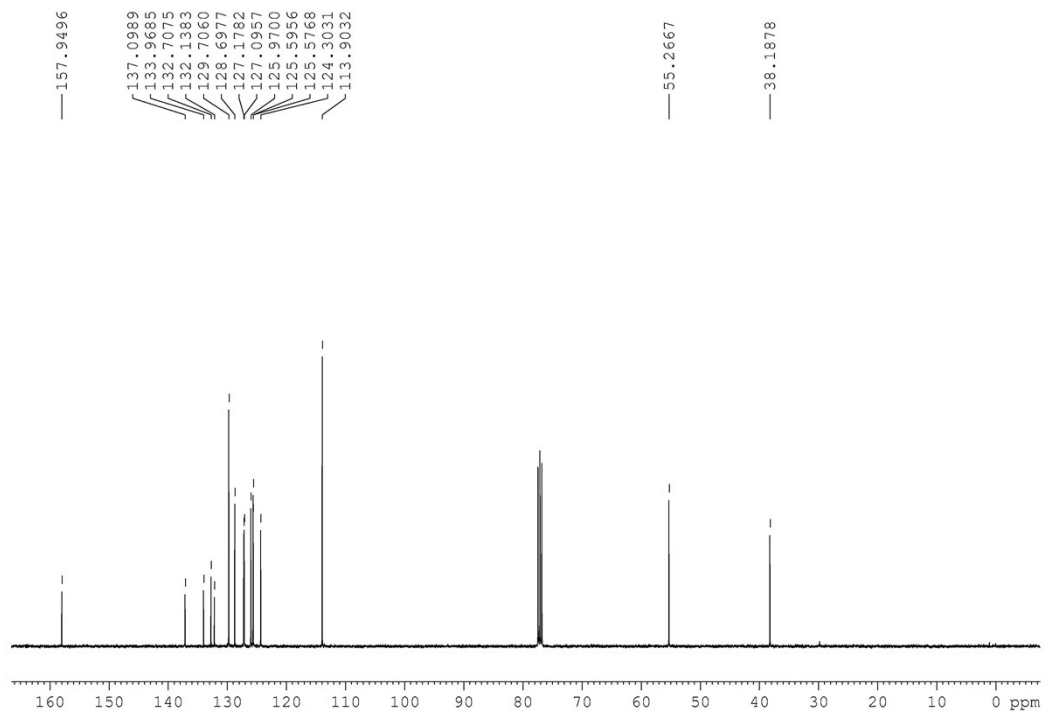
¹³C NMR(3bf)



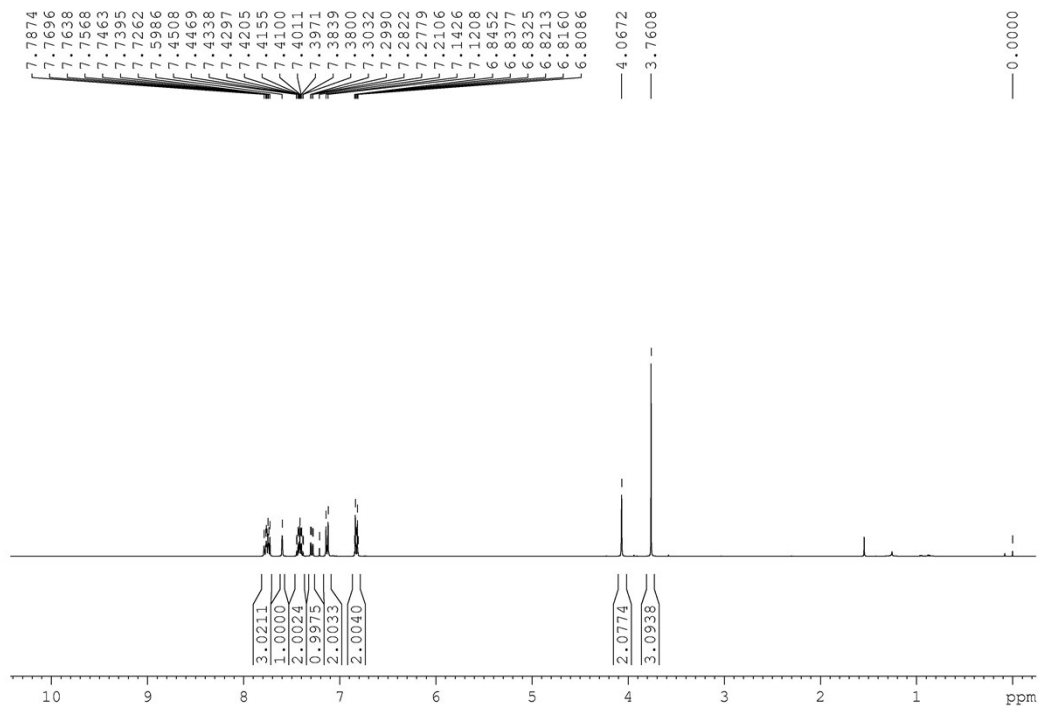
¹H NMR(3bg)



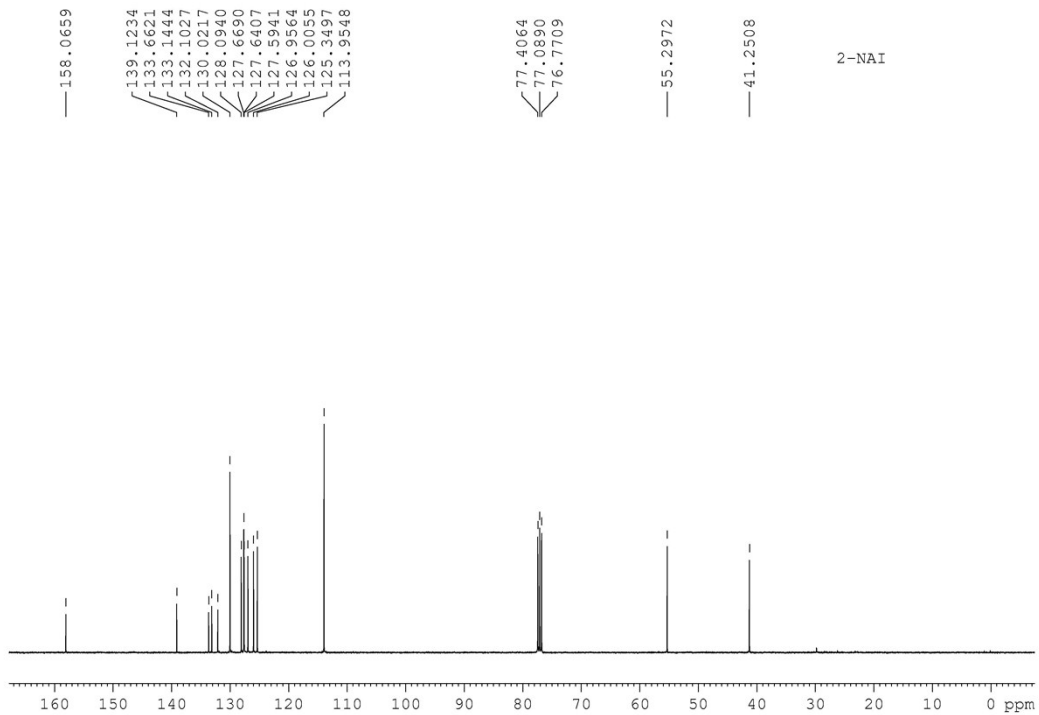
¹³C NMR(3bg)



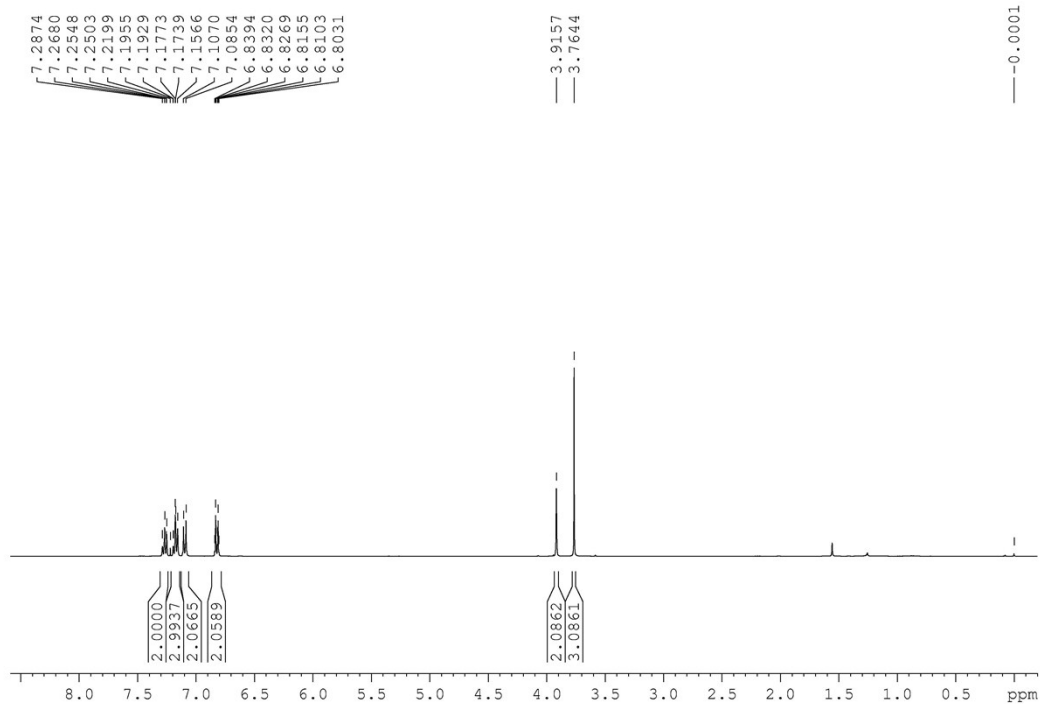
¹H NMR(3bh)



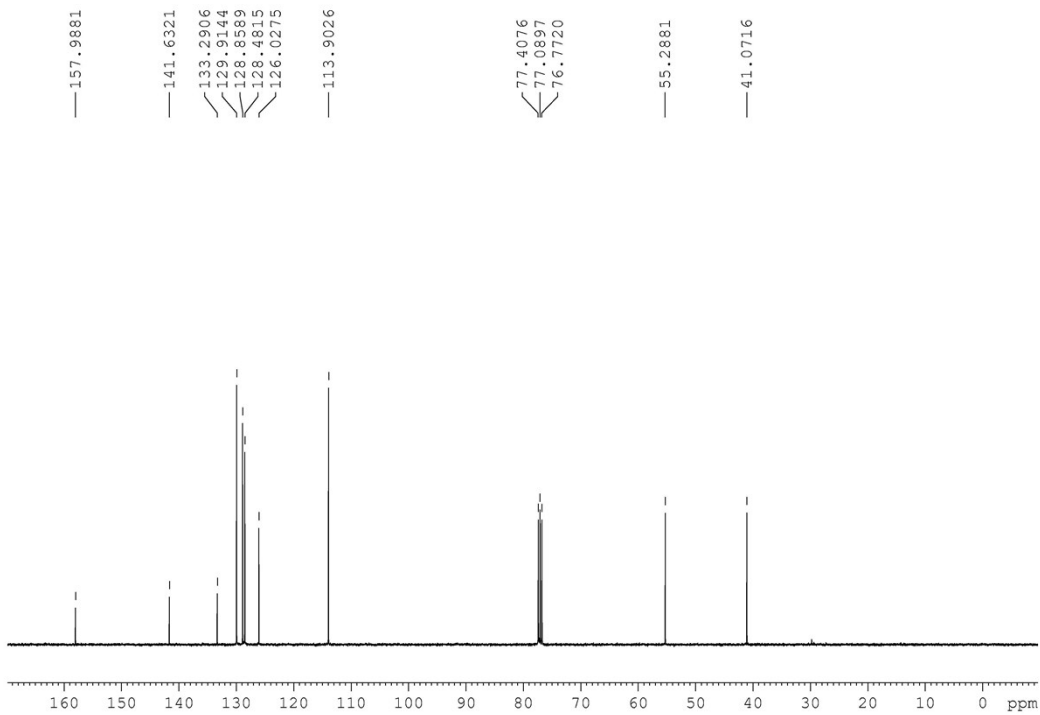
¹³C NMR(3bh)



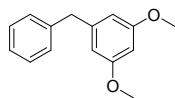
¹H NMR(3bi)



¹³C NMR(3bi)



Copies of the GC-MS Spectra of New Catalytic Products



3ad

Chemical Formula: C₁₅H₁₆O₂
Exact Mass: 228.1

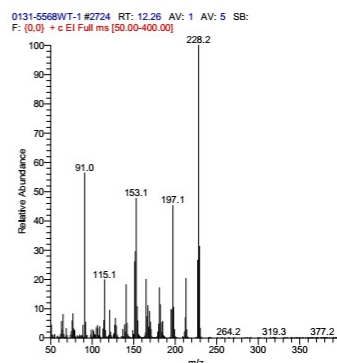
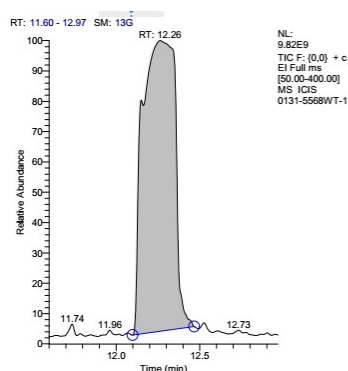


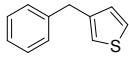
ChemLab Technologies - GC/MS Report

Data File:	0131-5568WT-1	Original Data Path:	E:\GCMS Data\ChemLab
Current Data Path:	E:\GCMS Data\ChemLab	Sample Type:	Unknown
Sample ID:	7	Sample Name:	
Operator:	W. T	Acquisition Date:	02/03/19 01:37:53 AM
Run Time(min):	14.10	Comments:	
Vial:	5	Injection Volume(μl):	10.00
Scans:	4148	Low Mass(m/z):	50
High Mass(m/z):	400	Sample Volume(μl):	0.00
Sample Weight:	0.00	ISTD Amount:	0.000
Calibration Level:		Dilution Factor:	1.00
Instrument Method:	E:\GCMS Methods\ChemLab\CLT	Original Processing Method:	
Current Processing Method:	N/A	Calibration File:	N/A

```

Method type: Acquisition - General
MS transfer line temperature: 270 °C
Ion source temperature: 220 °C
Use acquisition threshold: No
Ionization mode: EI
Run completion: GC run time
Segment #1:
Start time: 3 min
Filament/multiplier/dynode on: Yes
Chromatography filter on: Yes
Chrom. filter peak width time: 1 sec
Use tune file emission current: Yes
Use last tuned detector gain: Yes
Use tune file electron energy: No
Electron energy: 70 eV
Calibration gas: Off
Scan #1
Tune file: (Last Saved)
Ion polarity: Positive
Data type: Centroid
Start mass: 50 amu
End mass: 400 amu
Scan time: 0.2 sec
    
```





3am

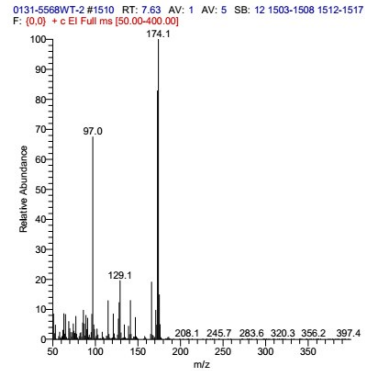
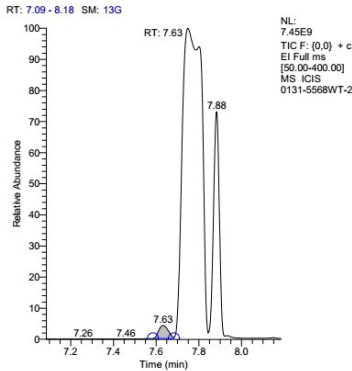
Chemical Formula: C₁₁H₁₀S
 Exact Mass: 174.1

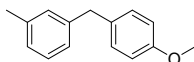


ChemLab Technologies - GC/MS Report

Data File:	0131-5568WT-2	Original Data Path:	E:\GCMS Data\ChemLab
Current Data Path:	E:\GCMS Data\ChemLab	Sample Type:	Unknown
Sample ID:	7	Sample Name:	
Operator:	W. T	Acquisition Date:	02/03/19 01:59:07 AM
Run Time(min):	15.58	Comments:	
Vial:	5	Injection Volume(μl):	10.00
Scans:	4582	Low Mass(m/z):	50
High Mass(m/z):	400	Sample Volume(μl):	0.00
Sample Weight:	0.00	ISTD Amount:	0.000
Calibration Level:		Dilution Factor:	1.00
Instrument Method:	E:\GCMS Methods\ChemLab\CLT	Original Processing Method:	
Current Processing Method:	N/A	Calibration File:	N/A

Method type: Acquisition - General
 MS transfer line temperature: 270 °C
 Ion source temperature: 220 °C
 Use acquisition threshold: No
 Ionization mode: EI
 Run completion: GC run time
 Segment #1:
 Start time: 2.5 min
 Filament/multiplier/dynode on: Yes
 Chromatography filter on: Yes
 Chrom. filter peak width time: 1 sec
 Use tune file emission current: Yes
 Use last tuned detector gain: Yes
 Use tune file electron energy: No
 Electron energy: 70 eV
 Calibration gas: Off
 Scan #1
 Tune file: (Last Saved)
 Ion polarity: Positive
 Data type: Centroid
 Start mass: 50 amu
 End mass: 400 amu
 Scan time: 0.2 sec





3bb

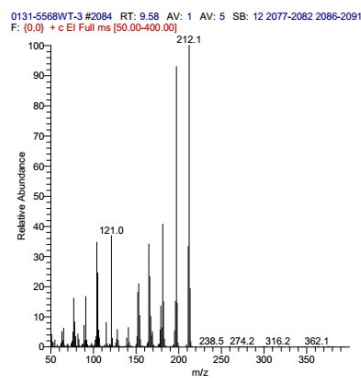
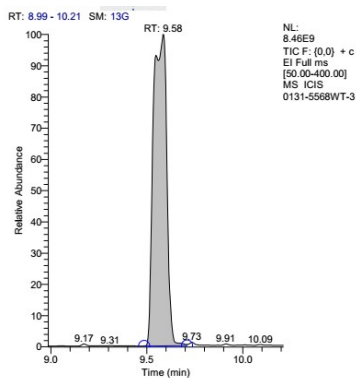
Chemical Formula: C₁₅H₁₆O
Exact Mass: 212.1

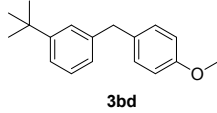


ChemLab Technologies - GC/MS Report

Data File:	0131-5568WT-3	Original Data Path:	E:\GCMS Data\ChemLab
Current Data Path:	E:\GCMS Data\ChemLab	Sample Type:	Unknown
Sample ID:	7	Sample Name:	
Operator:	W. T	Acquisition Date:	02/03/19 02:20:13 AM
Run Time(min):	15.60	Comments:	
Vial:	5	Injection Volume(μl):	10.00
Scans:	4588	Low Mass(m/z):	50
High Mass(m/z):	400	Sample Volume(μl):	0.00
Sample Weight:	0.00	ISTD Amount:	0.000
Calibration Level:		Dilution Factor:	1.00
Instrument Method:	E:\GCMS Methods\ChemLab\CLT	Original Processing Method:	
Current Processing Method:	N/A	Calibration File:	N/A

Method type:	Acquisition - General
MS transfer line temperature:	270 °C
Ion source temperature:	220 °C
Use acquisition threshold:	No
Ionization mode:	EI
Run completion:	GC run time
Segment #1:	
Start time:	2.5 min
Filament/multiplier/dynode on:	Yes
Chromatography filter on:	Yes
Chrom. filter peak width time:	1 sec
Use tune file emission current:	Yes
Use last tuned detector gain:	Yes
Use tune file electron energy:	No
Electron energy:	70 eV
Calibration gas:	Off
Scan #1:	
Tune file:	(Last Saved)
Ion polarity:	Positive
Data type:	Centroid
Start mass:	50 amu
End mass:	400 amu
Scan time:	0.2 sec





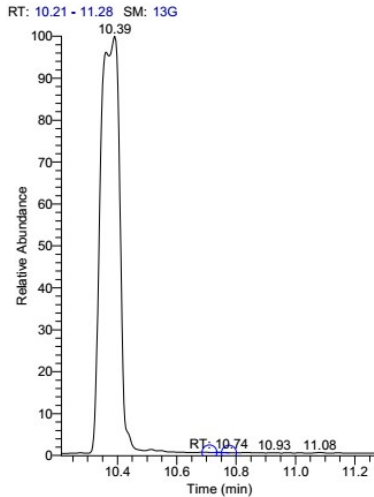
Chemical Formula: C₁₈H₂₂O
Exact Mass: 254.2



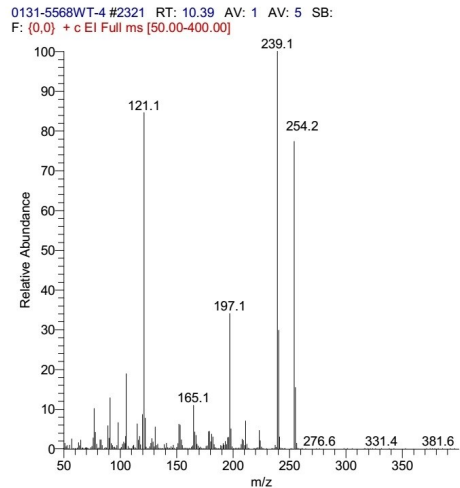
ChemLab Technologies - GC/MS Report

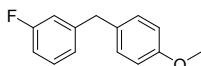
Data File:	0131-5568WT-4	Original Data Path:	E:\GCMS Data\ChemLab
Current Data Path:	E:\GCMS Data\ChemLab	Sample Type:	Unknown
Sample ID:	7	Sample Name:	
Operator:	W. T	Acquisition Date:	02/03/19 02:41:34 AM
Run Time(min):	15.59	Comments:	
Vial:	5	Injection Volume(μl):	10.00
Scans:	4584	Low Mass(m/z):	50
High Mass(m/z):	400	Sample Volume(μl):	0.00
Sample Weight:	0.00	ISTD Amount:	0.000
Calibration Level:		Dilution Factor:	1.00
Instrument Method:	E:\GCMS Methods\ChemLab\CLT	Original Processing Method:	
Current Processing Method:	N/A	Calibration File:	N/A

Method type: Acquisition - General
MS transfer line temperature: 270 °C
Ion source temperature: 220 °C
Use acquisition threshold: No
Ionization mode: EI
Run completion: GC run time
Segment #1:
Start time: 2.5 min
Filament/multiplier/dynode on: Yes
Chromatography filter on: Yes
Chrom. filter peak width time: 1 sec
Use tune file emission current: Yes
Use last tuned detector gain: Yes
Use tune file electron energy: No
Electron energy: 70 eV
Calibration gas: Off
Scan #1
Tune file: (Last Saved)
Ion polarity: Positive
Data type: Centroid
Start mass: 50 amu
End mass: 400 amu
Scan time: 0.2 sec



NL:
7.54E9
TIC F: {0.0} + c
EI Full ms
[50.00-400.00]
MS ICIS
0131-5568WT-4





3be

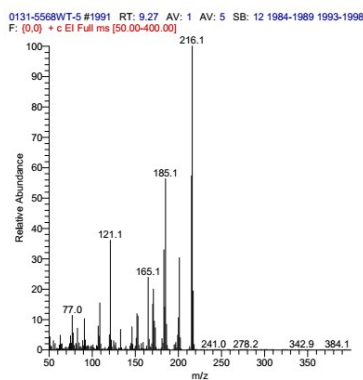
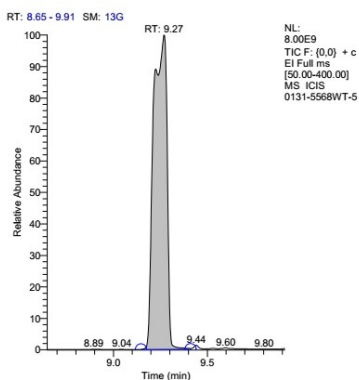
Chemical Formula: C₁₄H₁₃FO
Exact Mass: 216.1

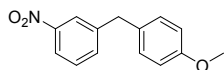


ChemLab Technologies - GC/MS Report

Data File:	0131-5568WT-5	Original Data Path:	E:\GCMS Data\ChemLab
Current Data Path:	E:\GCMS Data\ChemLab	Sample Type:	Unknown
Sample ID:	7	Sample Name:	
Operator:	W. T	Acquisition Date:	02/03/19 03:03:00 AM
Run Time(min):	15.60	Comments:	
Vial:	5	Injection Volume(μl):	10.00
Scans:	4589	Low Mass(m/z):	50
High Mass(m/z):	400	Sample Volume(μl):	0.00
Sample Weight:	0.00	ISTD Amount:	0.000
Calibration Level:		Dilution Factor:	1.00
Instrument Method:	E:\GCMS Methods\ChemLab\CLT	Original Processing Method:	
Current Processing Method:	N/A	Calibration File:	N/A

Method type: Acquisition - General
 MS transfer line temperature: 270 °C
 Ion source temperature: 220 °C
 Use acquisition threshold: No
 Ionization mode: EI
 Run completion: GC run time
 Segment #1:
 Start time: 2.5 min
 Filament/multiplier/dynode on: Yes
 Chromatography filter on: Yes
 Chrom. filter peak width time: 1 sec
 Use tune file emission current: Yes
 Use last tuned detector gain: Yes
 Use tune file electron energy: No
 Electron energy: 70 eV
 Calibration gas: Off
 Scan #1
 Tune file: (Last Saved)
 Ion polarity: Positive
 Data type: Centroid
 Start mass: 50 amu
 End mass: 400 amu
 Scan time: 0.2 sec





3bf

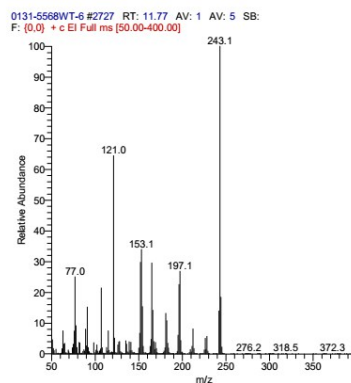
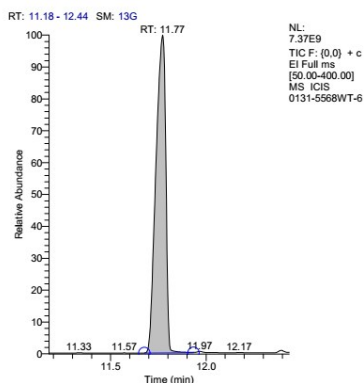
Chemical Formula: C₁₄H₁₃NO₃
Exact Mass: 243.1

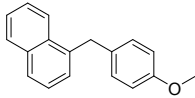


ChemLab Technologies - GC/MS Report

Data File:	0131-5568WT-6	Original Data Path:	E:\GCMS Data\ChemLab
Current Data Path:	E:\GCMS Data\ChemLab	Sample Type:	Unknown
Sample ID:	7	Sample Name:	
Operator:	W. T	Acquisition Date:	02/03/19 03:24:26 AM
Run Time(min):	15.60	Comments:	
Vial:	5	Injection Volume(μl):	10.00
Scans:	4589	Low Mass(m/z):	50
High Mass(m/z):	400	Sample Volume(μl):	0.00
Sample Weight:	0.00	ISTD Amount:	0.000
Calibration Level:		Dilution Factor:	1.00
Instrument Method:	E:\GCMS Methods\ChemLab\CLT	Original Processing Method:	
Current Processing Method:	N/A	Calibration File:	N/A

Method type:	Acquisition - General
MS transfer line temperature:	270 °C
Ion source temperature:	220 °C
Use acquisition threshold:	No
Ionization mode:	EI
Run completion:	GC run time
Segment #1:	
Start time:	2.5 min
Filament/multiplier/dynode on:	Yes
Chromatography filter on:	Yes
Chrom. filter peak width time:	1 sec
Use tune file emission current:	Yes
Use last tuned detector gain:	Yes
Use tune file electron energy:	No
Electron energy:	70 eV
Calibration gas:	Off
Scan #1	
Tune file:	(Last Saved)
Ion polarity:	Positive
Data type:	Centroid
Start mass:	50 amu
End mass:	400 amu
Scan time:	0.2 sec





3bg

Chemical Formula: C₁₈H₁₆O
Exact Mass: 248.1



ChemLab Technologies - GC/MS Report

Data File:	0131-5568WT-7	Original Data Path:	E:\GCMS Data\ChemLab
Current Data Path:	E:\GCMS Data\ChemLab	Sample Type:	Unknown
Sample ID:	7	Sample Name:	
Operator:	W. T	Acquisition Date:	02/03/19 03:45:52 AM
Run Time(min):	10.25	Comments:	
Vial:	5	Injection Volume(μl):	10.00
Scans:	3016	Low Mass(m/z):	50
High Mass(m/z):	400	Sample Volume(μl):	0.00
Sample Weight:	0.00	ISTD Amount:	0.000
Calibration Level:		Dilution Factor:	1.00
Instrument Method:	E:\GCMS Methods\ChemLab\CLT	Original Processing Method:	
Current Processing Method:	N/A	Calibration File:	N/A

```

Method type: Acquisition - General
MS transfer line temperature: 270 °C
Ion source temperature: 220 °C
Use acquisition threshold: No
Ionization mode: EI
Run completion: GC run time
Segment #1:
Start time: 2.5 min
Filament/multiplier/dynode on: Yes
Chromatography filter on: Yes
Chrom. filter peak width time: 1 sec
Use tune file emission current: Yes
Use last tuned detector gain: Yes
Use tune file electron energy: No
Electron energy: 70 eV
Calibration gas: Off
Scan #1
Tune file: (Last Saved)
Ion polarity: Positive
Data type: Centroid
Start mass: 50 amu
End mass: 400 amu
Scan time: 0.2 sec
  
```

