

Chan–Evans–Lam Amination of Boronic Acid Pinacol (BPin) Esters:

Overcoming the Aryl Amine Problem

Supporting Information

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Watson^{*a}

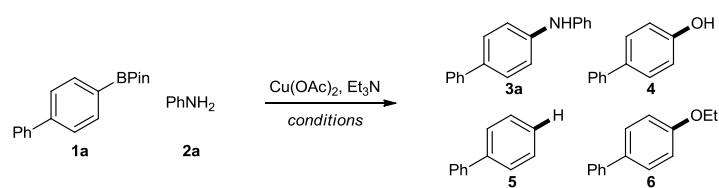
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^b GlaxoSmithKline, Medicines Research Centre, Gunnels Wood Road, Stevenage, SG1 2NY (UK).

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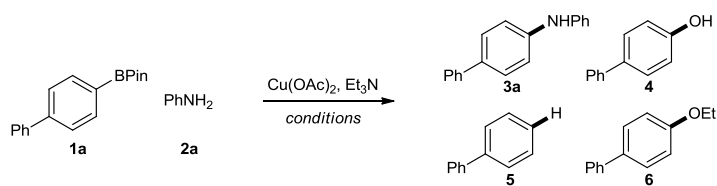
1. Data from solvent optimisation.



entry	reaction conditions	3a:4:5:6 (%) ^b
1	CH ₂ Cl ₂ , 0.25 M, 40 °C	31:2:5:--
2	MeCN, 0.25 M, 60 °C	39:8:6:--
3	EtOH, 0.25 M, 60 °C	43:12:15:38
4	EtOAc, 0.25 M, 60 °C	3:1:0:--
5	Toluene, 0.25 M, 60 °C	2:7:12:--
6	DMSO, 0.25 M, 60 °C	7:4:5:--
7	Acetone, 0.25 M, 60 °C	5:6:3:--
8	DMF, 0.25 M, 60 °C	16:6:7:--
9	THF, 0.25 M, 60 °C	5:1:0:--
10	MeCN:EtOH (1:1), 0.25 M, 60 °C	47:14:12:20
11	MeCN:EtOH (2:1), 0.25 M, 60 °C	46:15:11:14
12	MeCN:EtOH (5:1), 0.25 M, 60 °C	46:14:13:12
13	MeCN:EtOH (10:1), 0.25 M, 60 °C	47:14:13:9
14	MeCN:EtOH (20:1), 0.25 M, 60 °C	45:13:10:1
15	MeCN:EtOH (30:1), 0.25 M, 60 °C	38:11:7:0

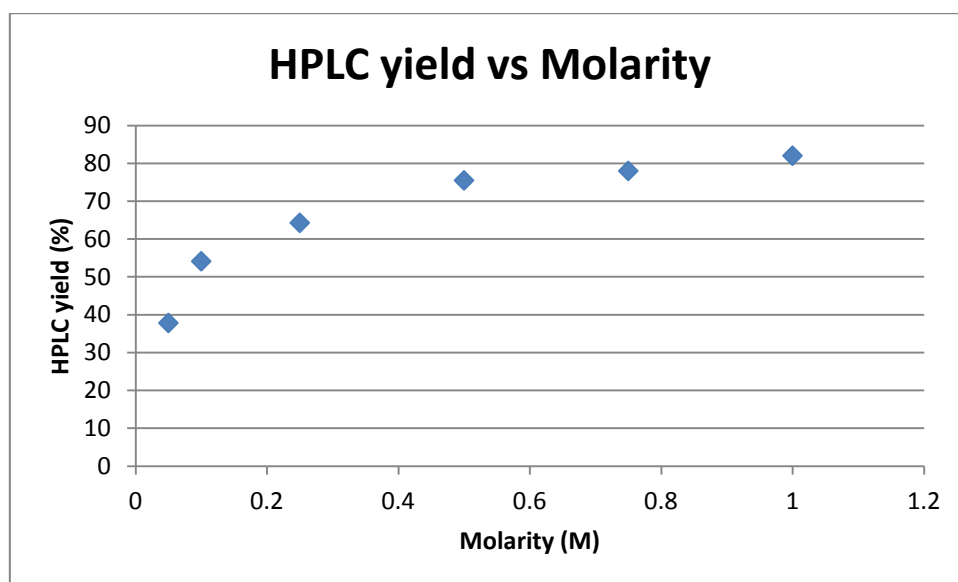
^a **1a** (1.0 equiv, 0.3 mmol), **2a** (2 equiv, 0.6 mmol), Cu(OAc)₂ (1 equiv, 0.3 mmol), Et₃N (2 equiv, 0.6 mmol), solvent, air, 24 h. ^b Determined by HPLC analysis using an internal standard. Mass balance is returned starting material.

2. Data from concentration optimization.



entry	reaction conditions	3a (%) ^b
1	MeCN:EtOH (20:1), 1 M, 3 Å MS, 80 °C	82
2	MeCN:EtOH (20:1), 0.75 M, 3 Å MS, 80 °C	78
3	MeCN:EtOH (20:1), 0.5 M, 3 Å MS, 80 °C	75
4	MeCN:EtOH (20:1), 0.25 M, 3 Å MS, 80 °C	64
5	MeCN:EtOH (20:1), 0.1 M, 3 Å MS, 80 °C	54
6	MeCN:EtOH (20:1), 0.05 M, 3 Å MS, 80 °C	38

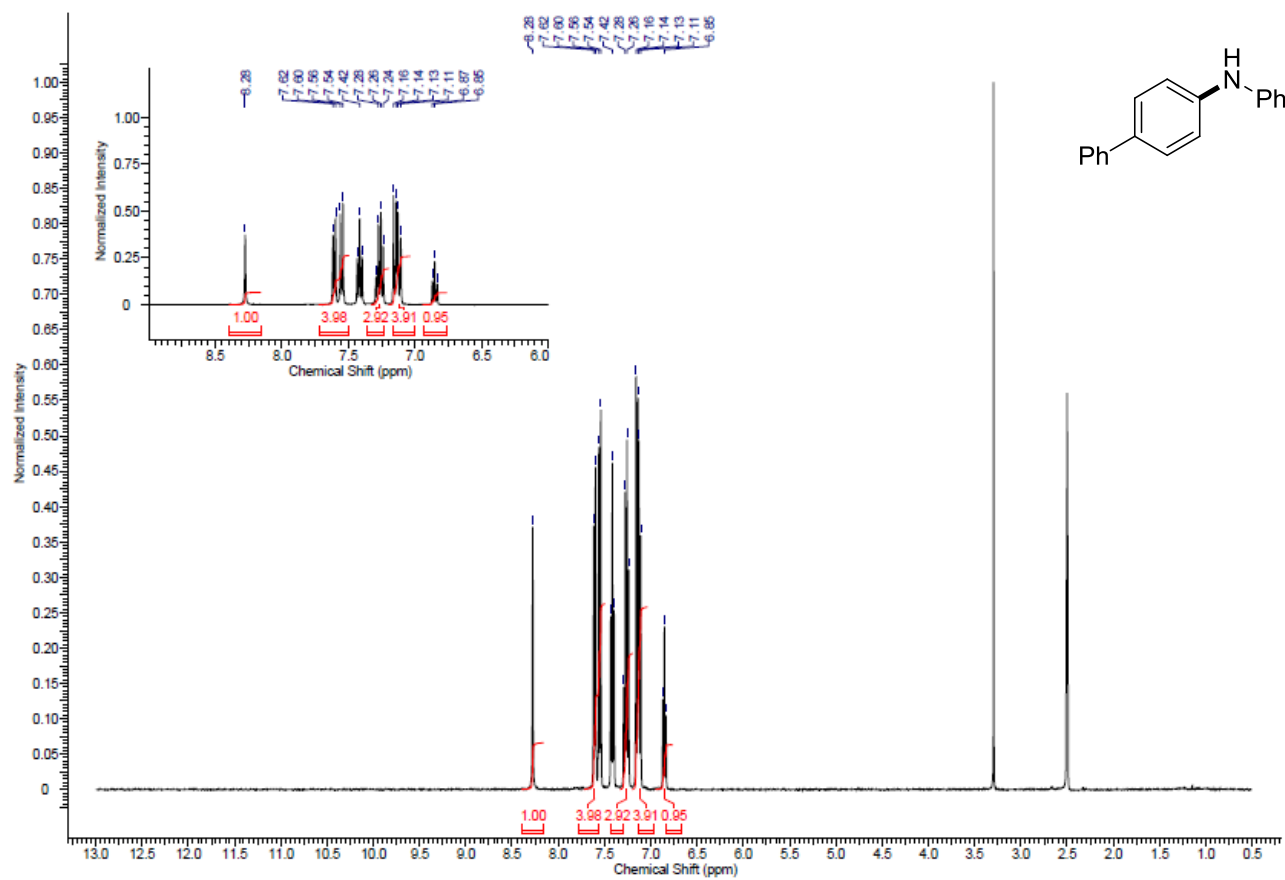
^a **1a** (1.0 equiv, 0.3 mmol), **2a** (2 equiv, 0.6 mmol), $\text{Cu}(\text{OAc})_2$ (1 equiv, 0.3 mmol), Et_3N (2 equiv, 0.6 mmol), 3 Å MS (75 mg), solvent, air, 24 h. ^b Determined by HPLC analysis using an internal standard. Mass balance is returned starting material.



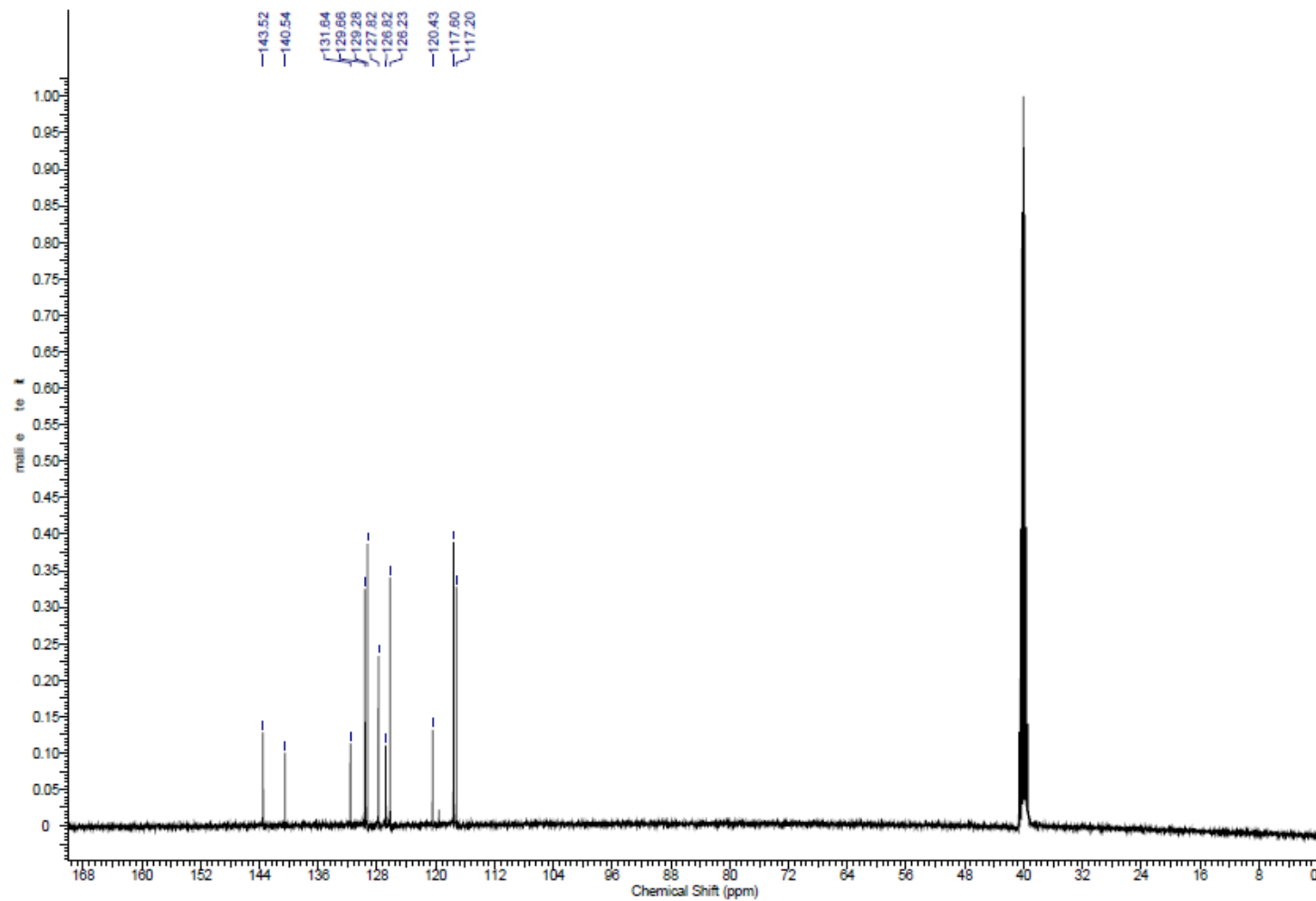
3. ^1H NMR, ^{13}C NMR, ^{19}F NMR, LCMS, HRMS, and IR spectra.

N-Phenyl-[1,1'-biphenyl]-4-amine (3a).

^1H -NMR Spectra

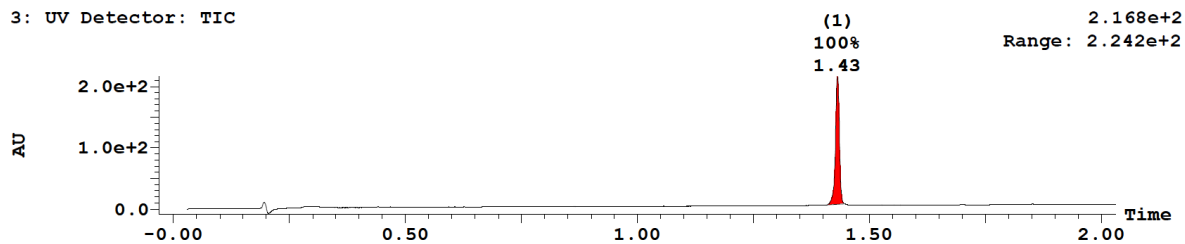


^{13}C -NMR Spectra



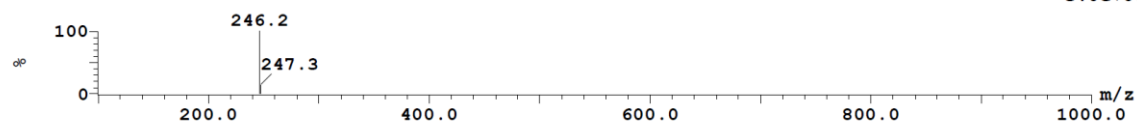
LCMS

3: UV Detector: TIC



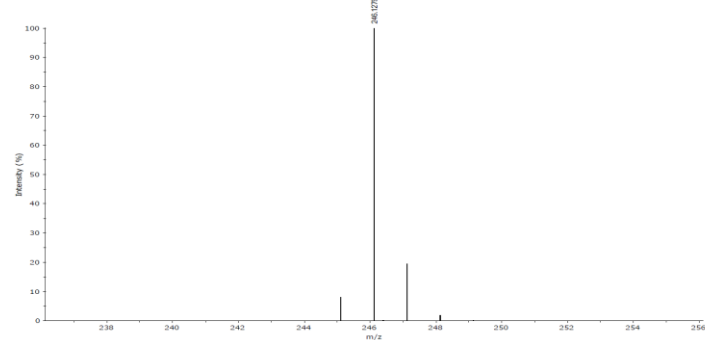
Peak Time
1 1.43
1: (Time: 1.43)

1: MS ES+
3.0e+007

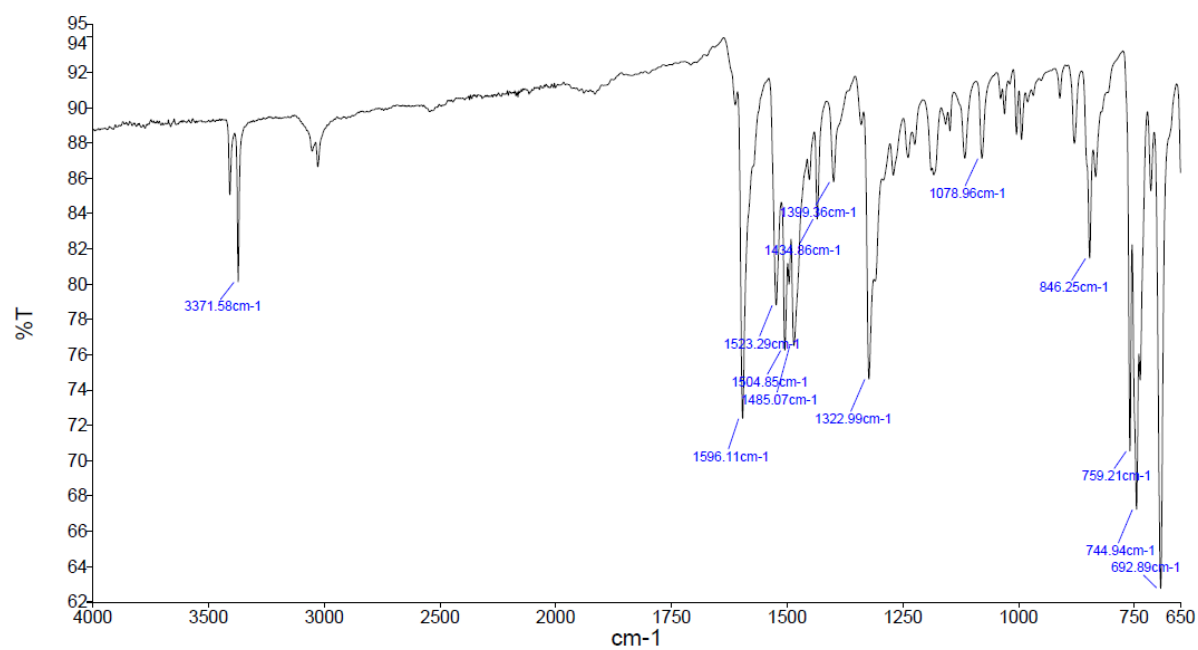


HRMS

Expanded Spectrum RT 5.10, Peak [1], Target Mass 246.1277

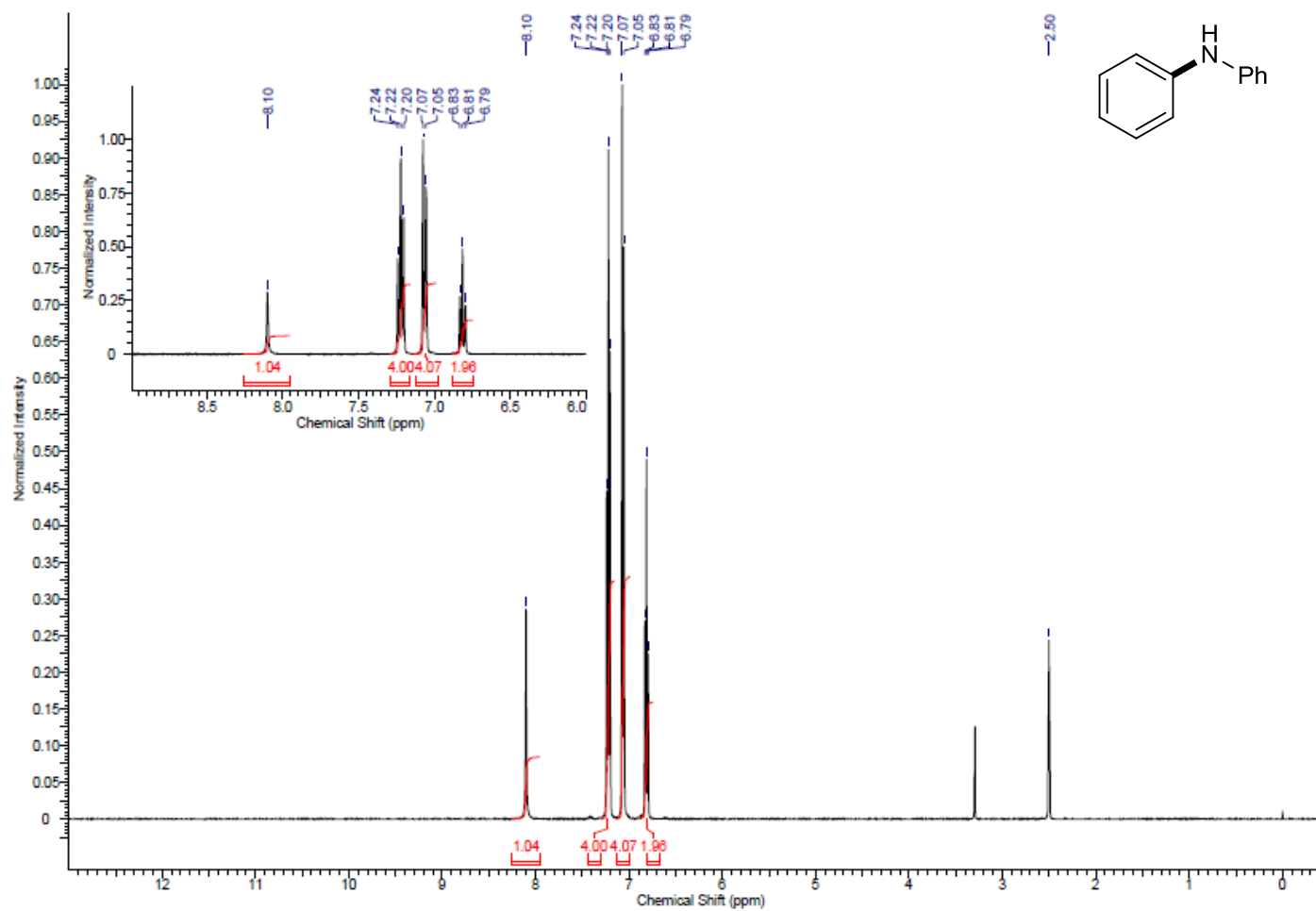


IR Spectra

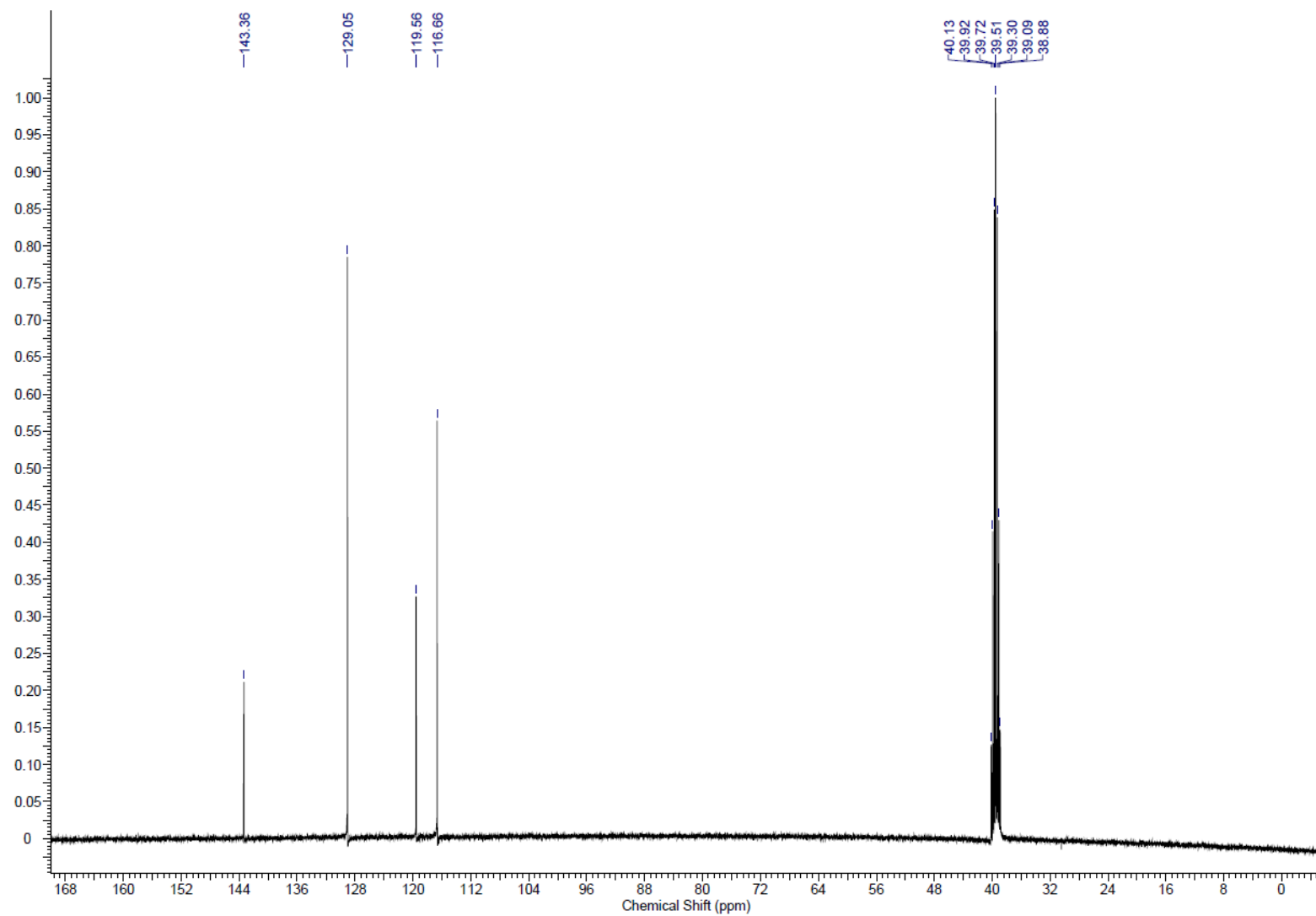


Diphenylamine (3b).

^1H -NMR Spectra

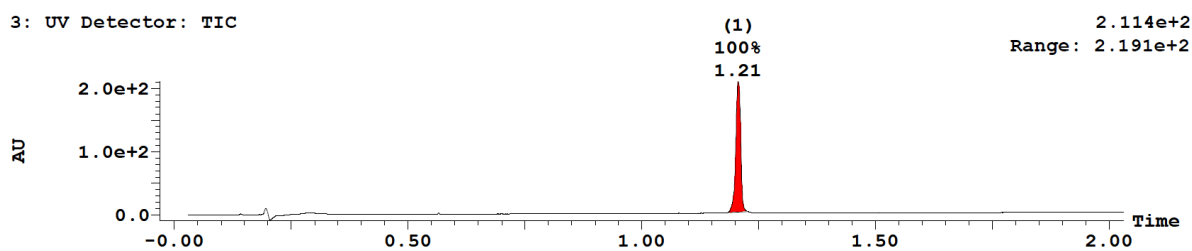


^{13}C -NMR Spectra



LCMS

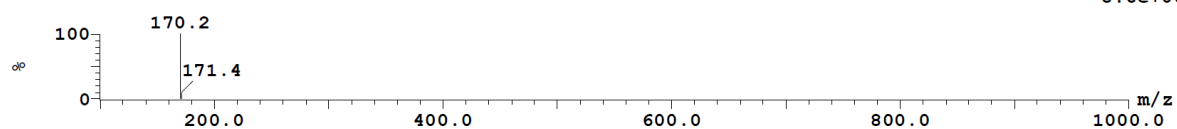
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Peak Time
1 1.21

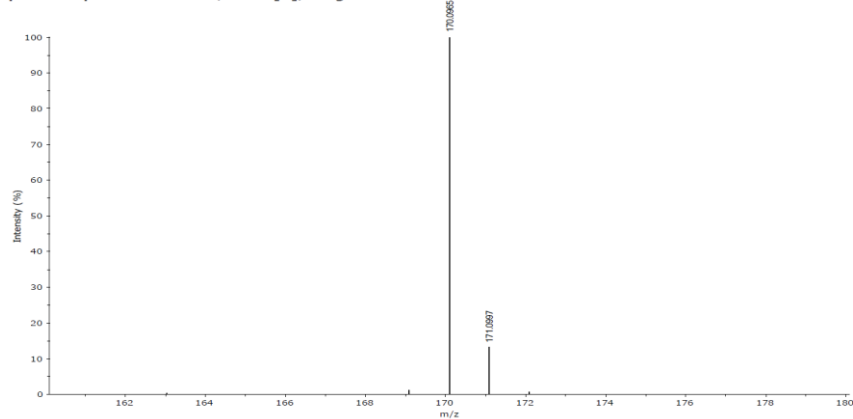
1: (Time: 1.21)

1: MS ES+
8.6e+007

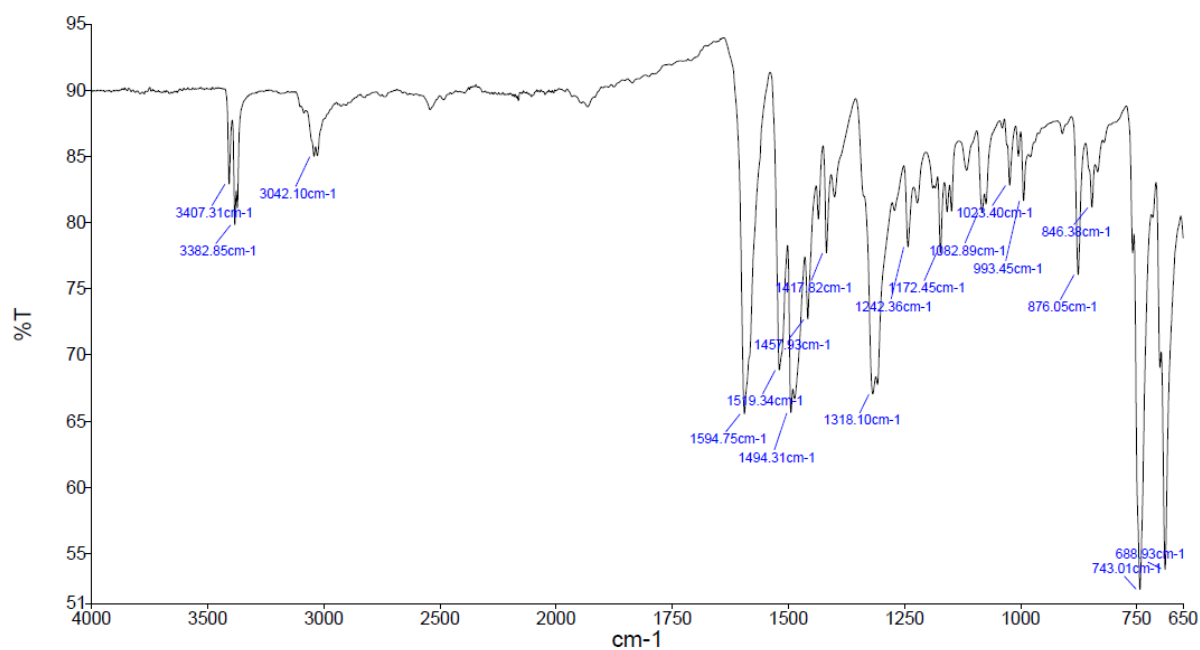


HRMS

Expanded Spectrum RT 3.90, Peak [1], Target Mass 170.0964

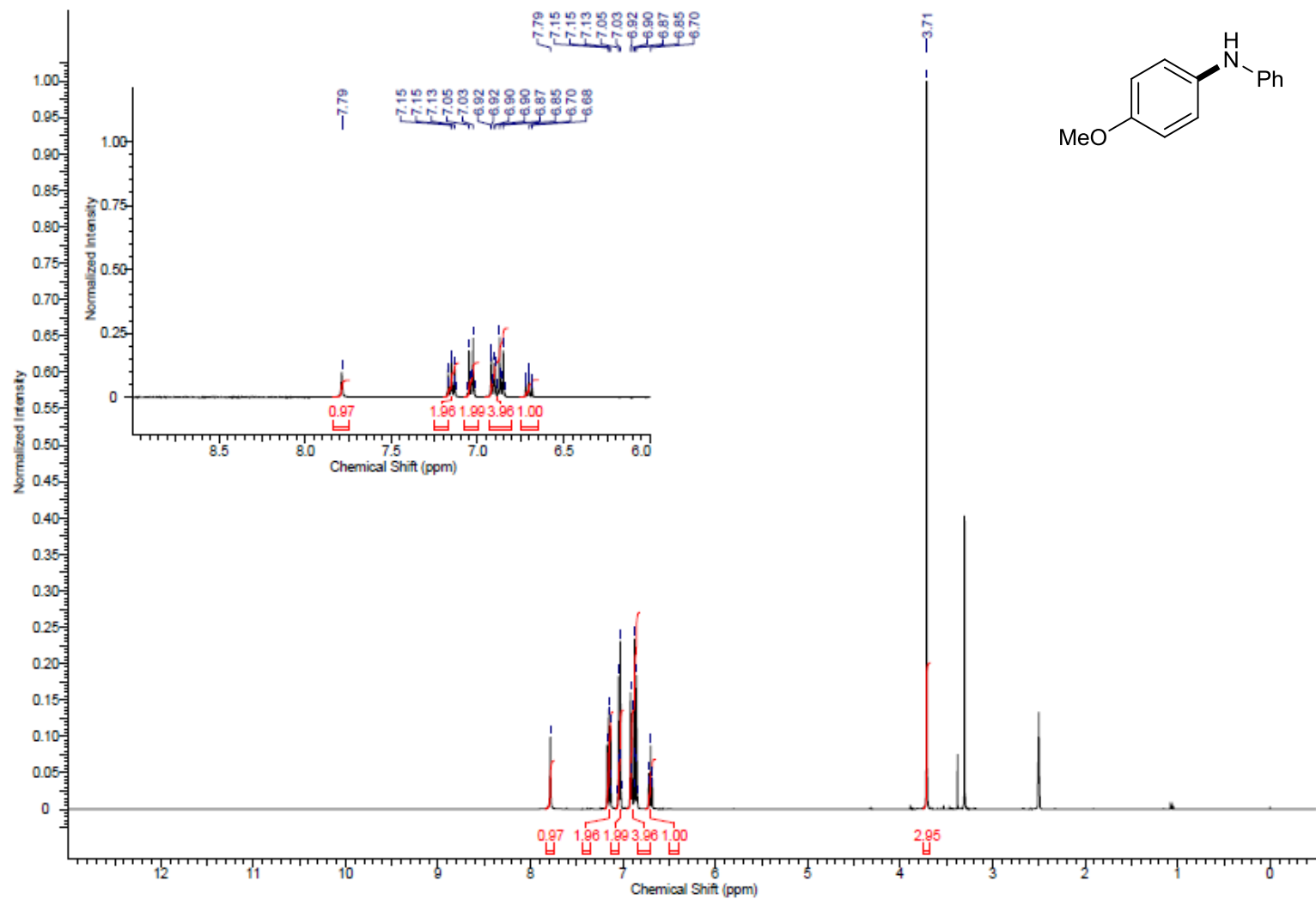


IR Spectra

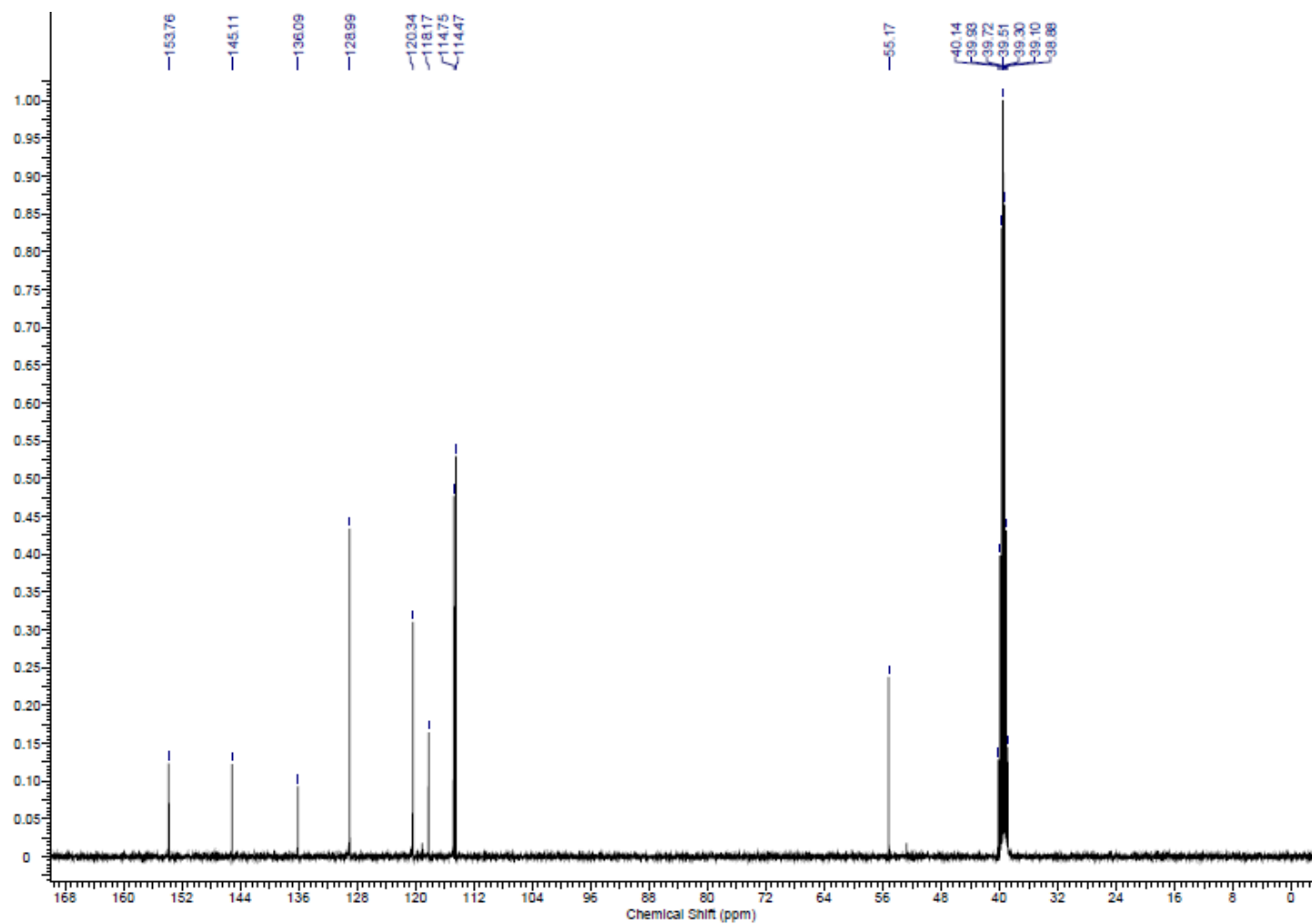


4-Methoxy-N-phenylaniline (3c).

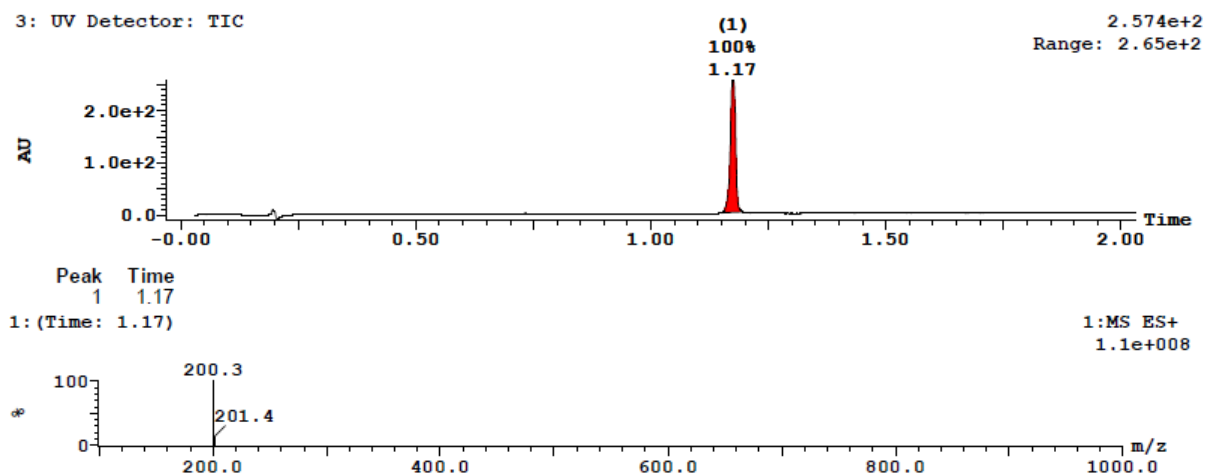
^1H NMR Spectra



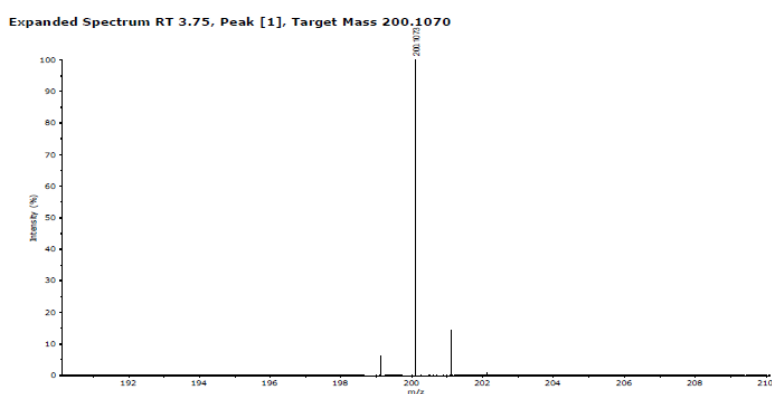
^{13}C NMR Spectra



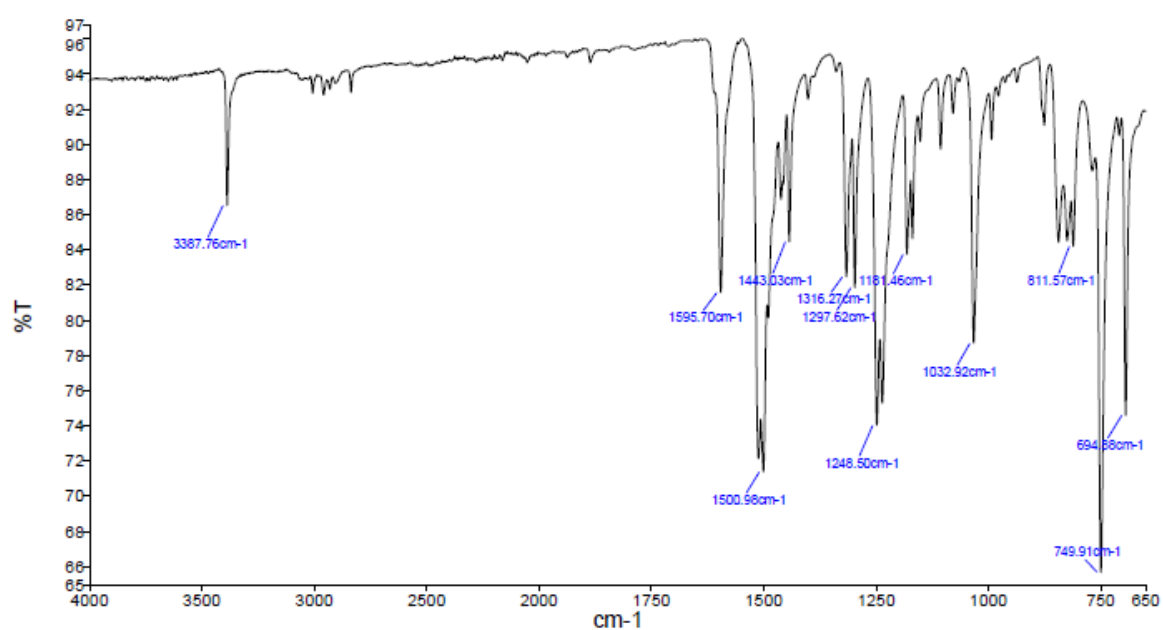
LCMS



HRMS

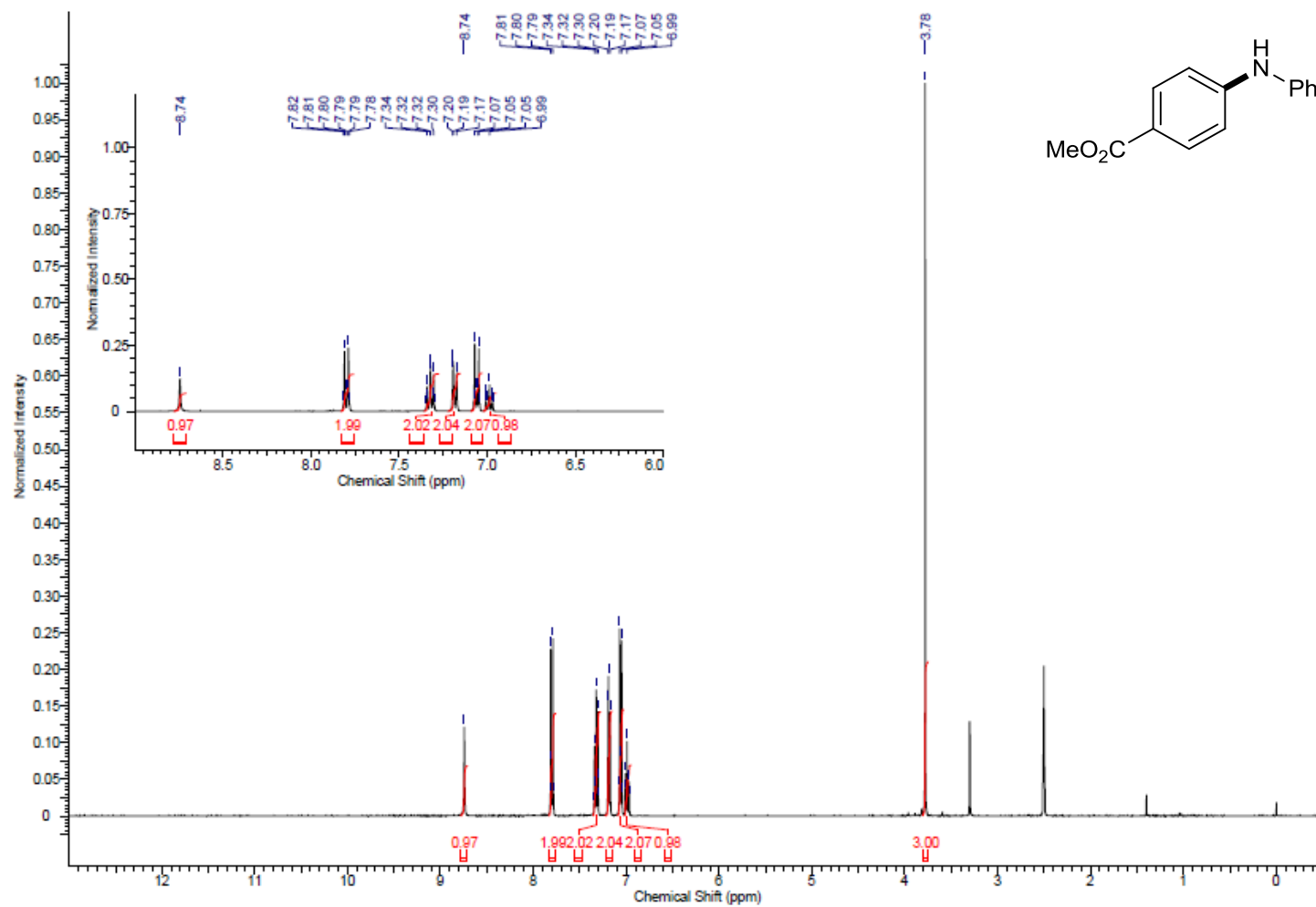


IR Spectra

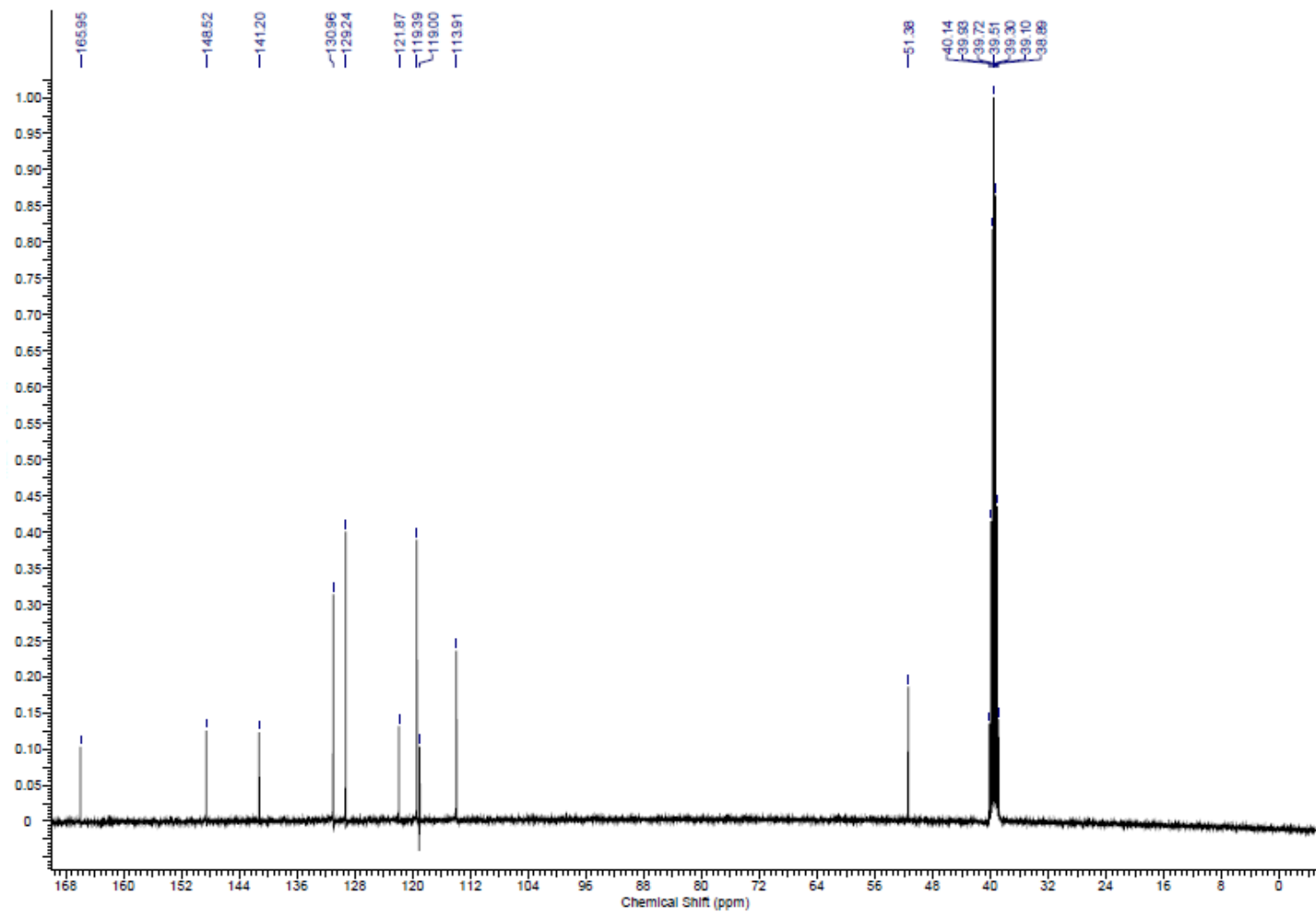


Methyl-4-(phenylamino)benzoate (3d).

¹H NMR SPECTRA

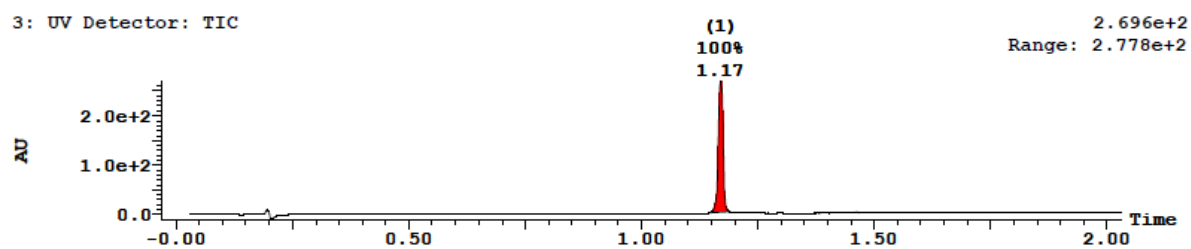


^{13}C NMR SPECTRA



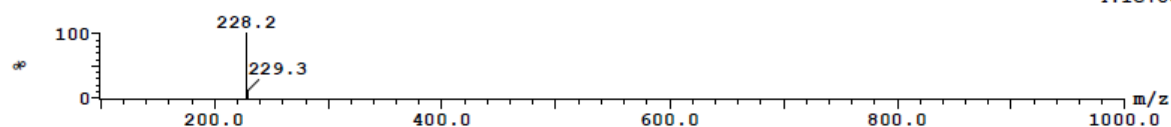
LCMS

3: UV Detector: TIC



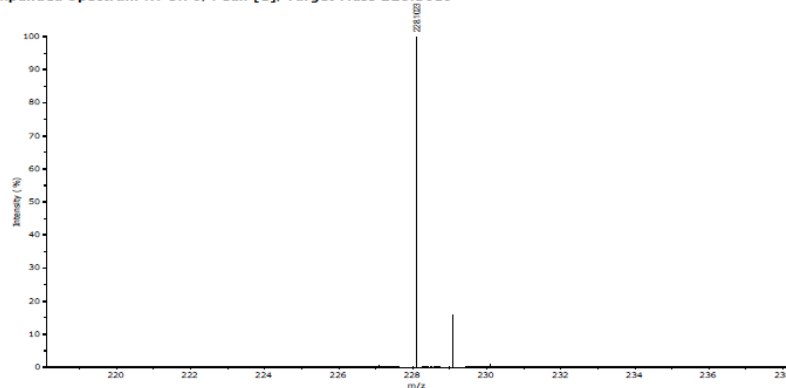
Peak Time
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1: (Time: 1.17)

1:MS ES+
4.1e+007

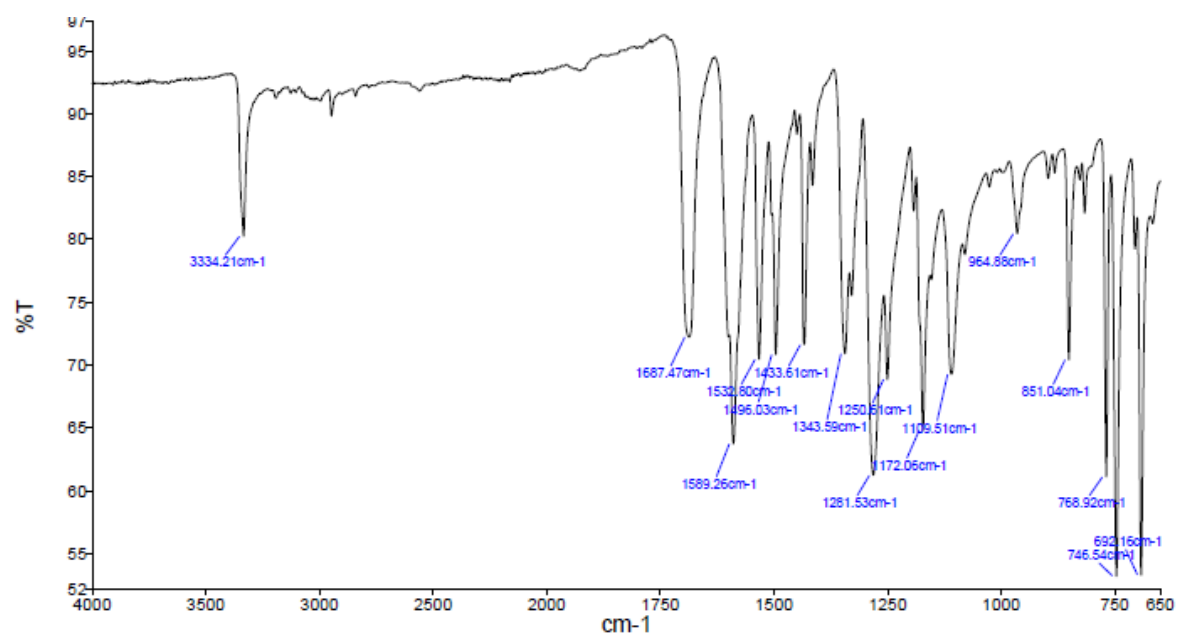


HRMS

Expanded Spectrum RT 3.76, Peak [1], Target Mass 228.1019

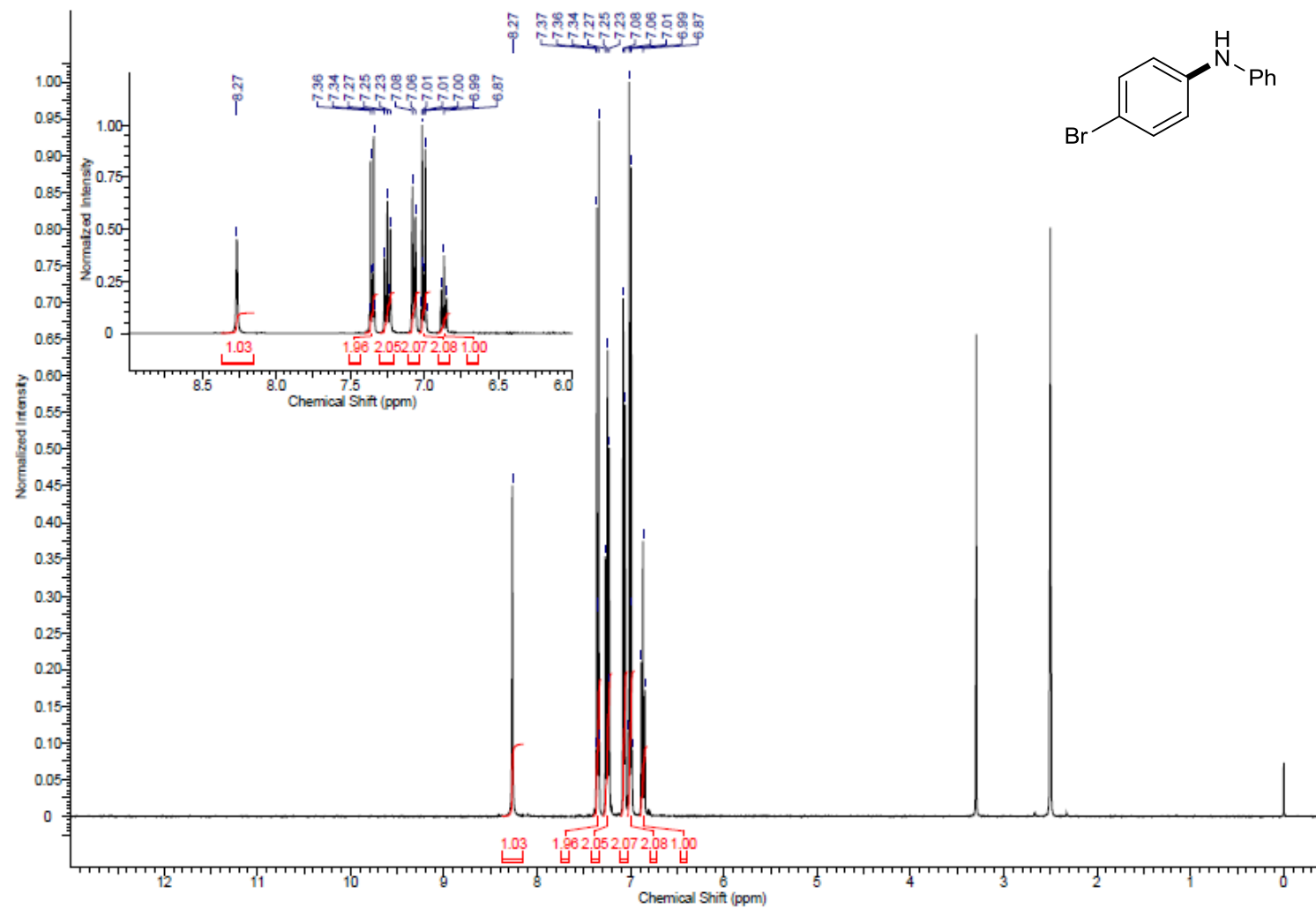


IR SPECTRA

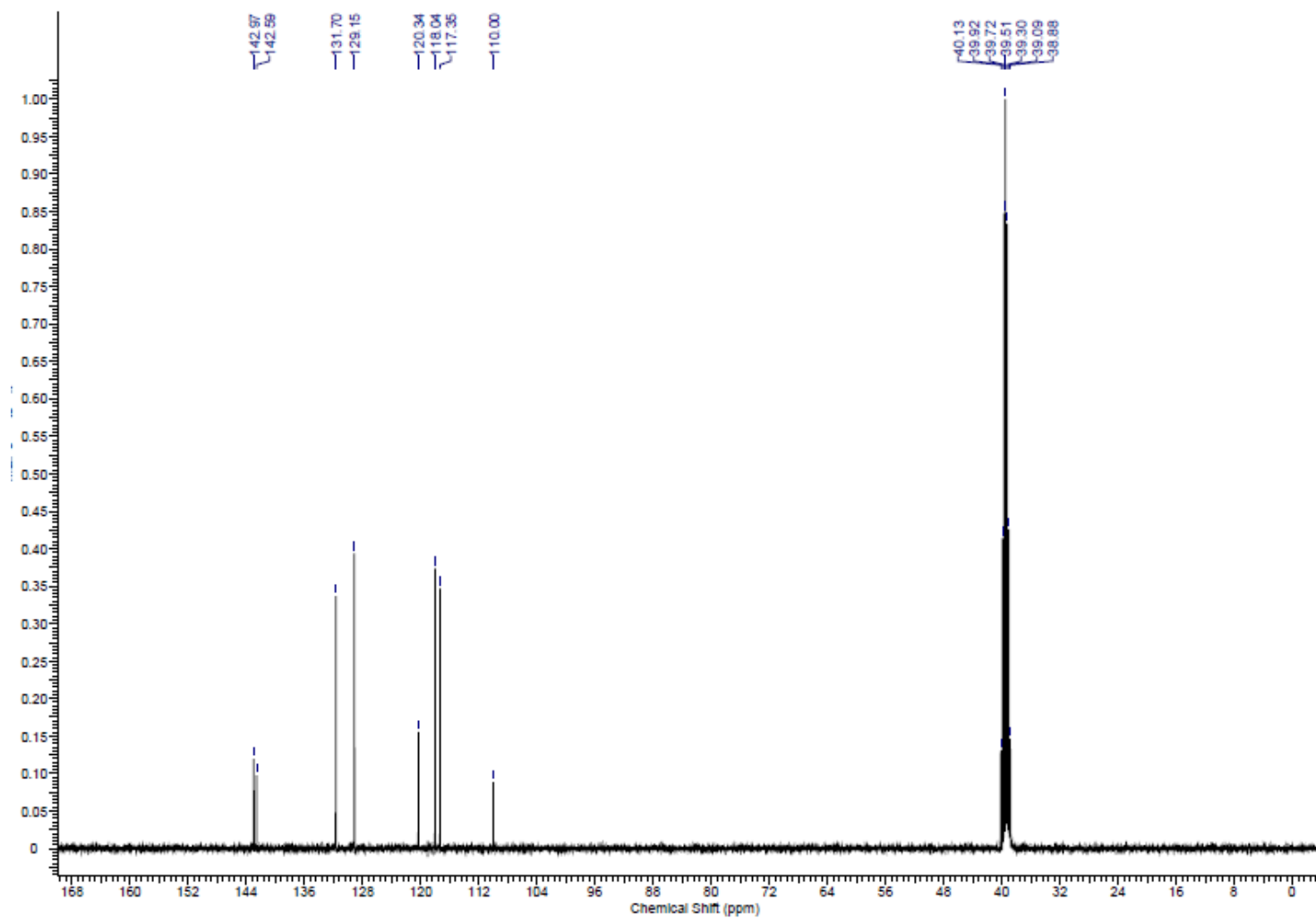


4-Bromo-*N*-phenylaniline (3e).

¹H NMR Spectra

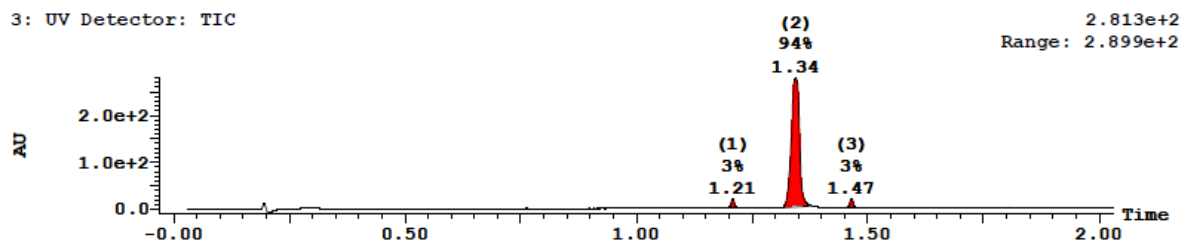


¹³C NMR Spectra



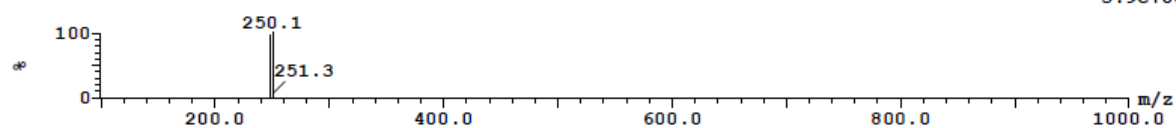
LCMS

3: UV Detector: TIC



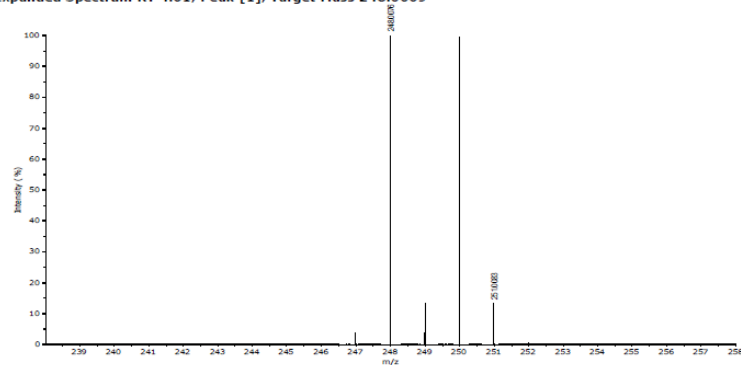
Peak Time
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2: (Time: 1.34)

1: MS ES+
3.9e+007

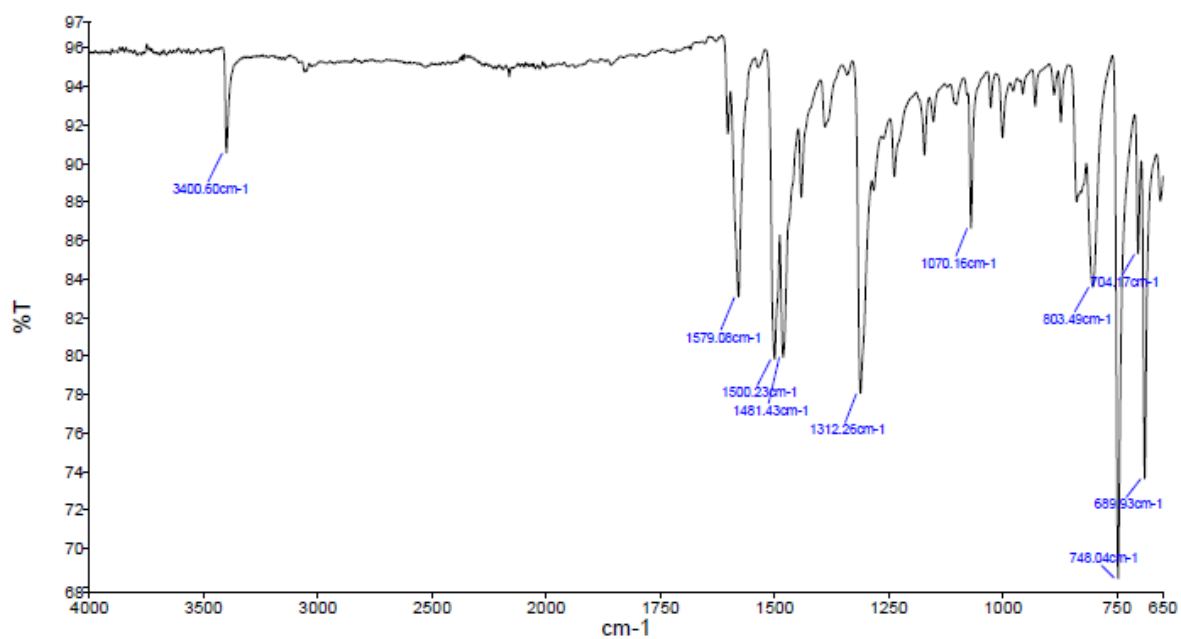


HRMS

Expanded Spectrum RT 4.61, Peak [1], Target Mass 248.0069

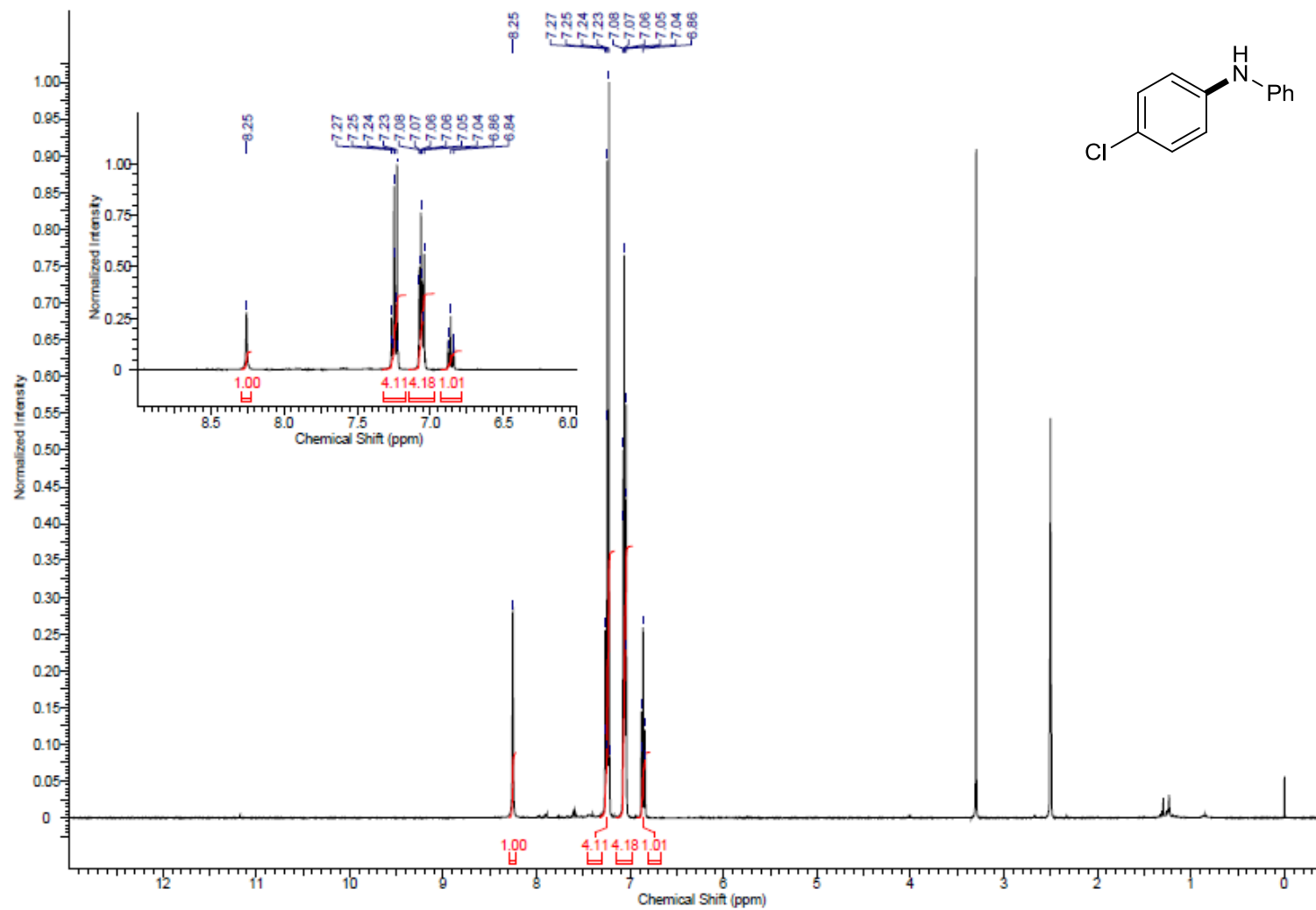


IR Spectra

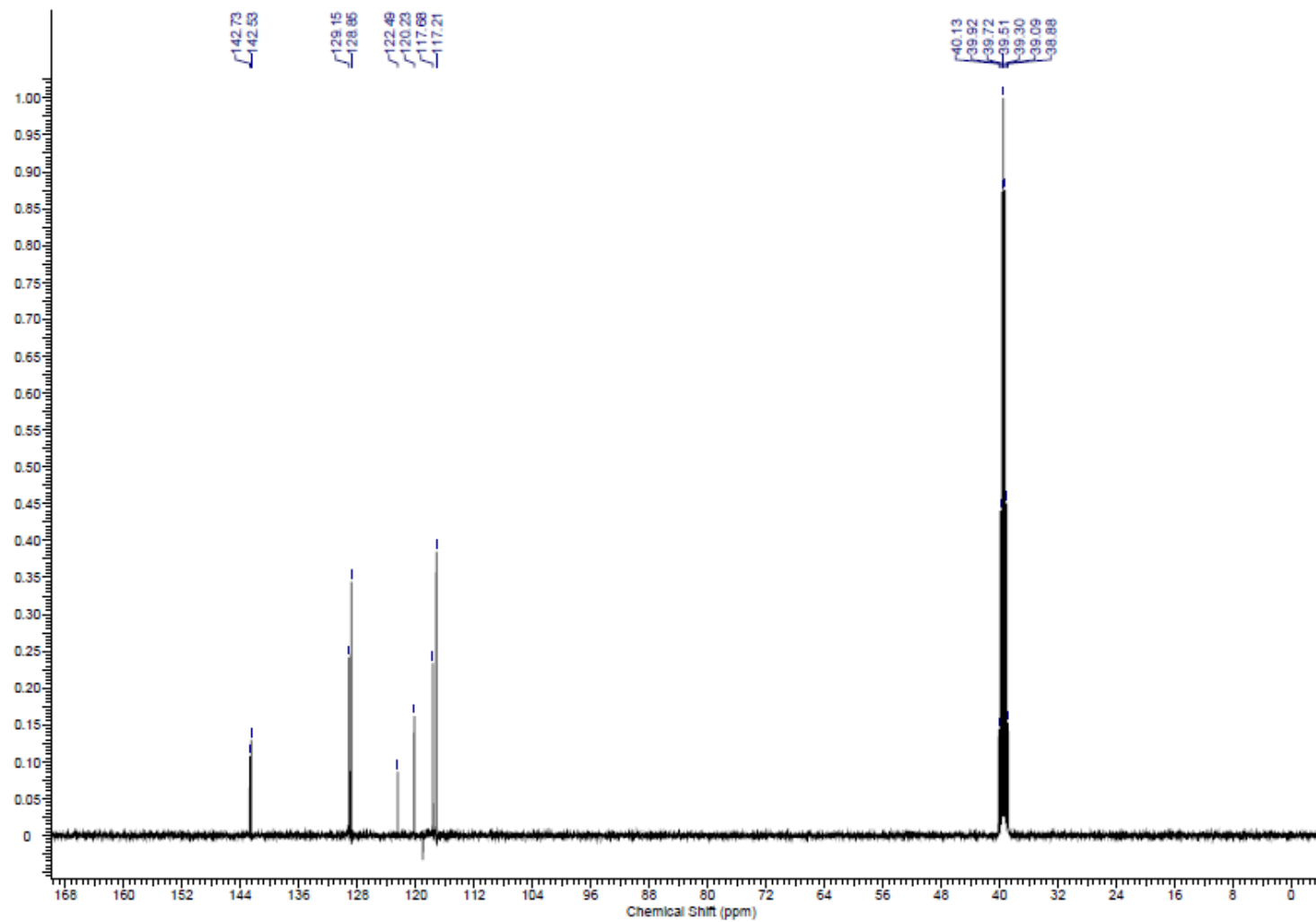


4-Chloro-*N*-phenylaniline (3f).

^1H NMR Spectra

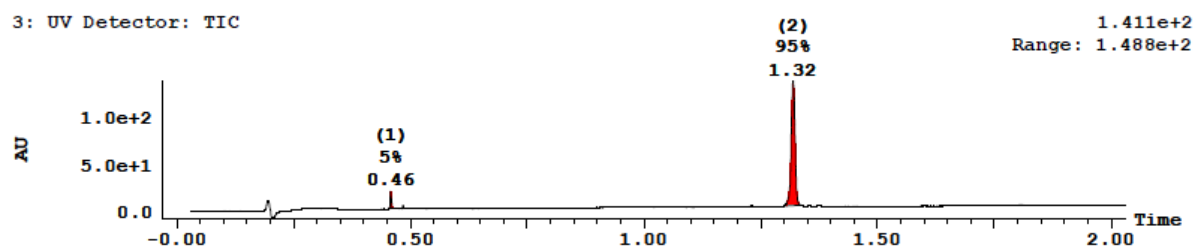


^{13}C NMR Spectra



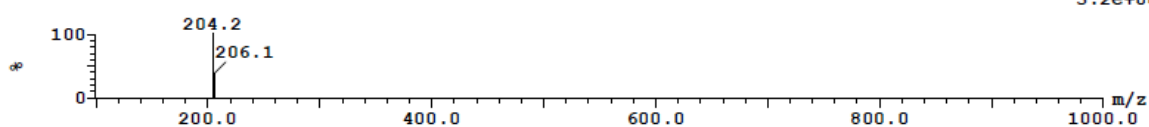
LCMS

3: UV Detector: TIC



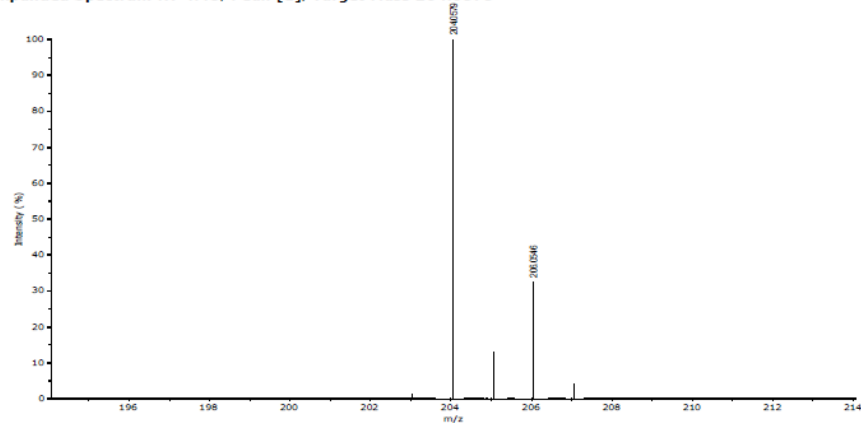
Peak Time
2 1.32
2: (Time: 1.32)

1:MS ES+
3.2e+007

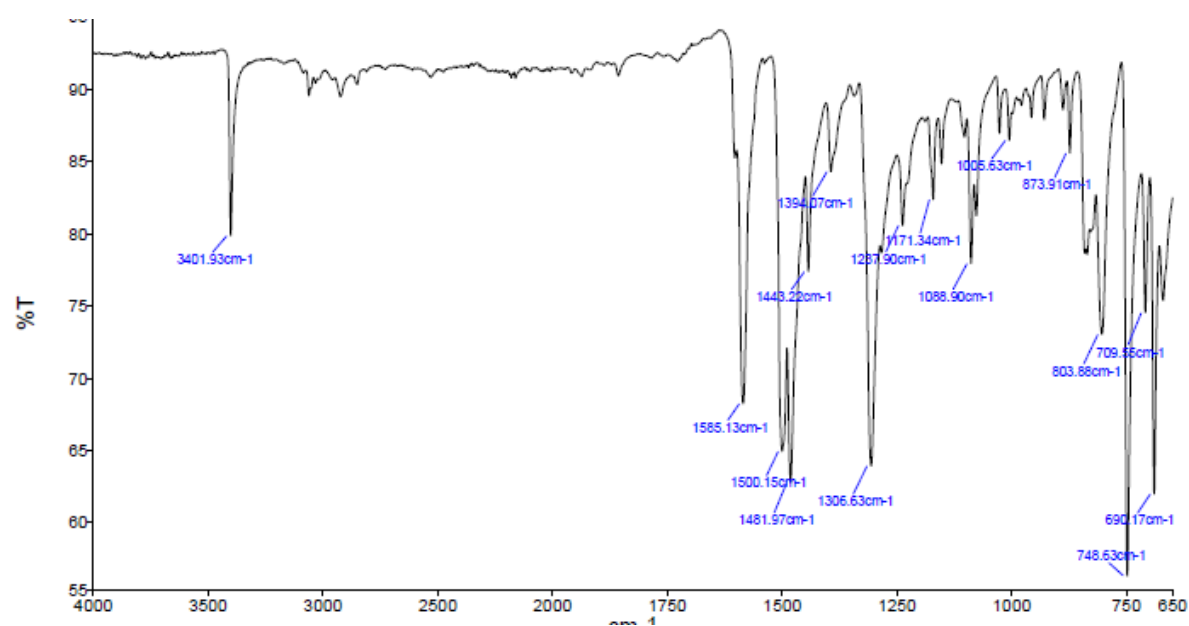


HRMS

Expanded Spectrum RT 4.48, Peak [1], Target Mass 204.0575

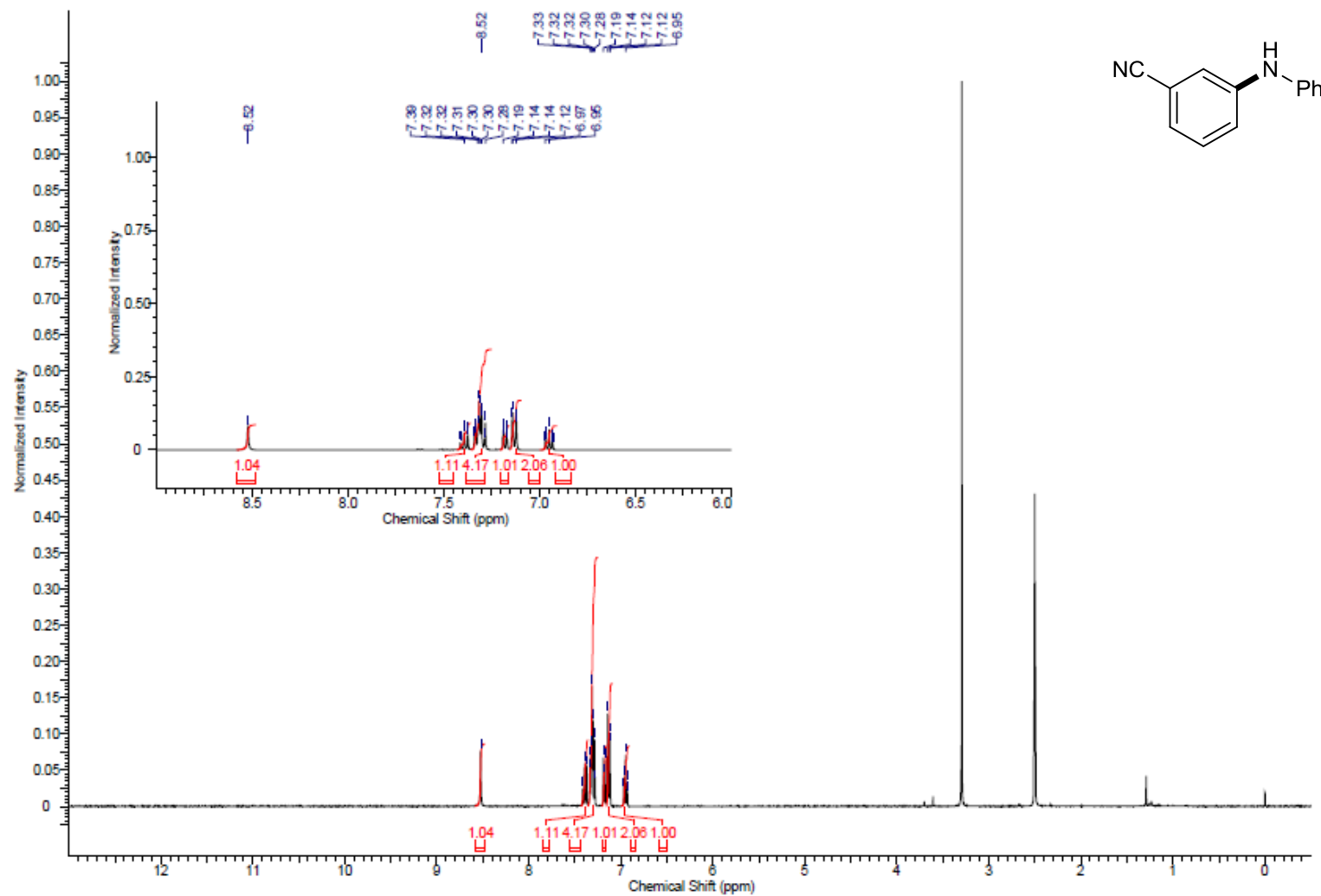


IR Spectra

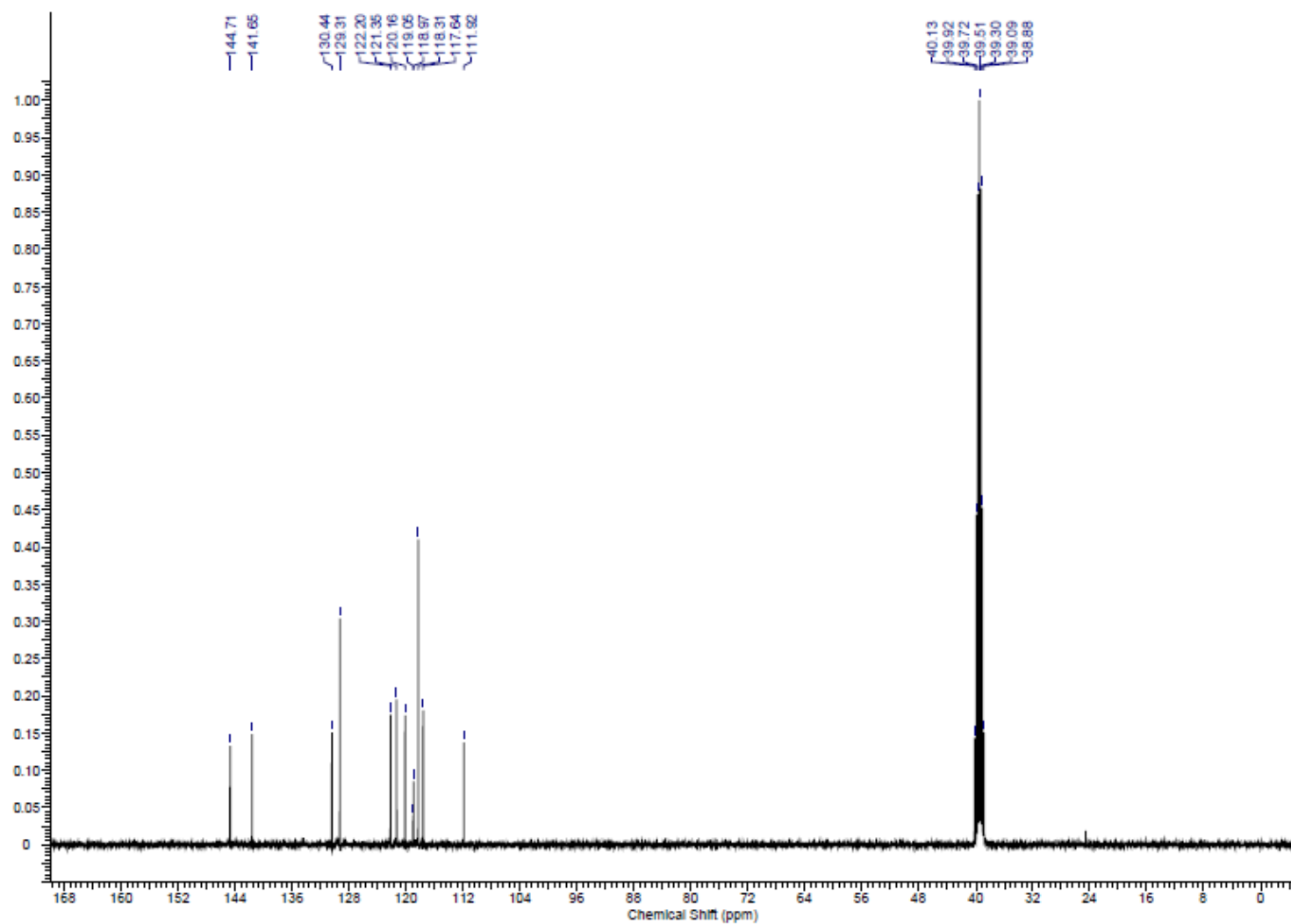


3-(Phenylamino)benzonitrile (3g).

¹H NMR Spectra

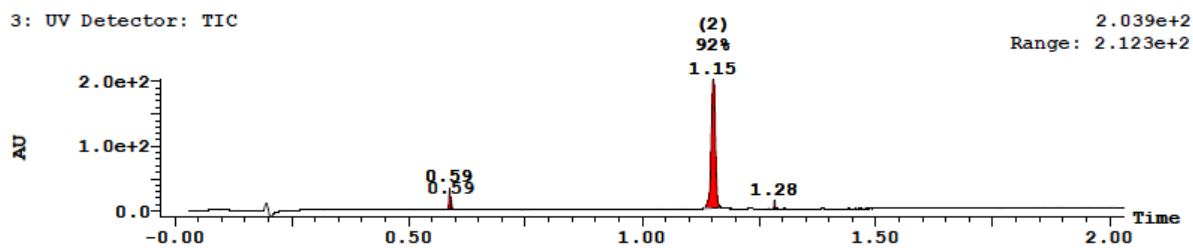


¹³C NMR Spectra



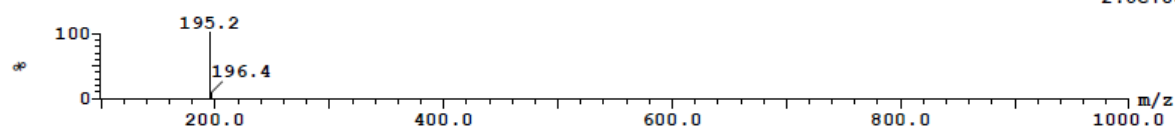
LCMS

3: UV Detector: TIC



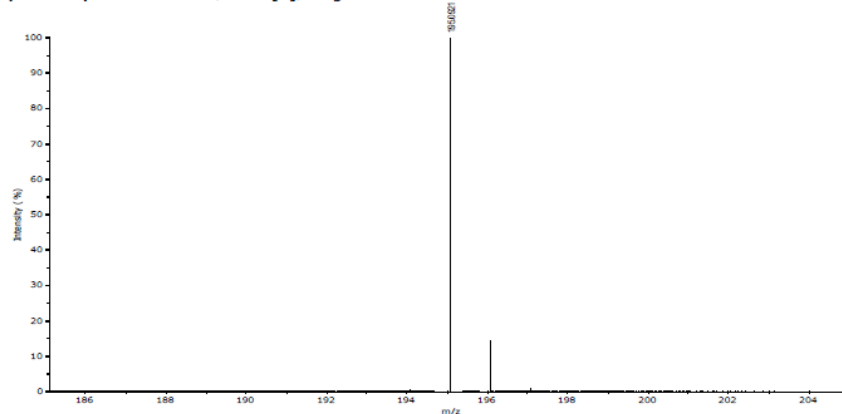
Peak Time
2 1.15
2: (Time: 1.15)

1:MS ES+
2.8e+007

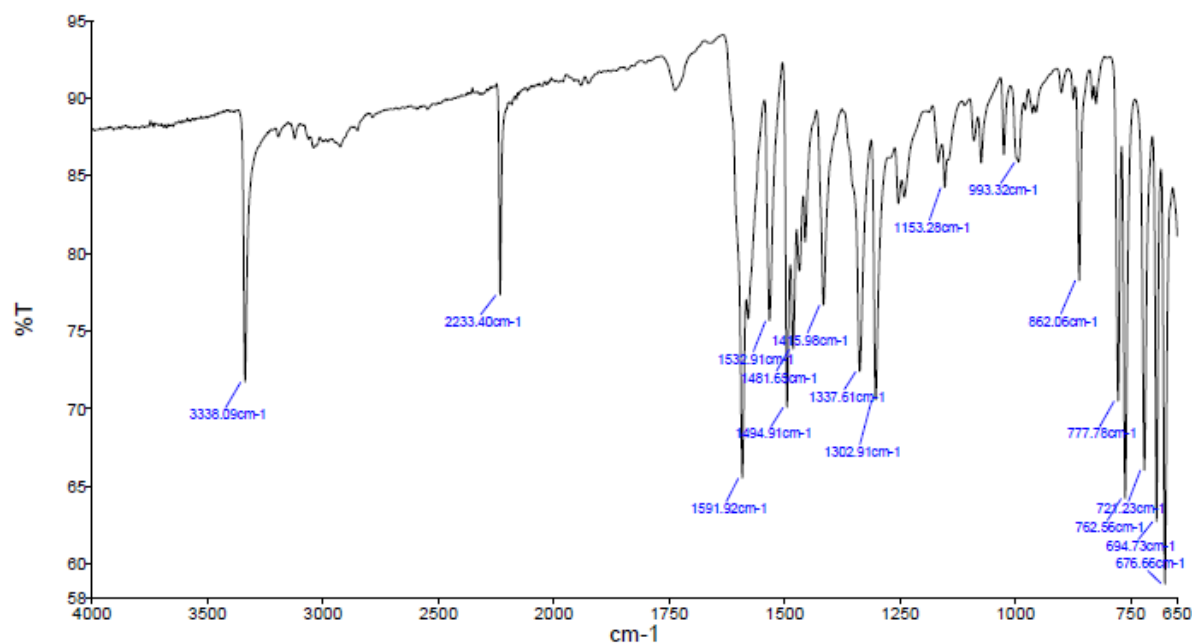


HRMS

Expanded Spectrum RT 3.66, Peak [1], Target Mass 195.0917

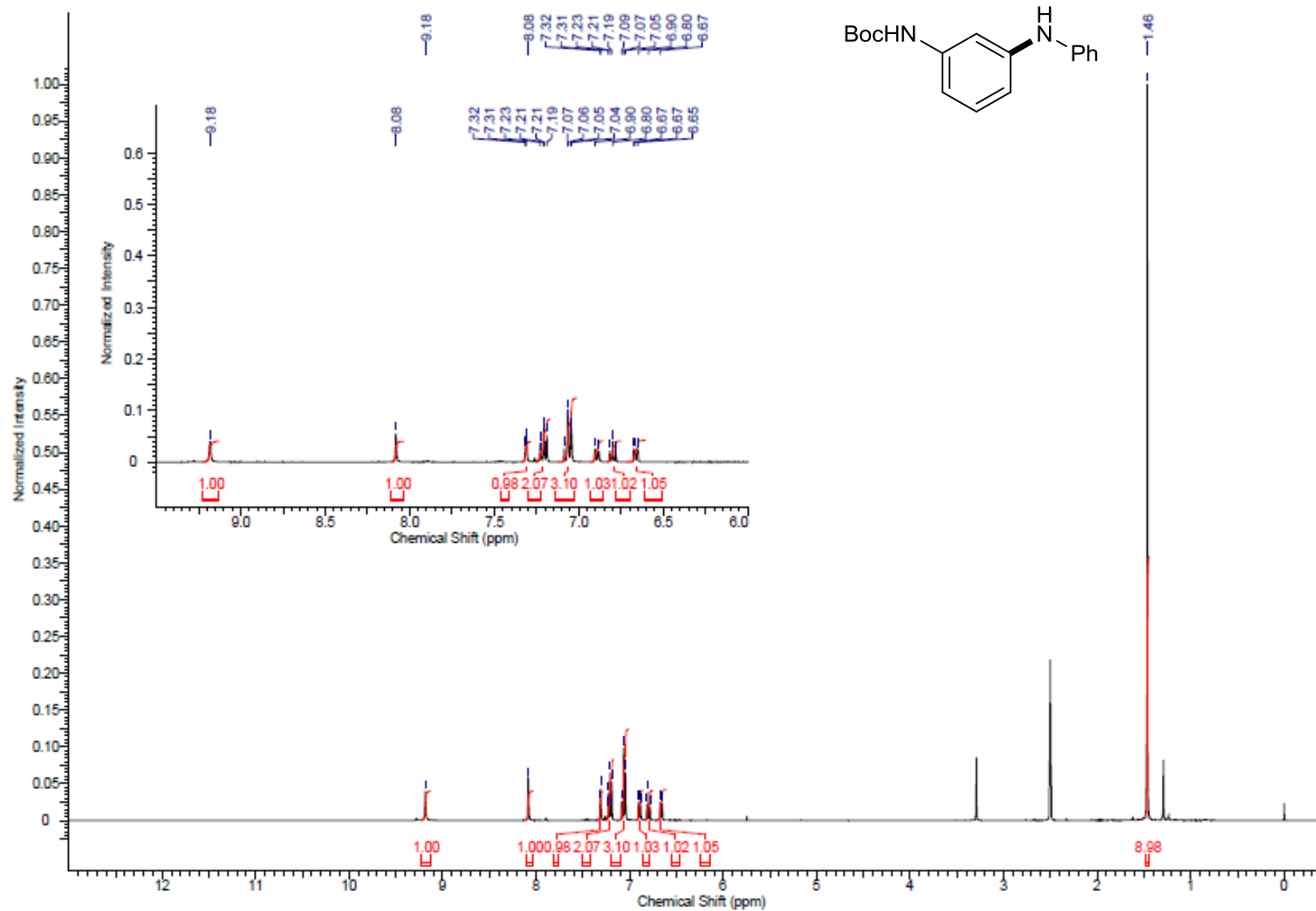


IR Spectra

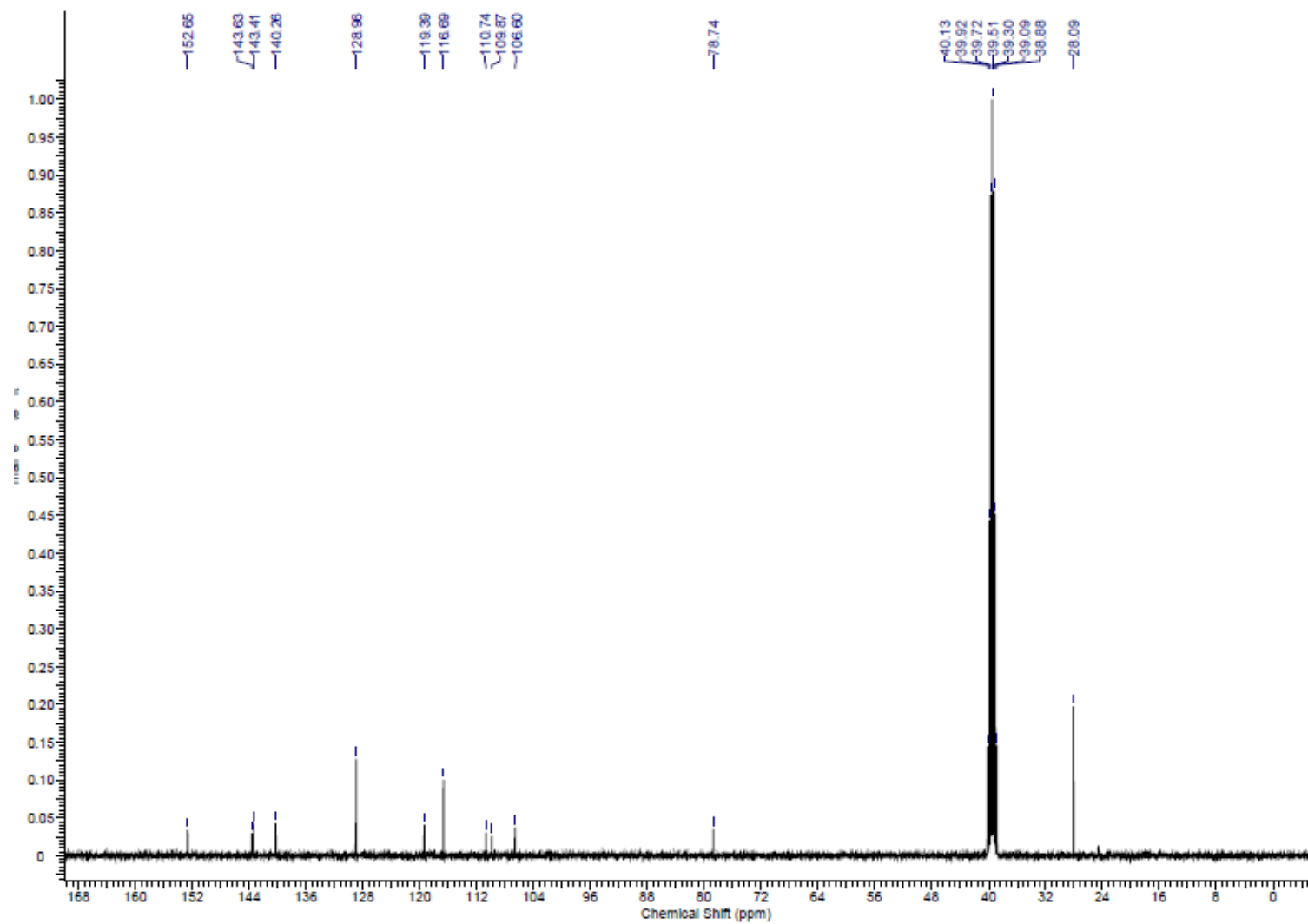


tert-Butyl-(3-(phenylamino)phenyl)carbamate (3h).

¹H NMR Spectra

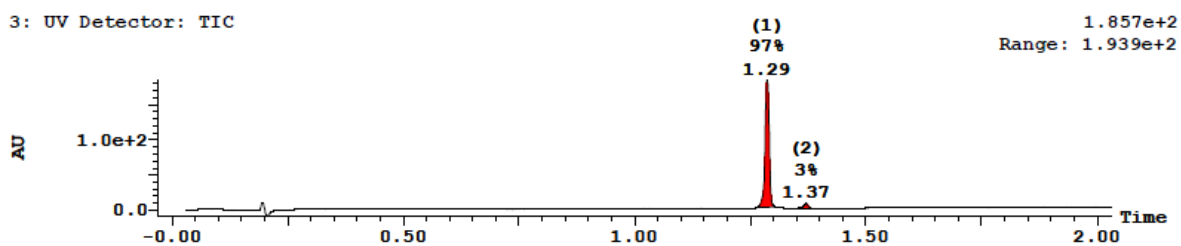


¹³C NMR Spectra



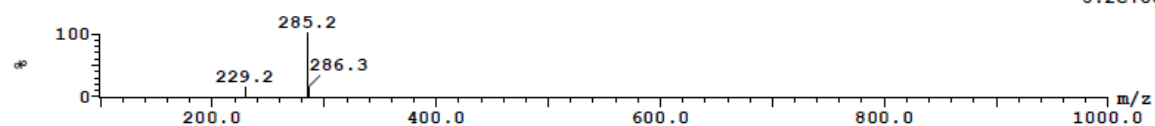
LCMS

3: UV Detector: TIC



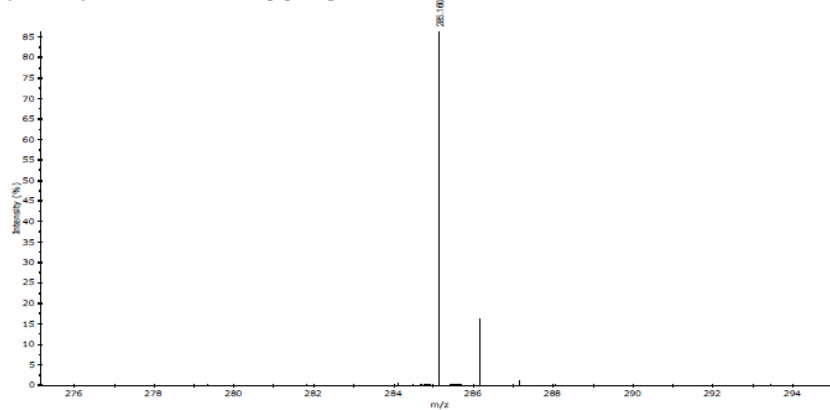
Peak Time
1 1.29
1: (Time: 1.29)

1: MS ES+
6.2e+007

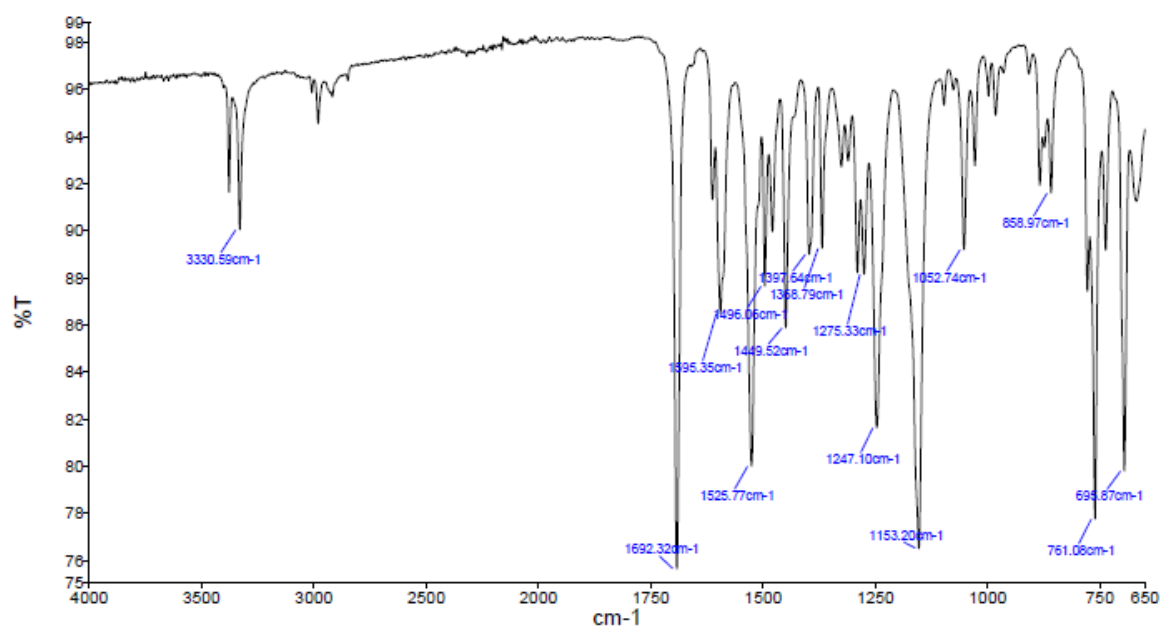


HRMS

Expanded Spectrum RT 4.45, Peak [1], Target Mass 285.1598

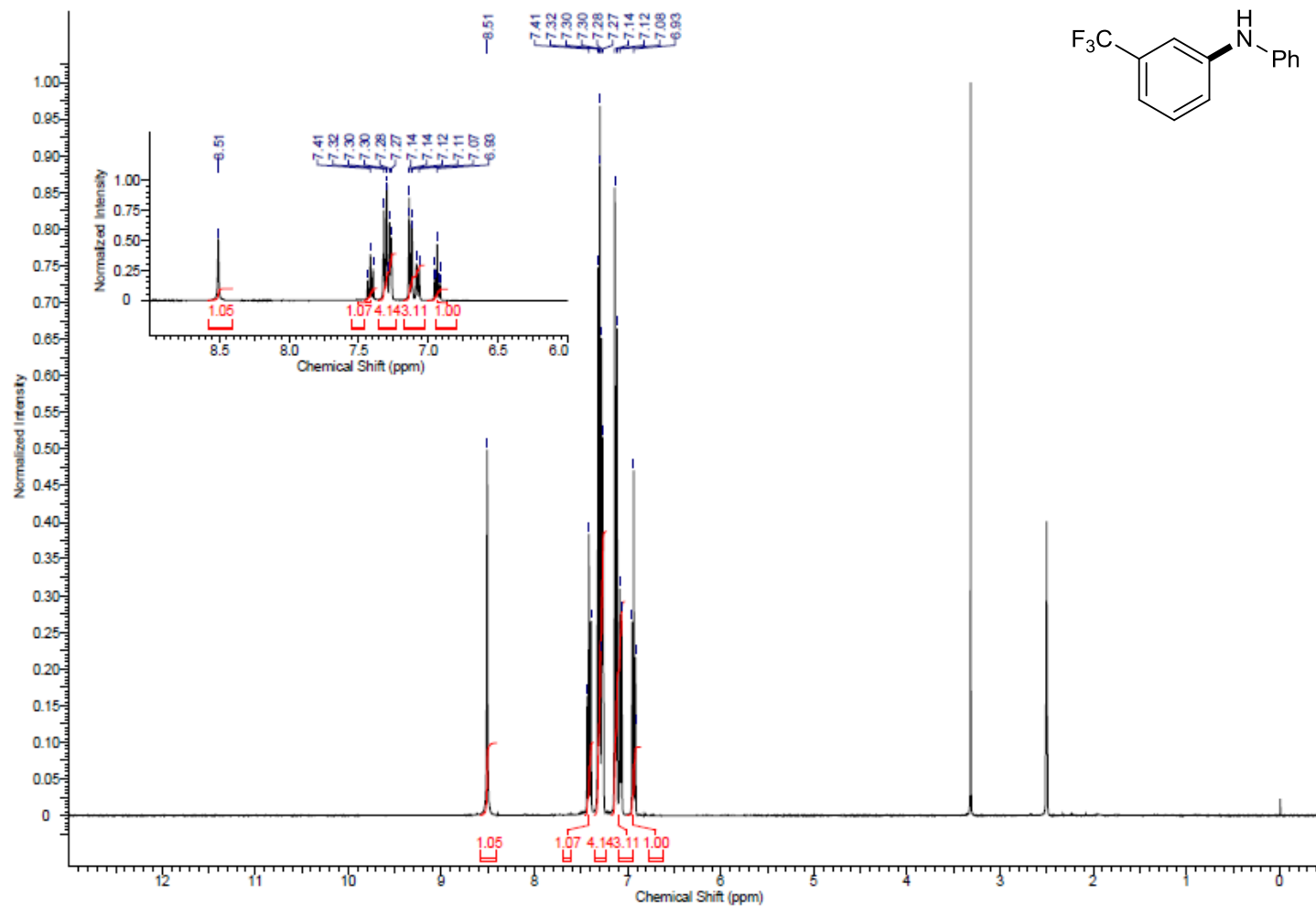


IR Spectra

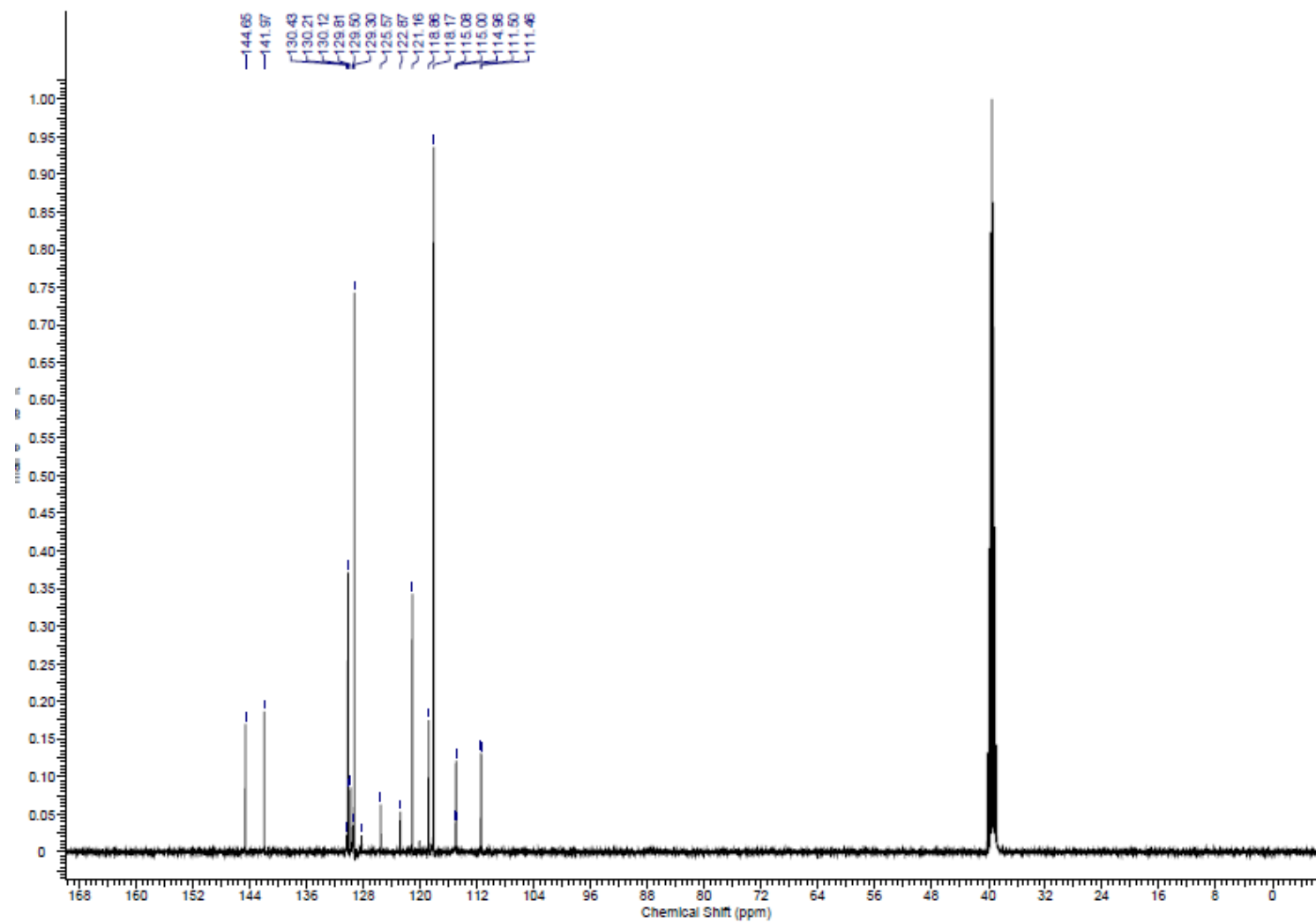


***N*-Phenyl-3-(trifluoromethyl)aniline (3i).**

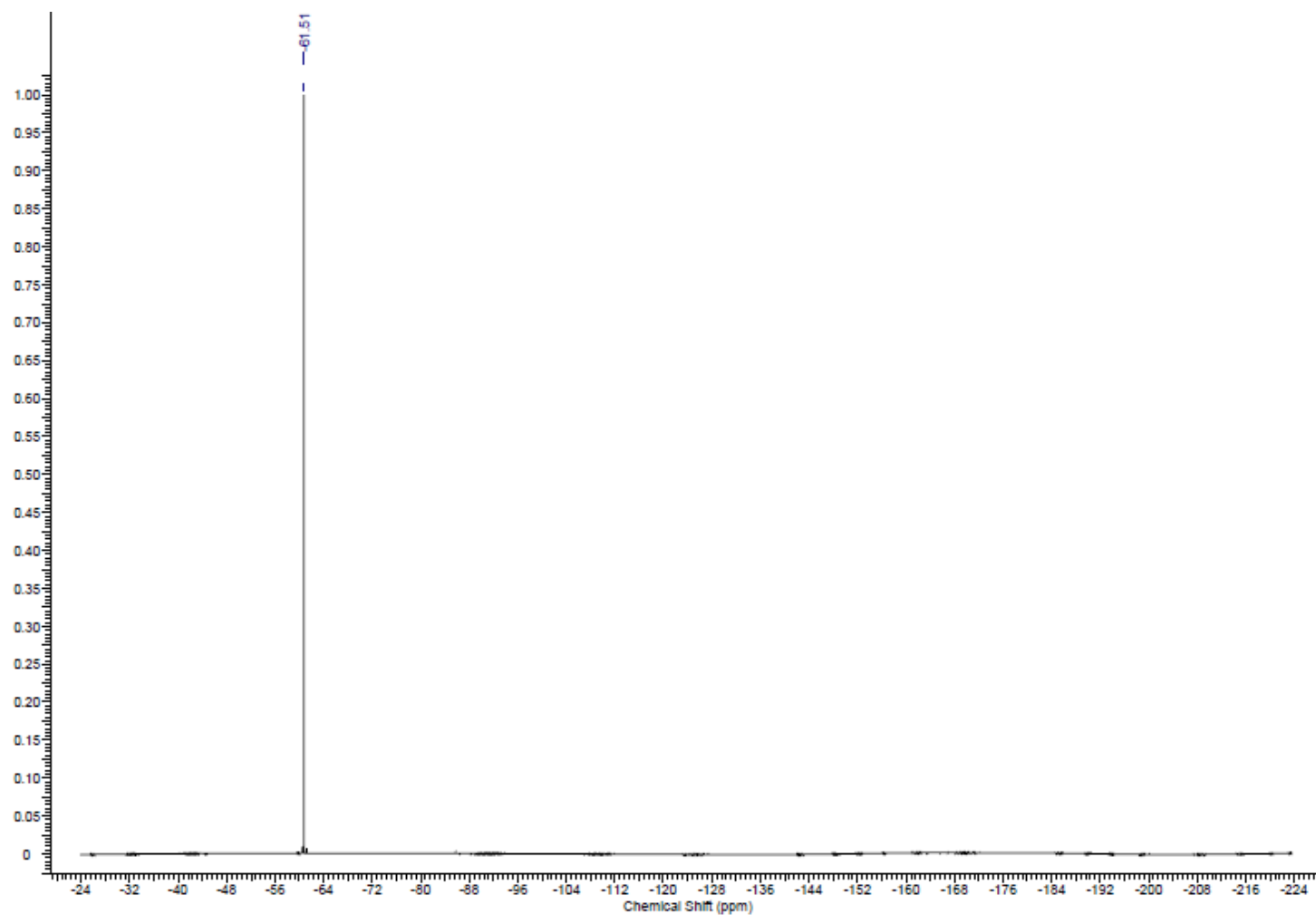
¹H NMR Spectra



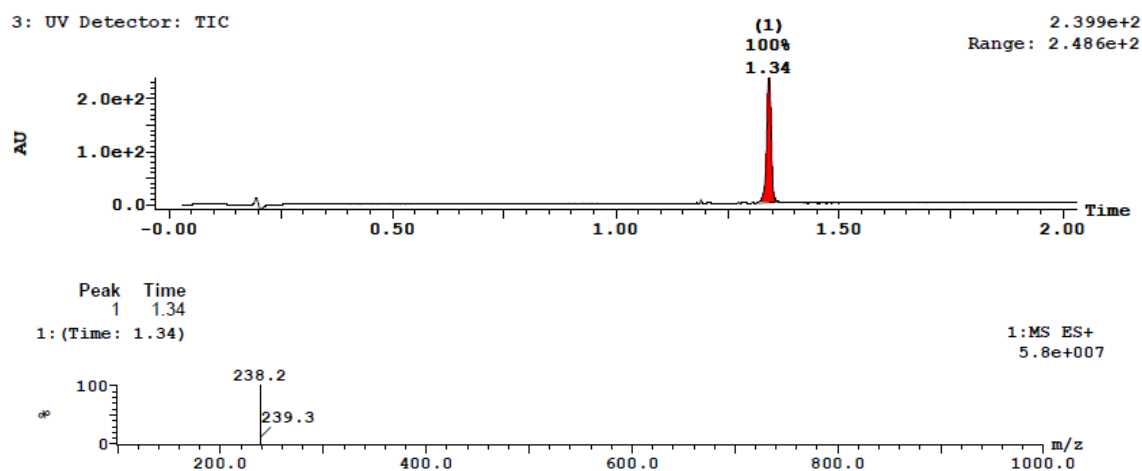
^{13}C NMR Spectra



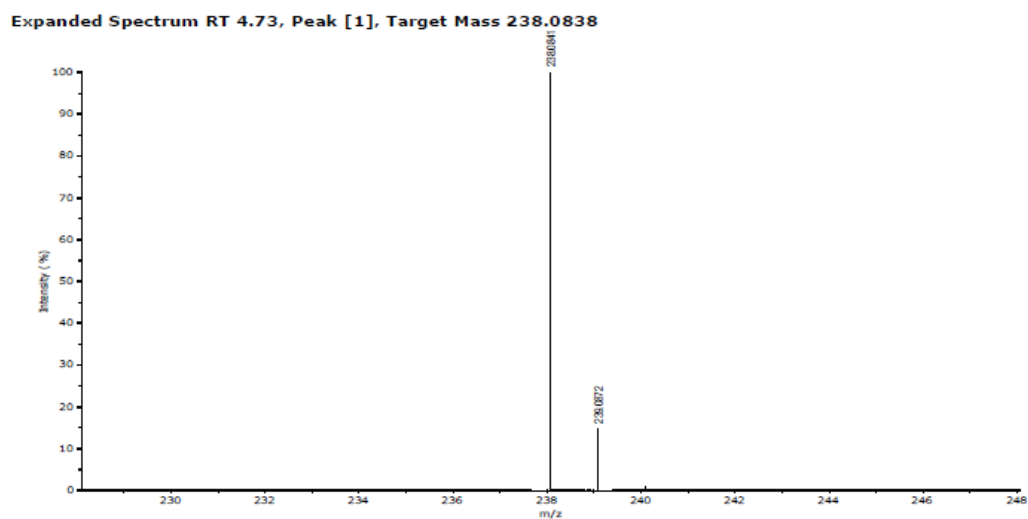
^{19}F NMR Spectra



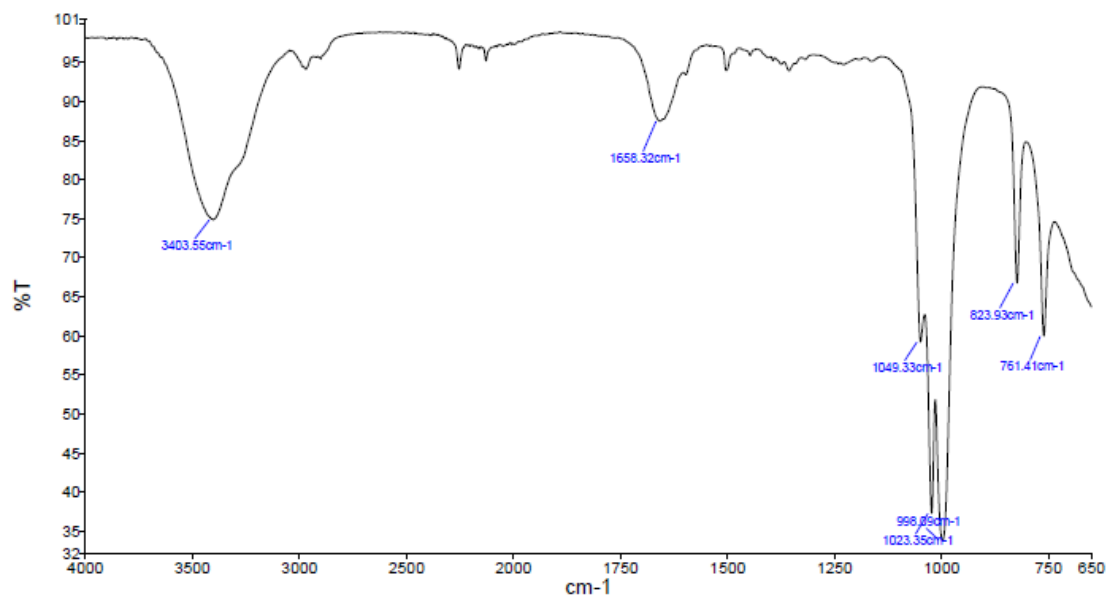
LCMS



HRMS

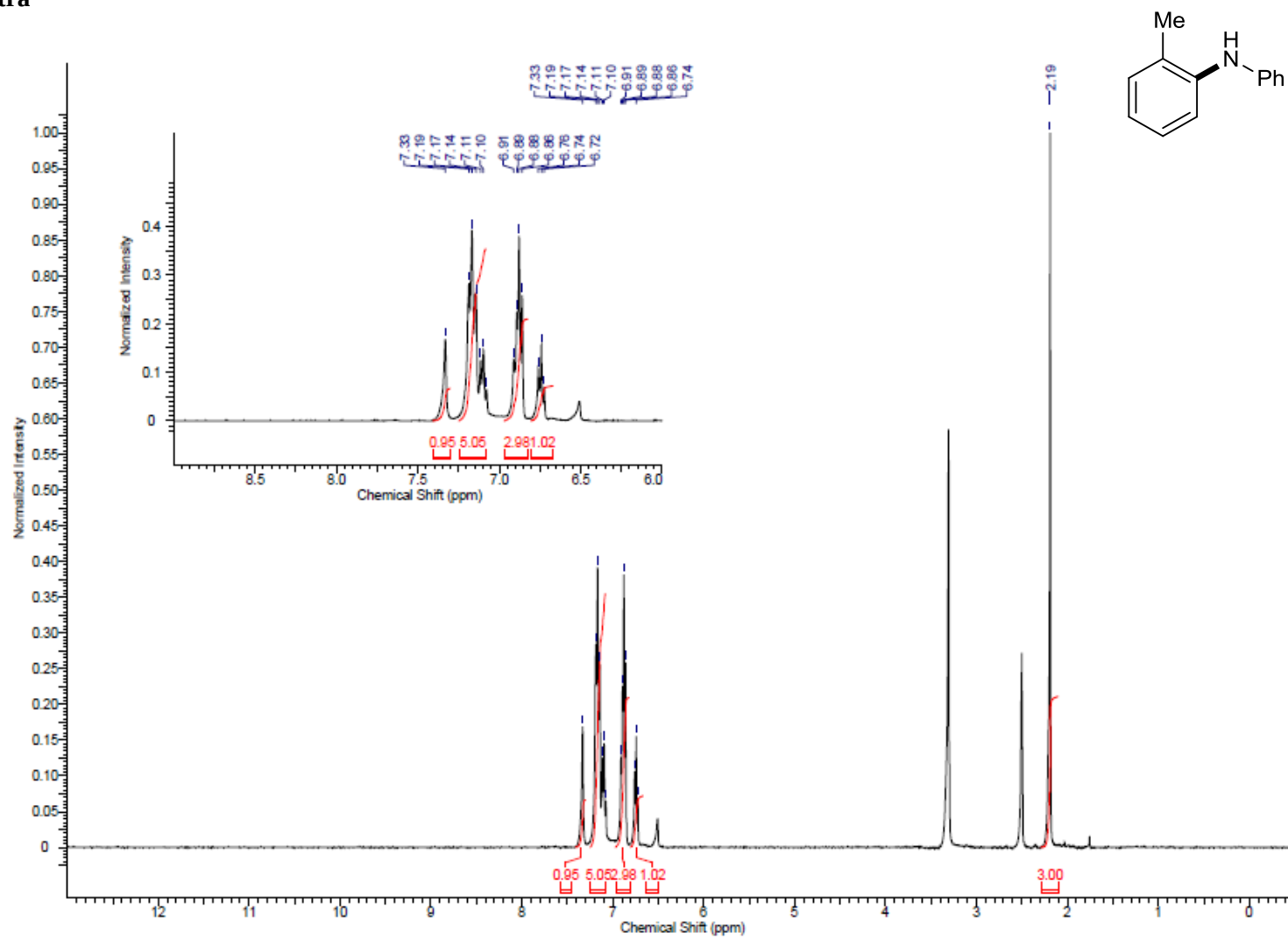


IR Spectra

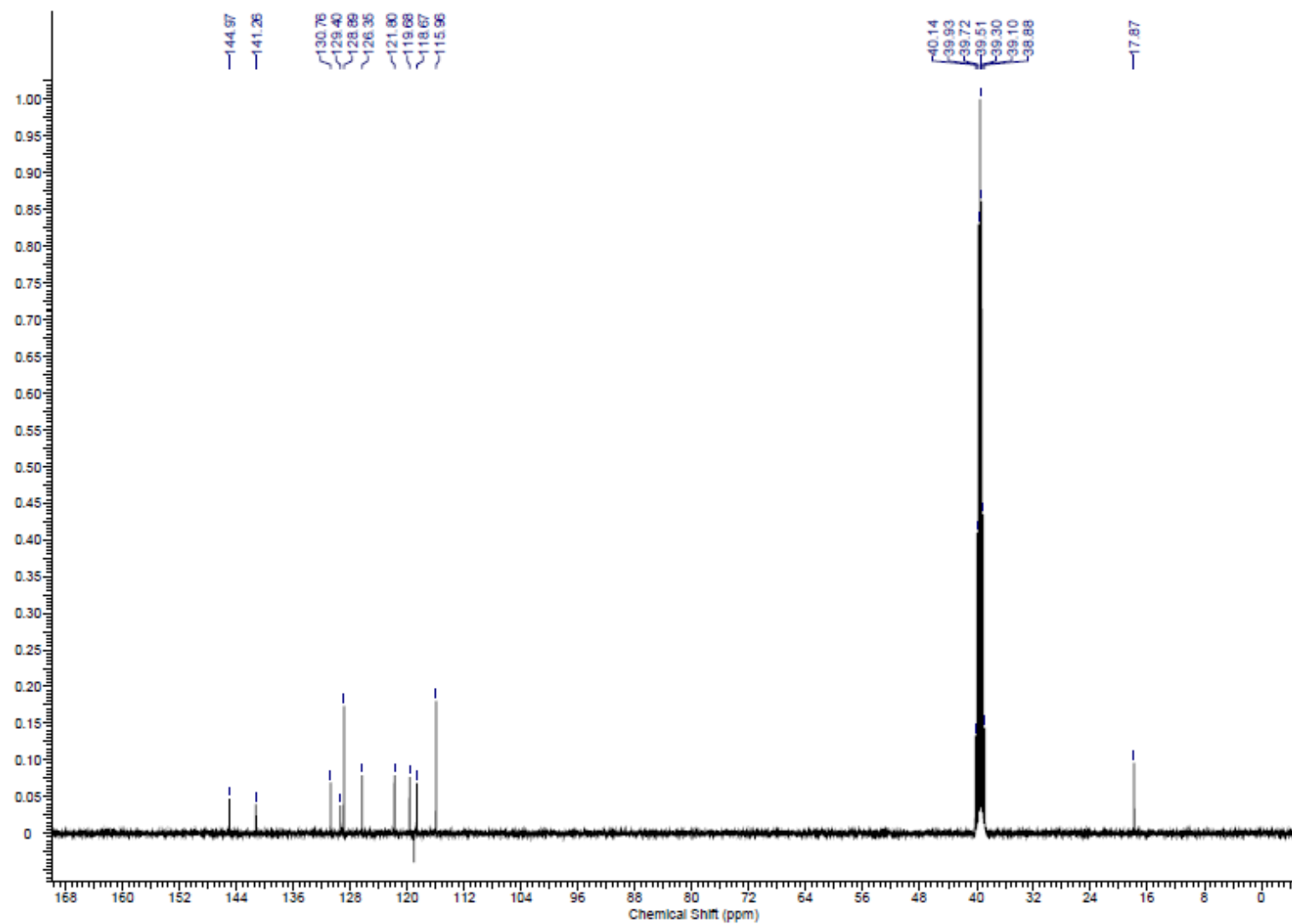


2-Methyl-N-phenylaniline (3j).

^1H NMR Spectra

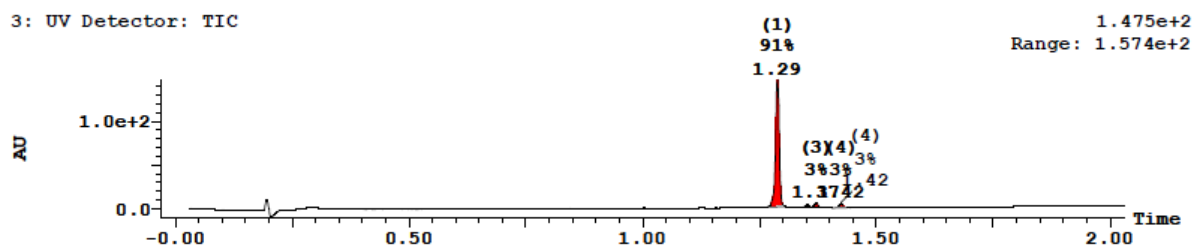


^{13}C NMR Spectra



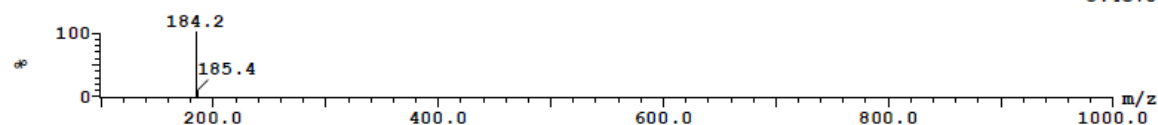
LCMS

3: UV Detector: TIC



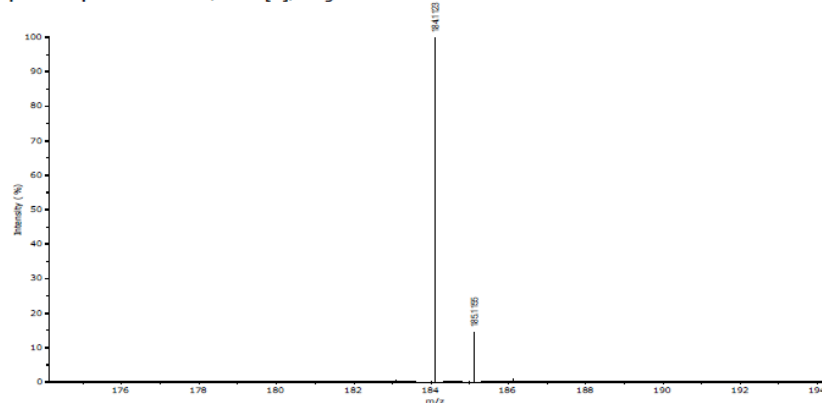
Peak Time
1 1.29
1: (Time: 1.29)

1: MS ES+
5.4e+007

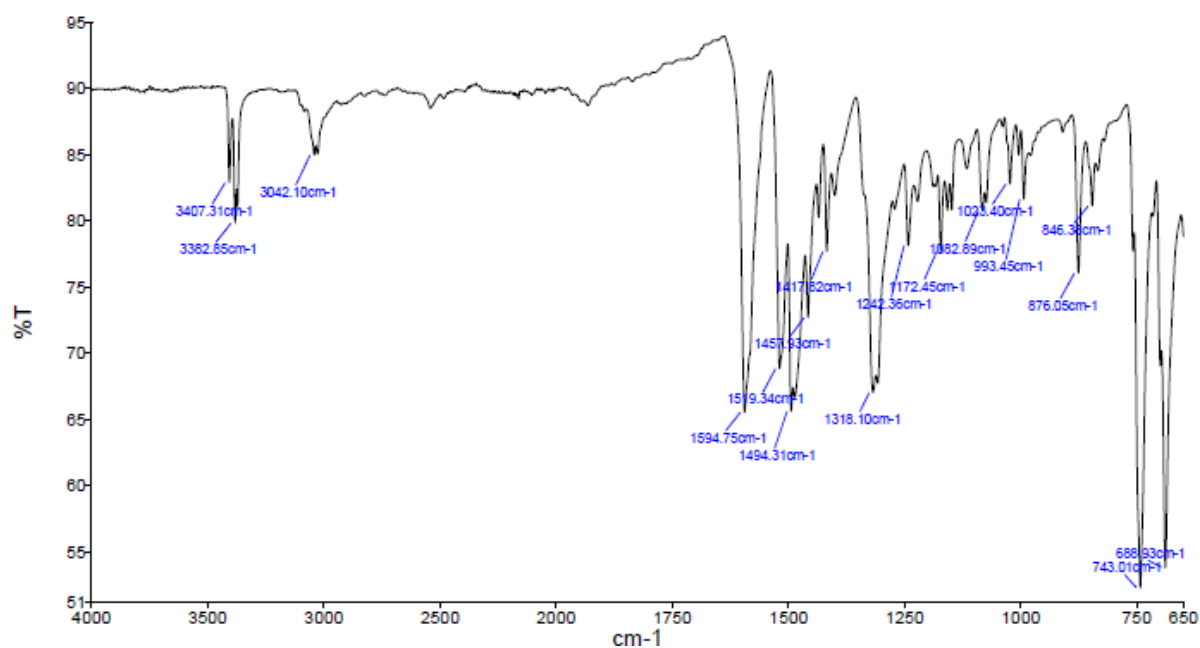


HRMS

Expanded Spectrum RT 4.35, Peak [1], Target Mass 184.1121

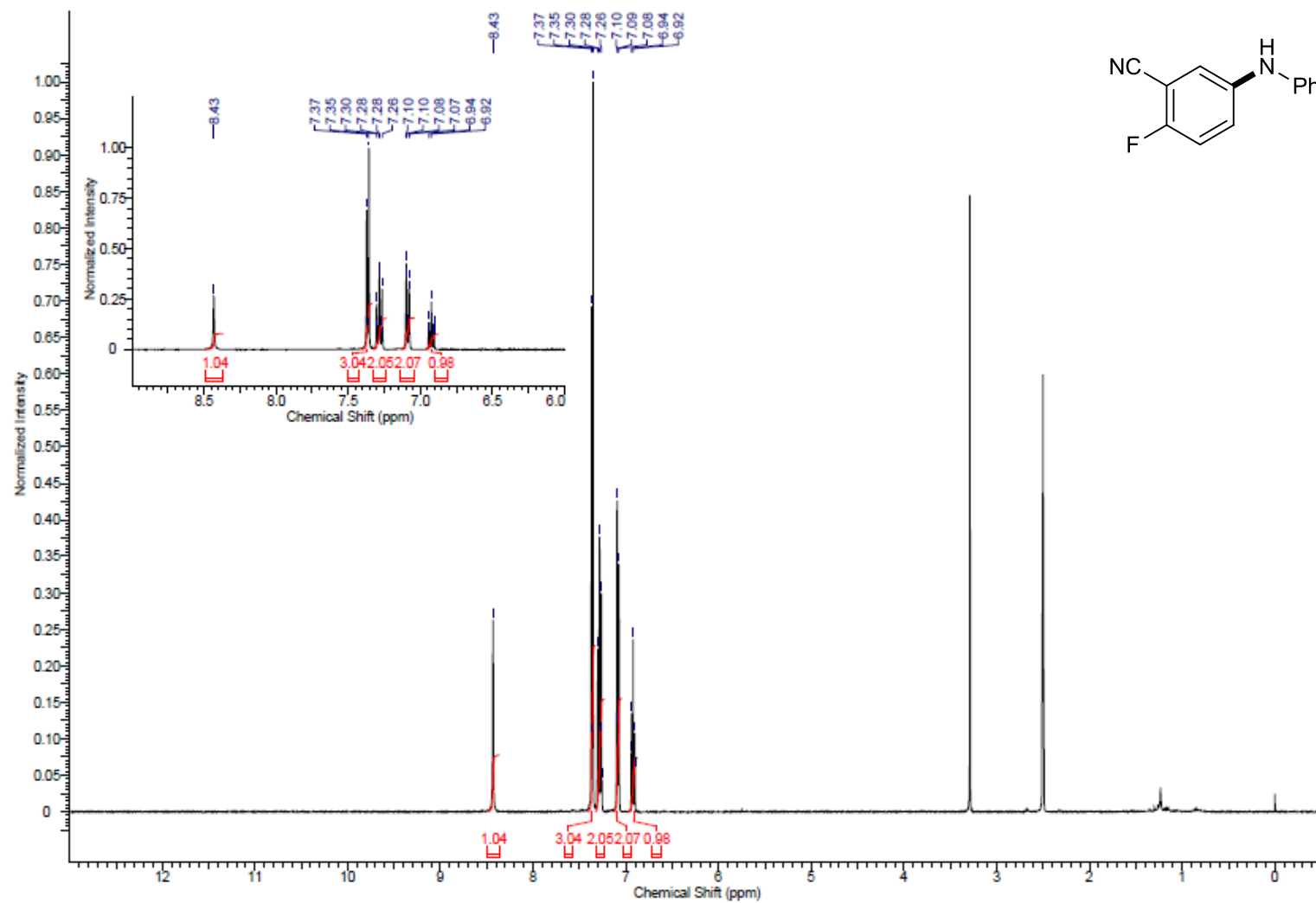


IR Spectra

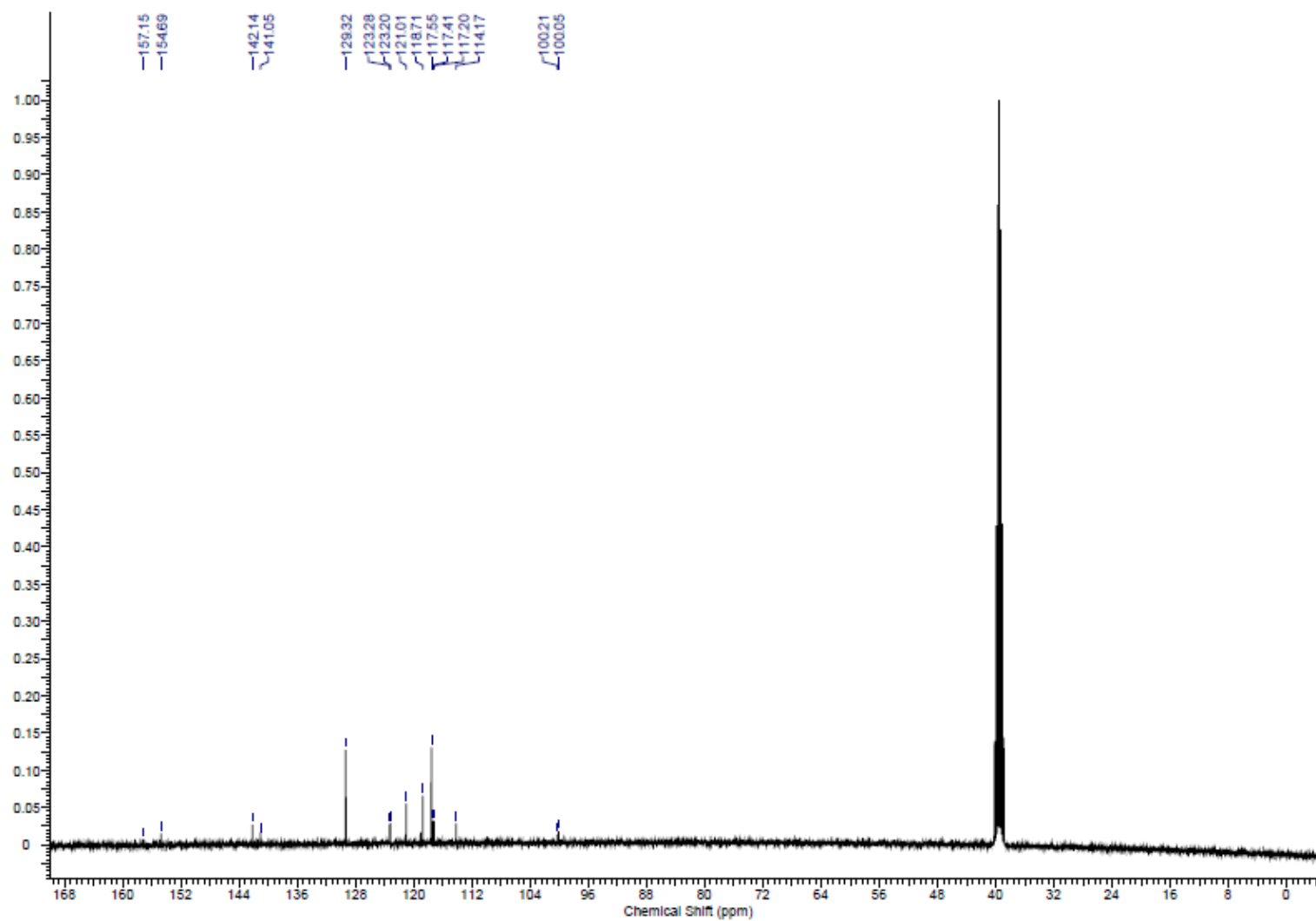


2-Fluoro-5-(phenylamino)benzonitrile (3k).

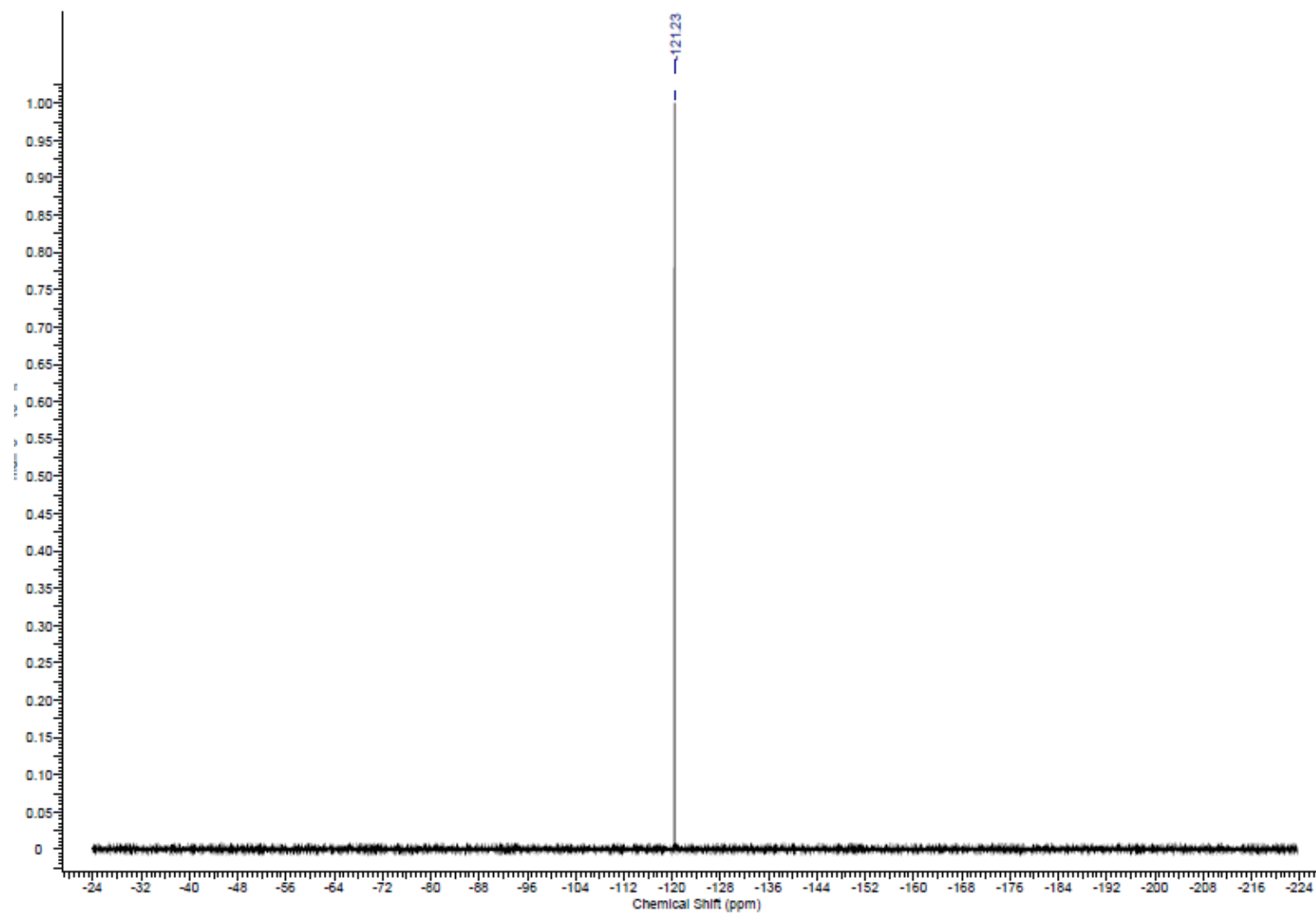
^1H NMR Spectra



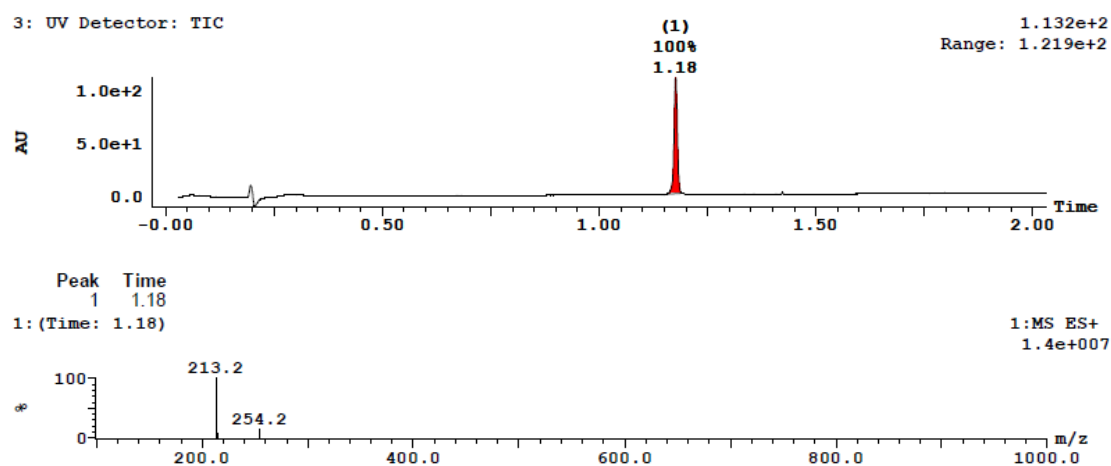
¹³C NMR Spectra



¹⁹F NMR Spectra

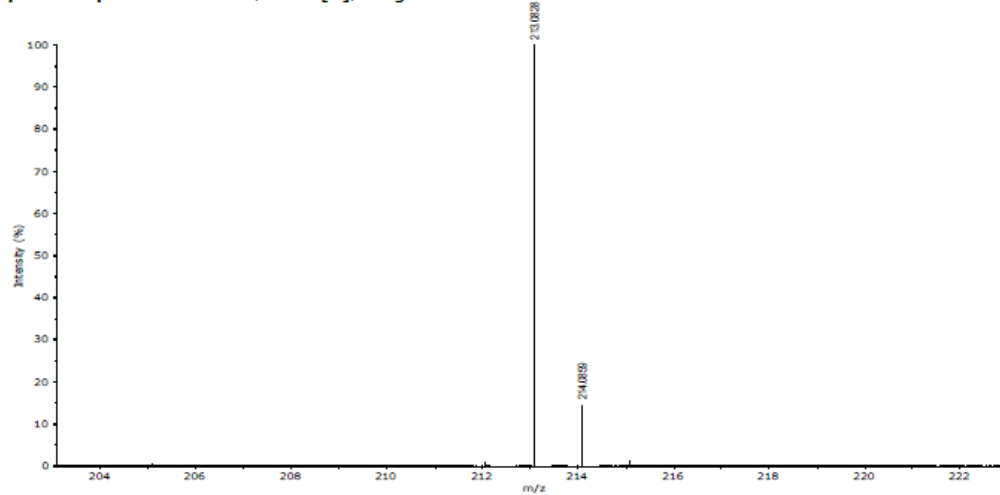


LCMS

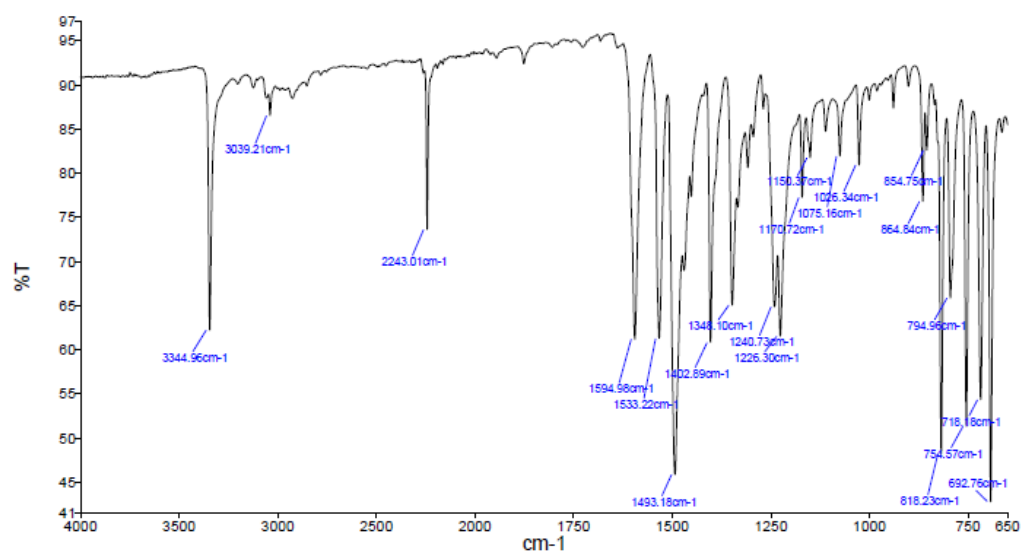


HRMS

Expanded Spectrum RT 3.83, Peak [1], Target Mass 213.0823

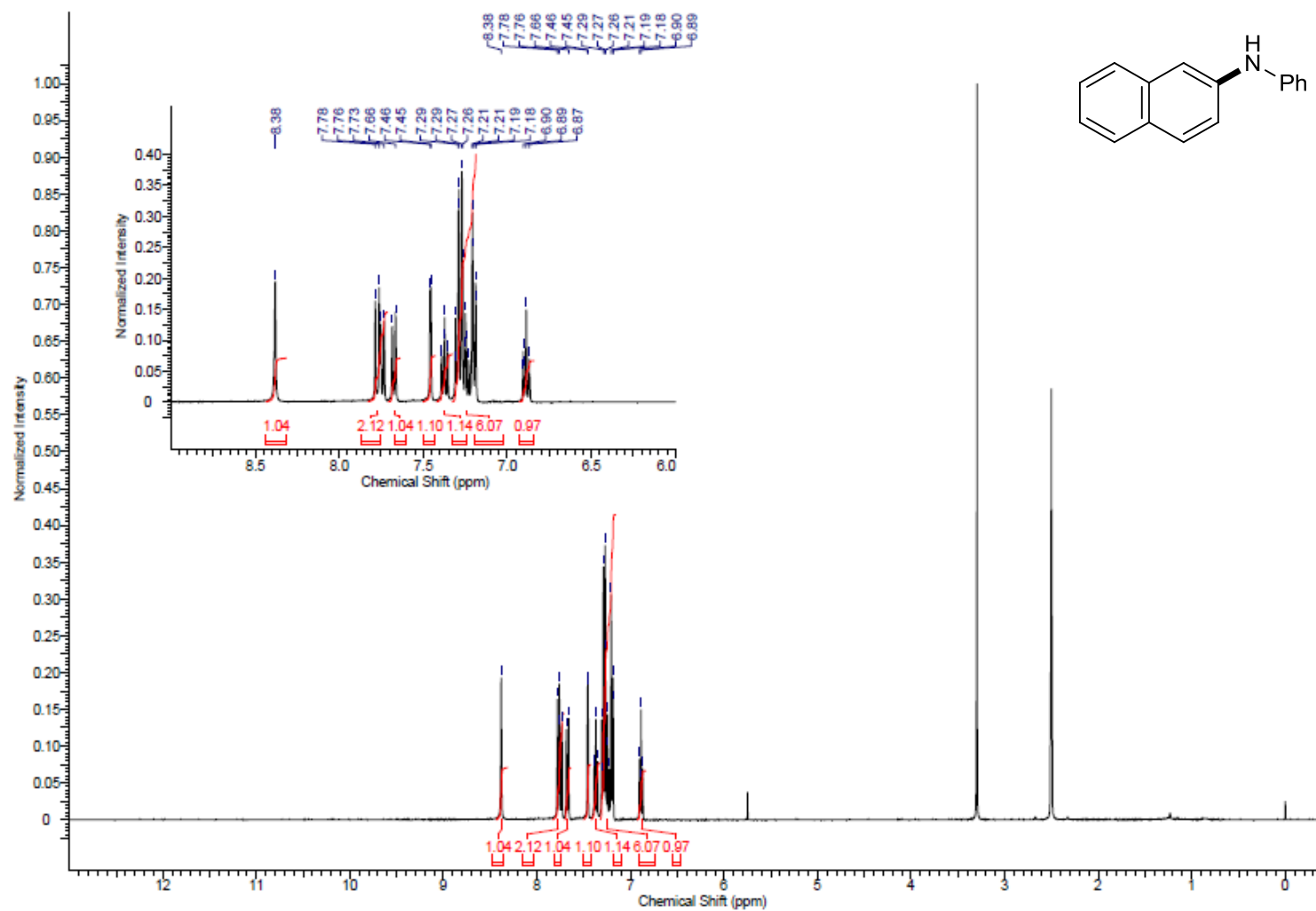


IR Spectra

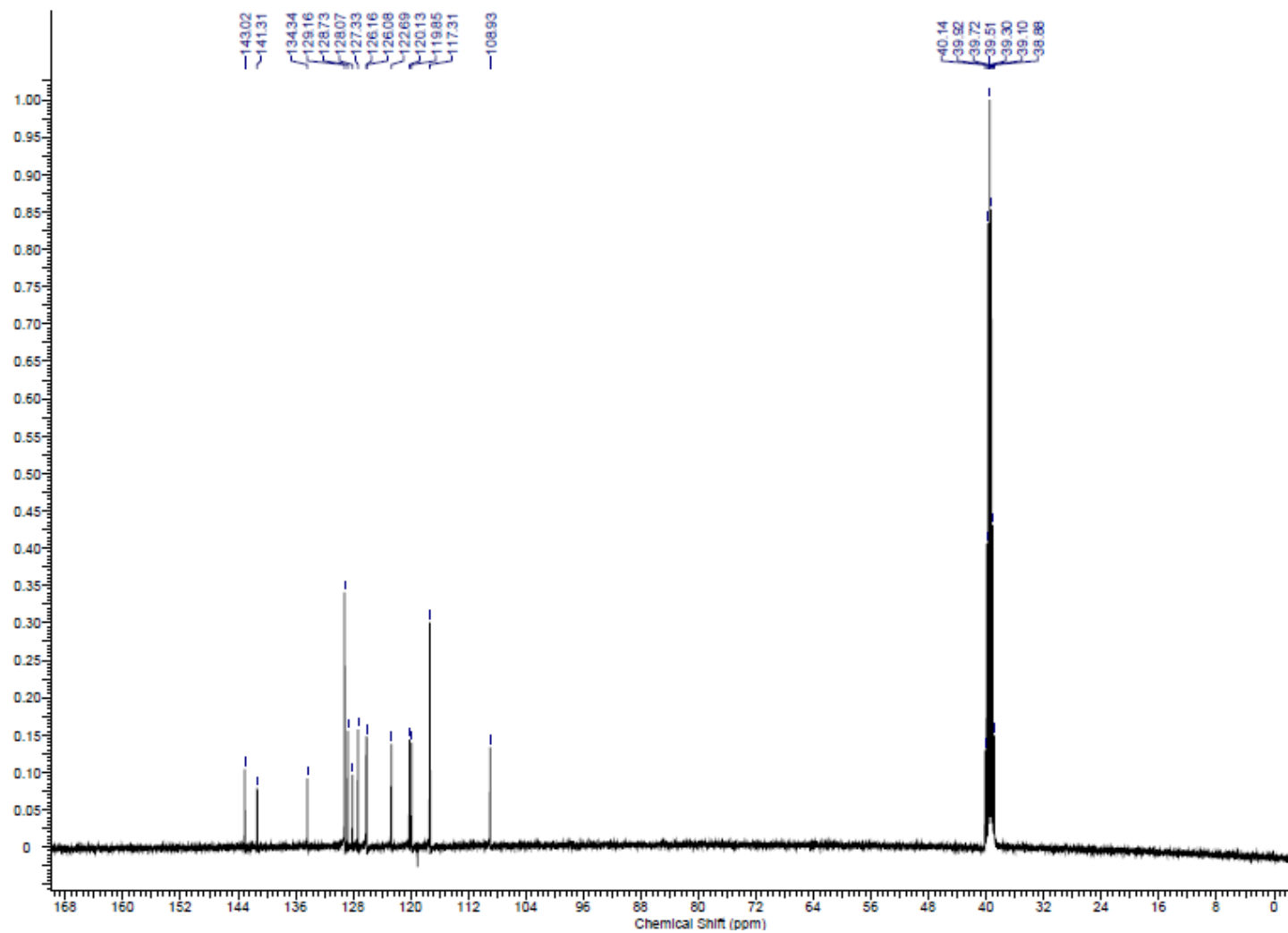


***N*-Phenylnaphthalen-2-amine (3l).**

¹H NMR Spectra

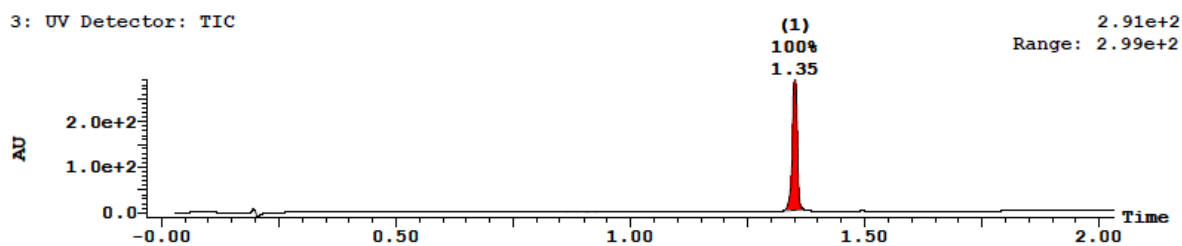


¹³C NMR Spectra



LCMS

3: UV Detector: TIC

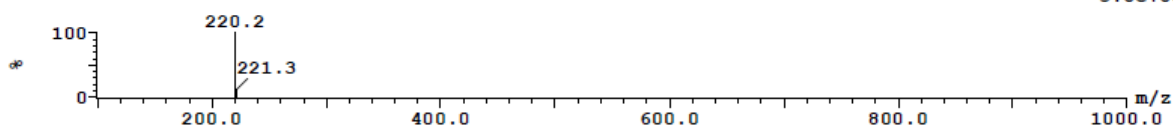


Peak Time
1 1.35

1: (Time: 1.35)

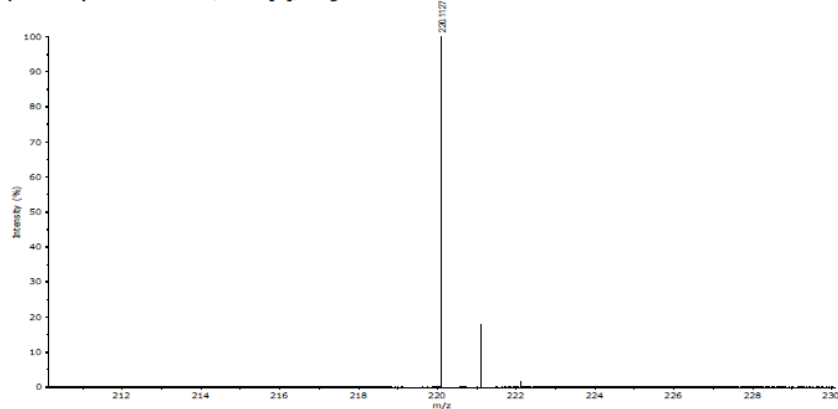
1: MS ES+

5.0e+007

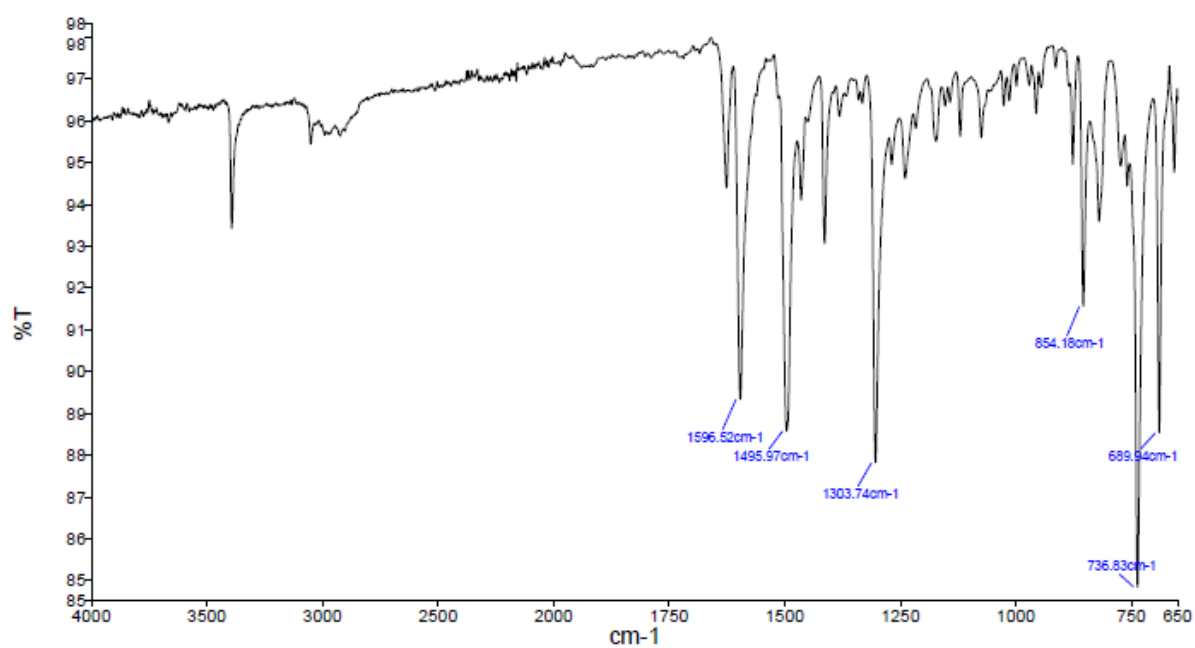


HRMS

Expanded Spectrum RT 4.67, Peak [1], Target Mass 220.1121

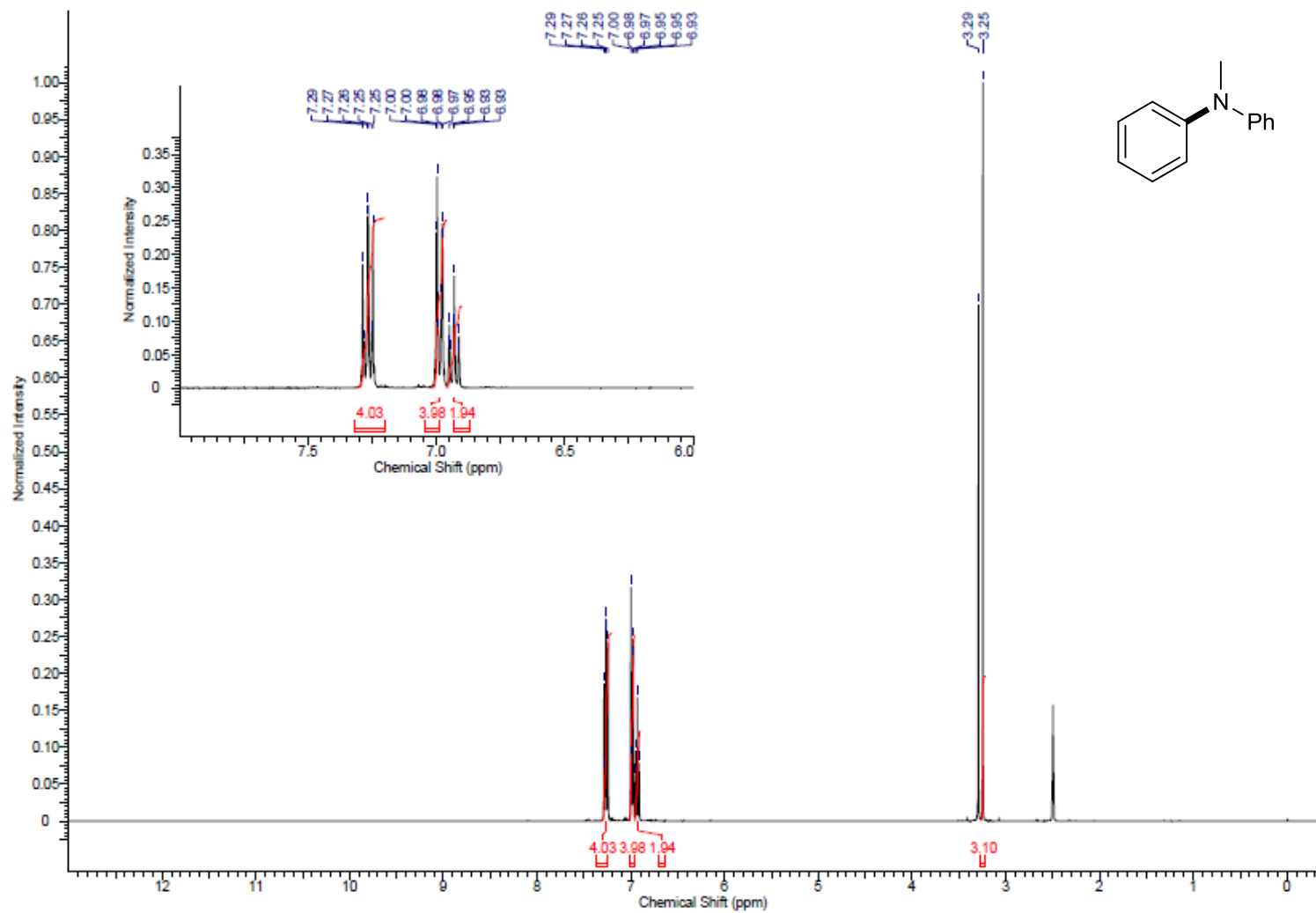


IR Spectra

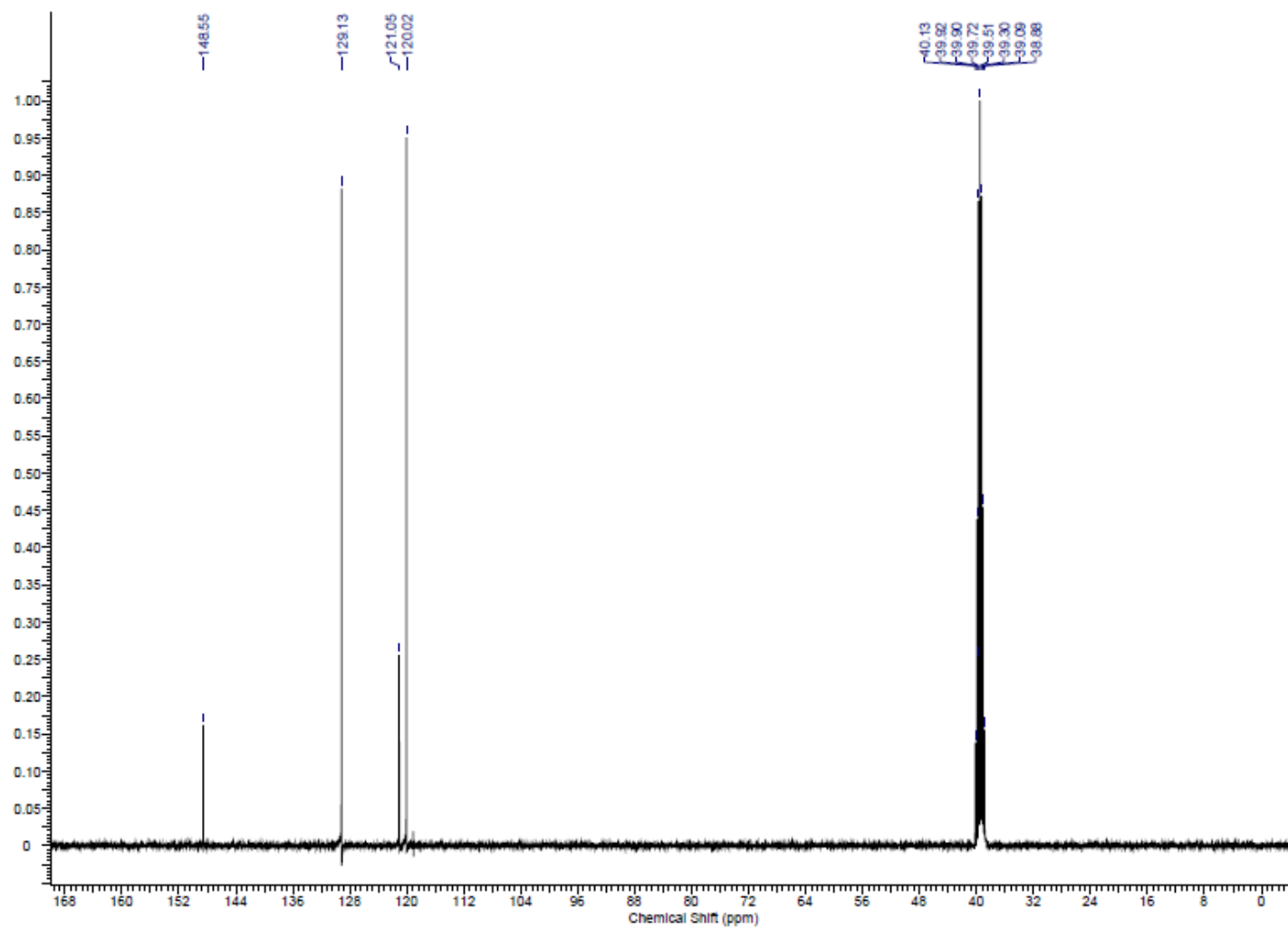


***N*-Methyl-*N*-phenylaniline (3m).**

¹H NMR Spectra

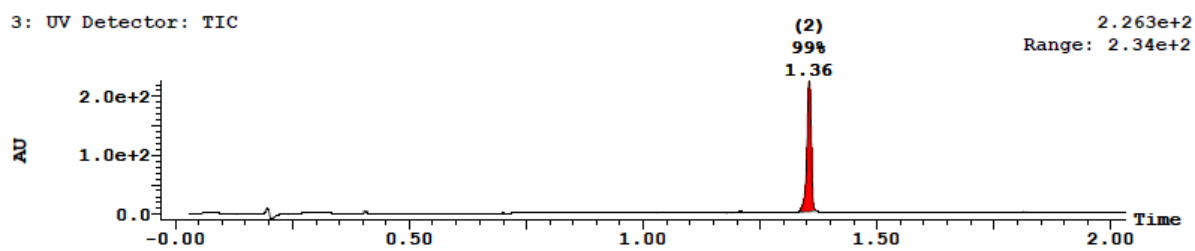


¹³C NMR Spectra



LCMS

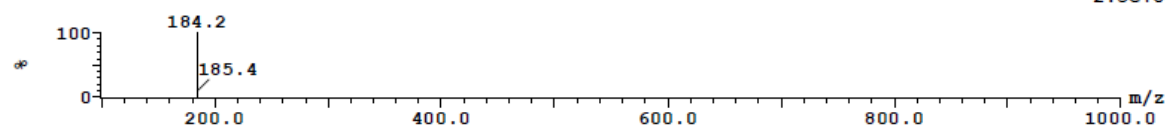
3: UV Detector: TIC



Peak Time
2 1.36

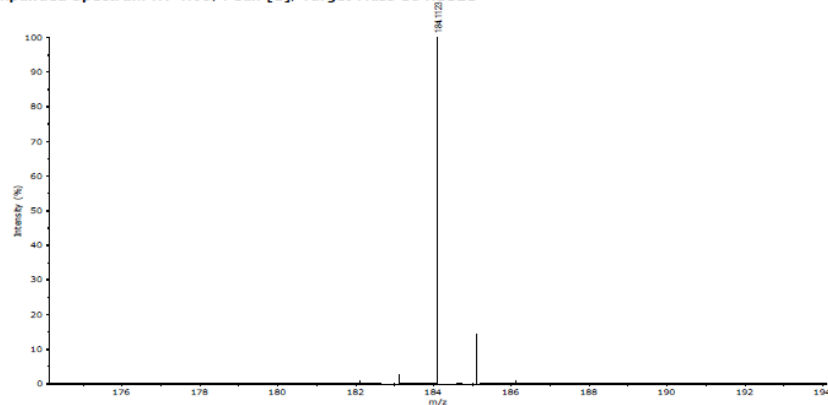
2: (Time: 1.36)

1:MS ES+
2.5e+007

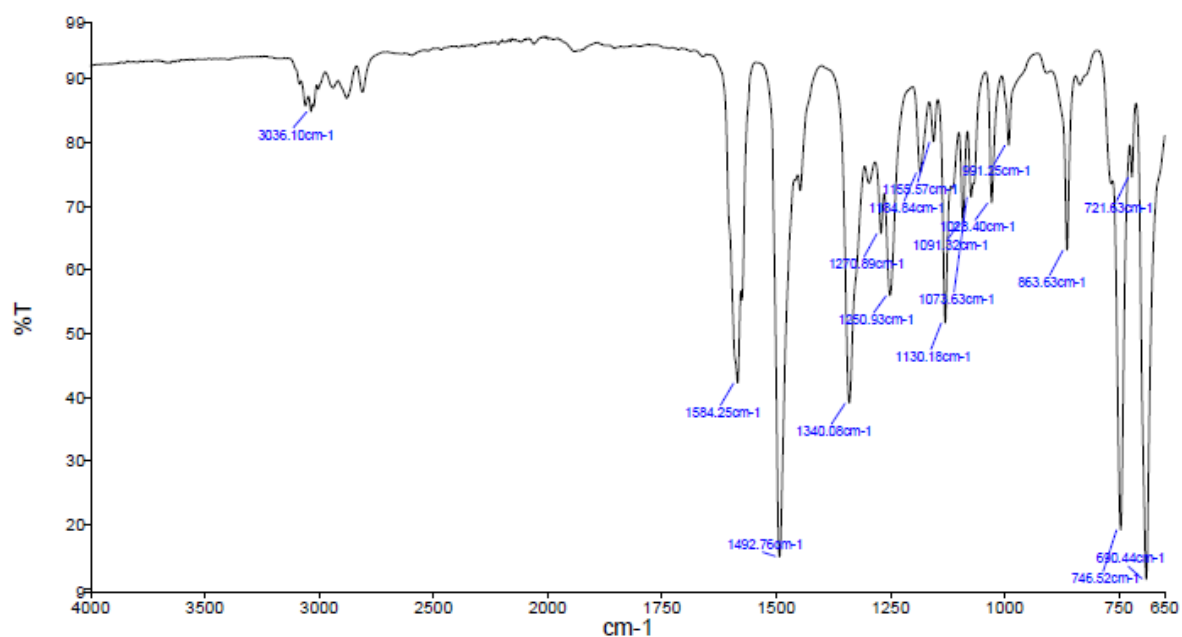


HRMS

Expanded Spectrum RT 4.65, Peak [1], Target Mass 184.1121

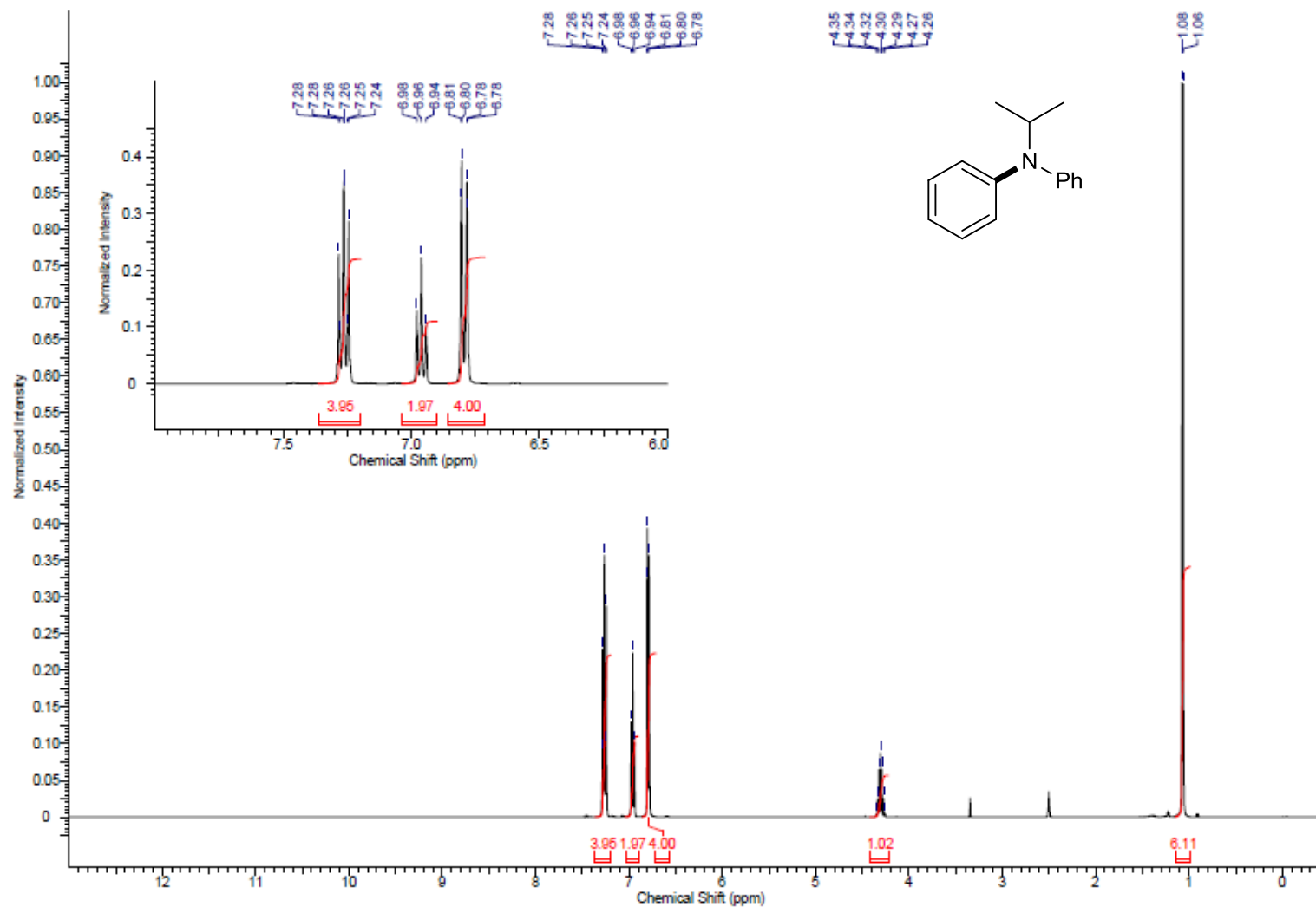


IR Spectra

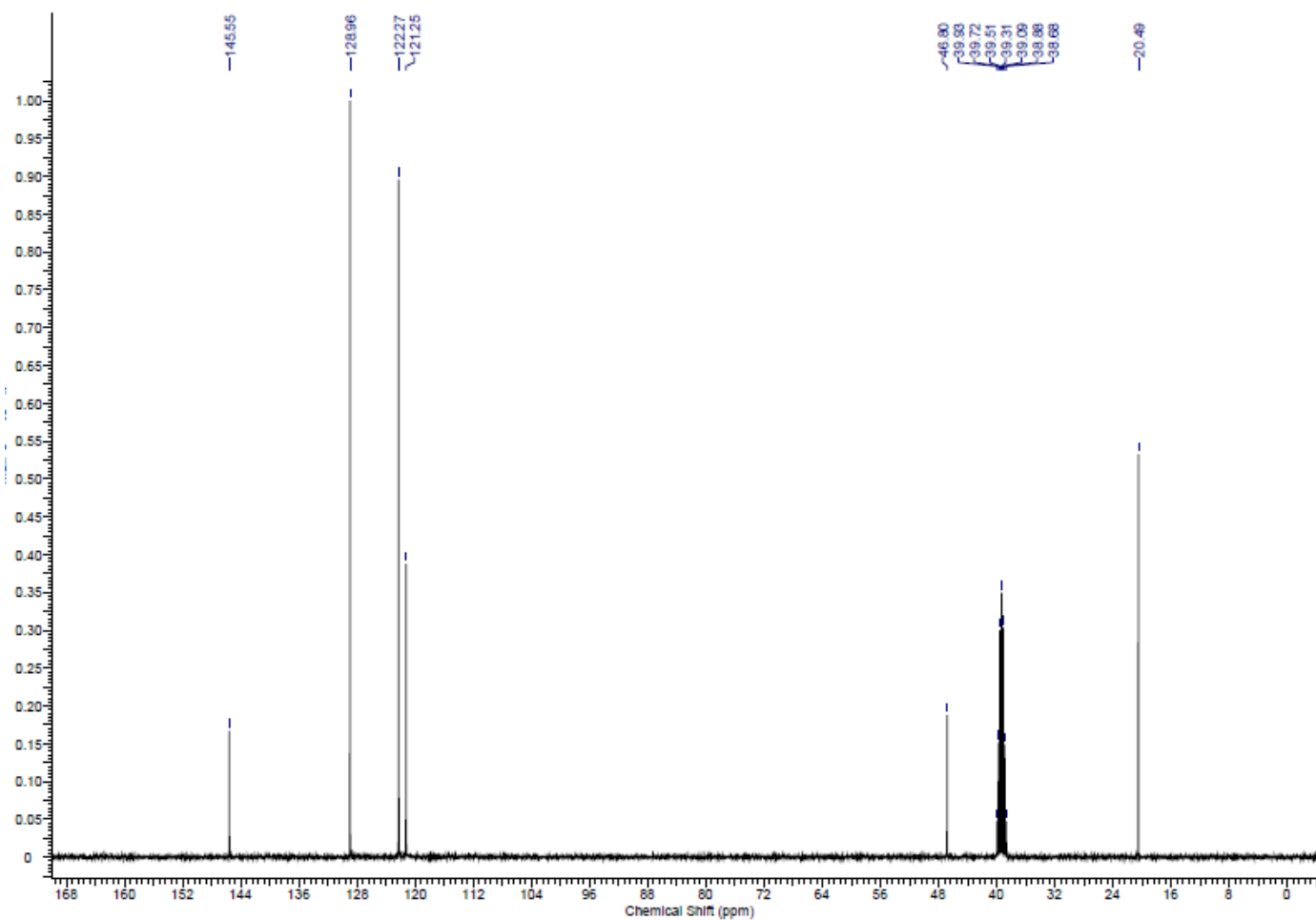


***N*-Isopropyl-*N*-phenylaniline (3n).**

¹H NMR Spectra

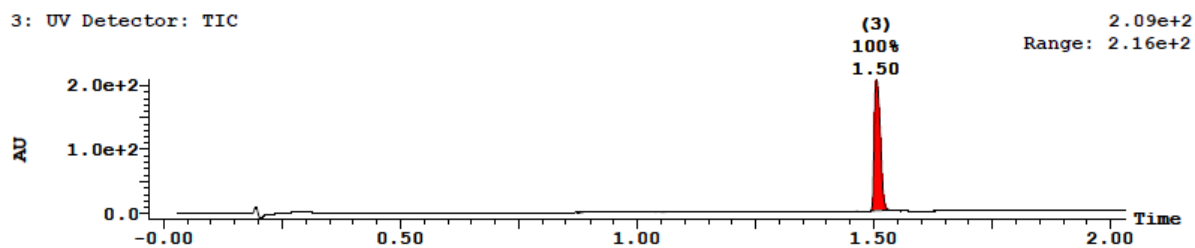


^{13}C NMR Spectra



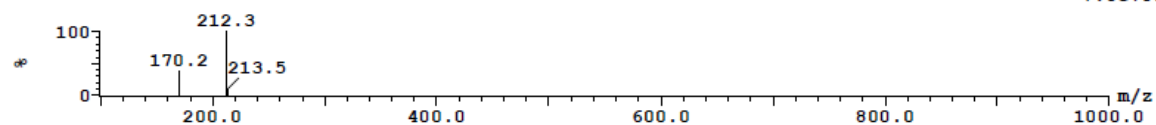
LCMS

3: UV Detector: TIC



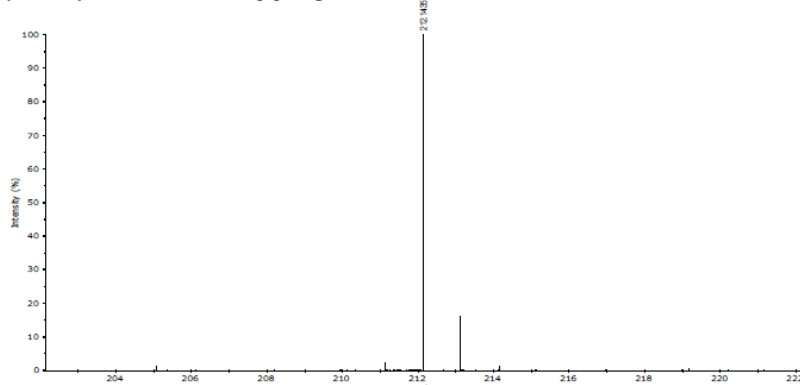
Peak Time
3 1.50
3: (Time: 1.50)

1: MS ES+
7.0e+007

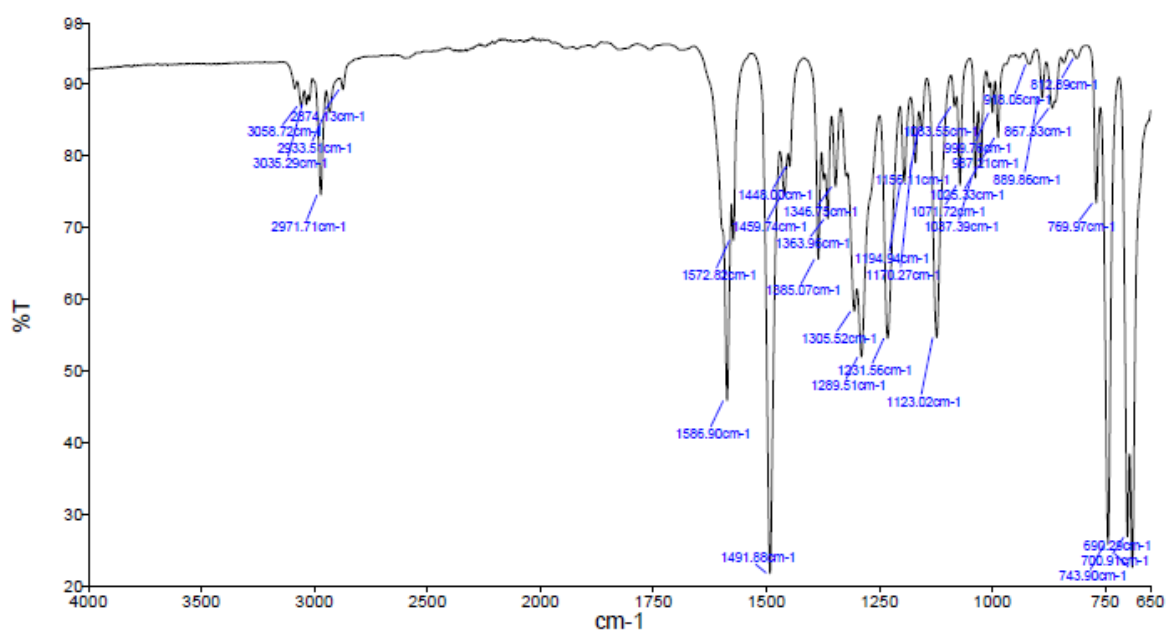


HRMS

Expanded Spectrum RT 5.31, Peak [1], Target Mass 212.1434

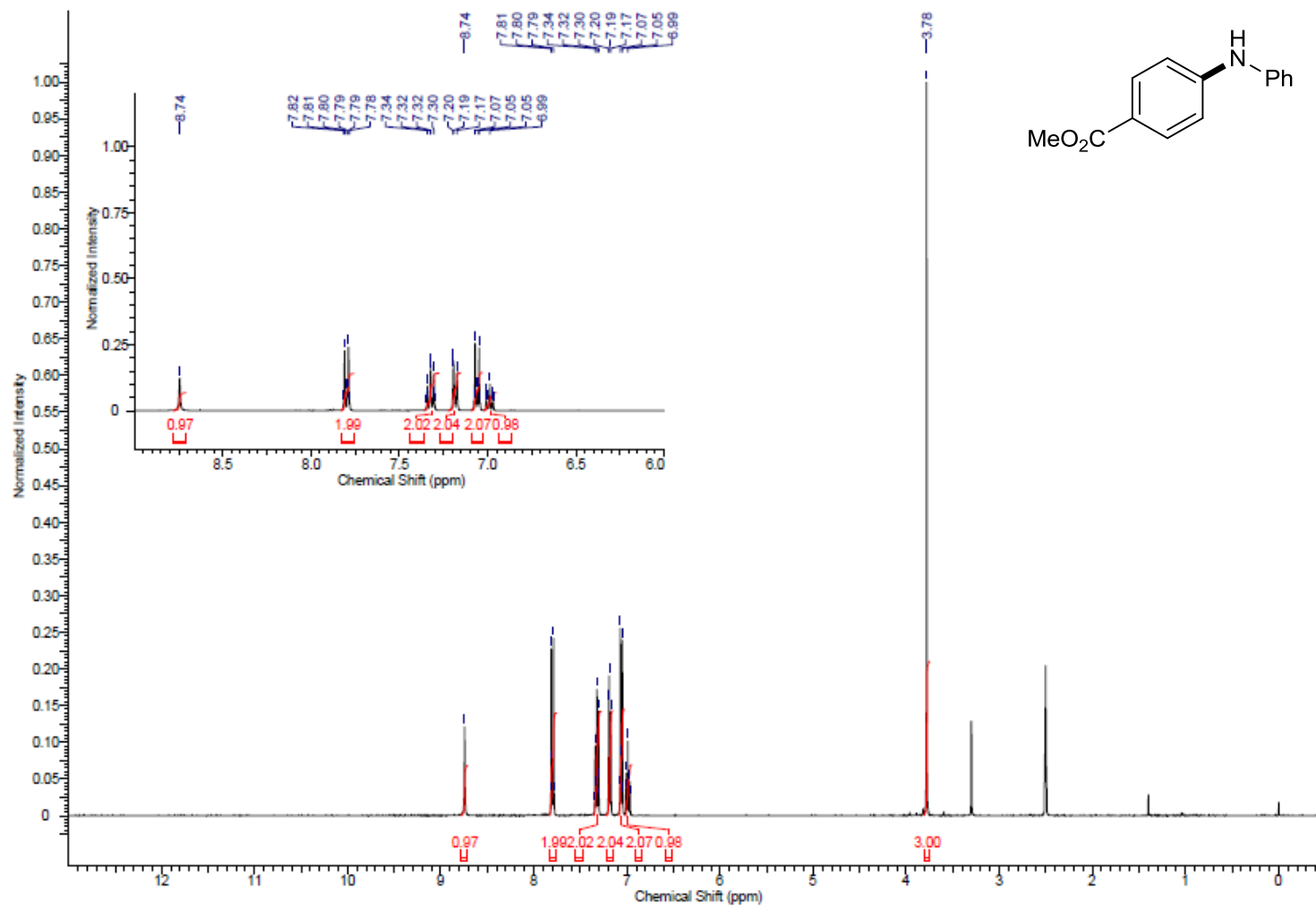


IR Spectra

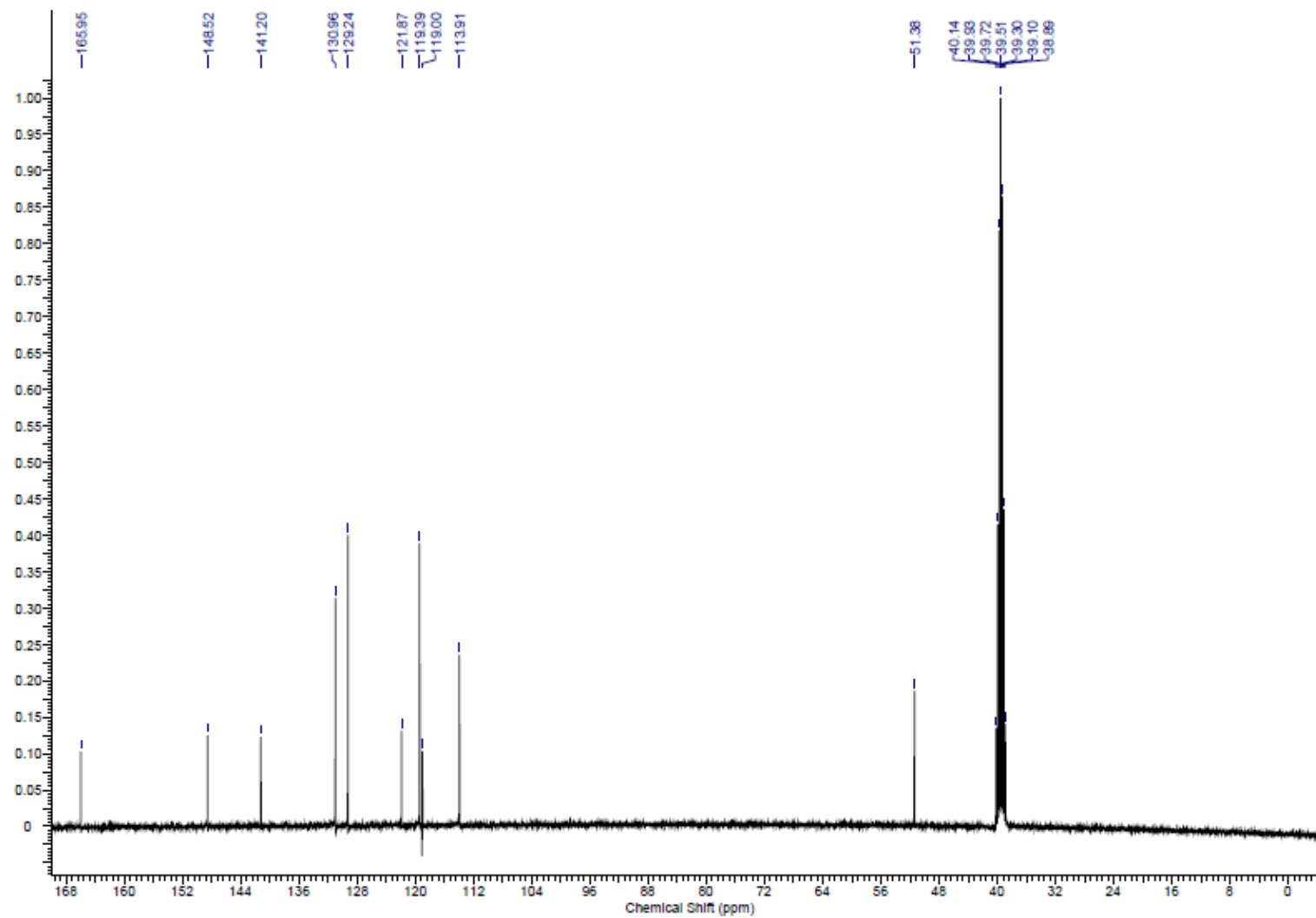


Methyl 4-(phenylamino)benzoate (3o).

¹H NMR SPECTRA

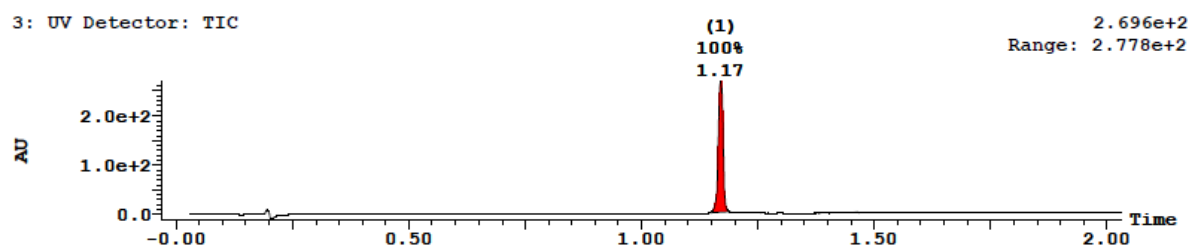


^{13}C NMR SPECTRA



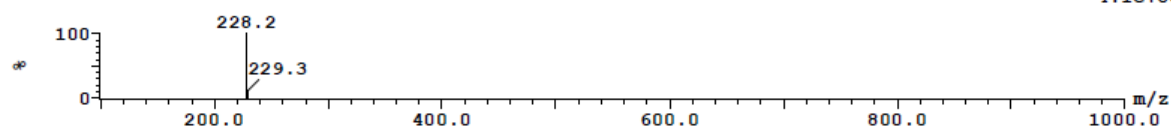
LCMS

3: UV Detector: TIC



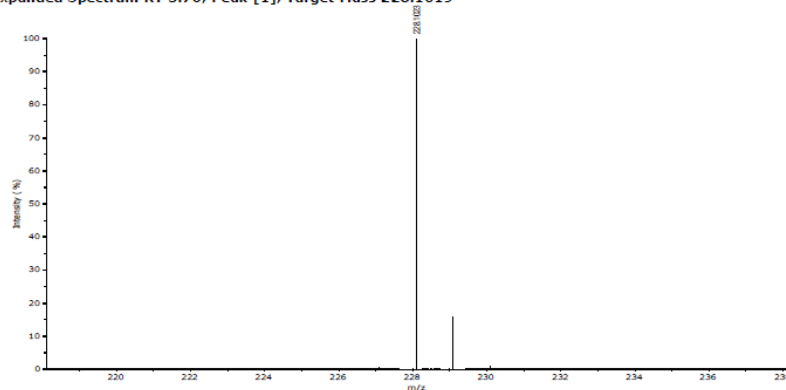
Peak Time
1 1.17
1: (Time: 1.17)

1:MS ES+
4.1e+007

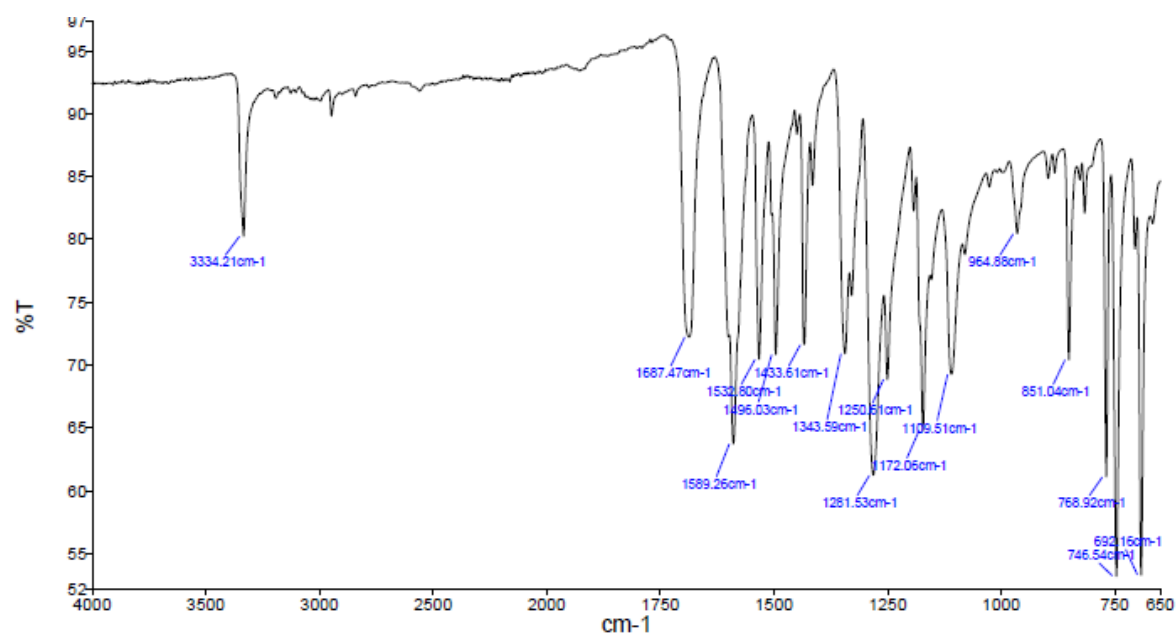


HRMS

Expanded Spectrum RT 3.76, Peak [1], Target Mass 228.1019

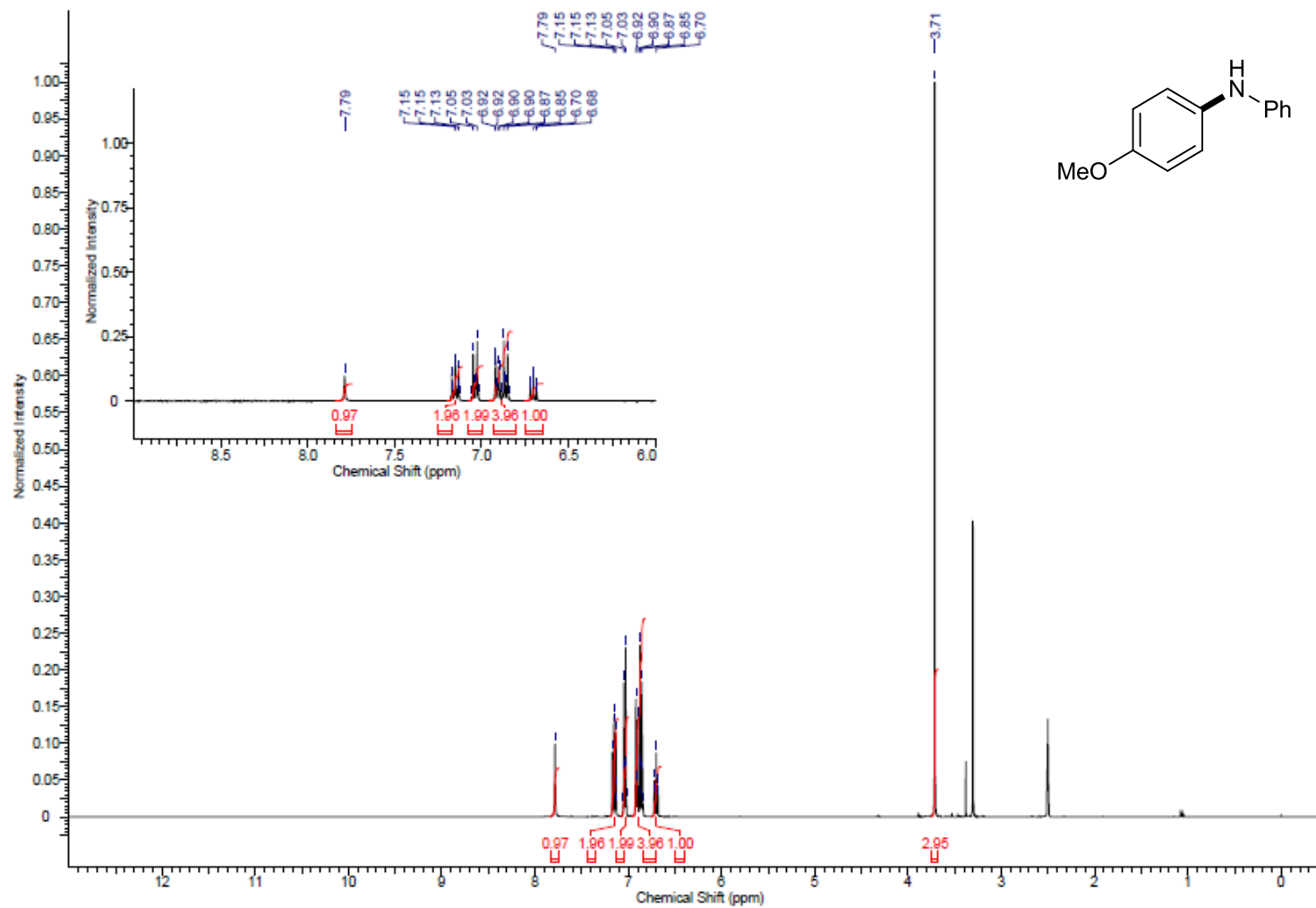


IR SPECTRA

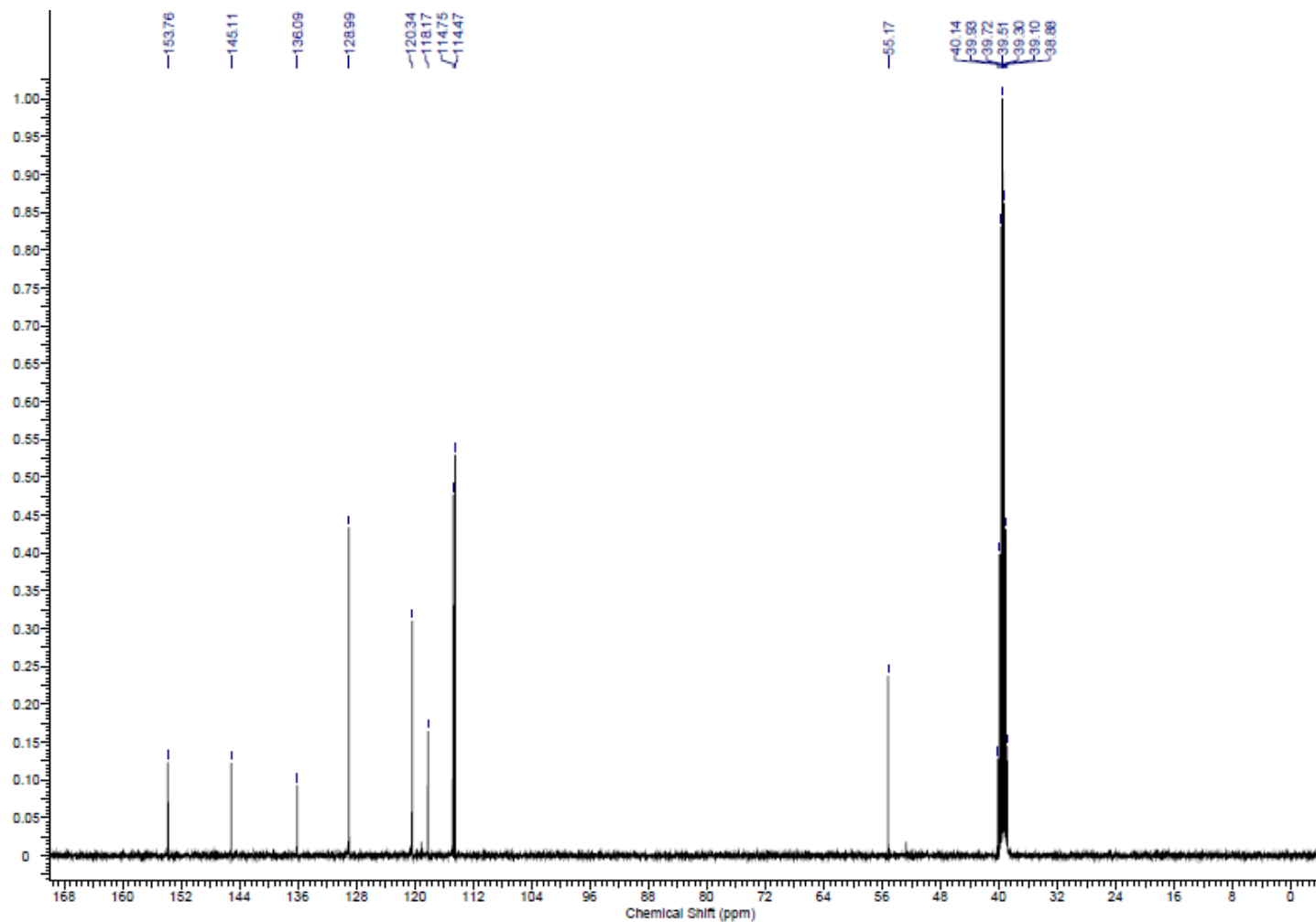


4-Methoxy-N-phenylaniline (3p).

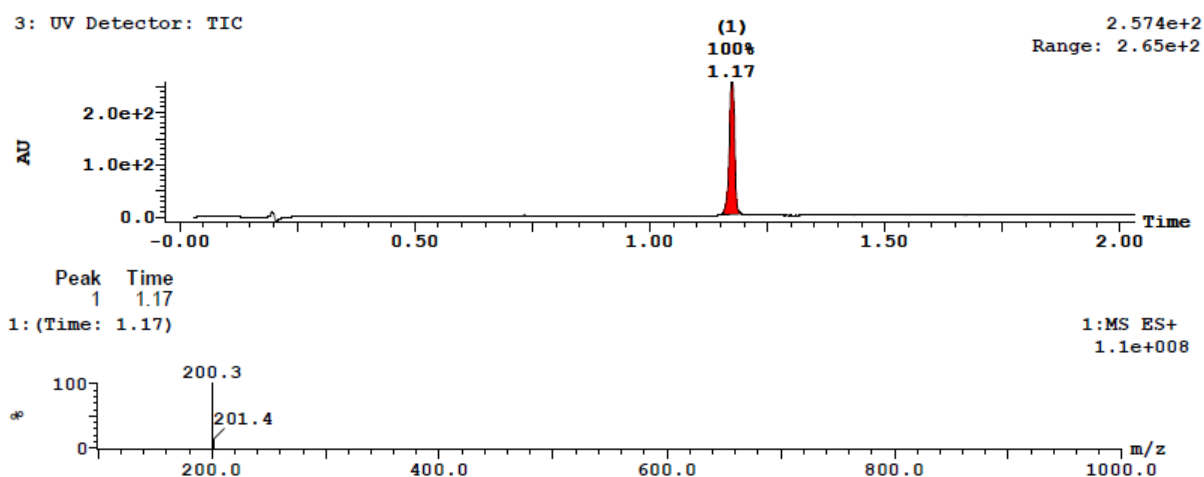
^1H NMR Spectra



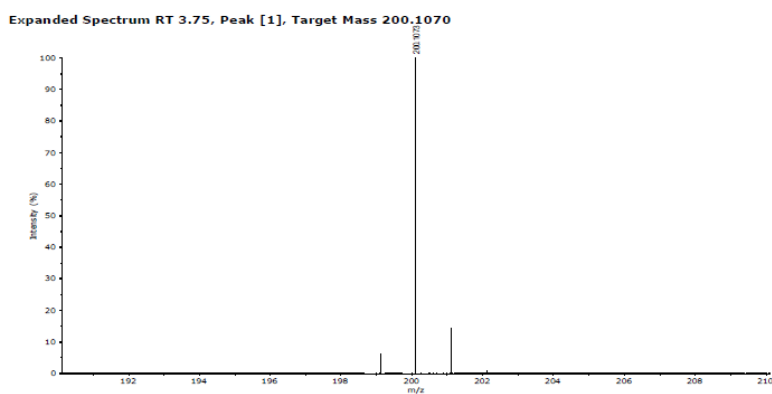
^{13}C NMR Spectra



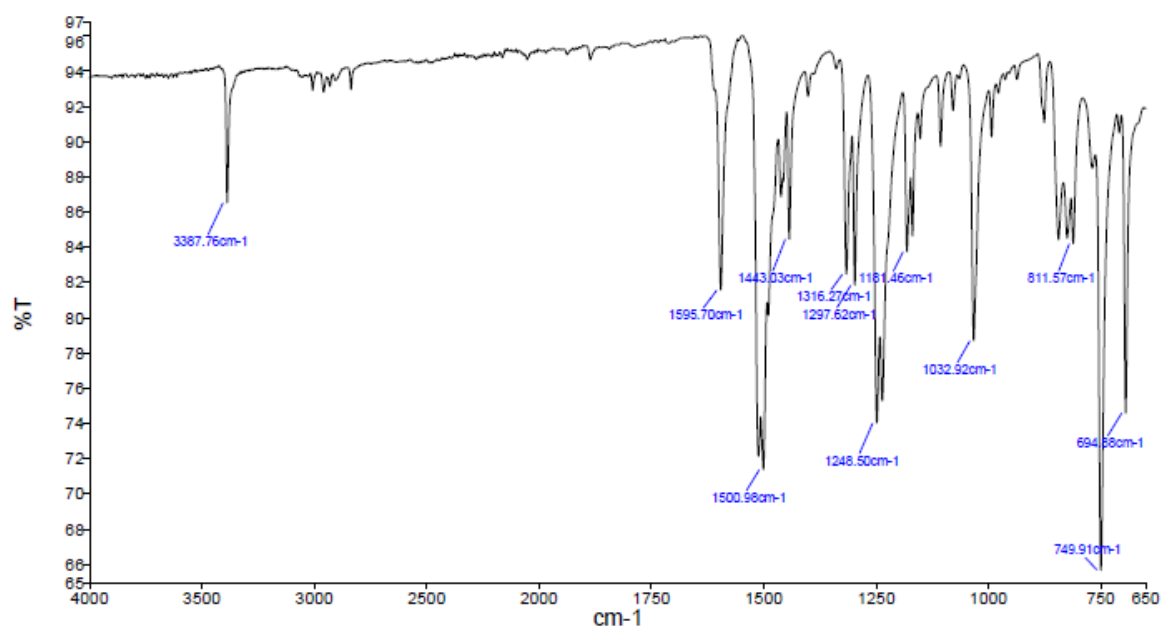
LCMS



HRMS

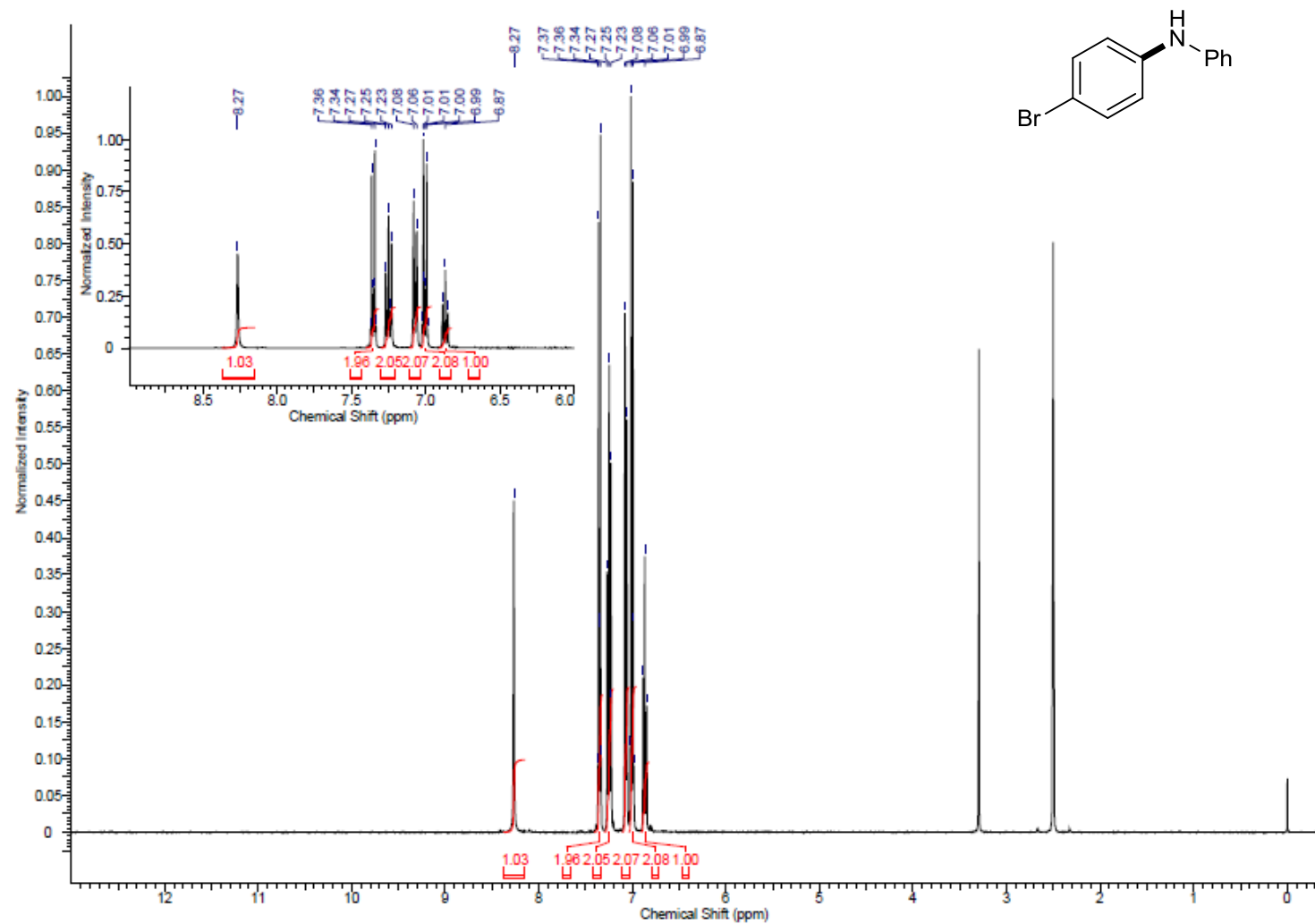


IR Spectra

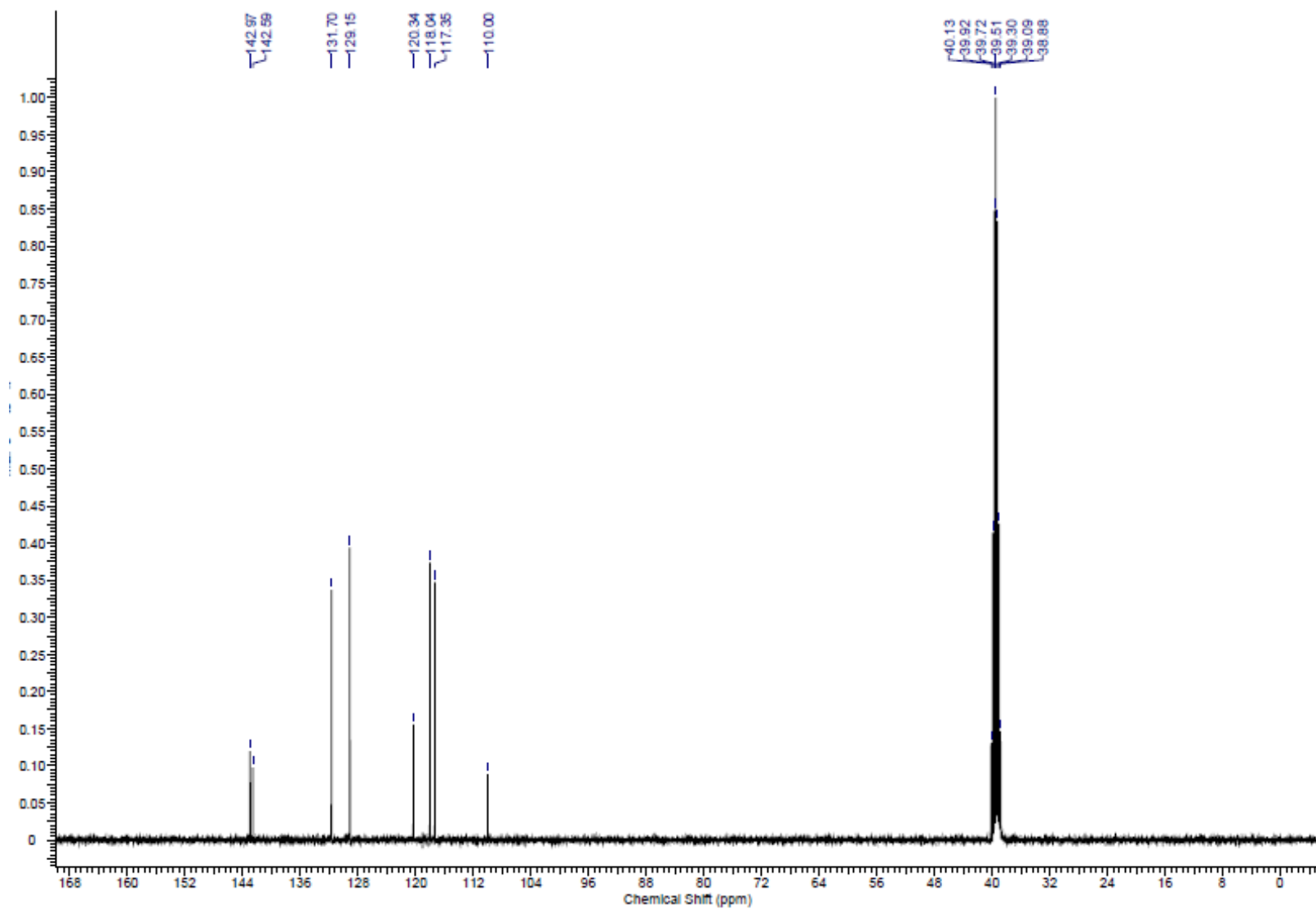


4-Bromo-*N*-phenylaniline (3q).

^1H NMR Spectra

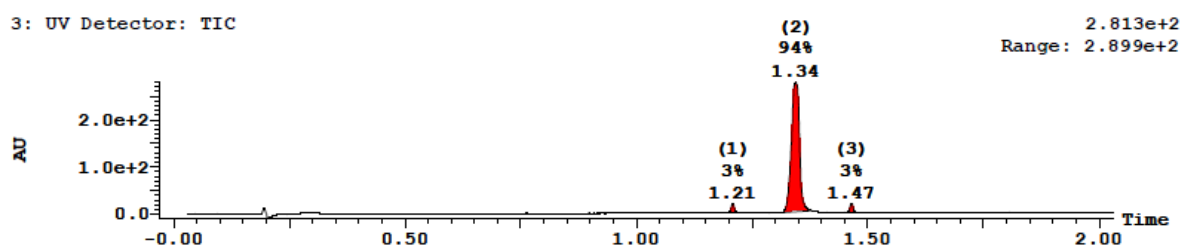


¹³C NMR Spectra

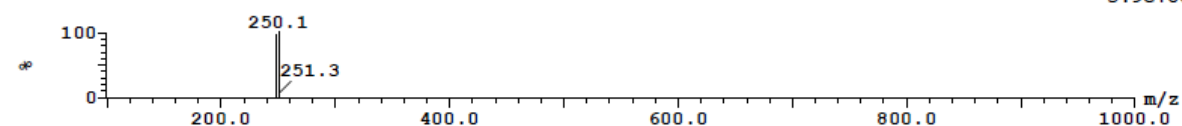


LCMS

3: UV Detector: TIC

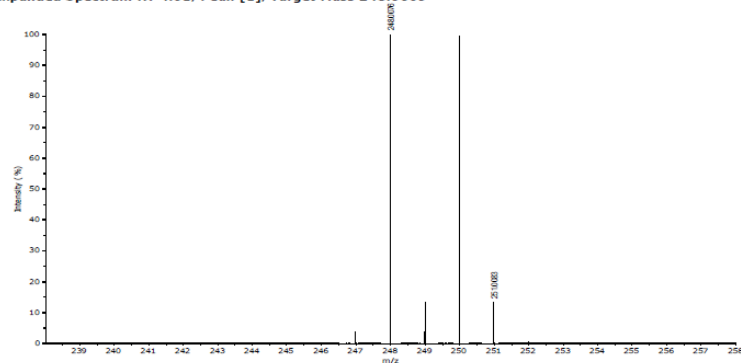


1: MS ES+
3.9e+007

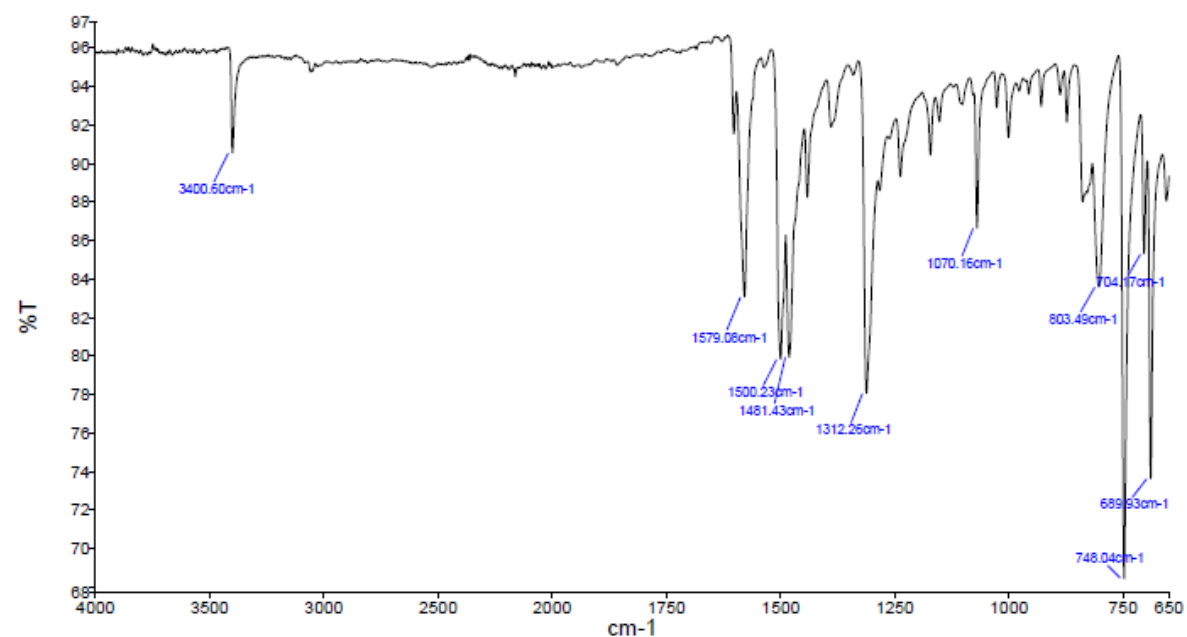


HRMS

Expanded Spectrum RT 4.61, Peak [1], Target Mass 248.0069

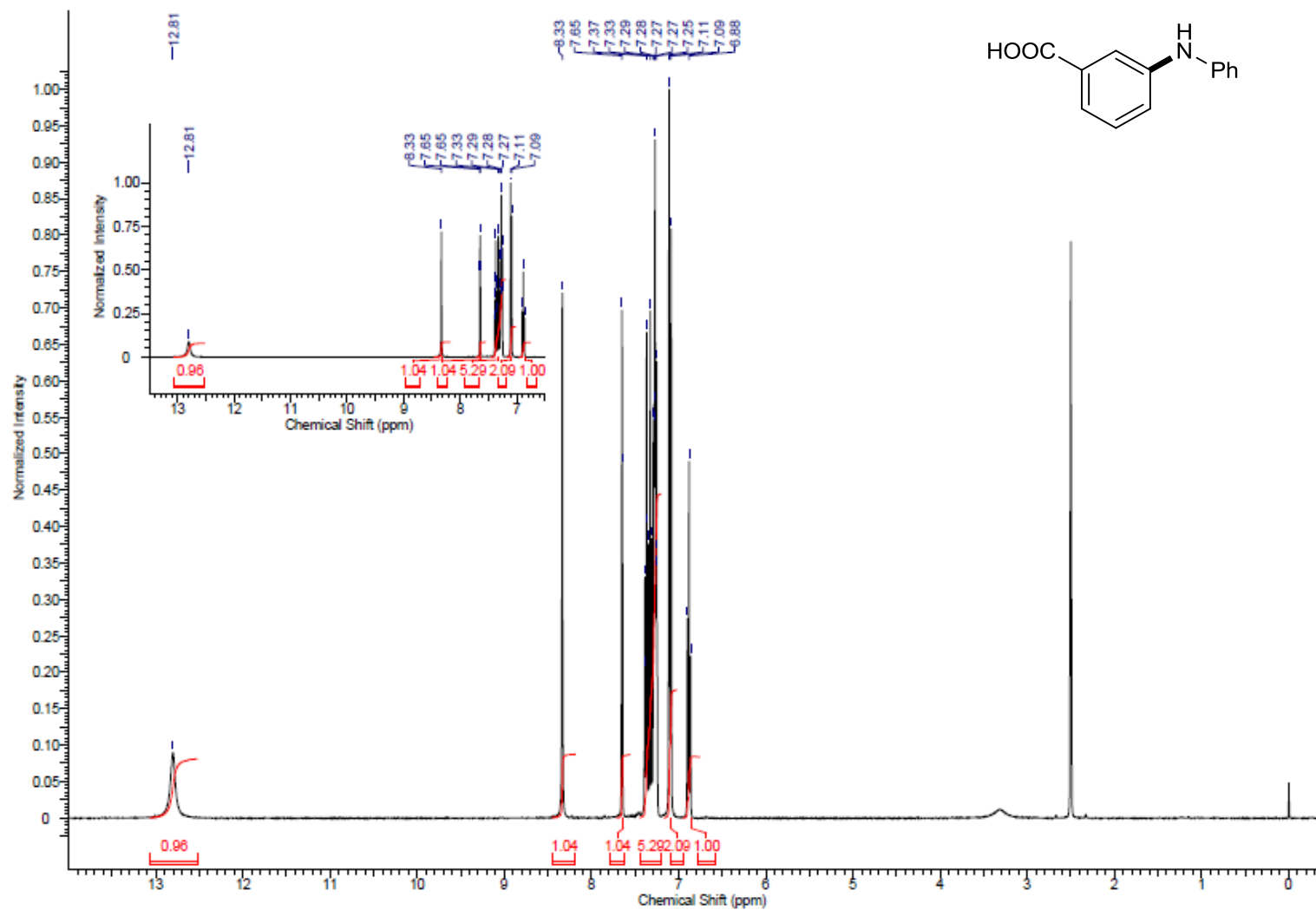


IR Spectra

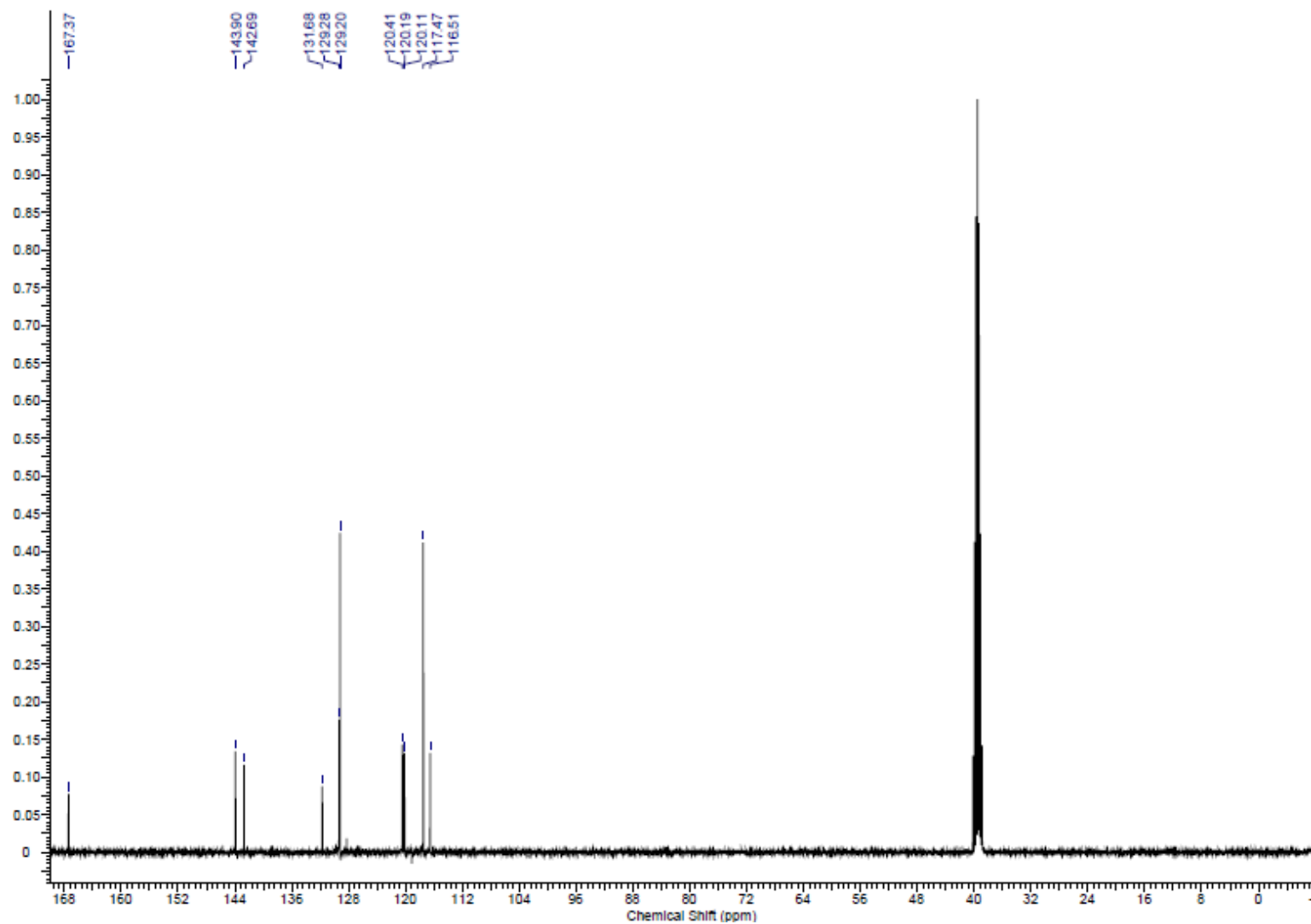


3-(Phenylamino)benzoic acid (3r).

^1H NMR Spectra

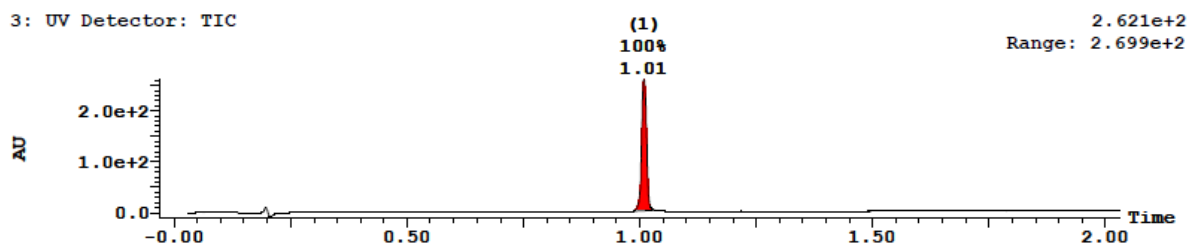


^{13}C NMR Spectra



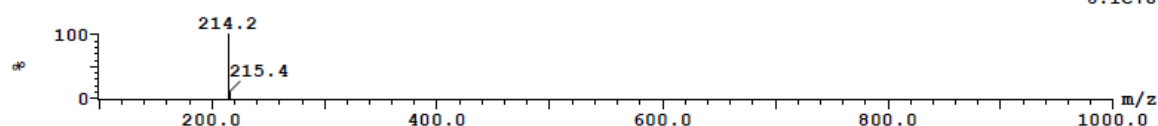
LCMS

3: UV Detector: TIC



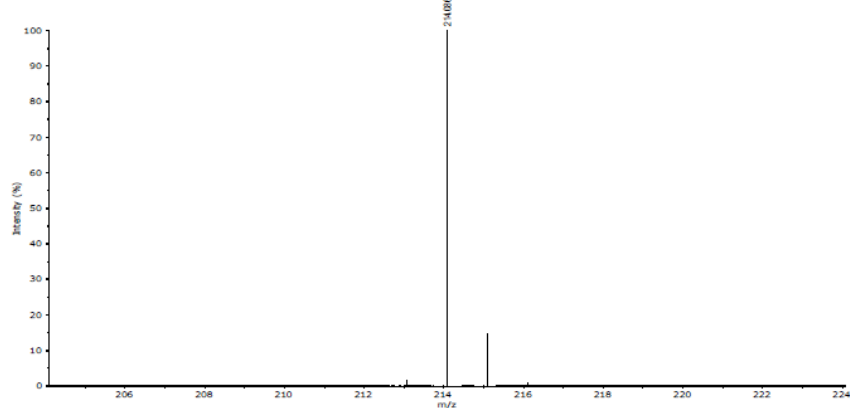
Peak Time
1 1.01
1: (Time: 1.01)

1:MS ES+
6.1e+007

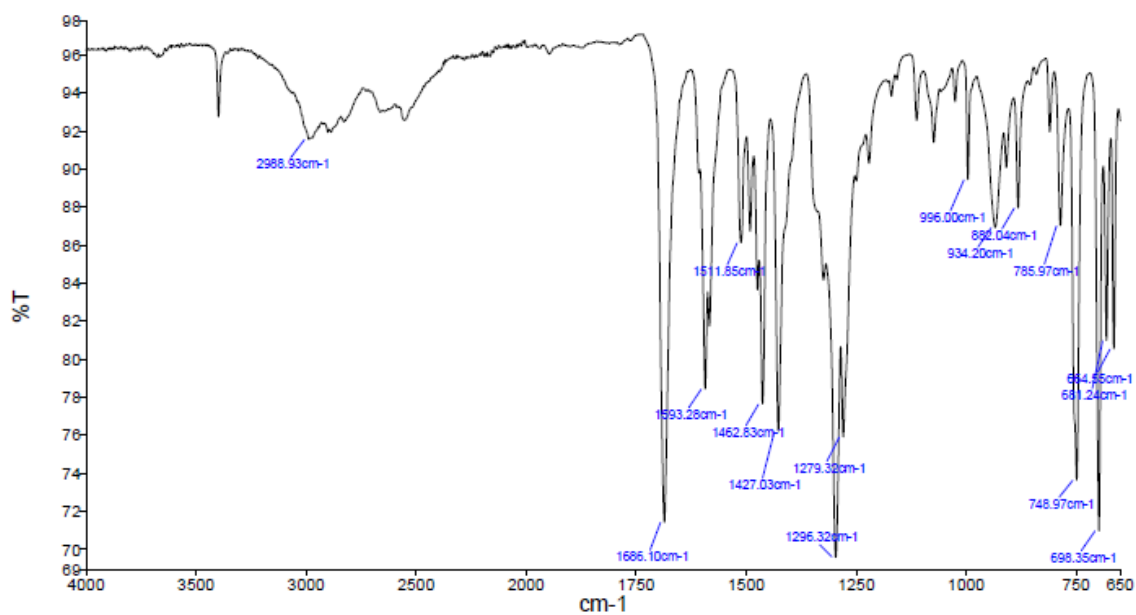


HRMS

Expanded Spectrum RT 2.92, Peak [1], Target Mass 214.0863

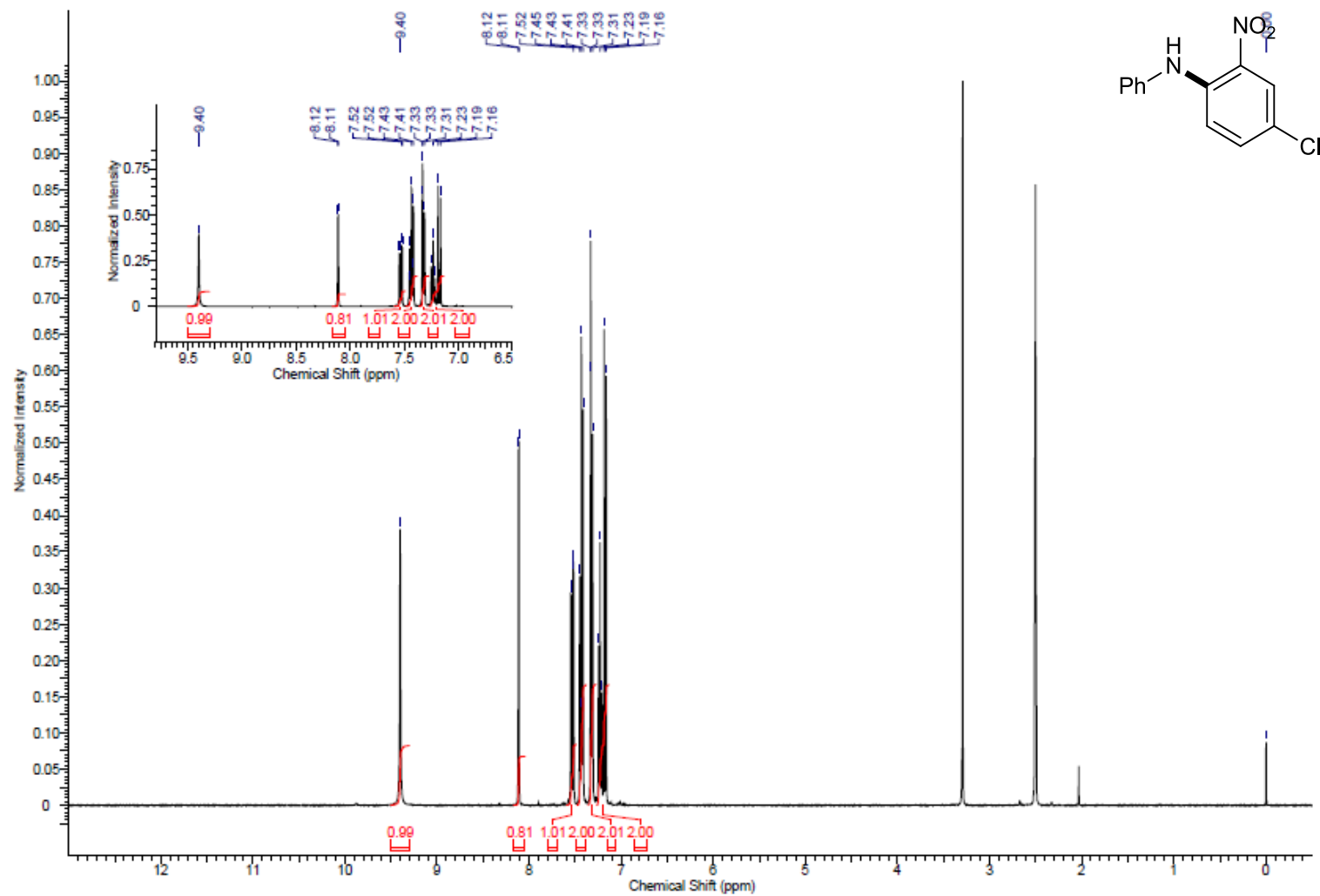


IR Spectra

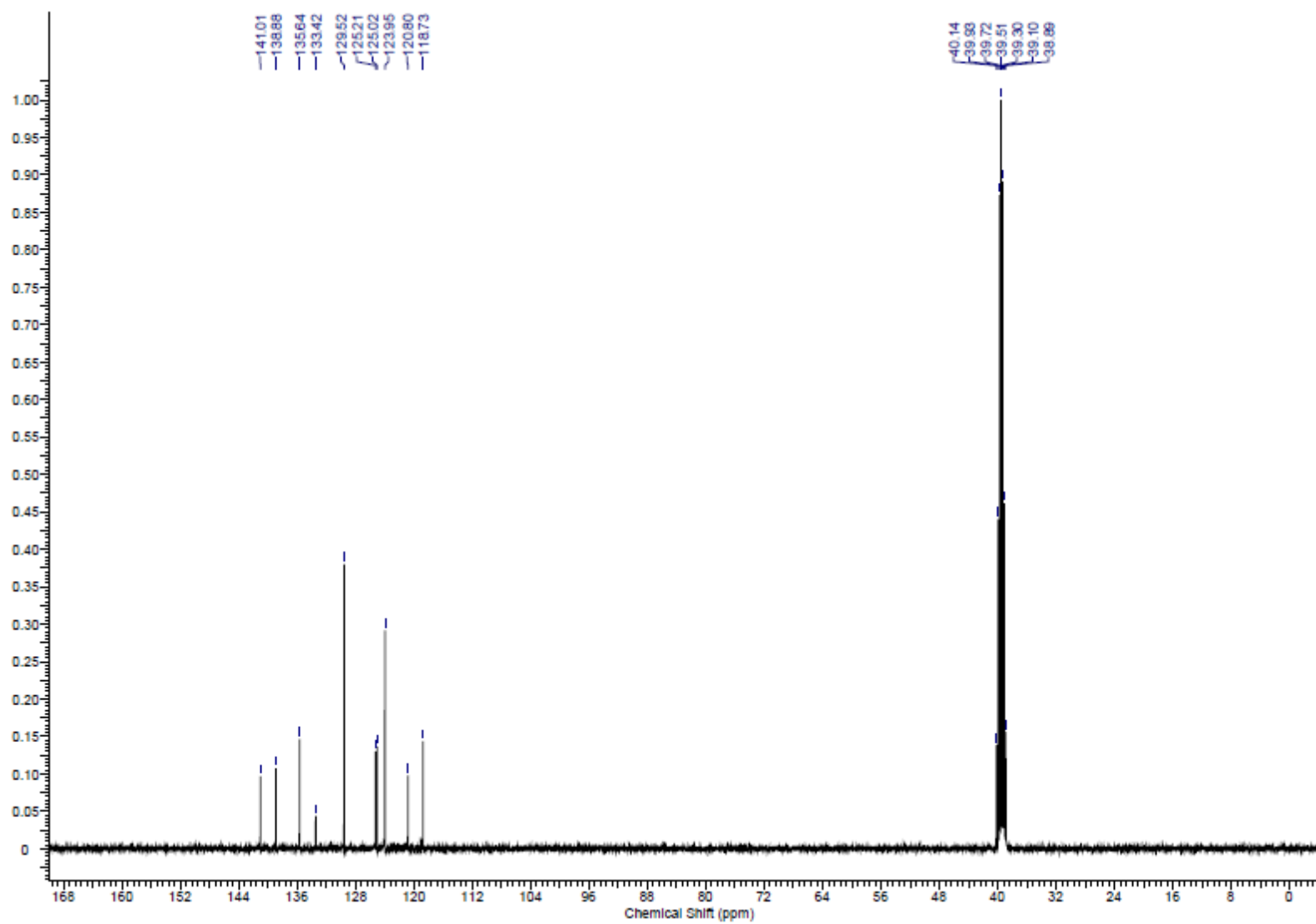


4-Chloro-2-nitro-*N*-phenylaniline (3s).

¹H NMR Spectra

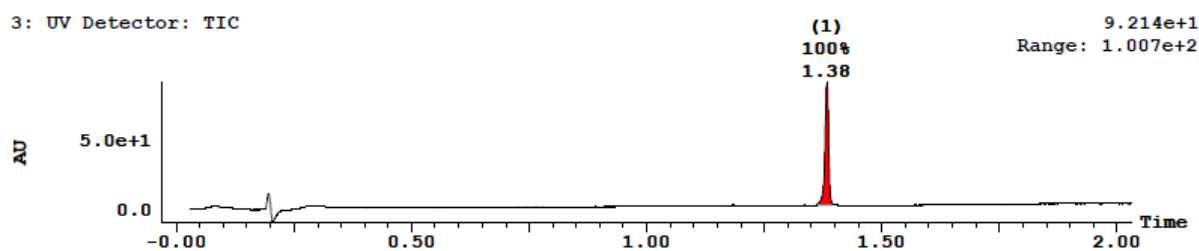


¹³C NMR Spectra



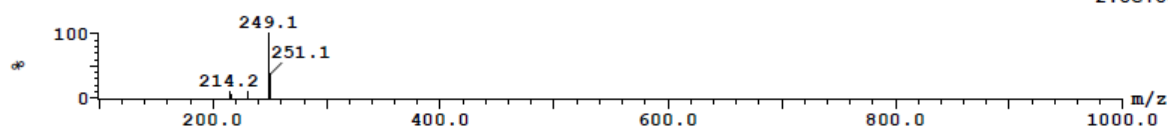
LCMS

3: UV Detector: TIC



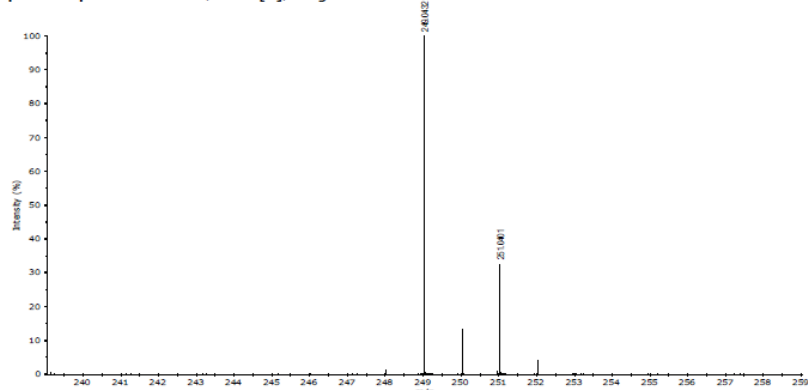
Peak Time
1 1.38
1: (Time: 1.38)

1:MS ES+
2.0e+006

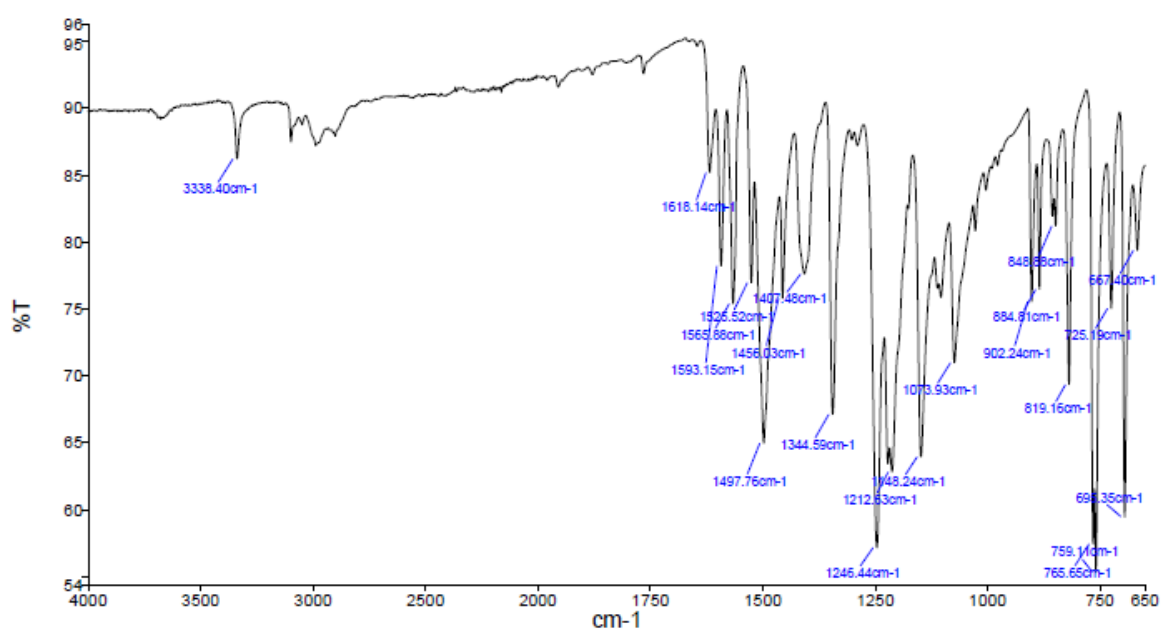


HRMS

Expanded Spectrum RT 4.80, Peak [1], Target Mass 249.0425

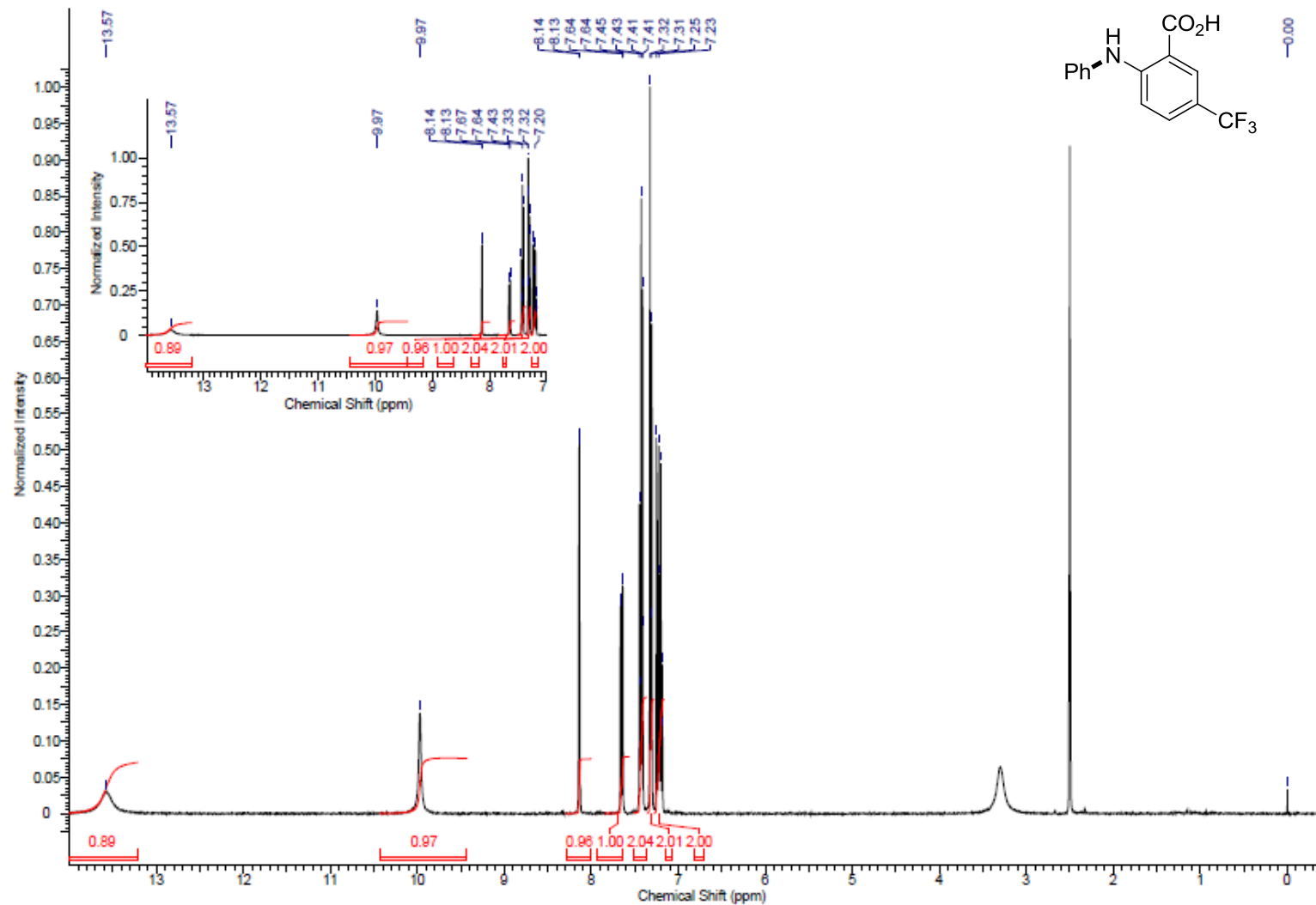


IR Spectra

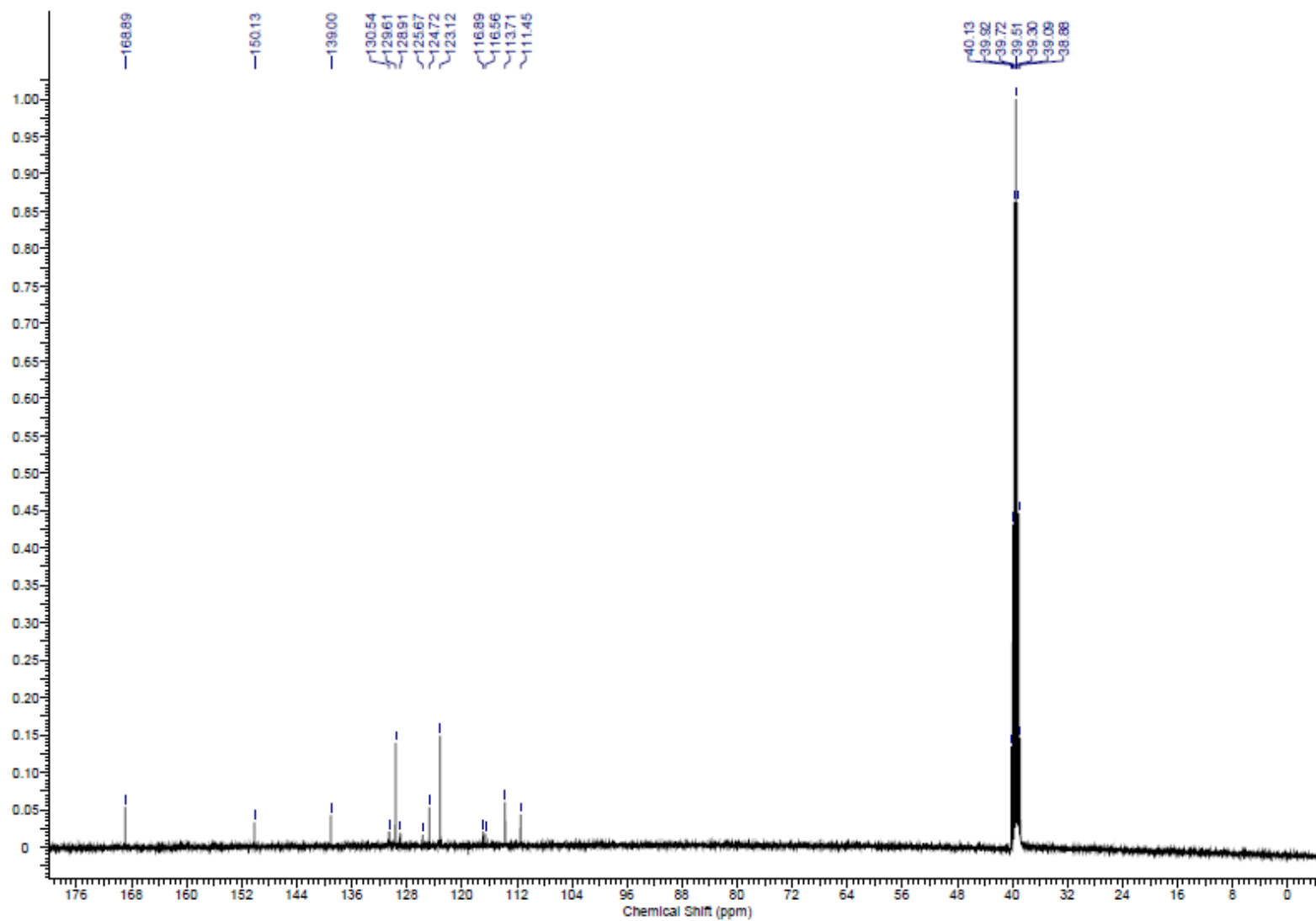


2-(Phenylamino)-5-(trifluoromethyl)benzoic acid (3t).

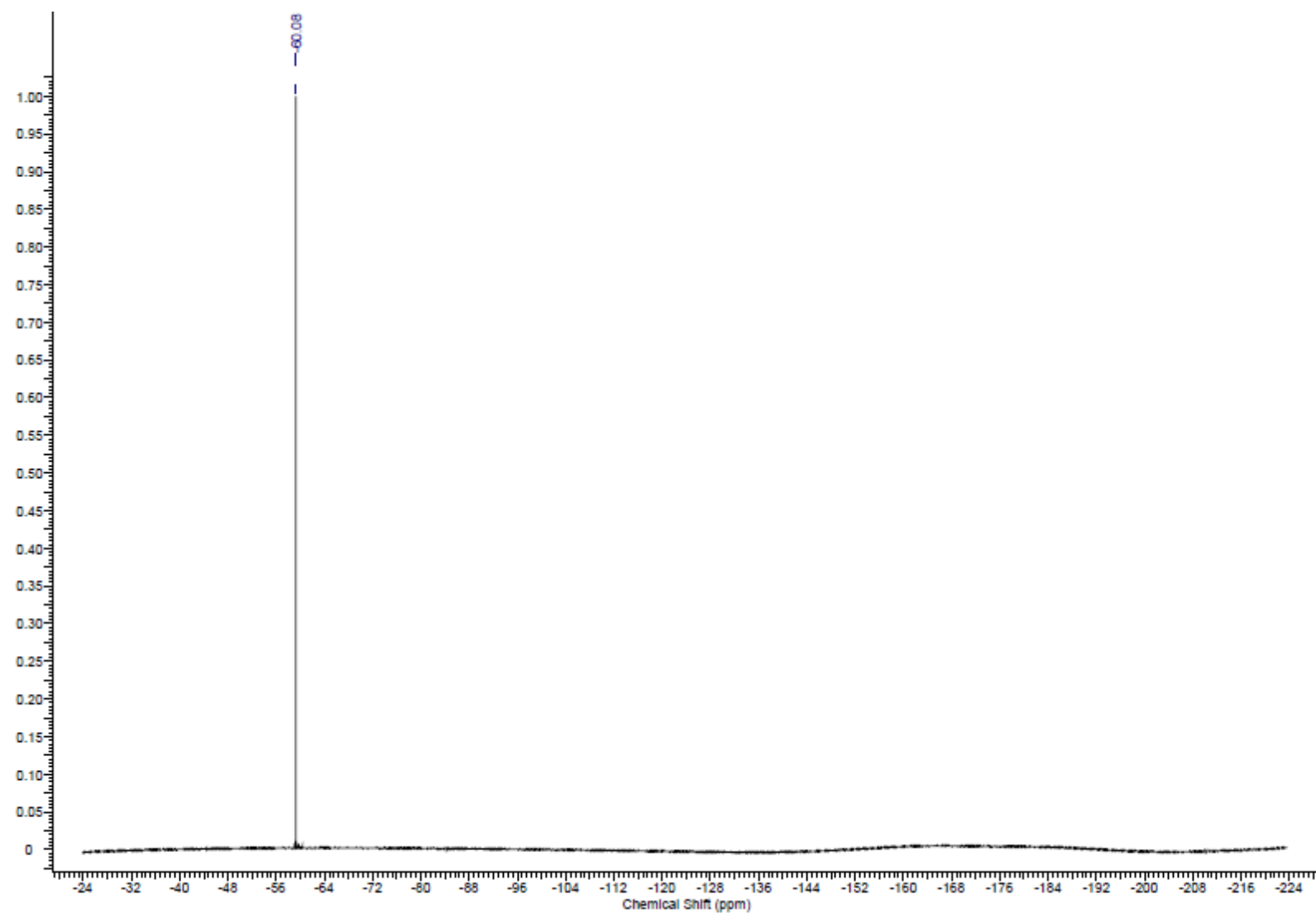
¹H NMR Spectra



^{13}C NMR Spectra

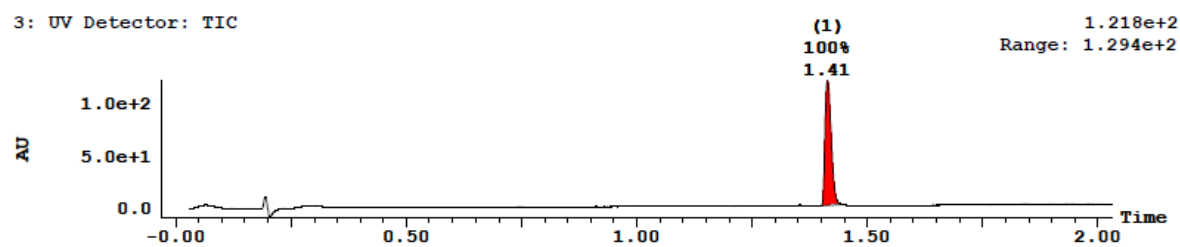


¹⁹F NMR Spectra



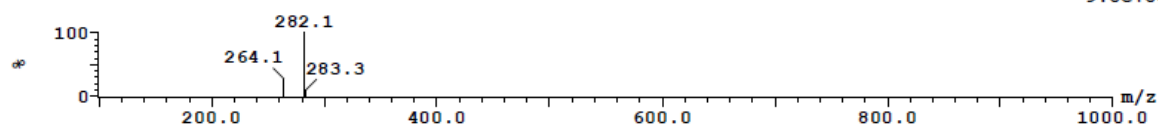
LCMS

3: UV Detector: TIC



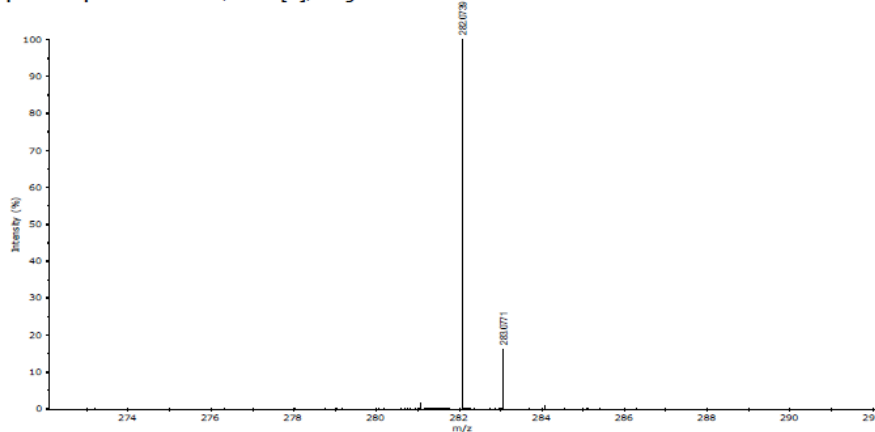
Peak Time
1 1.41
1: (Time: 1.41)

1: MS ES+
9.0e+006

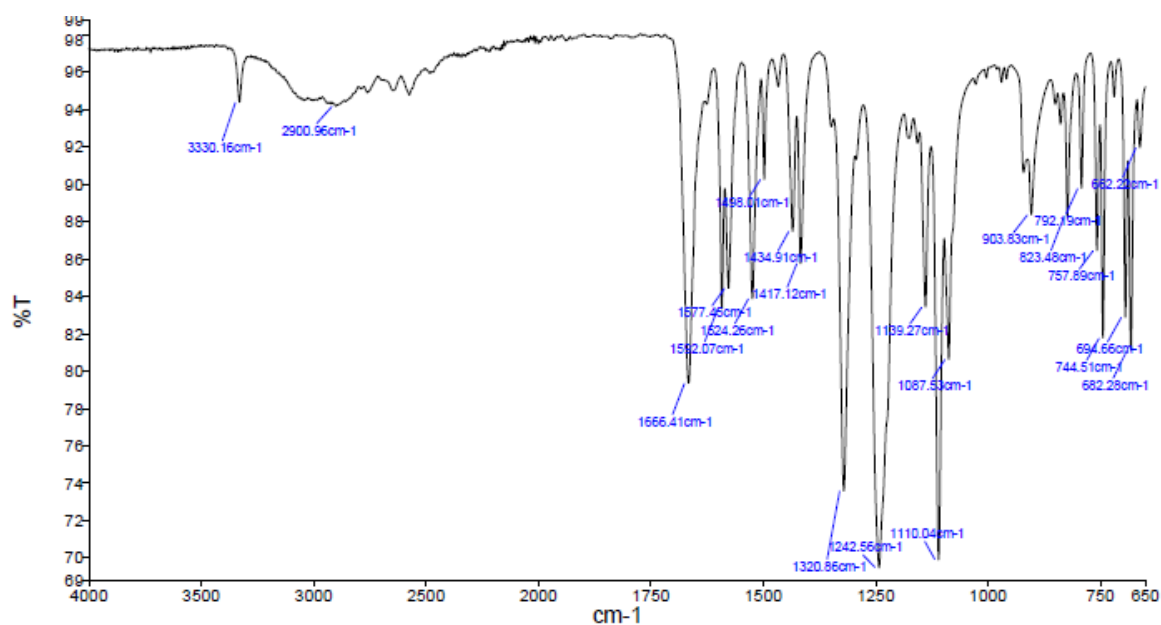


HRMS

Expanded Spectrum RT 4.40, Peak [1], Target Mass 282.0736

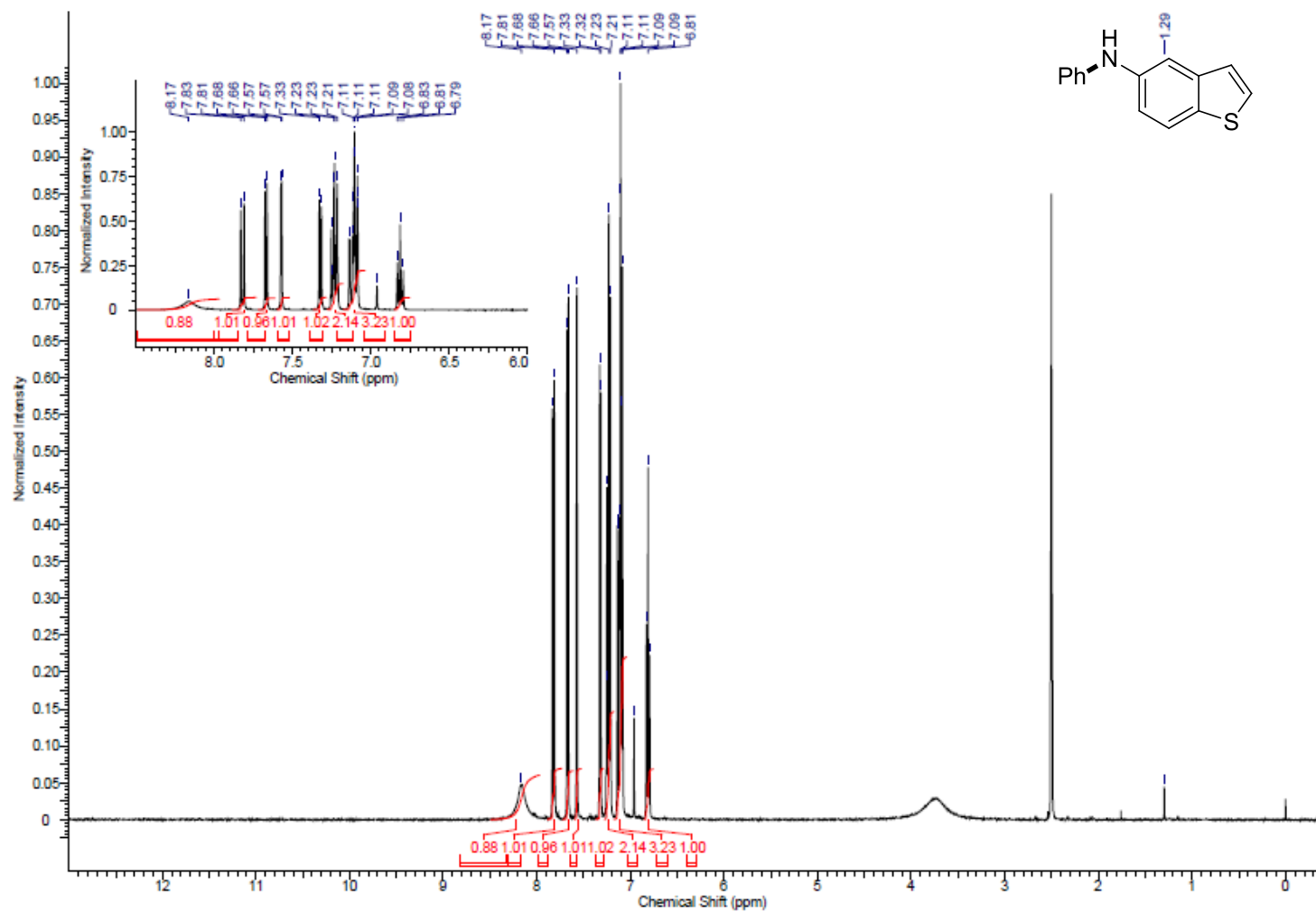


IR Spectra

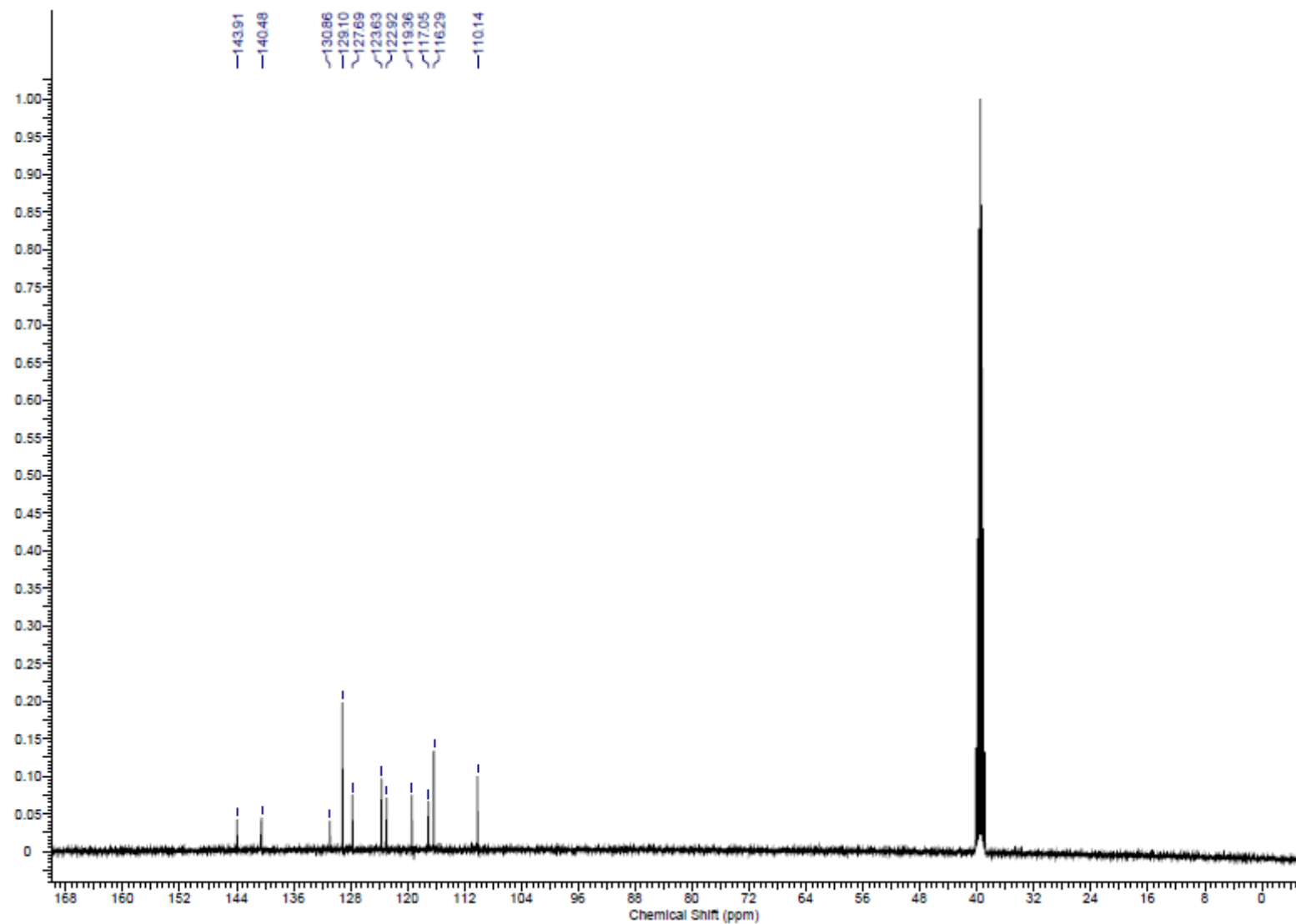


***N*-Phenylbenzo[*b*]thiophen-5-amine (3u).**

¹H NMR Spectra

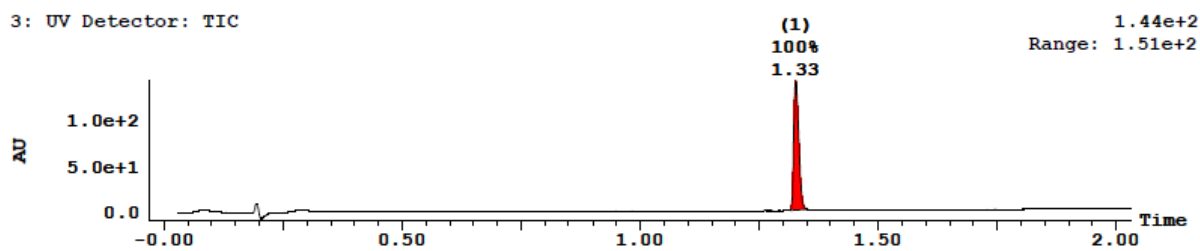


¹³C NMR Spectra



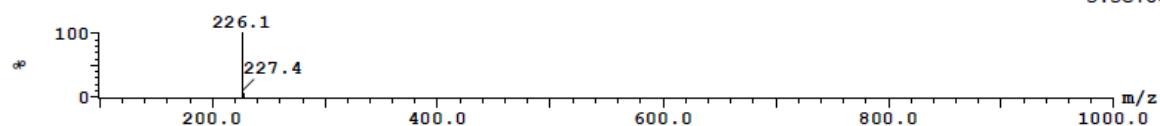
LCMS

3: UV Detector: TIC



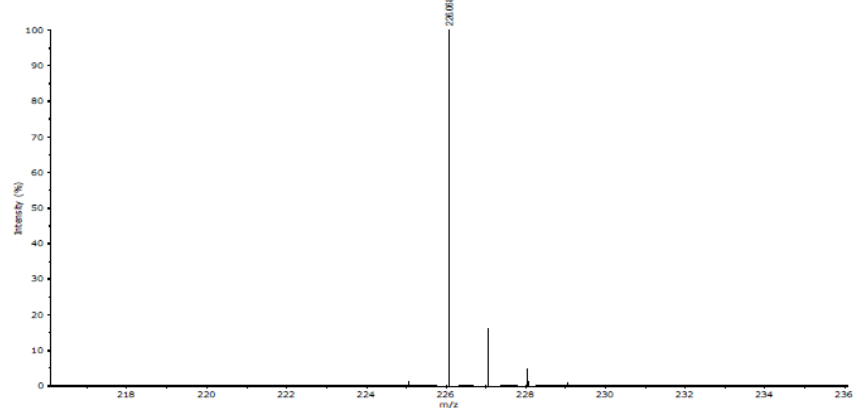
Peak Time
1 1.33
1: (Time: 1.33)

1:MS ES+
3.3e+007

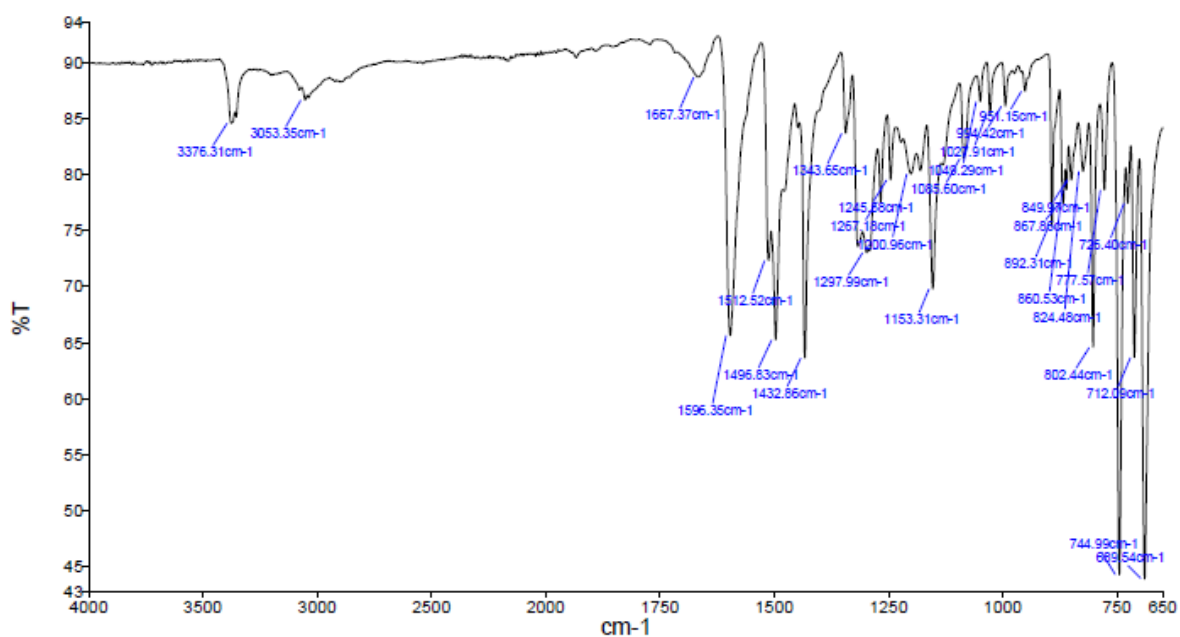


HRMS

Expanded Spectrum RT 4.47, Peak [1], Target Mass 226.0685

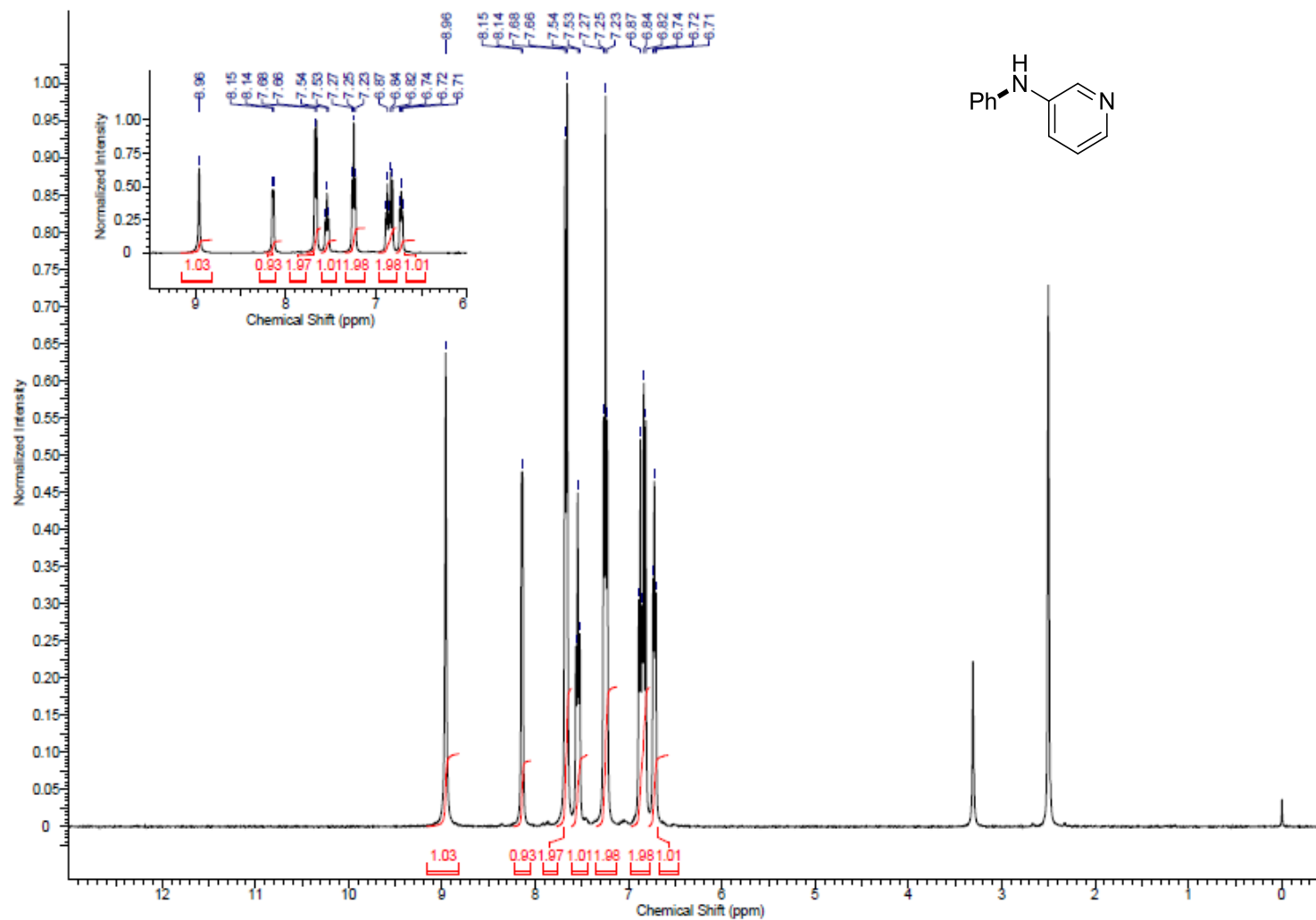


IR Spectra

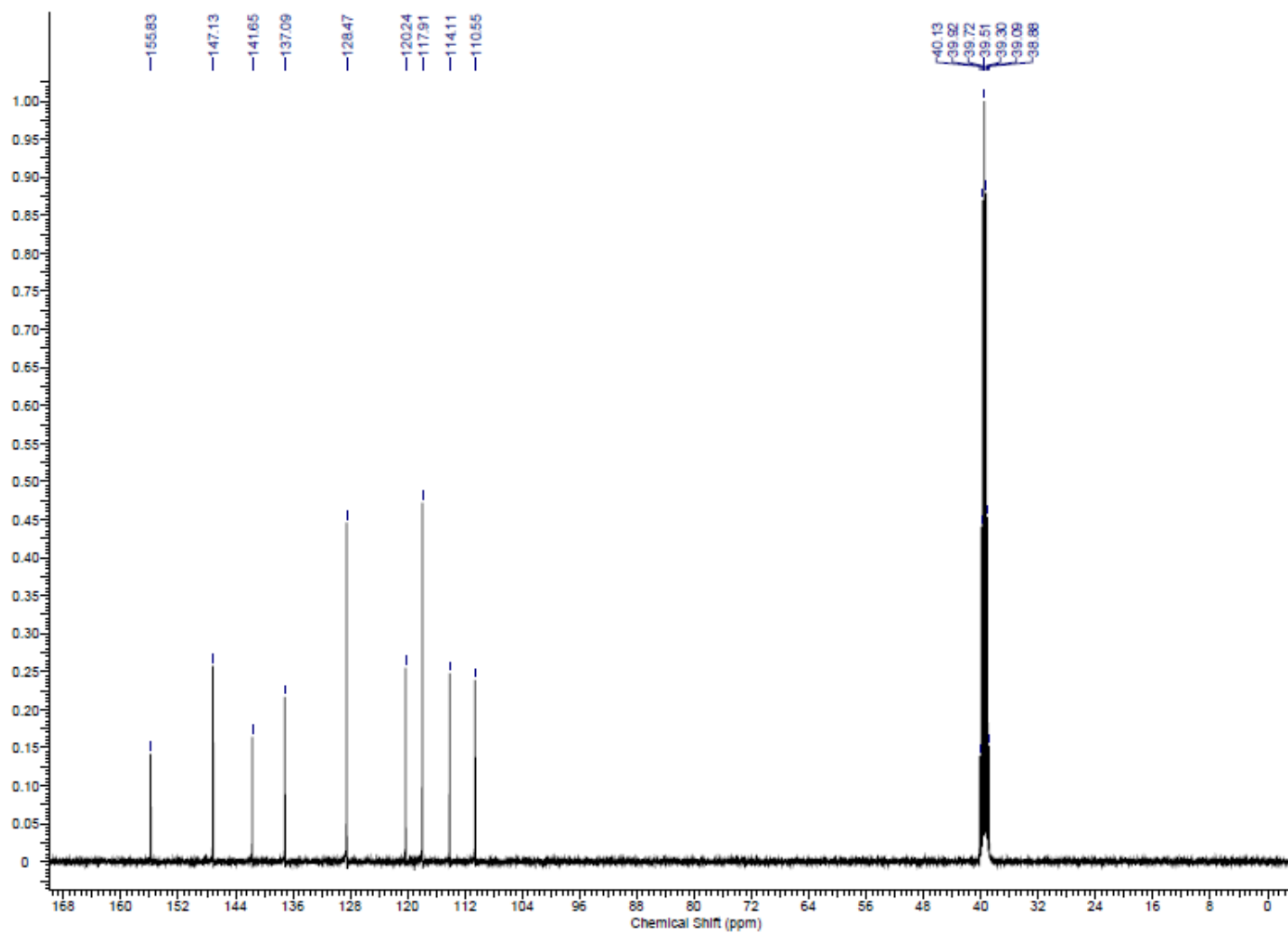


***N*-Phenylpyridin-3-amine (3v).**

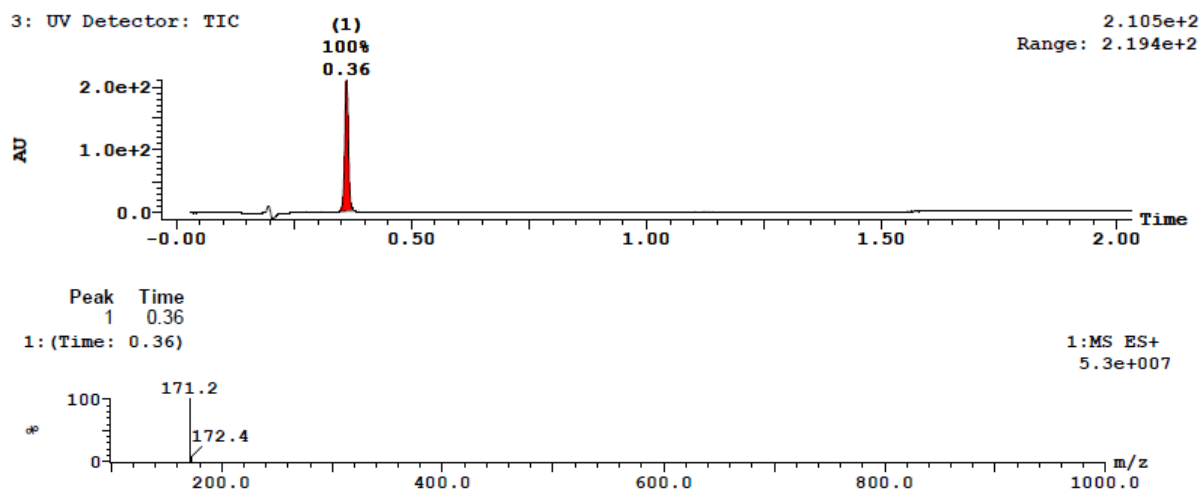
¹H NMR Spectra



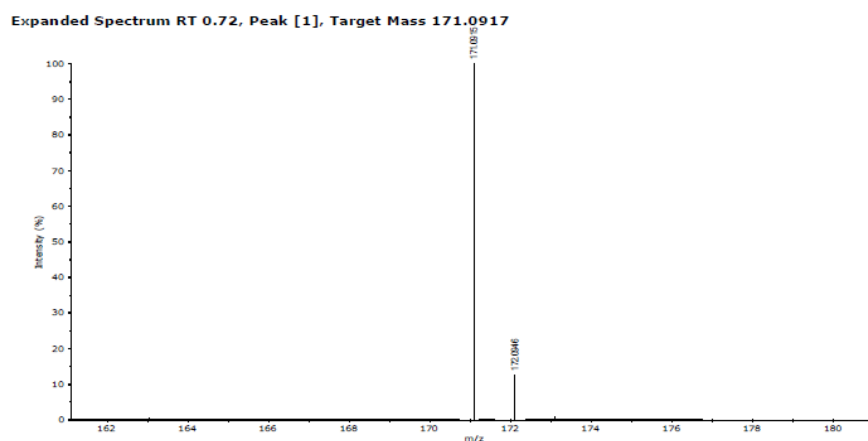
^{13}C NMR Spectra



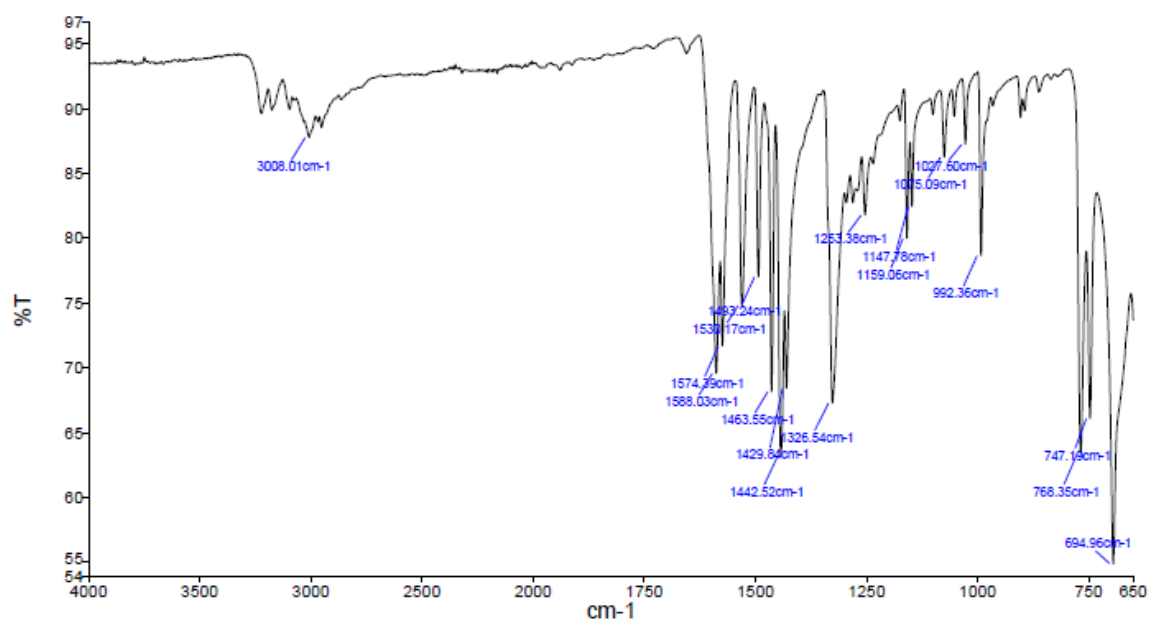
LCMS



HRMS

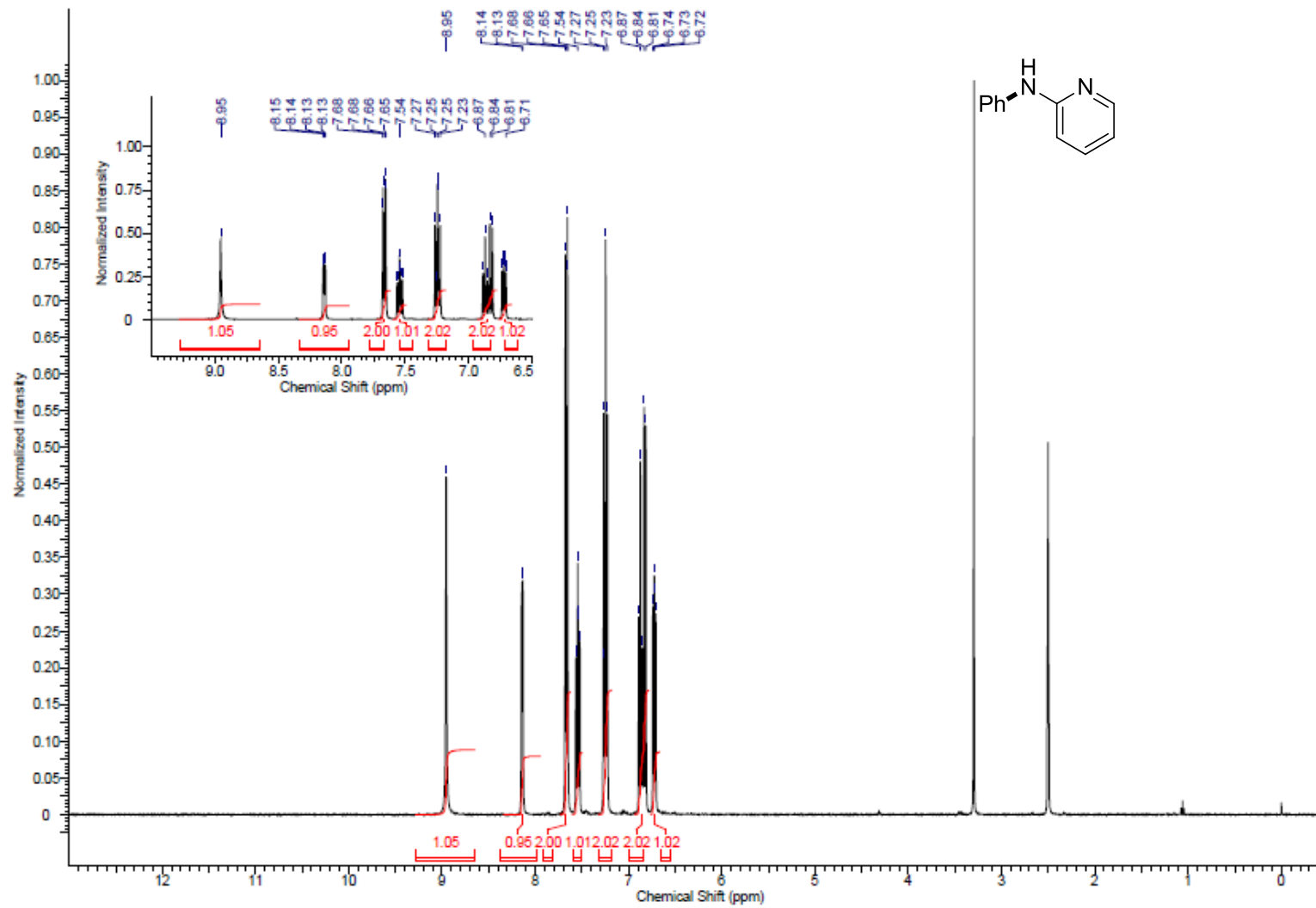


IR Spectra

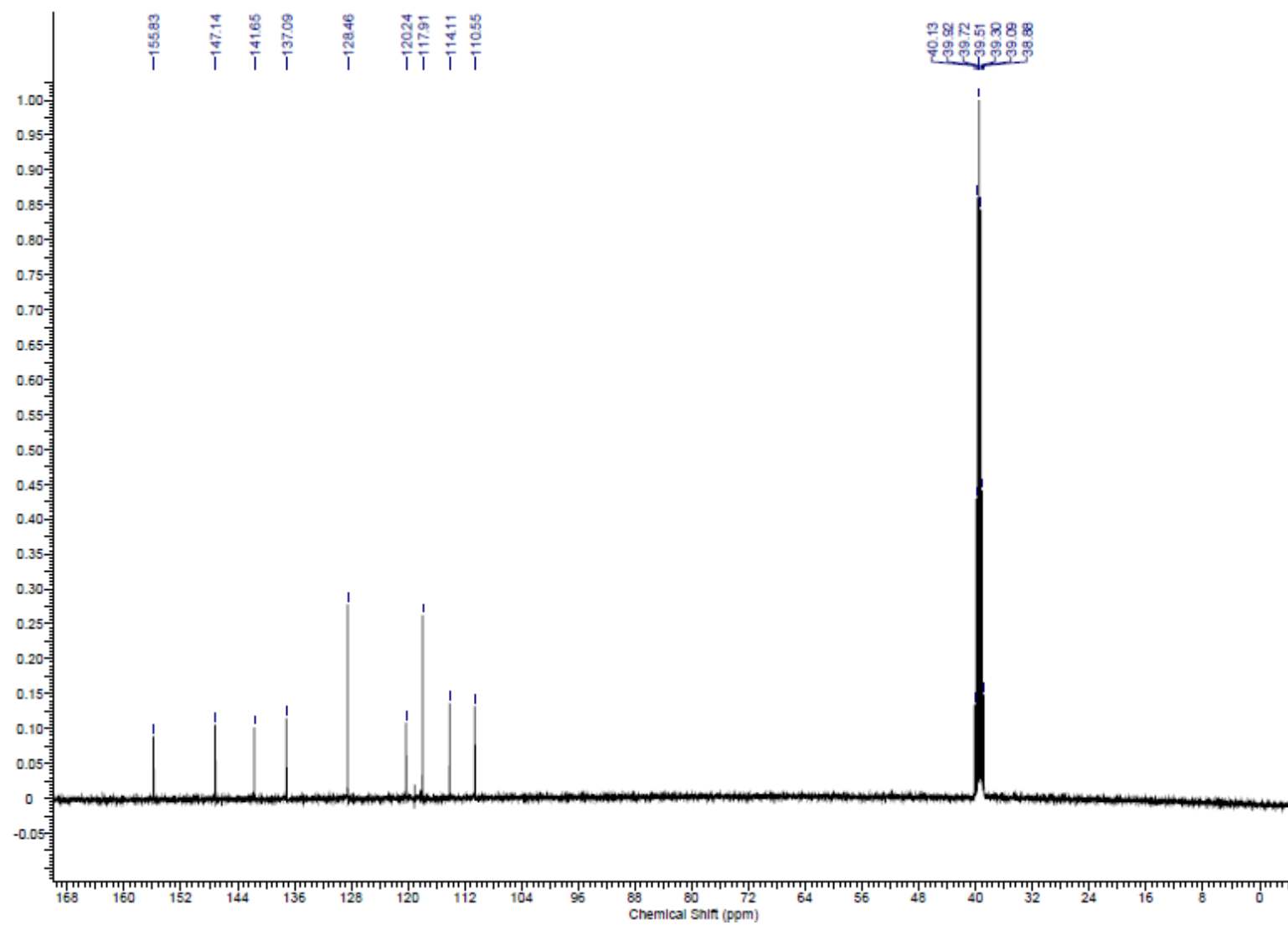


N-Phenylpyridin-2-amine (3w).

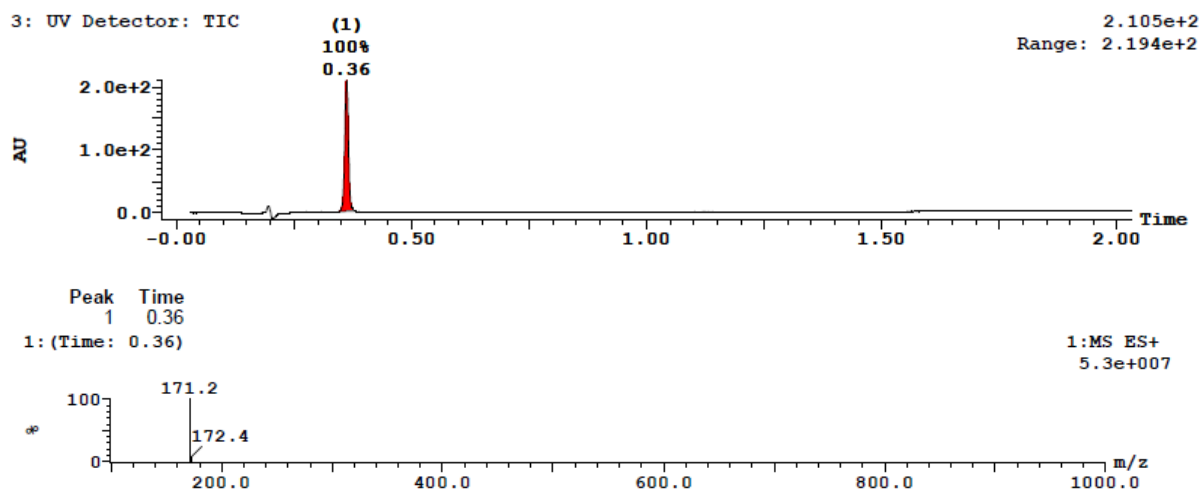
¹H NMR Spectra



^{13}C NMR Spectra

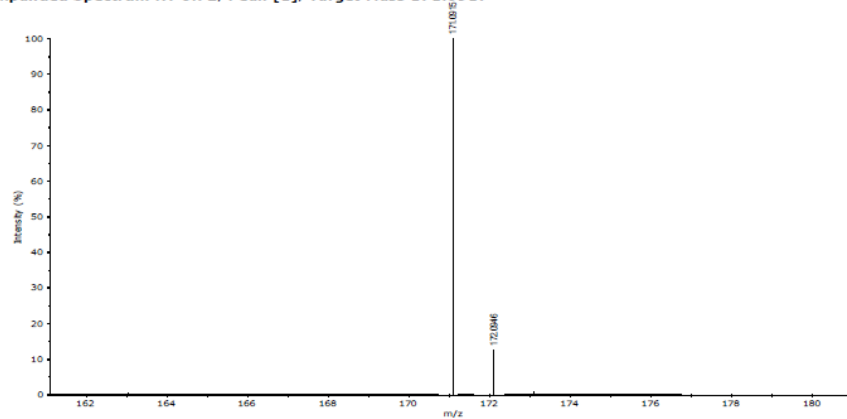


LCMS

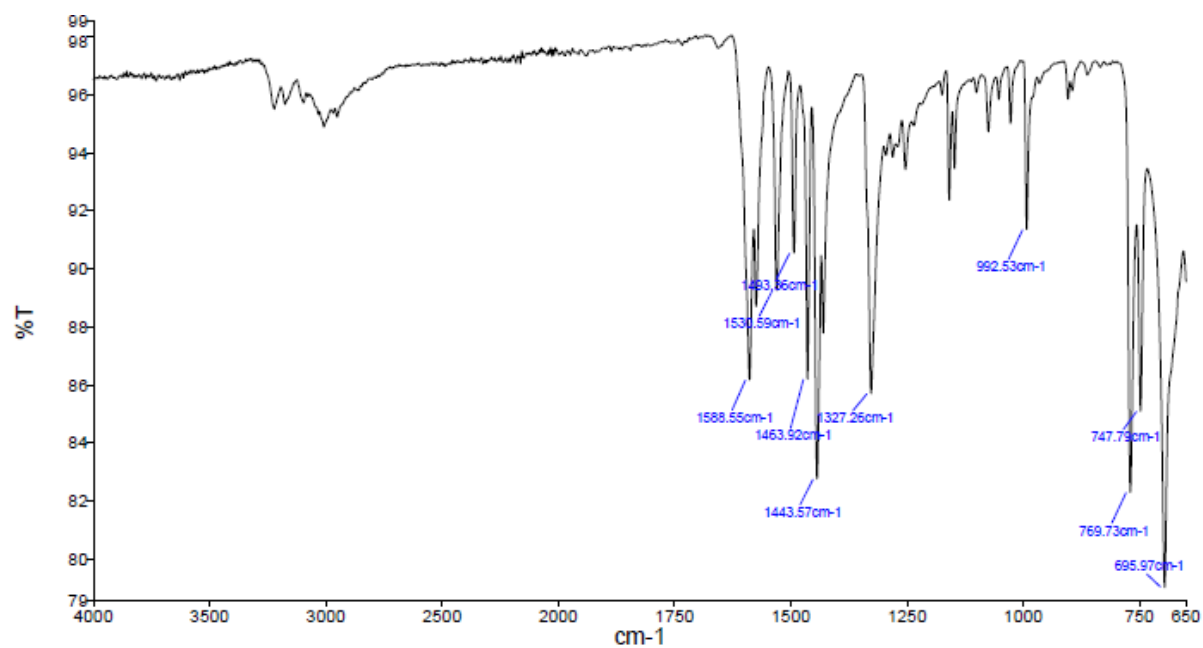


HRMS

Expanded Spectrum RT 0.72, Peak [1], Target Mass 171.0917

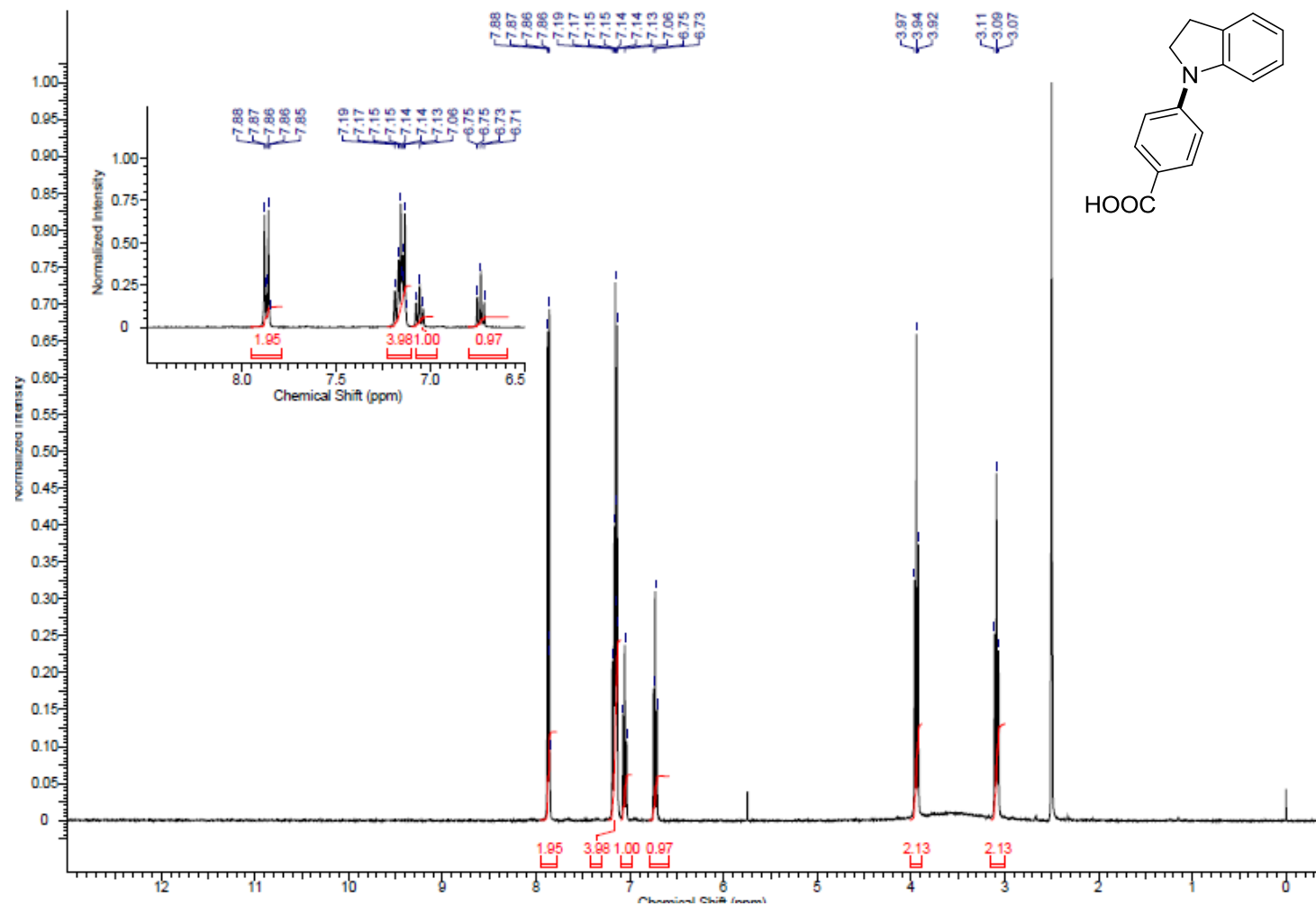


IR Spectra

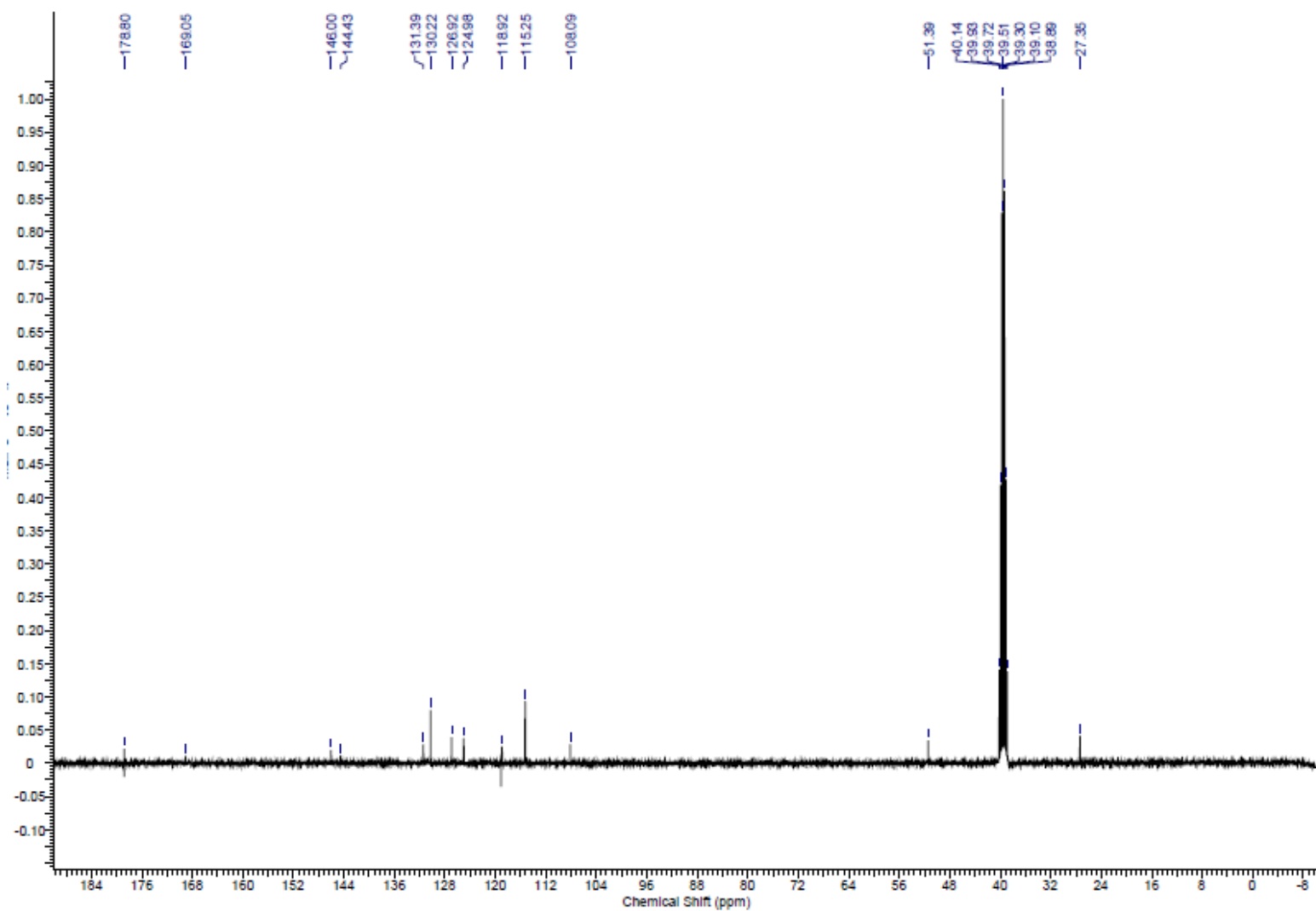


4-(indolin-1-yl)benzoic acid (3x).

^1H NMR Spectra

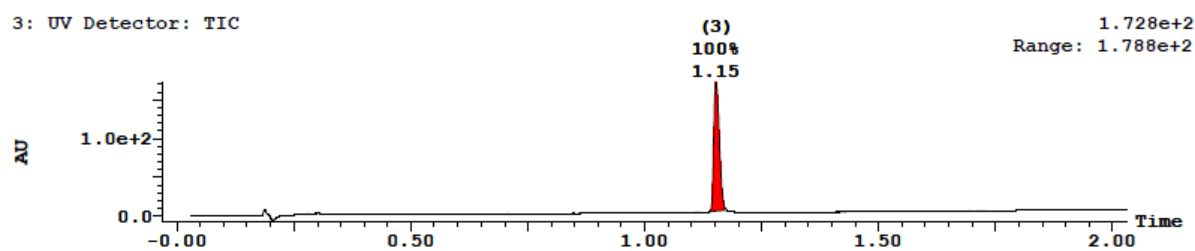


¹³C NMR Spectra



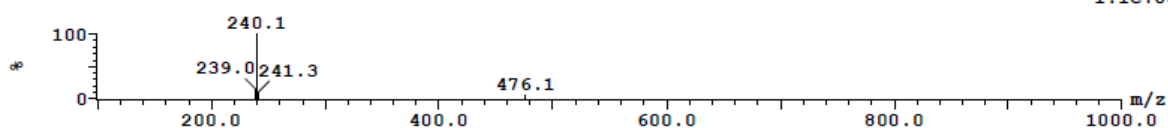
LCMS

3: UV Detector: TIC



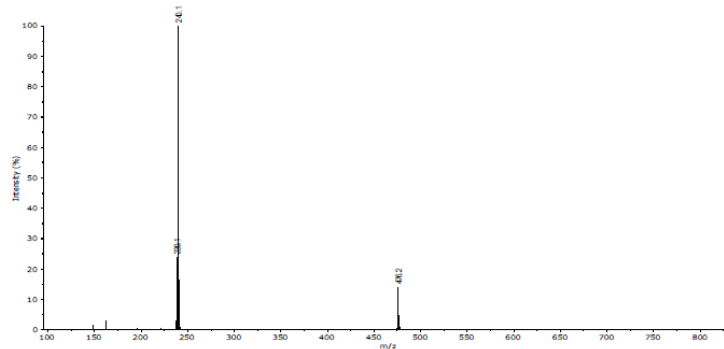
Peak Time
3 1.15
3: (Time: 1.15)

1:MS ES+
1.1e+007

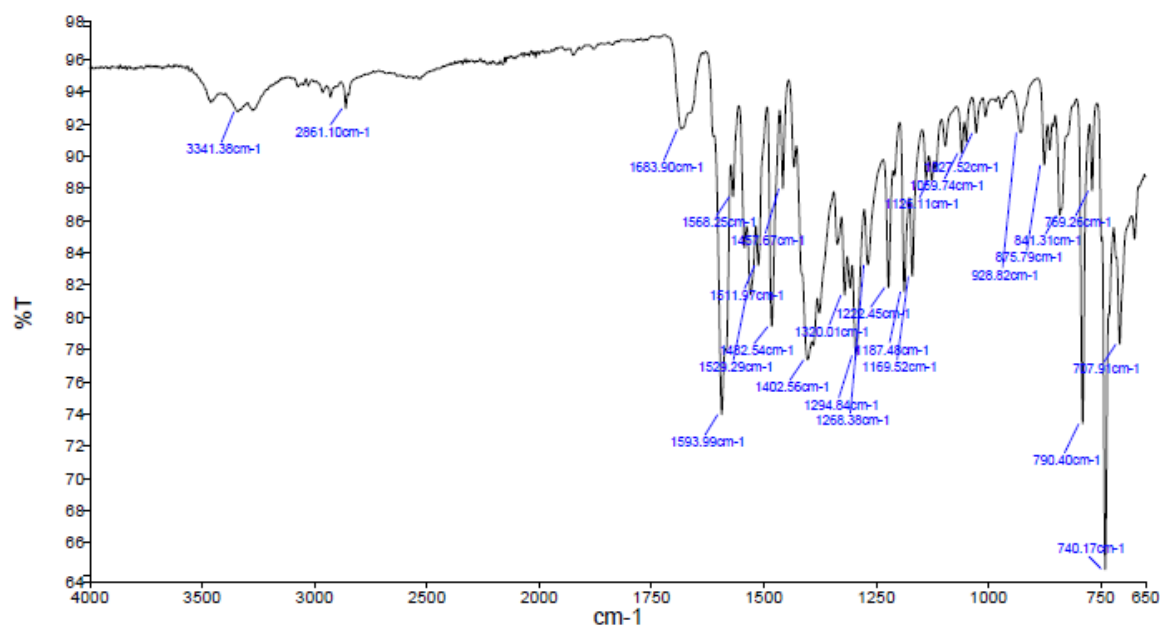


HRMS

Spectrum RT 3.50, Peak [1], Target Mass 221.1073



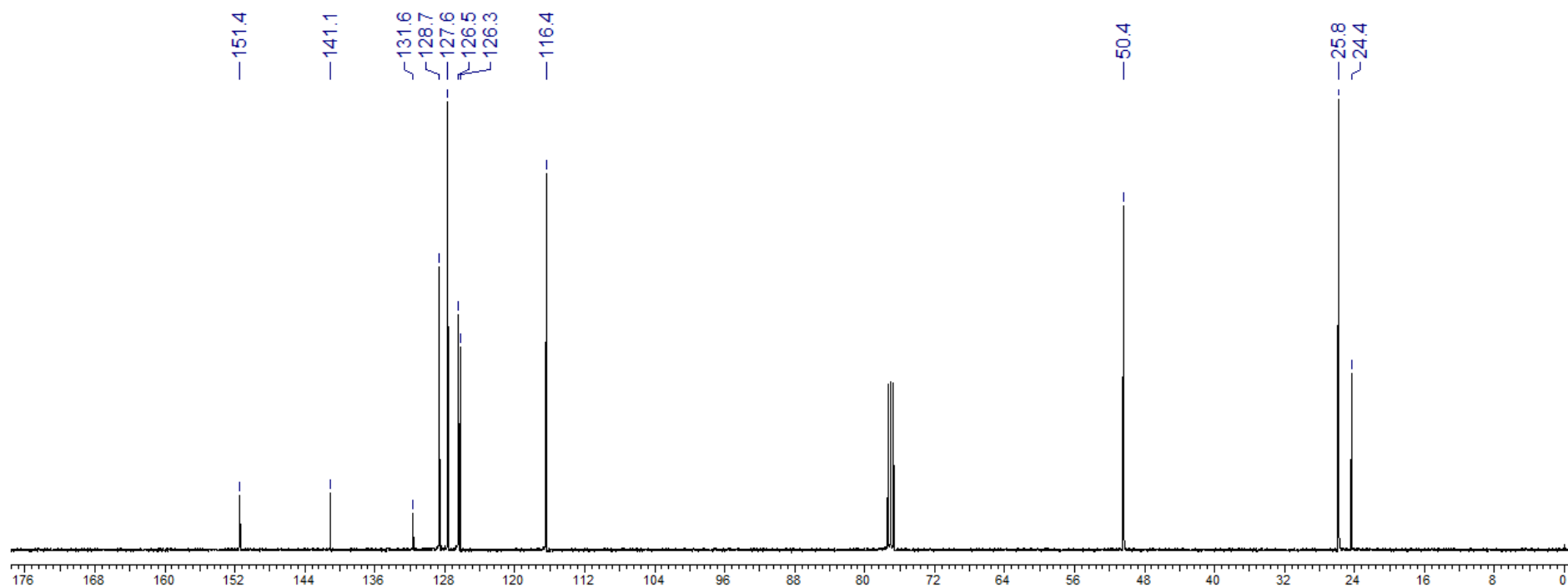
IR Spectra



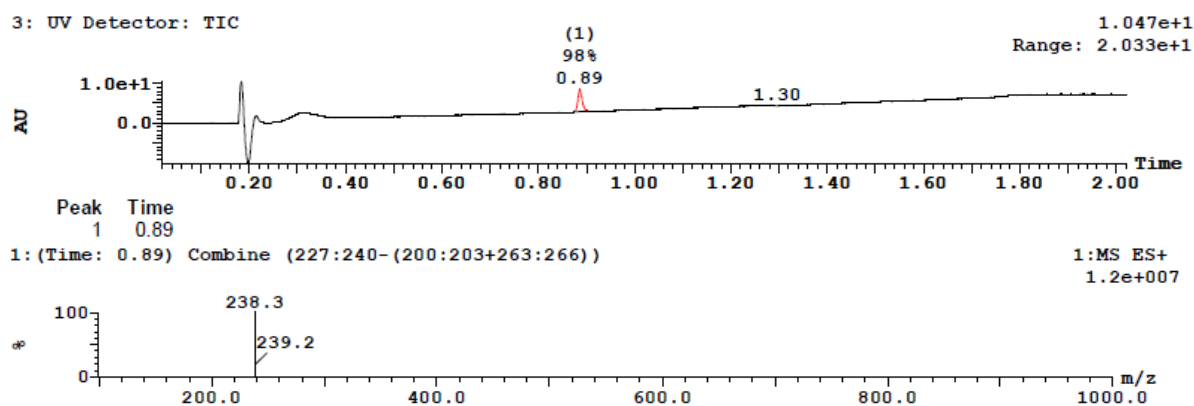
¹H NMR Spectra



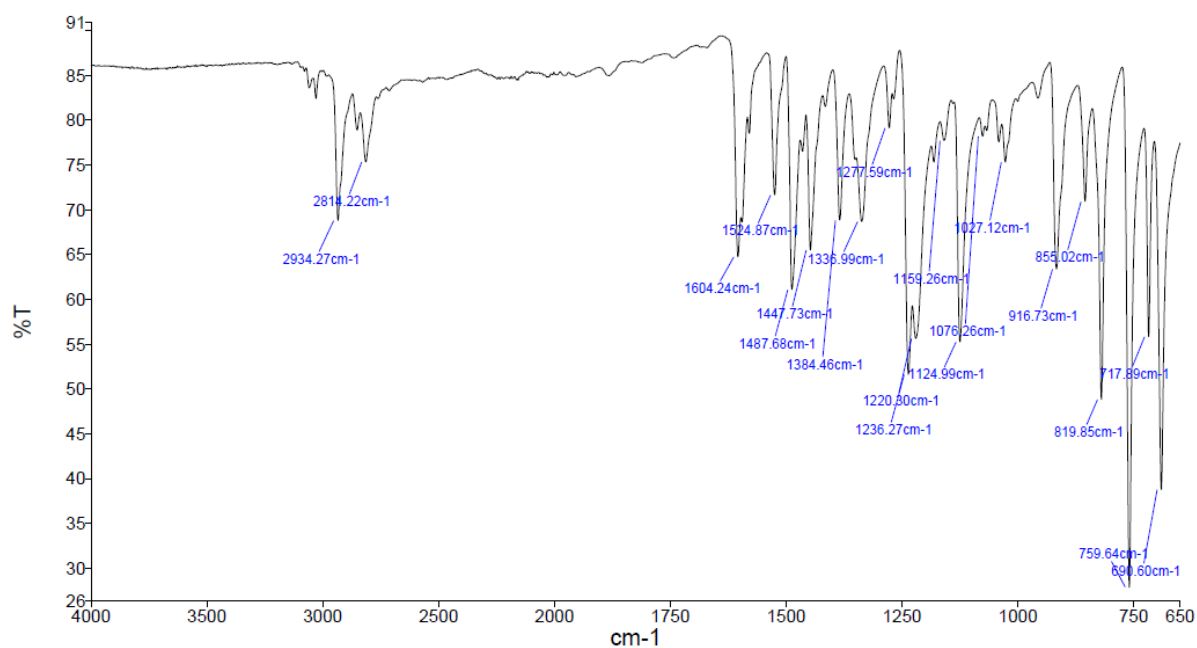
¹³C NMR Spectra



LCMS

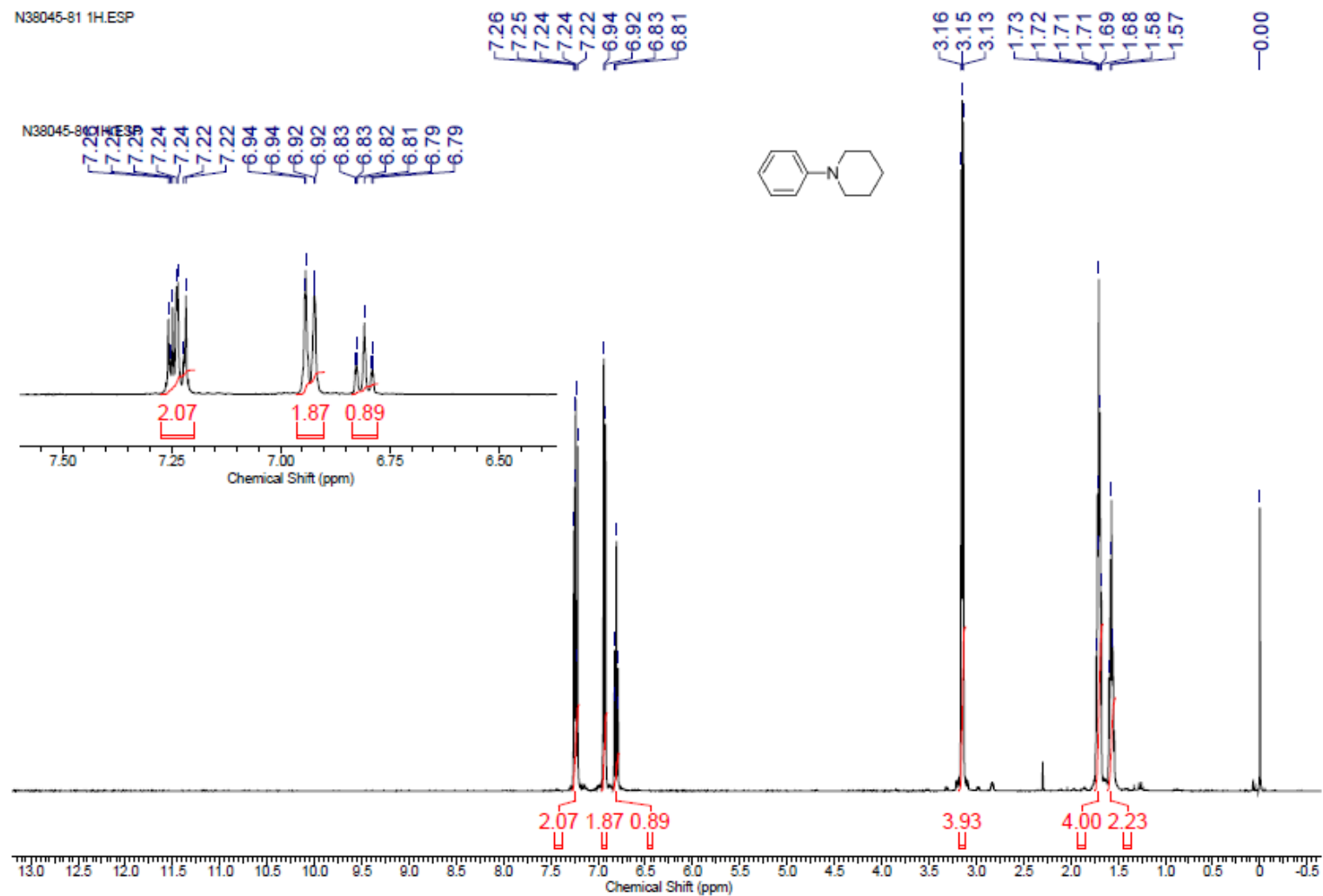


IR Spectra

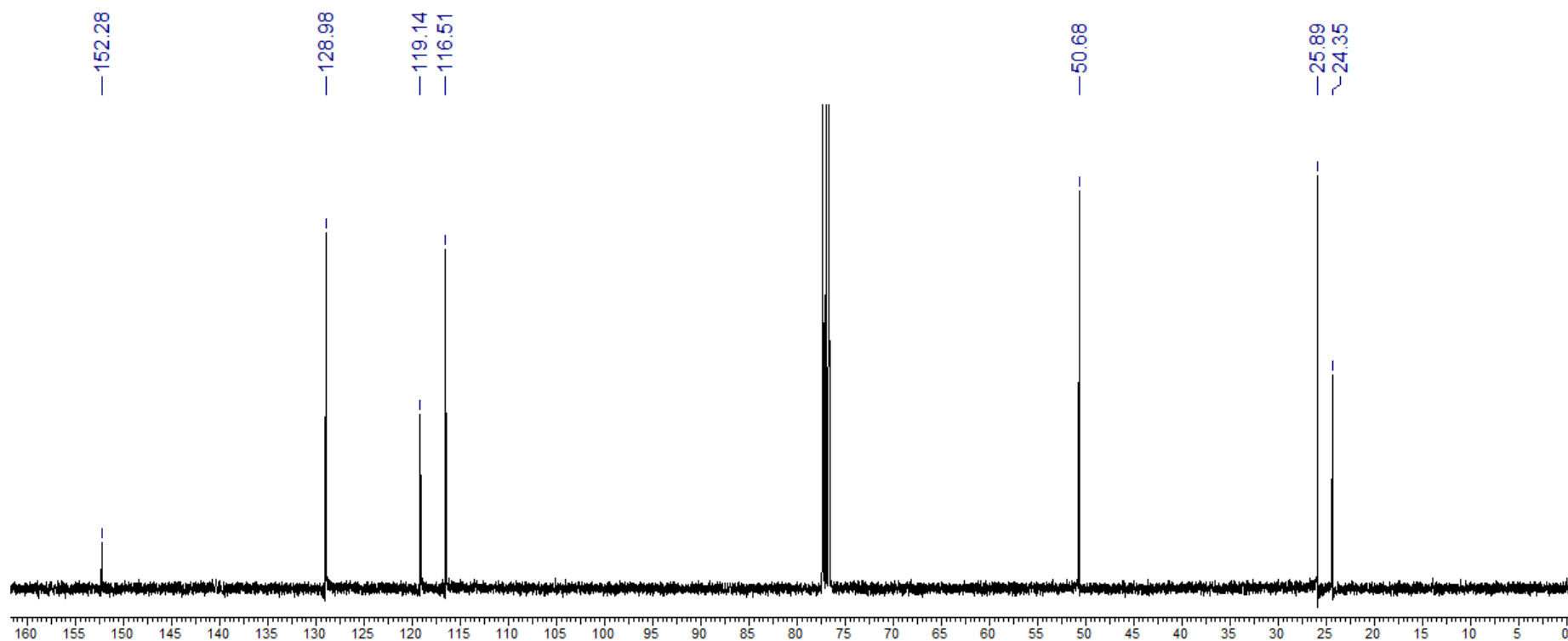


1-Phenylpiperidine (7b).

^1H NMR Spectra



¹³C NMR Spectra



LCMS

3: UV Detector: TAC :Wavelength Range: (210 - 350)

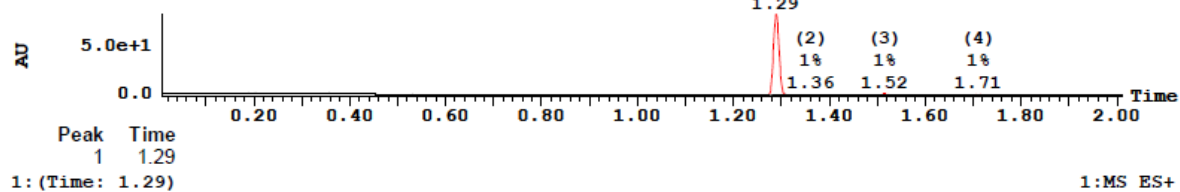
(1)

8.234e+1

Range: 8.481e+1

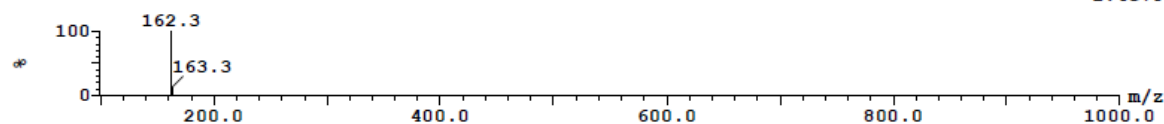
96%

1.29

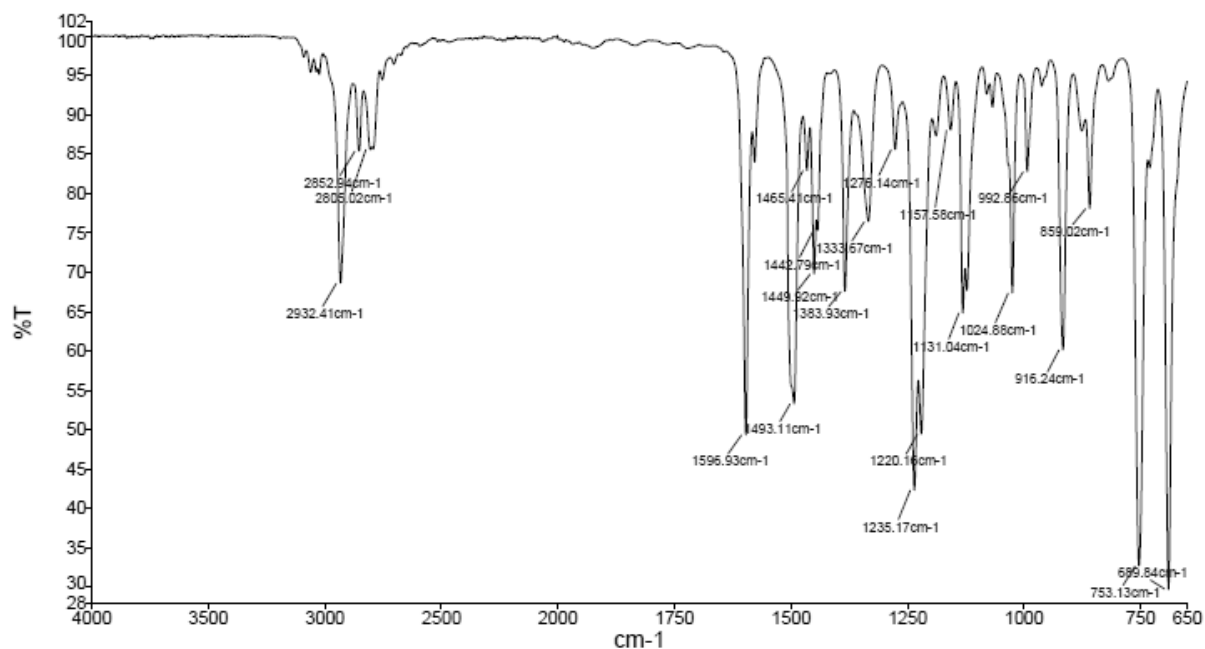


1:MS ES+

1.4e+007

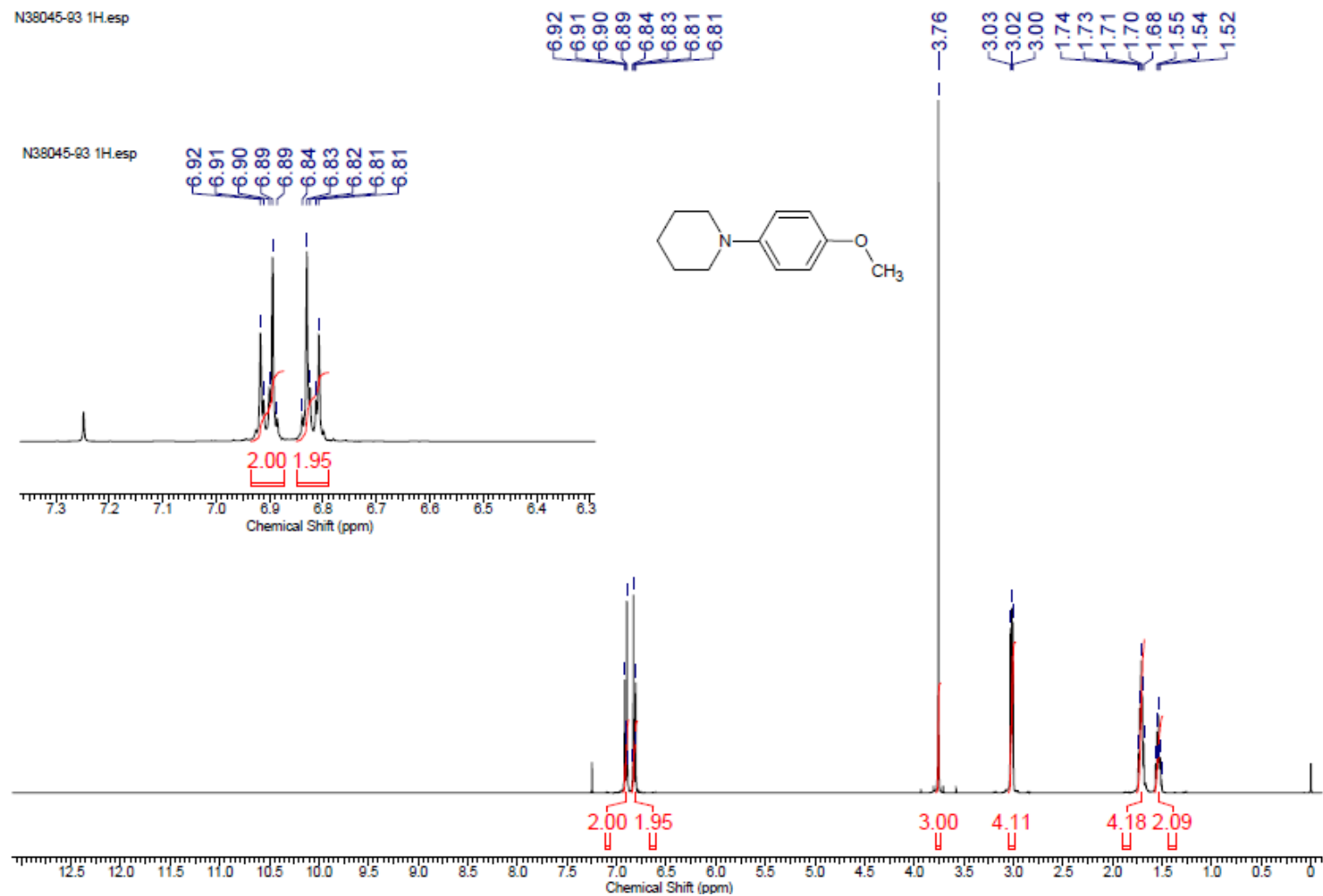


IR Spectra

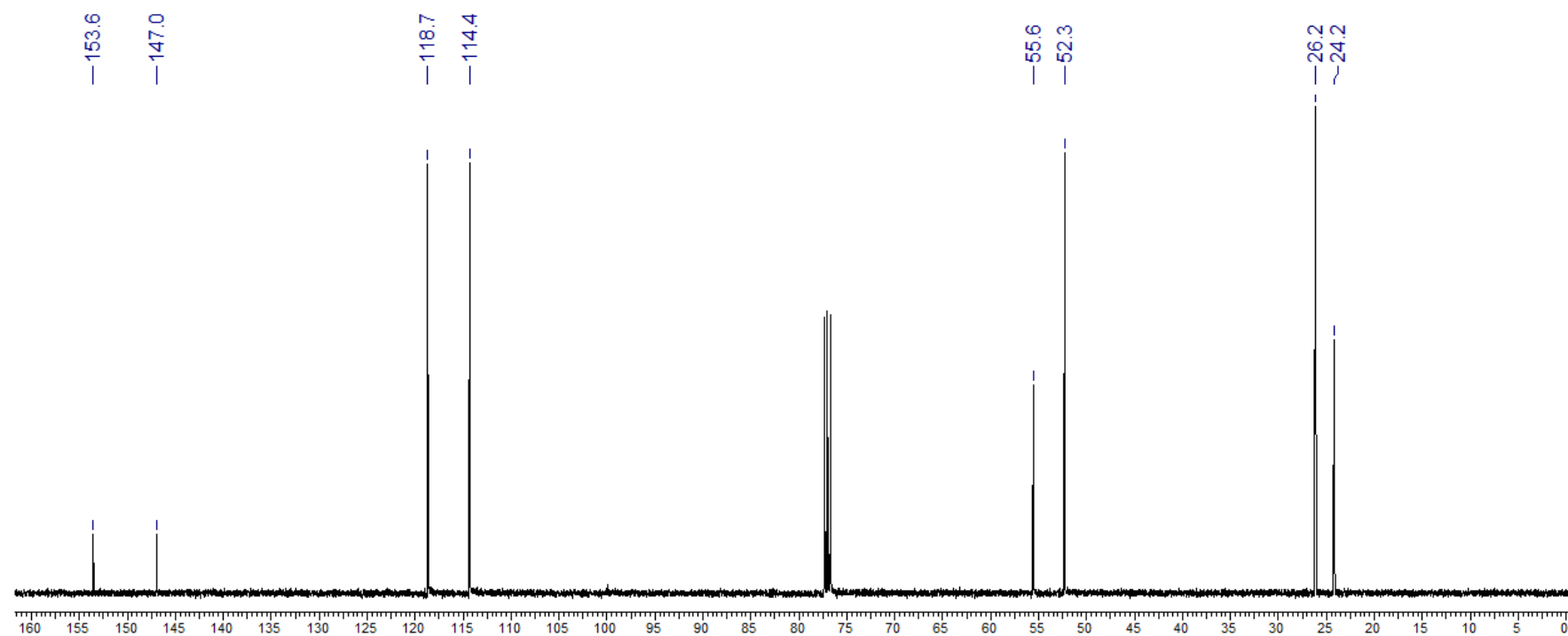


1-(4-Methoxyphenyl)piperidine (7c).

¹H NMR Spectra



¹³C NMR Spectra



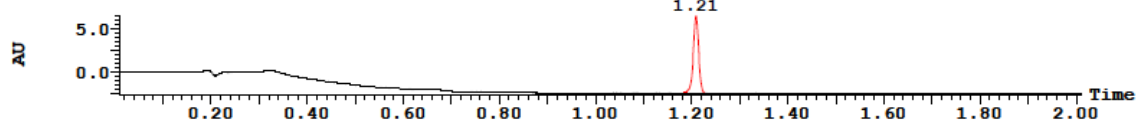
LCMS

3: UV Detector: TAC :Wavelength Range: (210 - 350)

(1)

6.536

Range: 9.048

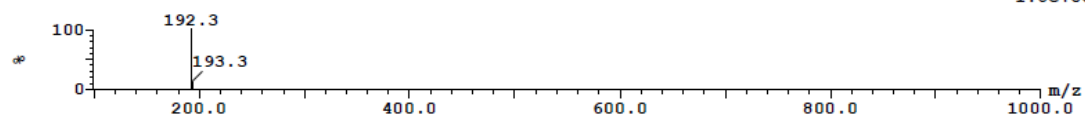


Peak Time
1 1.21

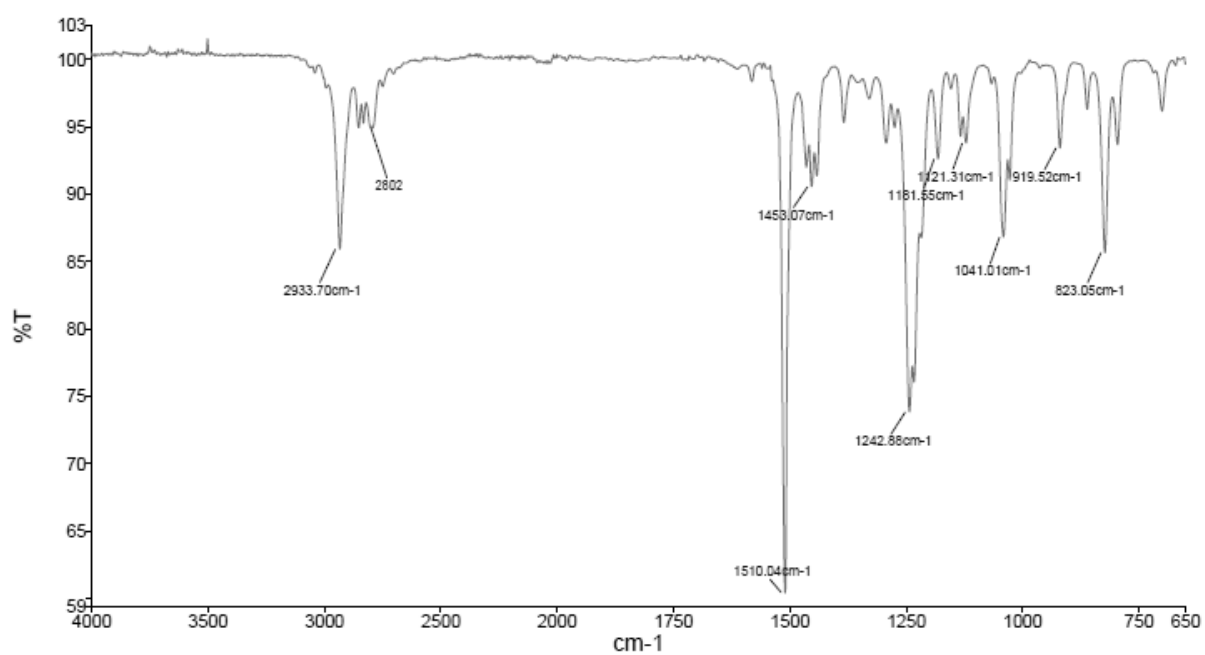
1: (Time: 1.21)

1:MS ES+

1.8e+007

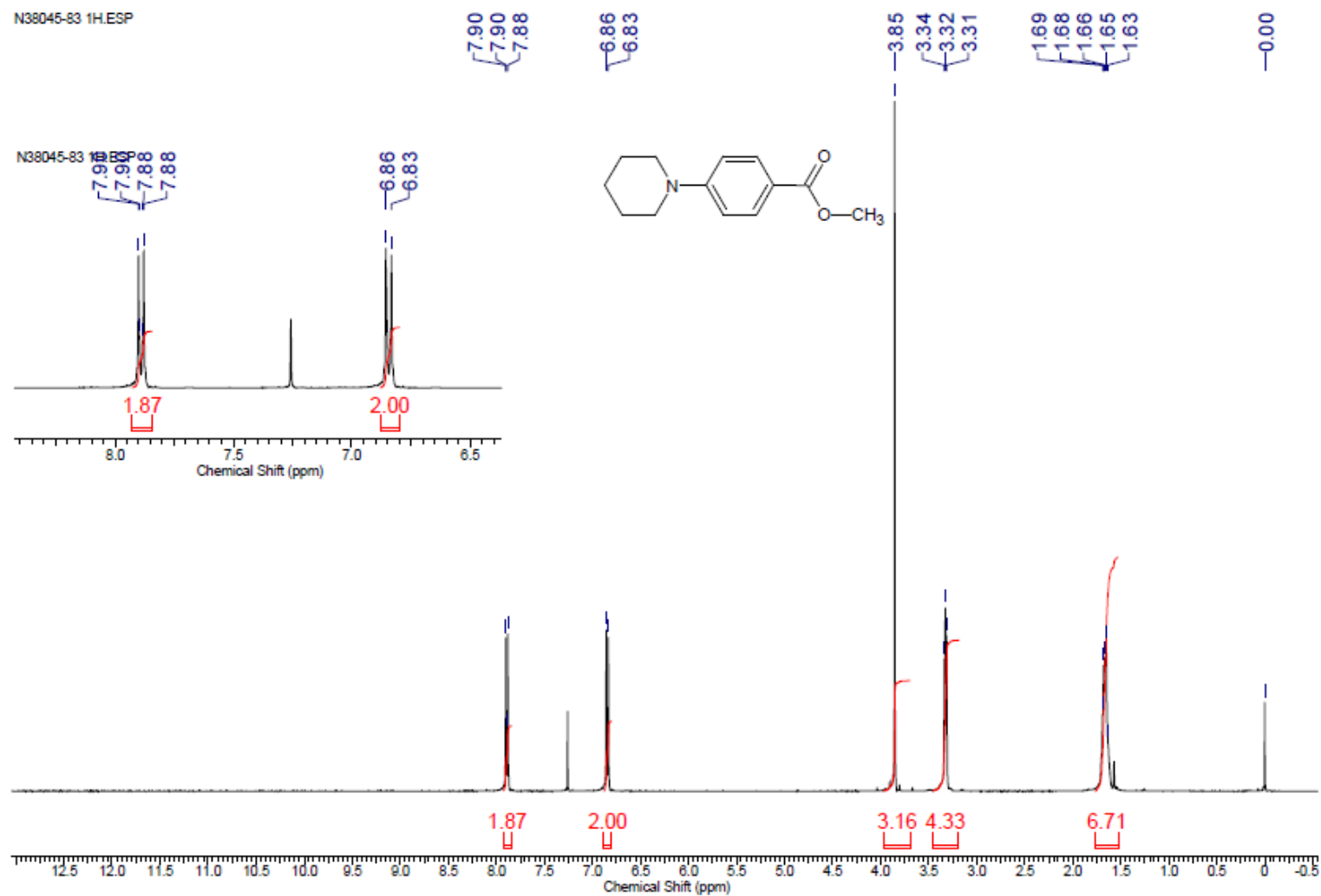


IR Spectra

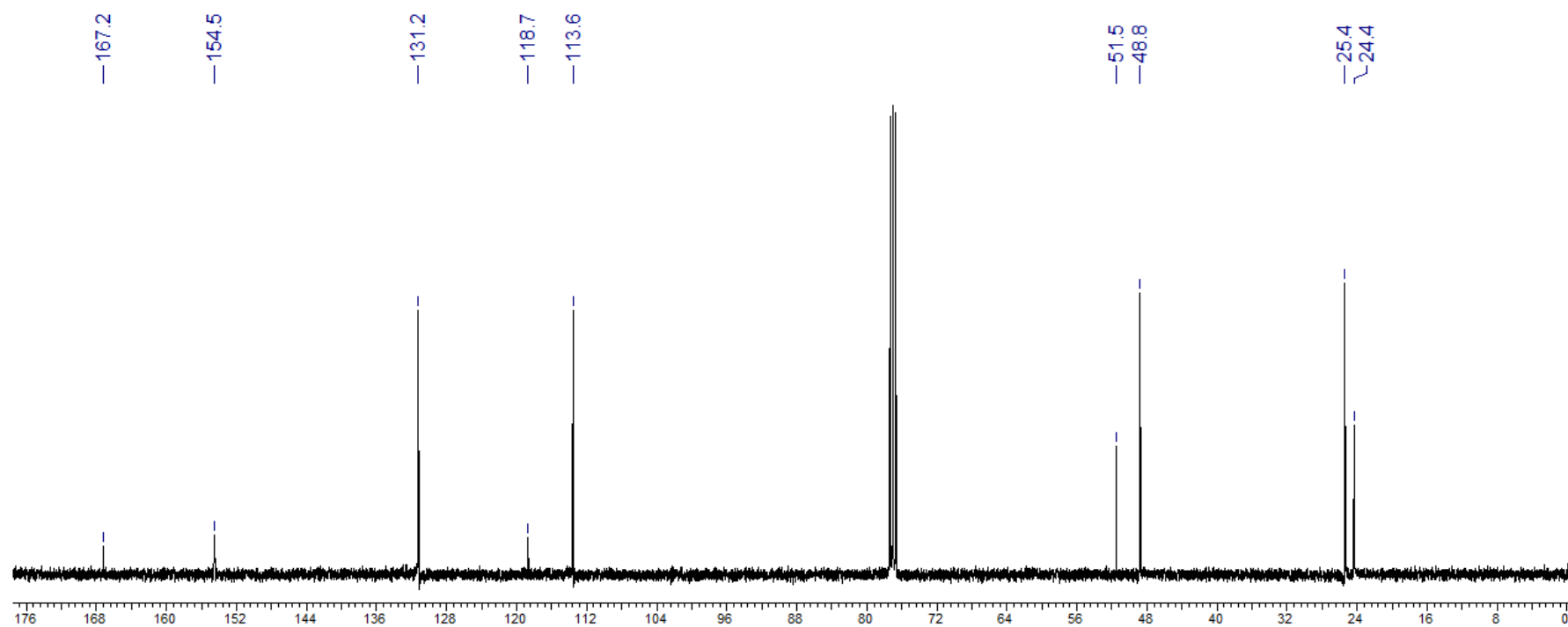


Methyl 4-(piperidin-1-yl)benzoate (7d).

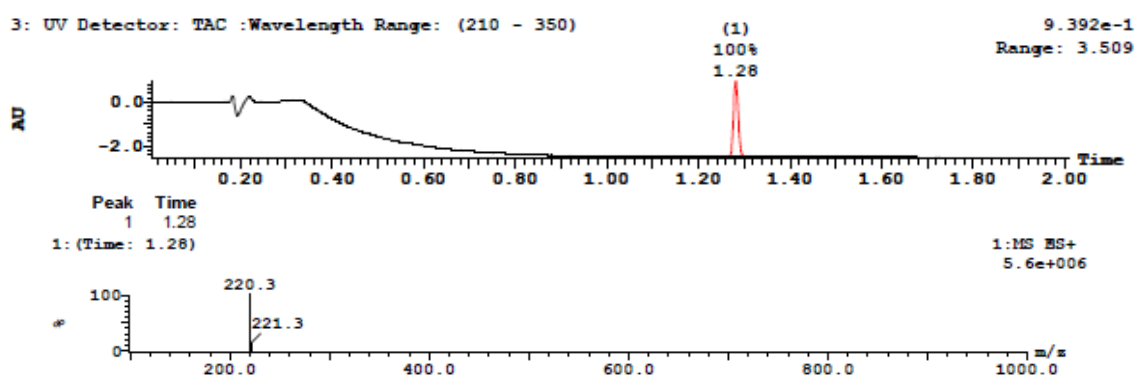
¹H NMR Spectra



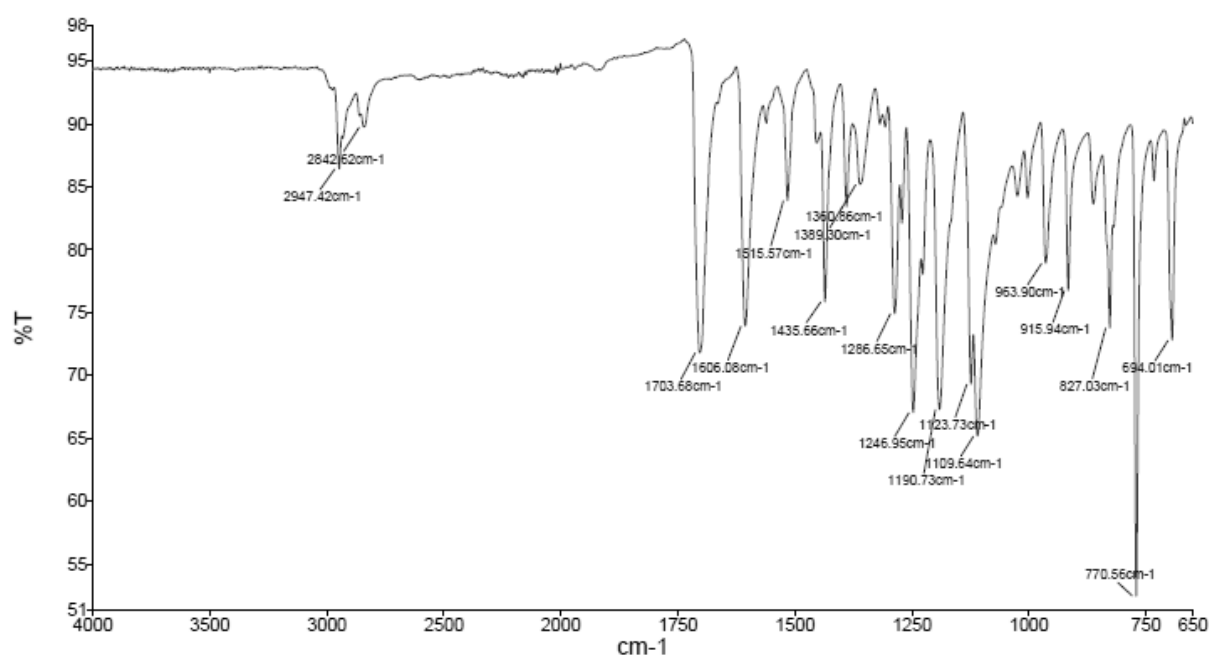
¹³C NMR Spectra



LCMS

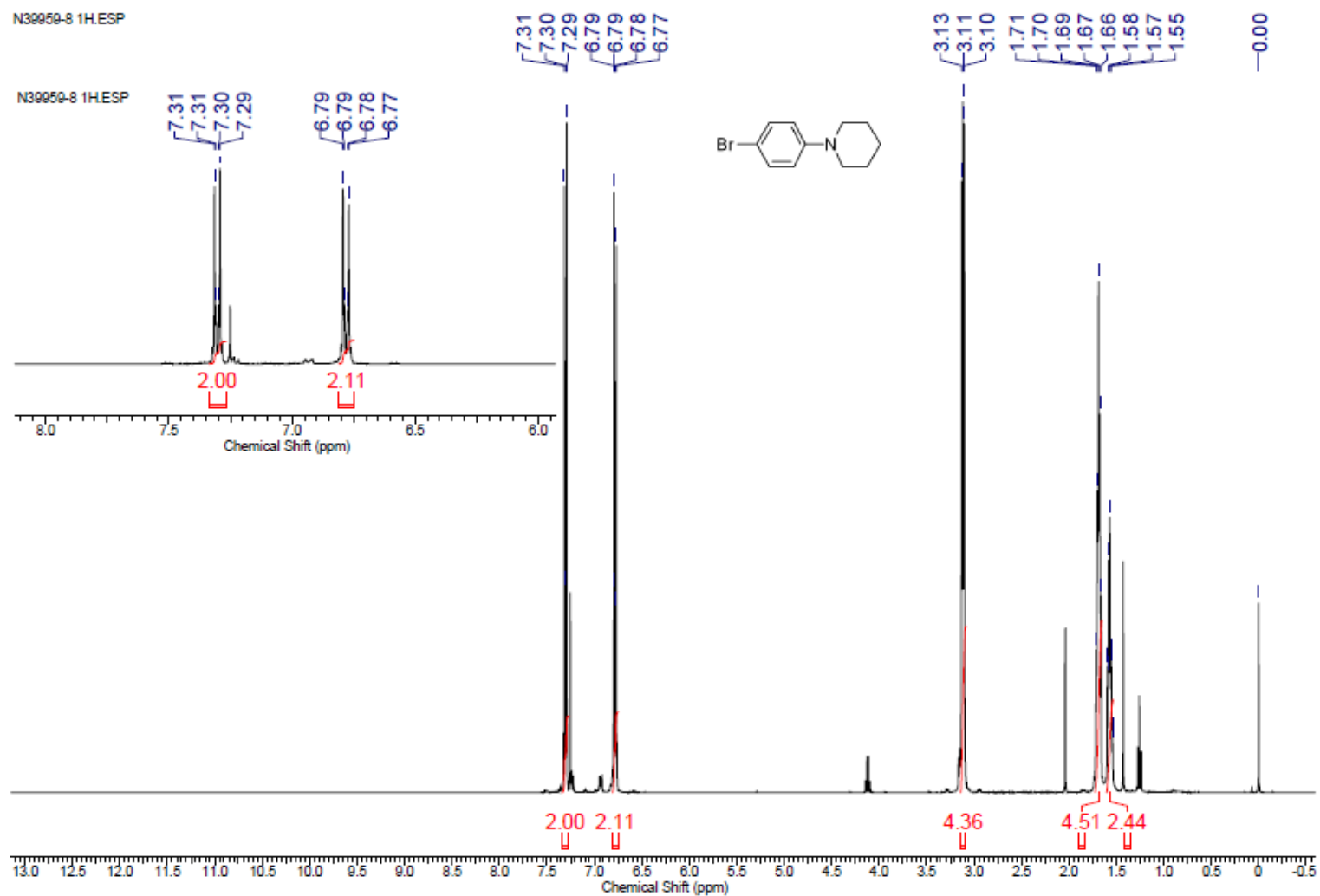


IR Spectra

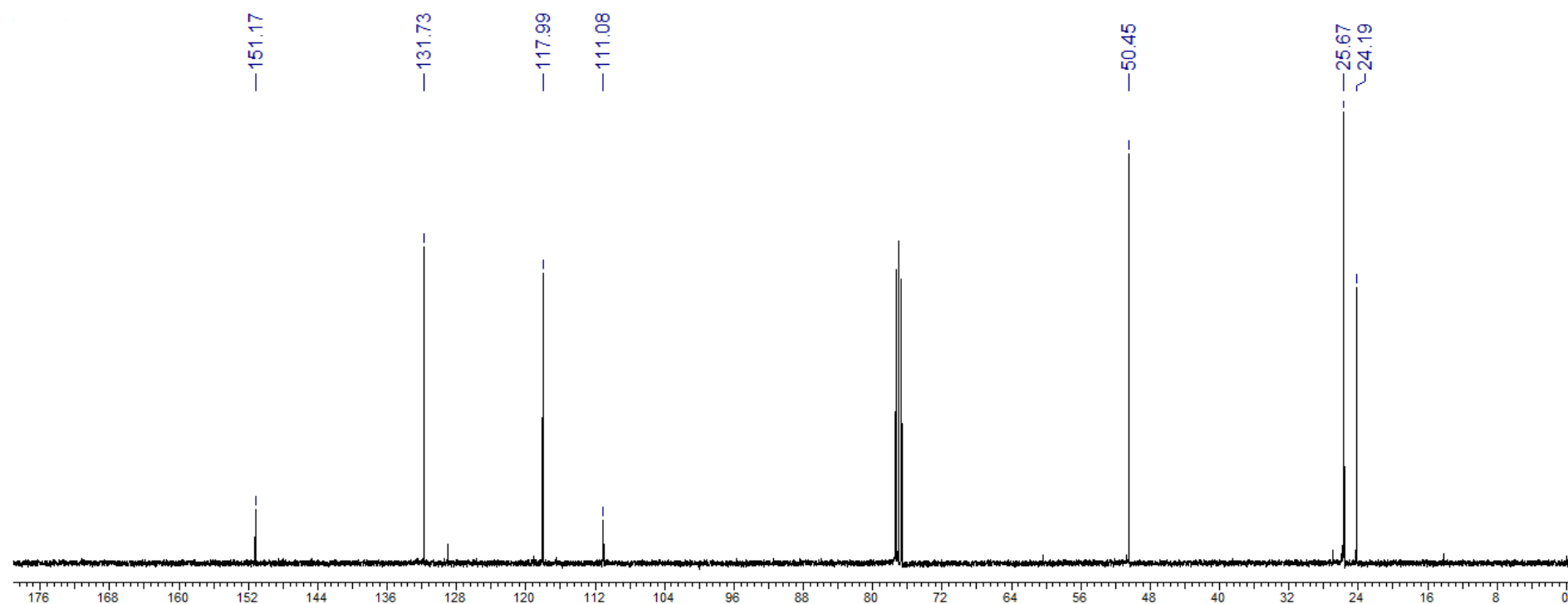


1-(4-Bromophenyl)piperidine (7e).

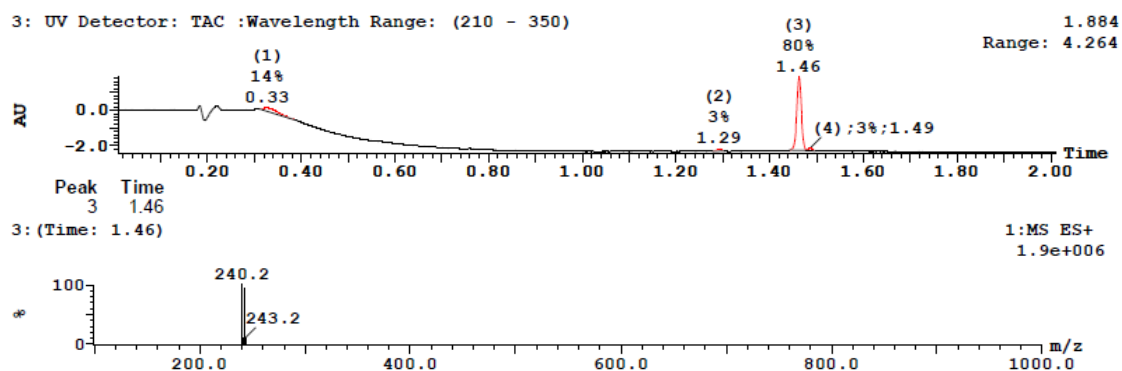
¹H NMR Spectra



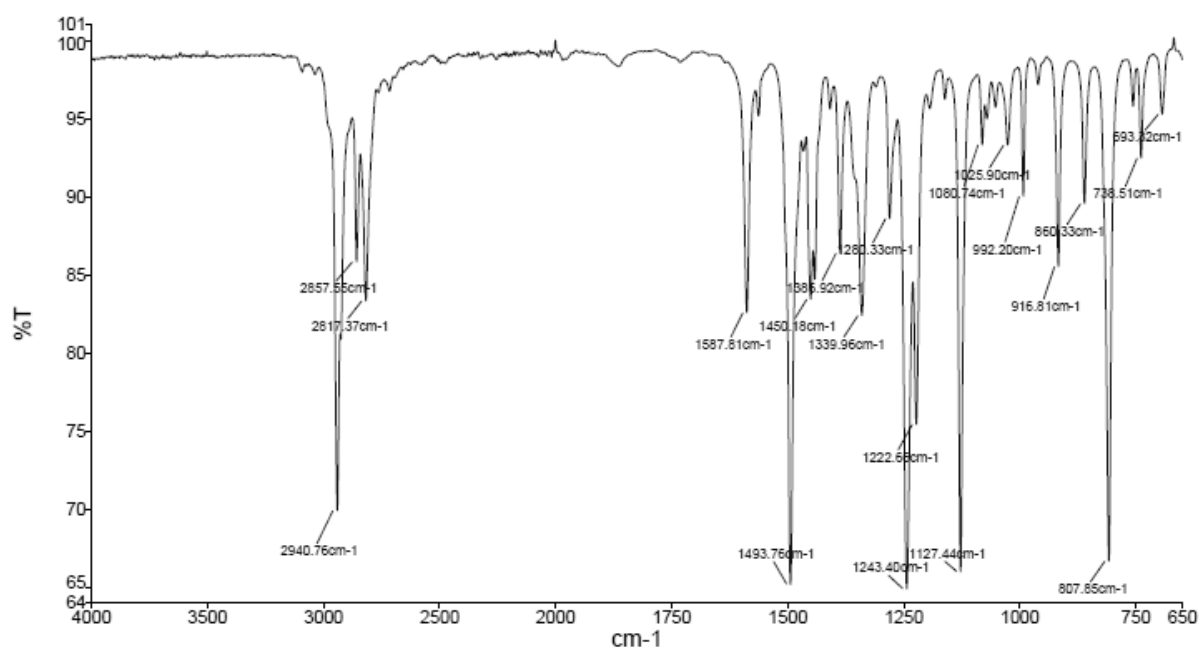
¹³C NMR Spectra



LCMS

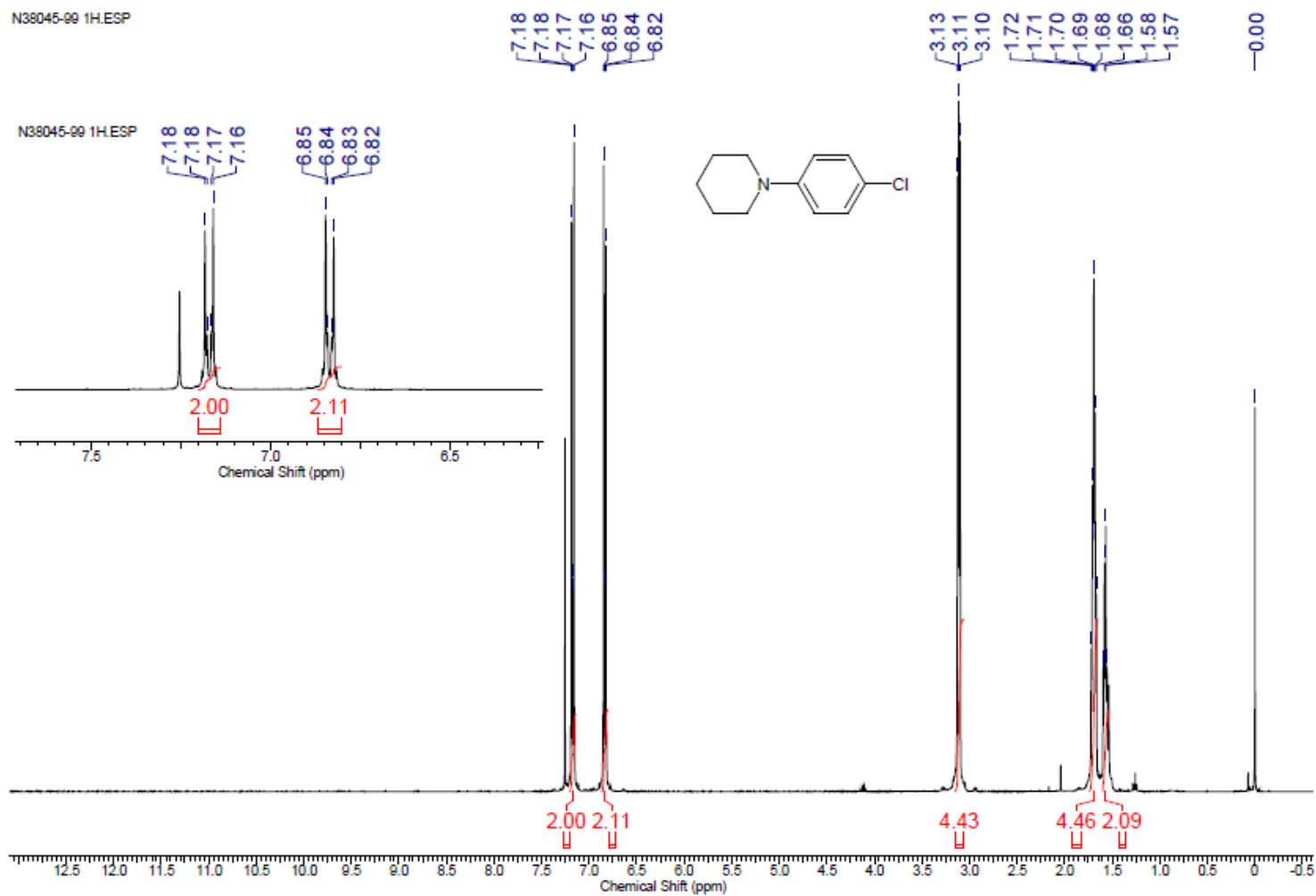


IR Spectra

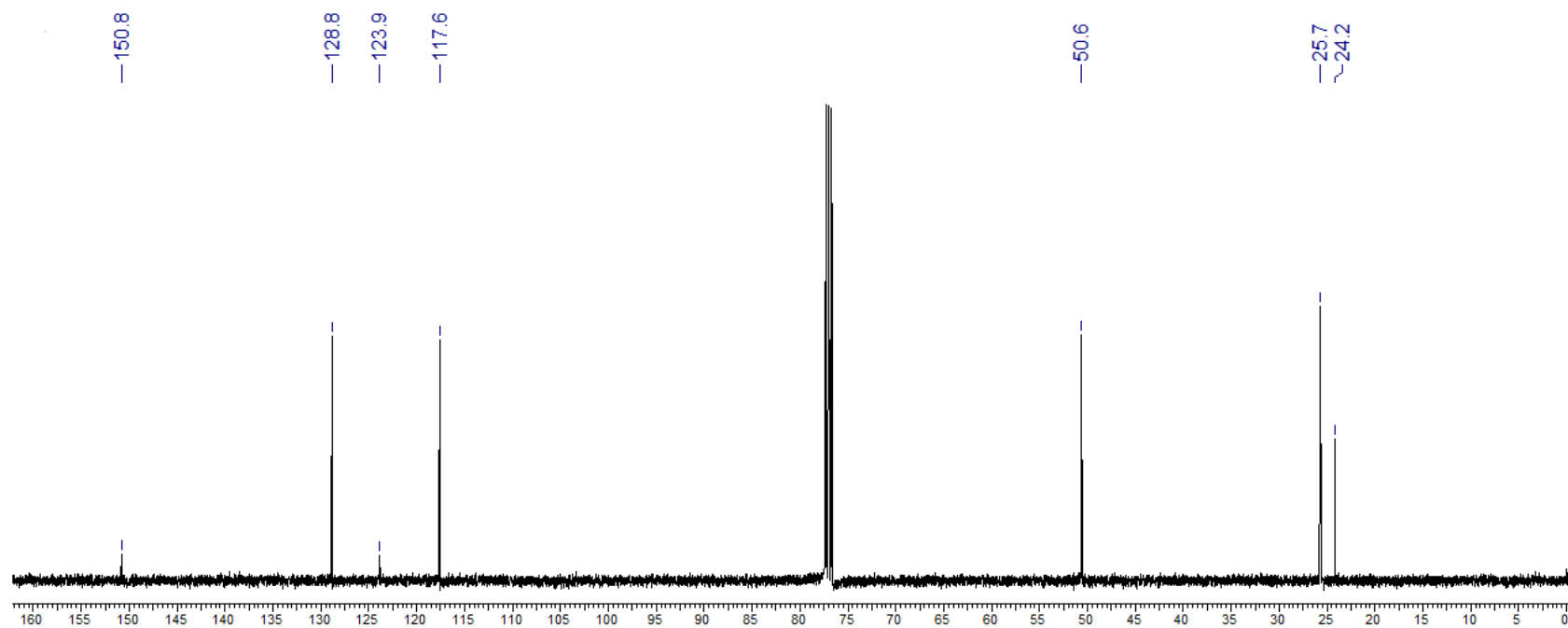


1-(4-Chlorophenyl)piperidine (7f).

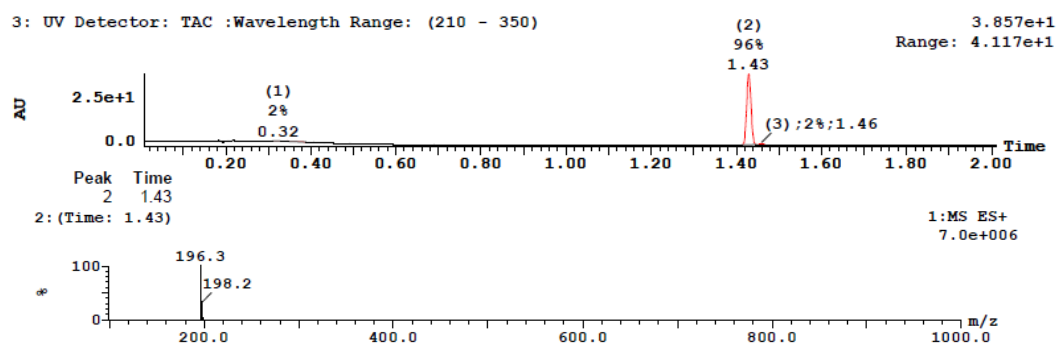
¹H NMR Spectra



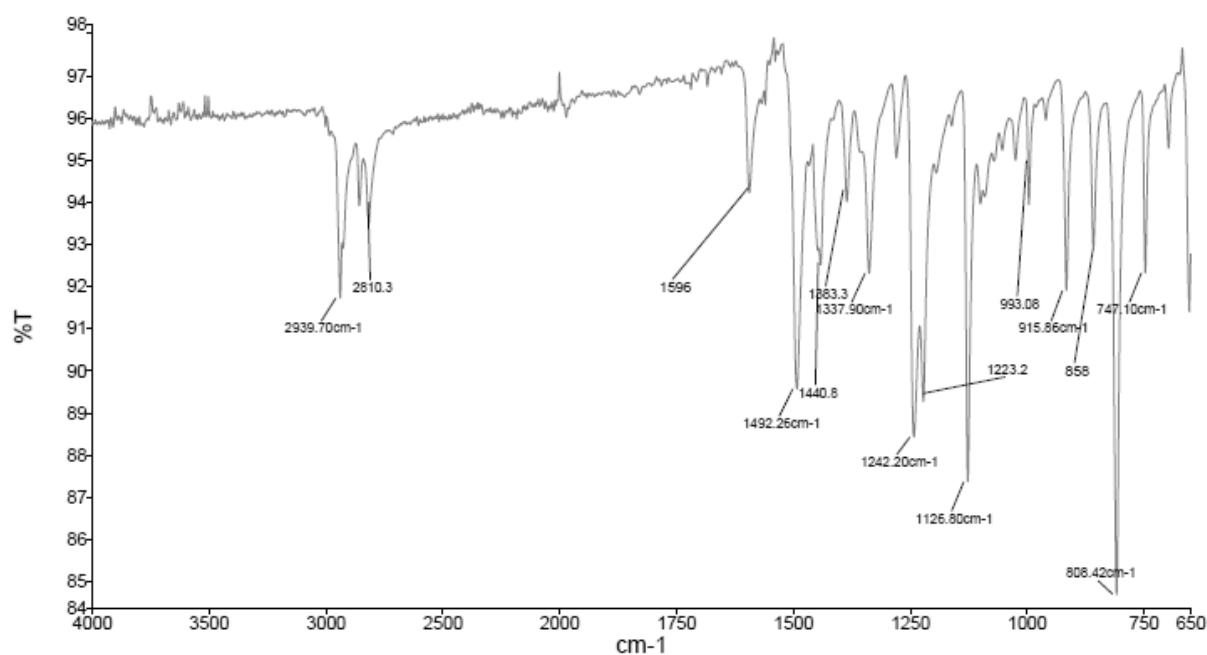
^{13}C NMR Spectra



LCMS



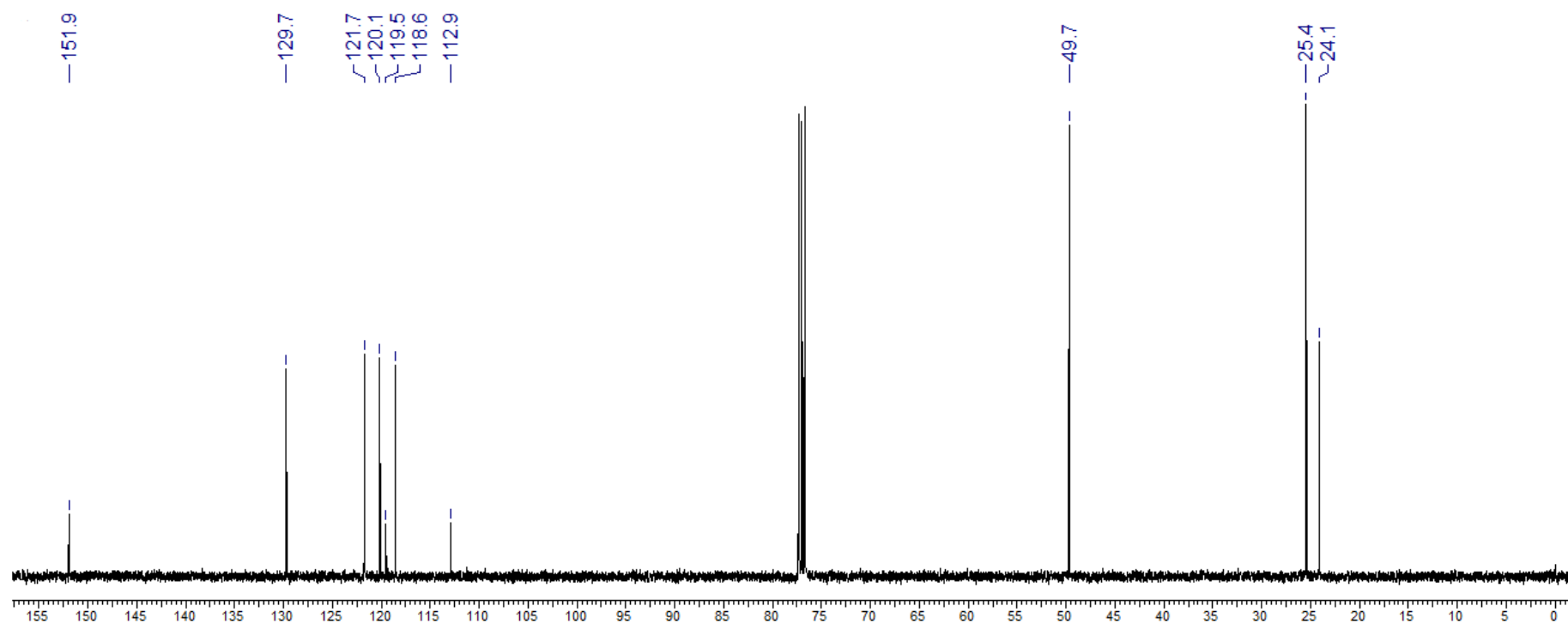
IR Spectra



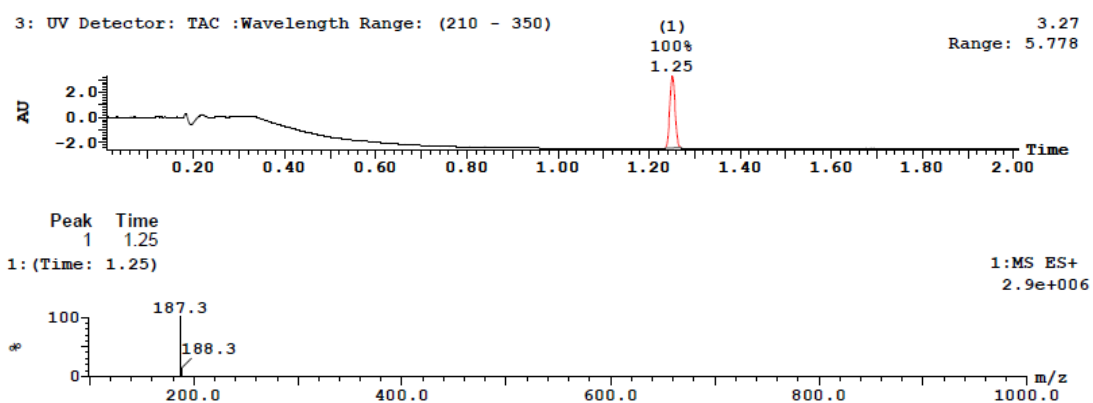
¹H NMR Spectra



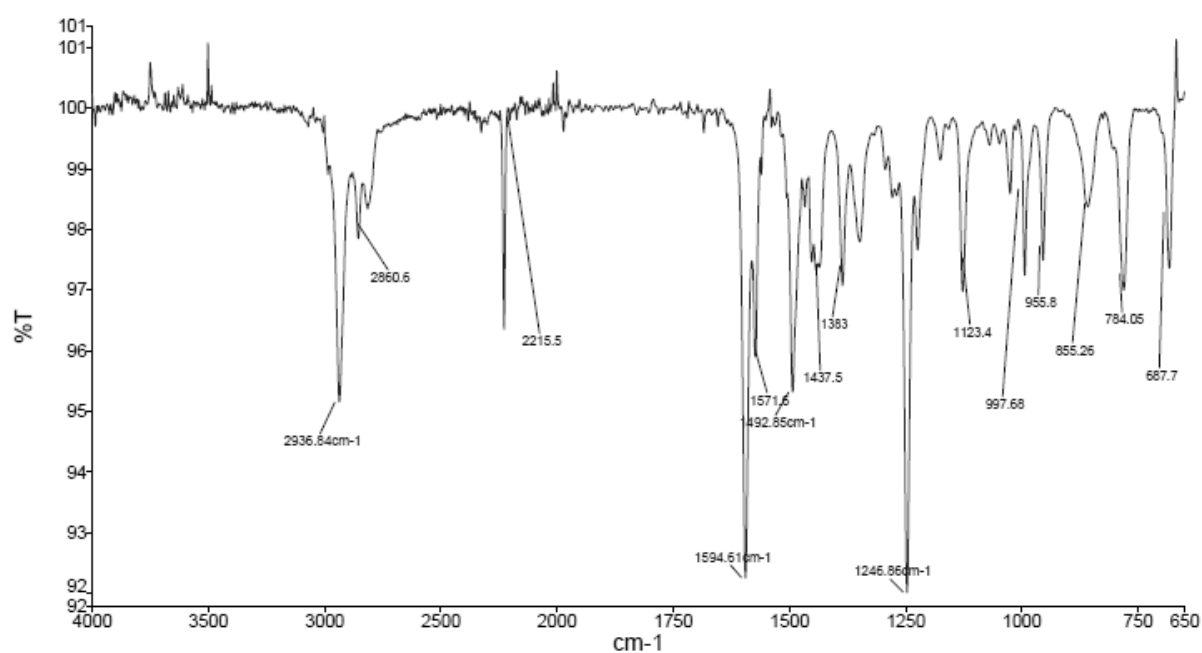
¹³C NMR Spectra



LCMS

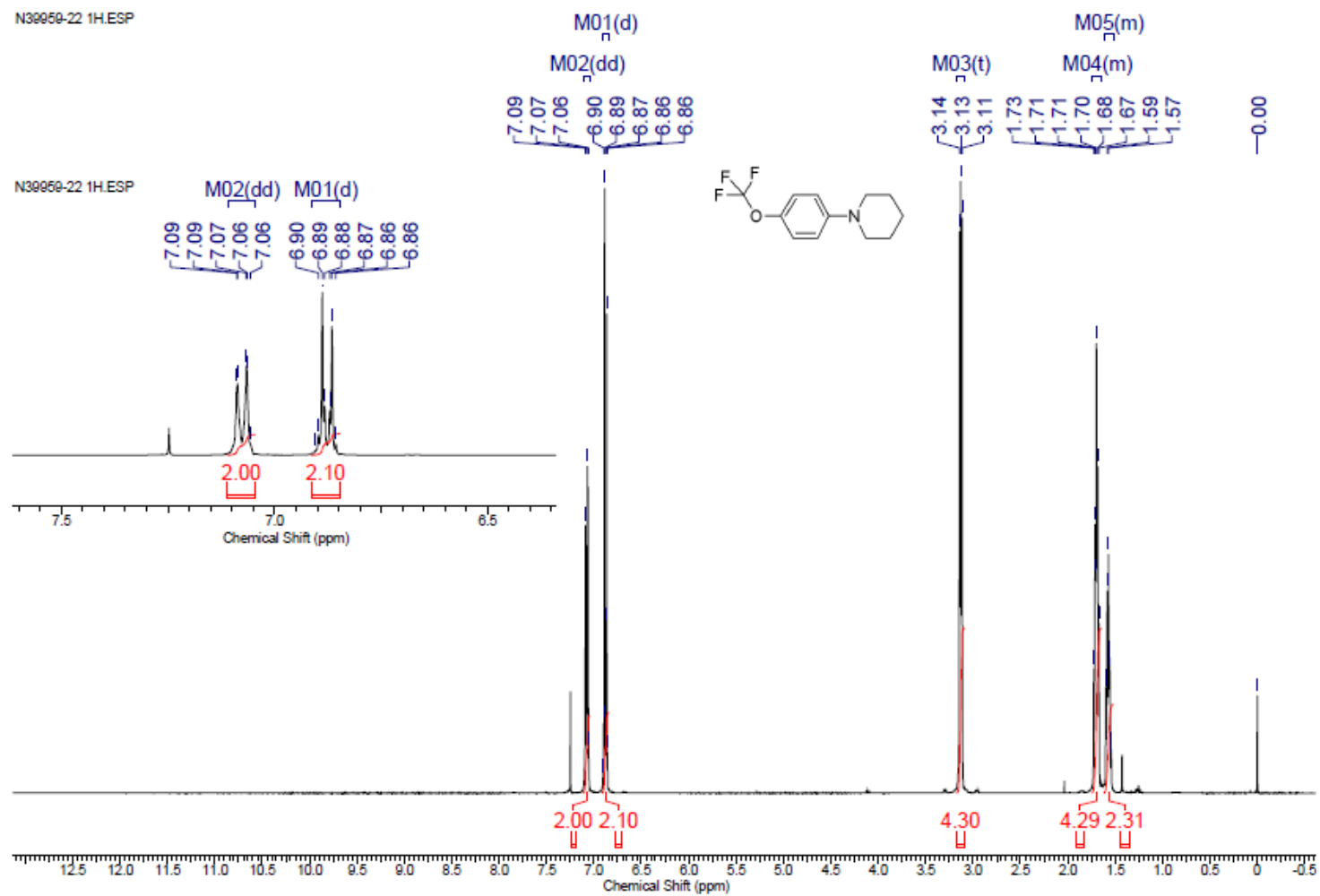


IR Spectra

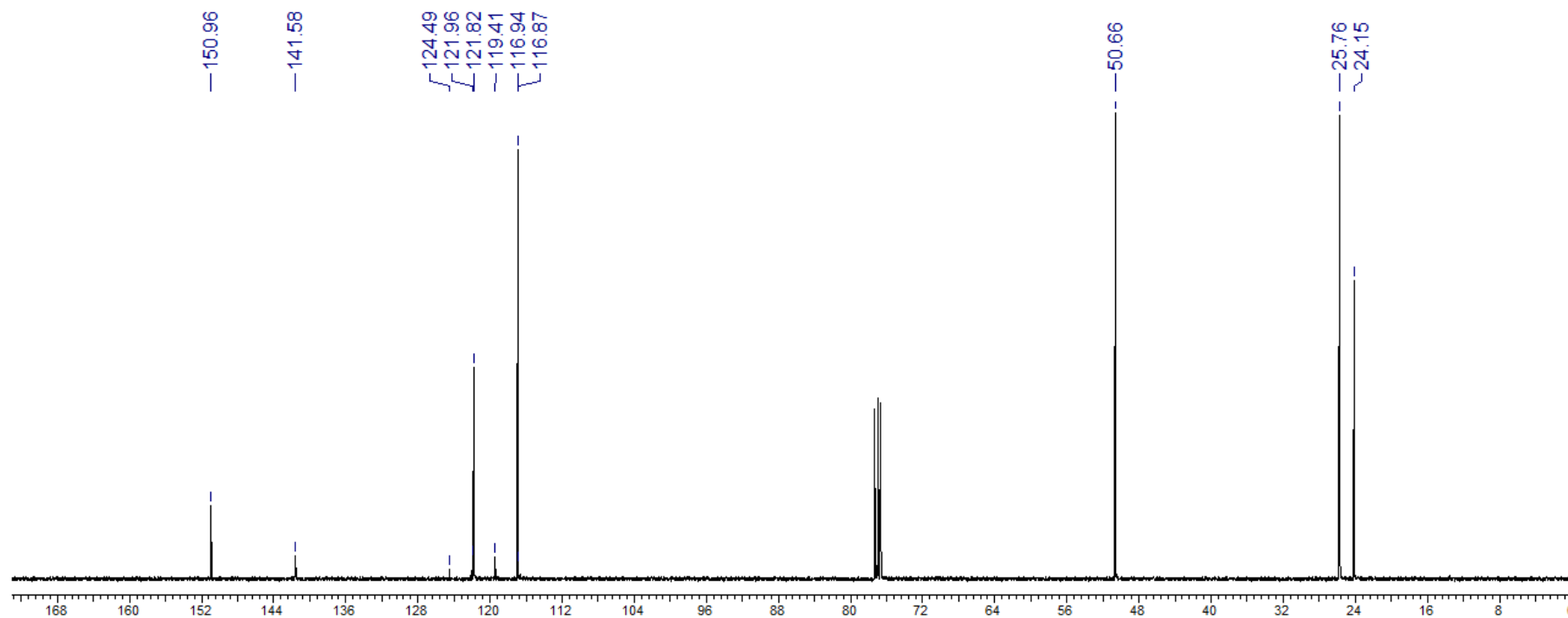


1-(4-(Trifluoromethoxy)phenyl)piperidine (7h).

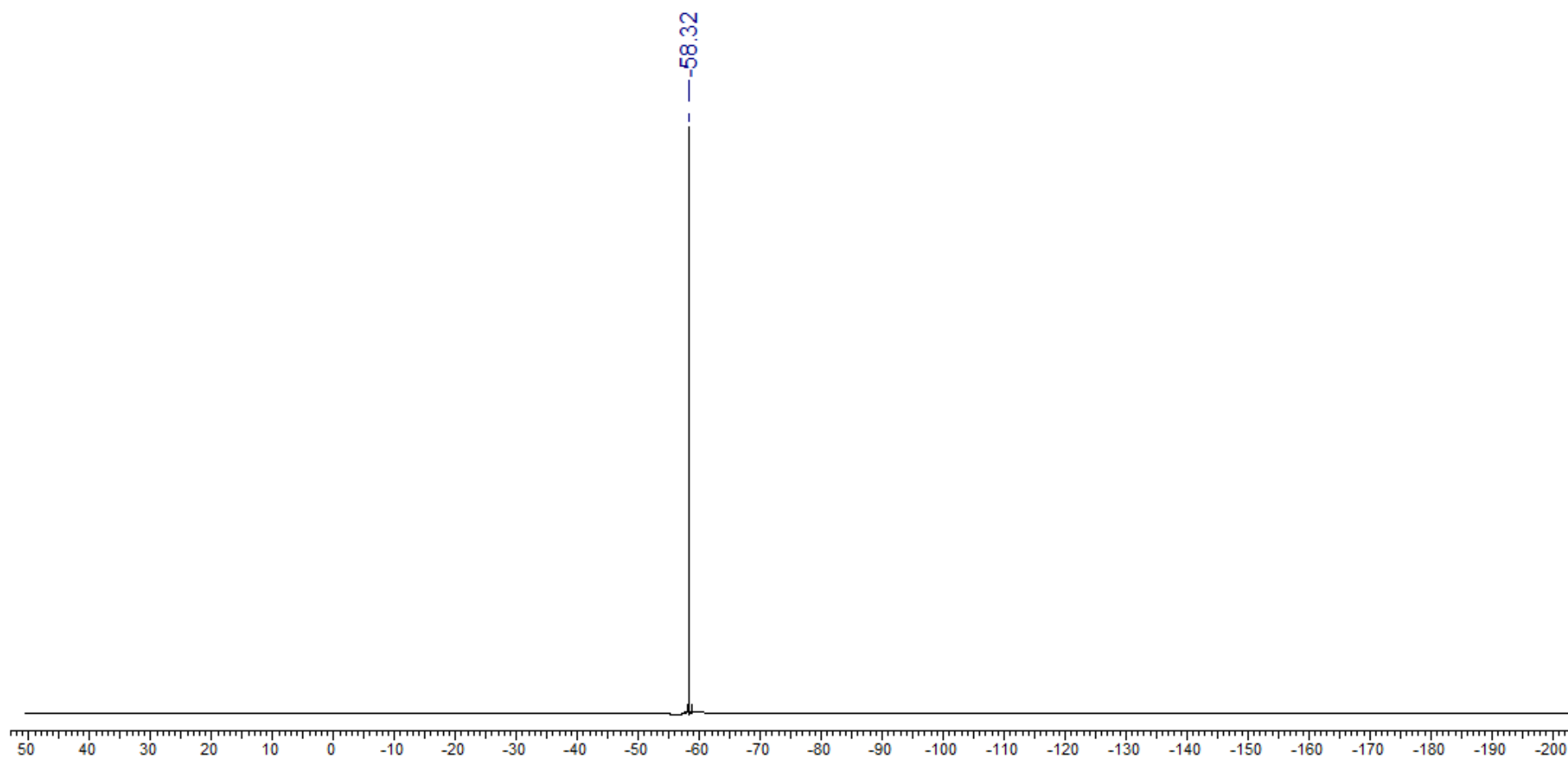
¹H NMR Spectra



^{13}C NMR Spectra

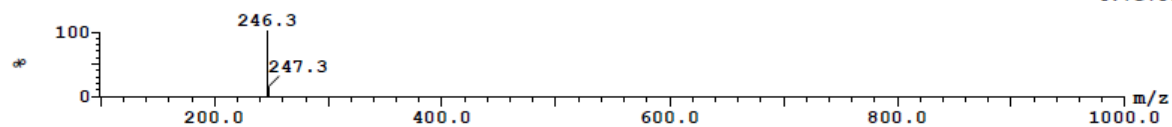
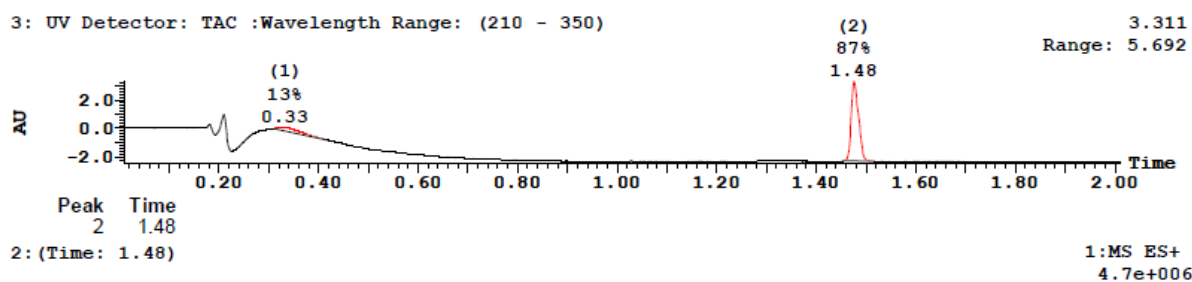


^{19}F NMR Spectra



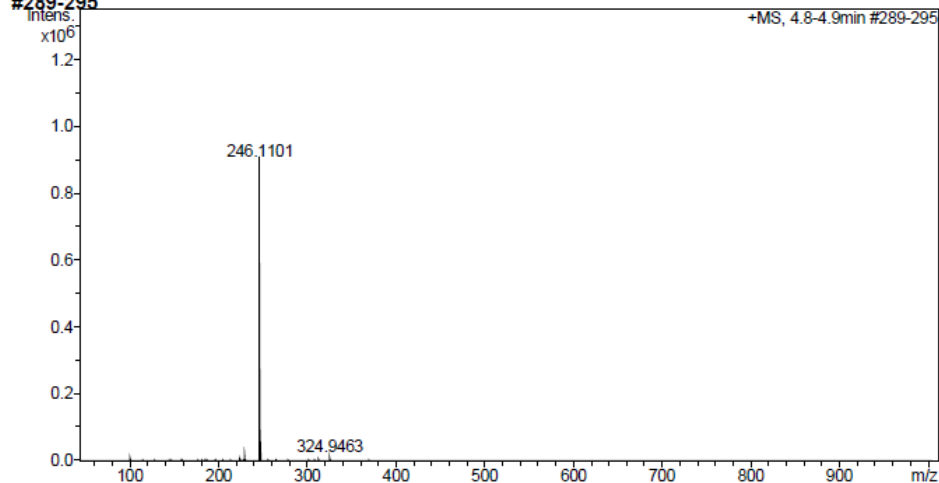
LCMS

3: UV Detector: TAC :Wavelength Range: (210 - 350)

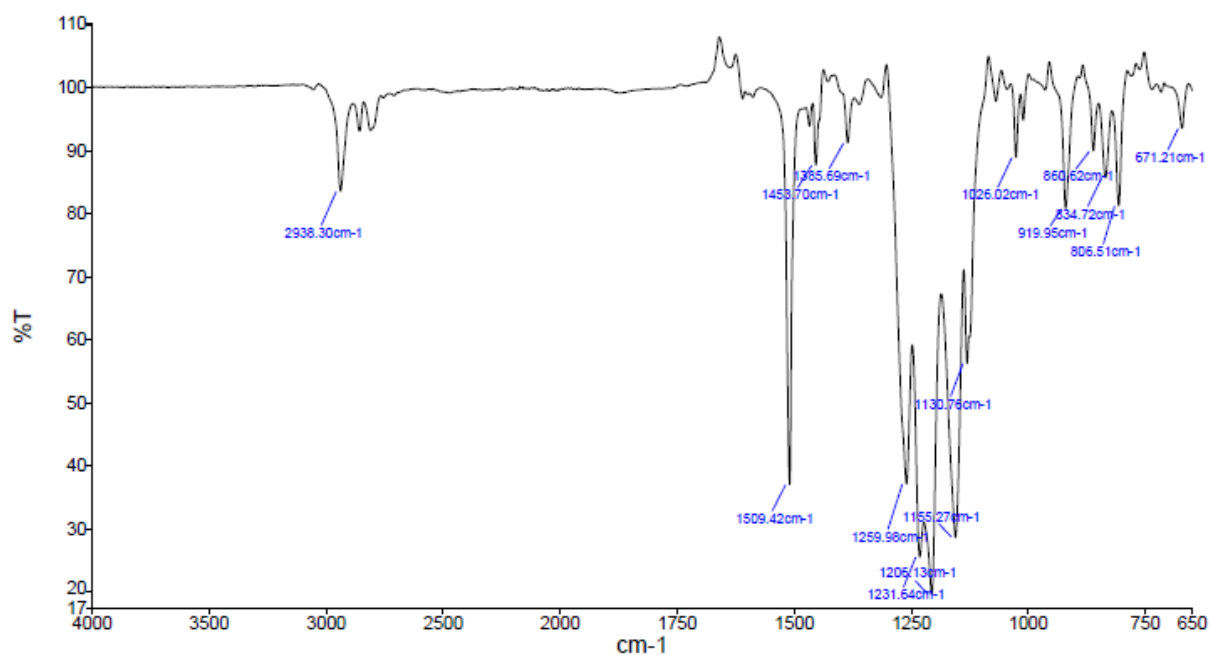


HRMS

+MS, 4.8-4.9min
#289-295

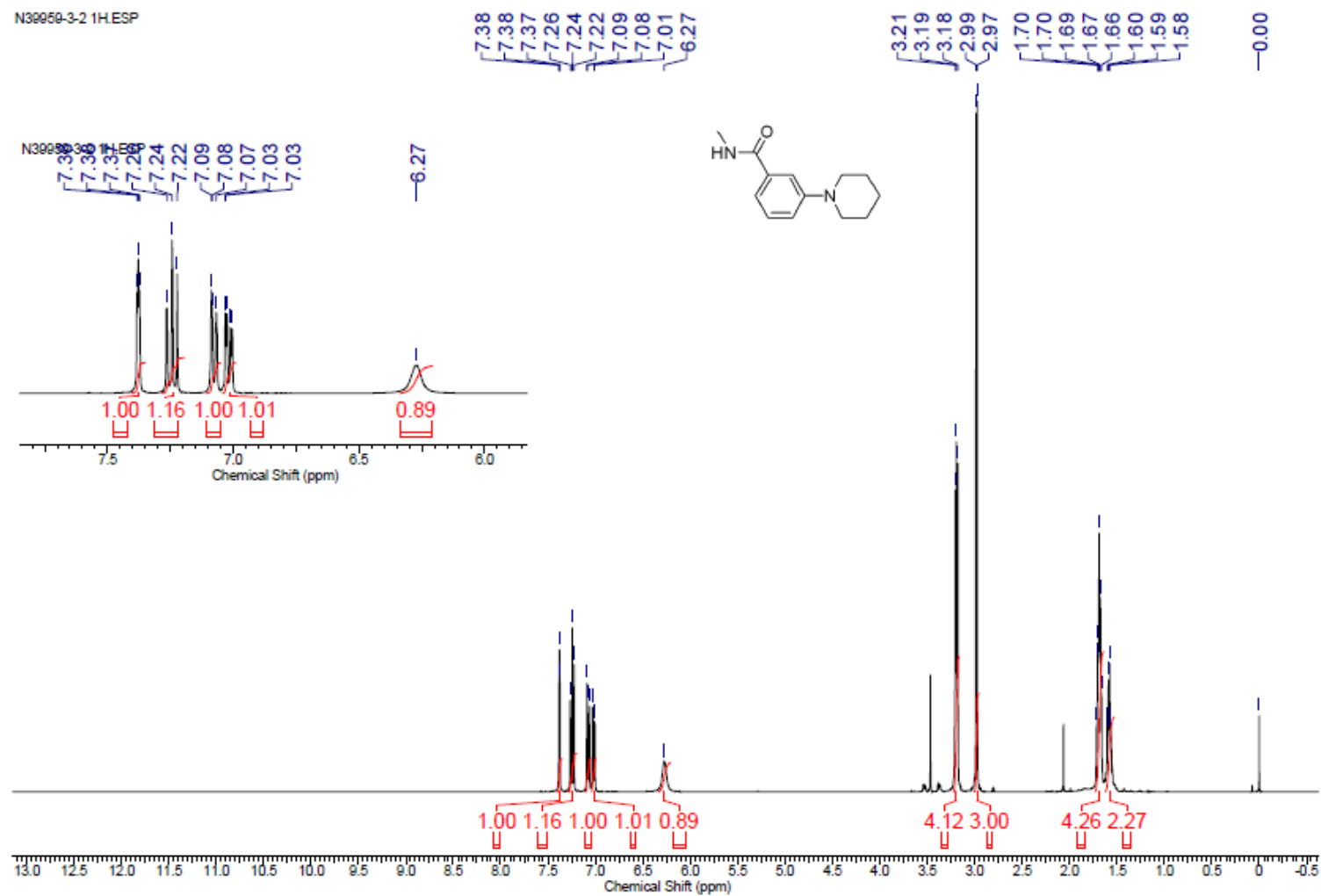


IR Spectra

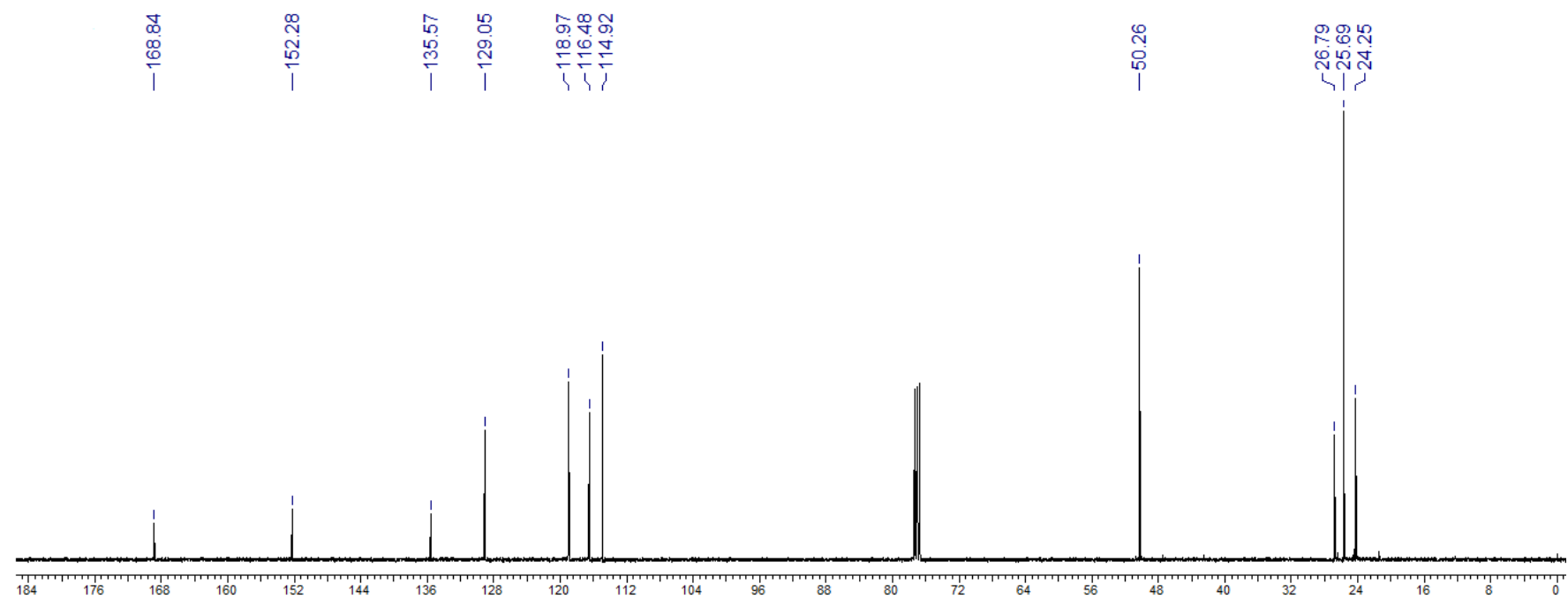


***N*-Methyl-3-(piperidin-1-yl)benzamide (7i).**

¹H NMR Spectra



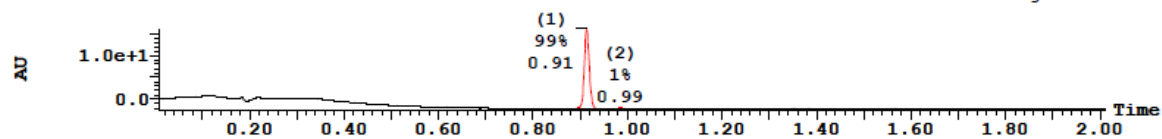
¹³C NMR Spectra



LCMS

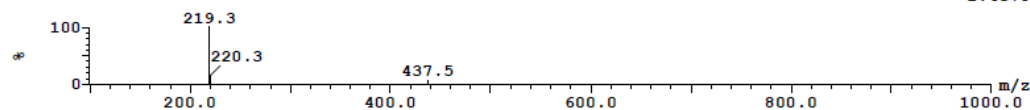
3: UV Detector: TAC :Wavelength Range: (210 - 350)

1.588e+1
Range: 1.812e+1



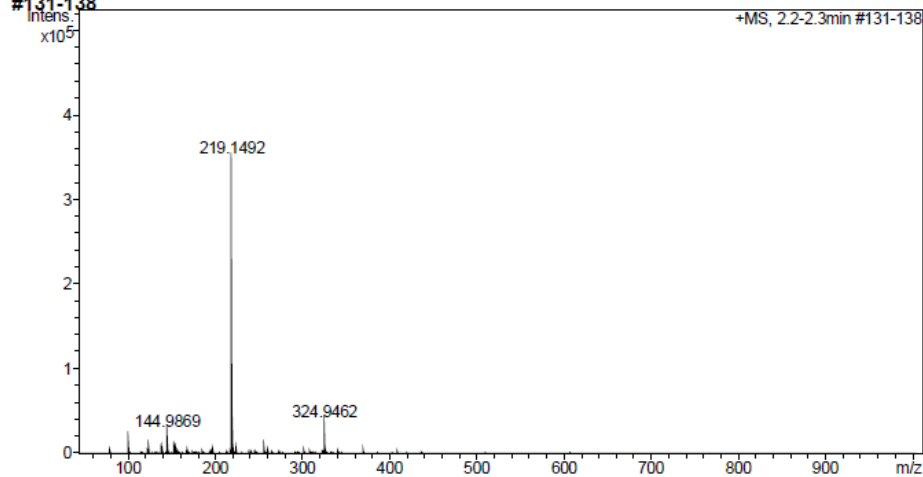
Peak Time
1 0.91
1: (Time: 0.91)

1:MS ES+
1.4e+007

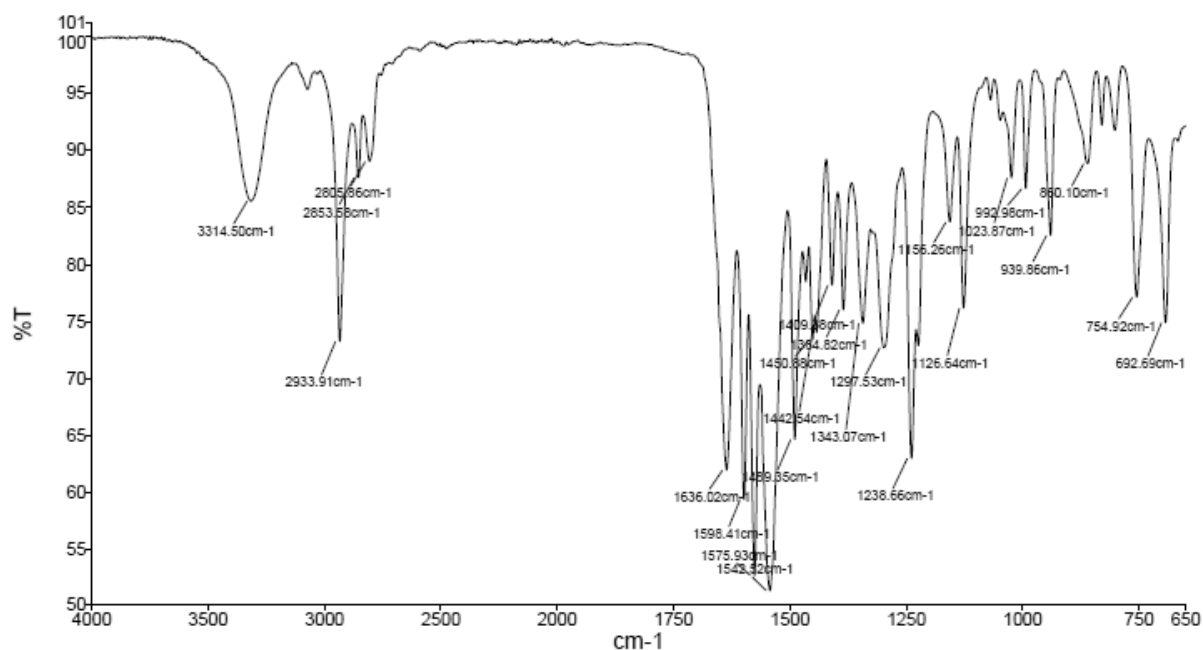


HRMS

+MS, 2.2-2.3min
#131-138

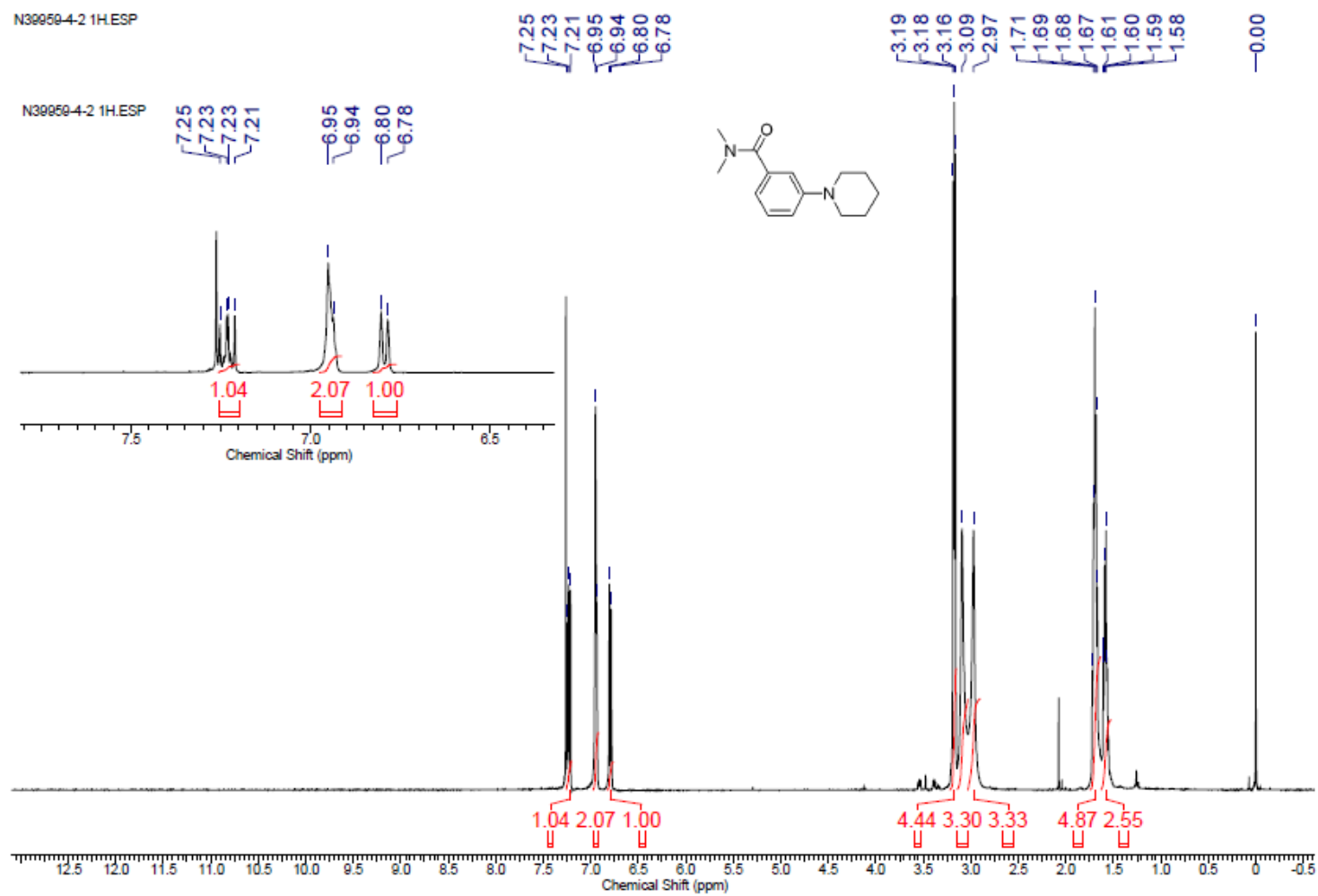


IR Spectra

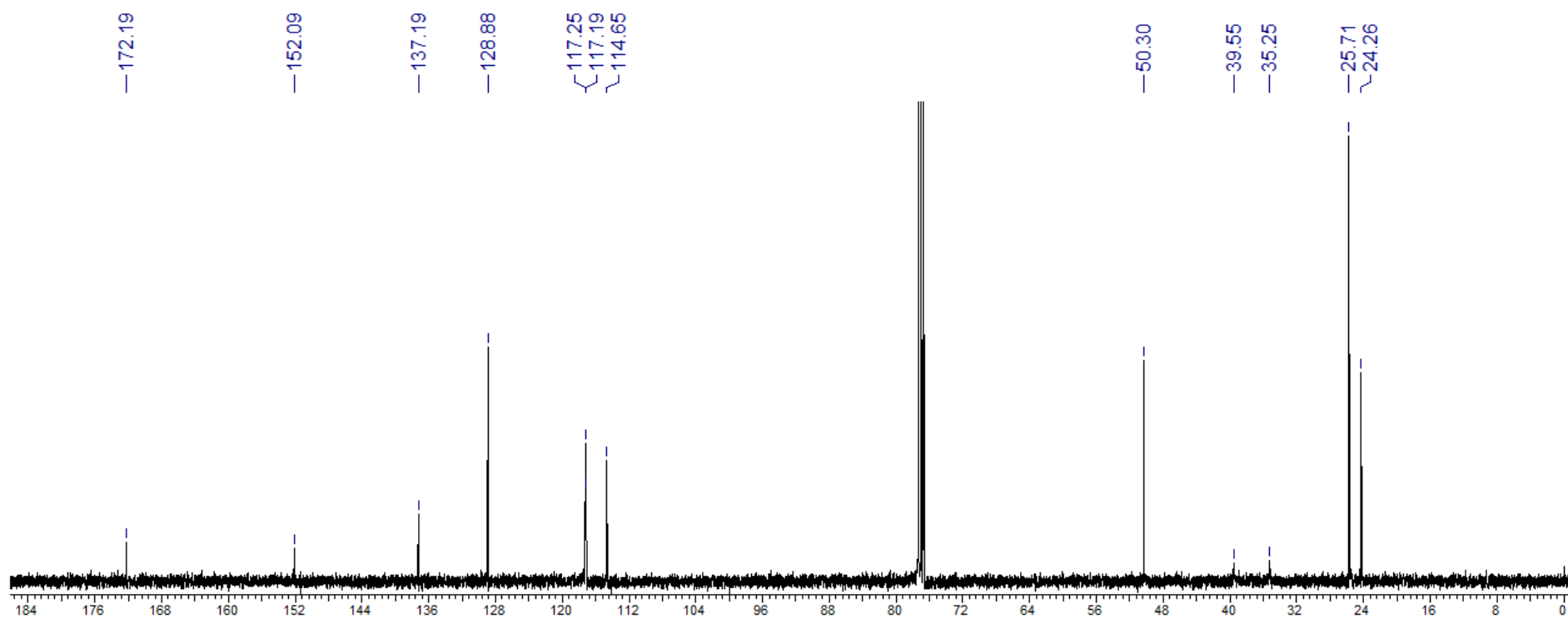


***N,N*-Dimethyl-3-(piperidin-1-yl)benzamide (7j).**

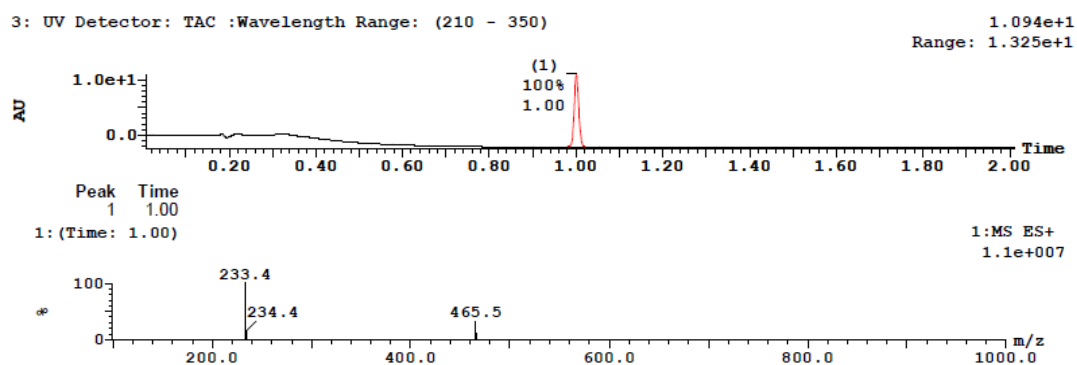
¹H NMR Spectra



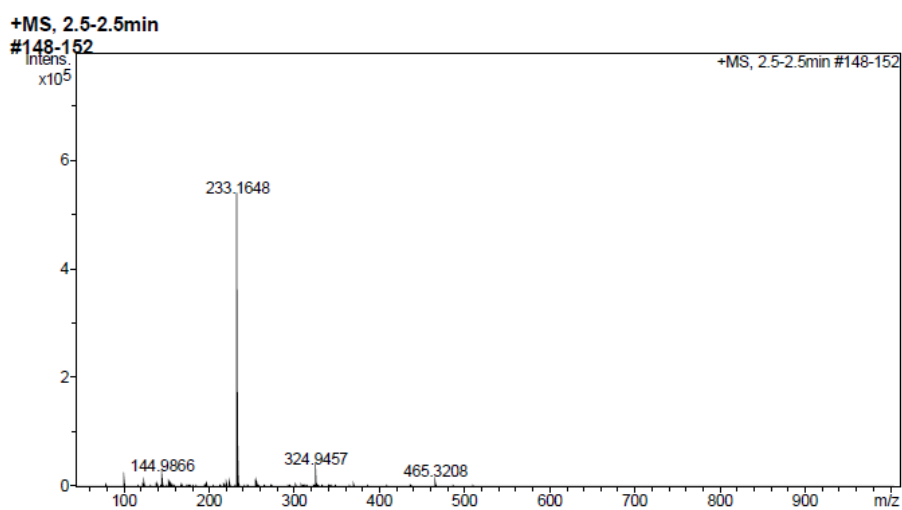
¹³C NMR Spectra



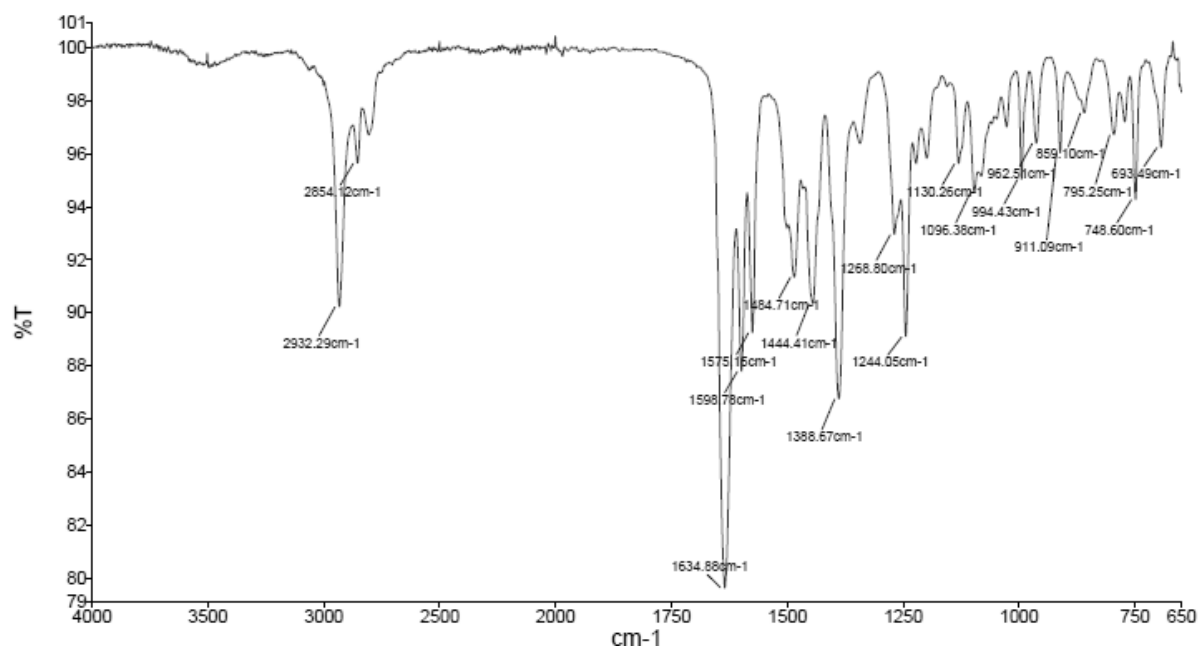
LCMS



HRMS

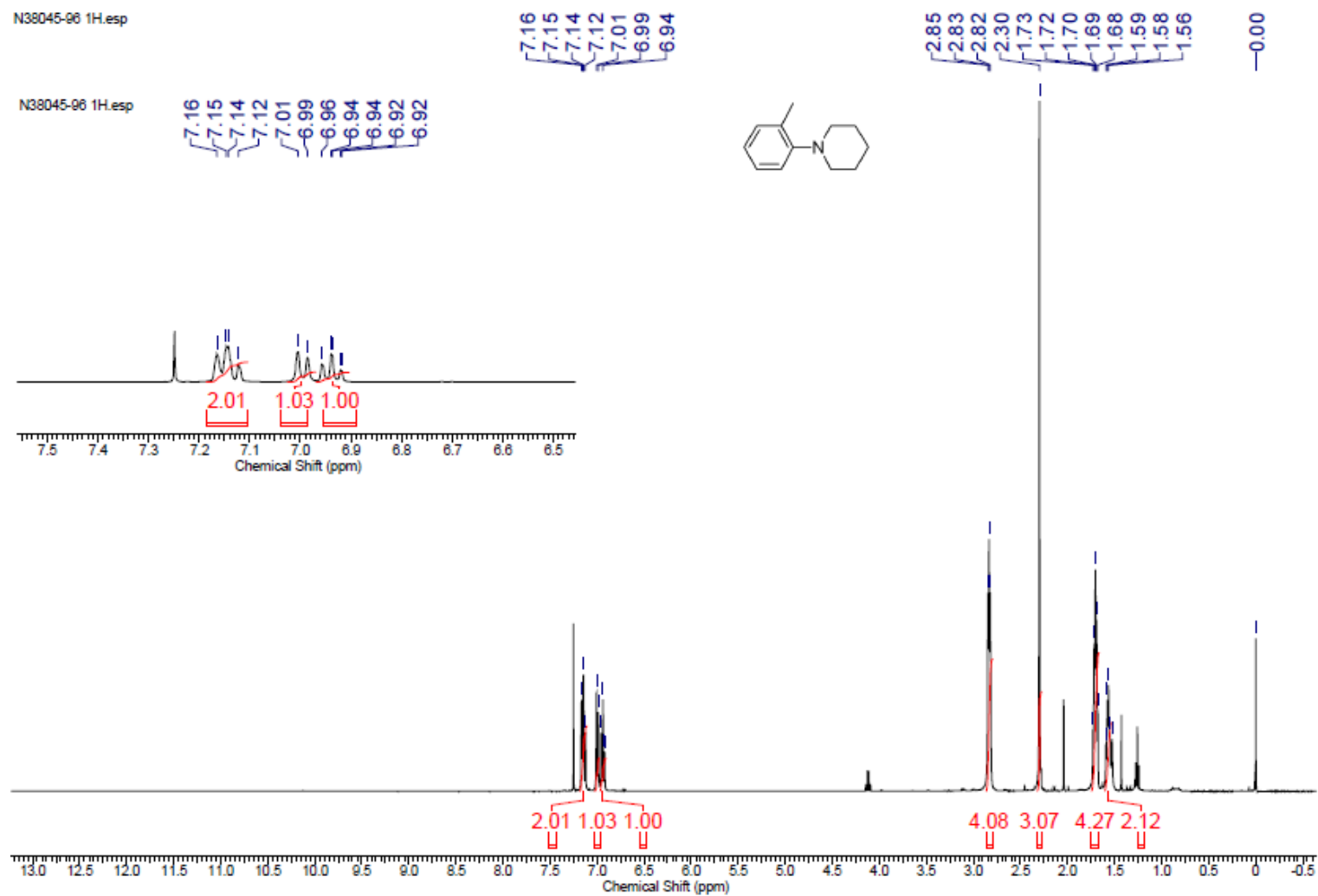


IR Spectra

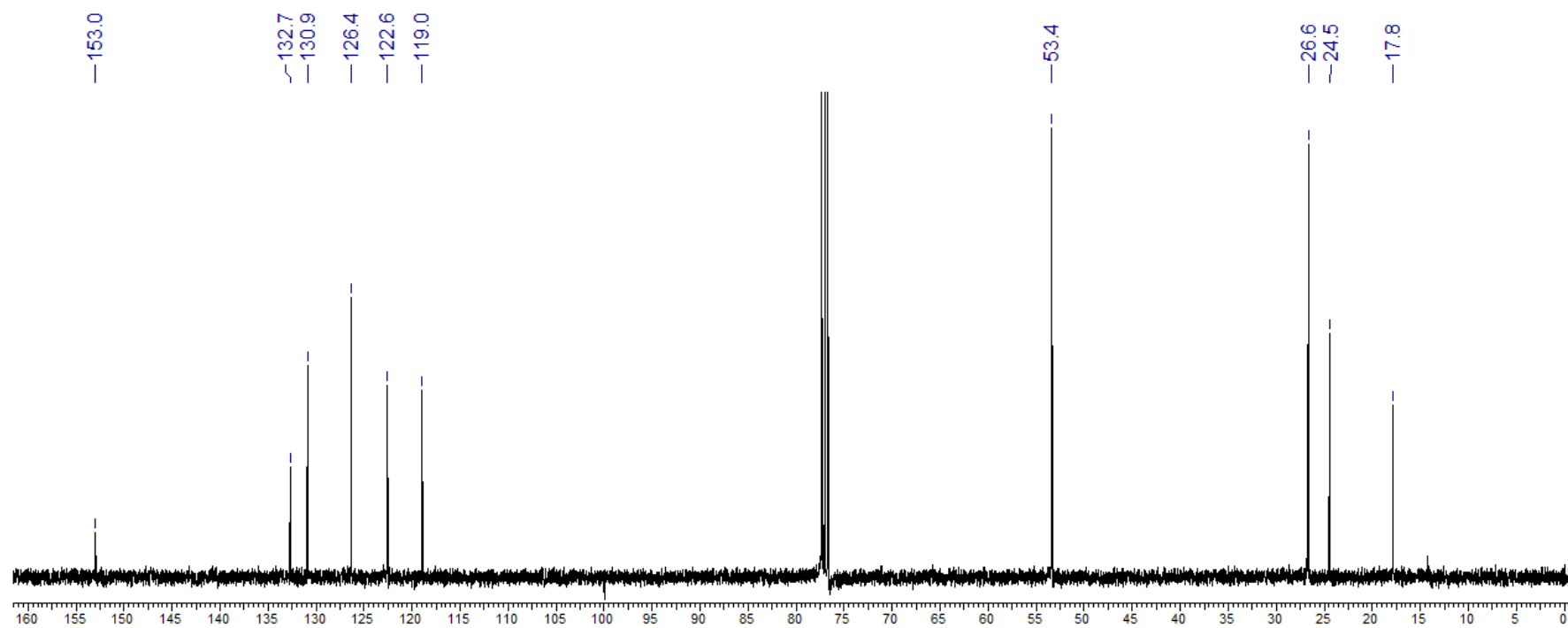


1-(*o*-Tolyl)piperidine (7k).

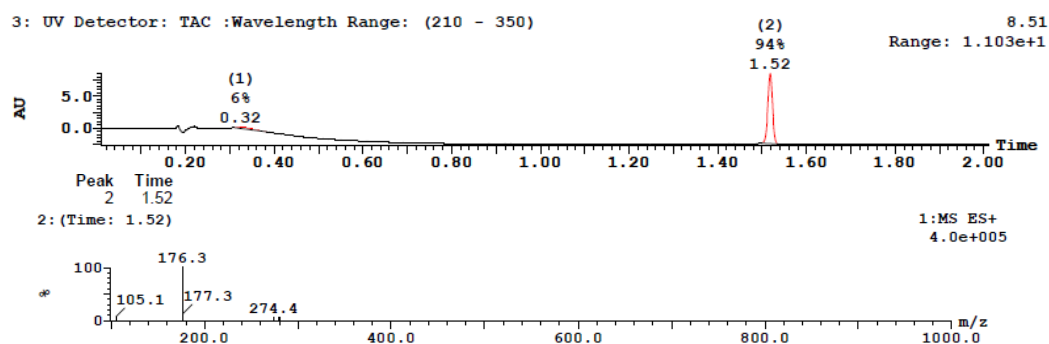
¹H NMR Spectra



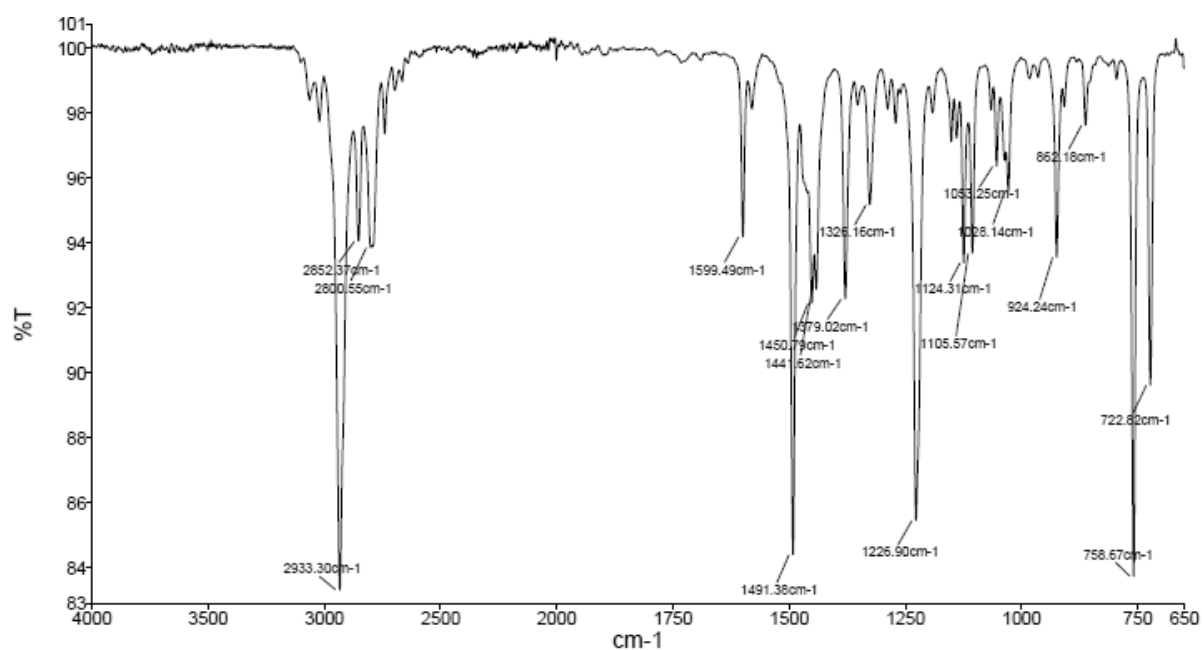
¹³C NMR Spectra



LCMS

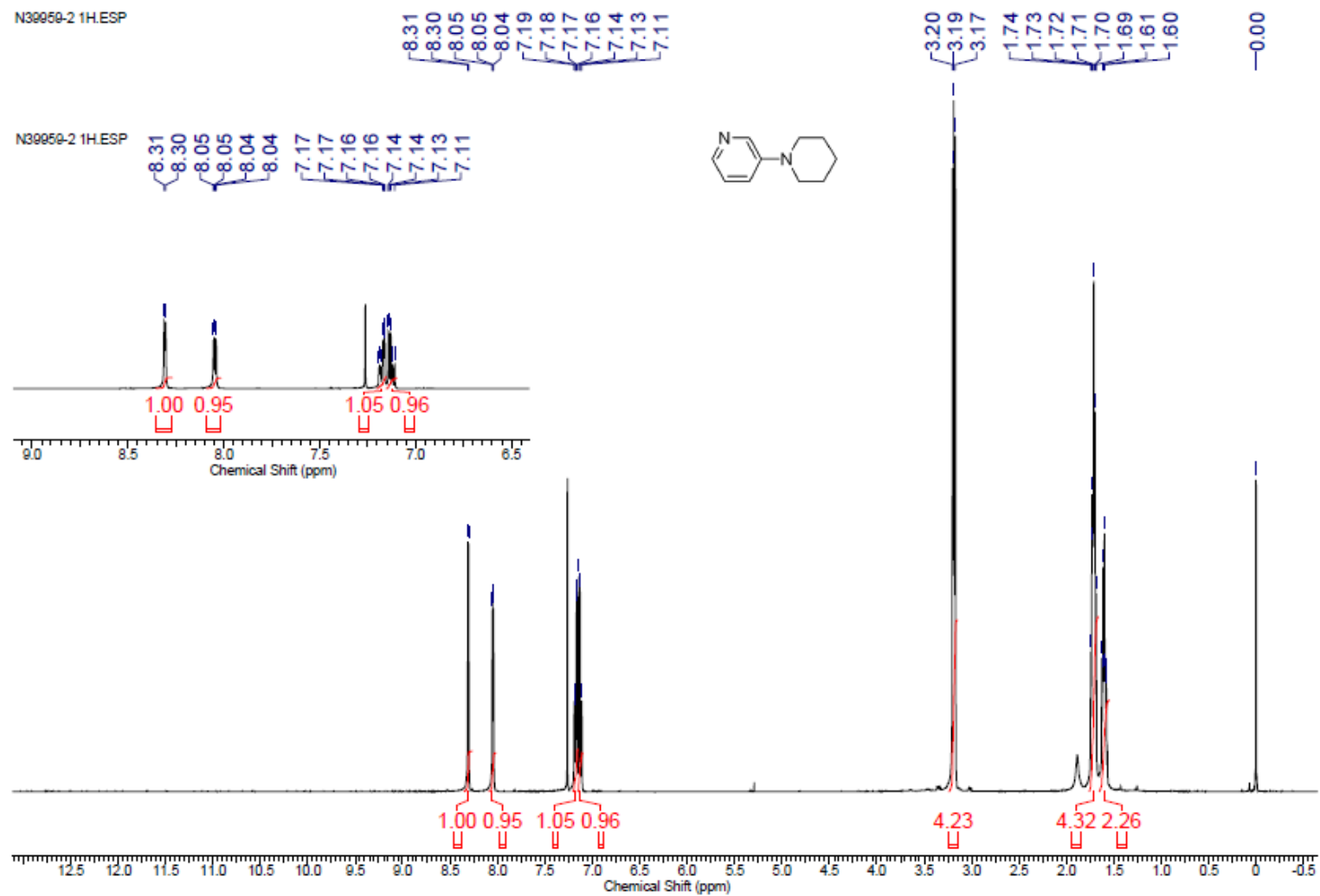


IR Spectra

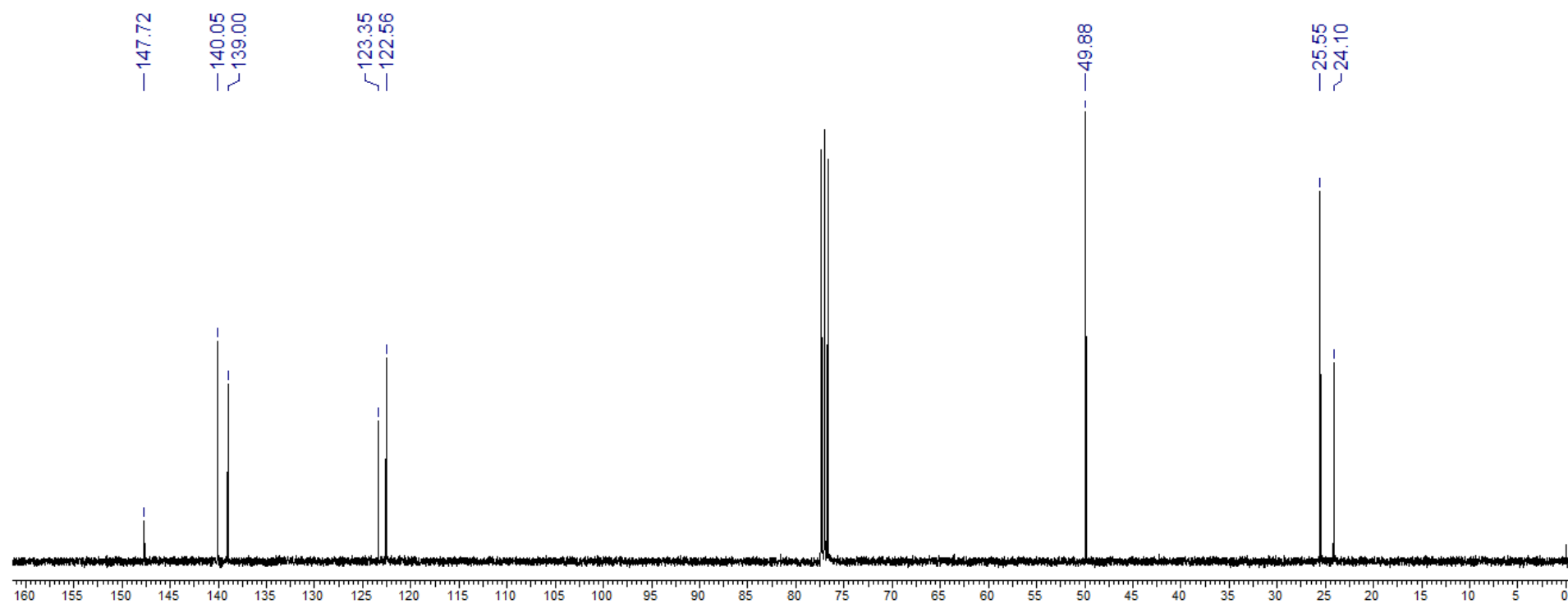


3-(Piperidin-1-yl)pyridine (7l).

¹H NMR Spectra



¹³C NMR Spectra

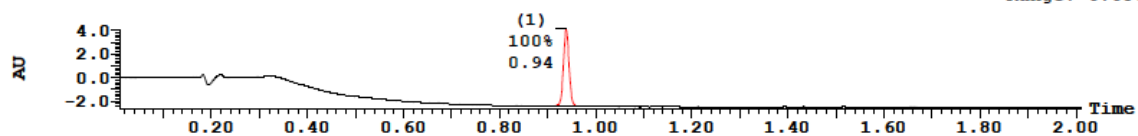


LCMS

3: UV Detector: TAC :Wavelength Range: (210 - 350)

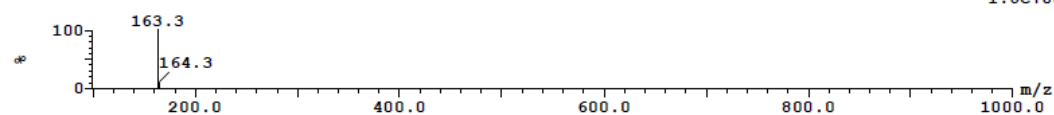
4.043

Range: 6.606

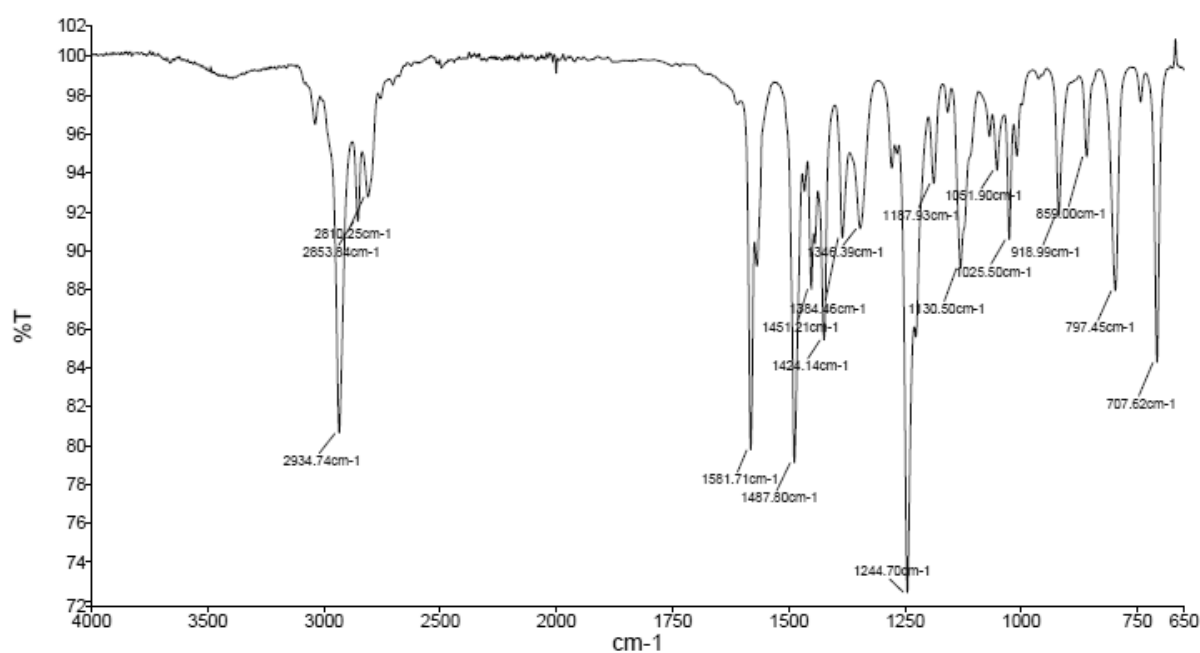


Peak Time
1 0.94
1: (Time: 0.94)

1:MS ES+
1.8e+007

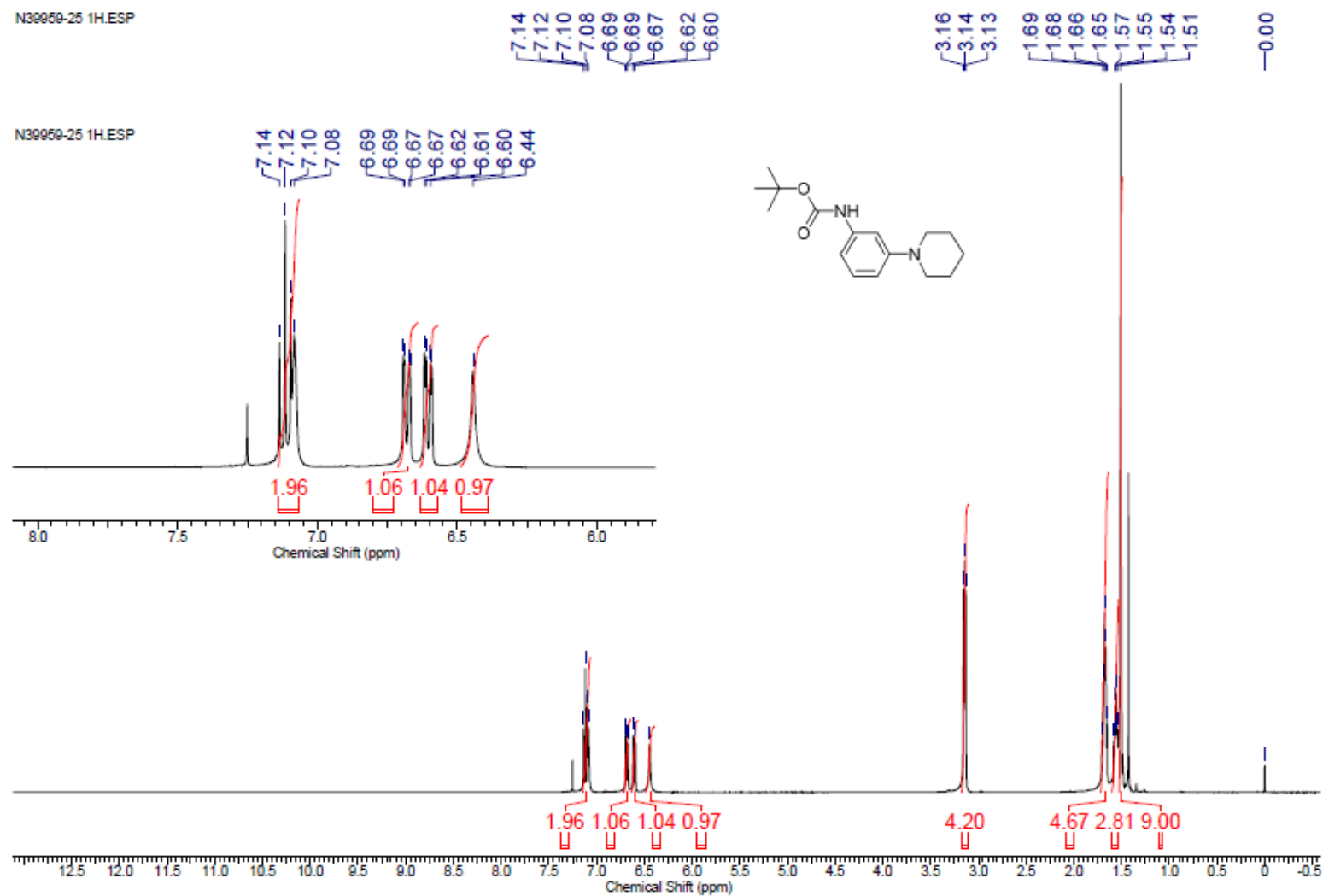


IR Spectra

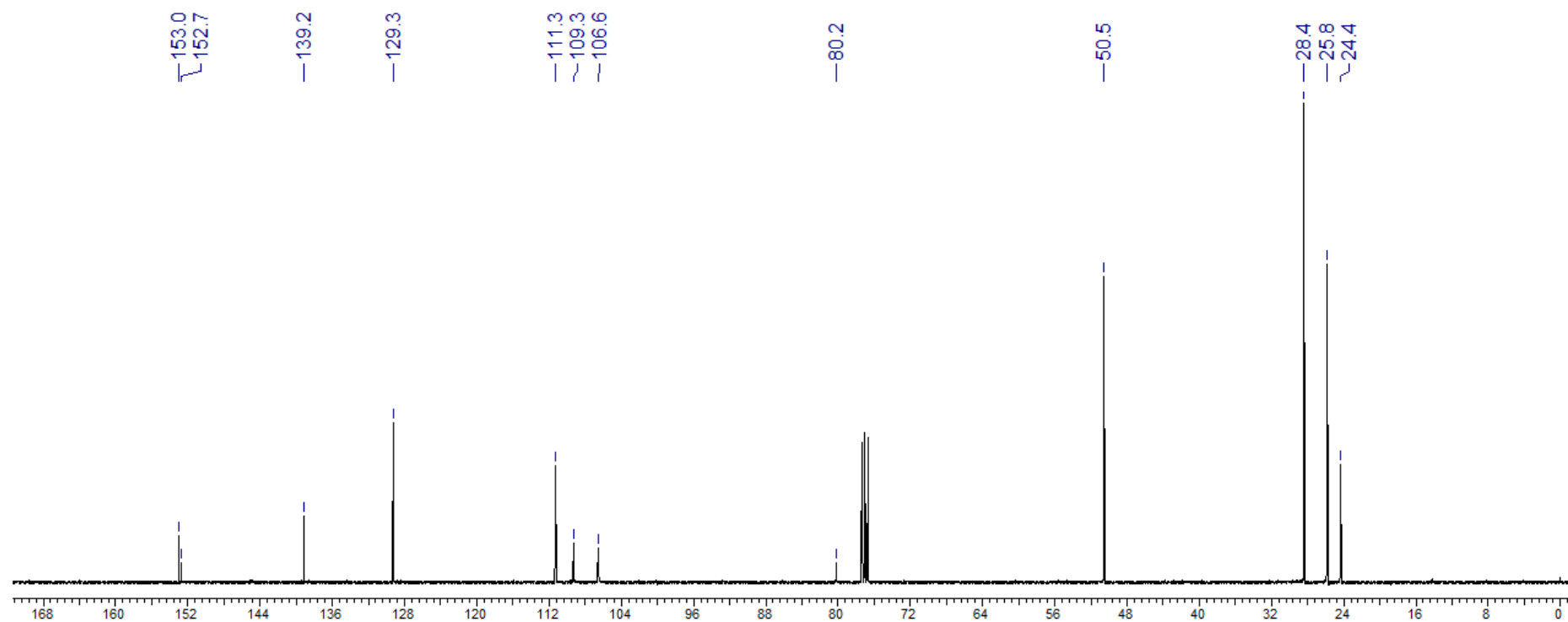


***tert*-Butyl (3-(piperidin-1-yl)phenyl)carbamate (7m).**

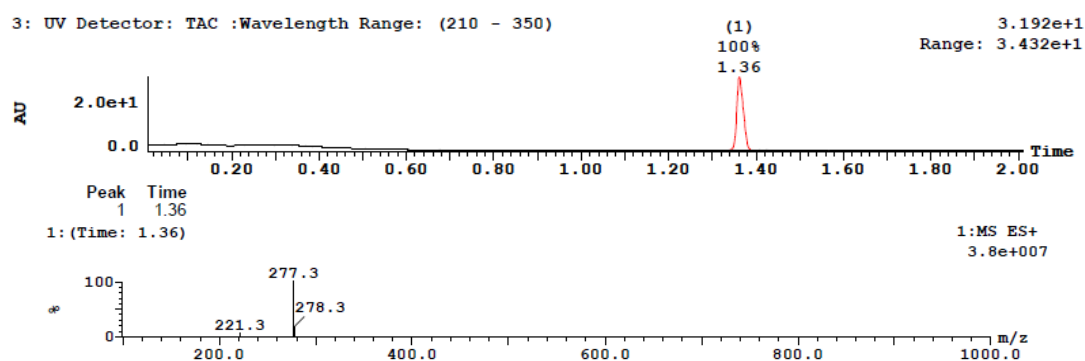
¹H NMR Spectra



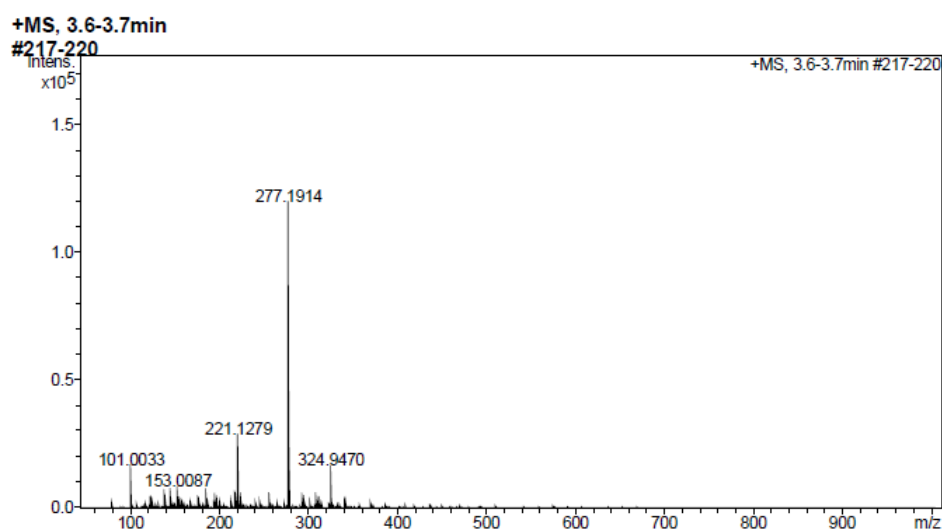
¹³C NMR Spectra



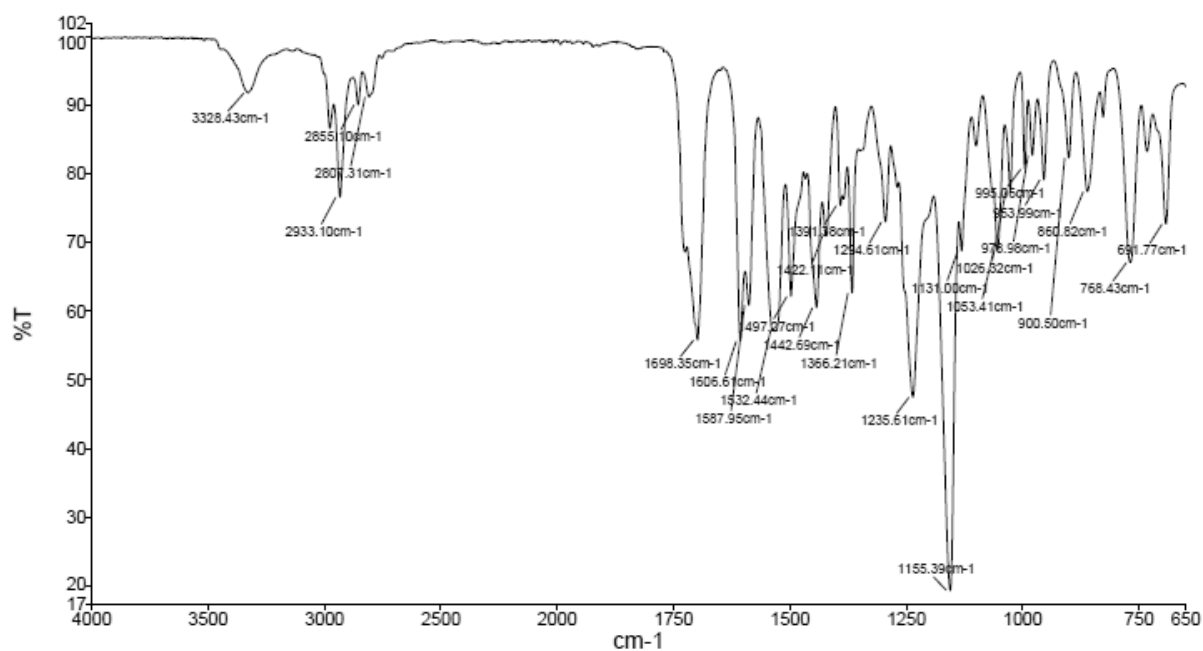
LCMS



HRMS

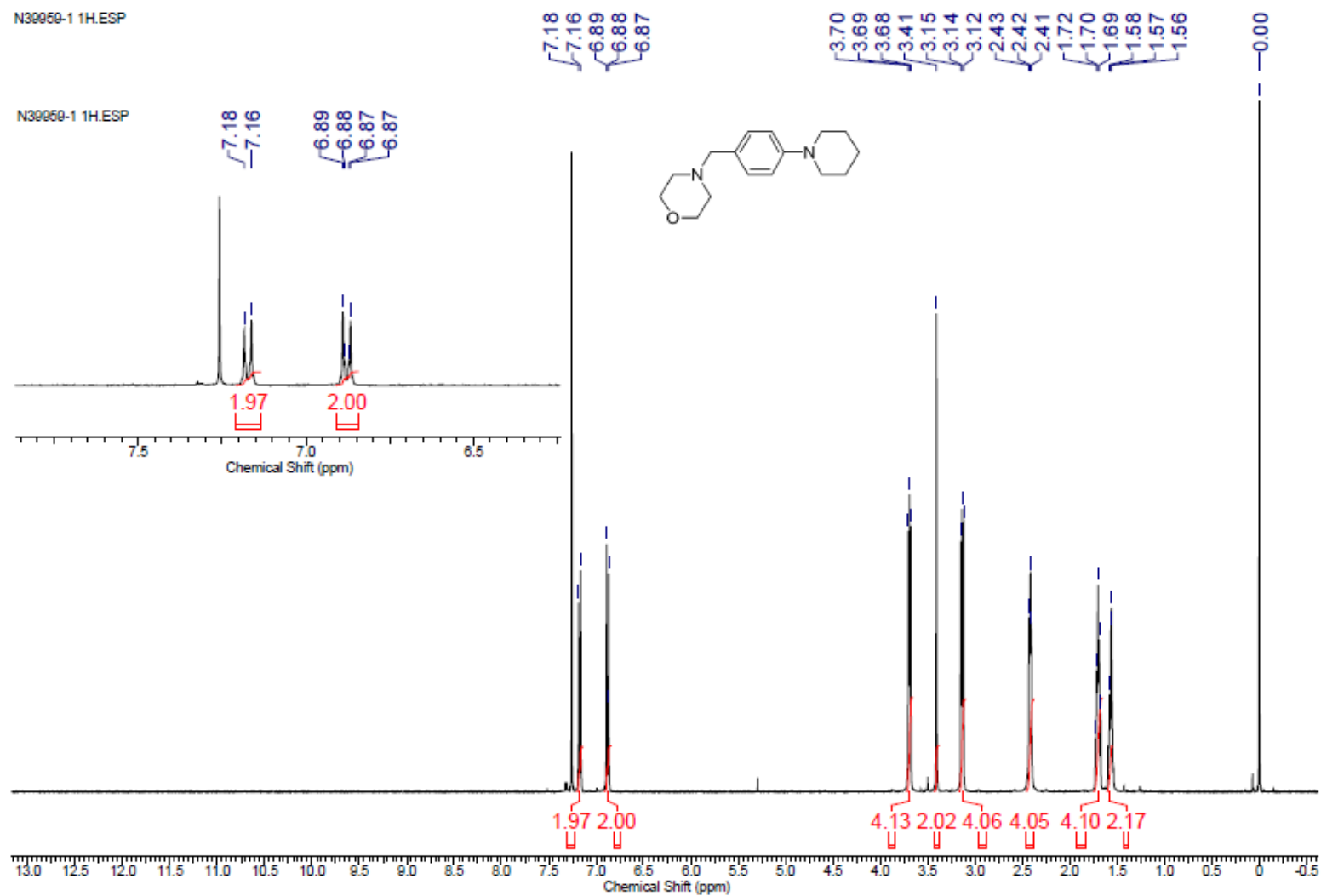


IR Spectra

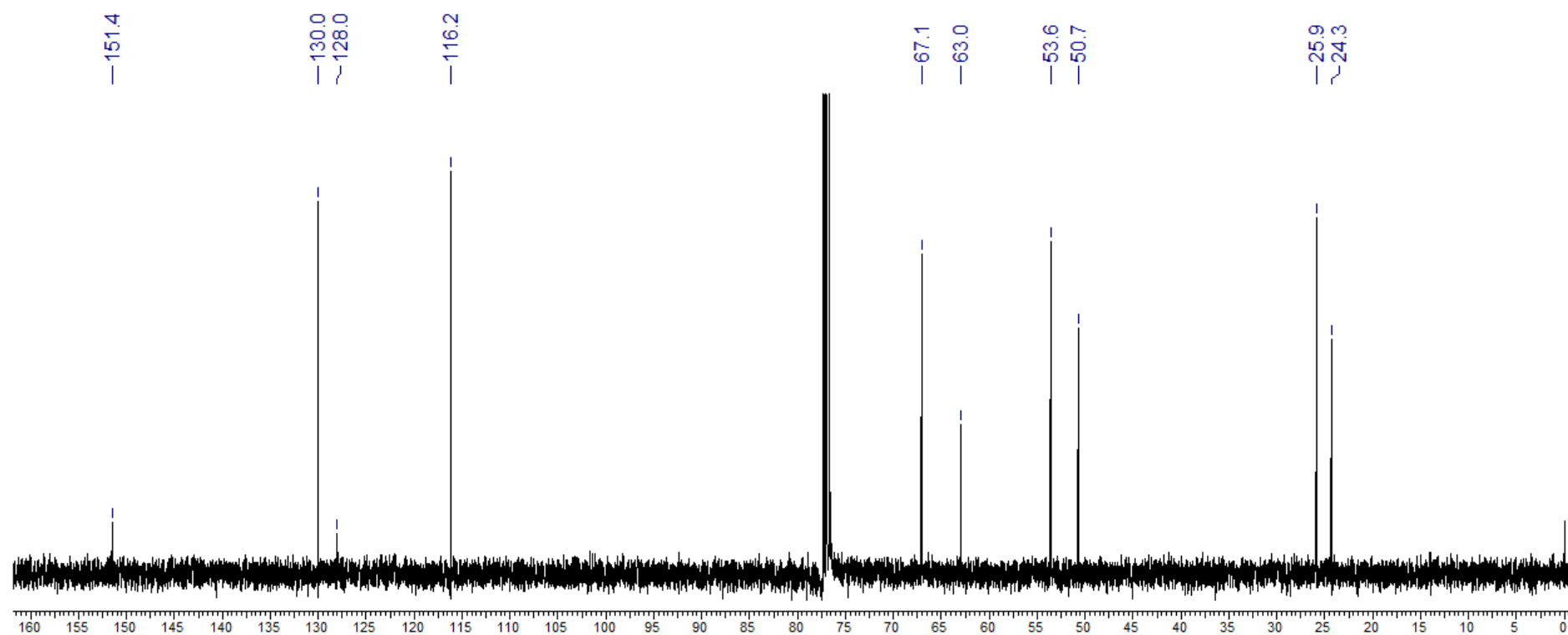


4-(4-(Piperidin-1-yl)benzyl)morpholine (7n).

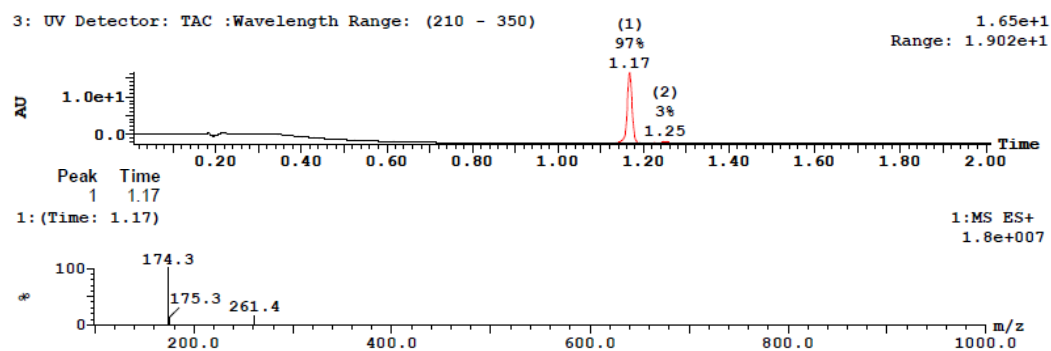
¹H NMR Spectra



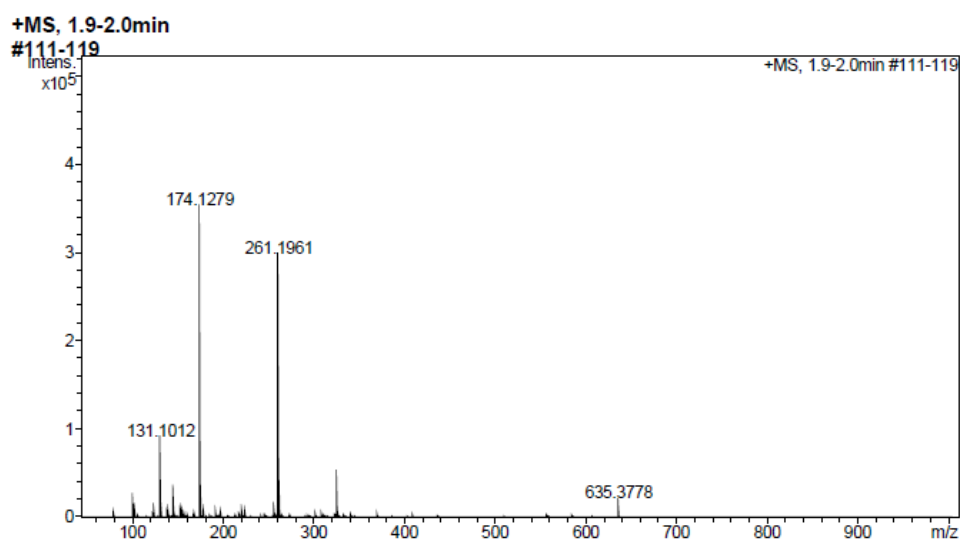
¹³C NMR Spectra



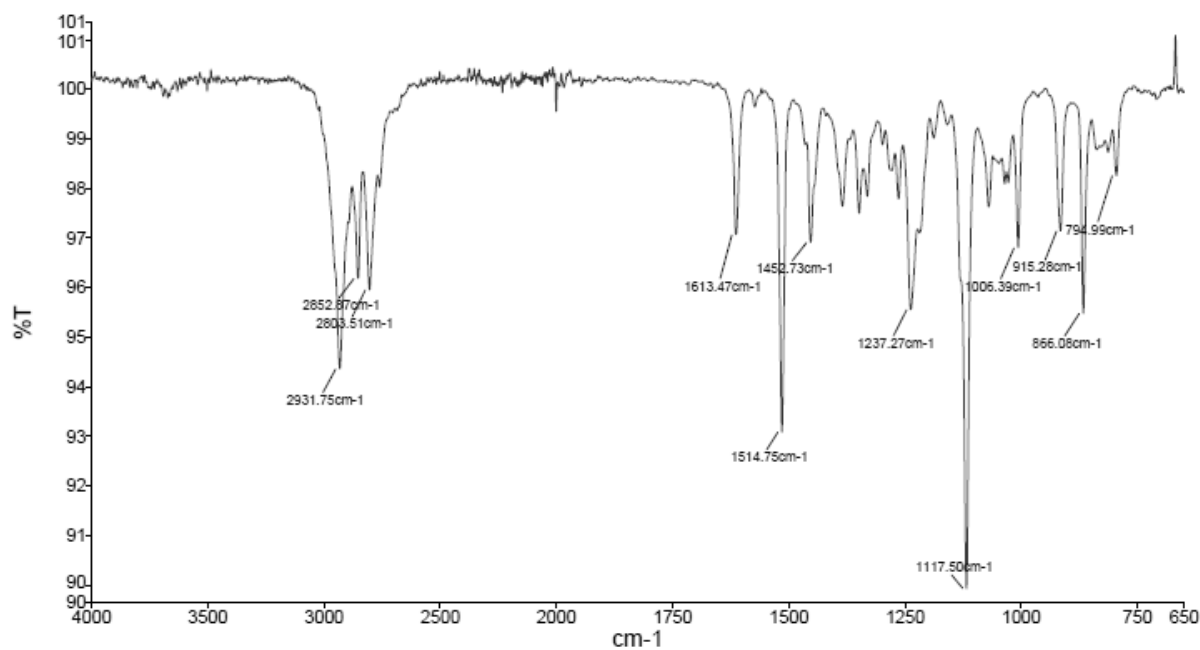
LCMS



HRMS

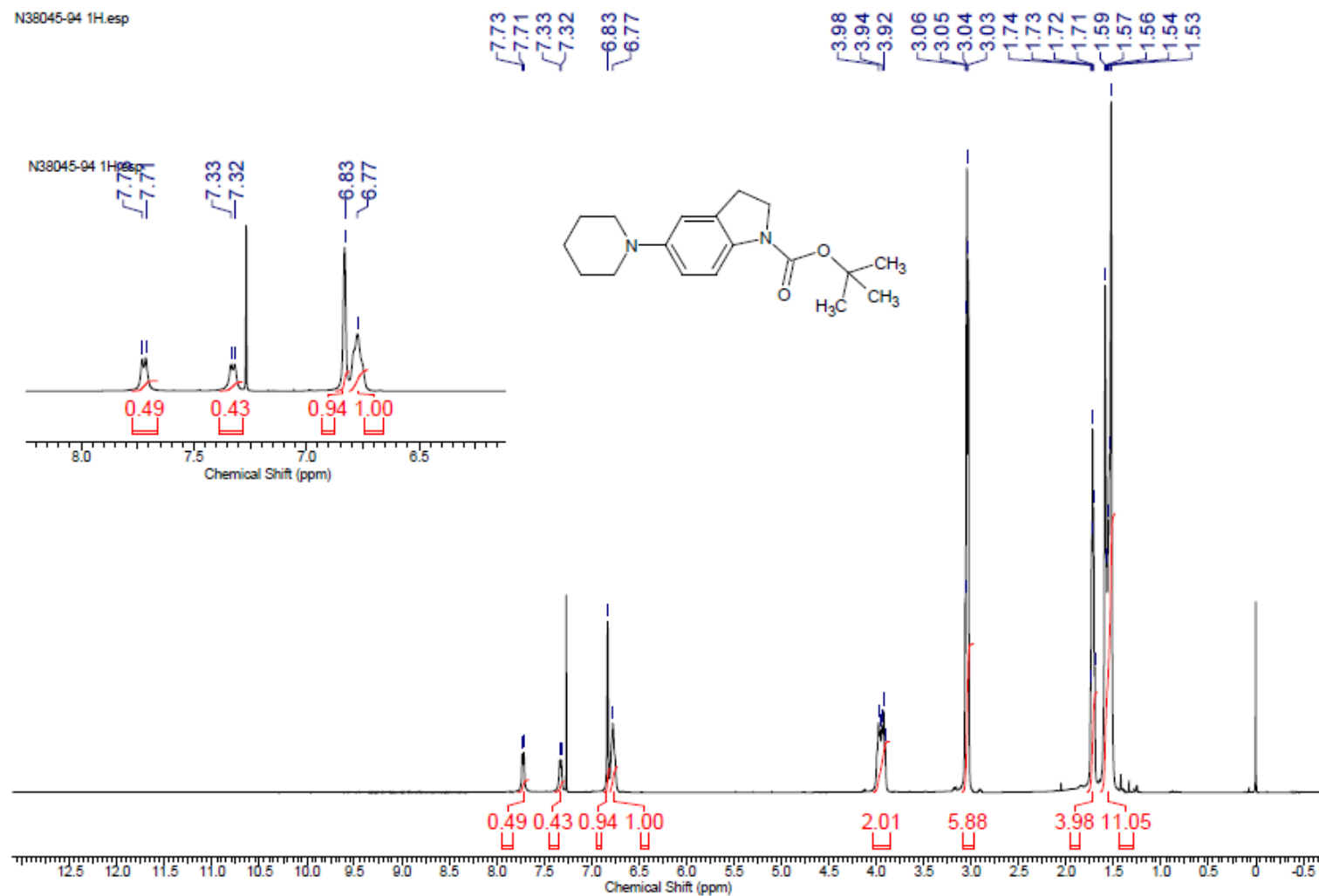


IR Spectra

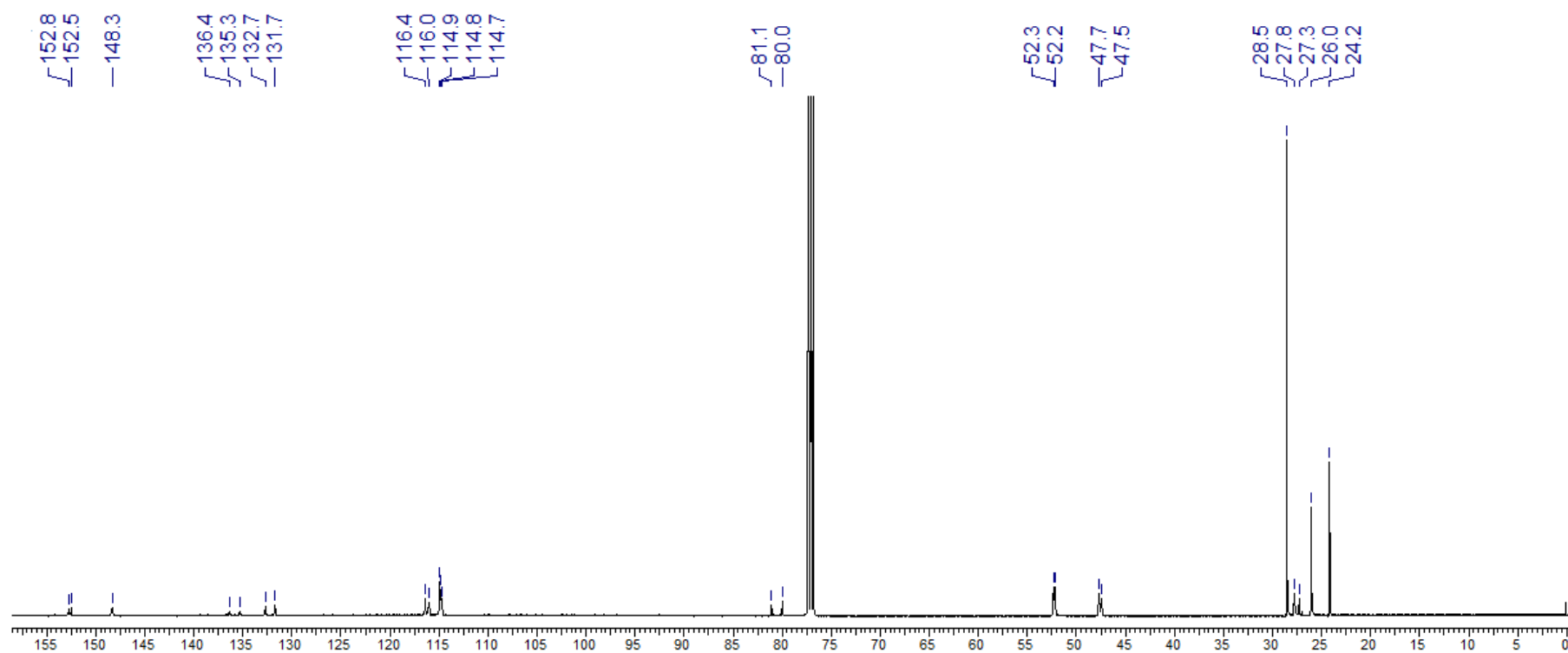


tert-Butyl 5-(piperidin-1-yl)indoline-1-carboxylate (7o).

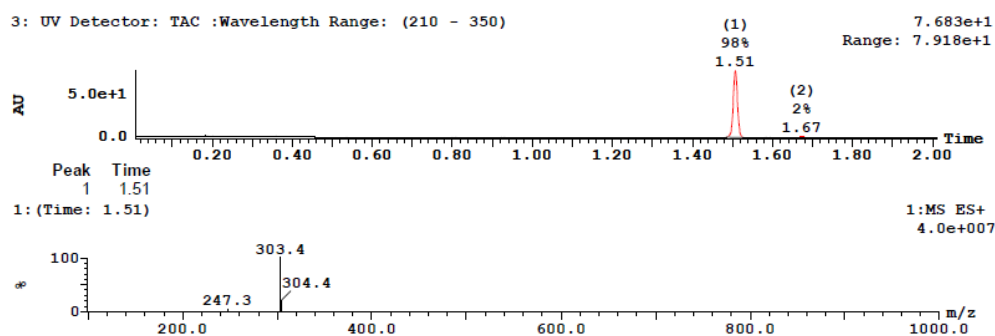
¹H NMR Spectra



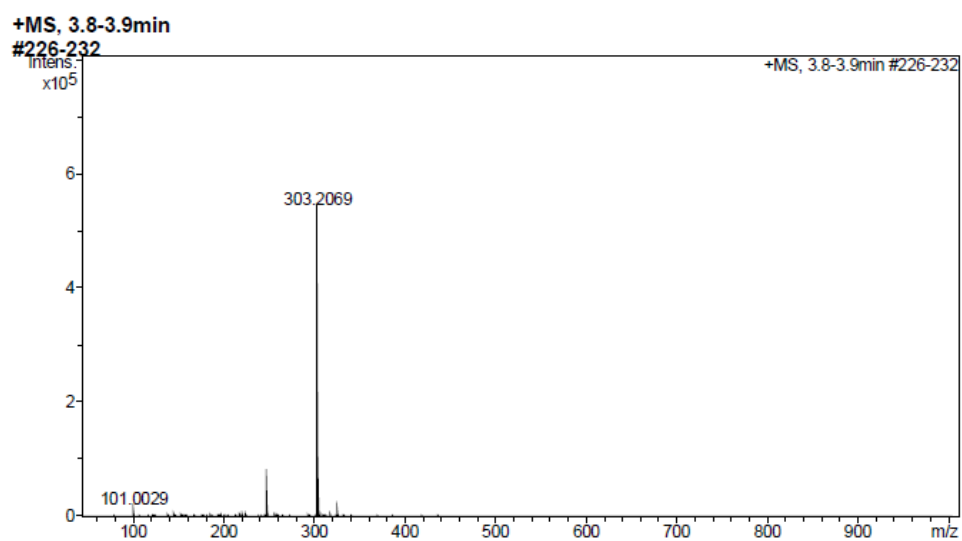
¹³C NMR Spectra



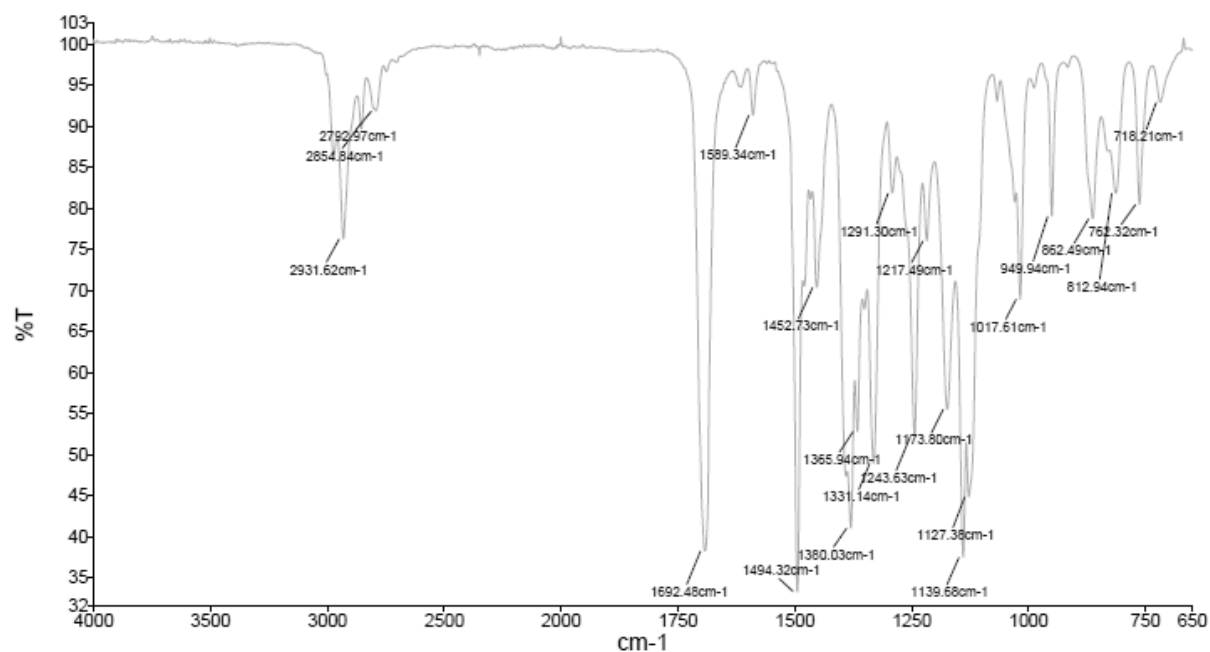
LCMS



HRMS

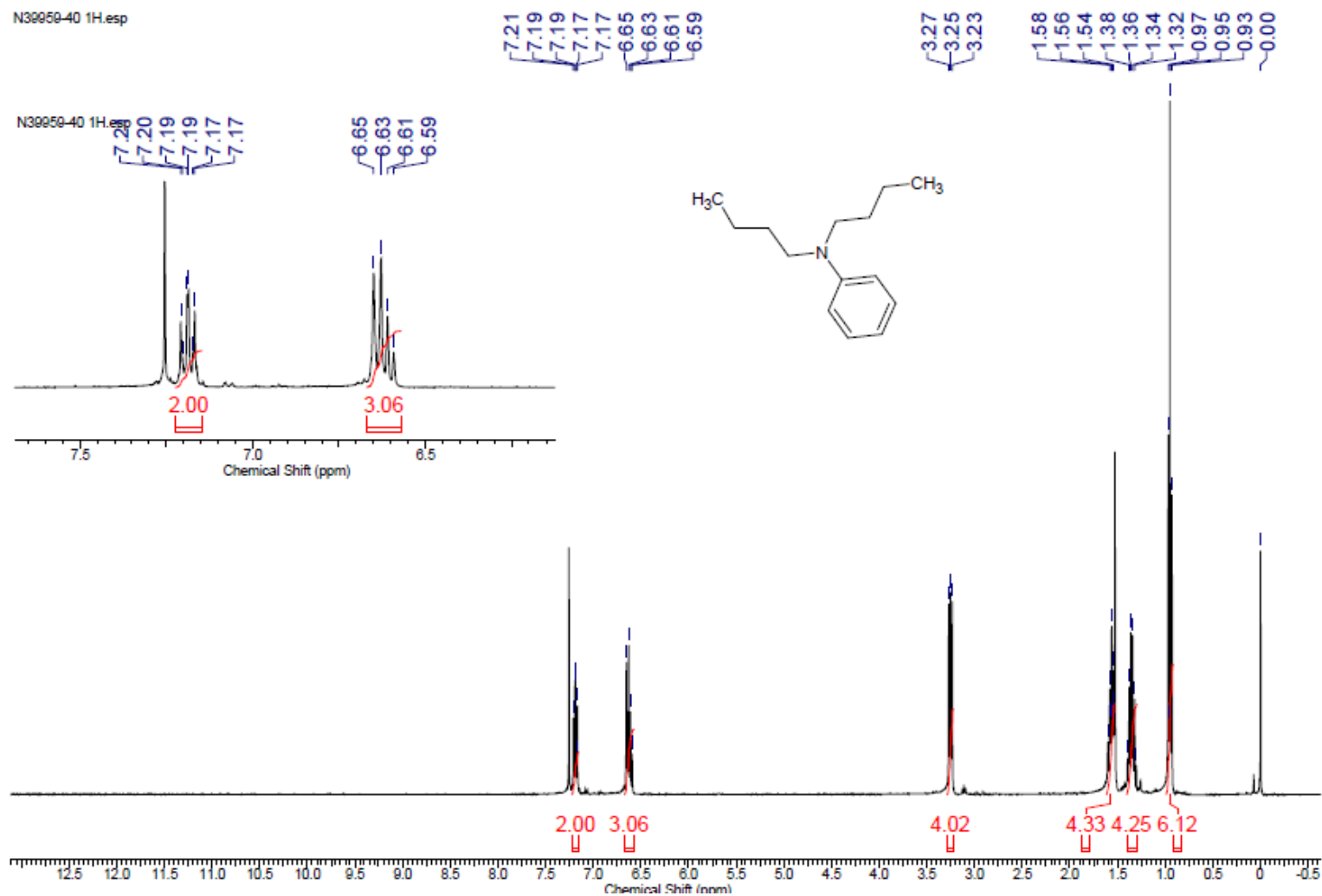


IR Spectra



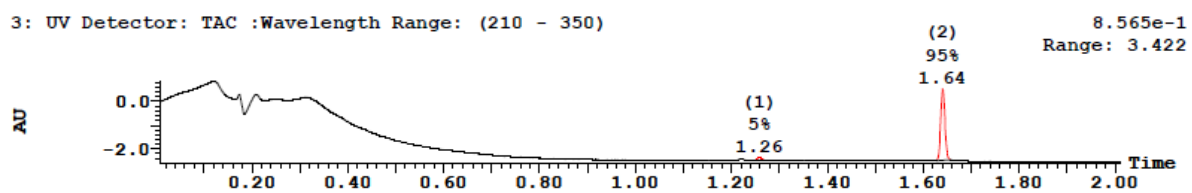
N,N-Dibutylaniline (7p).

¹H NMR Spectra



LCMS

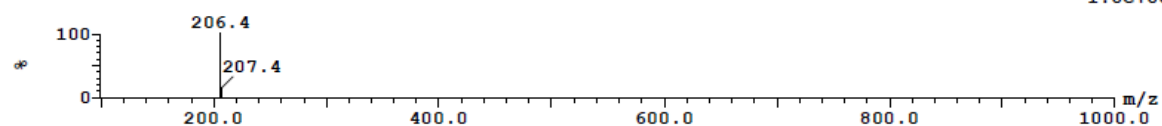
3: UV Detector: TAC :Wavelength Range: (210 - 350)



Peak Time
2 1.64

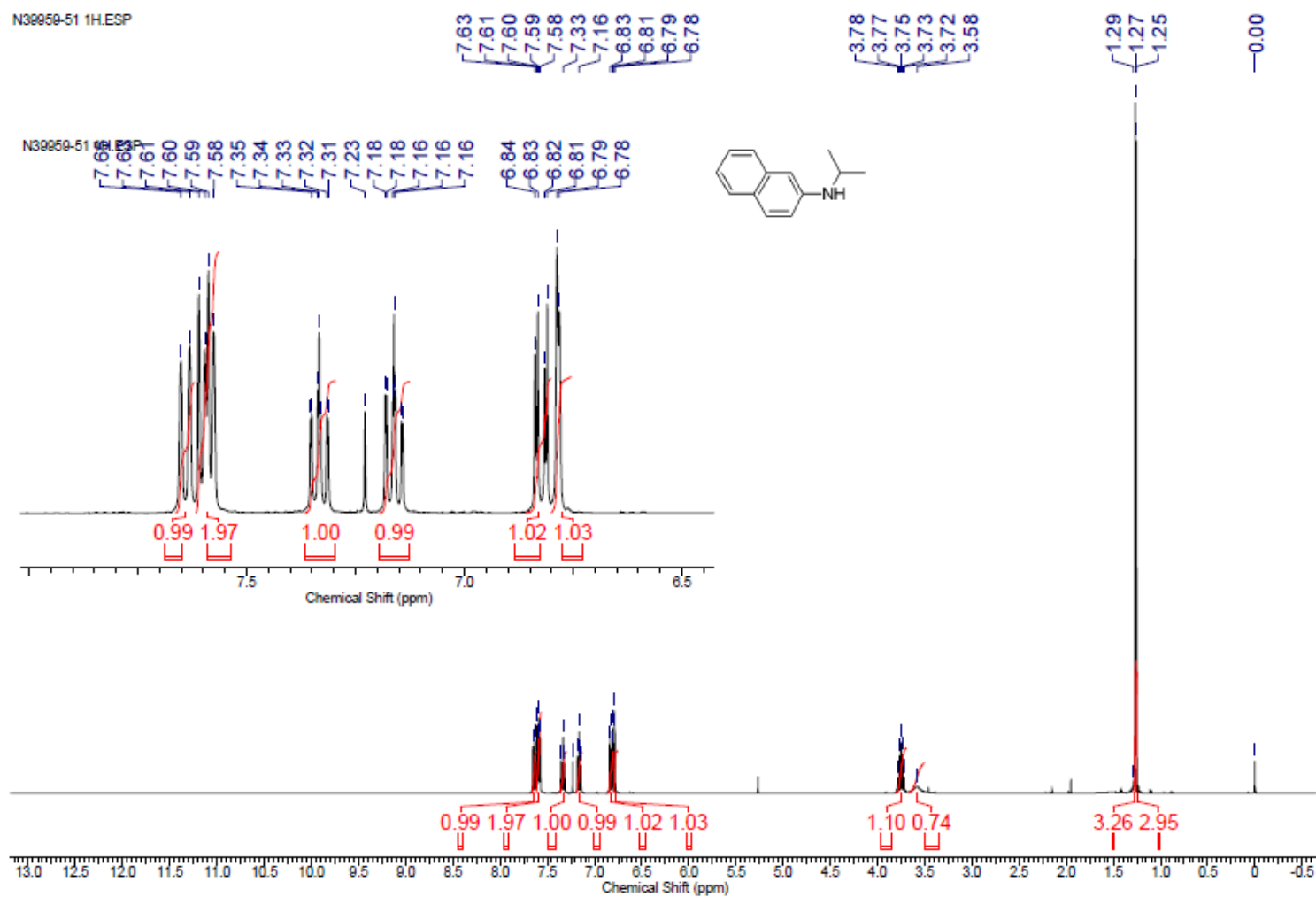
2: (Time: 1.64)

1:MS ES+
1.0e+007

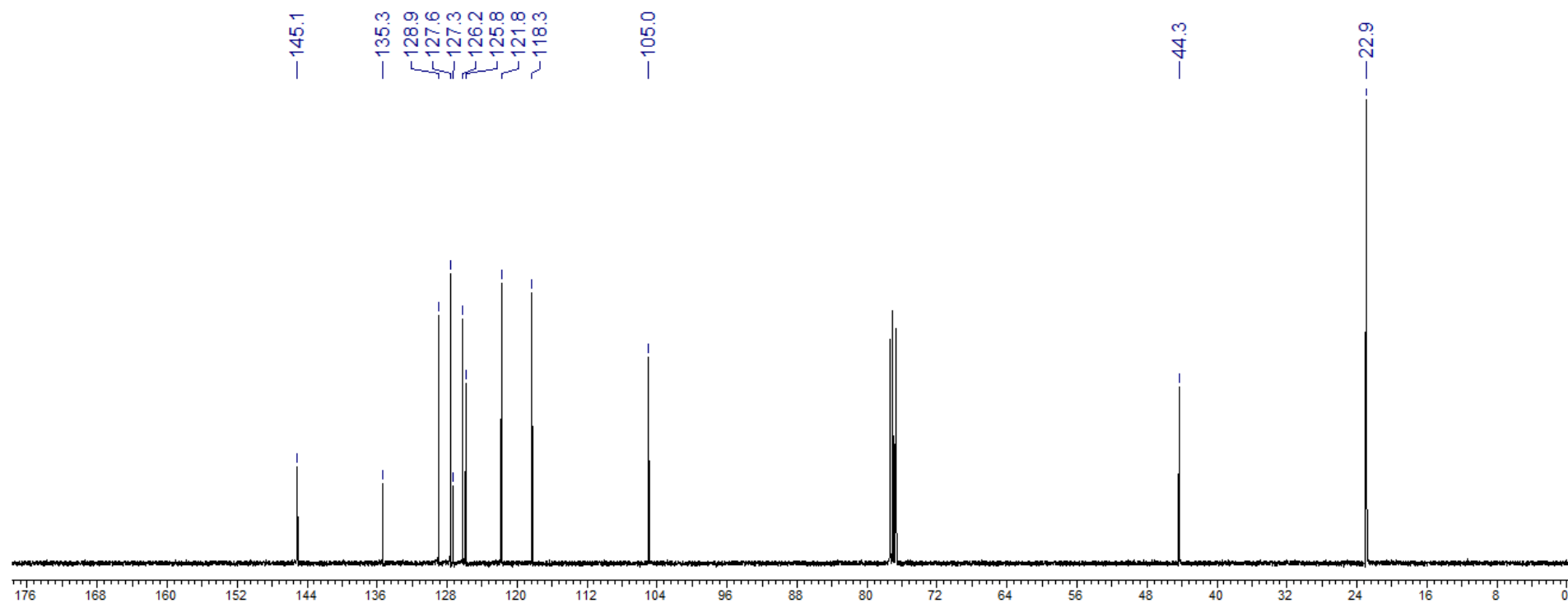


***N*-Isopropyl-naphthalen-2-amine (7q).**

¹H NMR Spectra

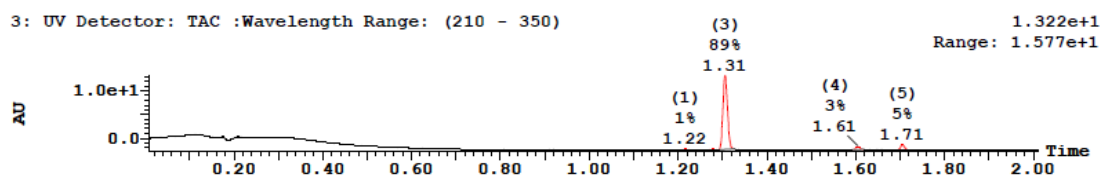


¹³C NMR Spectra



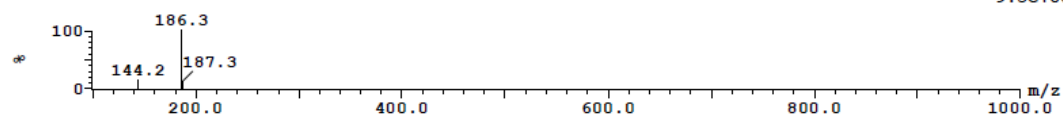
LCMS

3: UV Detector: TAC :Wavelength Range: (210 - 350)

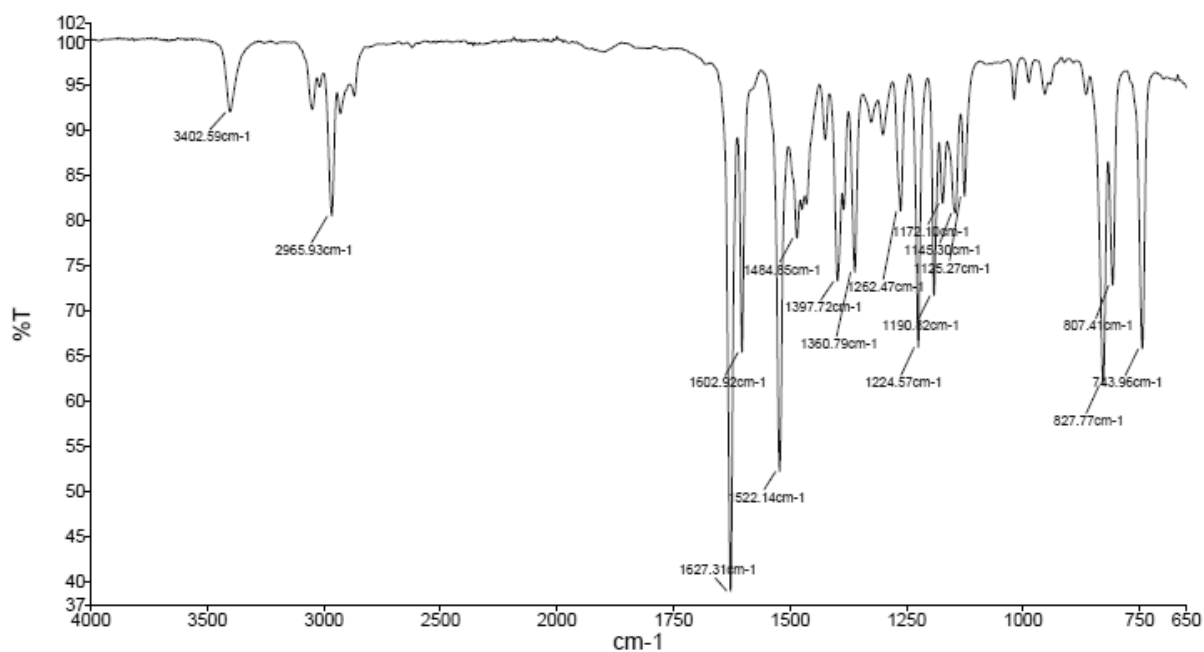


Peak Time
3 1.31
3: (Time: 1.31)

1:MS ES+
9.5e+006

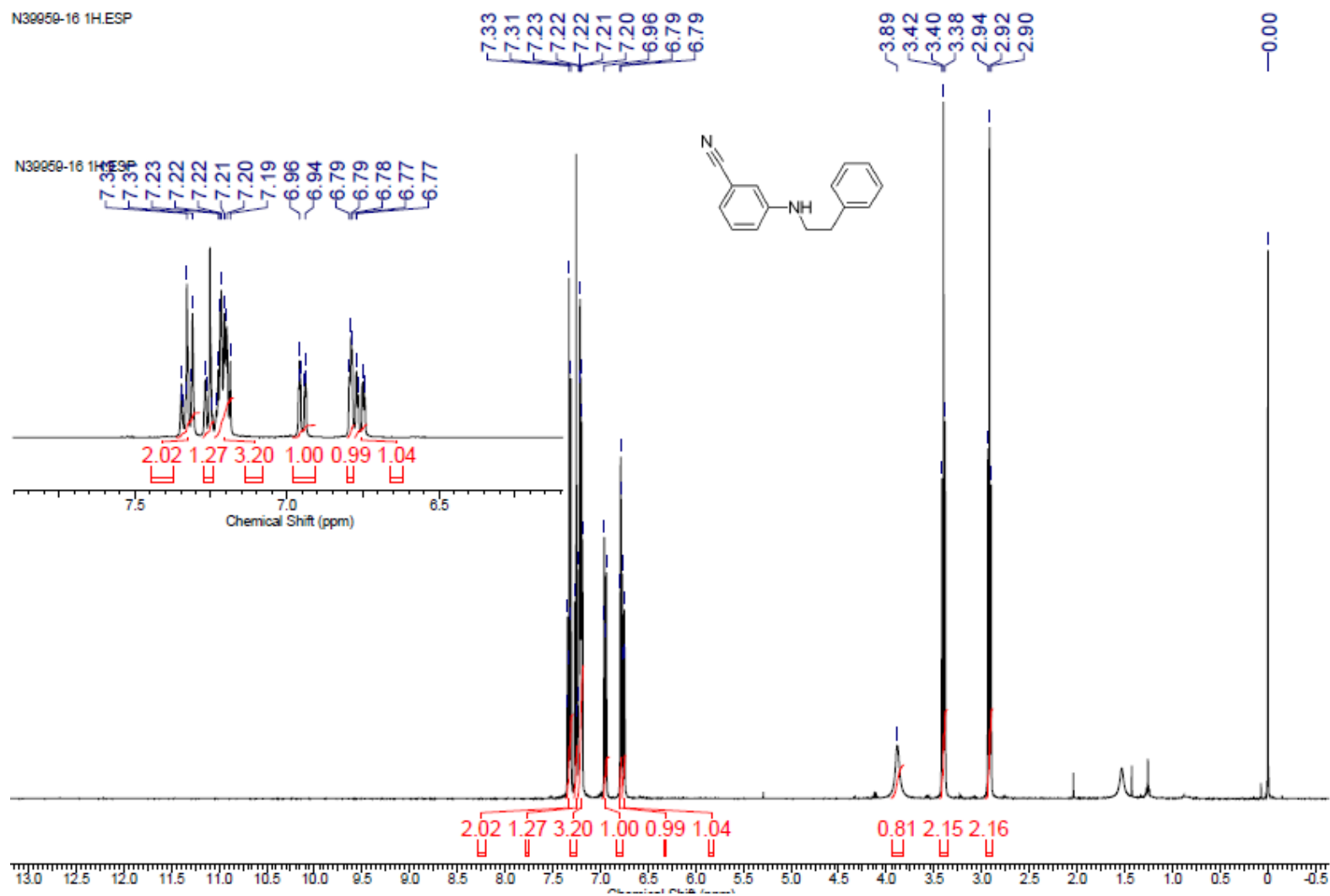


IR Spectra

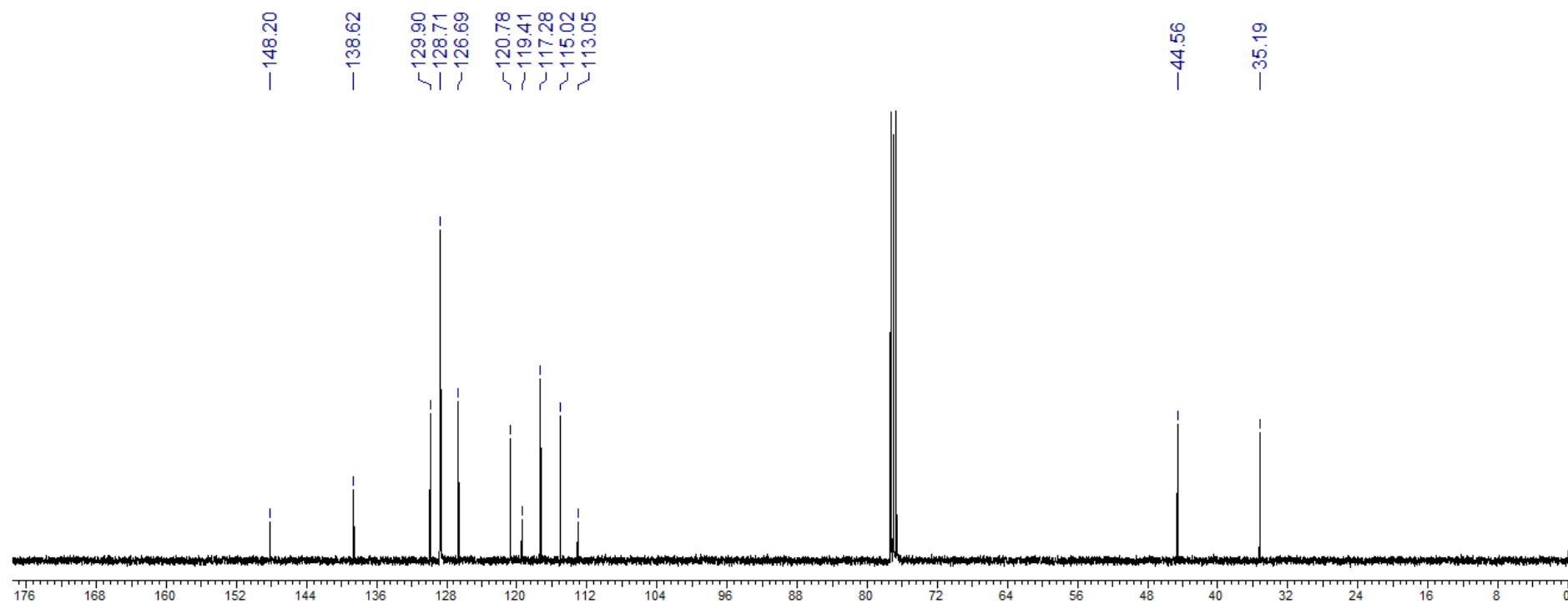


3-(Phenethylamino)benzonitrile (7r).

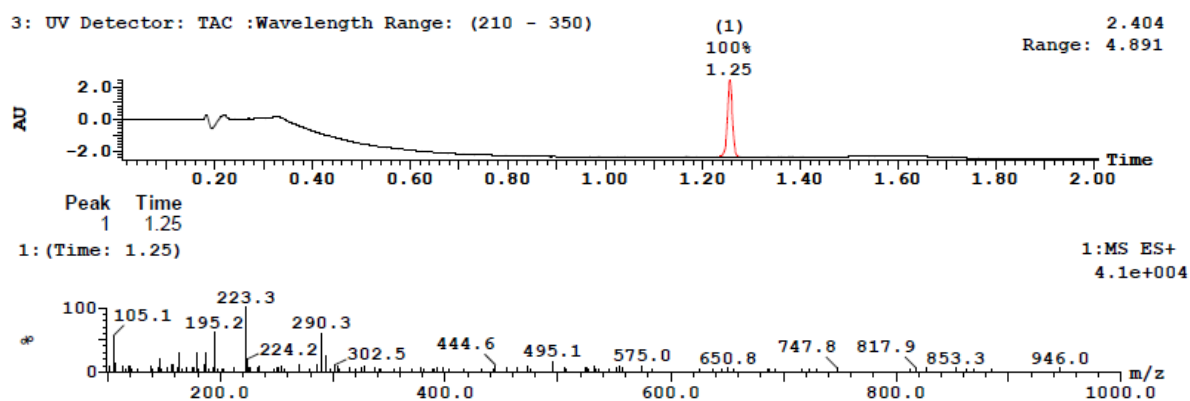
¹H NMR Spectra



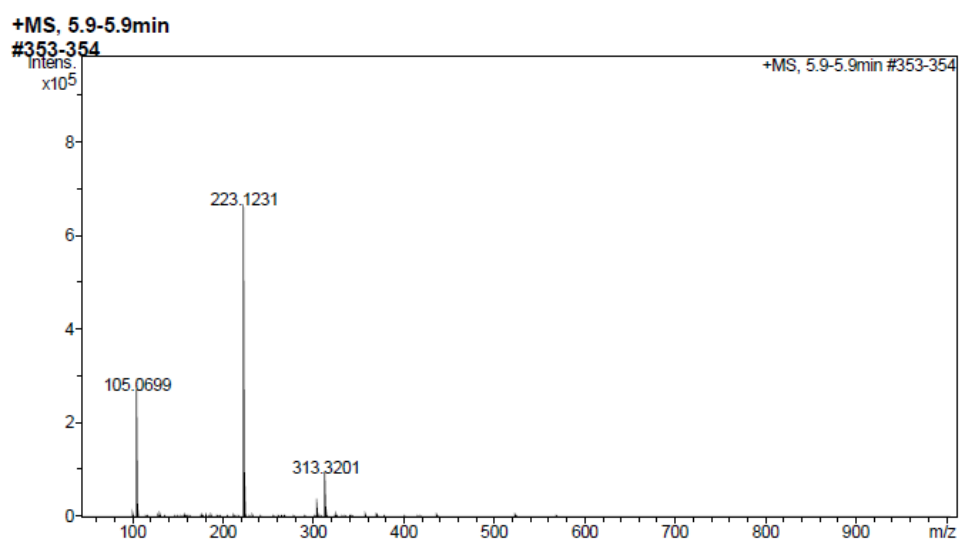
¹³C NMR Spectra



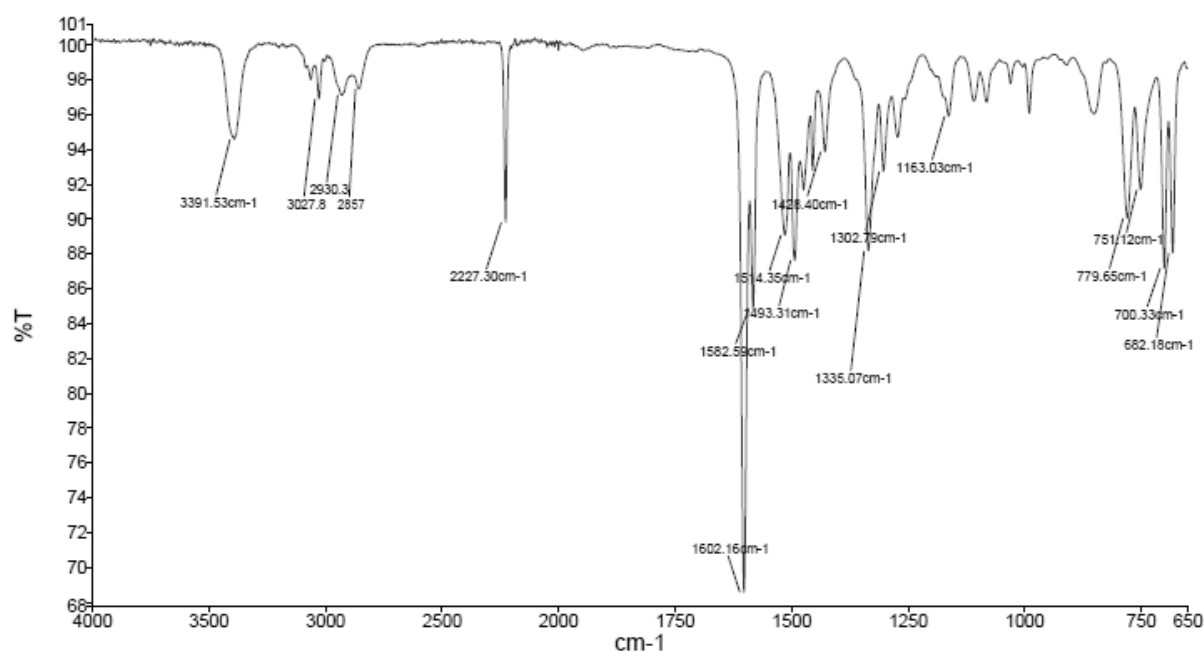
LCMS



HRMS

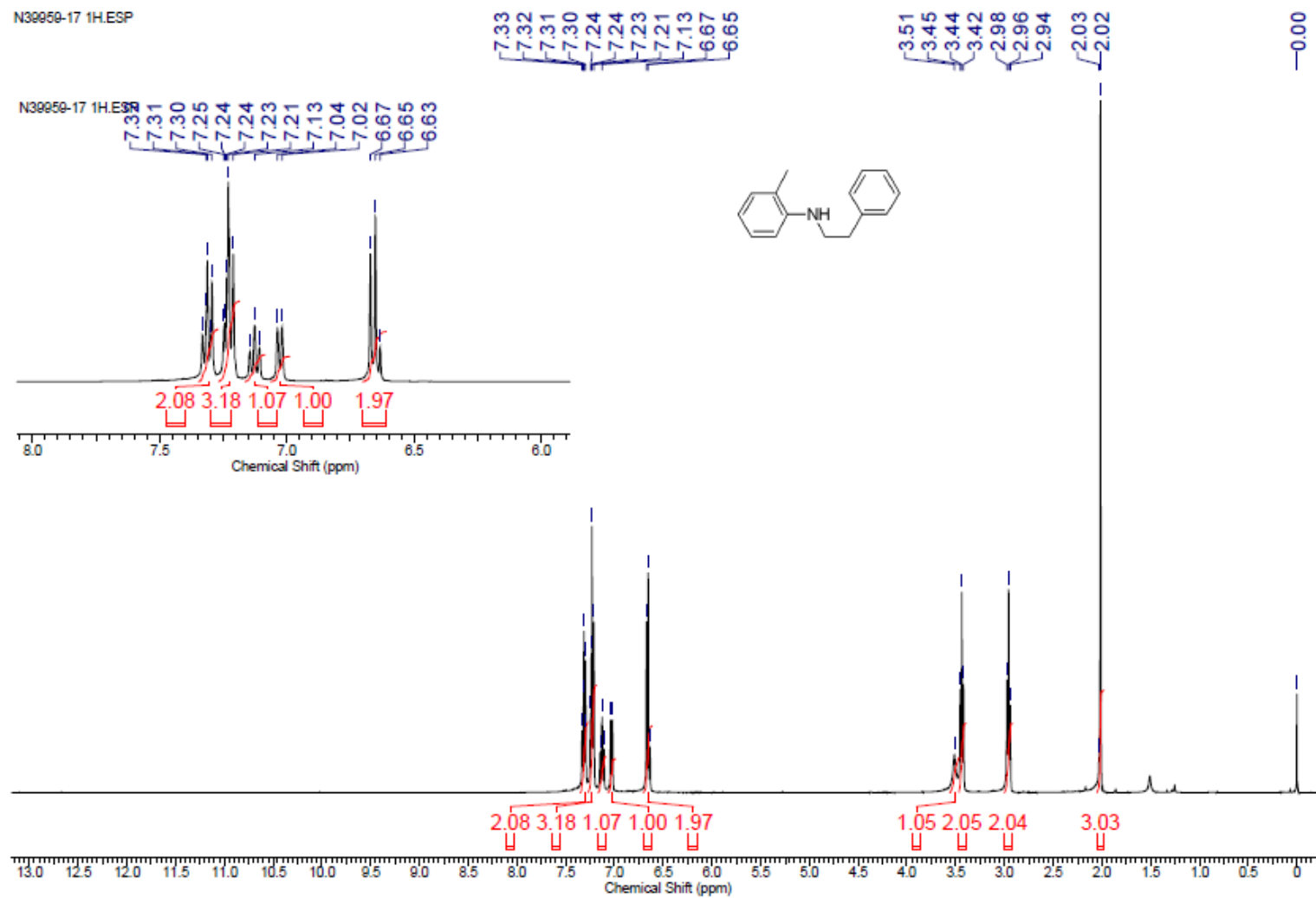


IR Spectra

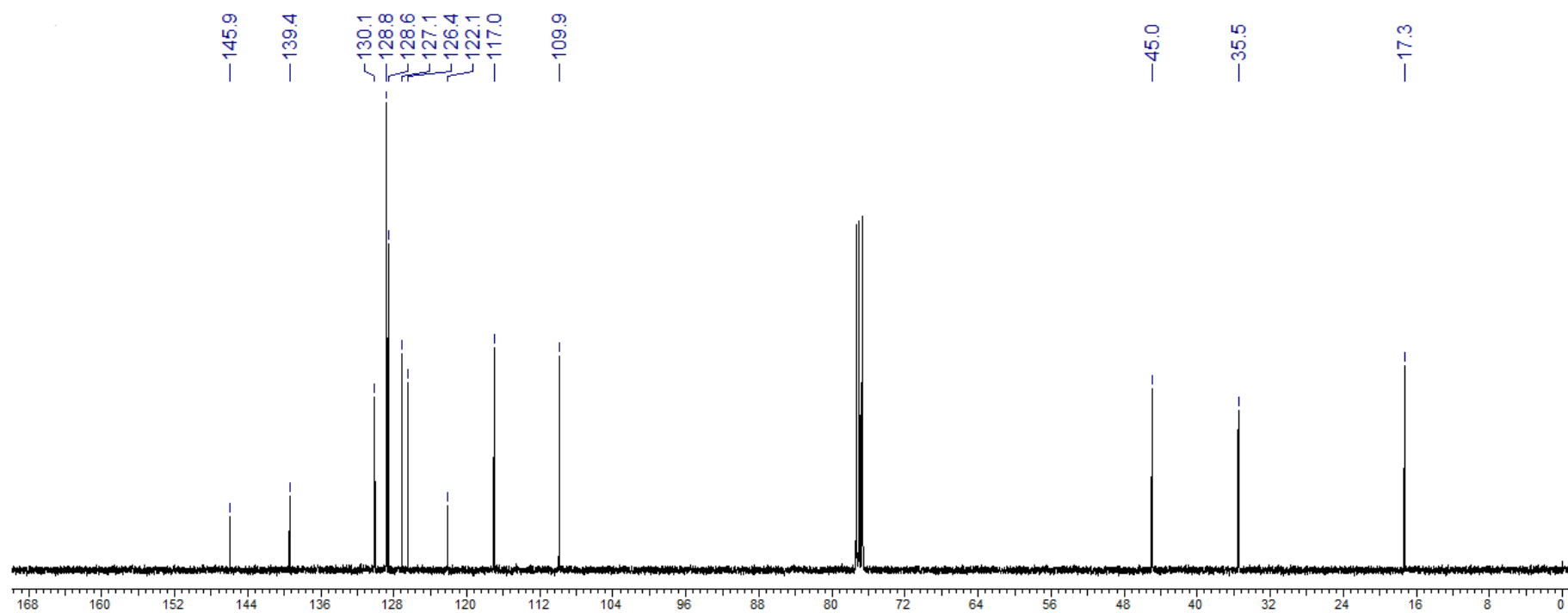


2-Methyl-N-phenethylamine (7s).

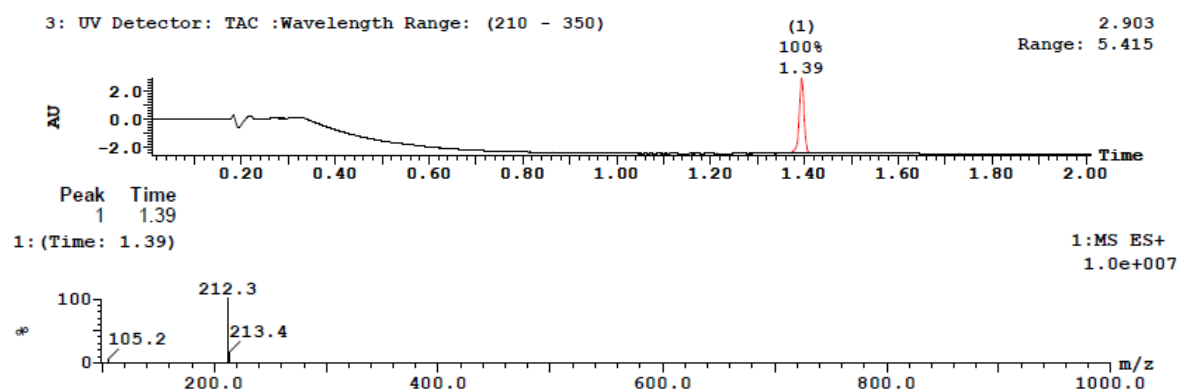
¹H NMR Spectra



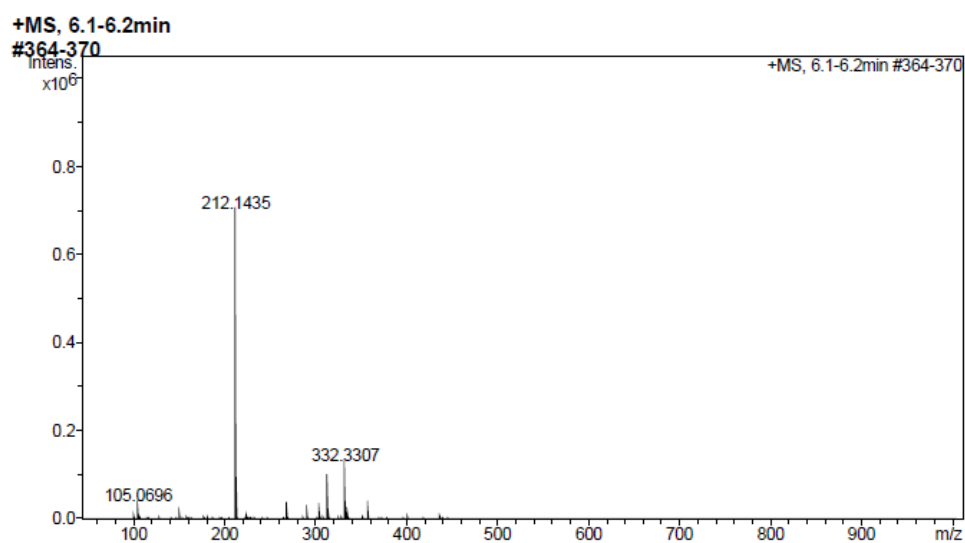
¹³C NMR Spectra



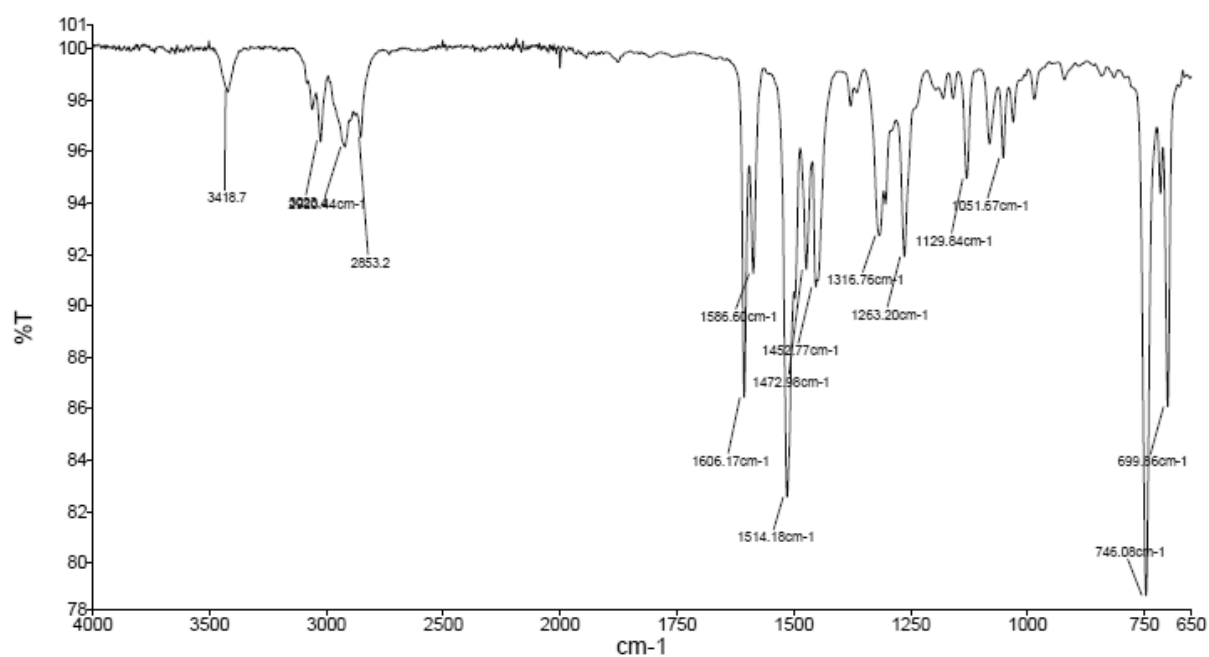
LCMS



HRMS



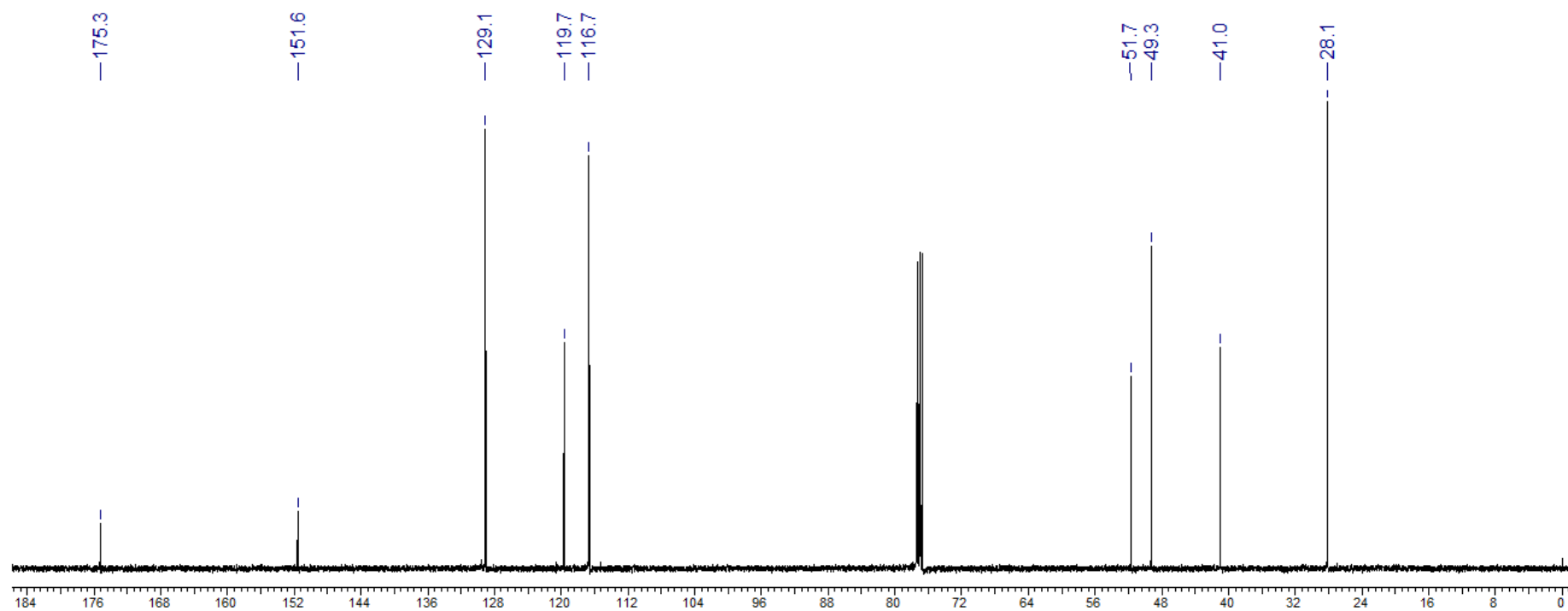
IR Spectra



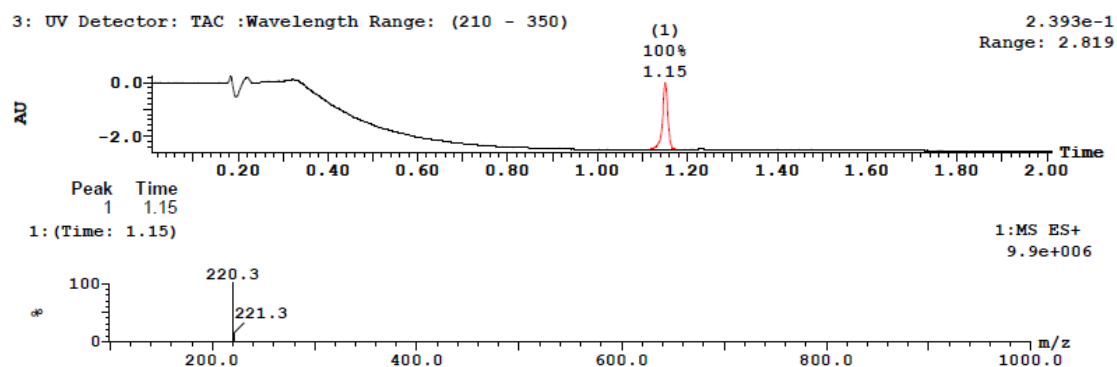
¹H NMR Spectra



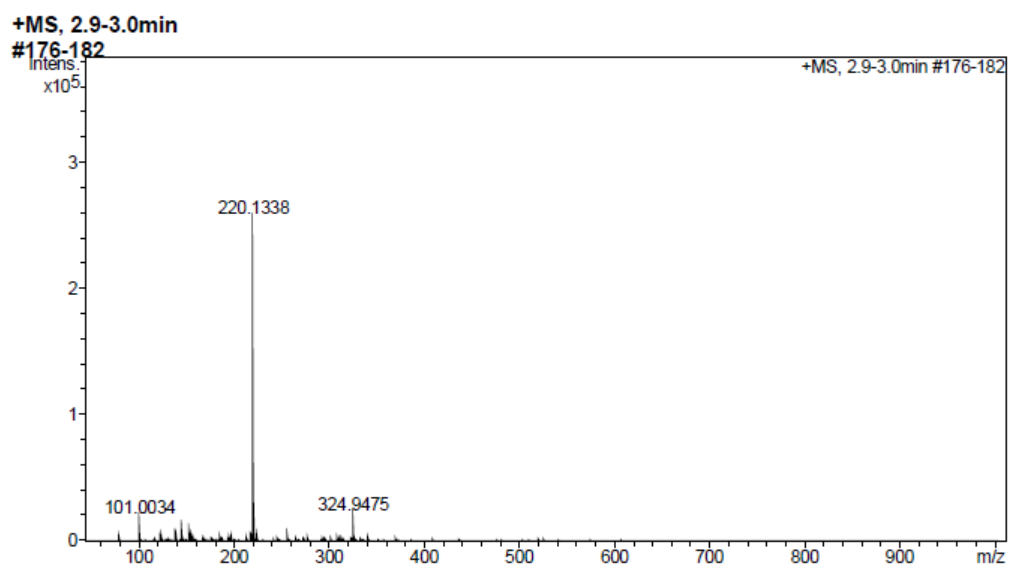
¹³C NMR Spectra



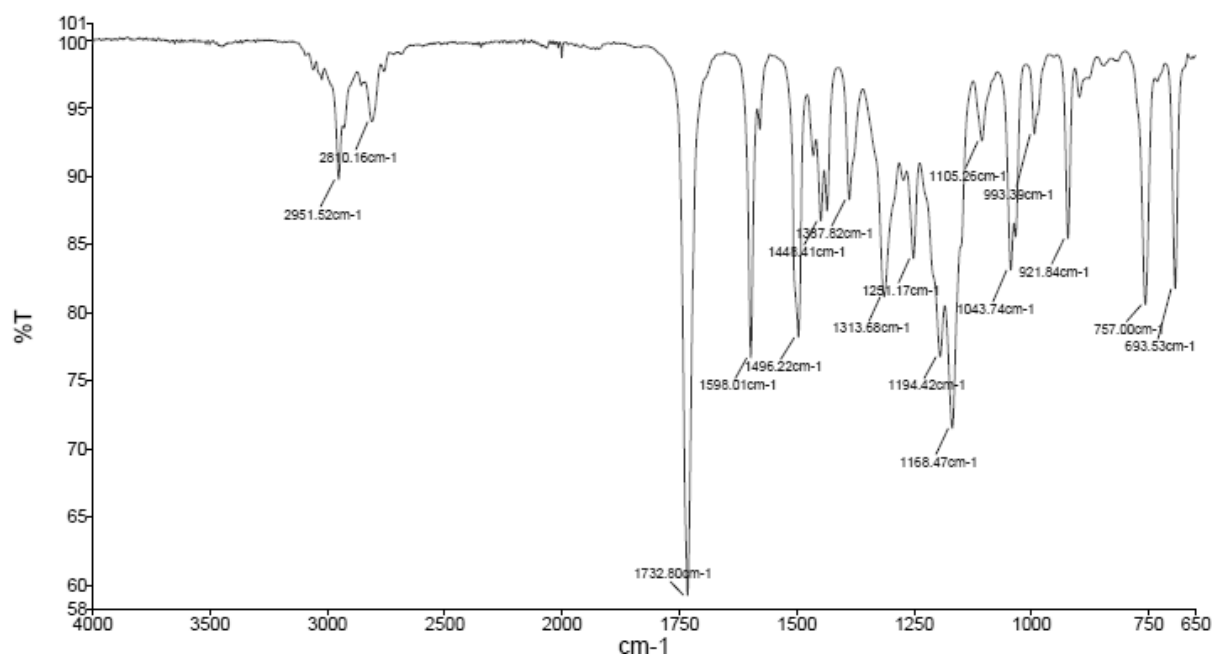
LCMS



HRMS

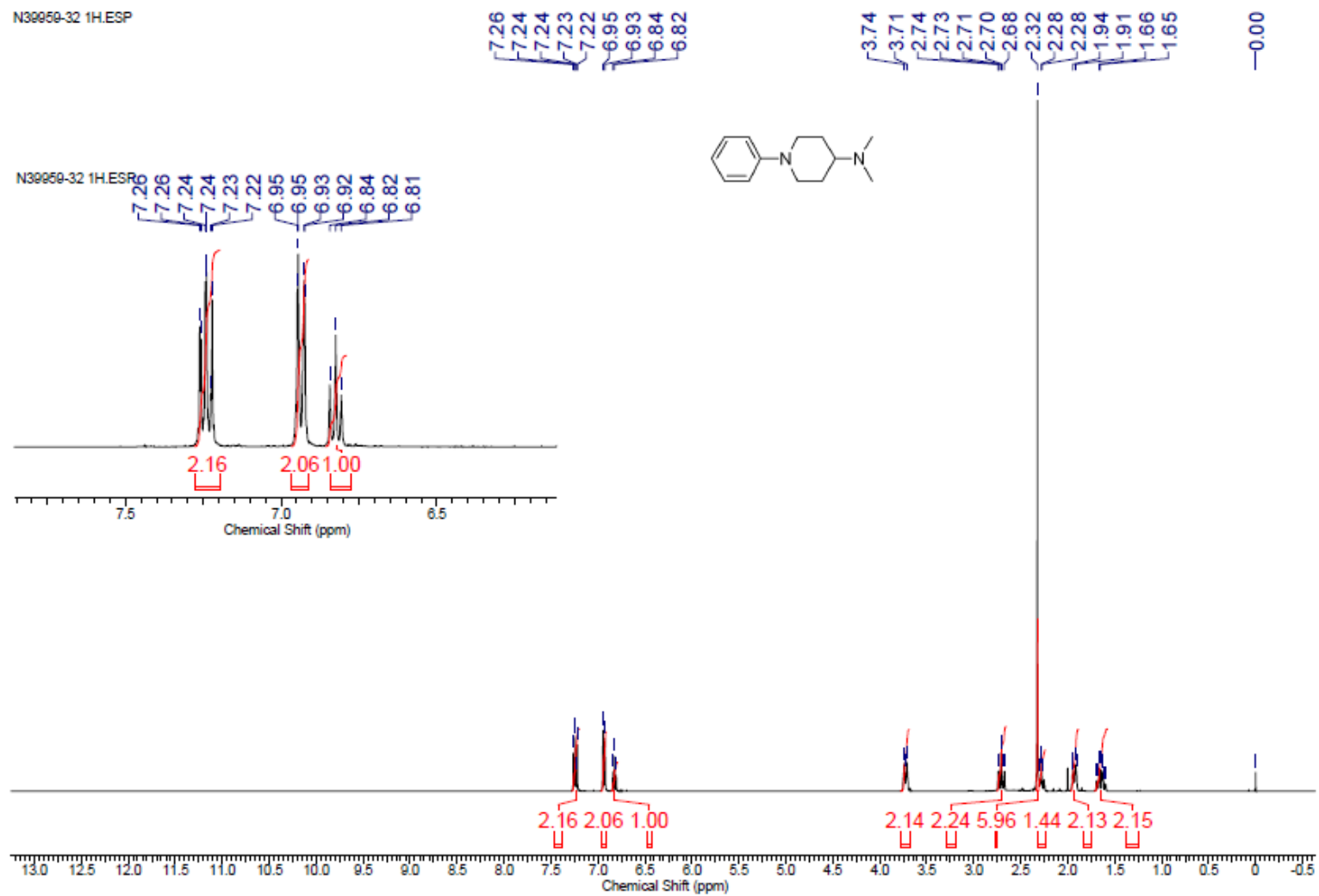


IR Spectra

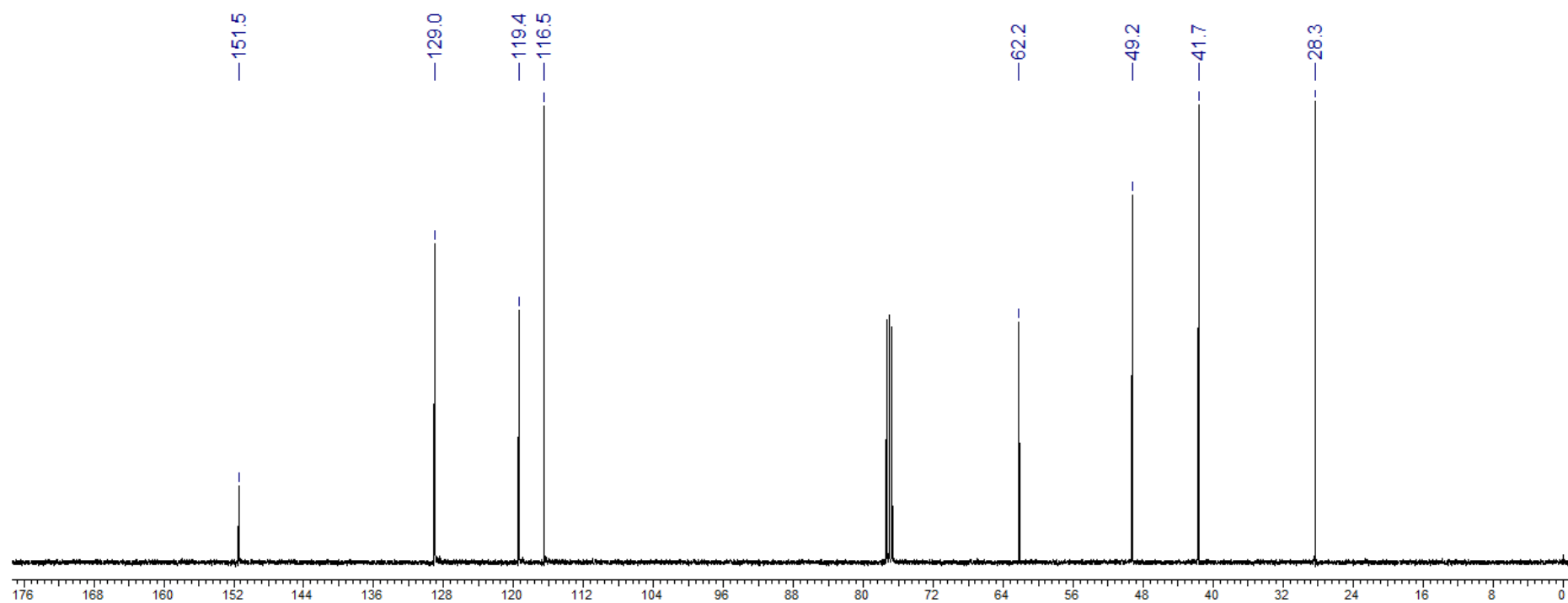


***N,N*-Dimethyl-1-phenylpiperidin-4-amine (7u).**

¹H NMR Spectra



¹³C NMR Spectra

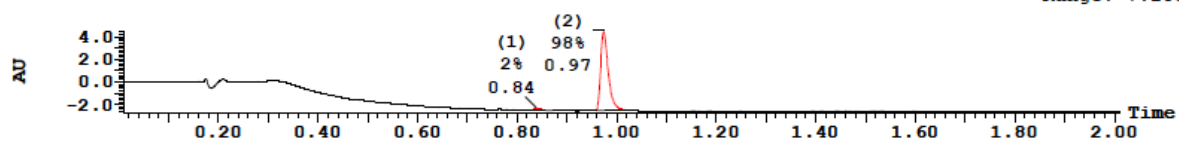


LCMS

3: UV Detector: TAC :Wavelength Range: (210 - 350)

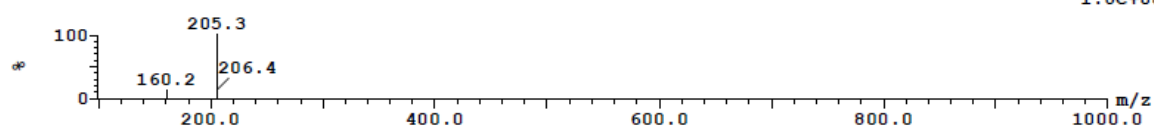
4.461

Range: 7.105



Peak Time
2 0.97
2: (Time: 0.97)

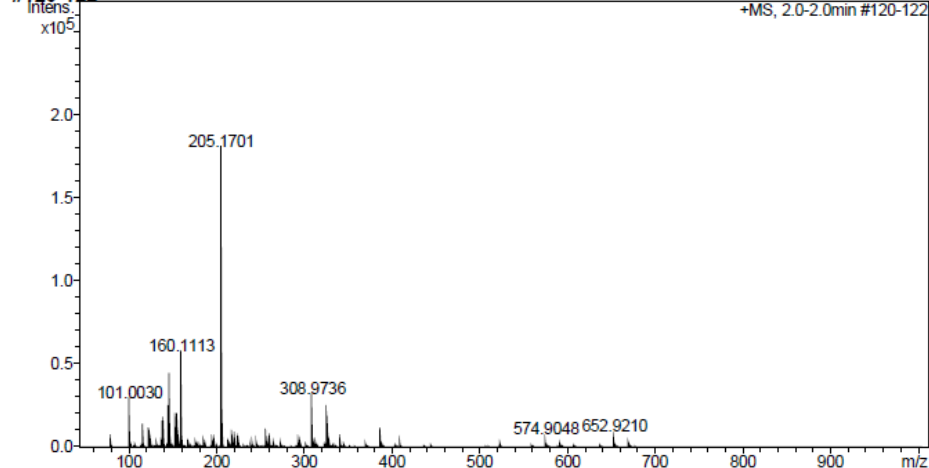
1:MS ES+
1.8e+007



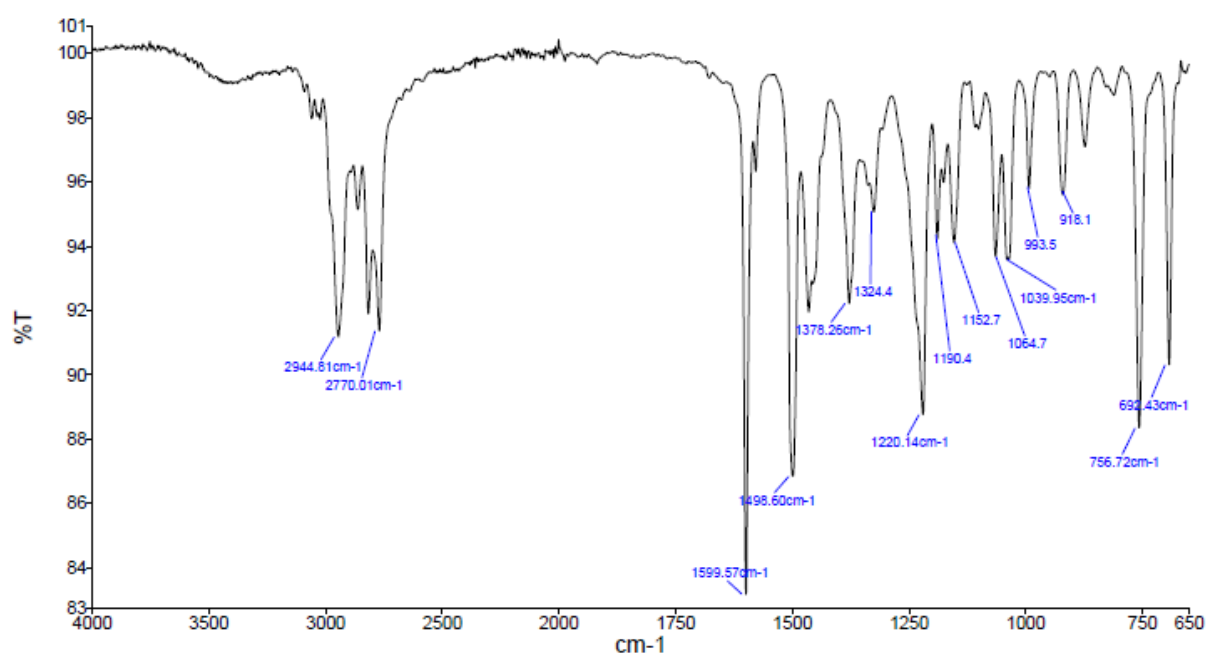
HRMS

+MS, 2.0-2.0min

#120-122

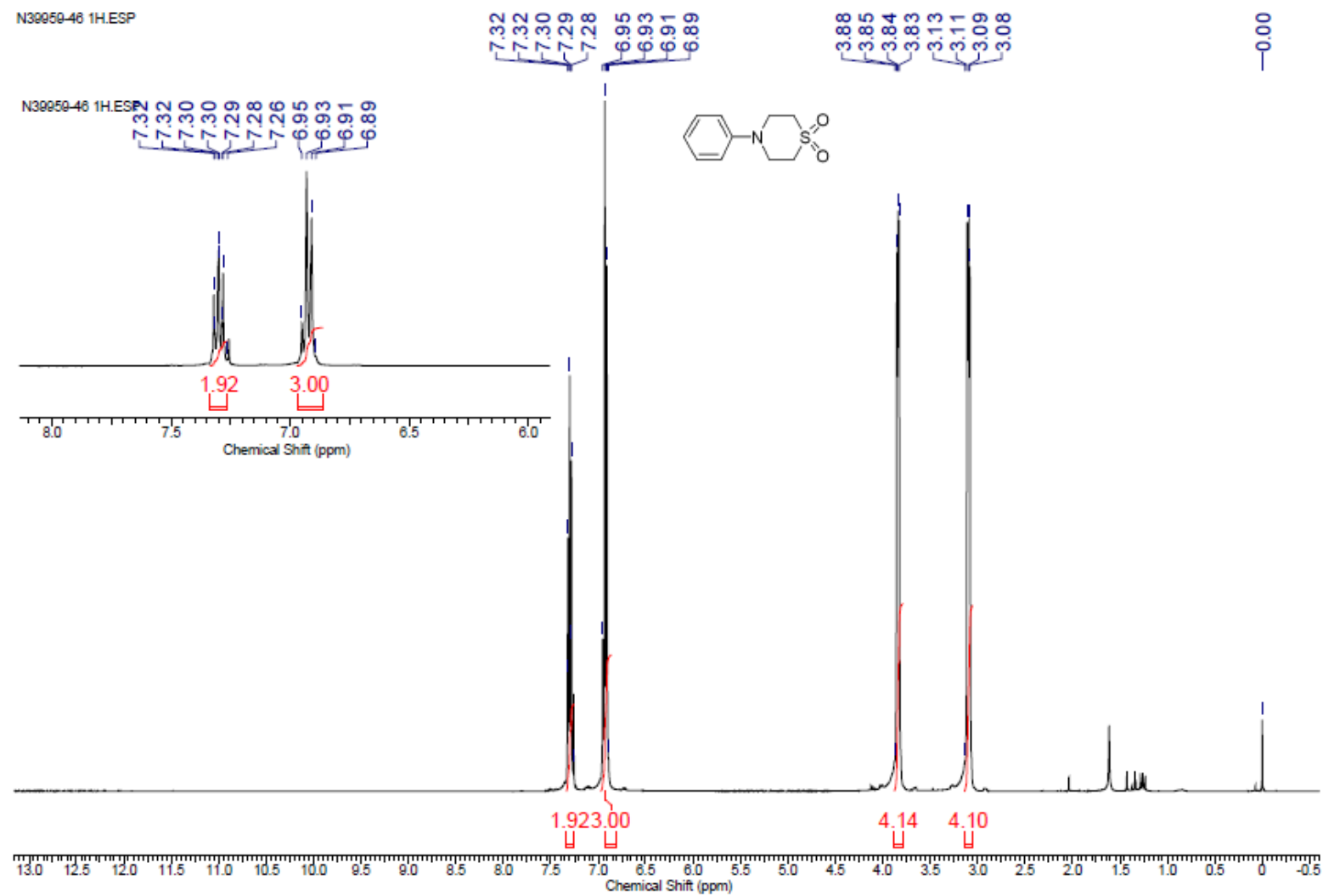


IR Spectra

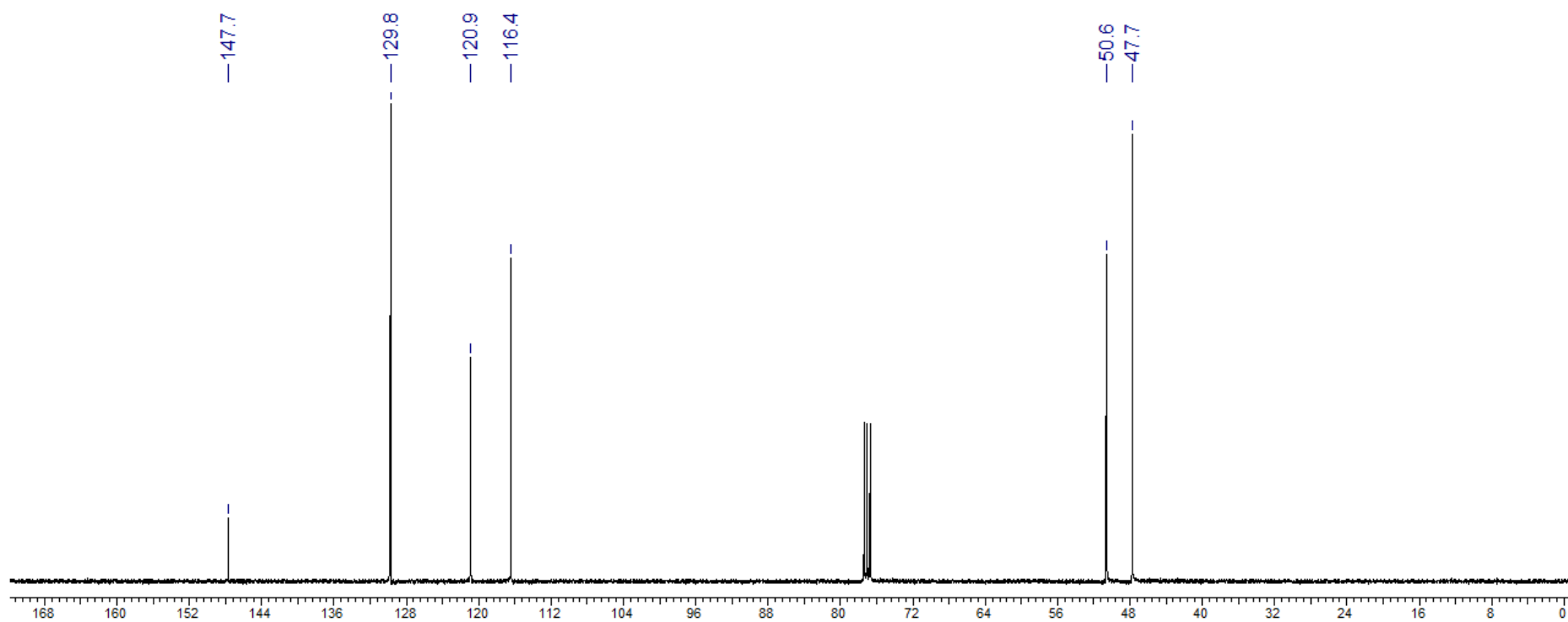


4-Phenylthiomorpholine 1,1-dioxide (7v).

¹H NMR Spectra



¹³C NMR Spectra

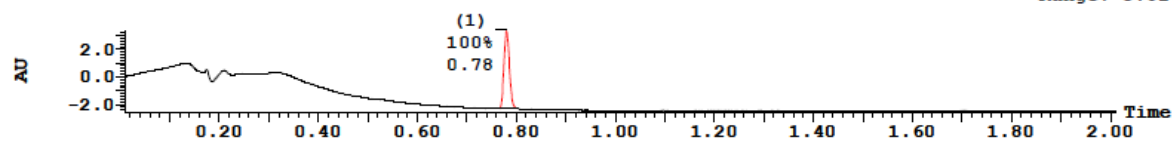


LCMS

3: UV Detector: TAC :Wavelength Range: (210 - 350)

3.321

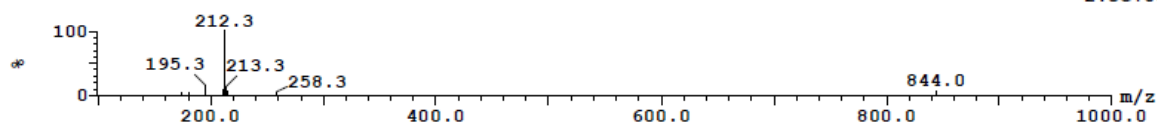
Range: 5.814



Peak Time
1 0.78
1: (Time: 0.78)

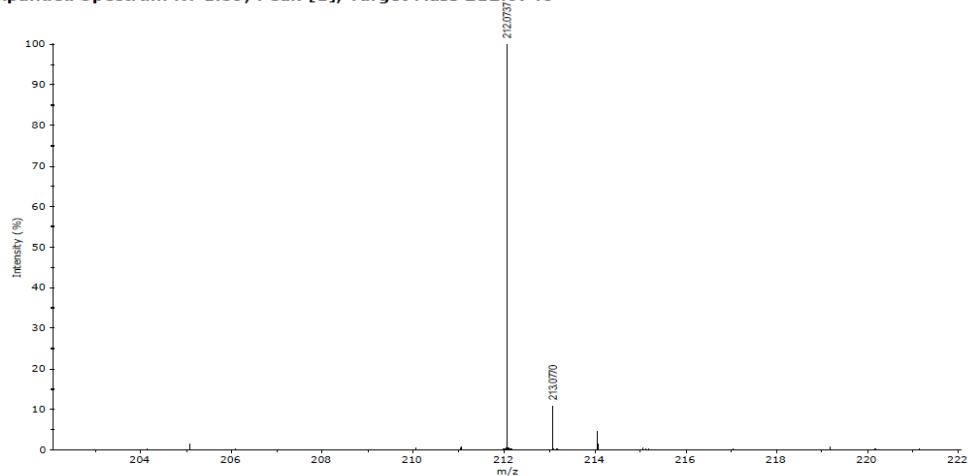
1:MS ES+

2.3e+005

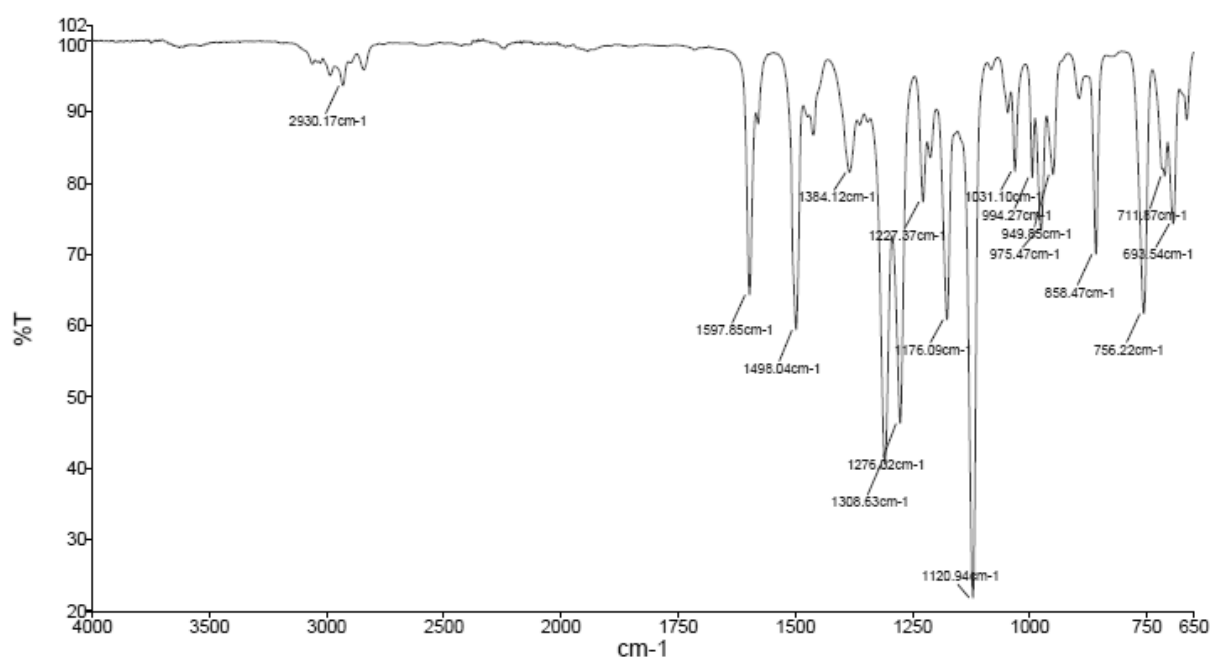


HRMS

Expanded Spectrum RT 1.69, Peak [1], Target Mass 212.0740

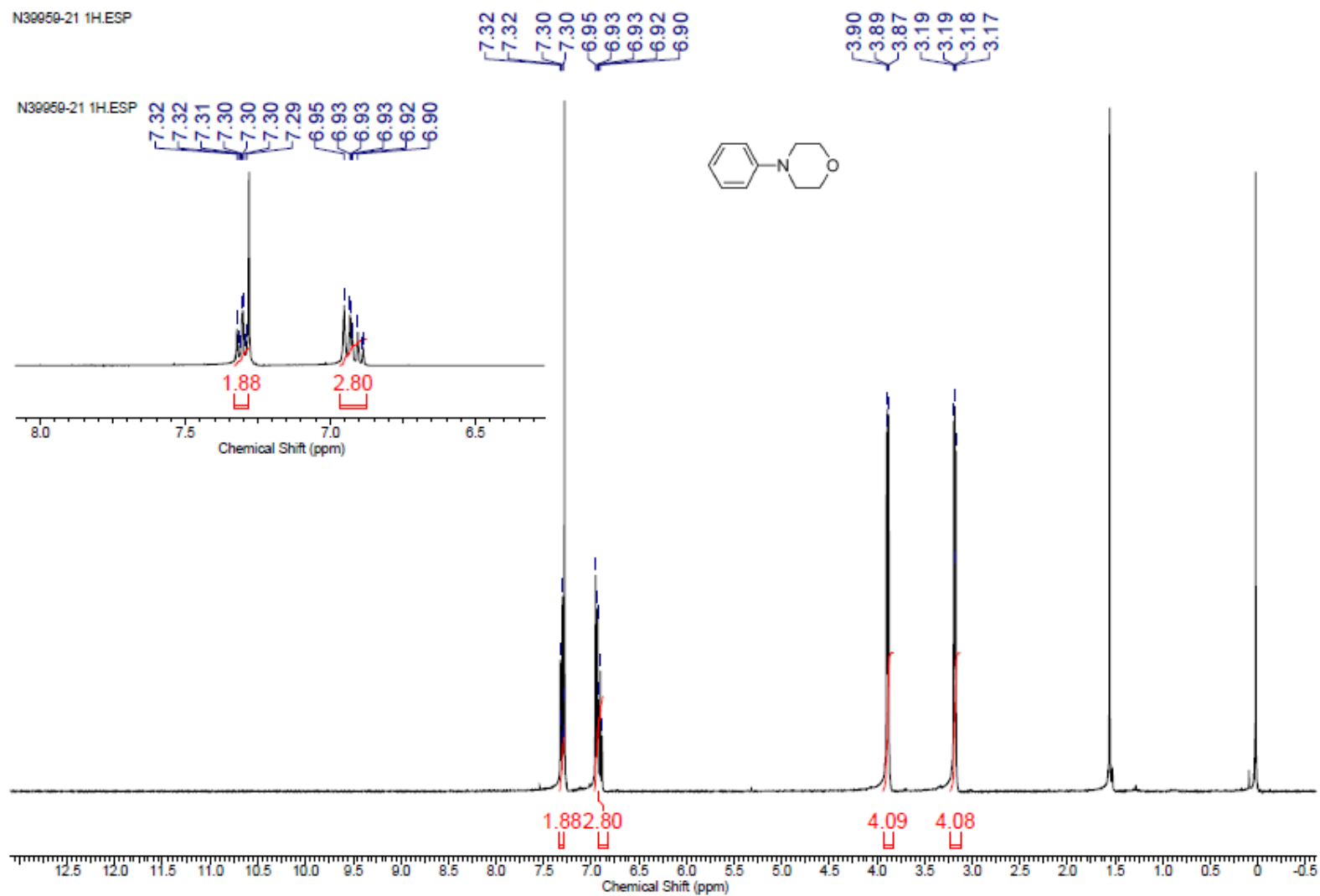


IR Spectra

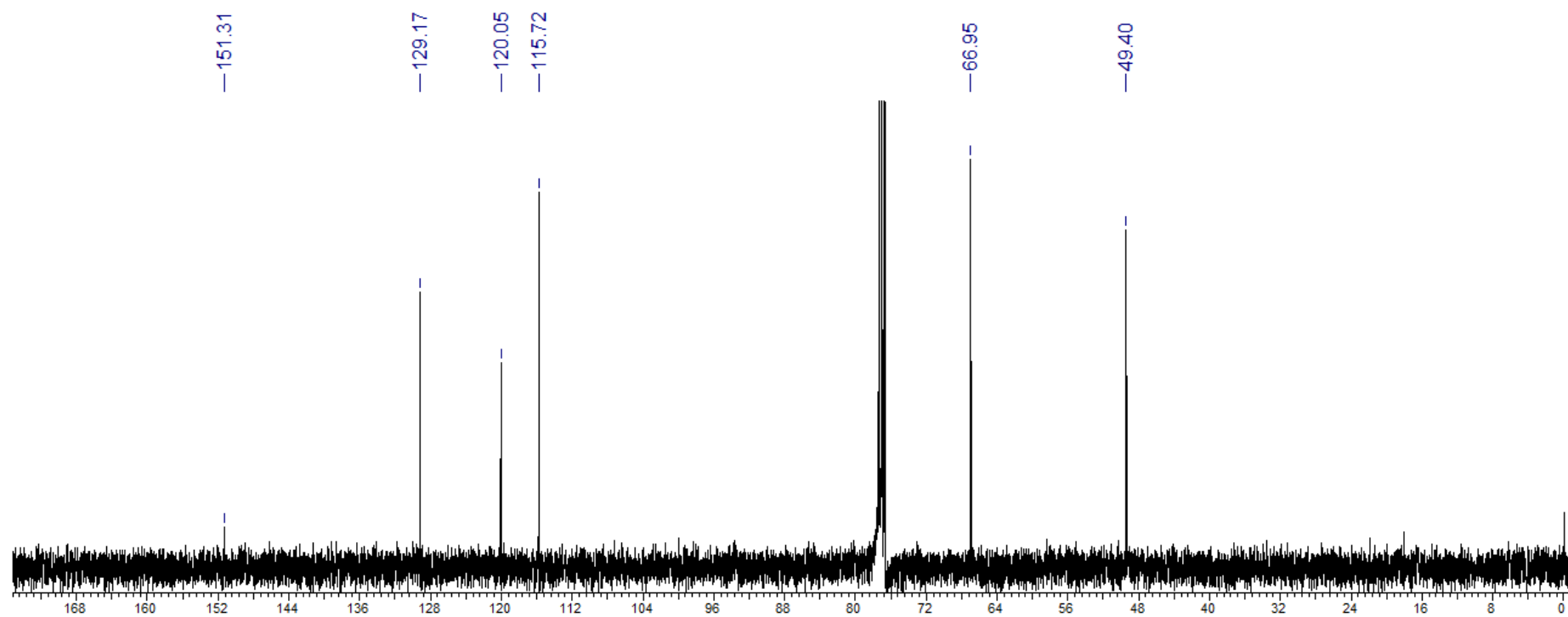


4-Phenylmorpholine (7w).

¹H NMR Spectra



¹³C NMR Spectra

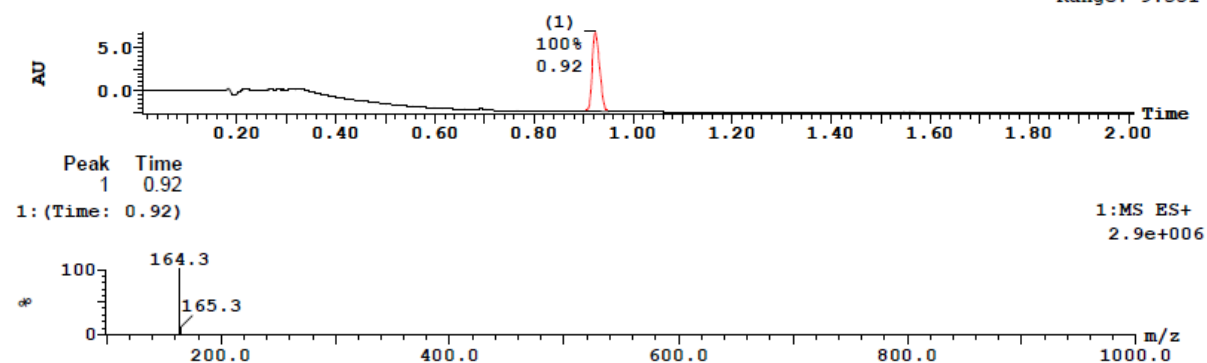


LCMS

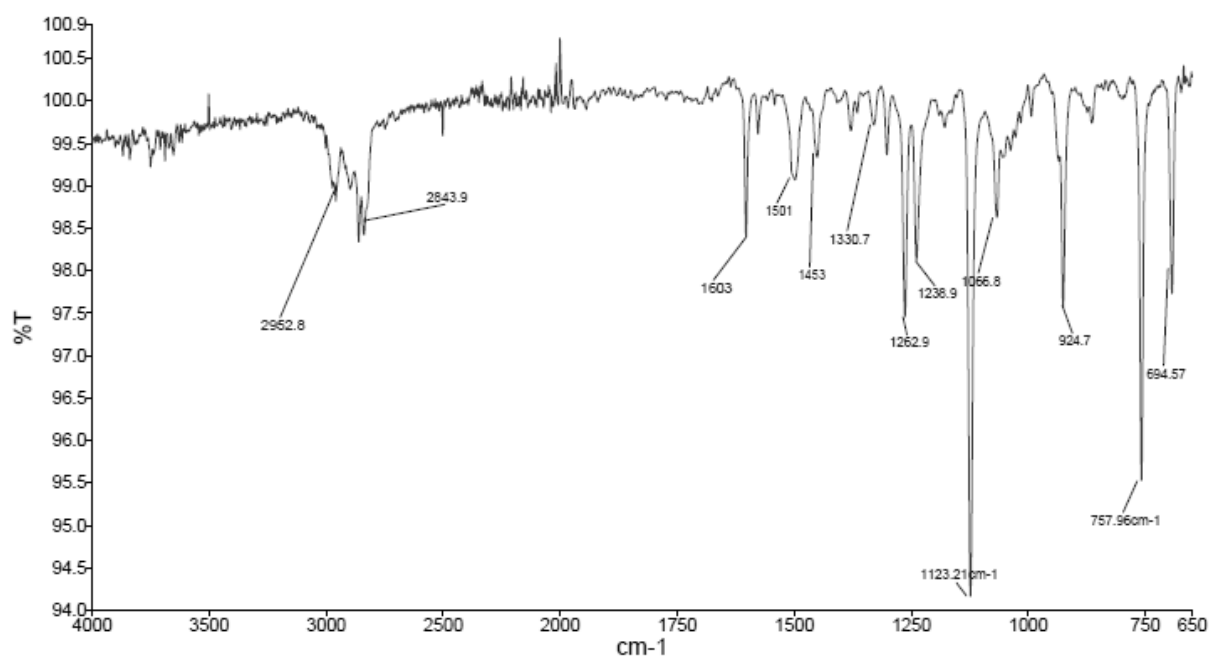
3: UV Detector: TAC :Wavelength Range: (210 - 350)

6.744

Range: 9.351

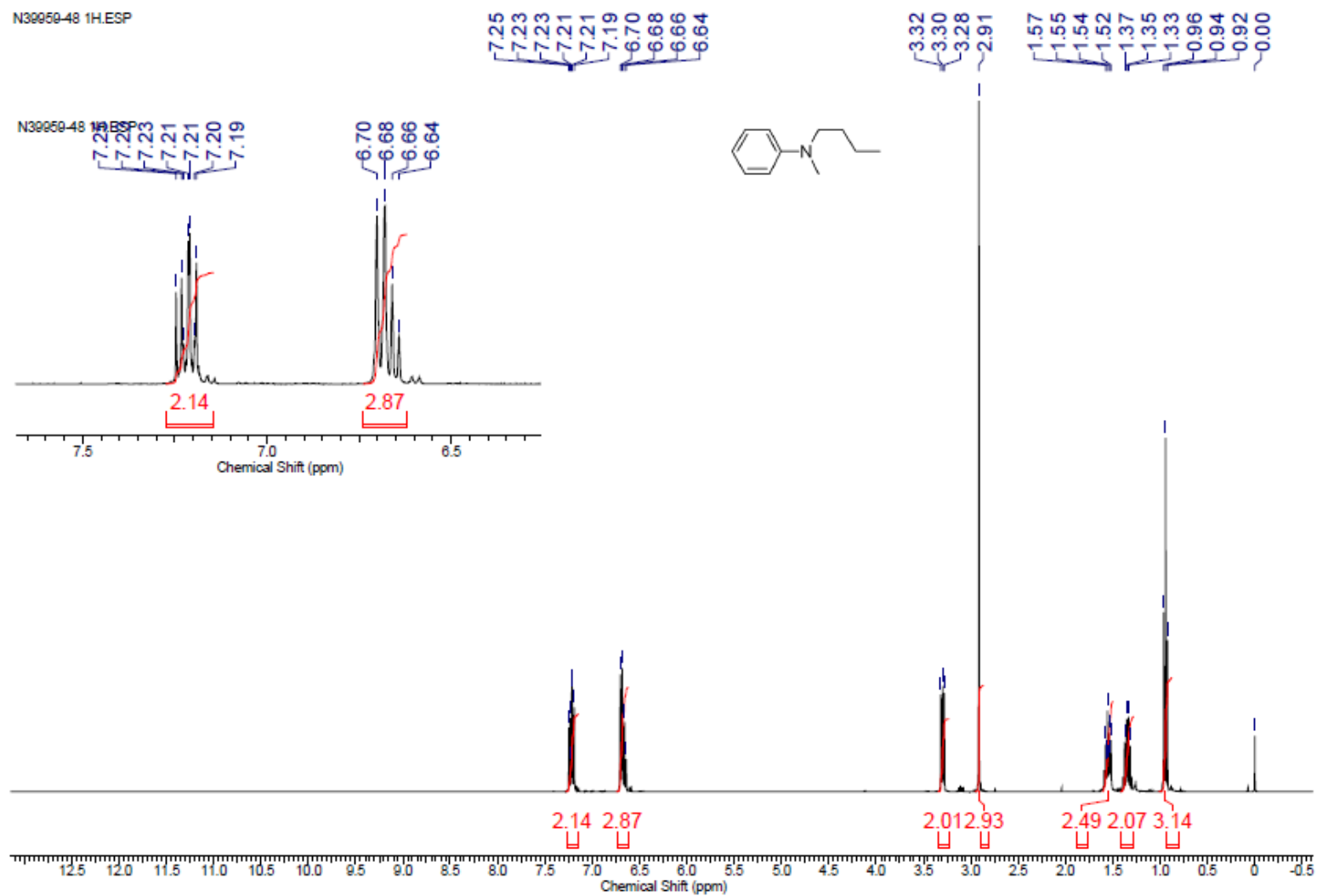


IR Spectra

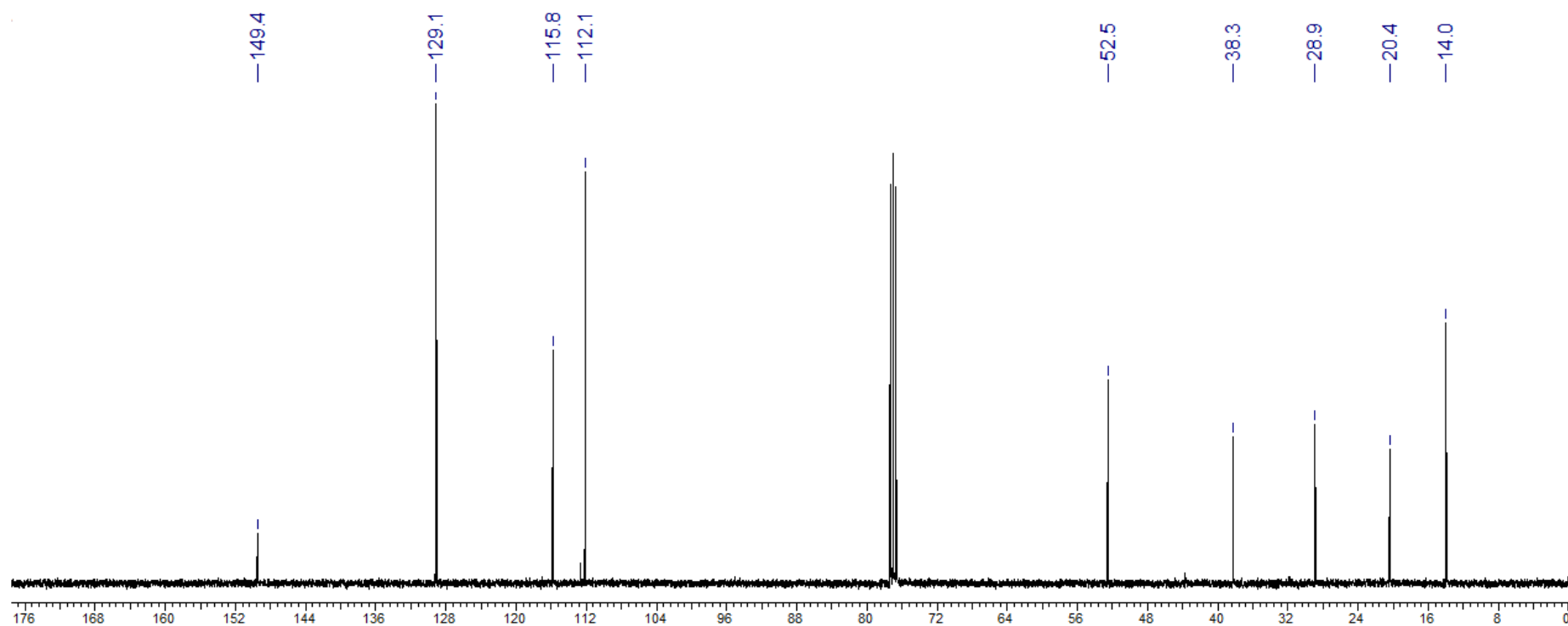


***N*-Butyl-*N*-methylaniline (7x).**

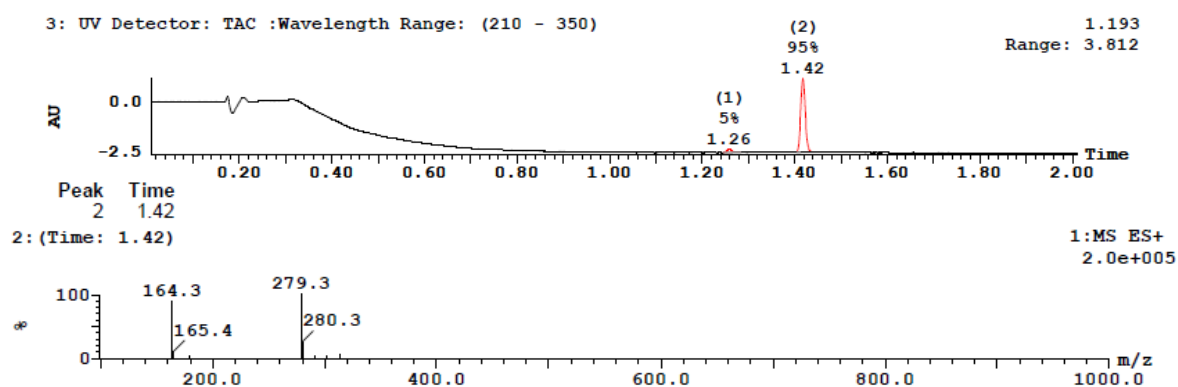
¹H NMR Spectra



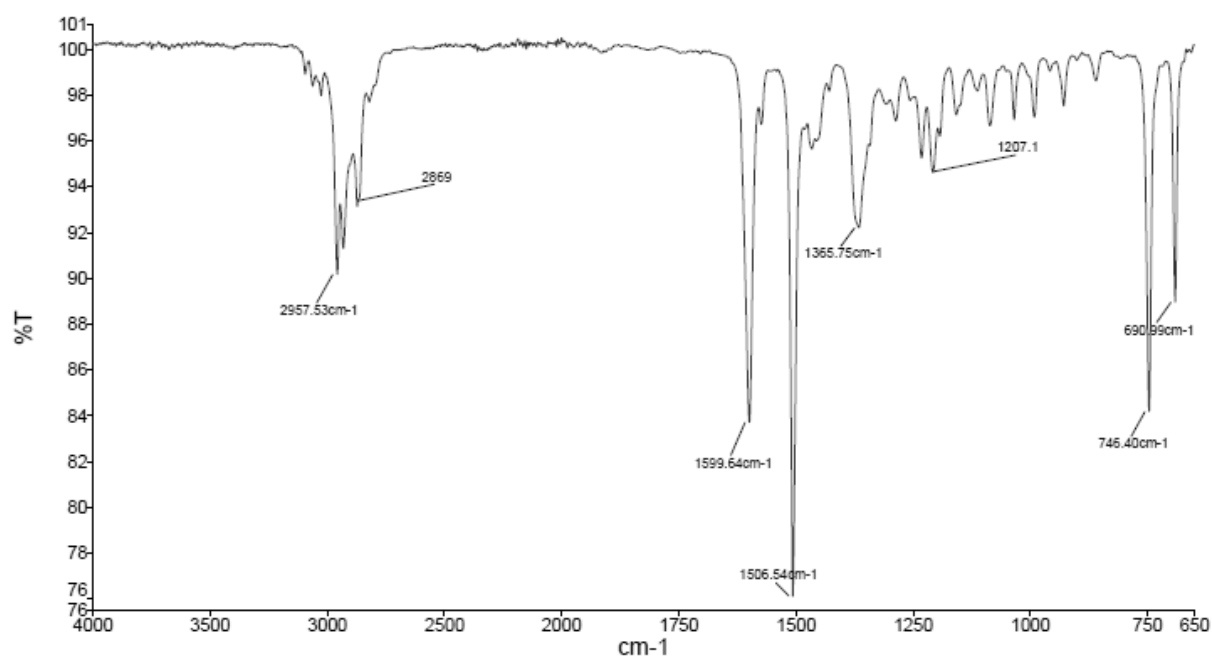
¹³C NMR Spectra



LCMS



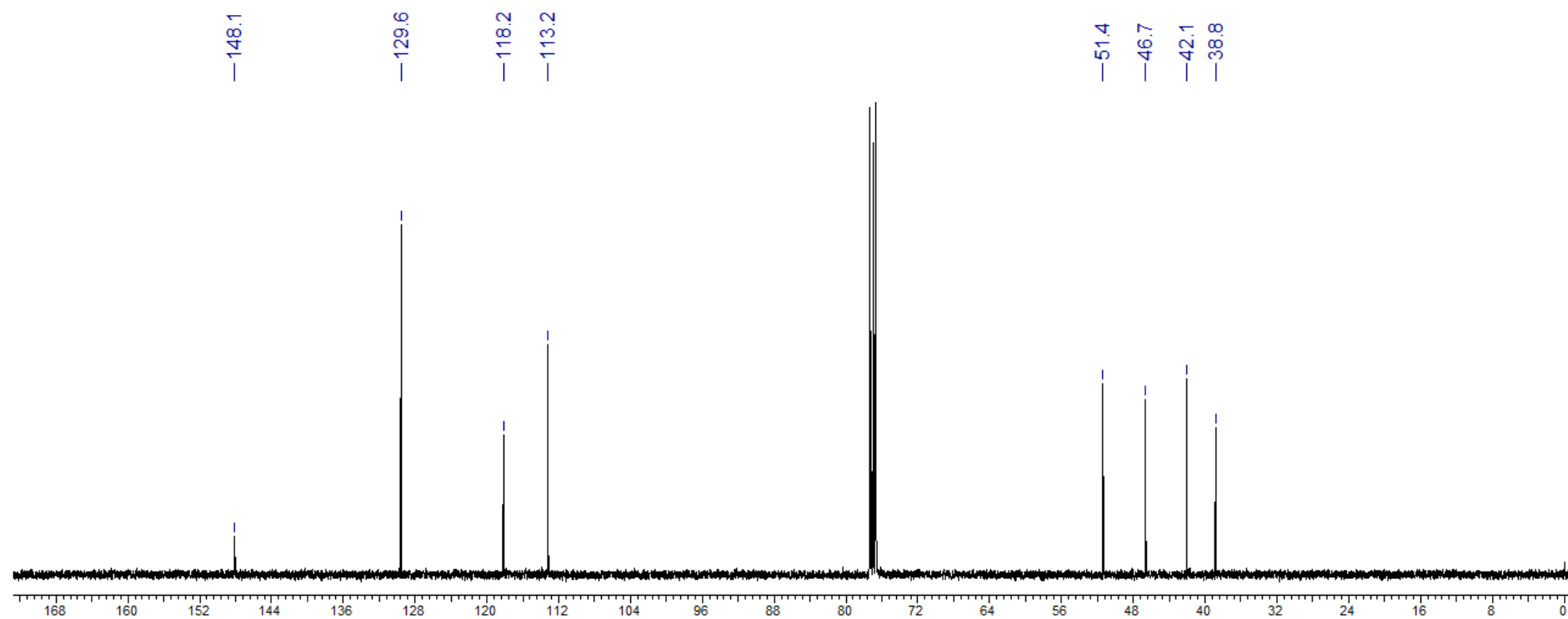
IR Spectra



¹H NMR Spectra



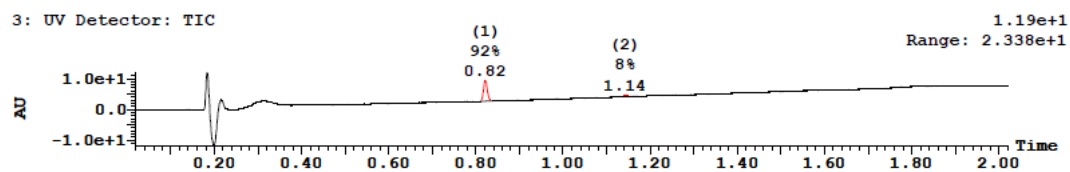
¹³C NMR Spectra



LCMS

Sample: 1

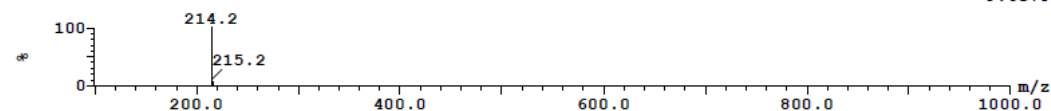
3: UV Detector: TIC



Peak Time
1 0.82

1: (Time: 0.82) Combine (210:223-(183:186+246:248))

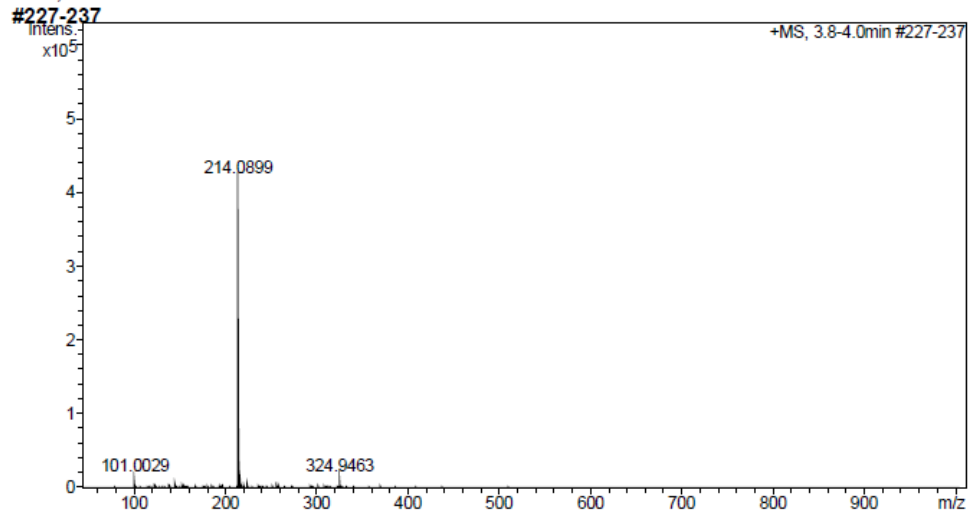
1:MS ES+
9.6e+006



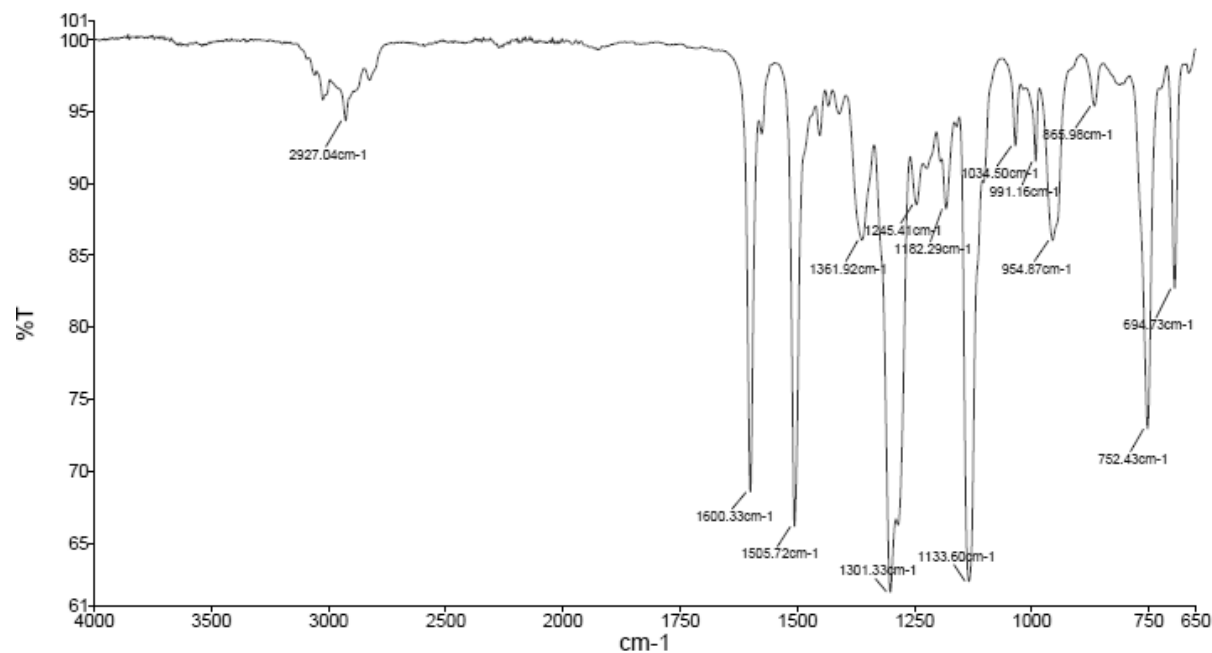
HRMS

+MS, 3.8-4.0min

#227-237

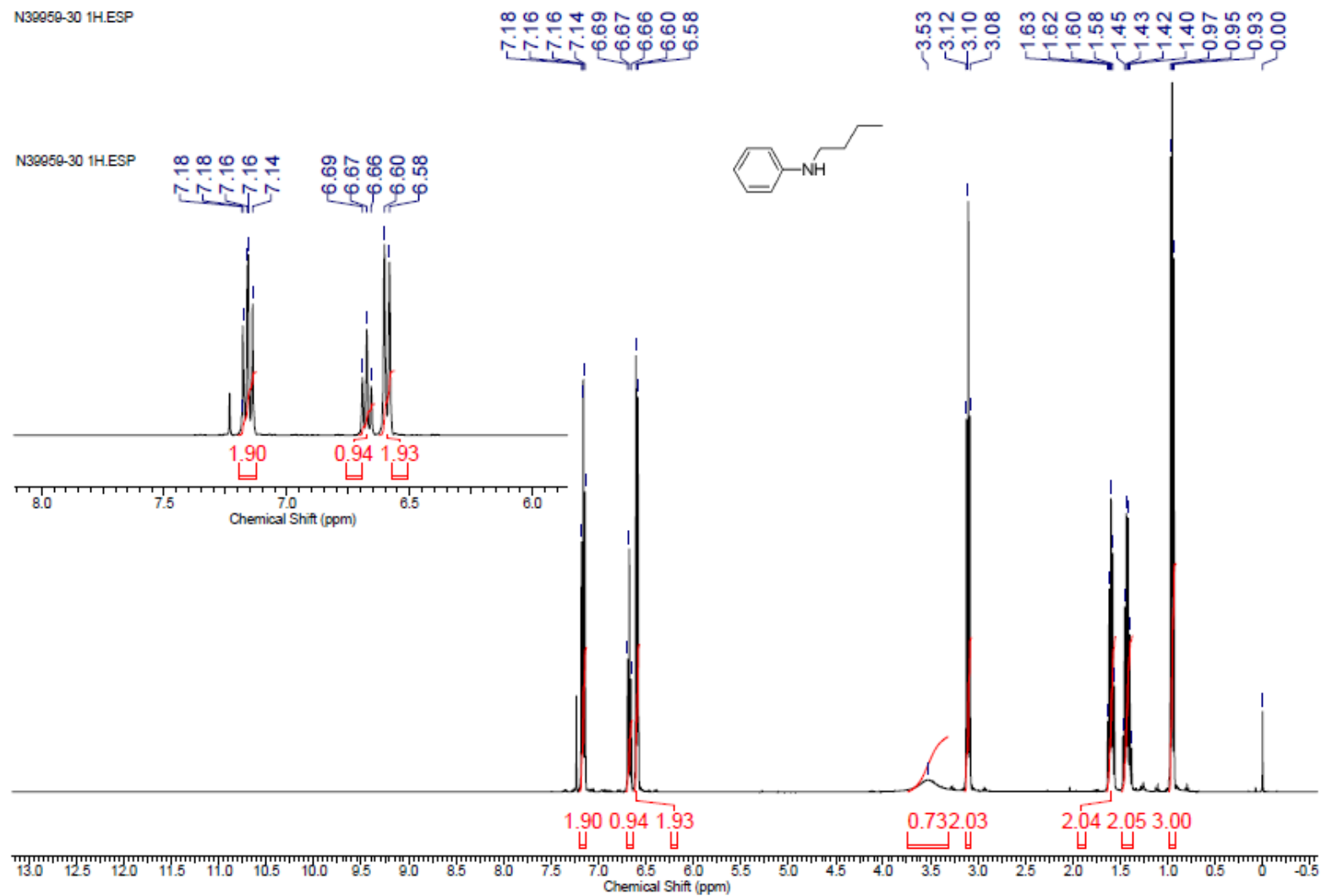


IR Spectra

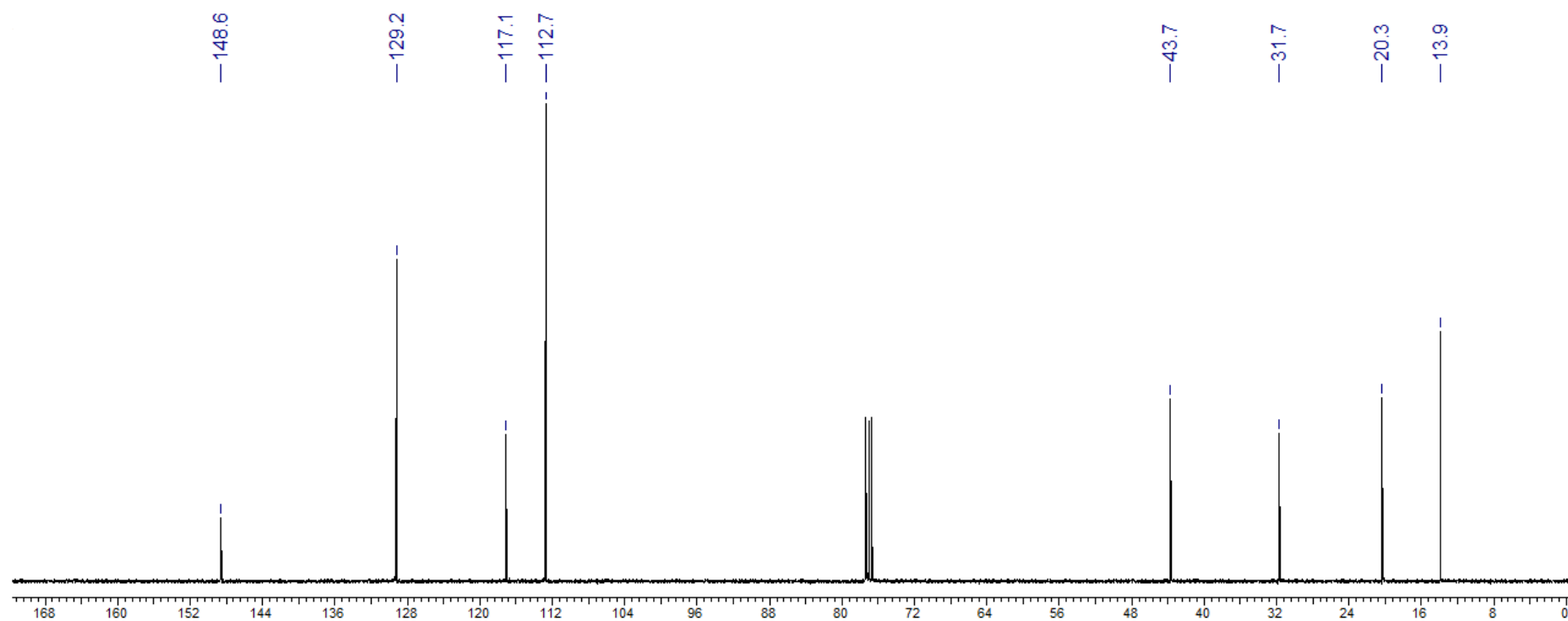


***N*-Butylaniline (7z).**

¹H NMR Spectra

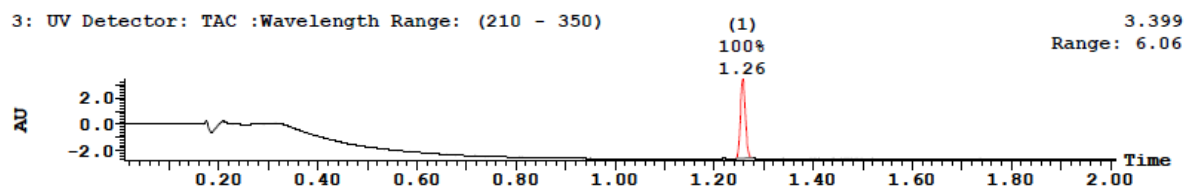


¹³C NMR Spectra



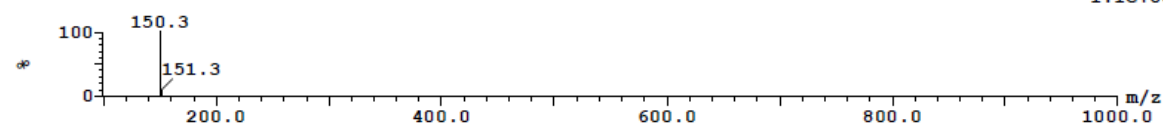
LCMS

3: UV Detector: TAC :Wavelength Range: (210 - 350)

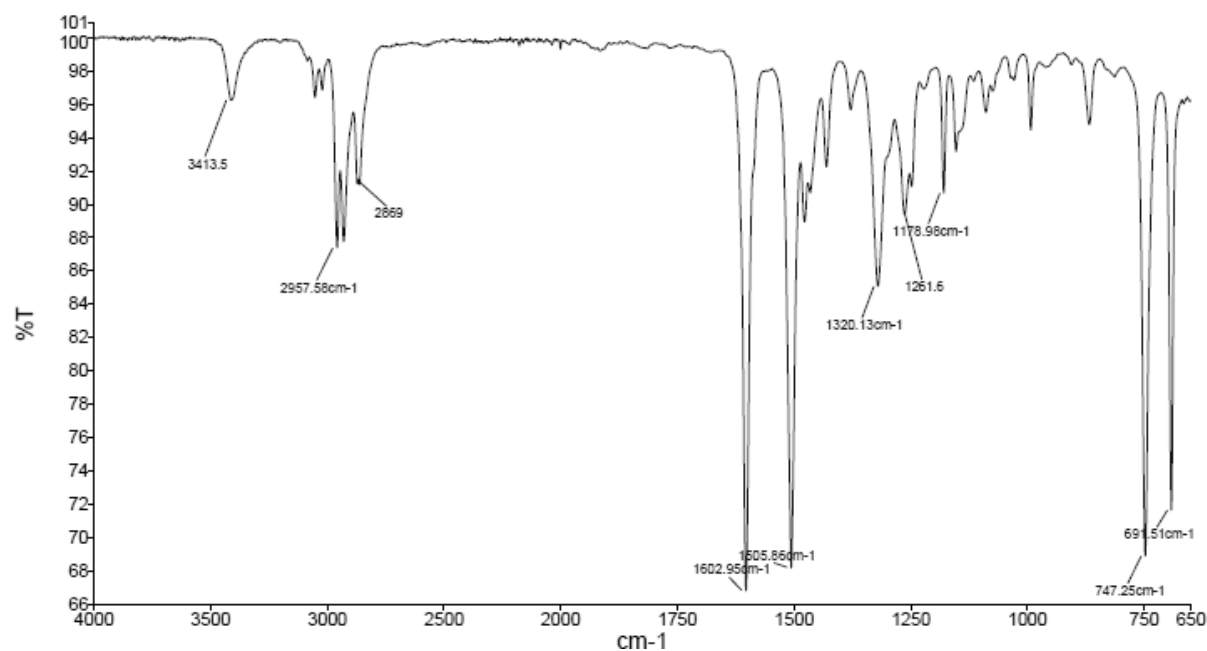


Peak Time
1 1.26
1: (Time: 1.26)

1:MS ES+
1.1e+006

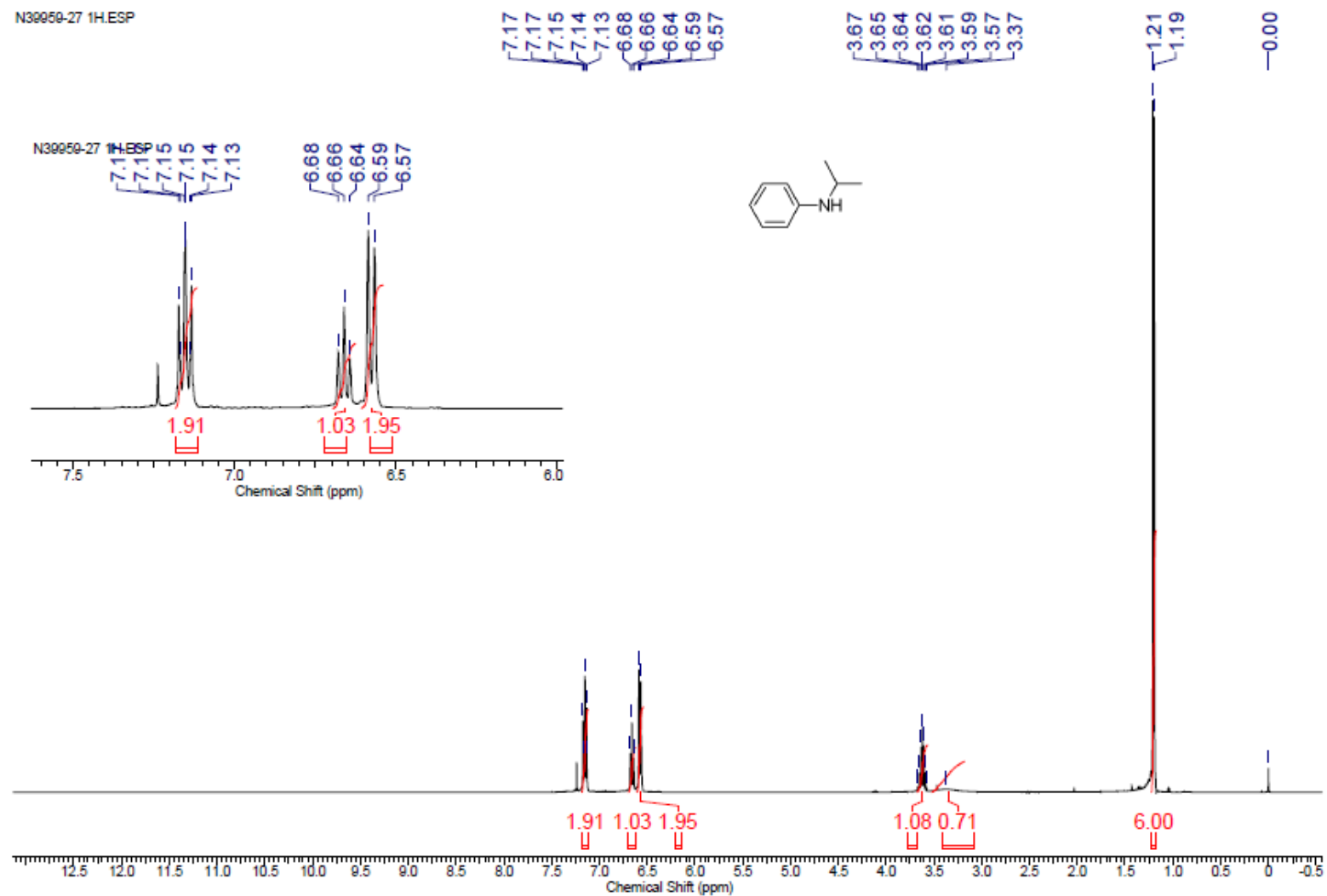


IR Spectra

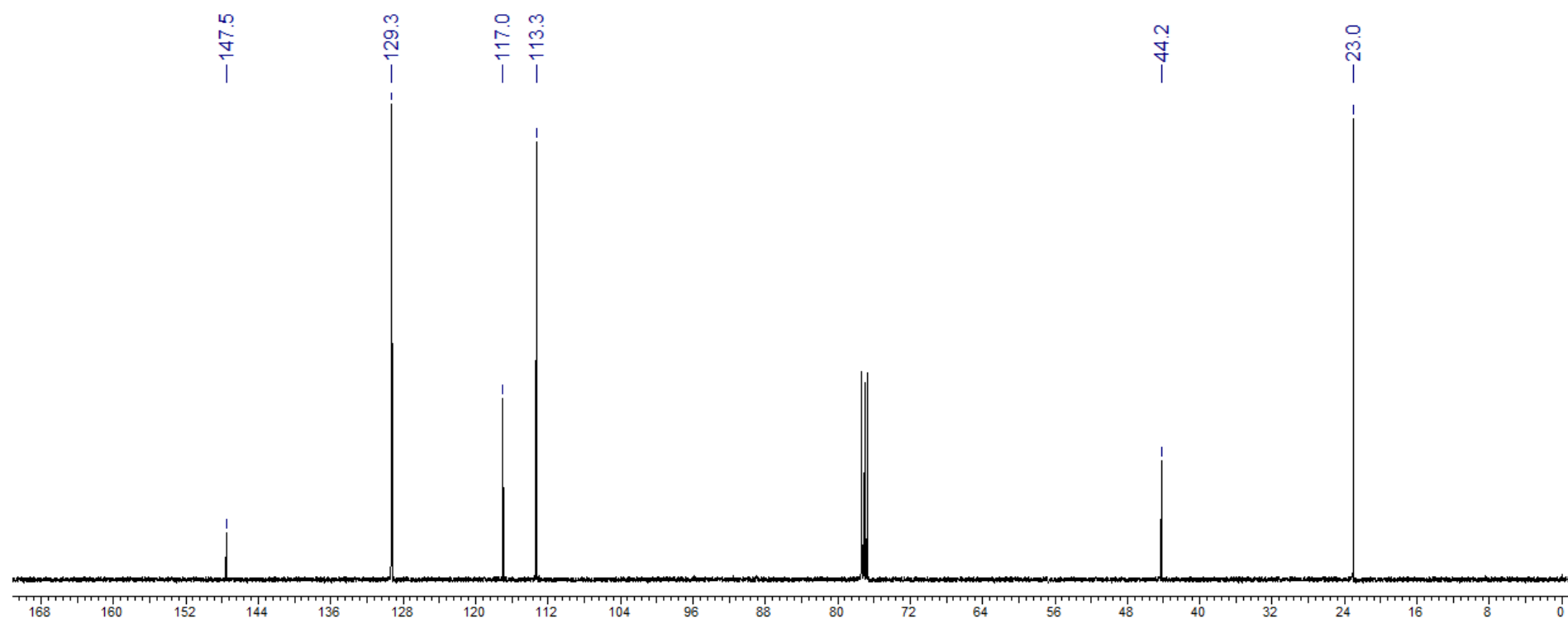


***N*-Isopropylaniline (7aa).**

¹H NMR Spectra



¹³C NMR Spectra

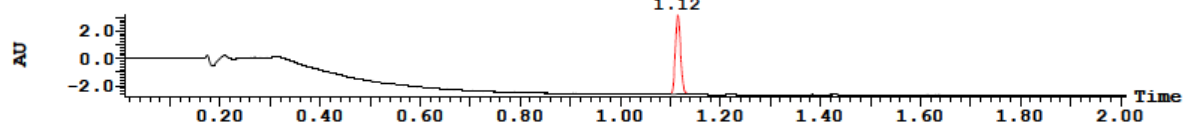


LCMS

3: UV Detector: TAC :Wavelength Range: (210 - 350)

(1)
100%
1.12

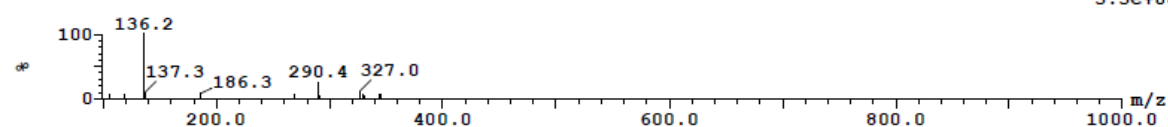
3.176
Range: 5.886



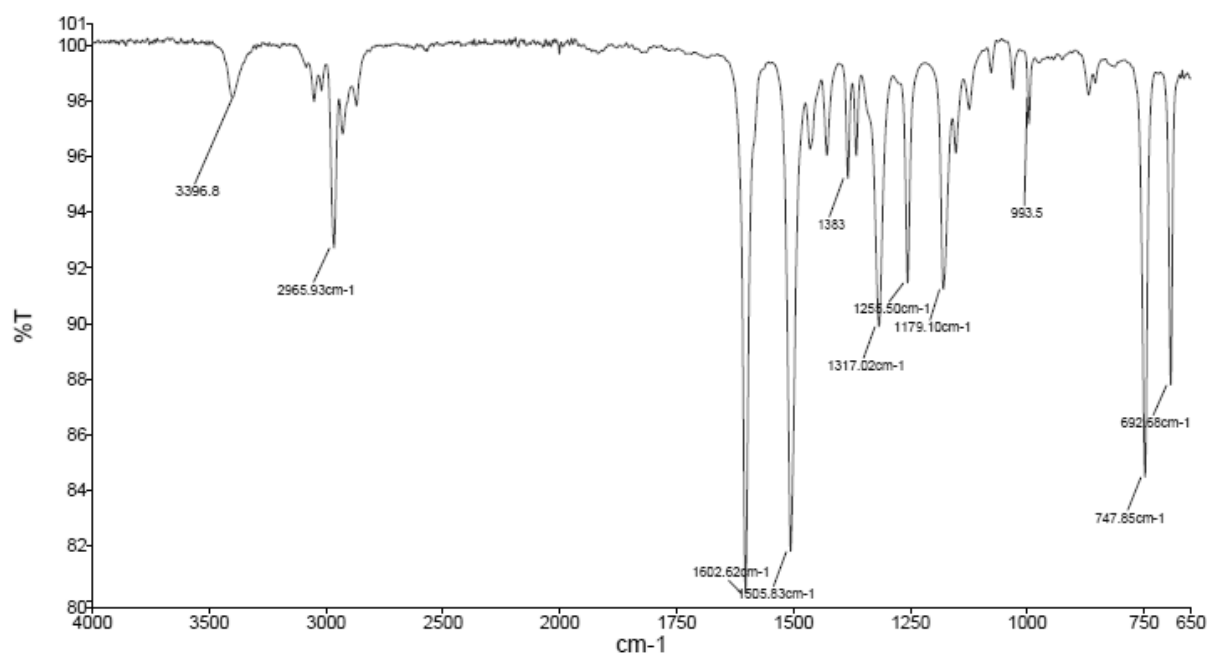
Peak Time
1 1.12

1: (Time: 1.12)

1:MS ES+
3.3e+005

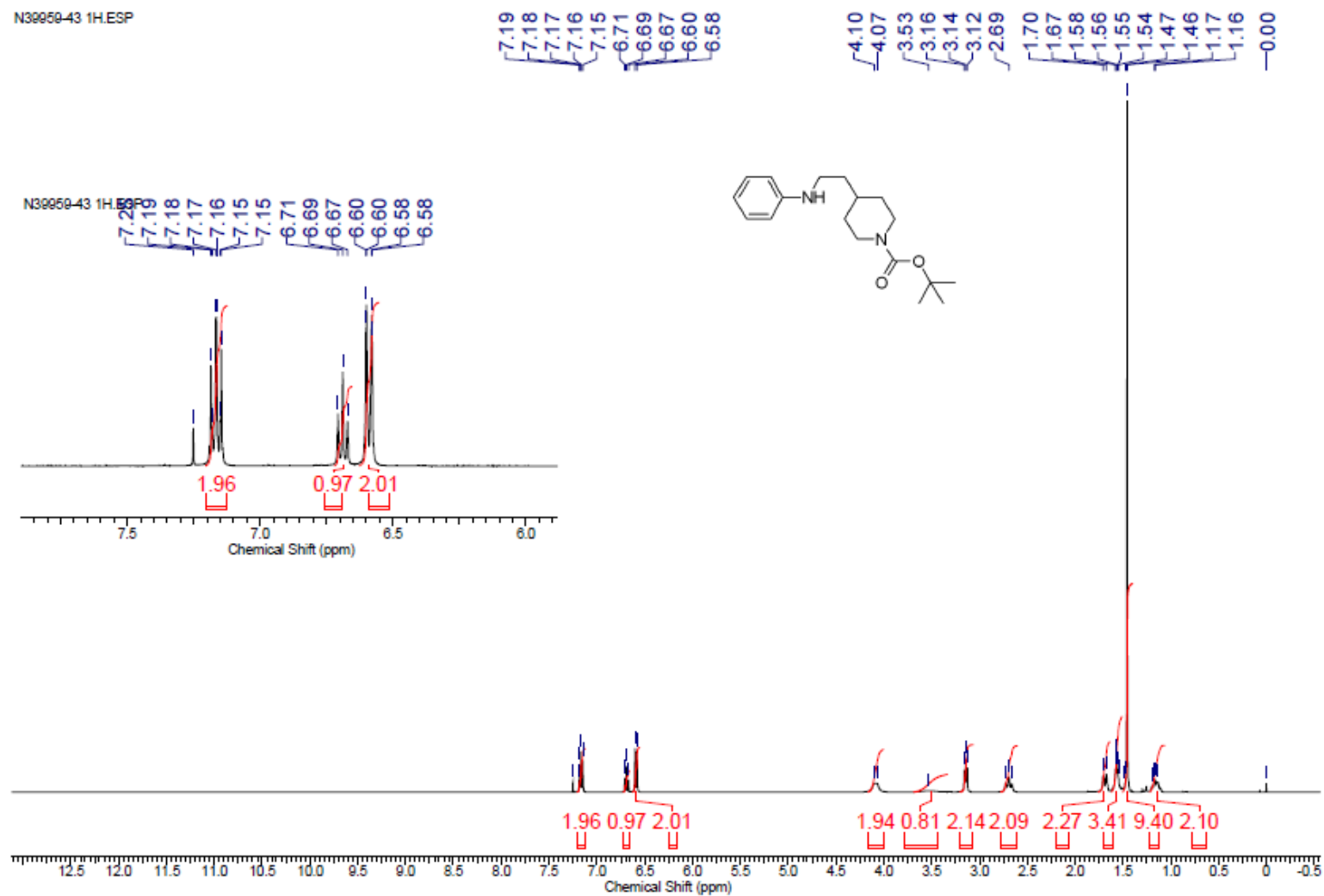


IR Spectra

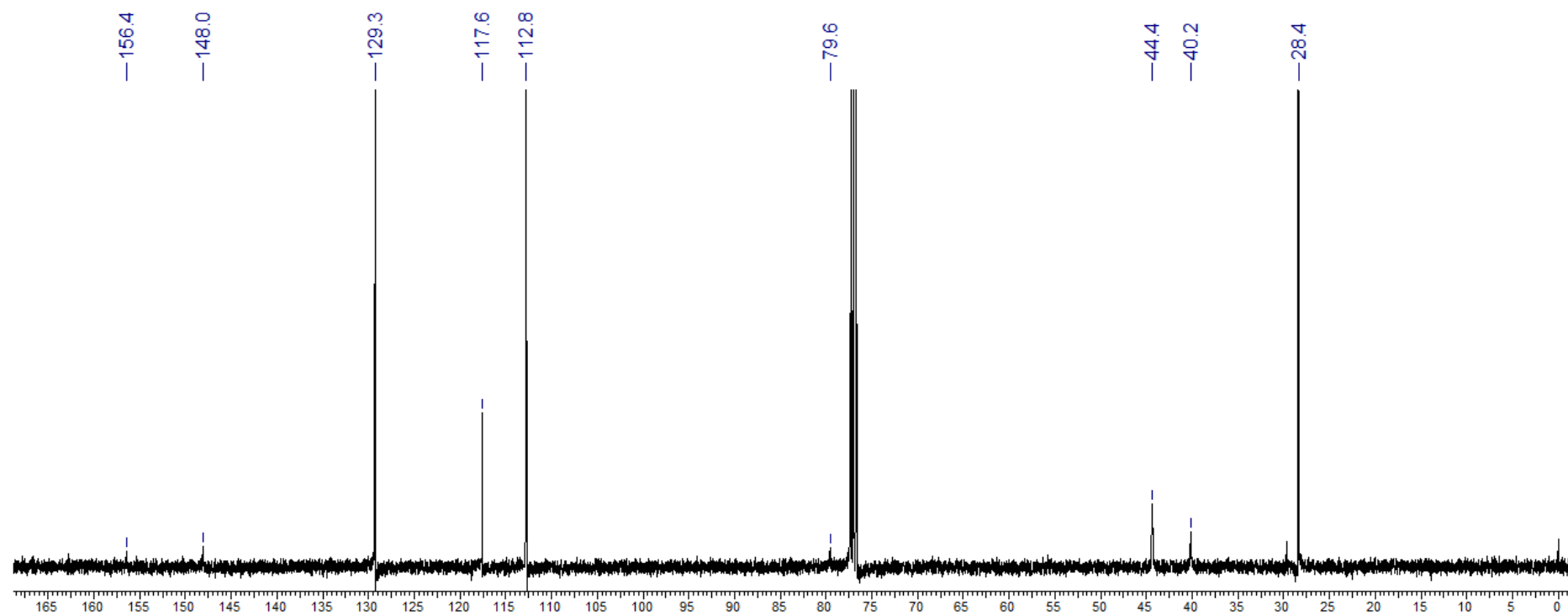


tert-Butyl 4-(2-(phenylamino)ethyl)piperidine-1-carboxylate (7ab).

¹H NMR Spectra



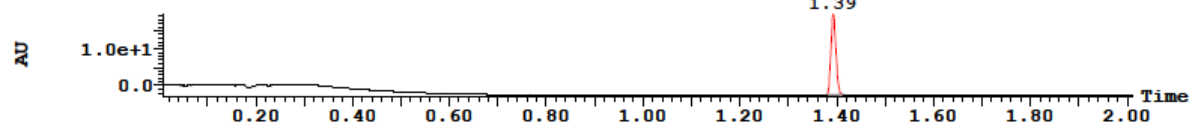
¹³C NMR Spectra



LCMS

3: UV Detector: TAC :Wavelength Range: (210 - 350)

(1) 1.959e+1
100% Range: 2.231e+1
1.39

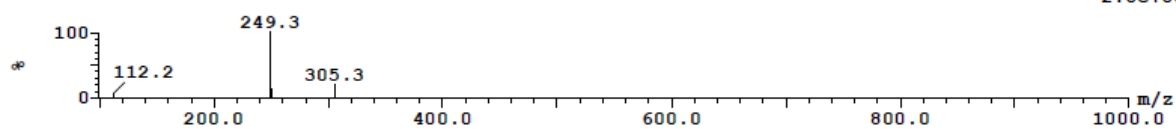


Peak Time
1 1.39

1: (Time: 1.39)

1:MS ES+

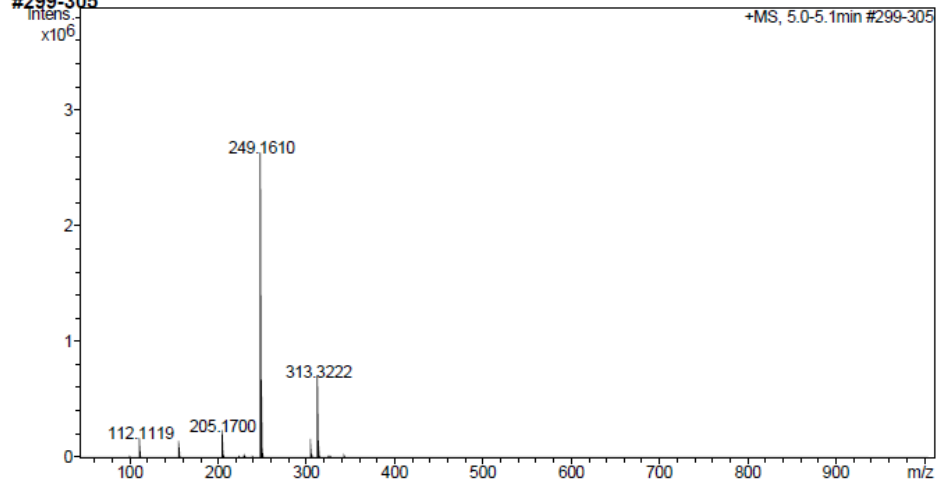
2.0e+007



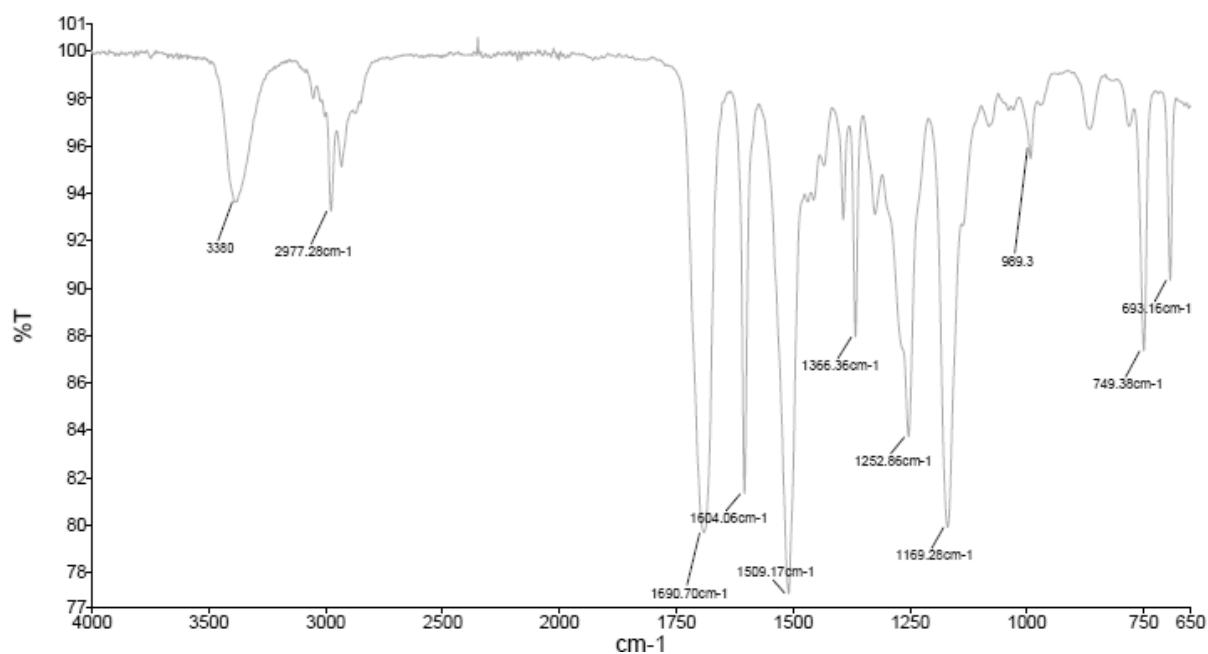
HRMS

+MS, 5.0-5.1min

#299-305

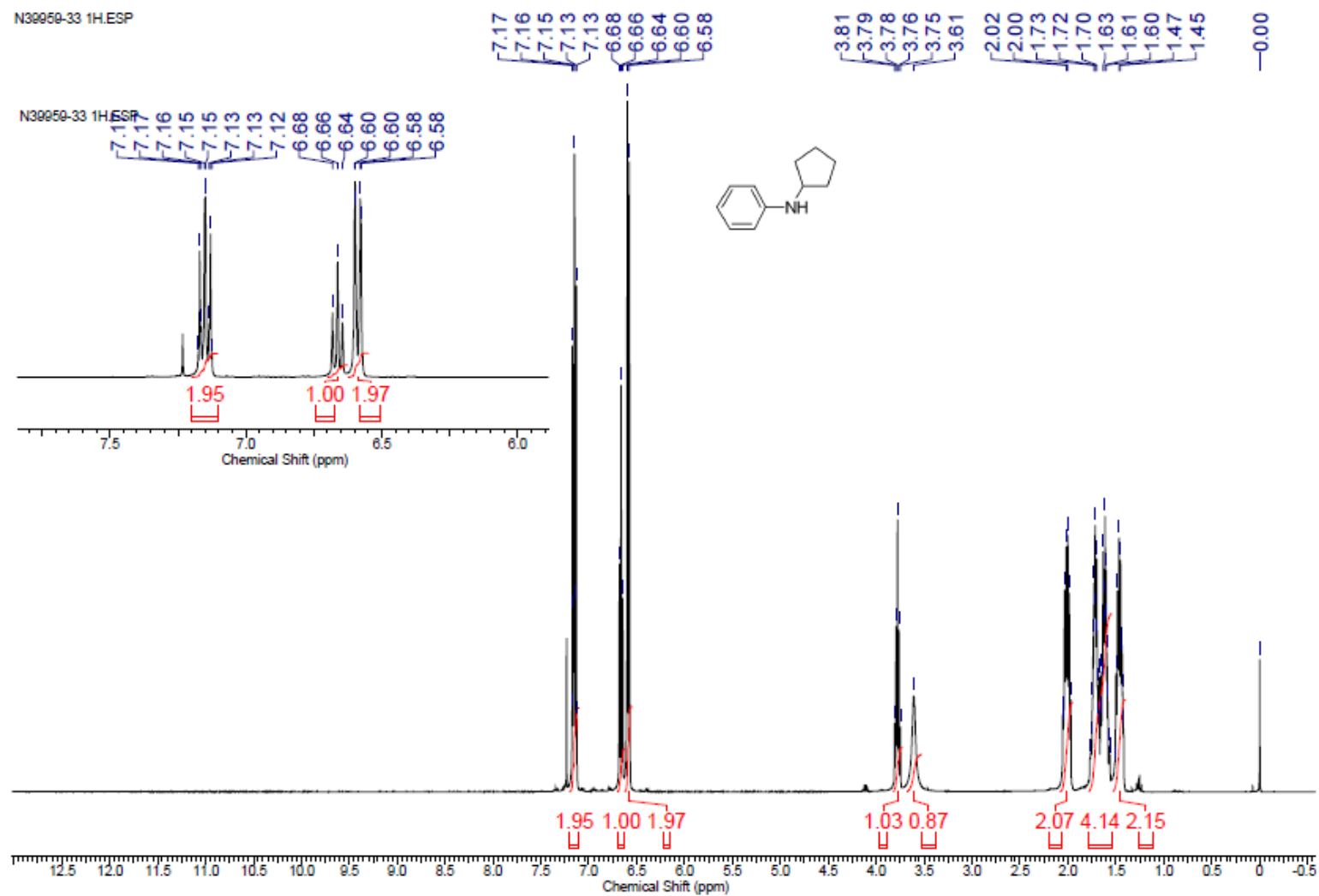


IR Spectra

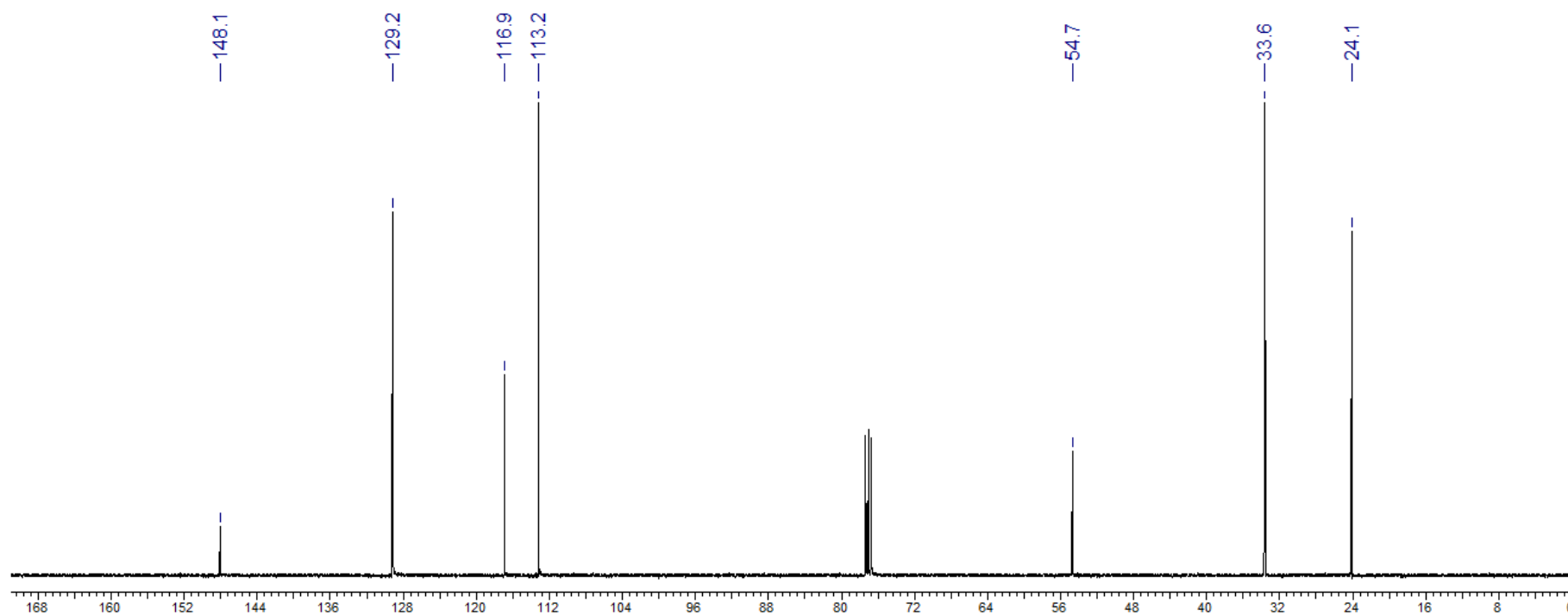


N-Cyclopentylaniline (7ac).

¹H NMR Spectra

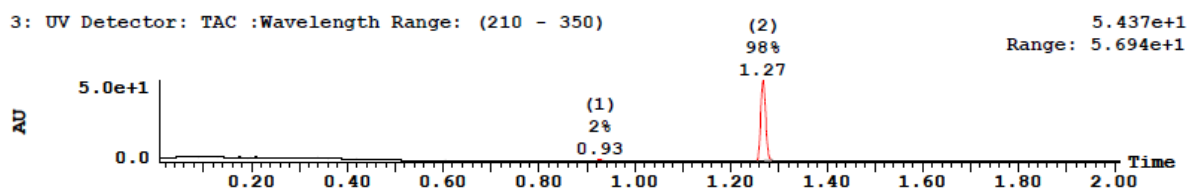


¹³C NMR Spectra



LCMS

3: UV Detector: TAC :Wavelength Range: (210 - 350)

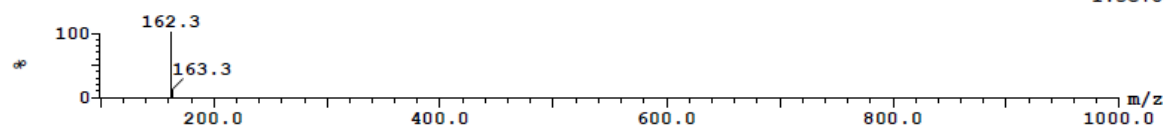


Peak Time
2 1.27

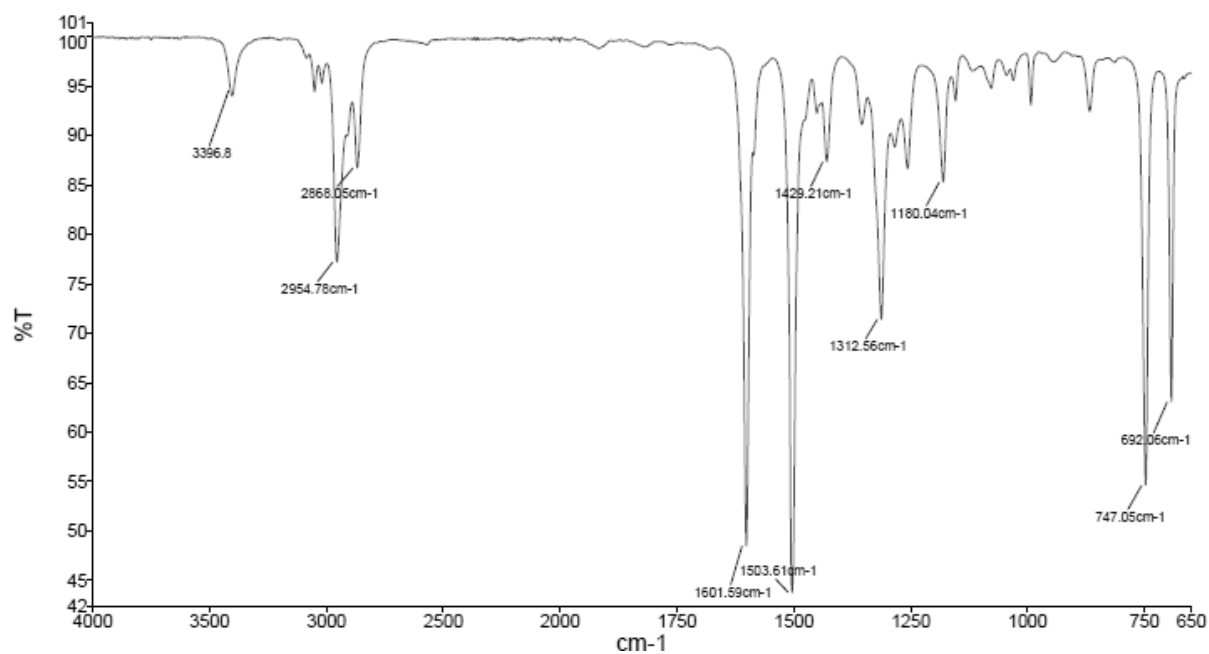
2: (Time: 1.27)

1:MS ES+

1.3e+007

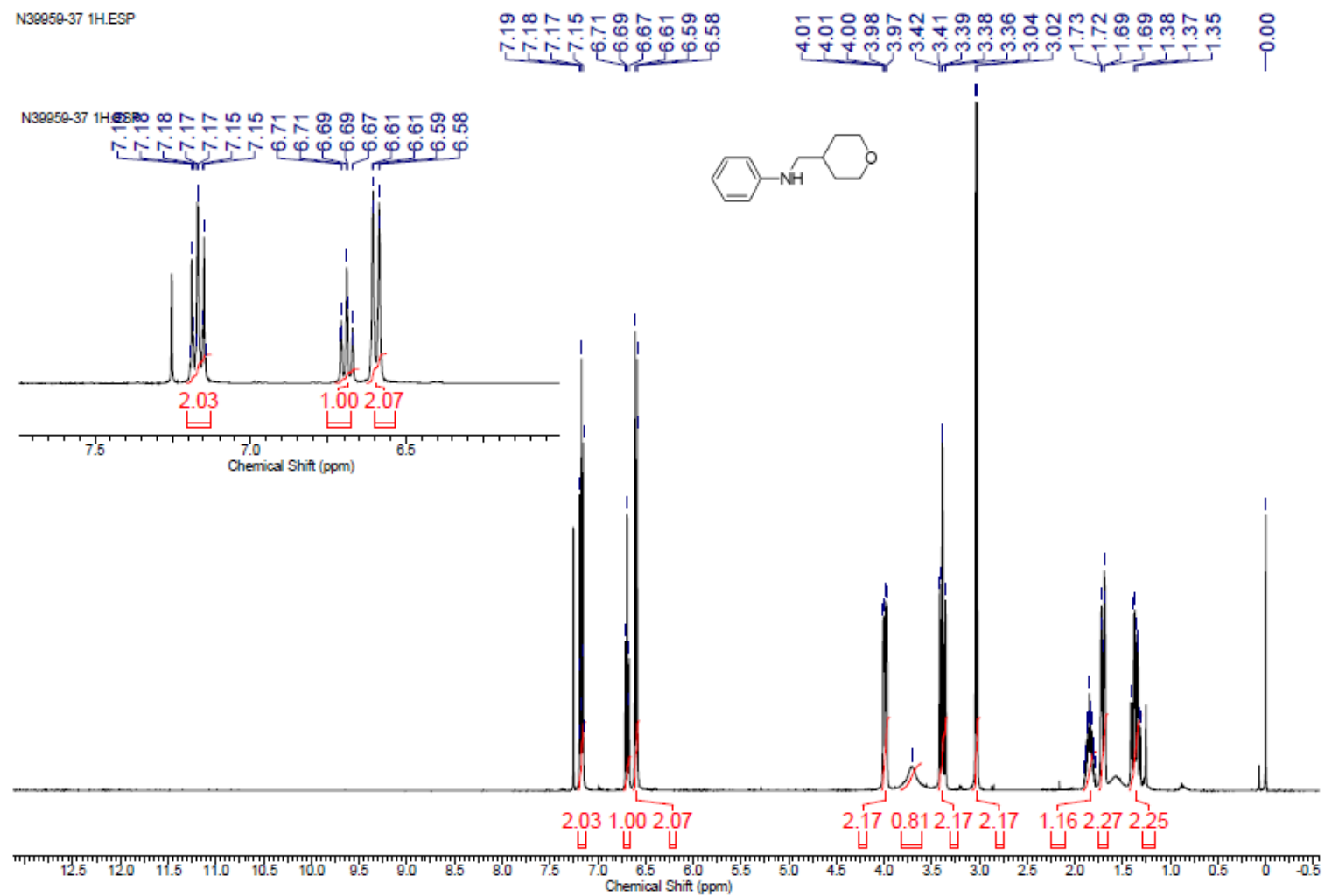


IR Spectra

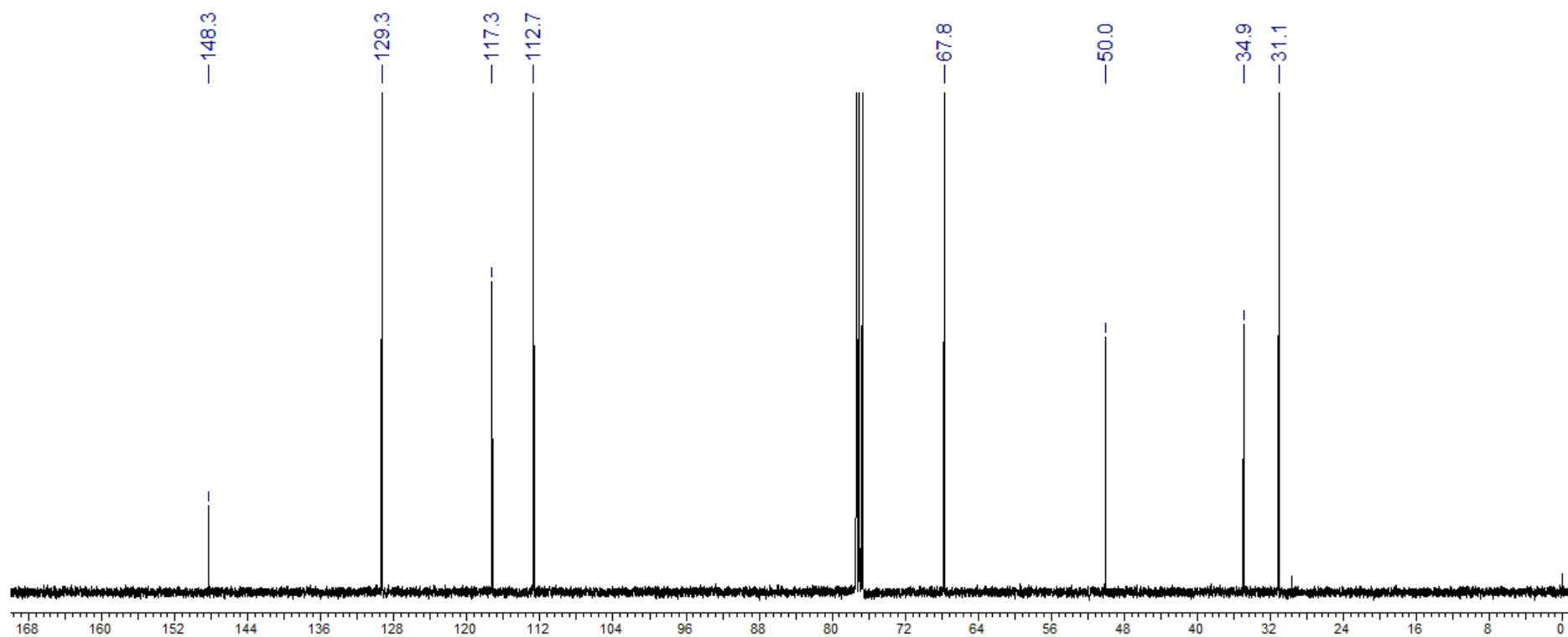


N-((Tetrahydro-2*H*-pyran-4-yl)methyl)aniline (7ad).

¹H NMR Spectra



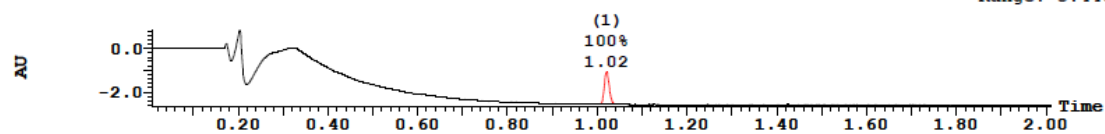
¹³C NMR Spectra



LCMS

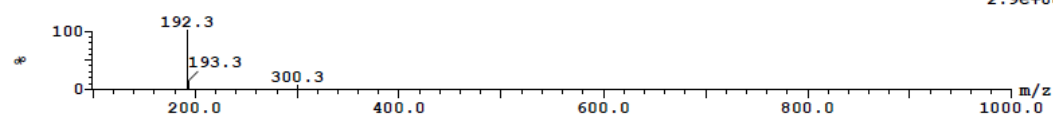
3: UV Detector: TAC :Wavelength Range: (210 - 350)

8.363e-1
Range: 3.448

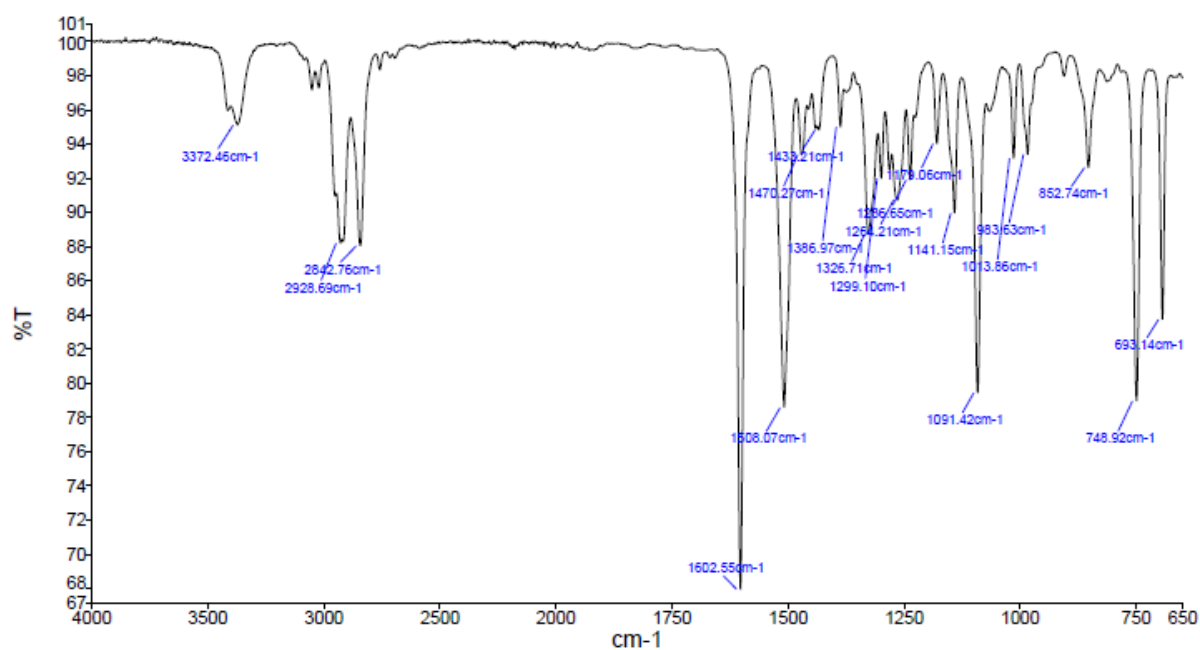


Peak Time
1 1.02
1: (Time: 1.02)

1:MS ES+
2.9e+006

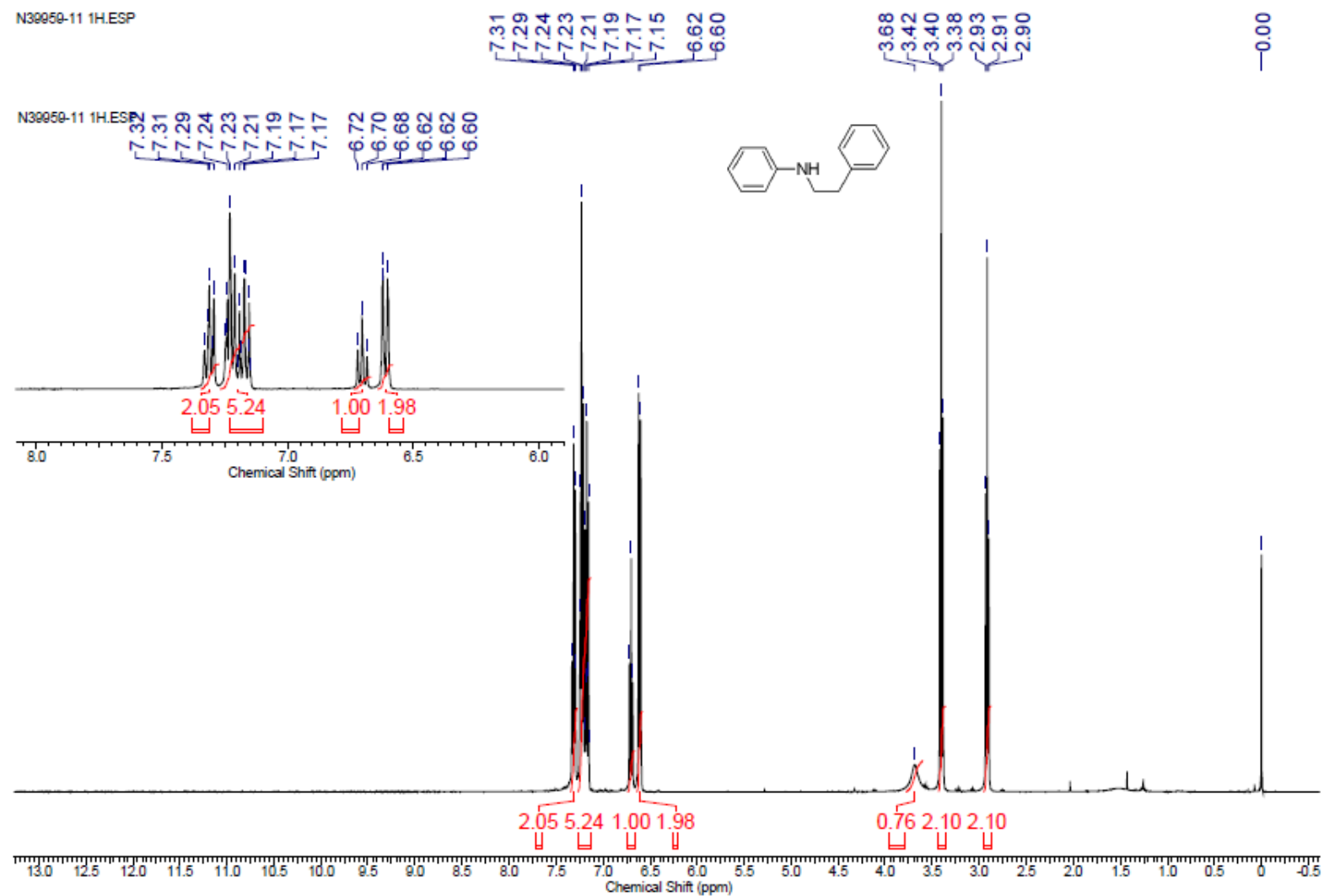


IR Spectra

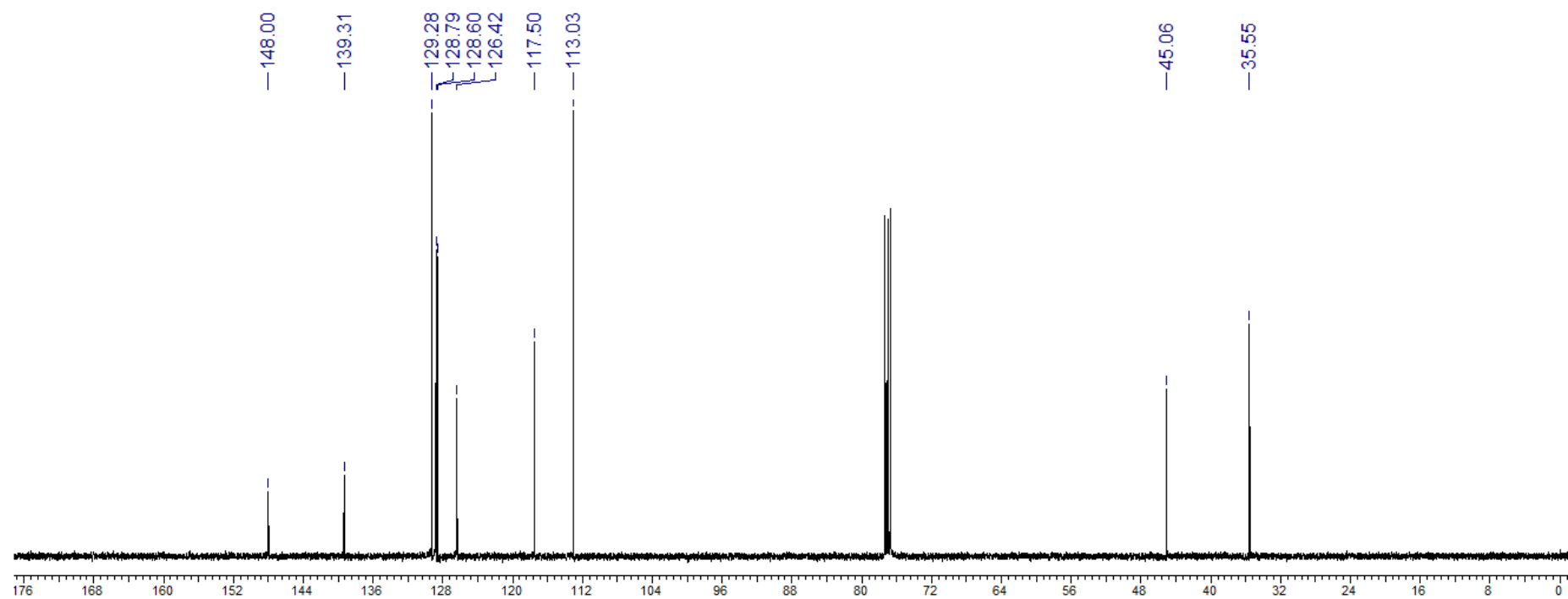


***N*-Phenethylaniline (7ae).**

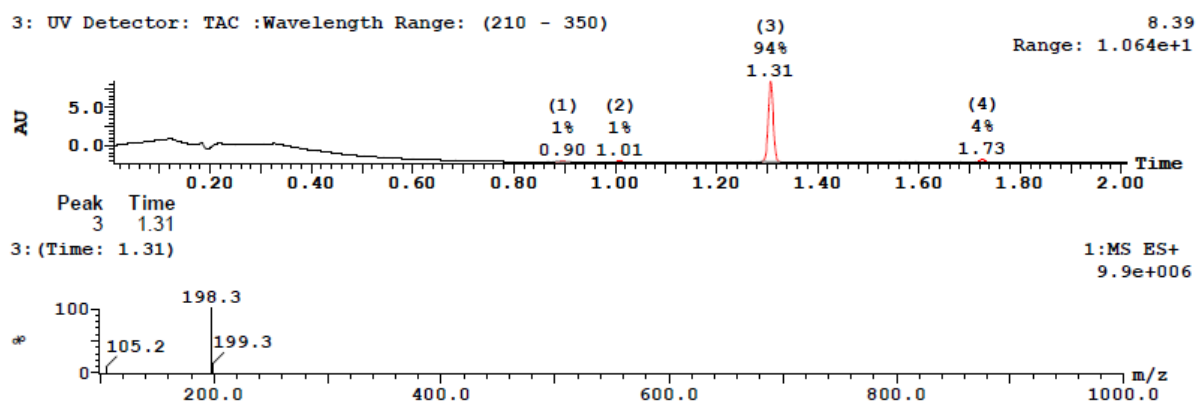
¹H NMR Spectra



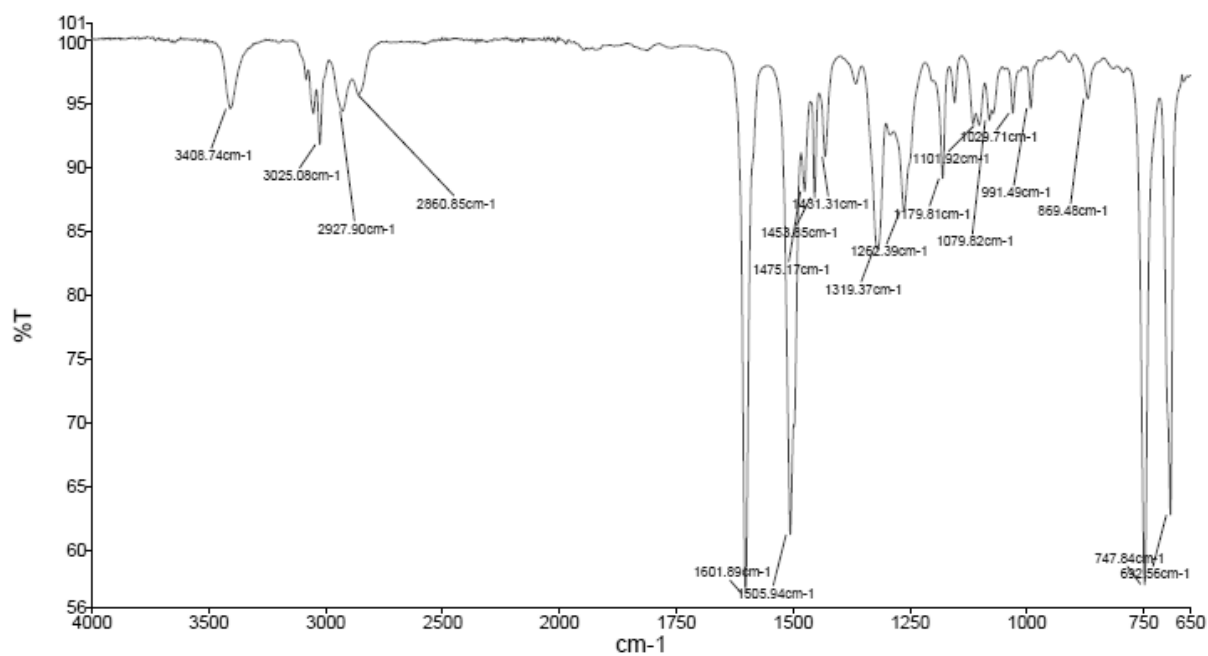
¹³C NMR Spectra



LCMS

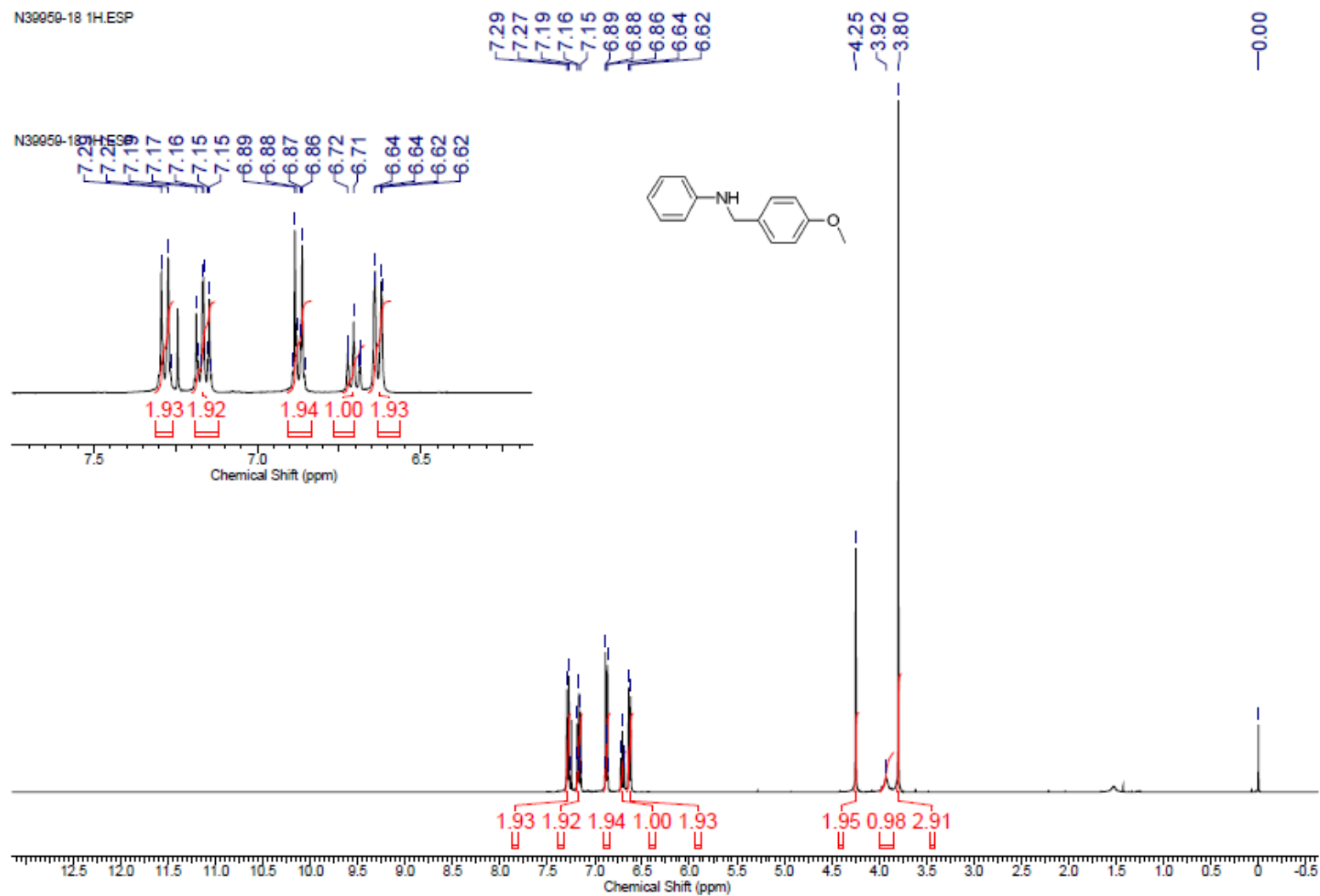


IR Spectra

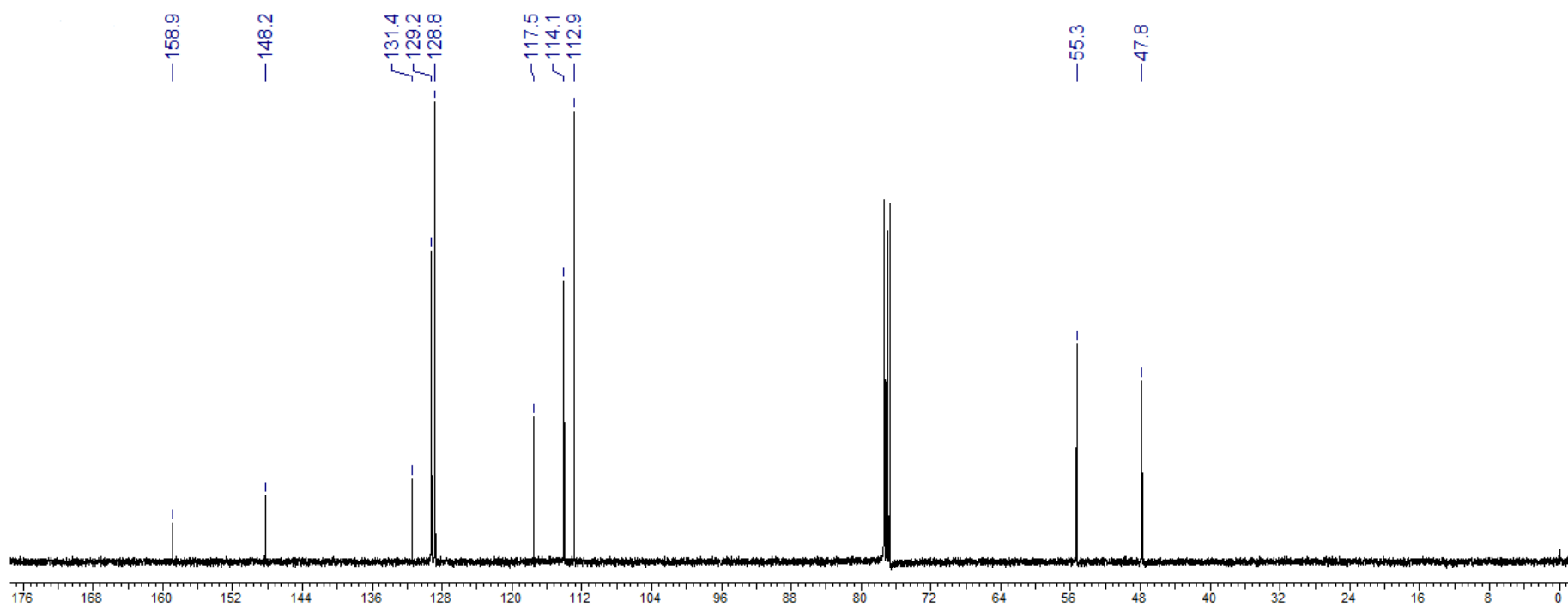


***N*-(4-Methoxybenzyl)aniline (7af).**

¹H NMR Spectra

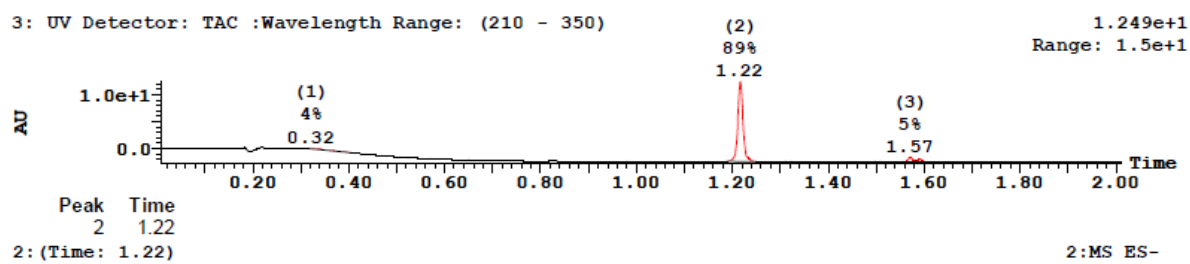


¹³C NMR Spectra



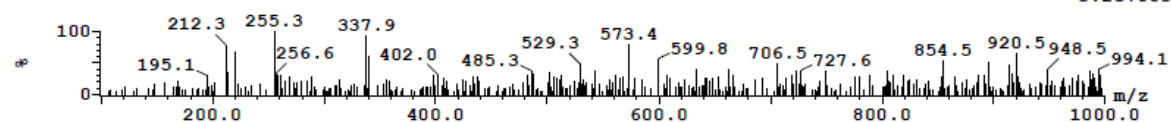
LCMS

3: UV Detector: TAC :Wavelength Range: (210 - 350)

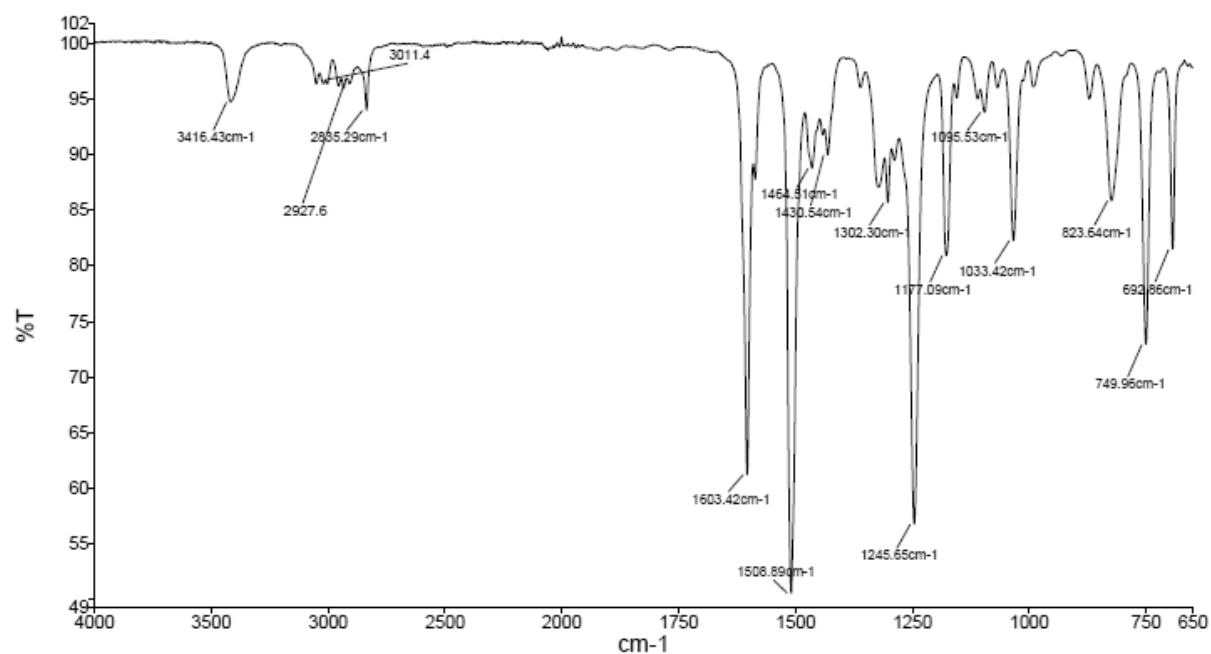


2: (Time: 1.22)

2:MS ES-
3.2e+003



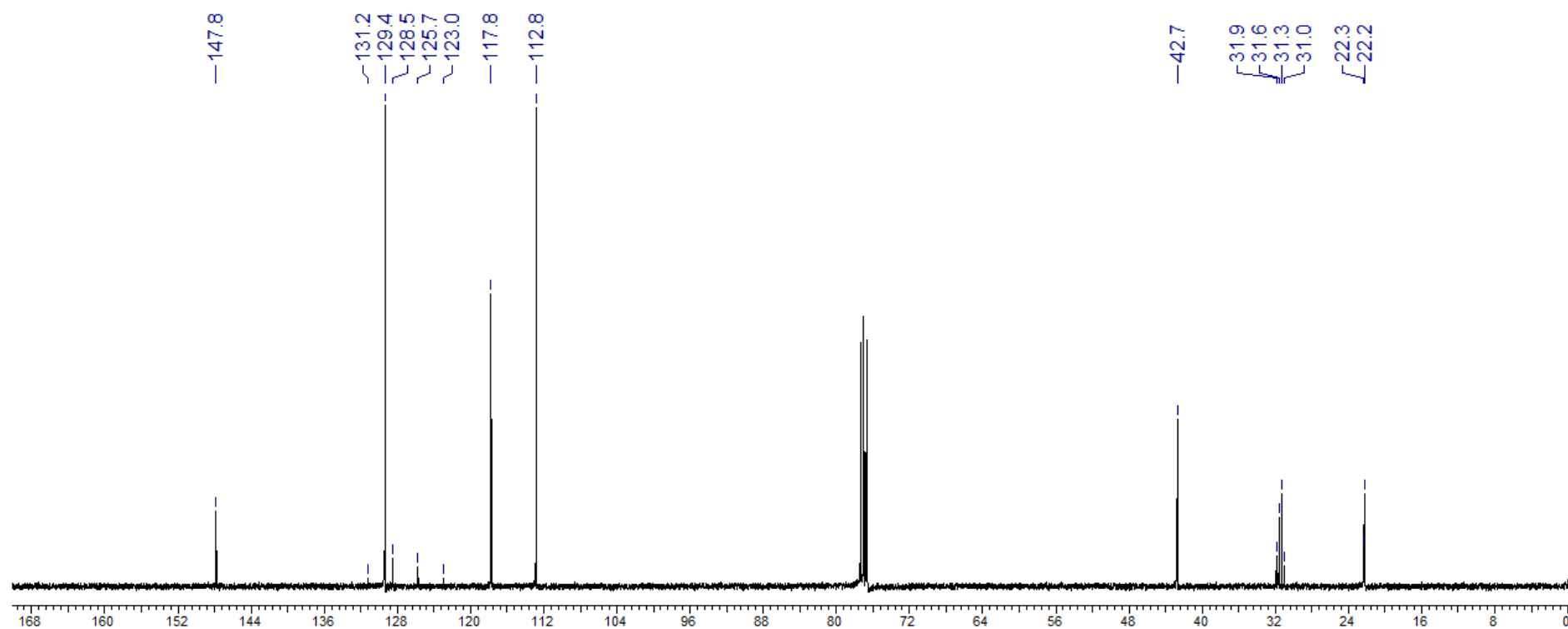
IR Spectra



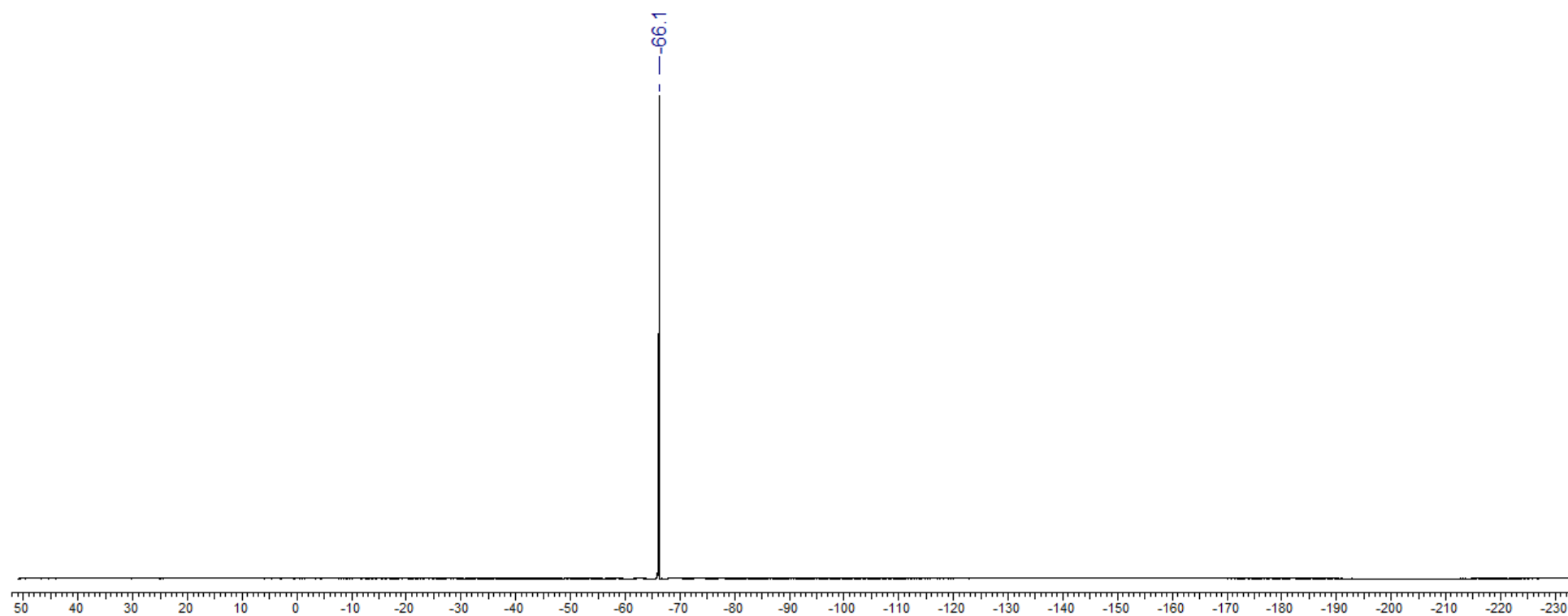
¹H NMR Spectra



¹³C NMR Spectra

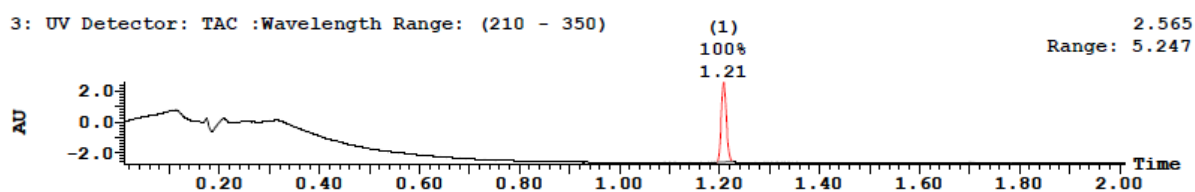


^{19}F NMR Spectra



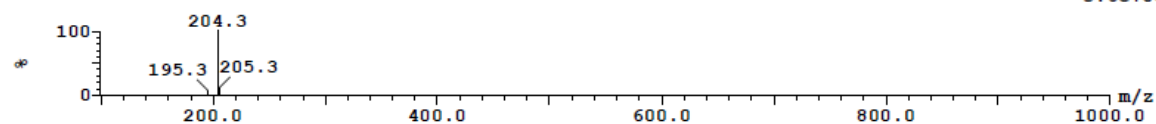
LCMS

3: UV Detector: TAC :Wavelength Range: (210 - 350)

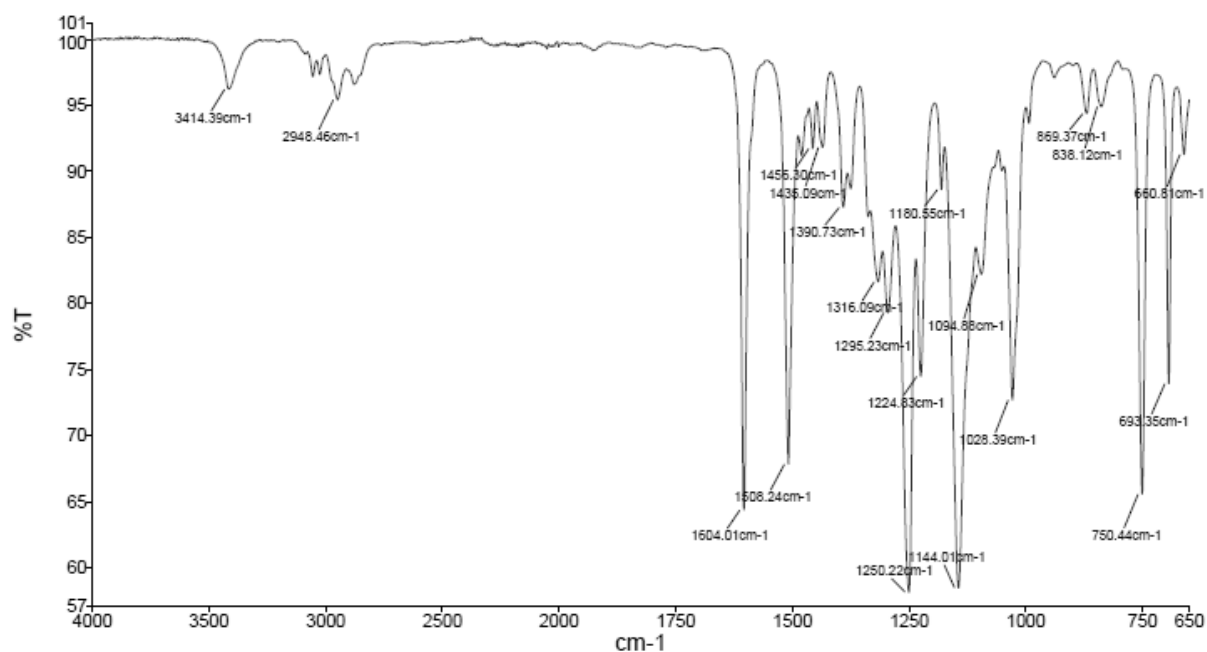


Peak Time
1 1.21
1: (Time: 1.21)

1:MS ES+
3.6e+005

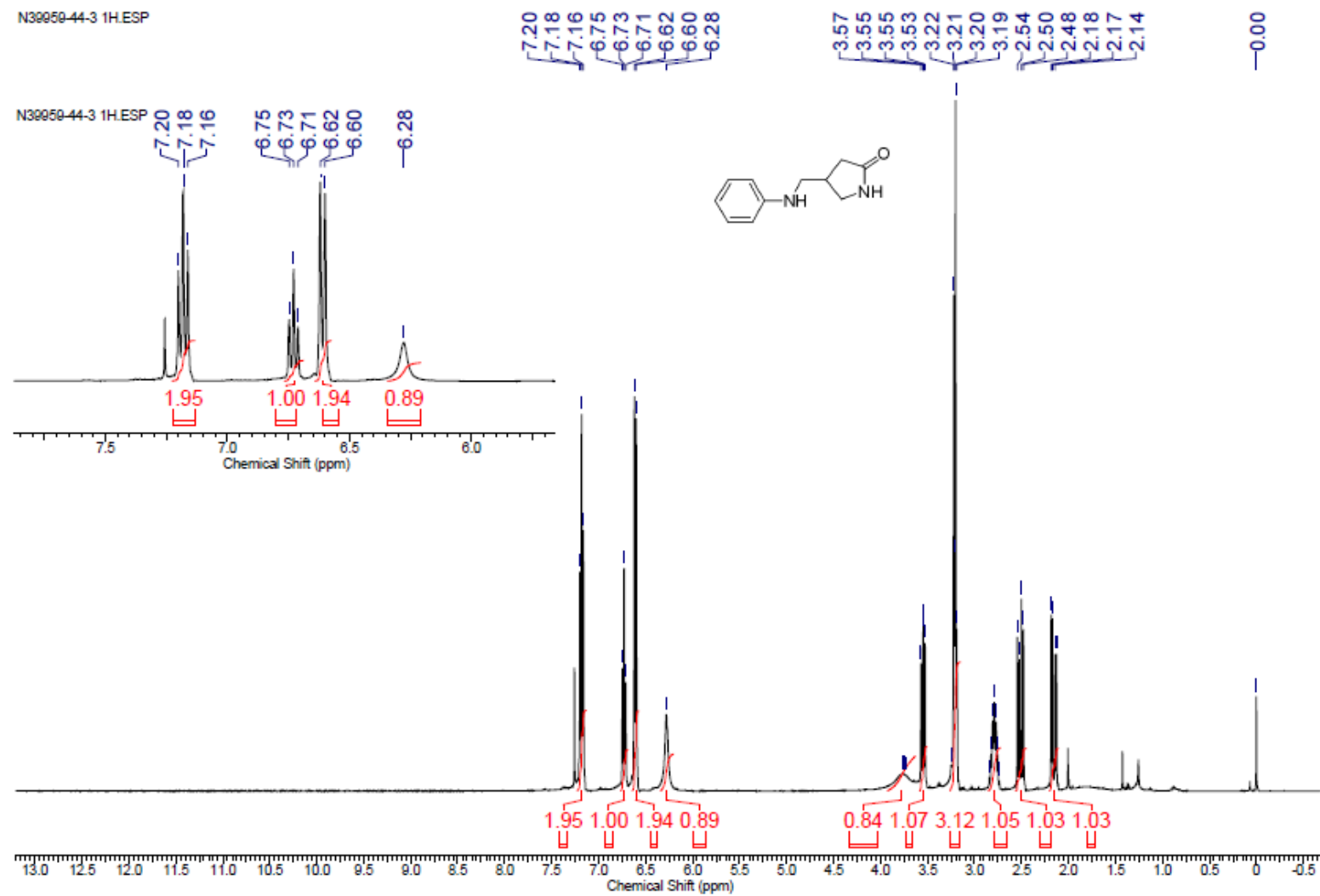


IR Spectra

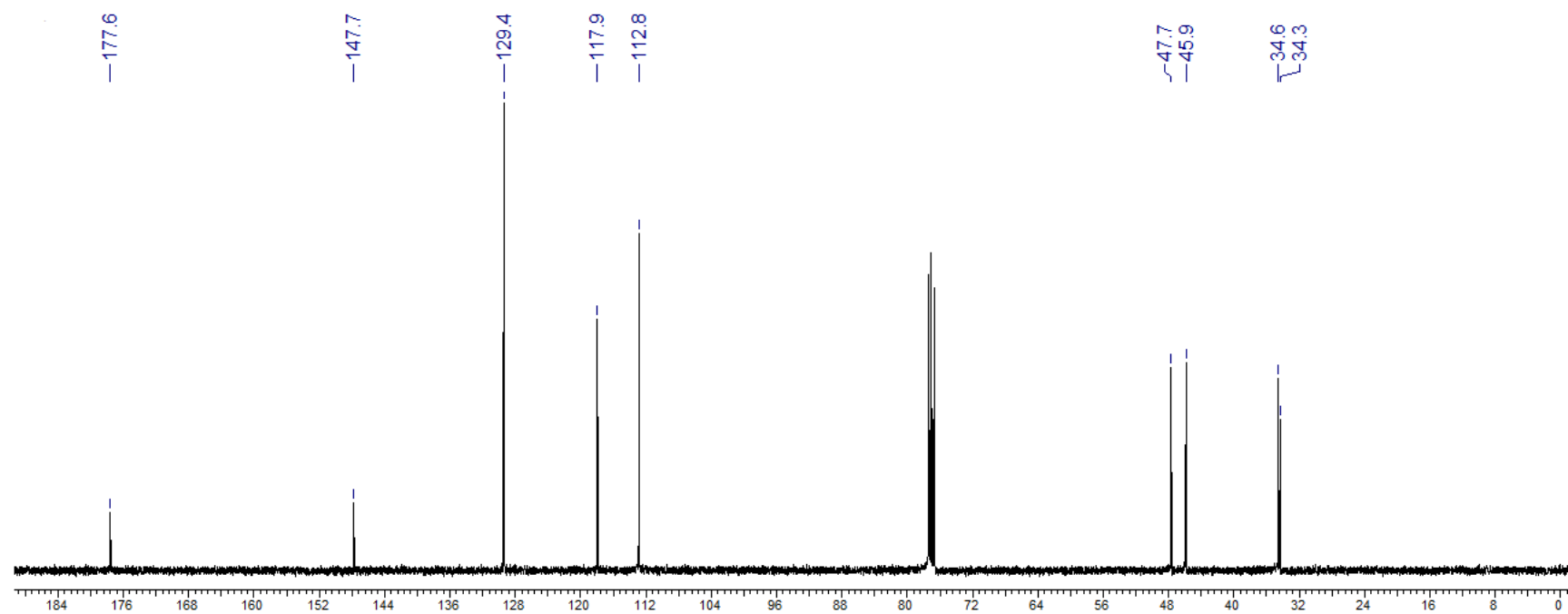


4-((Phenylamino)methyl)pyrrolidin-2-one (7ah).

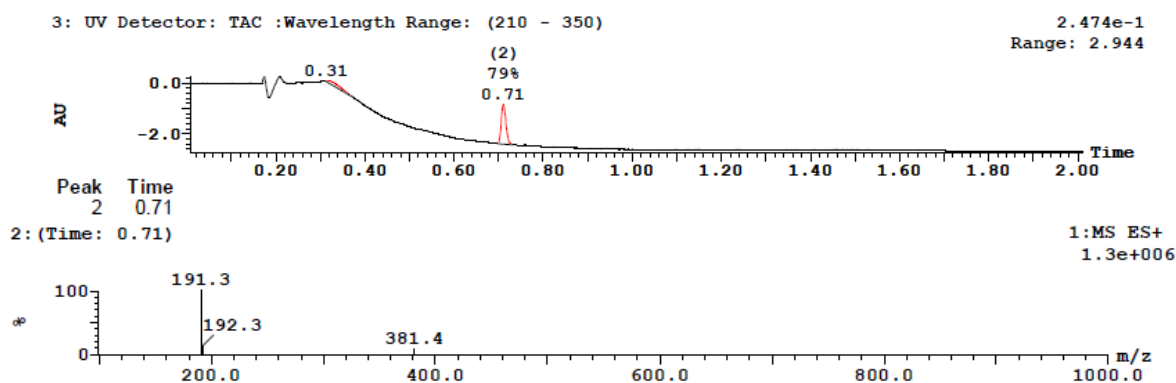
¹H NMR Spectra



¹³C NMR Spectra

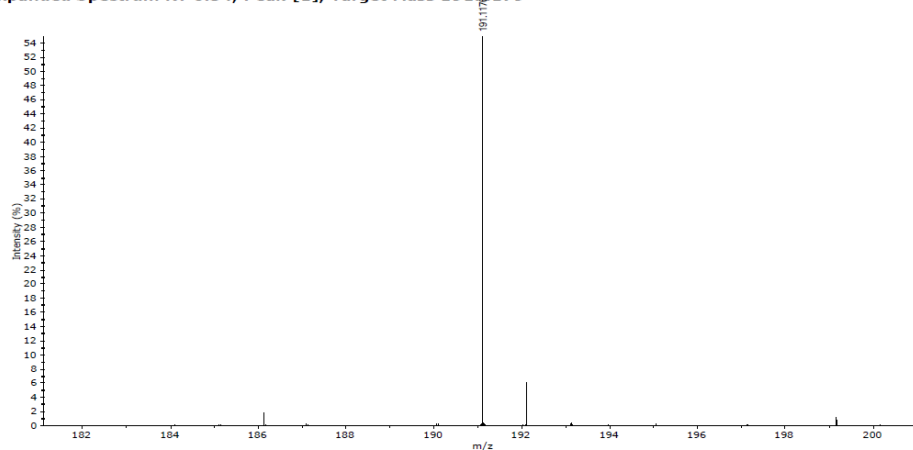


LCMS

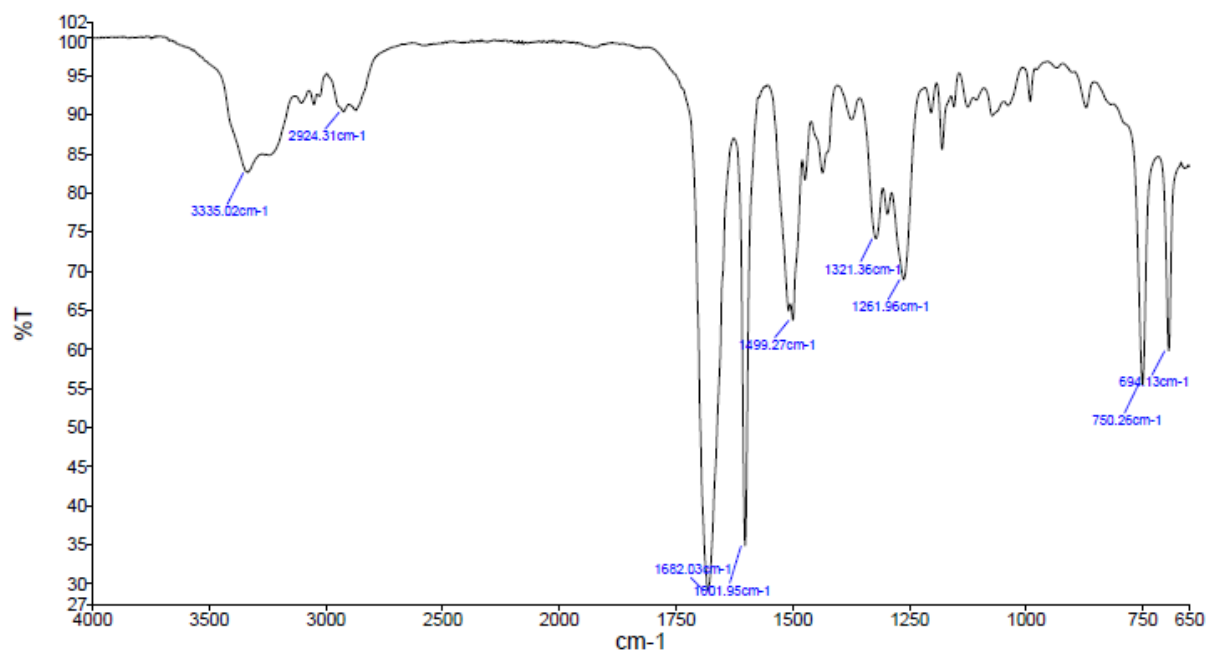


HRMS

Expanded Spectrum RT 0.34, Peak [1], Target Mass 191.1179

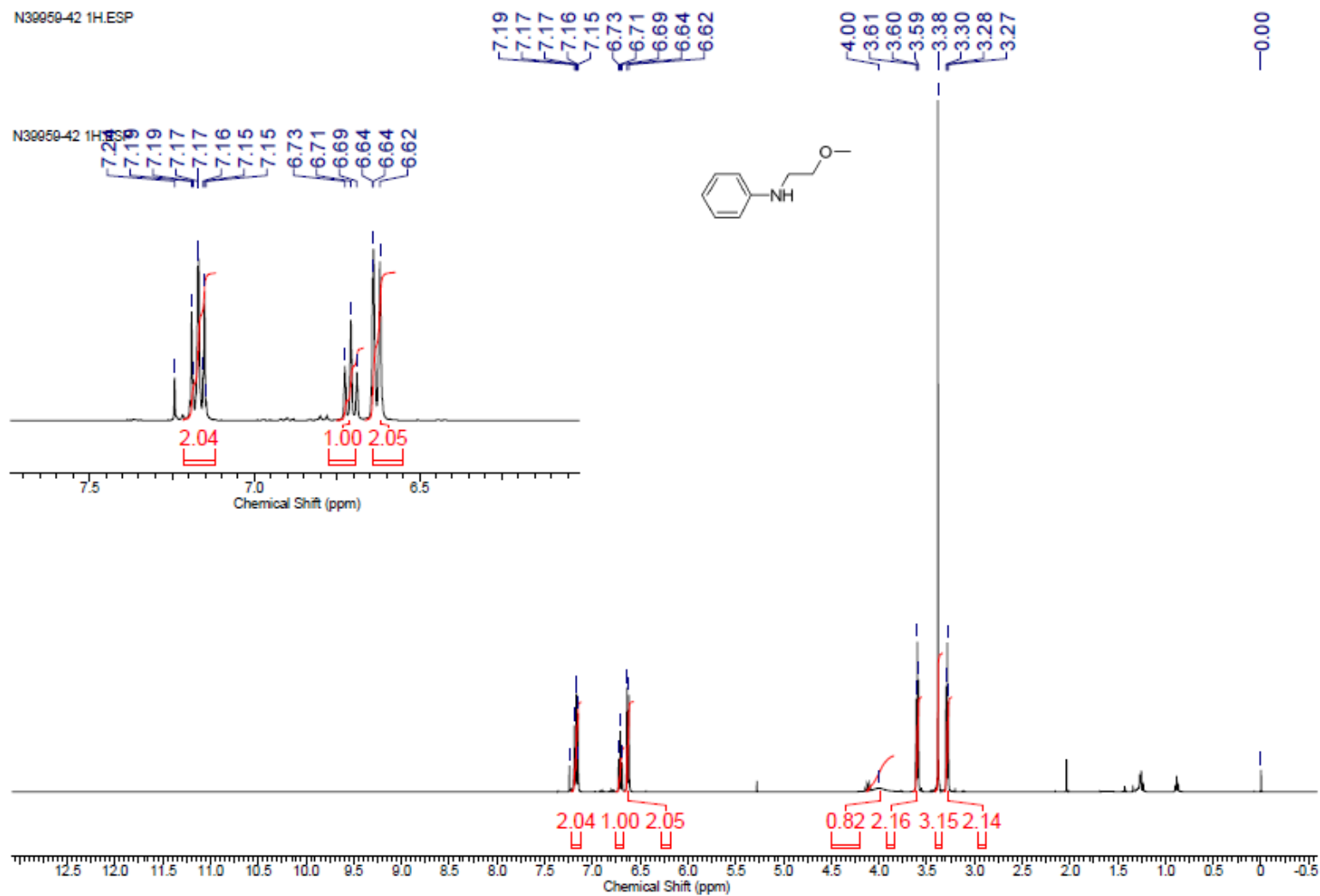


IR Spectra

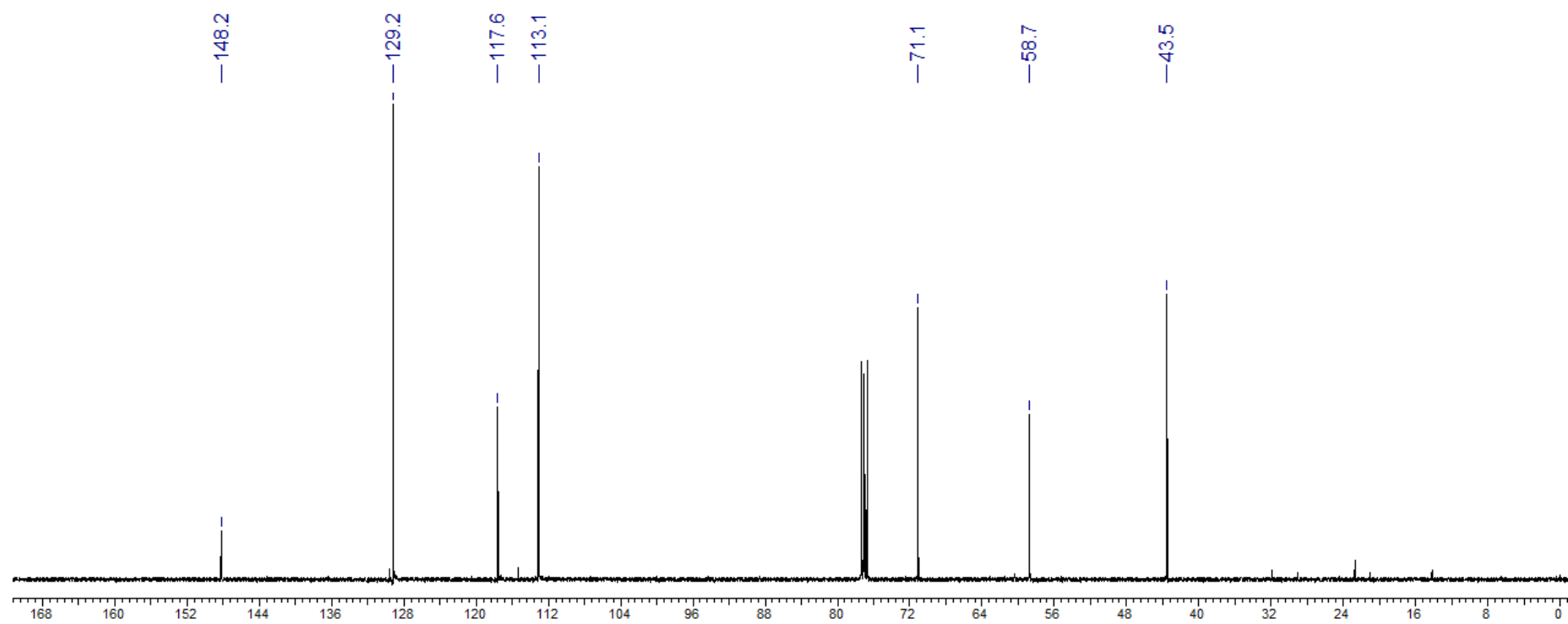


N-(2-Methoxyethyl)aniline (7ai).

¹H NMR Spectra



¹³C NMR Spectra



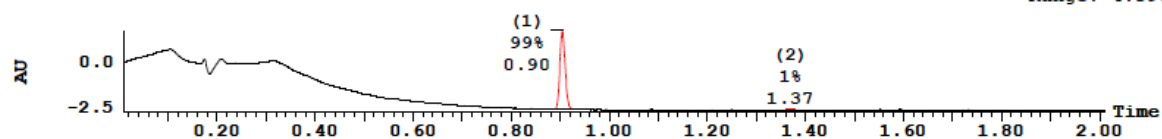
LCMS

Sample: 3

3: UV Detector: TAC :Wavelength Range: (210 - 350)

1.696

Range: 4.398

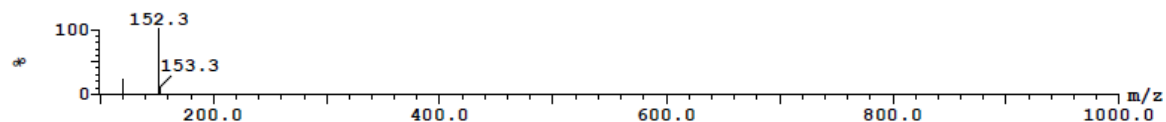


Peak Time
1 0.90

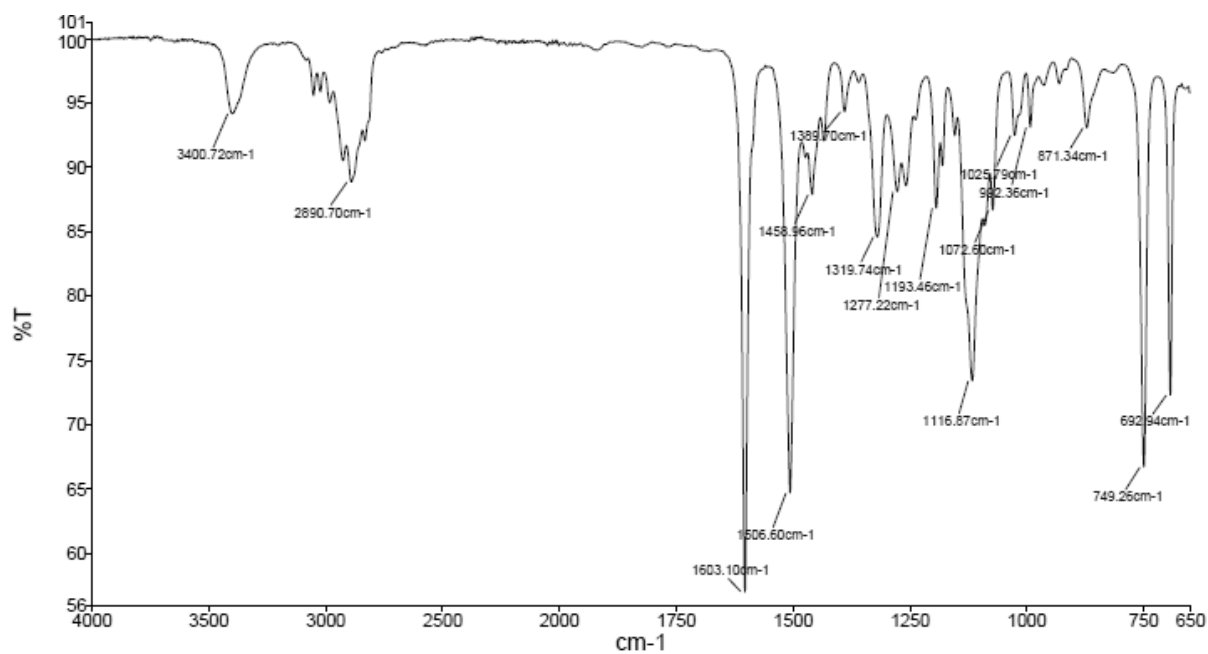
1: (Time: 0.90)

1: MS ES+

2.6e+006

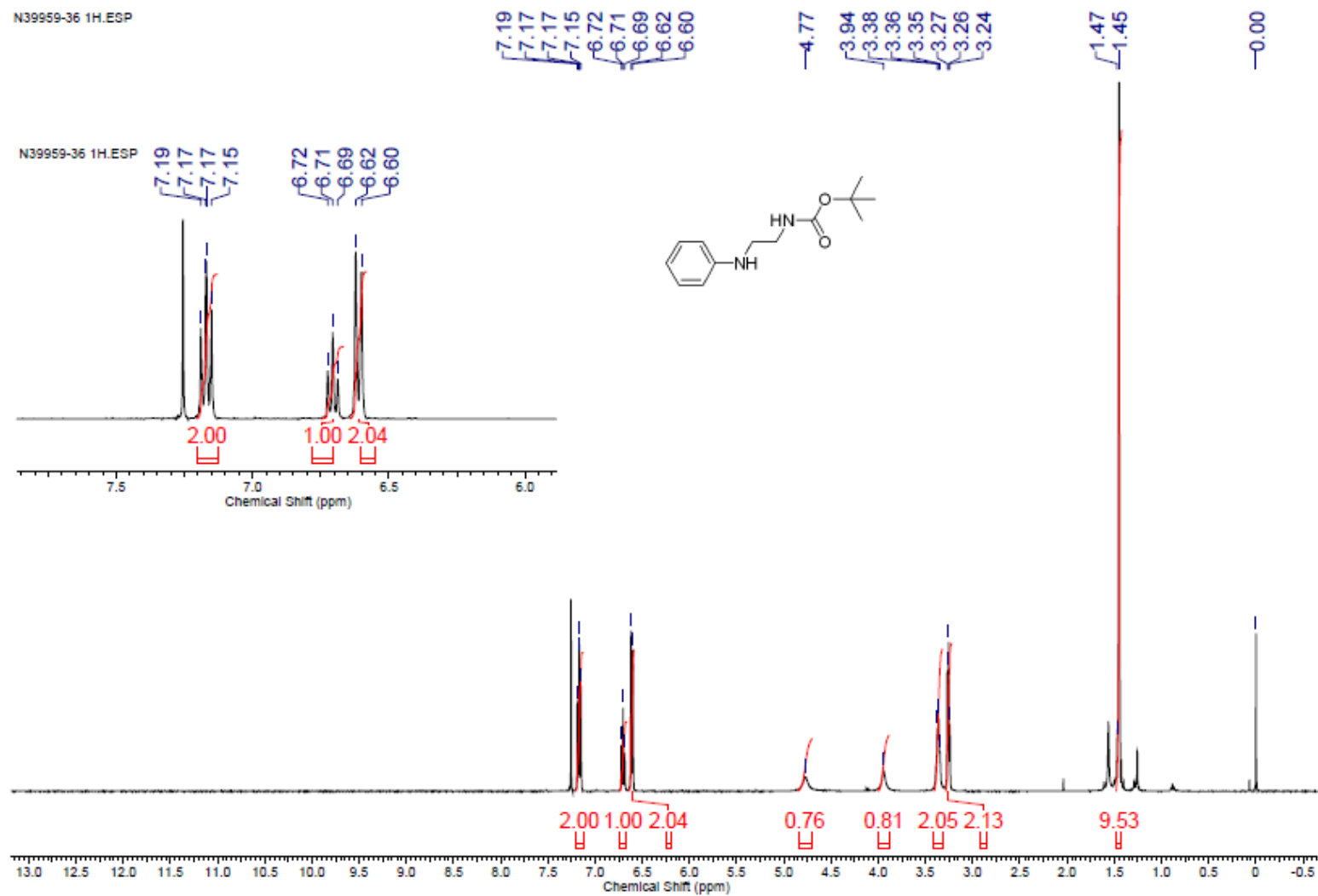


IR Spectra

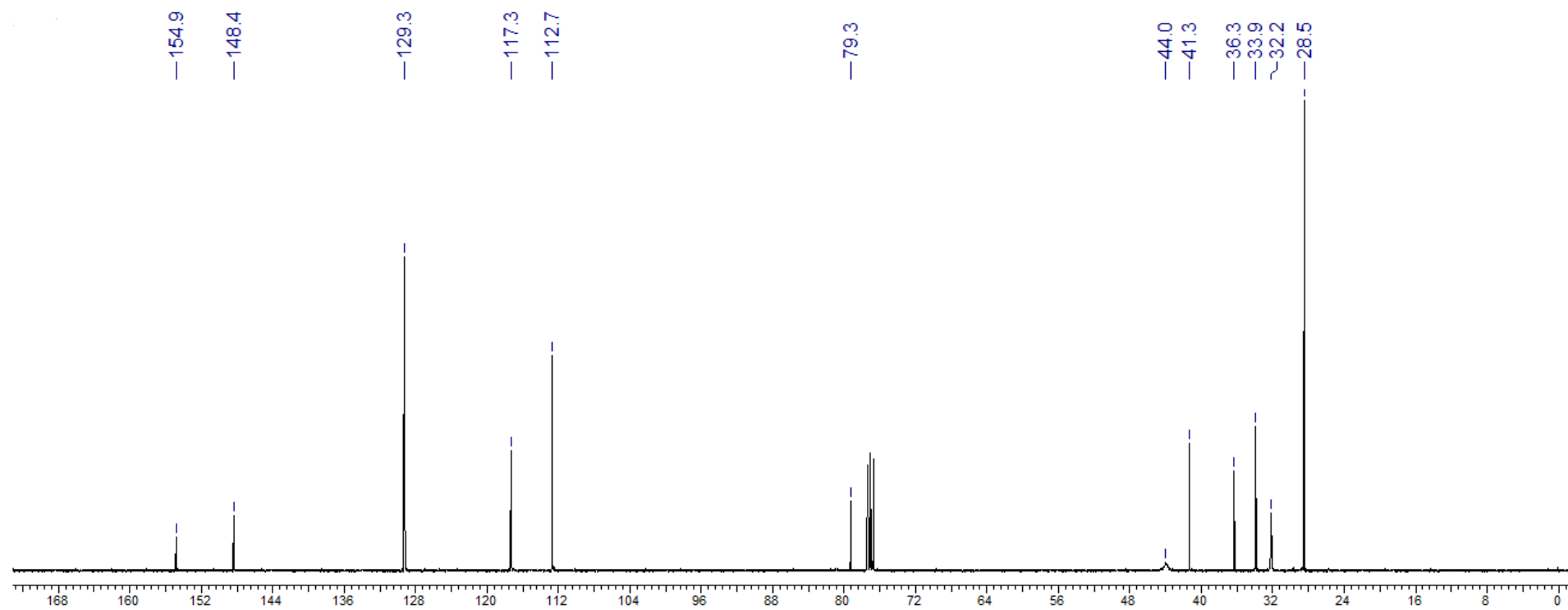


***tert*-Butyl (2-(phenylamino)ethyl)carbamate (7aj).**

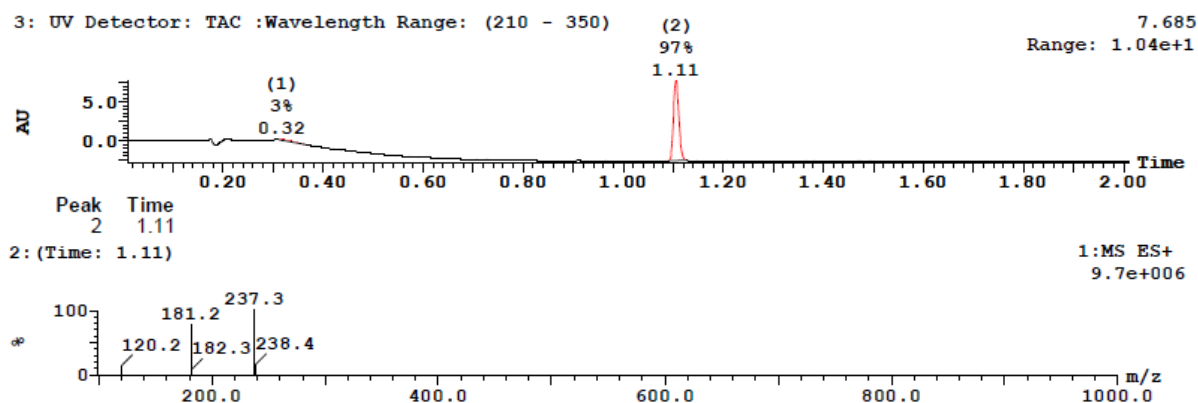
¹H NMR Spectra



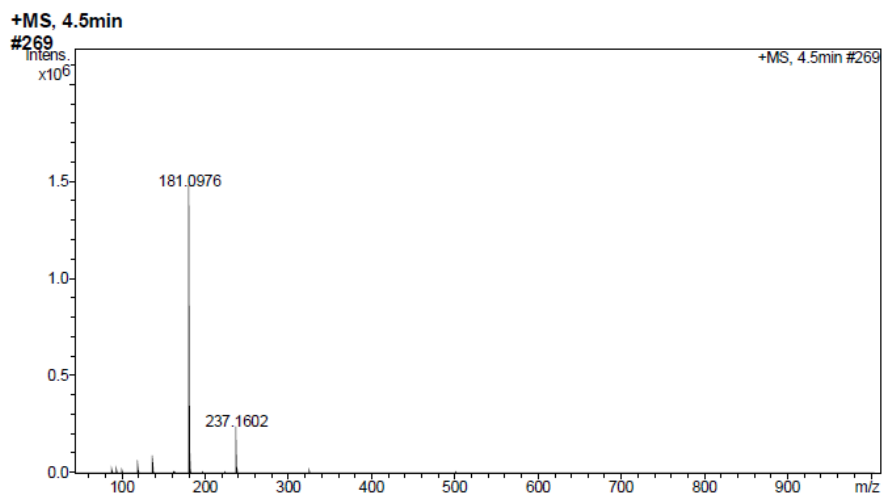
¹³C NMR Spectra



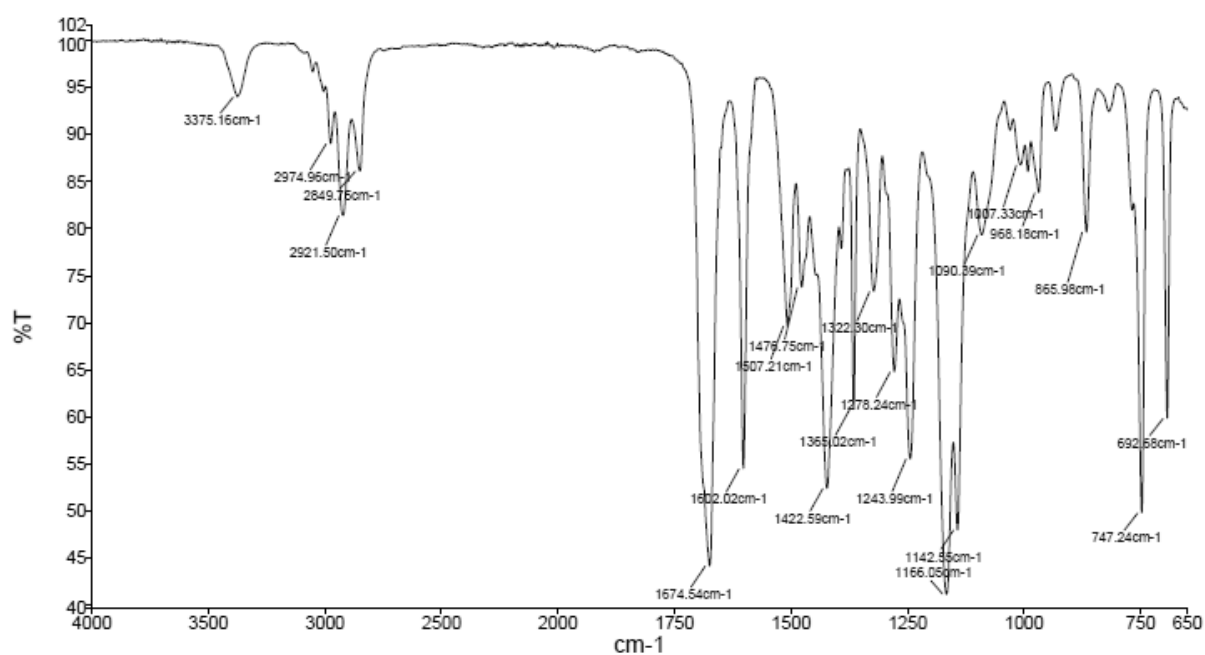
LCMS



HRMS

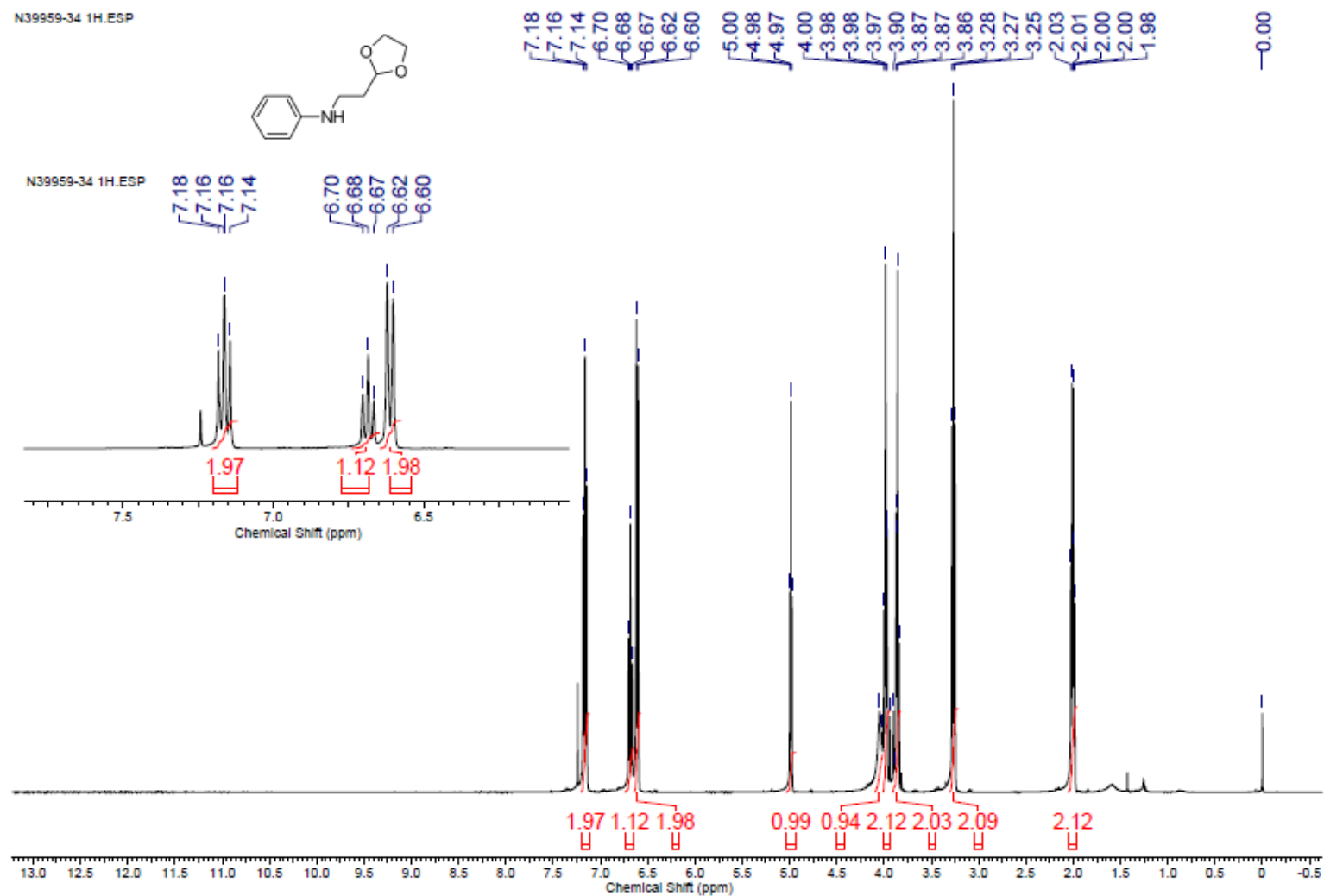


IR Spectra

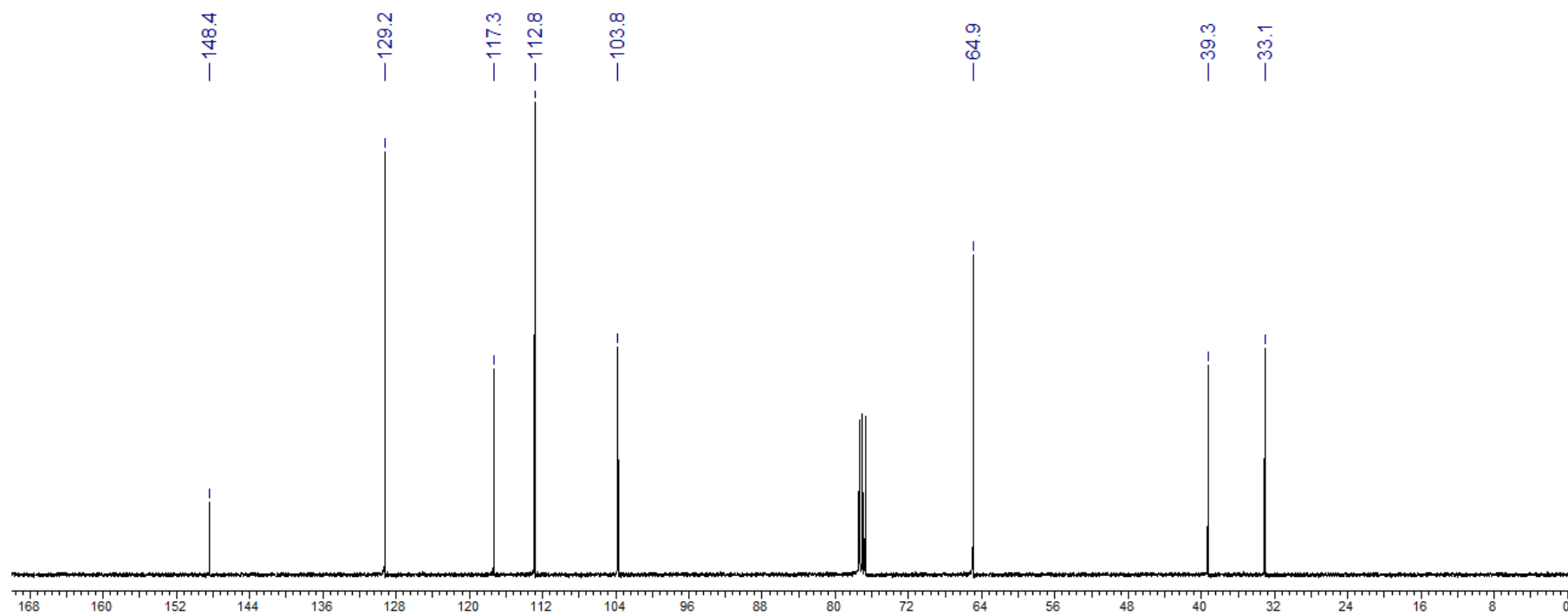


N-(2-(1,3-Dioxolan-2-yl)ethyl)aniline (7ak).

¹H NMR Spectra



¹³C NMR Spectra

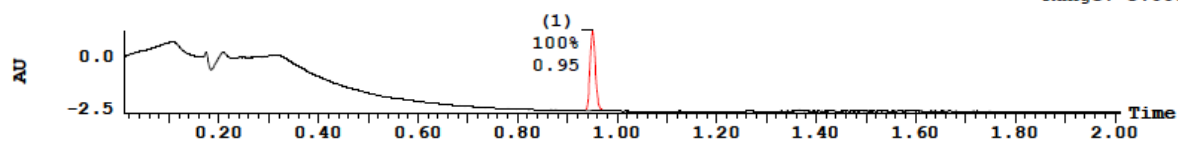


LCMS

3: UV Detector: TAC :Wavelength Range: (210 - 350)

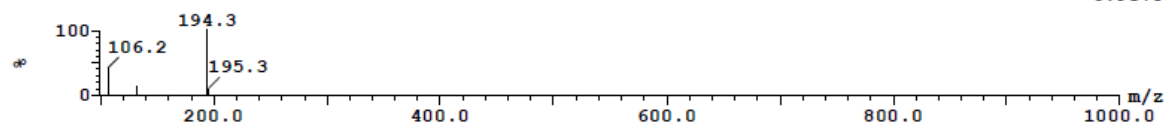
1.211

Range: 3.889



Peak Time
1 0.95
1: (Time: 0.95)

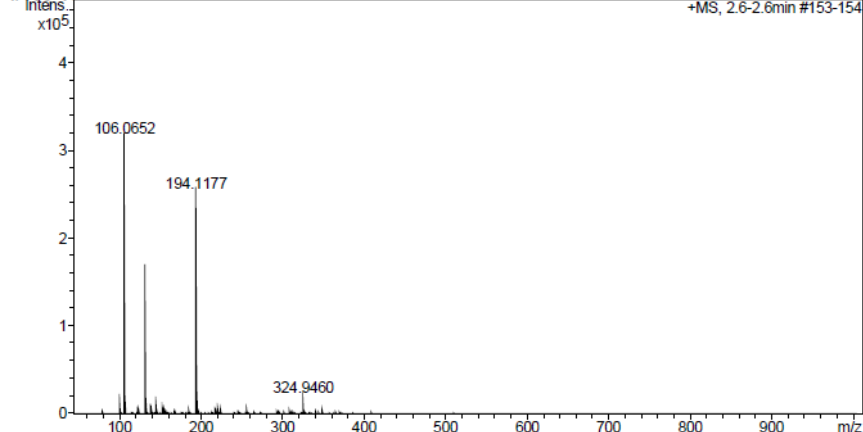
1:MS ES+
6.9e+006



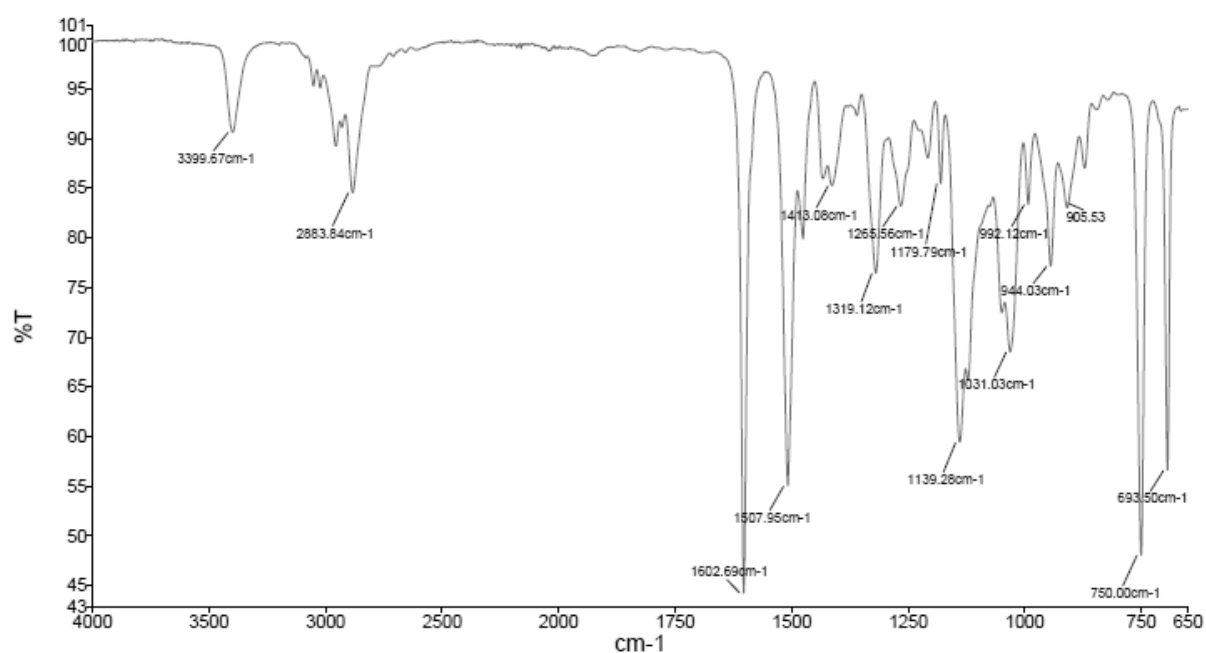
HRMS

+MS, 2.6-2.6min

#153-154

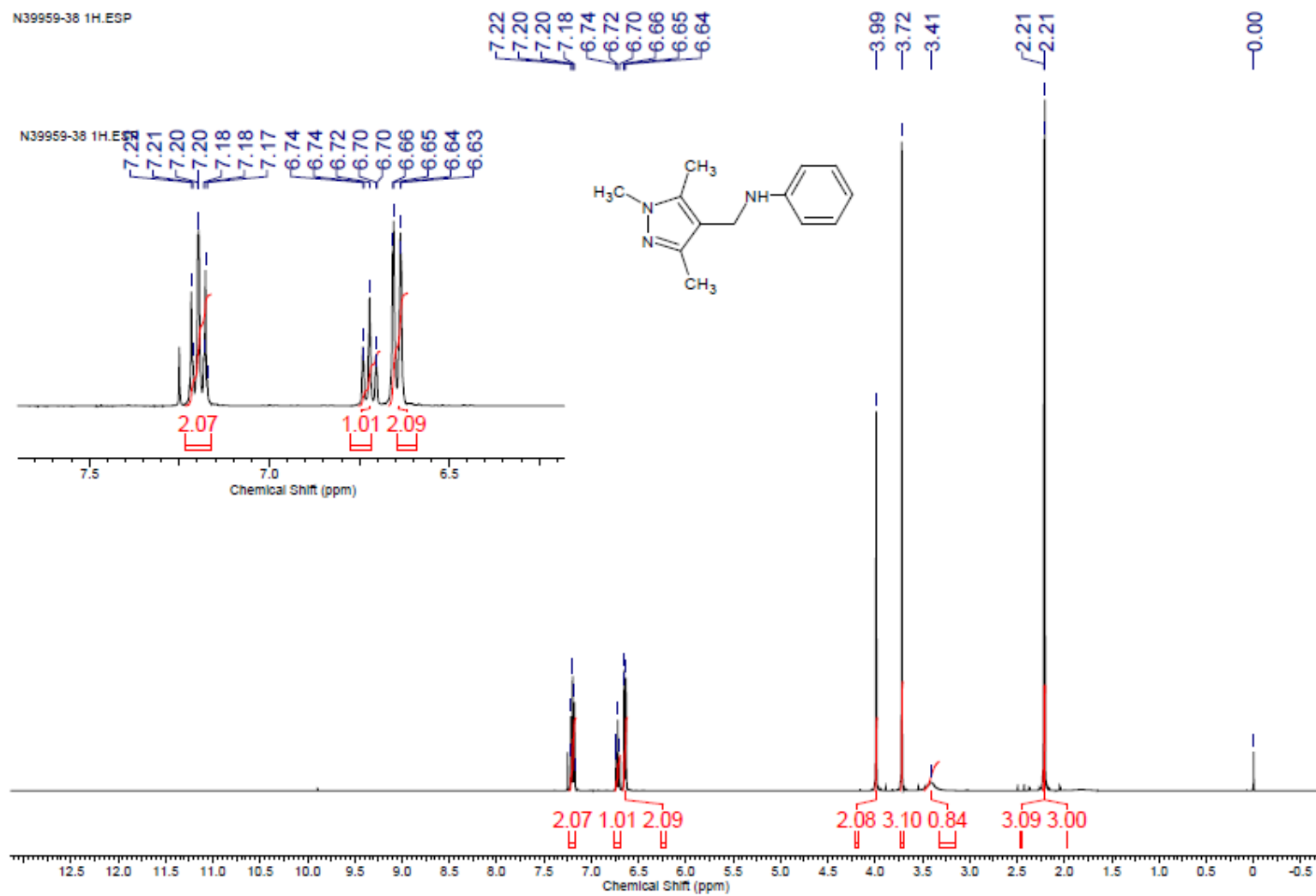


IR Spectra

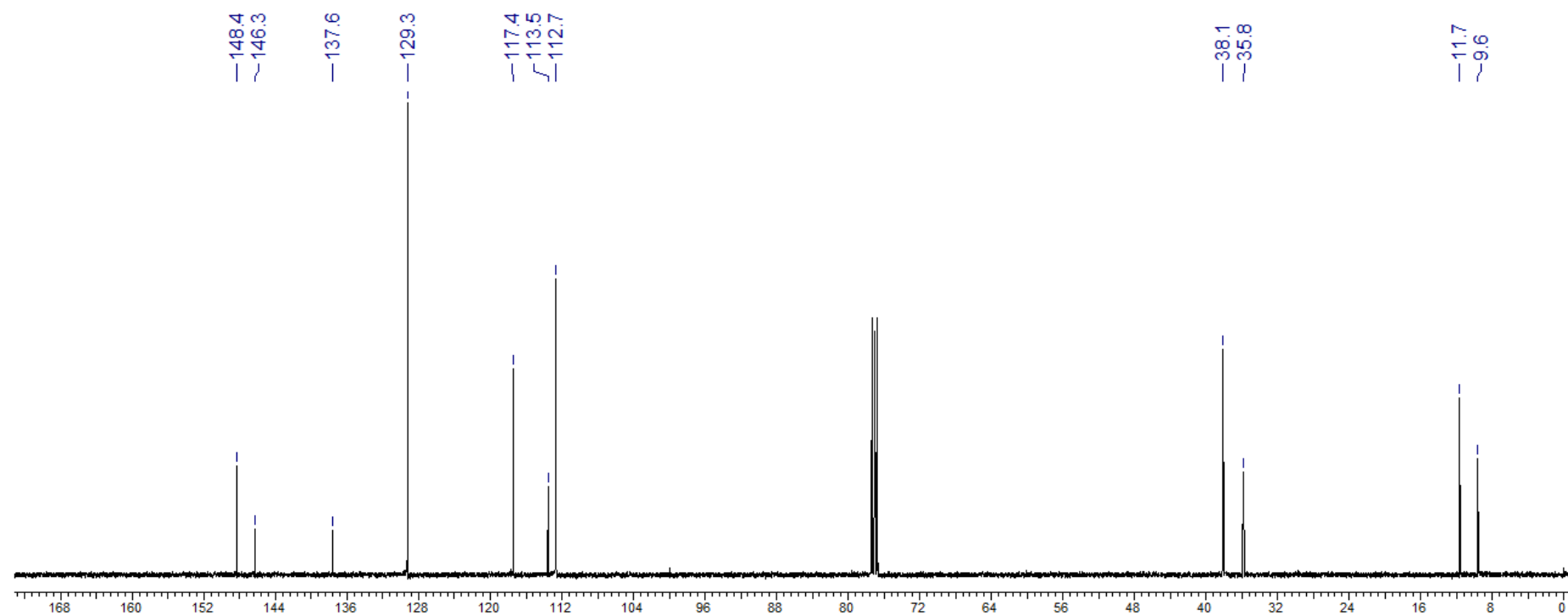


***N*-((1,3,5-Trimethyl-1*H*-pyrazol-4-yl)methyl)aniline (7al).**

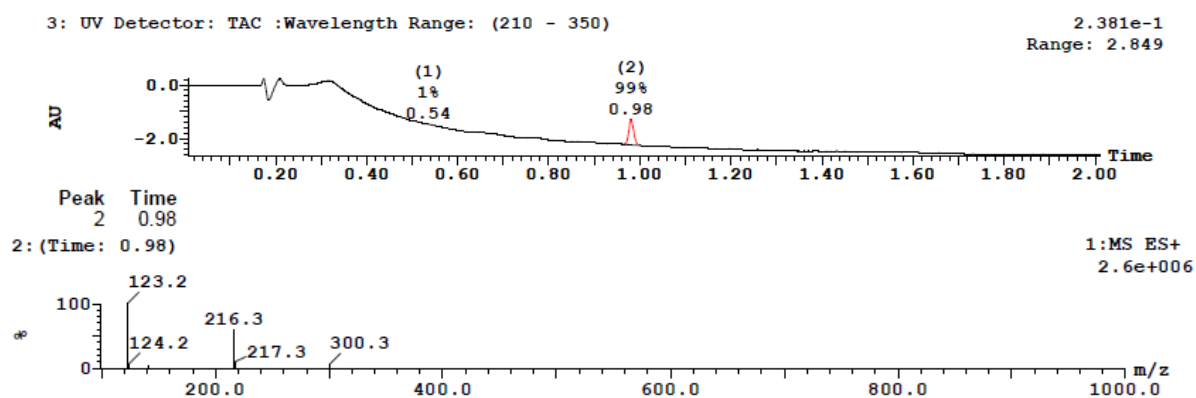
¹H NMR Spectra



¹³C NMR Spectra



LCMS



IR Spectra

