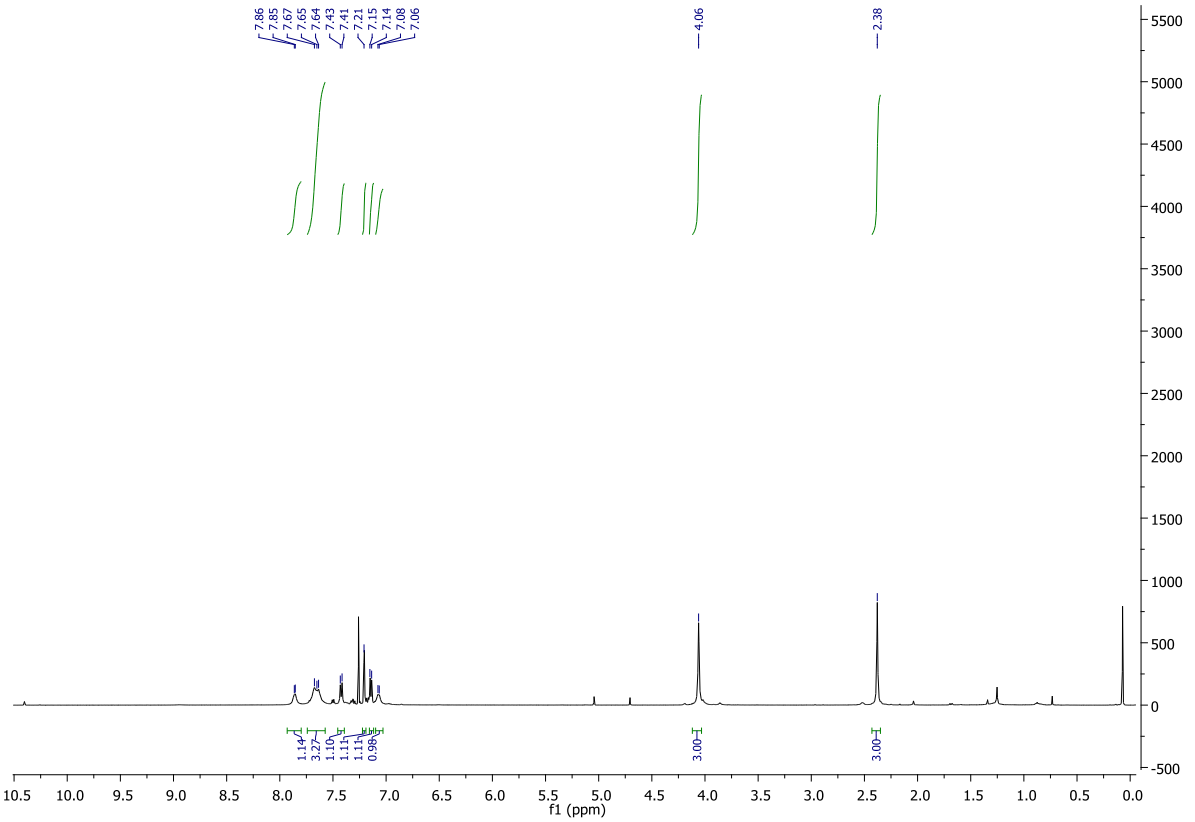
Table of Contents

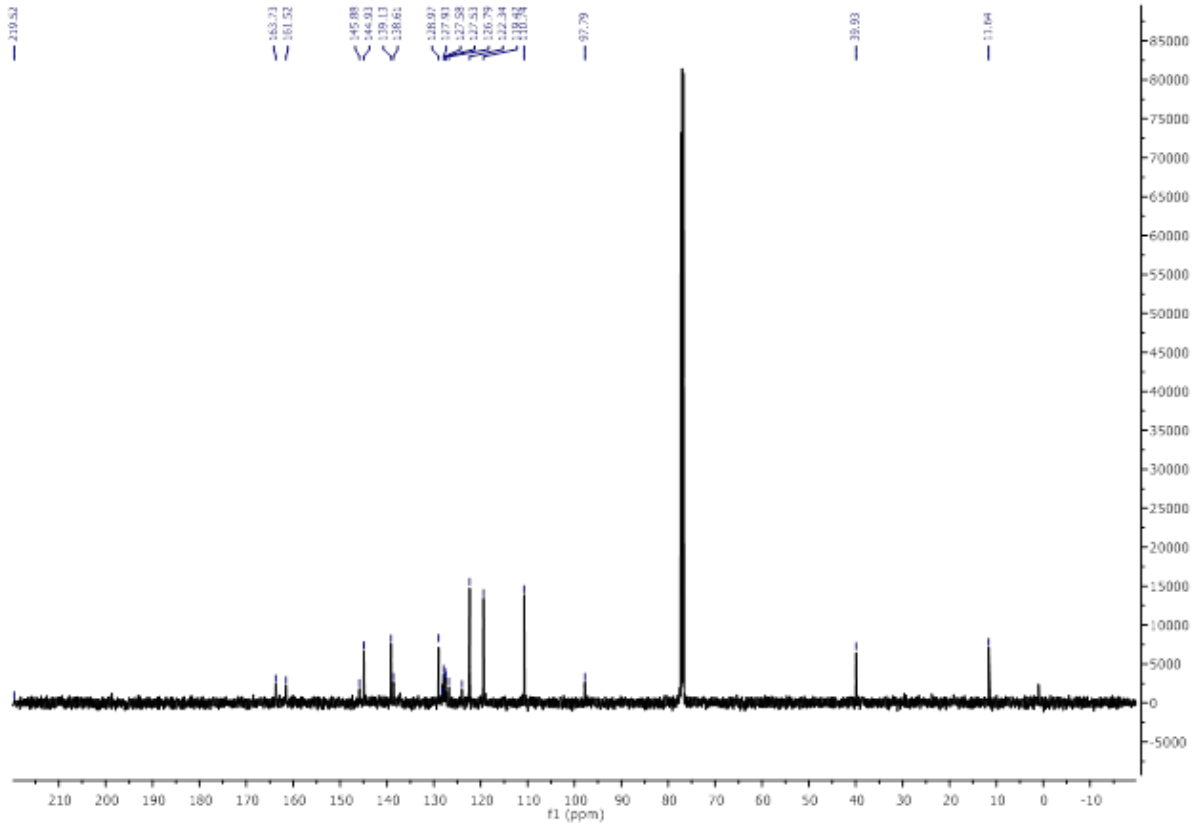
1. ^{1}H, ^{13}C, IR, and HRMS Spectra

Compound 18

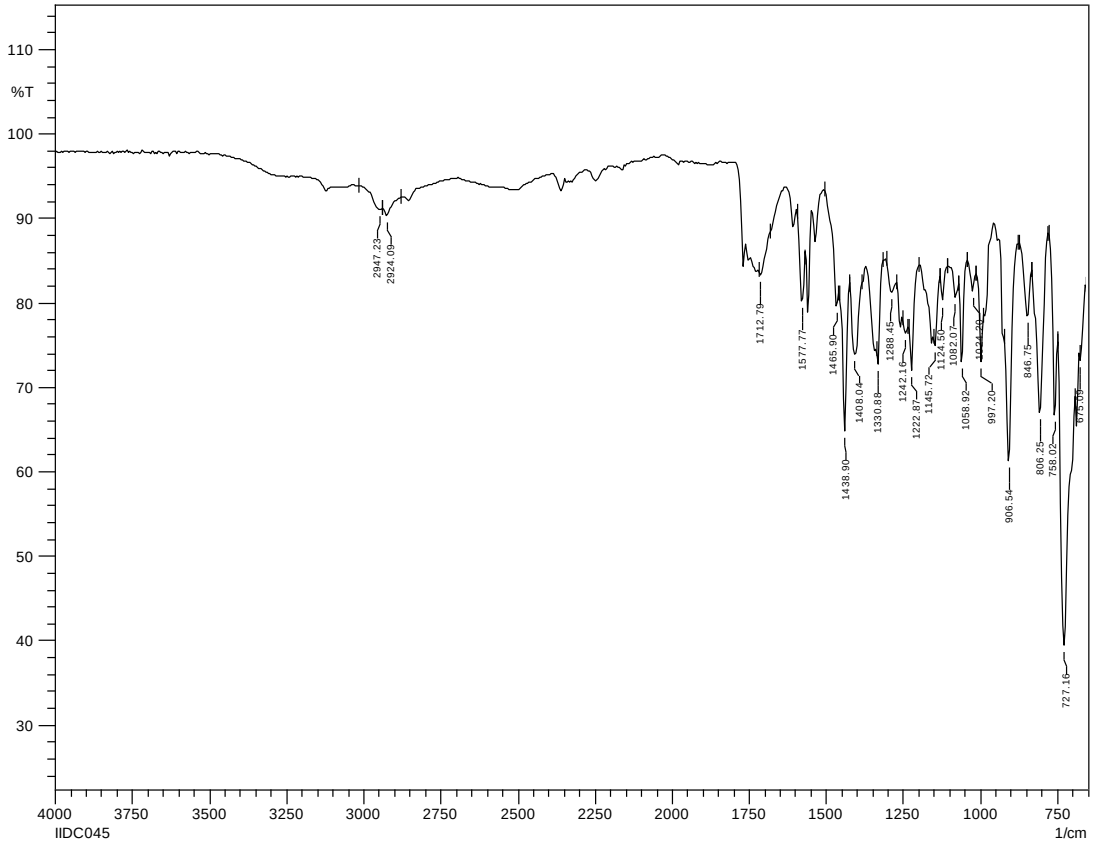
^{1}H NMR



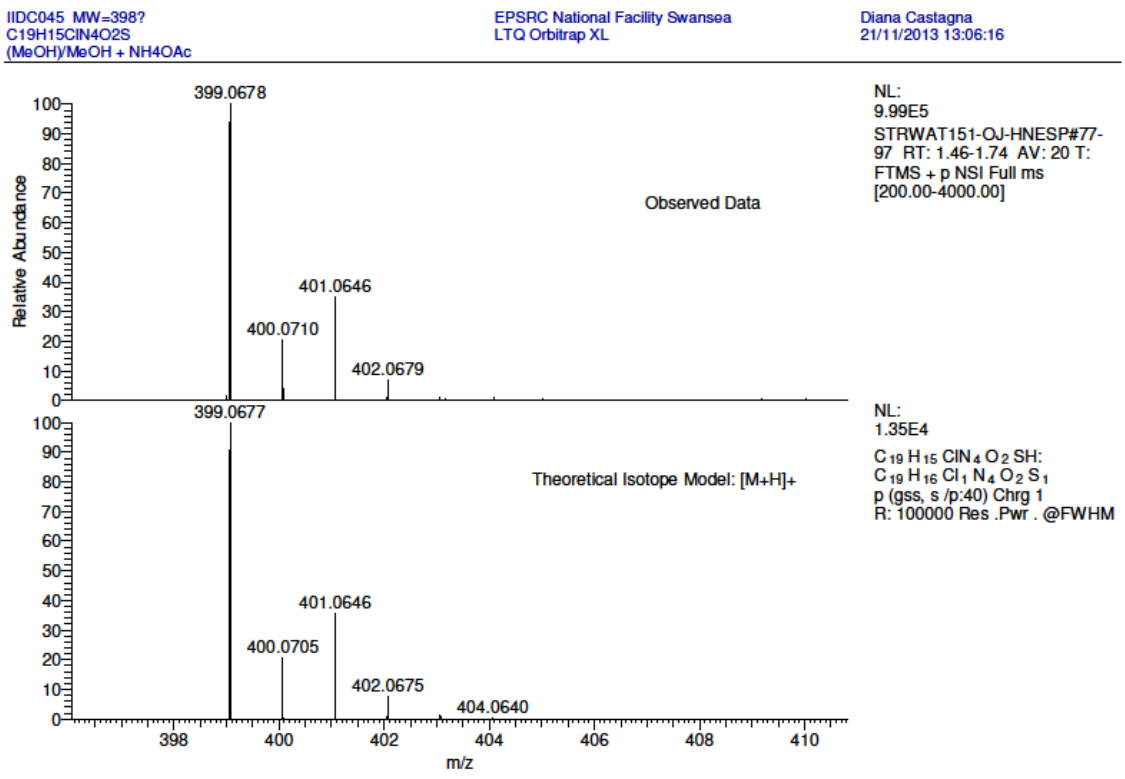
^{13}C NMR



IR

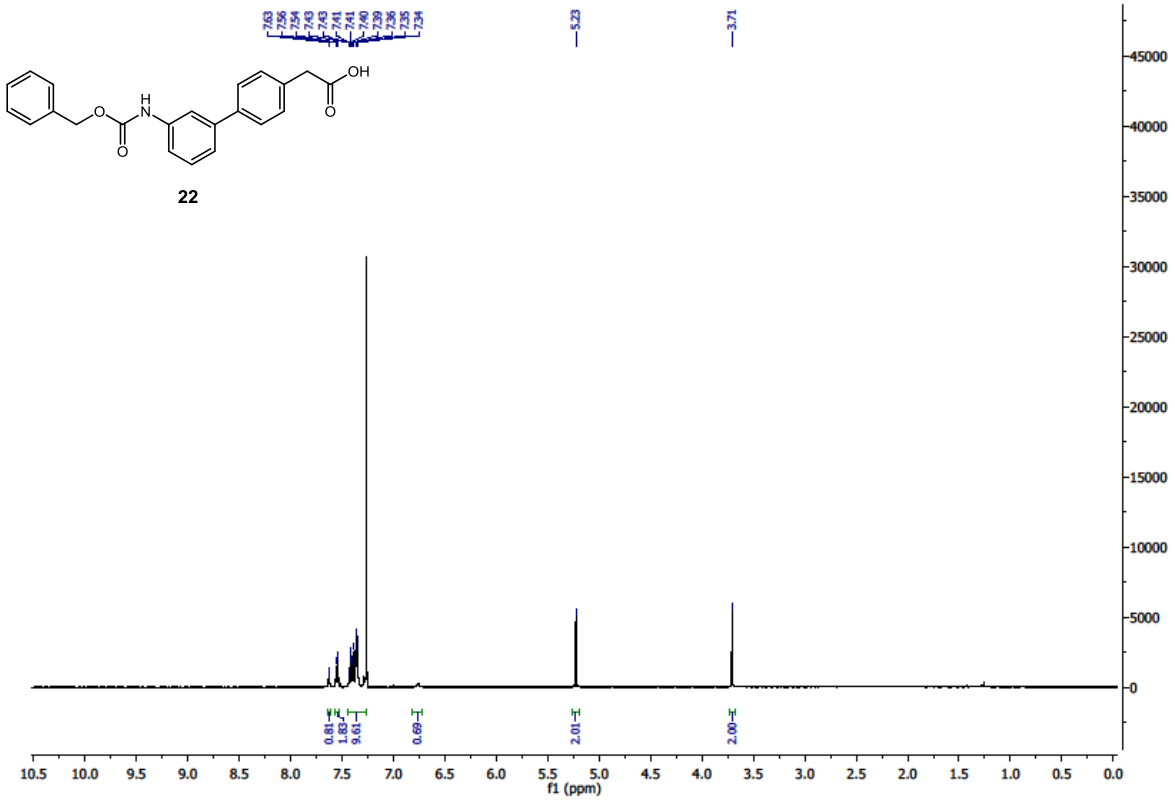

%T
110
100
90
80
70
60
50
40
30
2947.23
2924.09
1712.79
1577.77
1465.90
1438.90
1408.04
1330.88
1288.45
1242.16
1222.87
1145.72
1124.50
1082.07
1058.92
997.20
906.54
846.75
806.25
758.02
727.16
675.09
4000
3750
3500
3250
3000
2750
2500
2250
2000
1750
1500
1250
1000
750
IIDC045
1/cm

HRMS

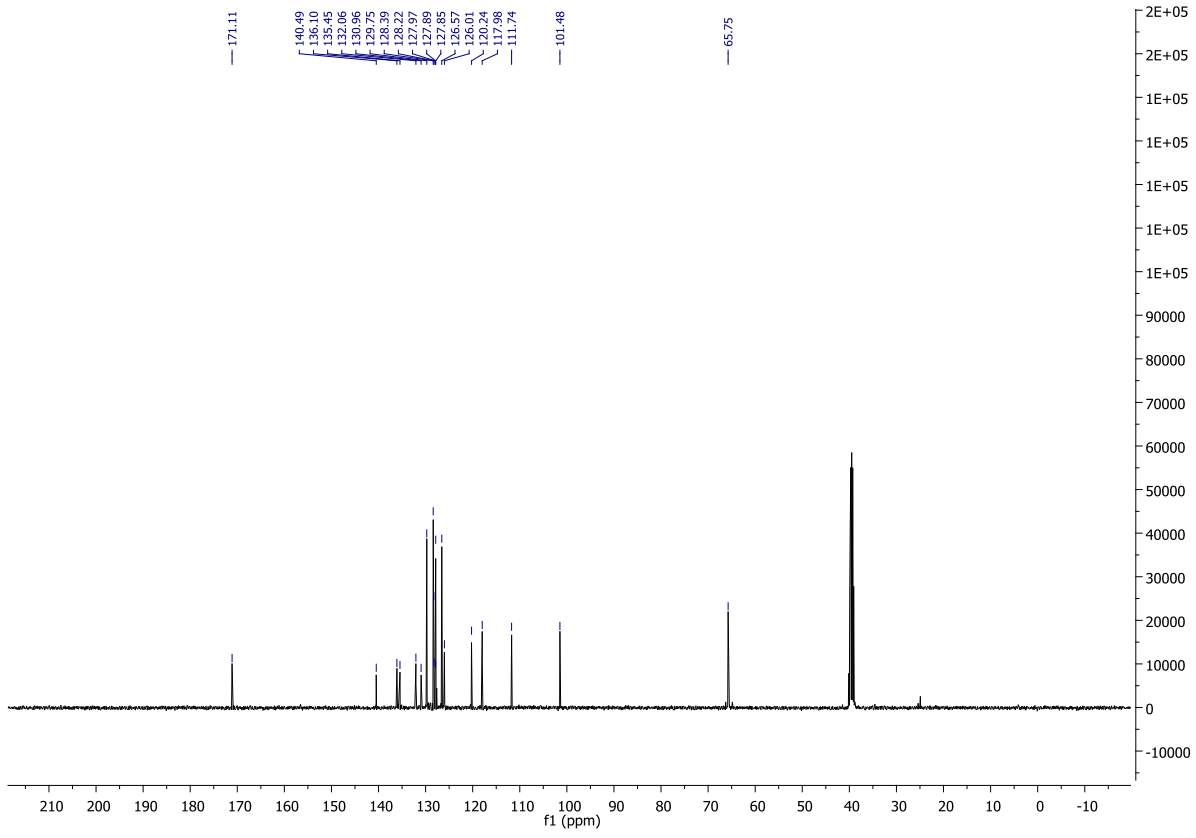

IIDC045 MW=398?
C19H15ClN4O2S
(MeOH)/MeOH + NH4OAc
EPSRC National Facility Swansea
LTQ Orbitrap XL
Diana Castagna
21/11/2013 13:06:16
399.0678
401.0646
400.0710
402.0679
Observed Data
NL:
9.99E5
STRWAT151-OJ-HNESP#77-97 RT: 1.46-1.74 AV: 20 T: FTMS + p NSI Full ms [200.00-4000.00]
Relative Abundance
399.0677
401.0646
400.0705
402.0675
404.0640
Theoretical Isotope Model: [M+H]+
NL:
1.35E4
C19 H15 ClN4 O2 SH:
C19 H16 Cl1 N4 O2 S1
p (gss, s /p:40) Chrg 1
R: 100000 Res .Pwr . @FWHM
398
400
402
404
406
408
410
m/z

Compound 22

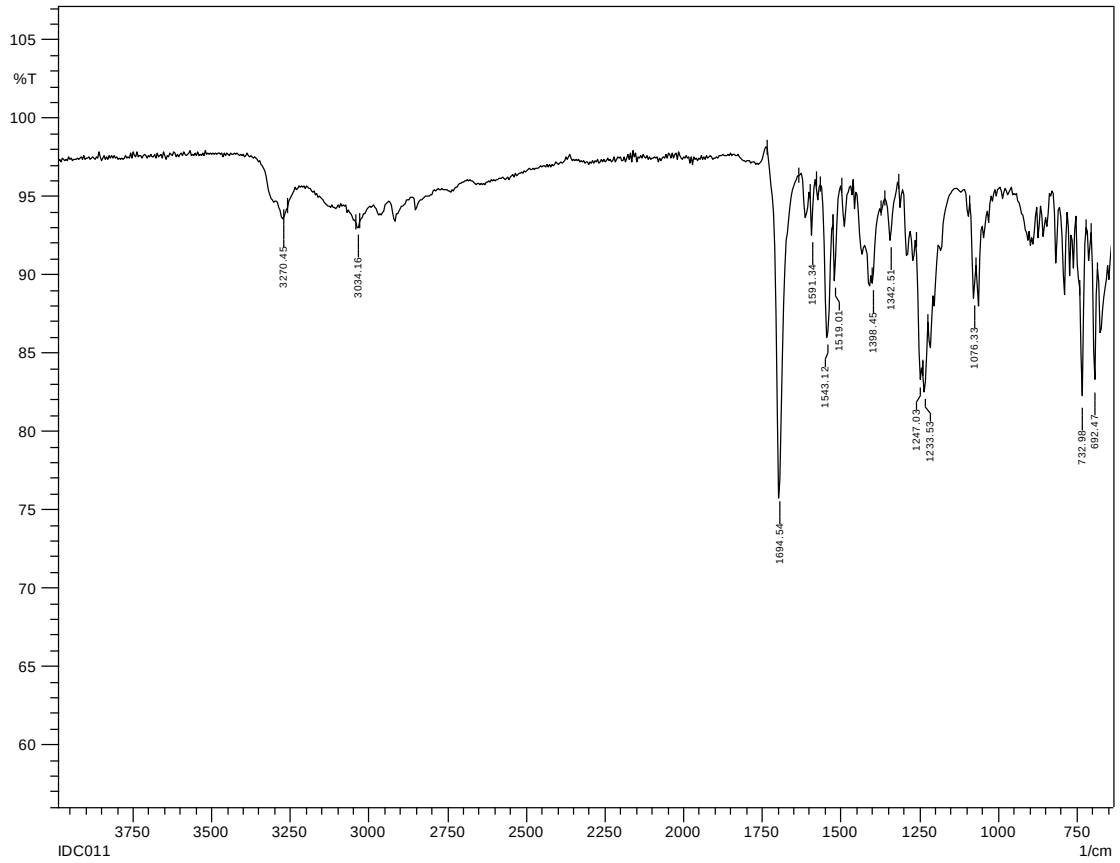
^{1}H NMR



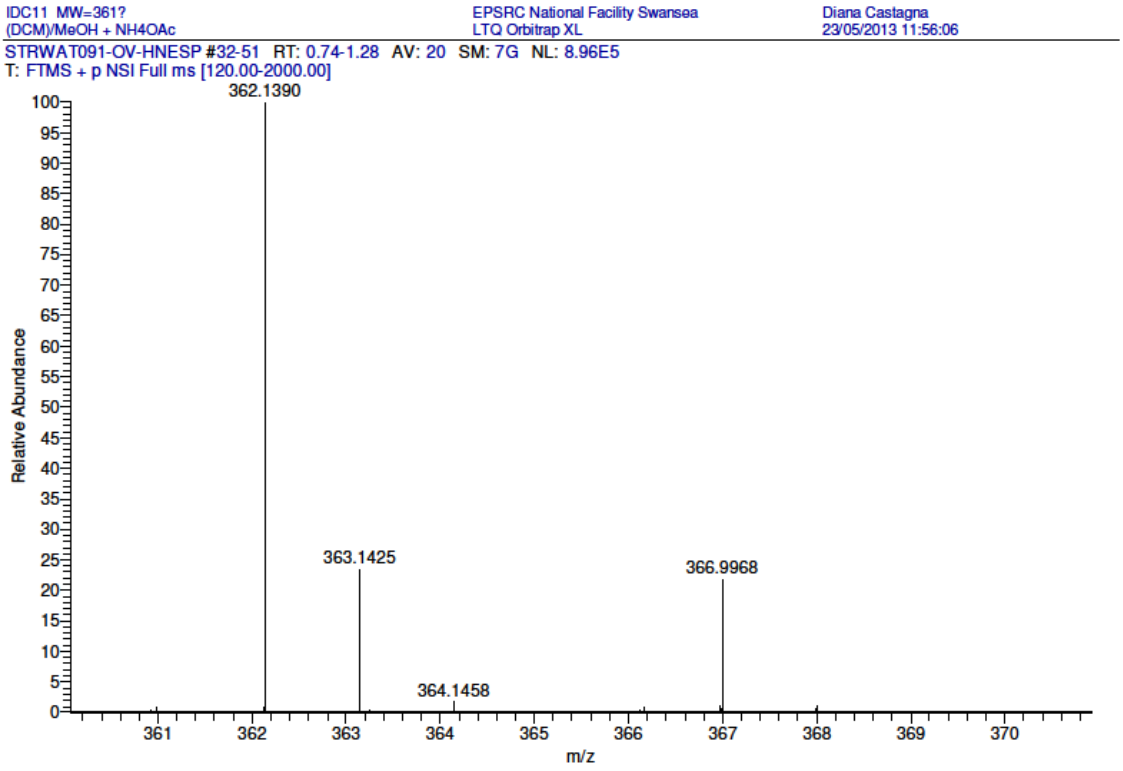
^{13}C NMR of 22



IR of 22

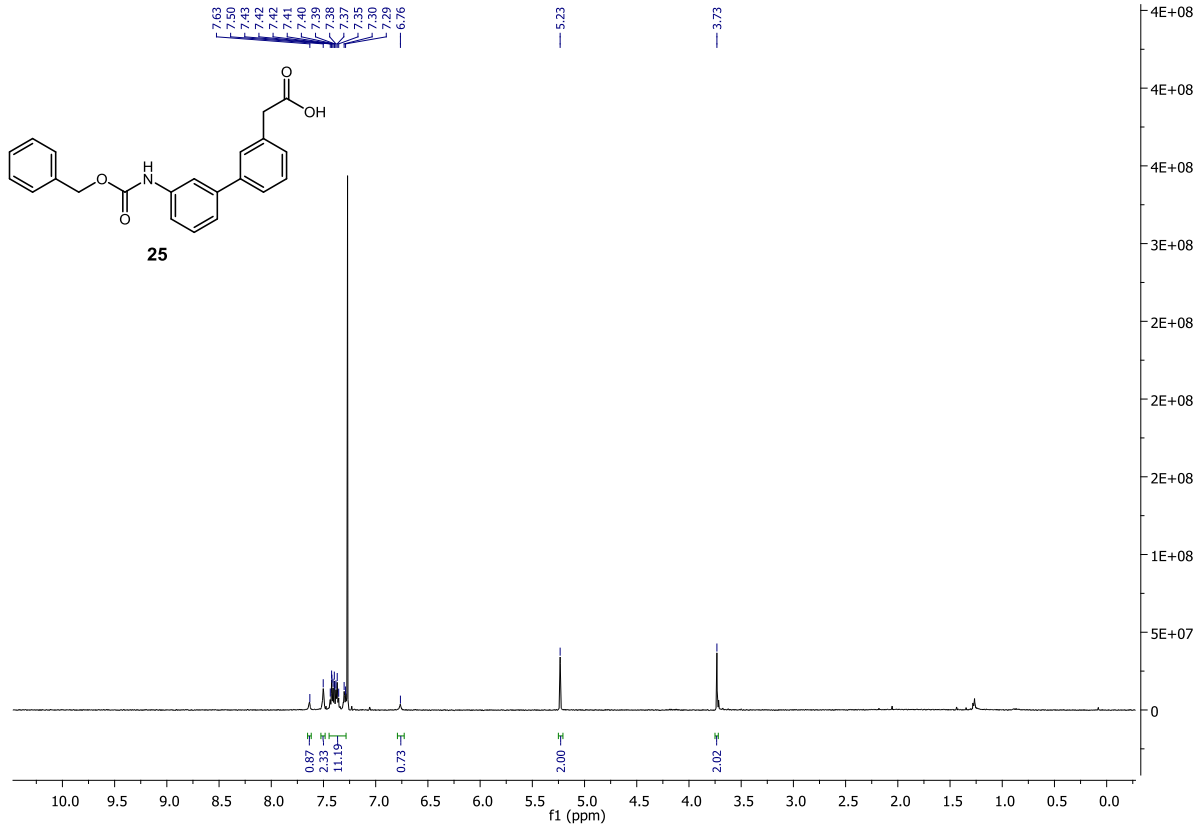


HRMS of 22

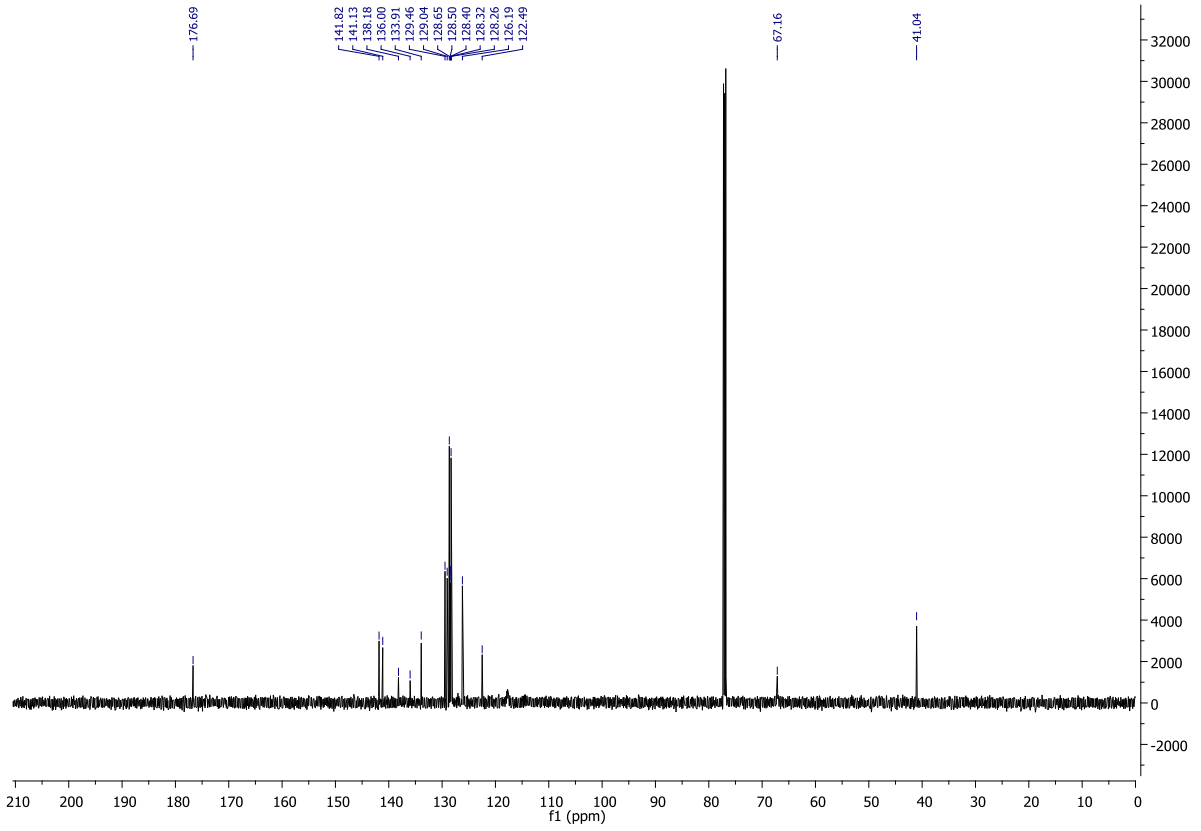


Compound 25

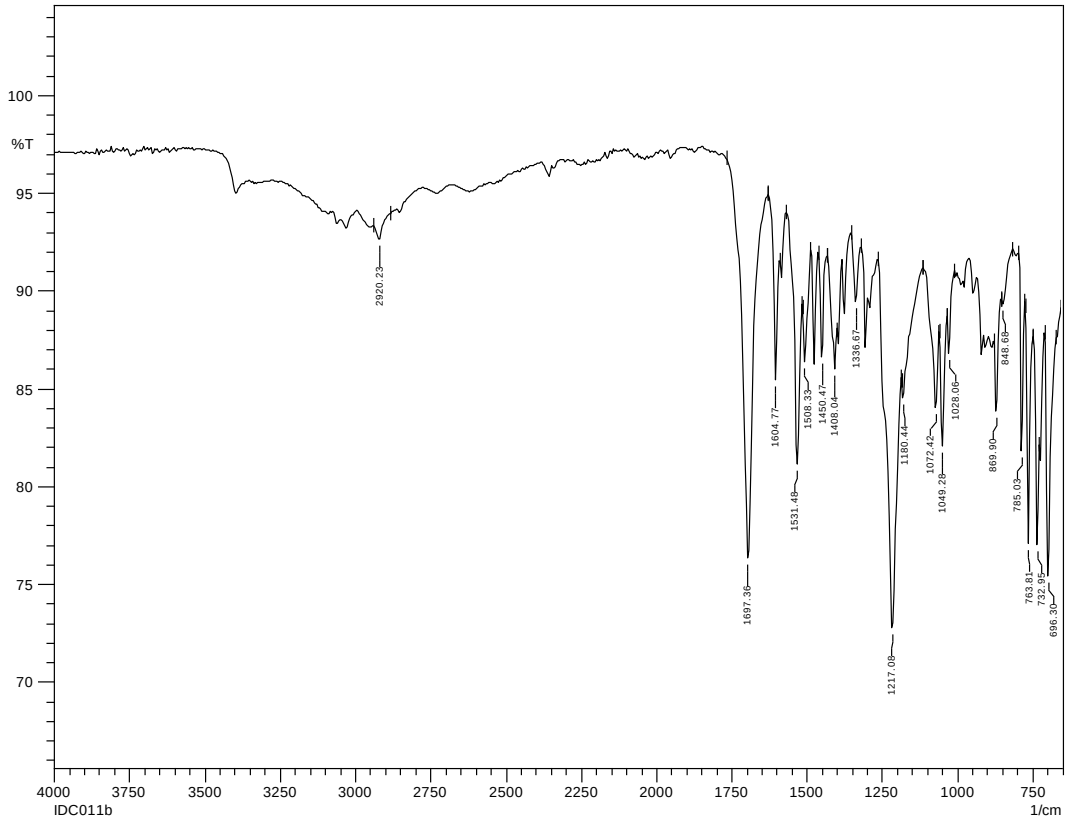
^{1}H NMR



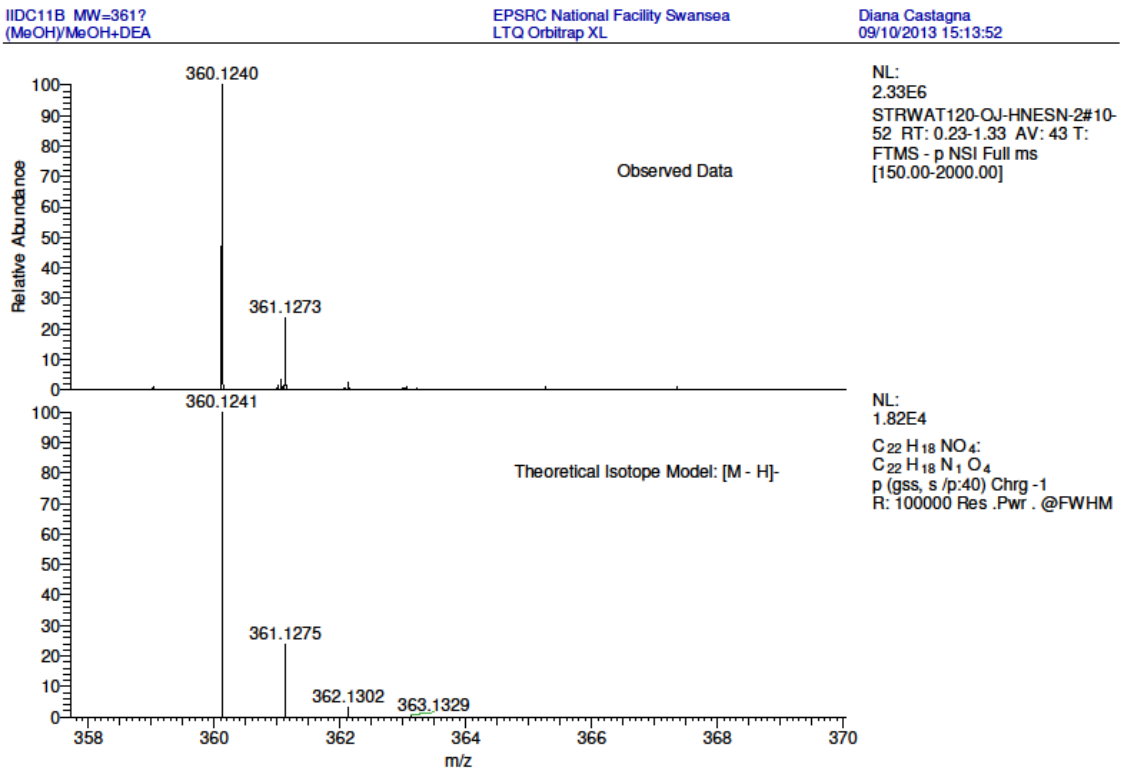
^{13}C NMR of 25



IR of 25

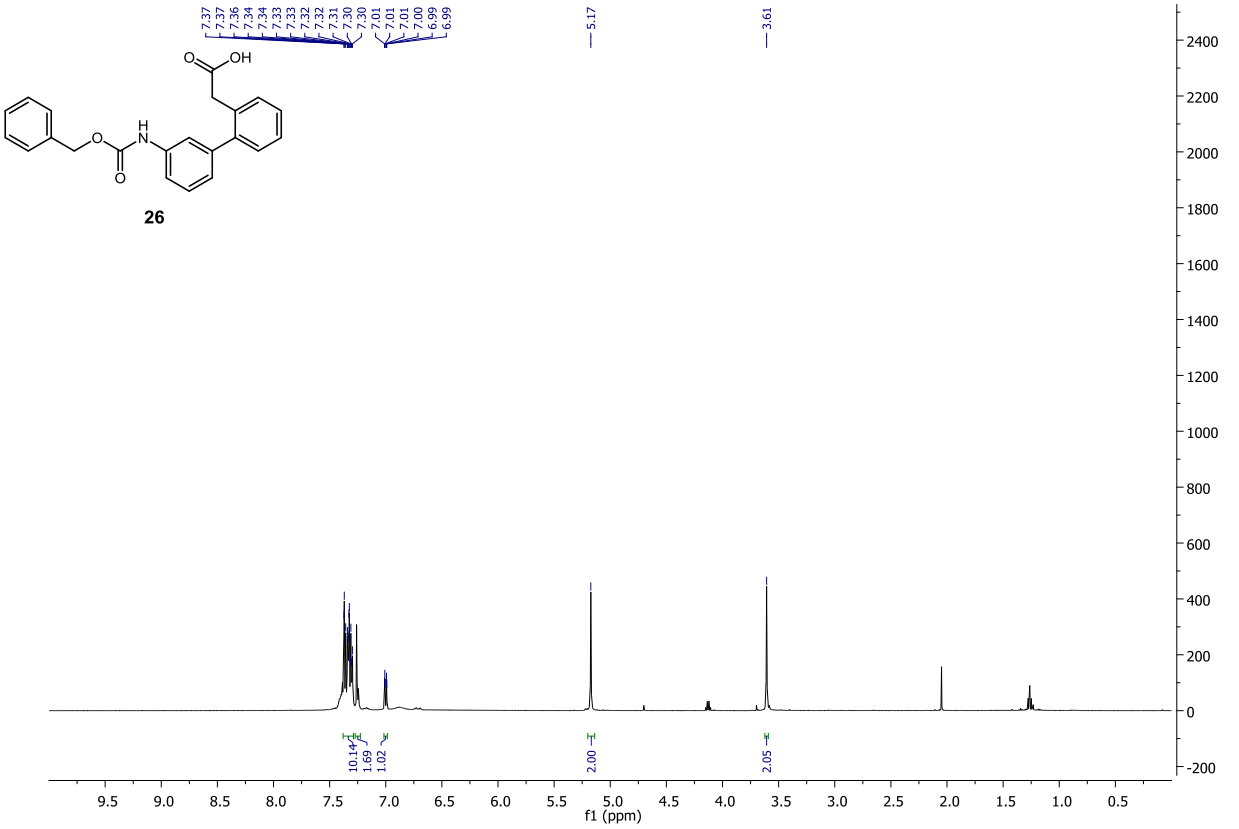


HRMS of 25

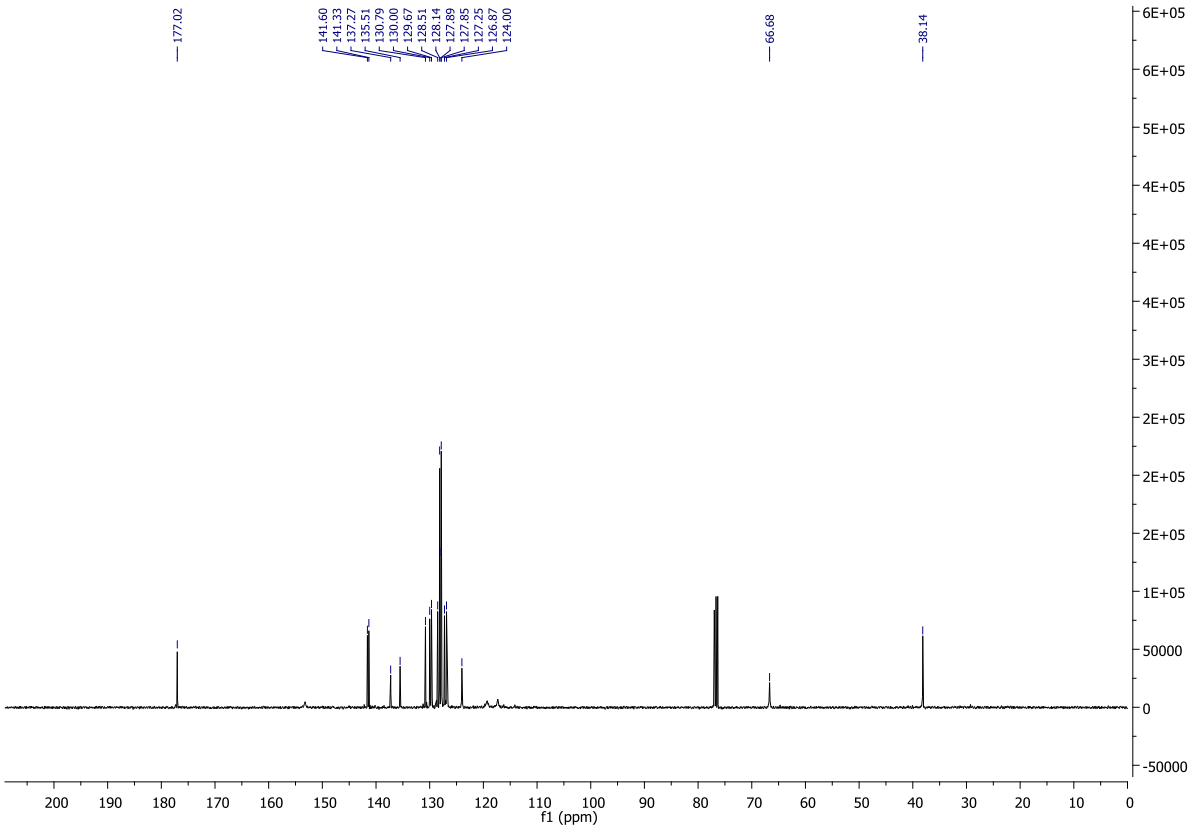


Compound 26

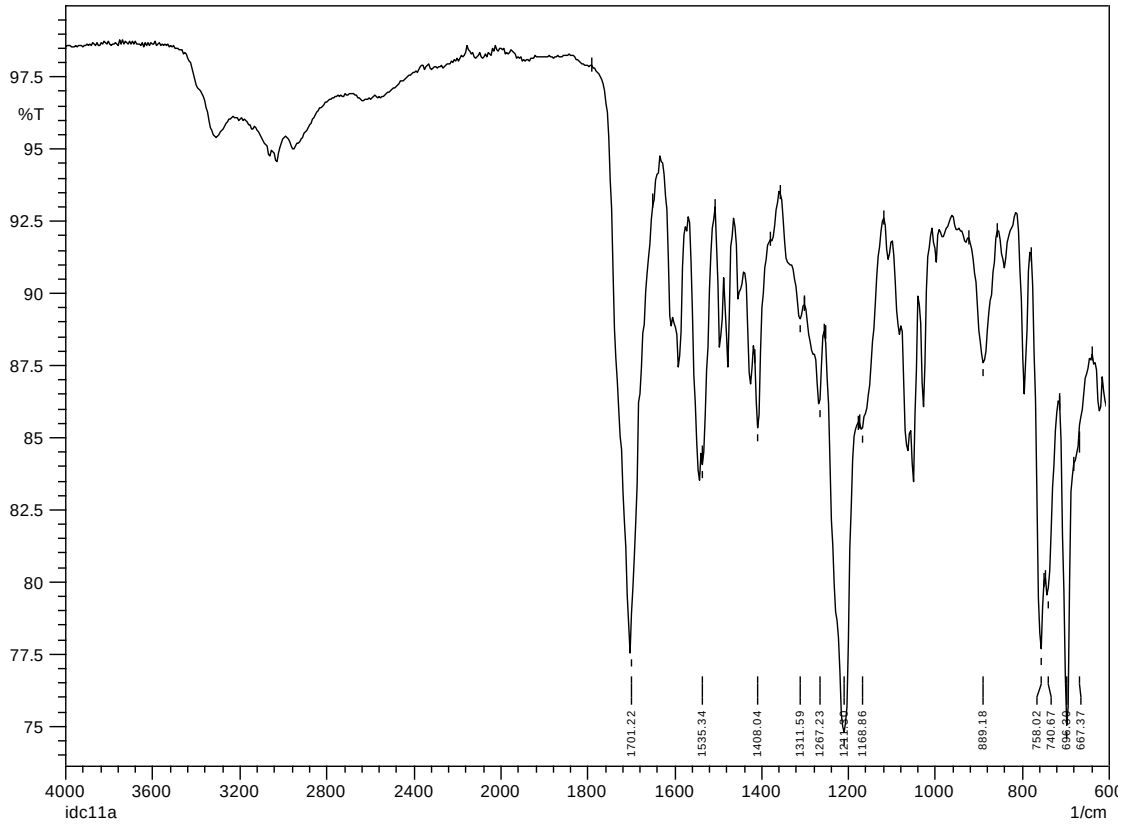
^{1}H NMR



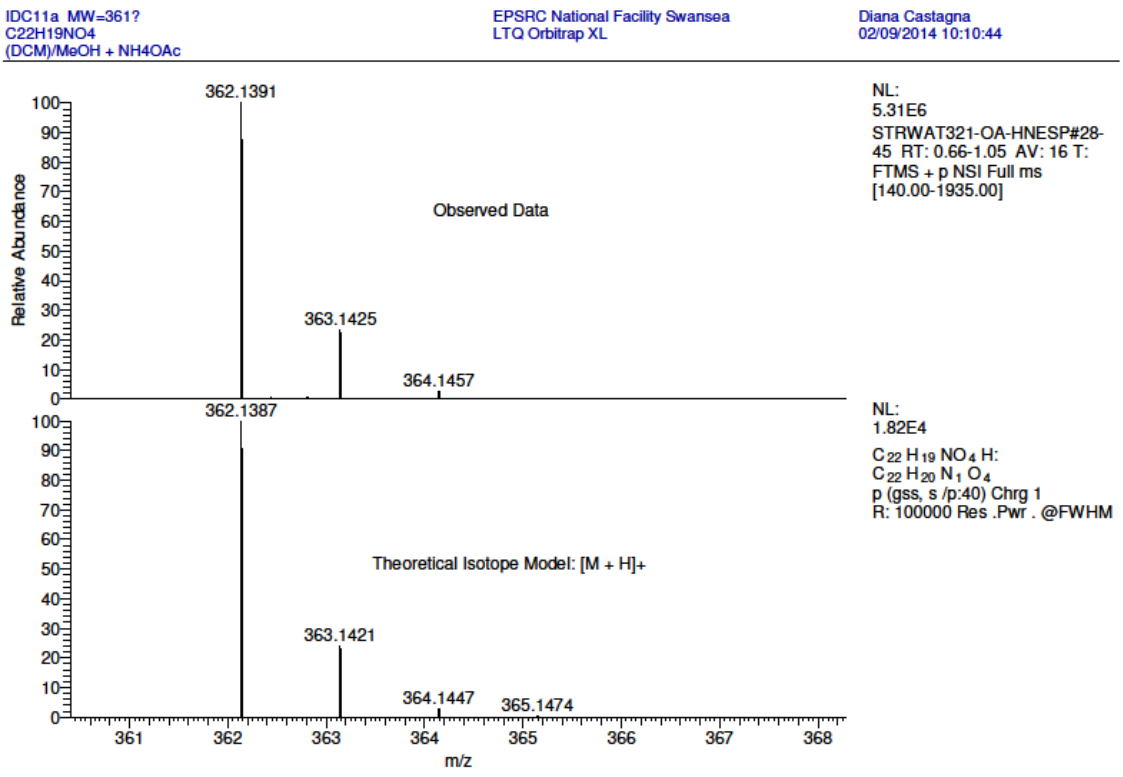
^{13}C NMR of 26



IR of 26

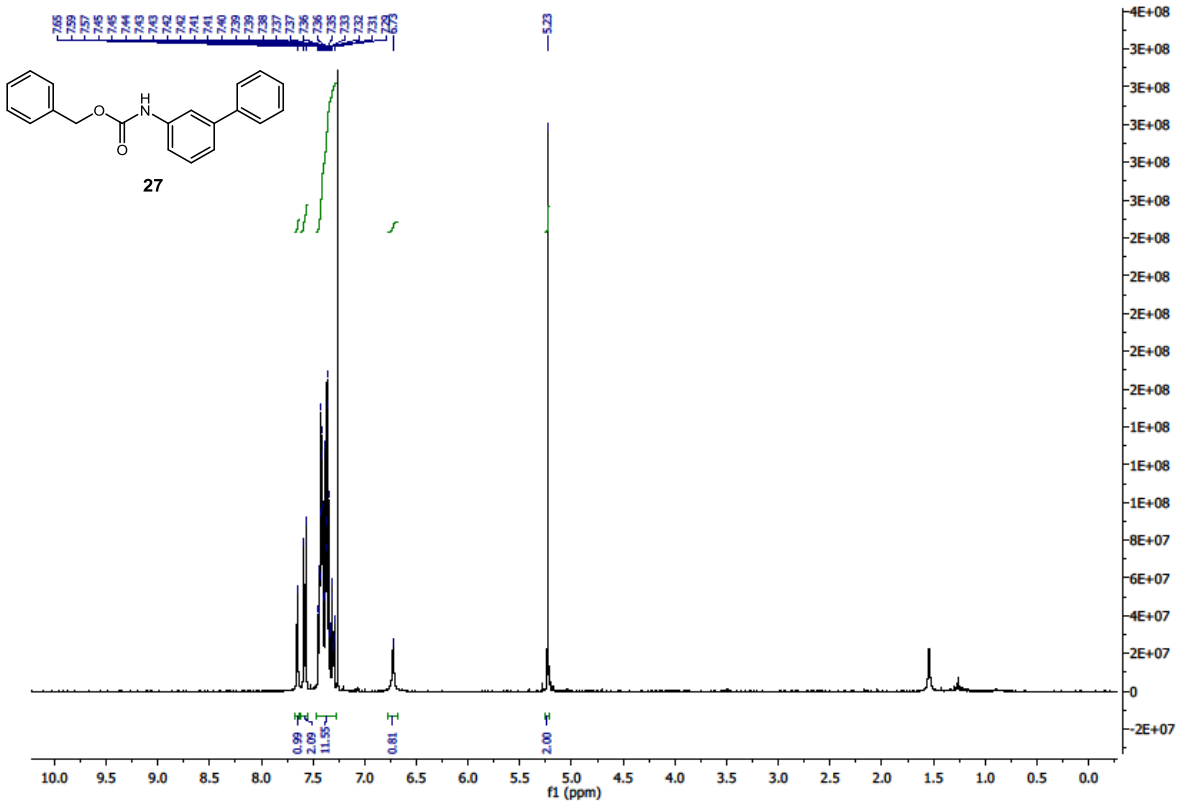


HRMS of 26

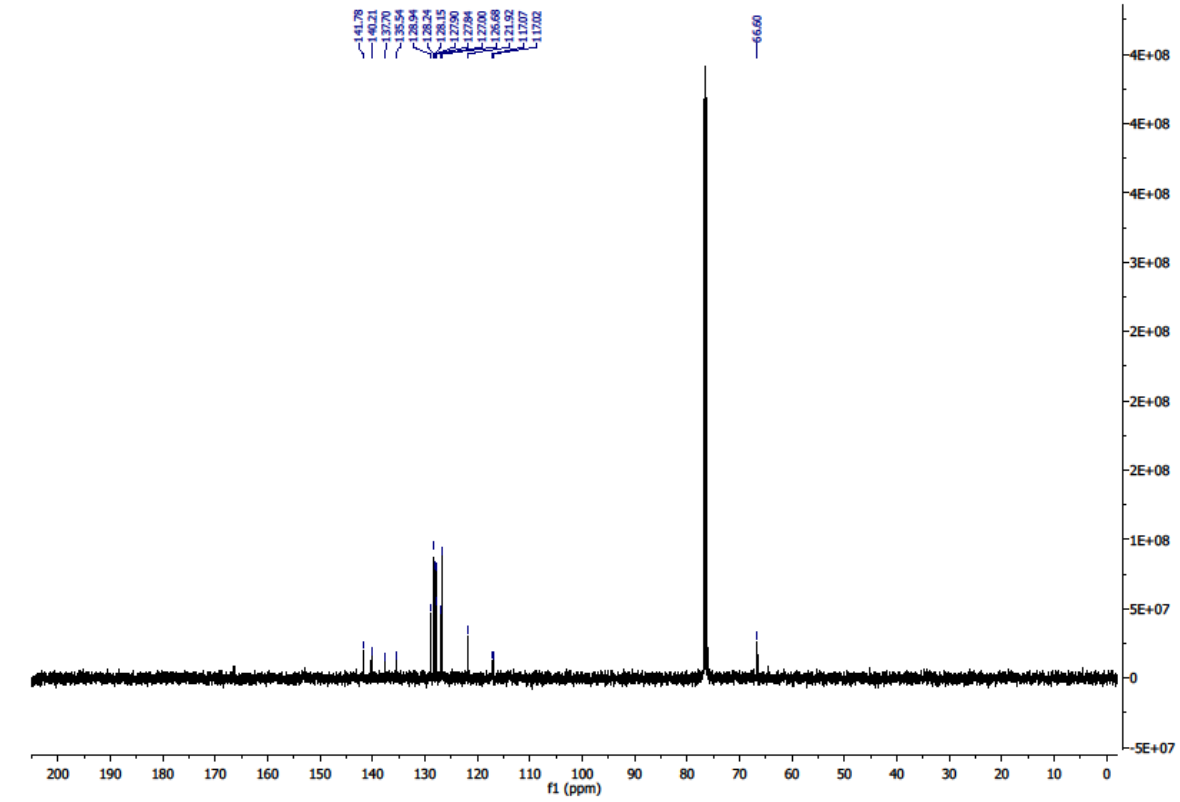


Compound 27

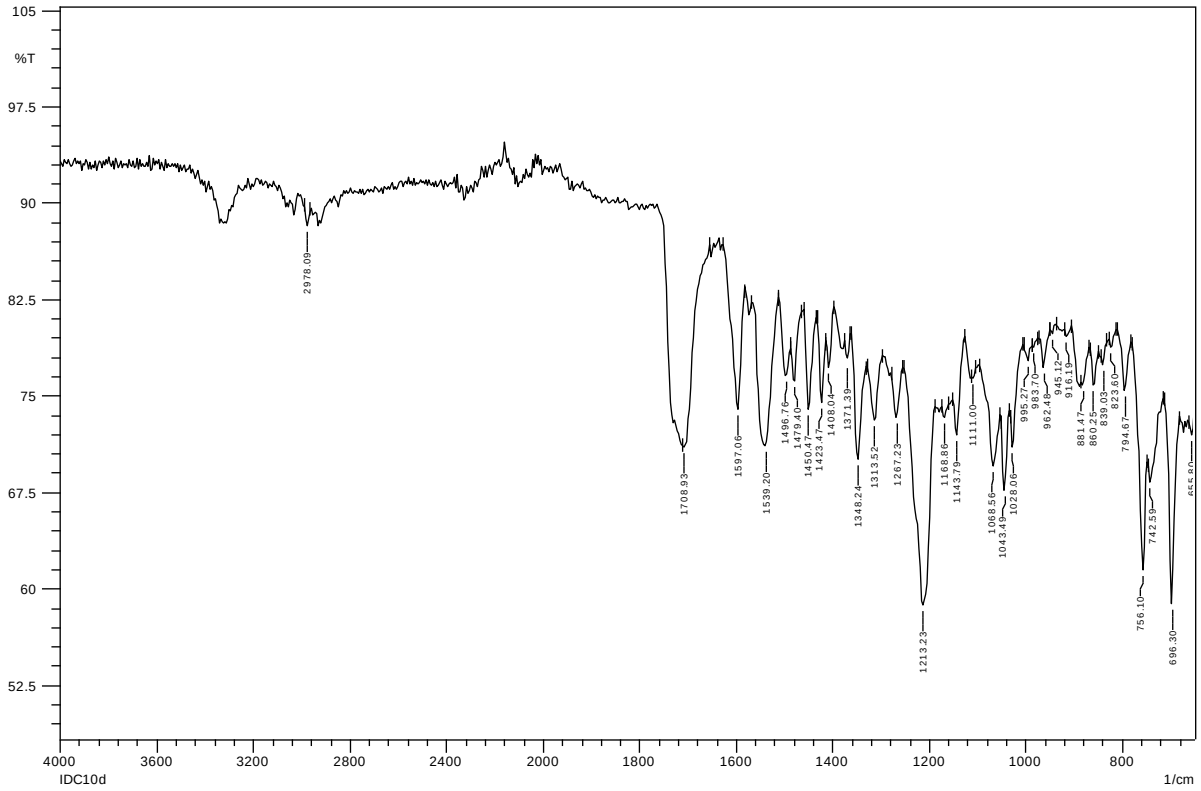
^{1}H NMR



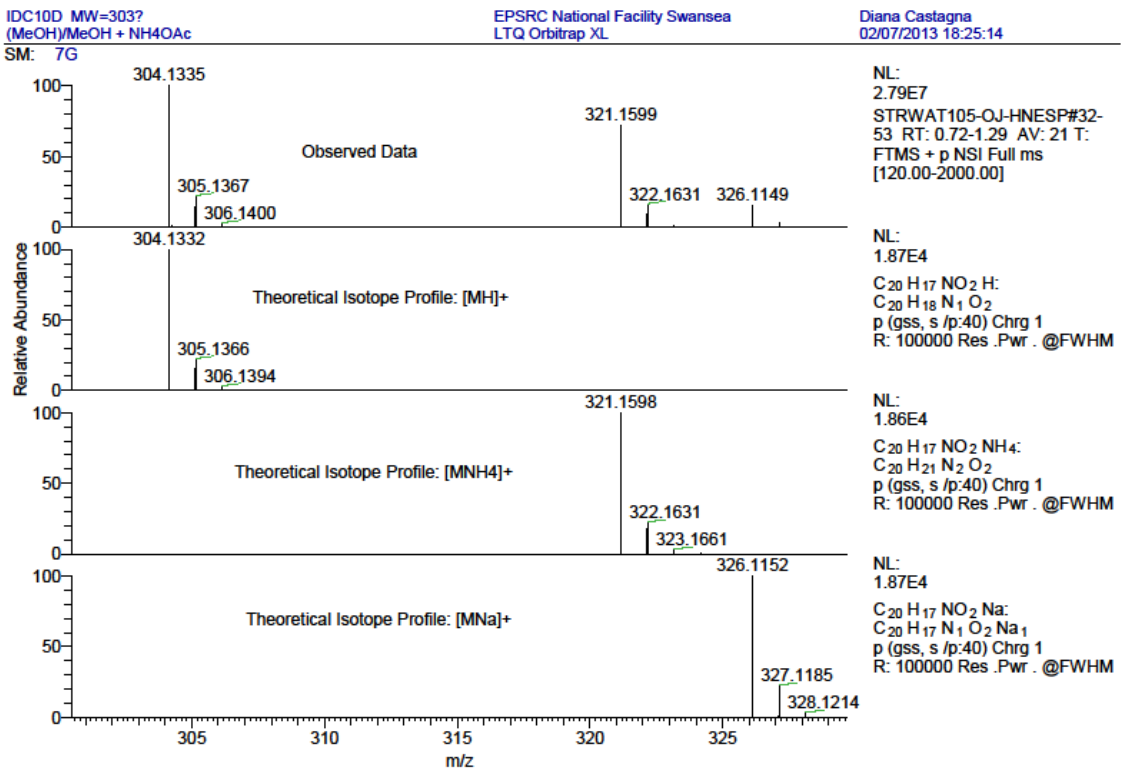
^{13}C NMR of 27



IR of 27

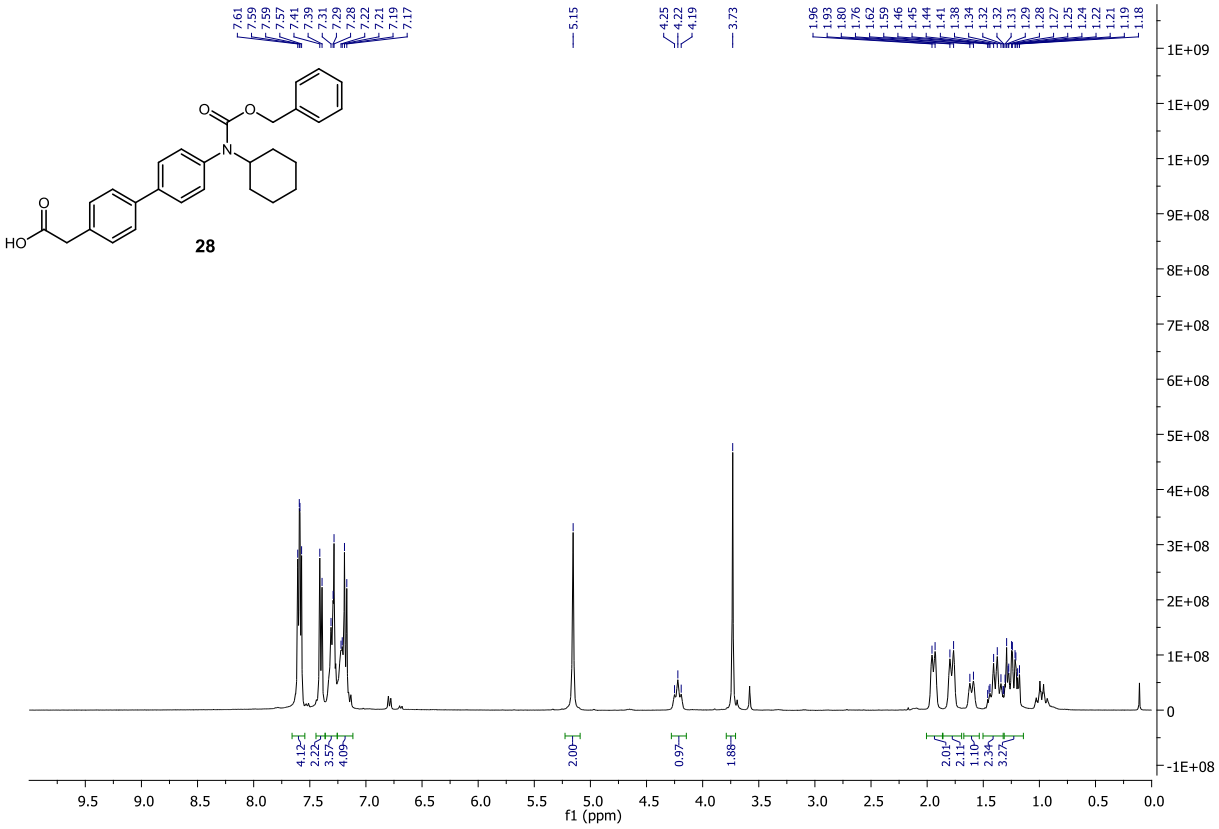


HRMS of 27

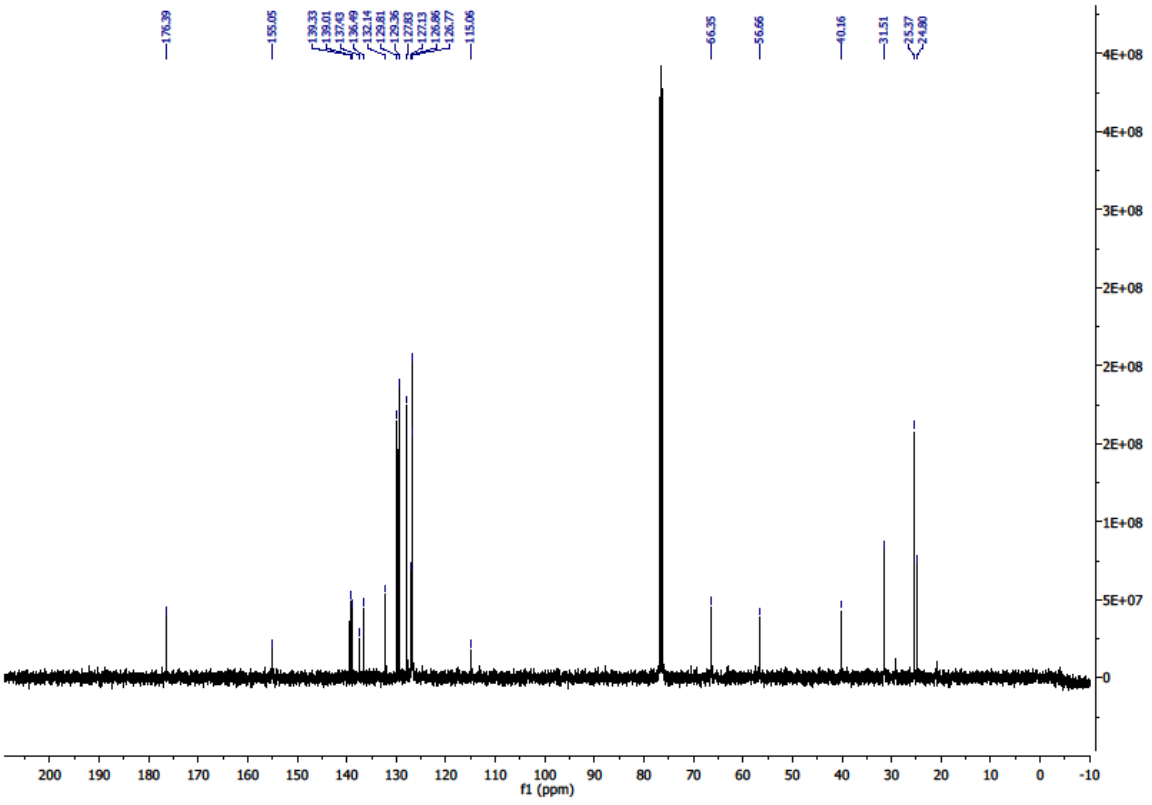


Compound 28

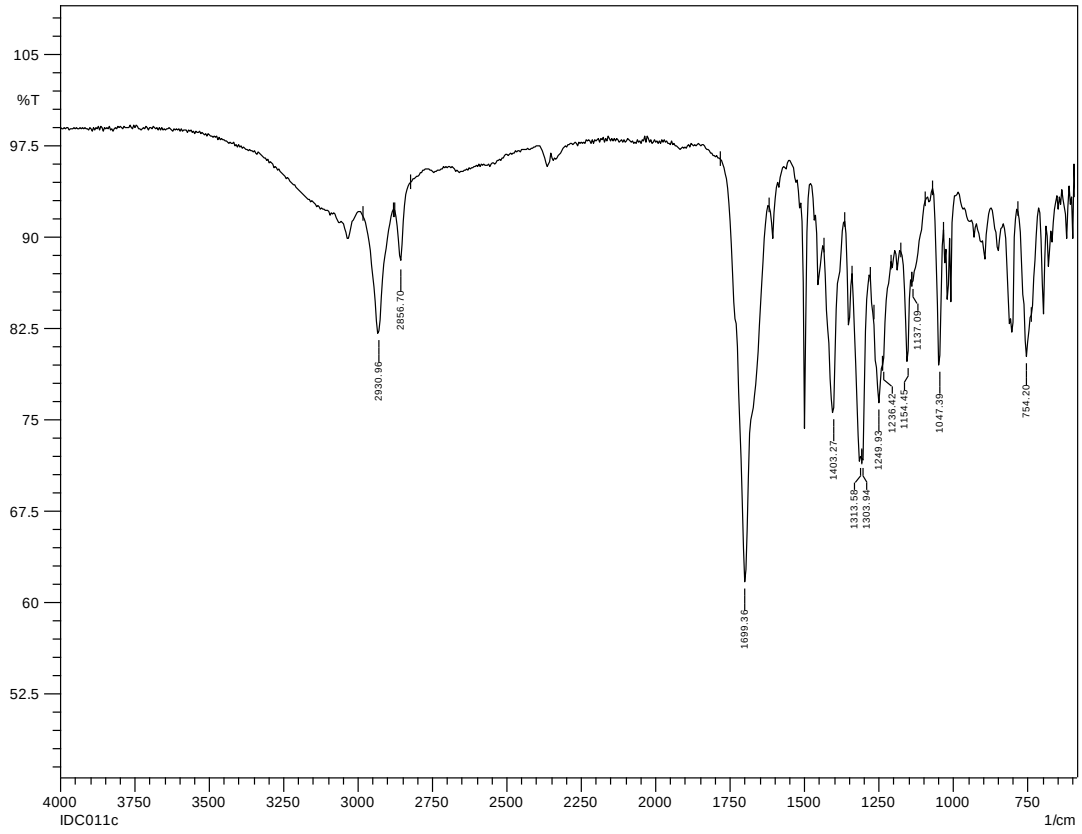
^{1}H NMR



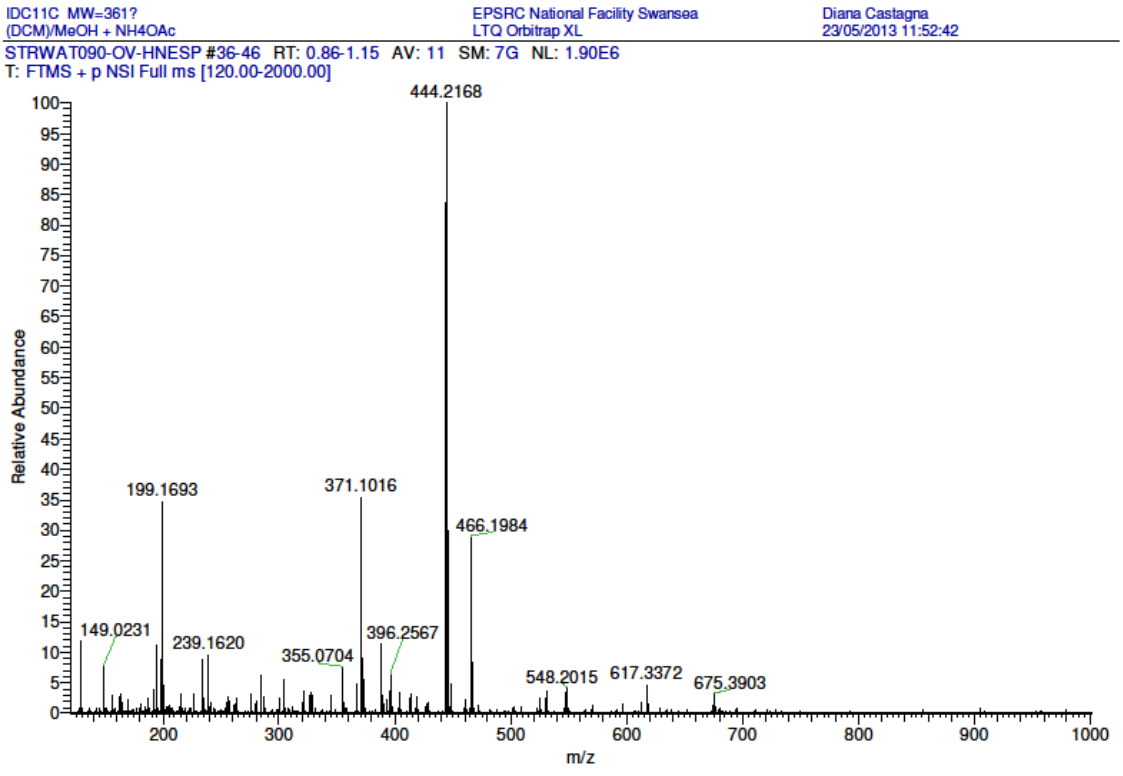
^{13}C NMR of 28



IR of 28

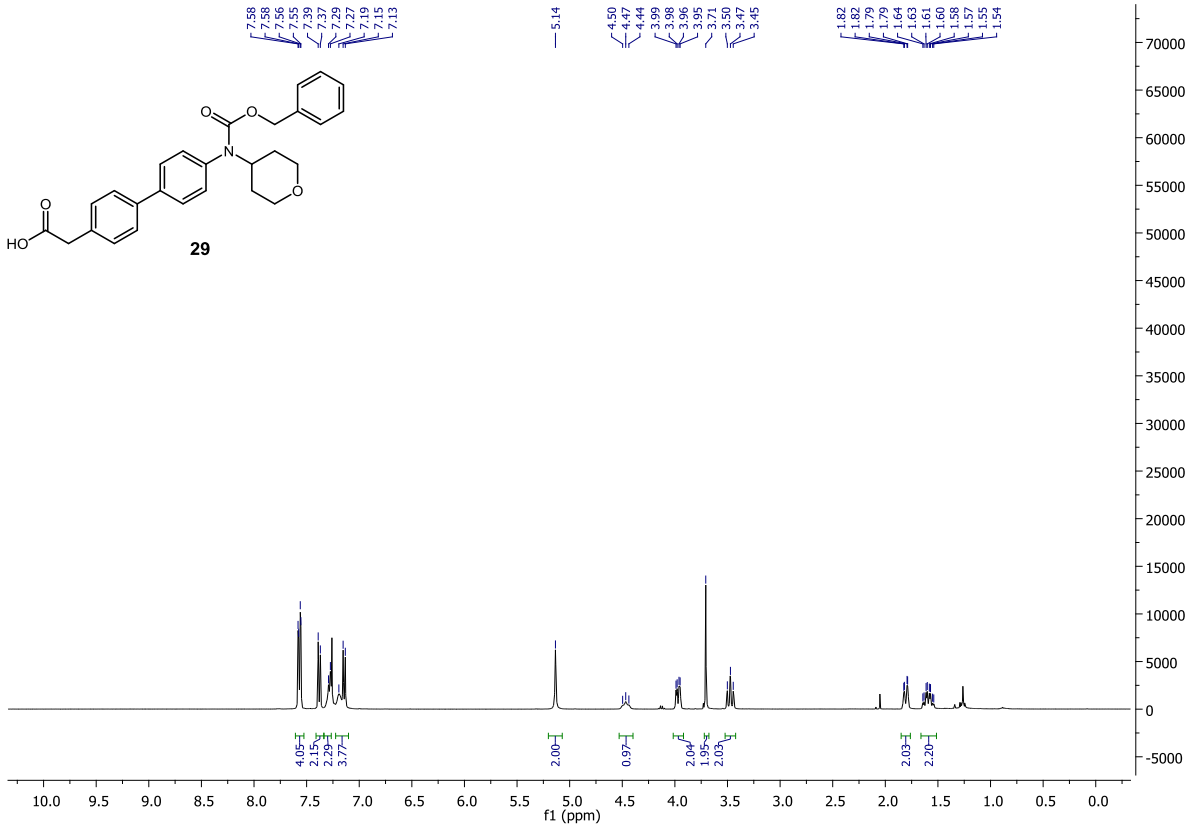


HRMS of 28



Compound 29

^{1}H NMR



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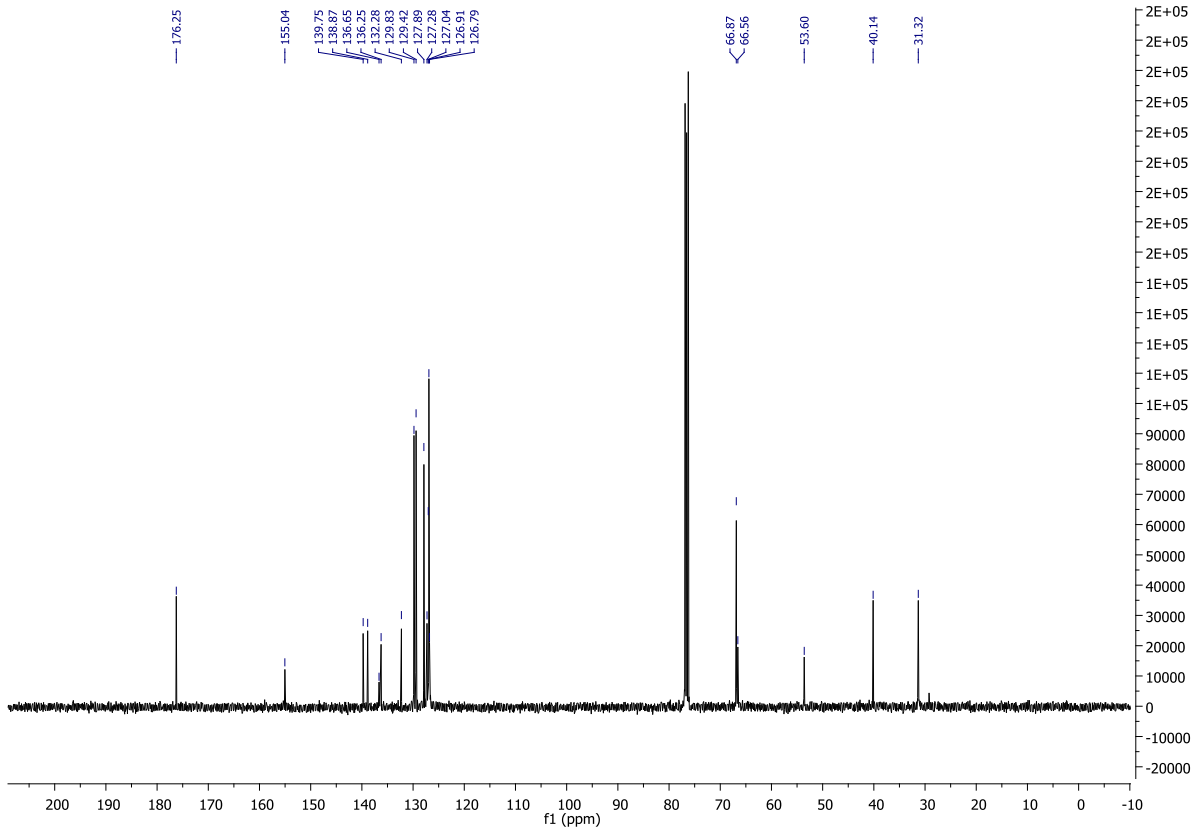
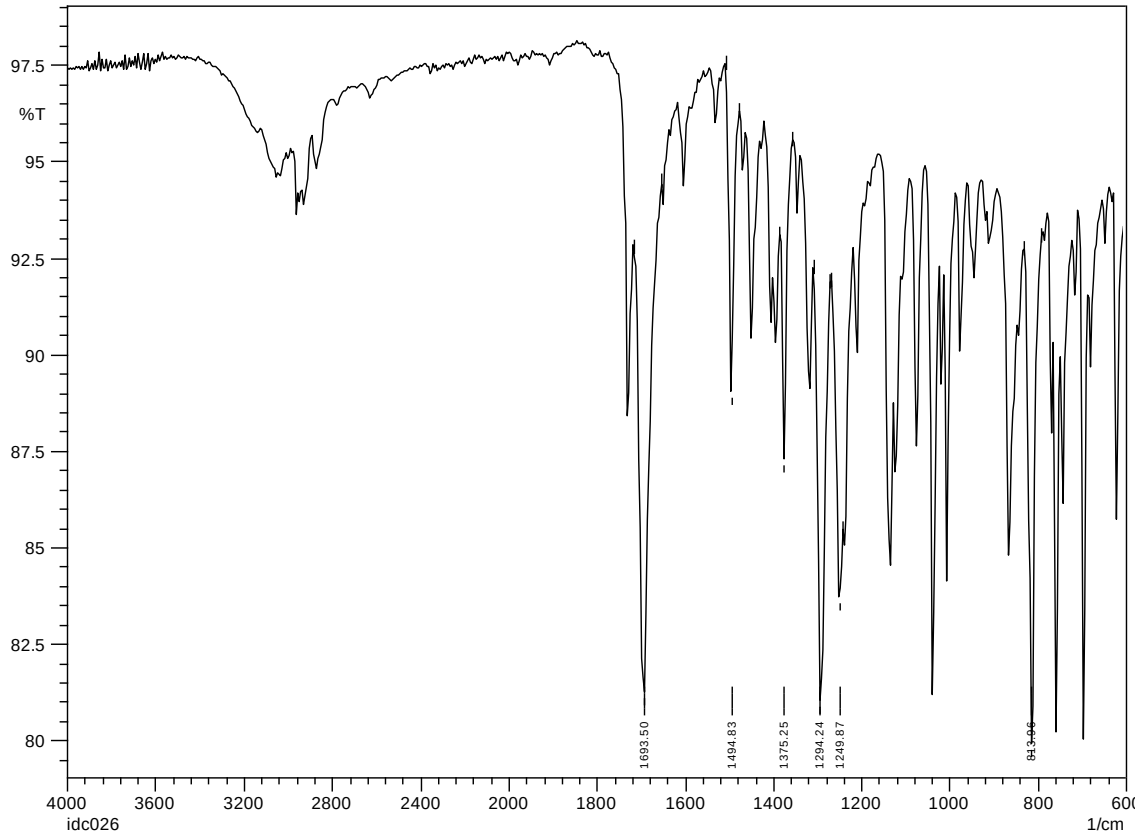
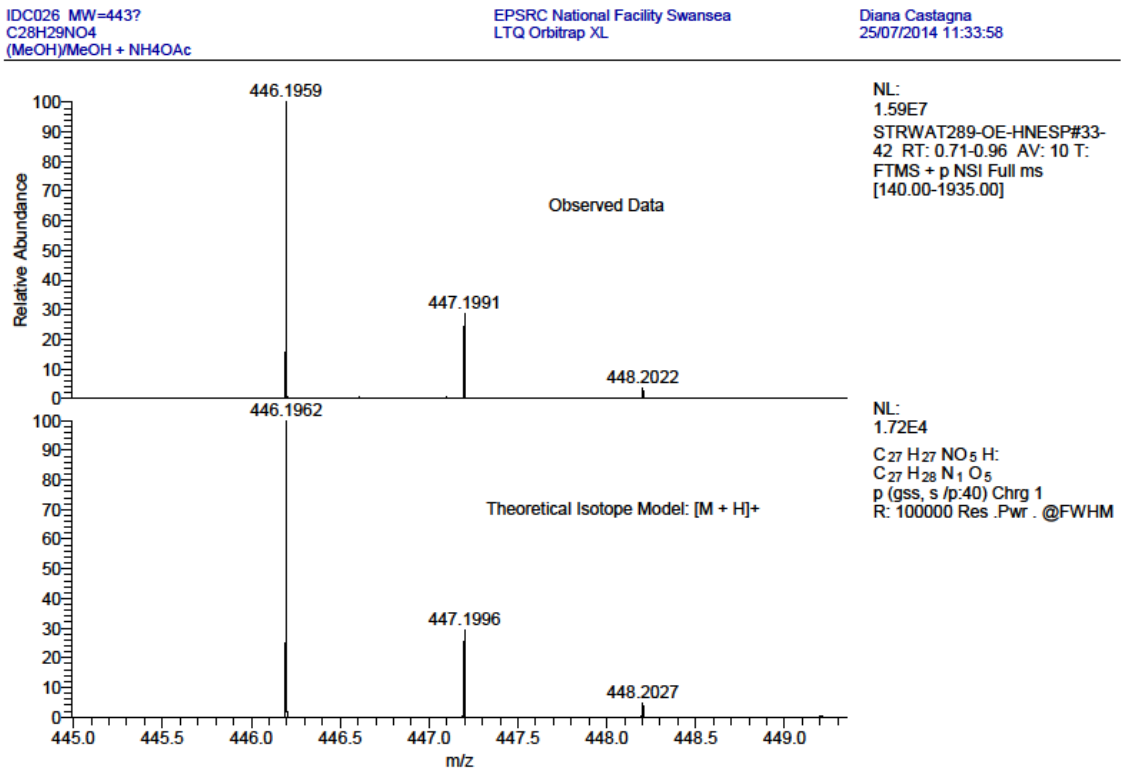


IR of 29

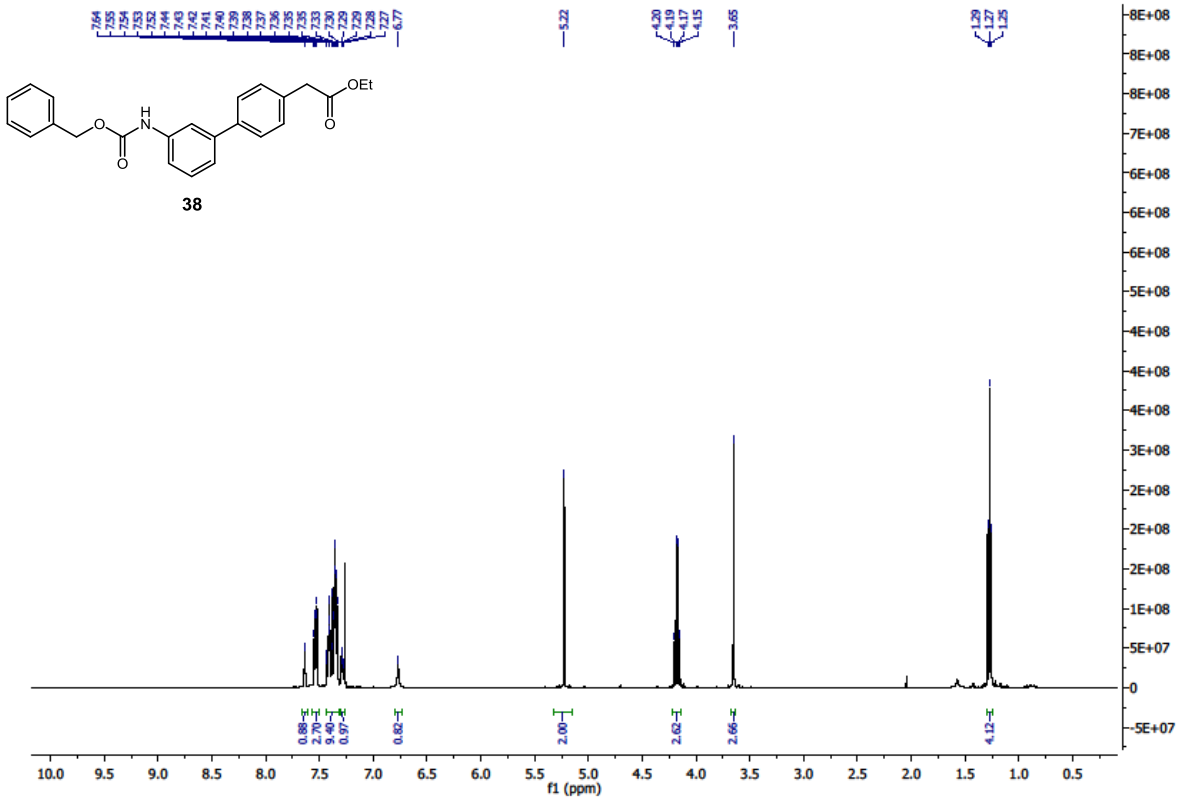


HRMS of 29

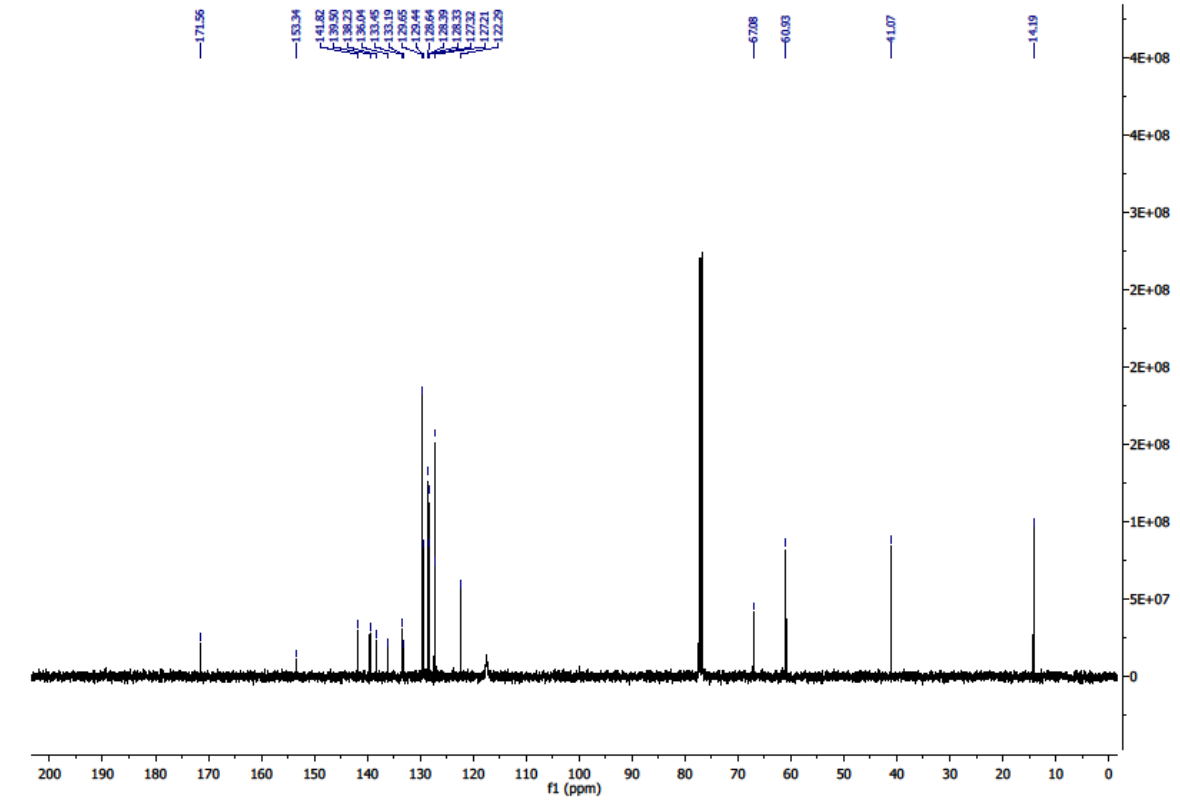


Compound 38

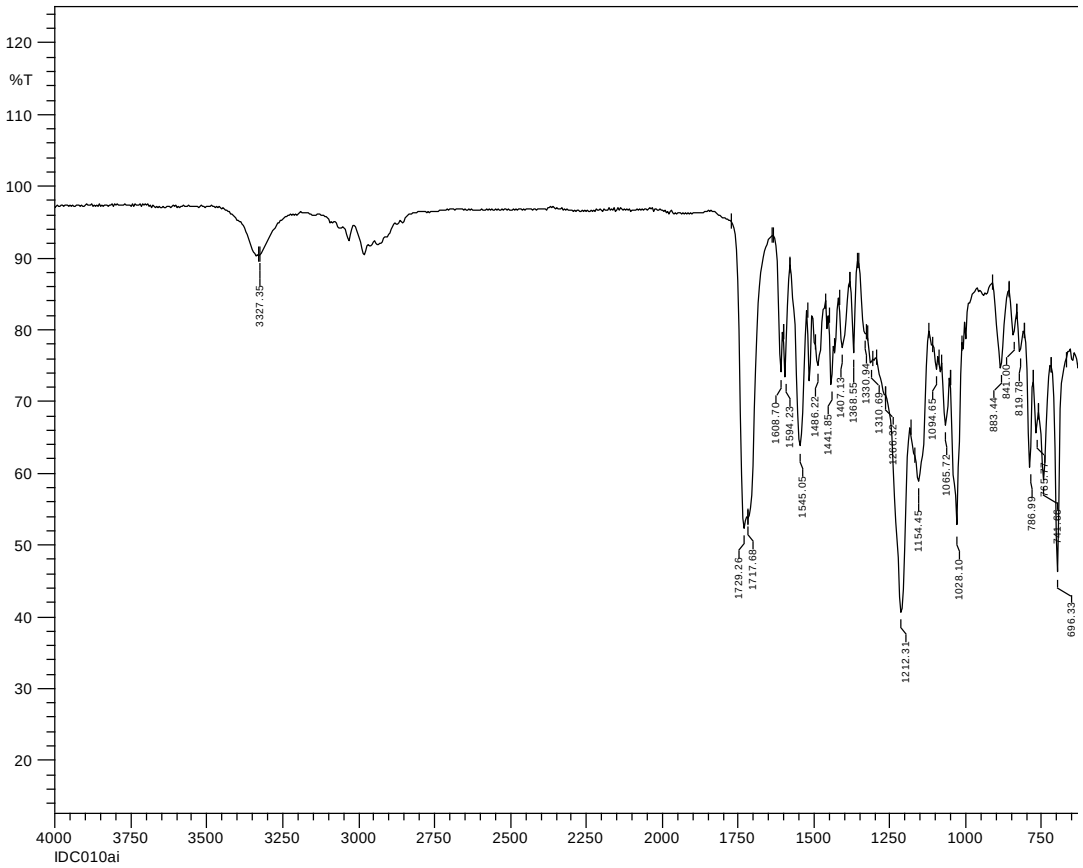
^{1}H NMR



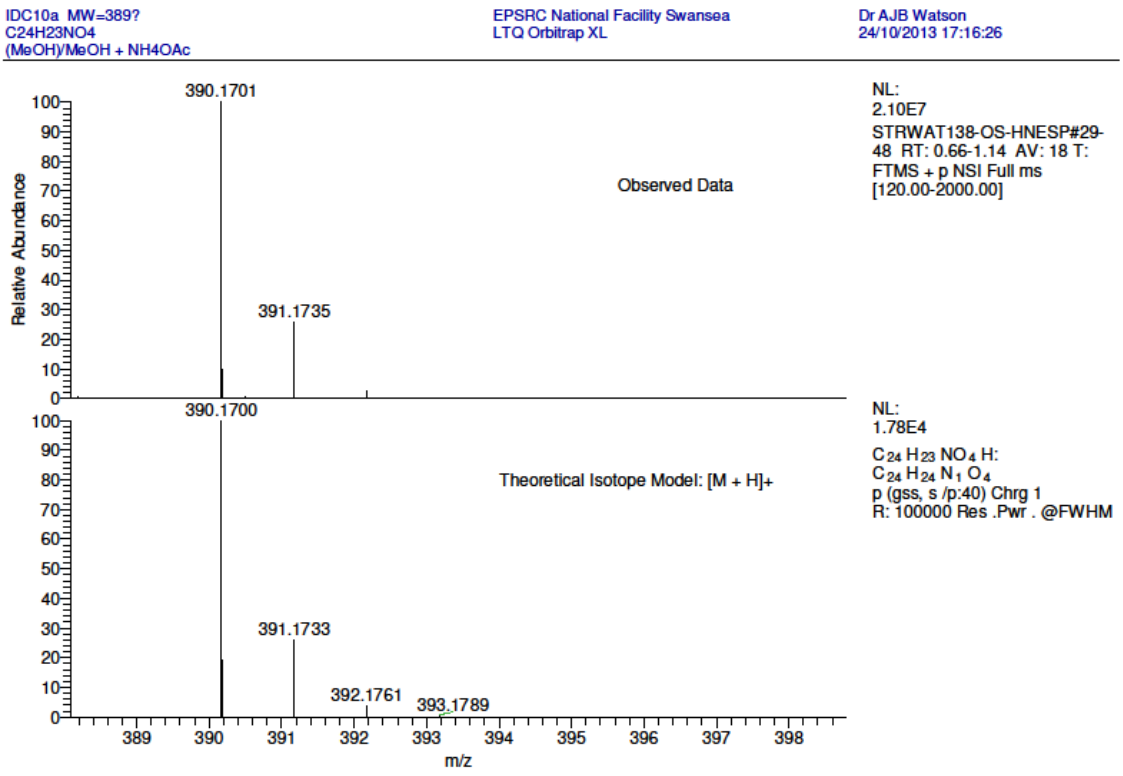
^{13}C NMR of 38



IR of 38

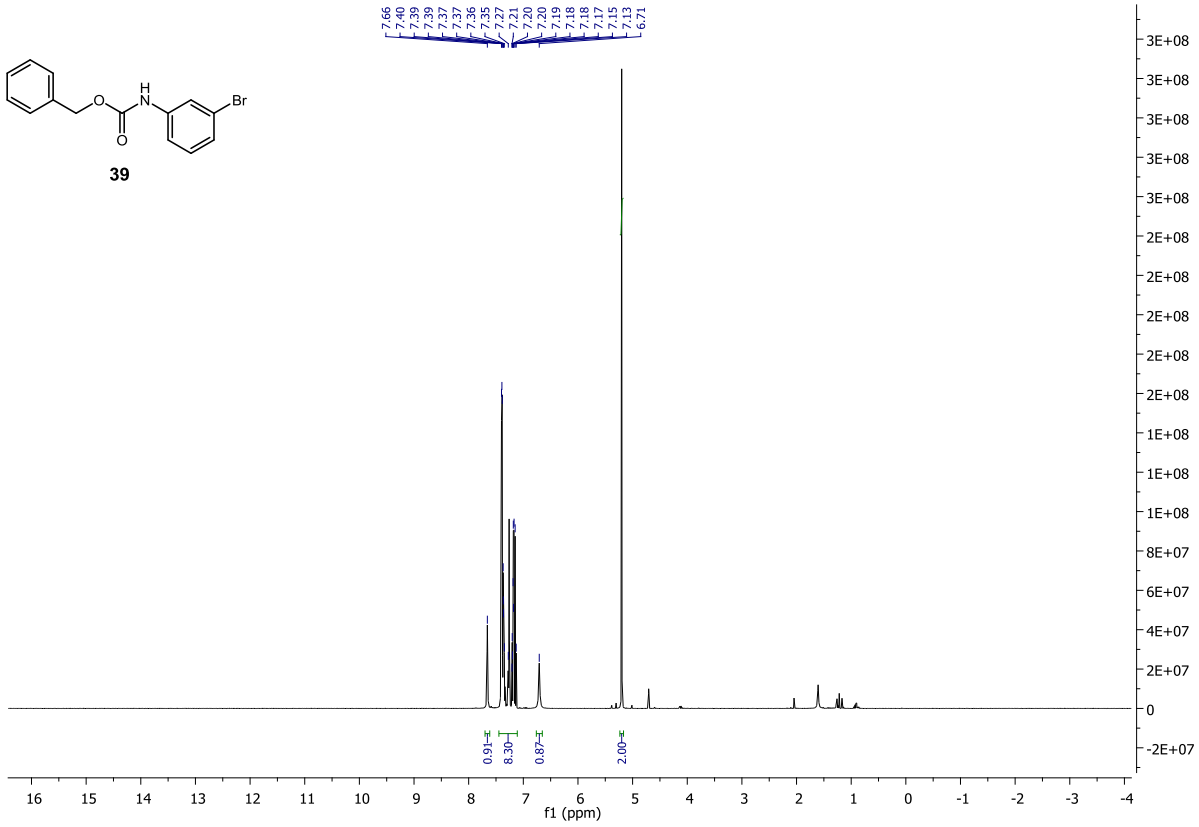


HRMS of 38

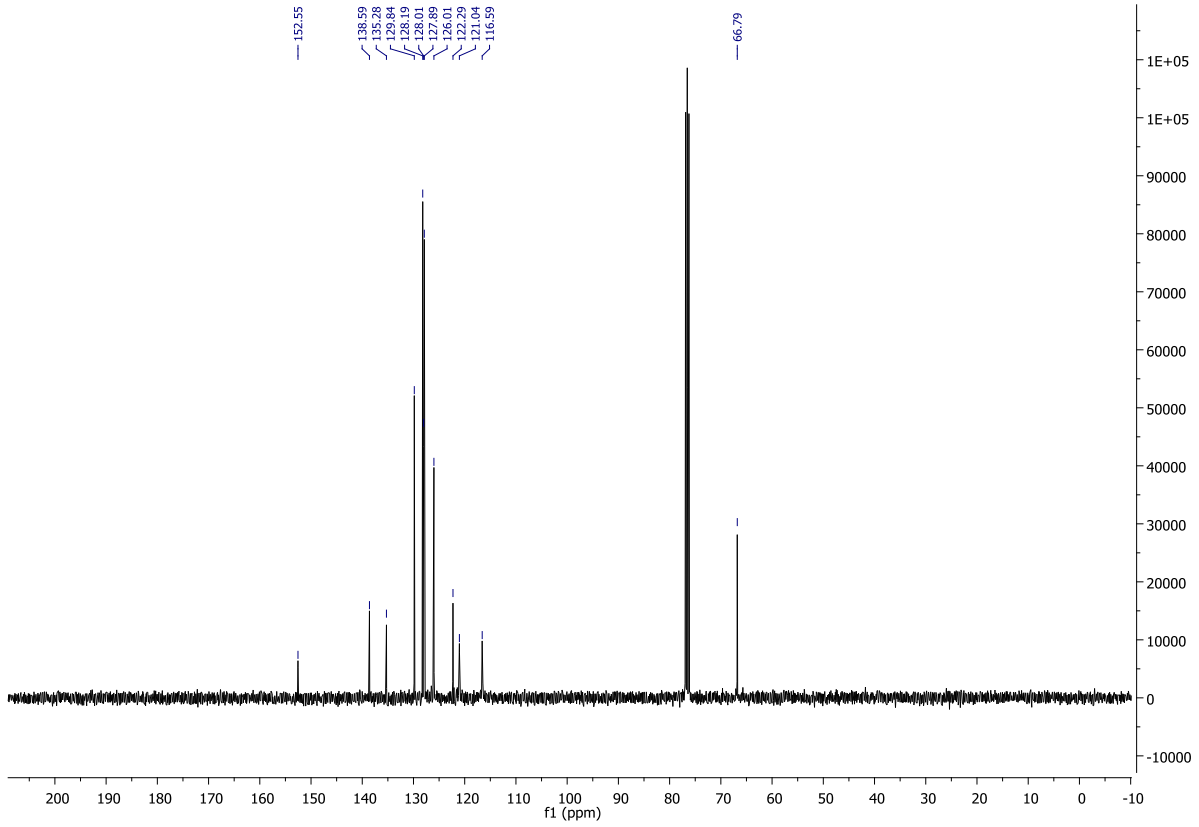


Compound 39

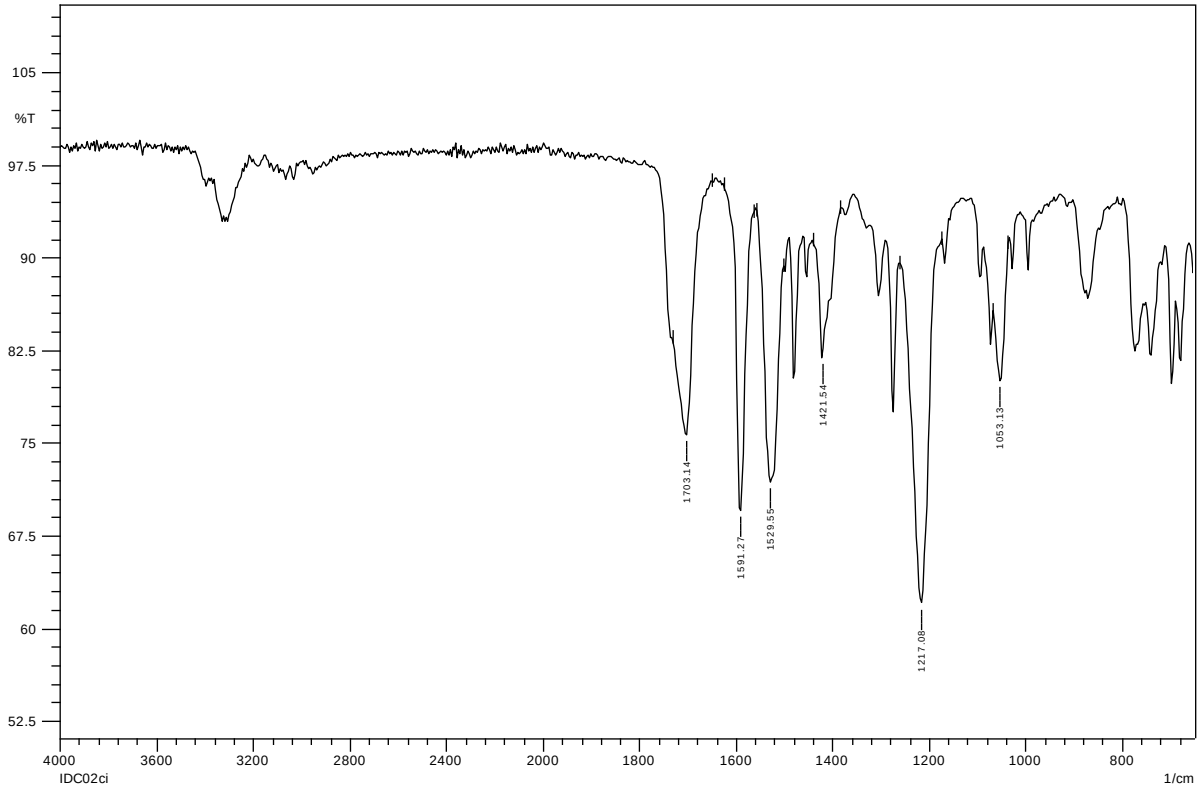
^{1}H NMR



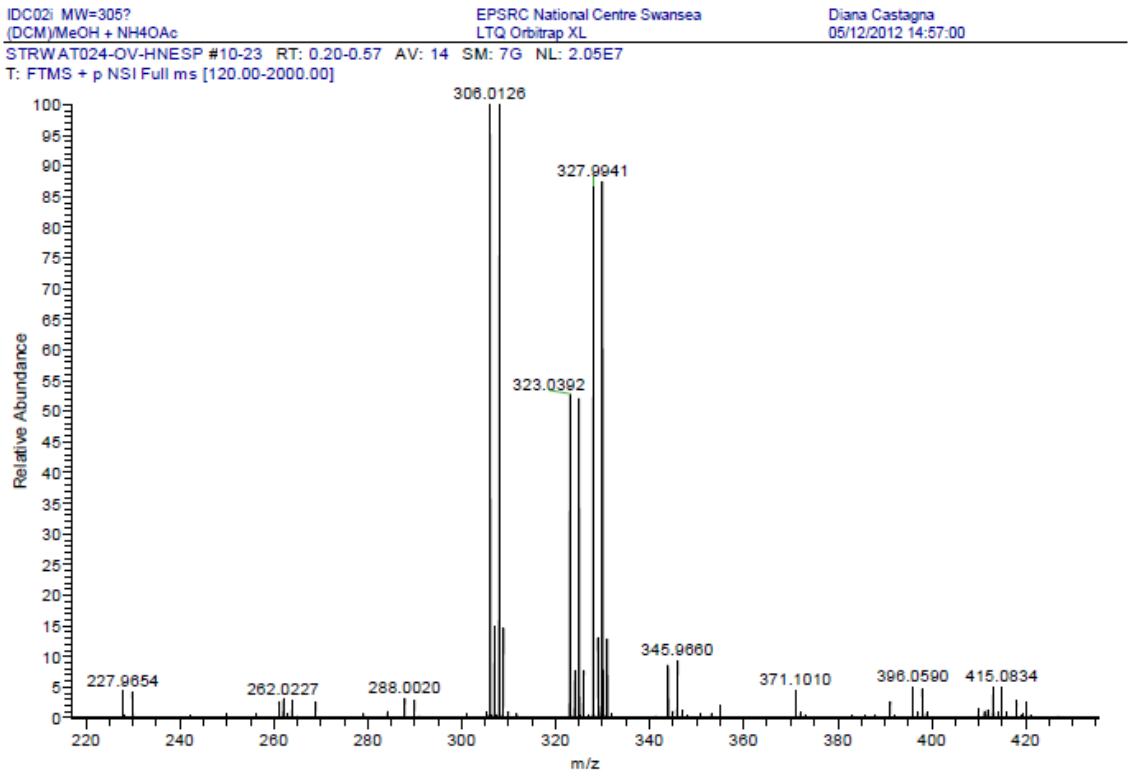
^{13}C NMR of 39



IR of 39

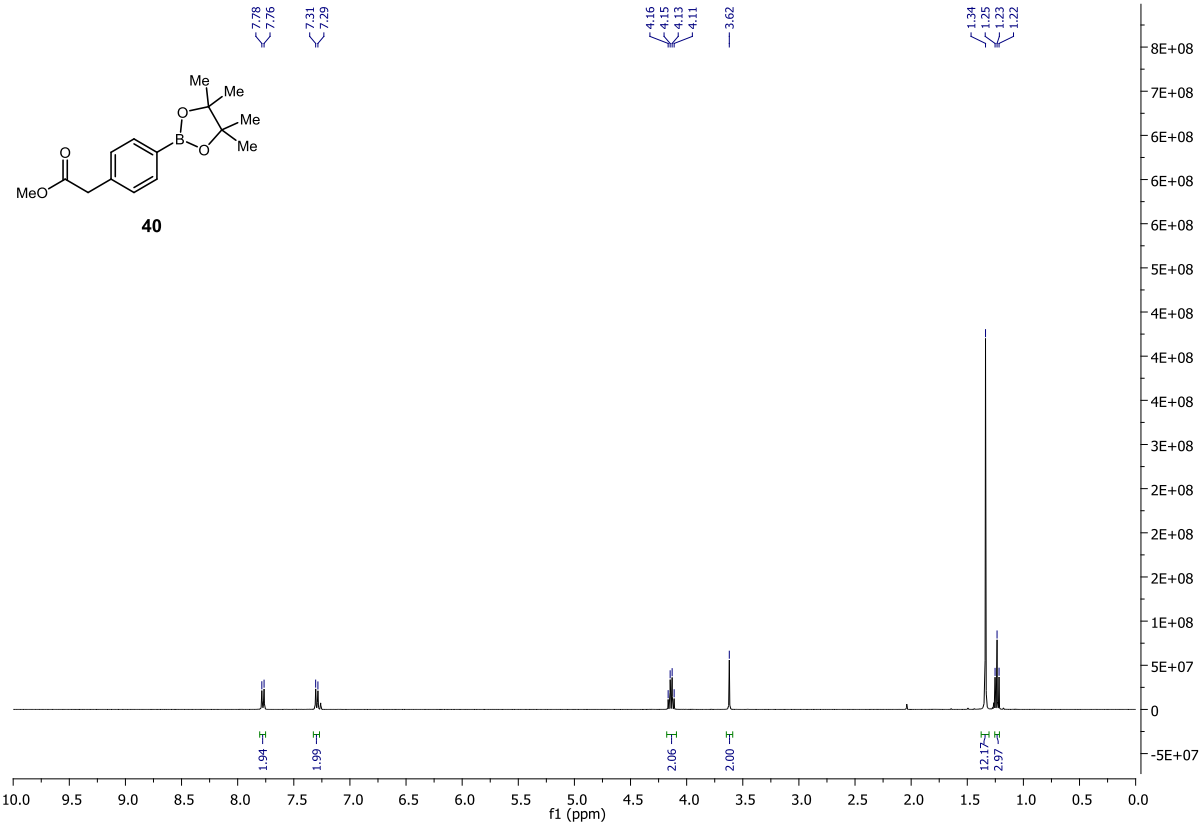


HRMS of 39

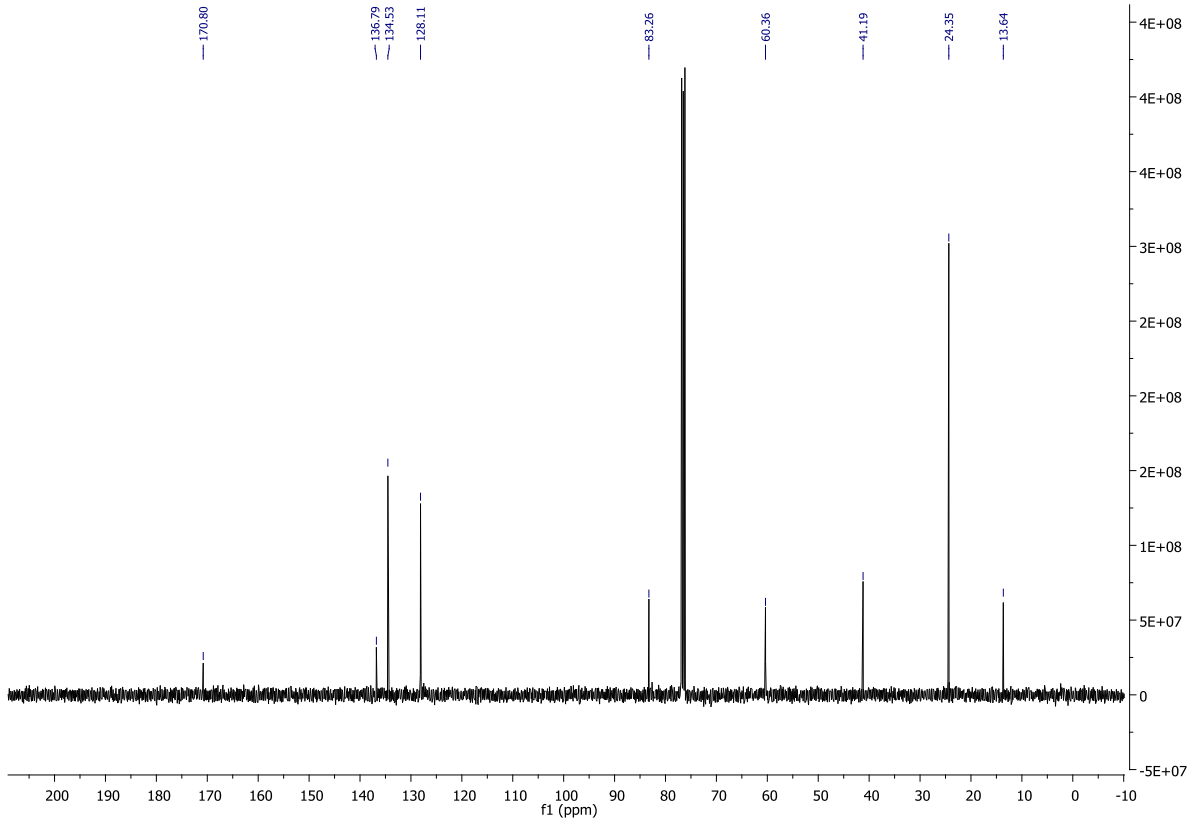


Compound 40

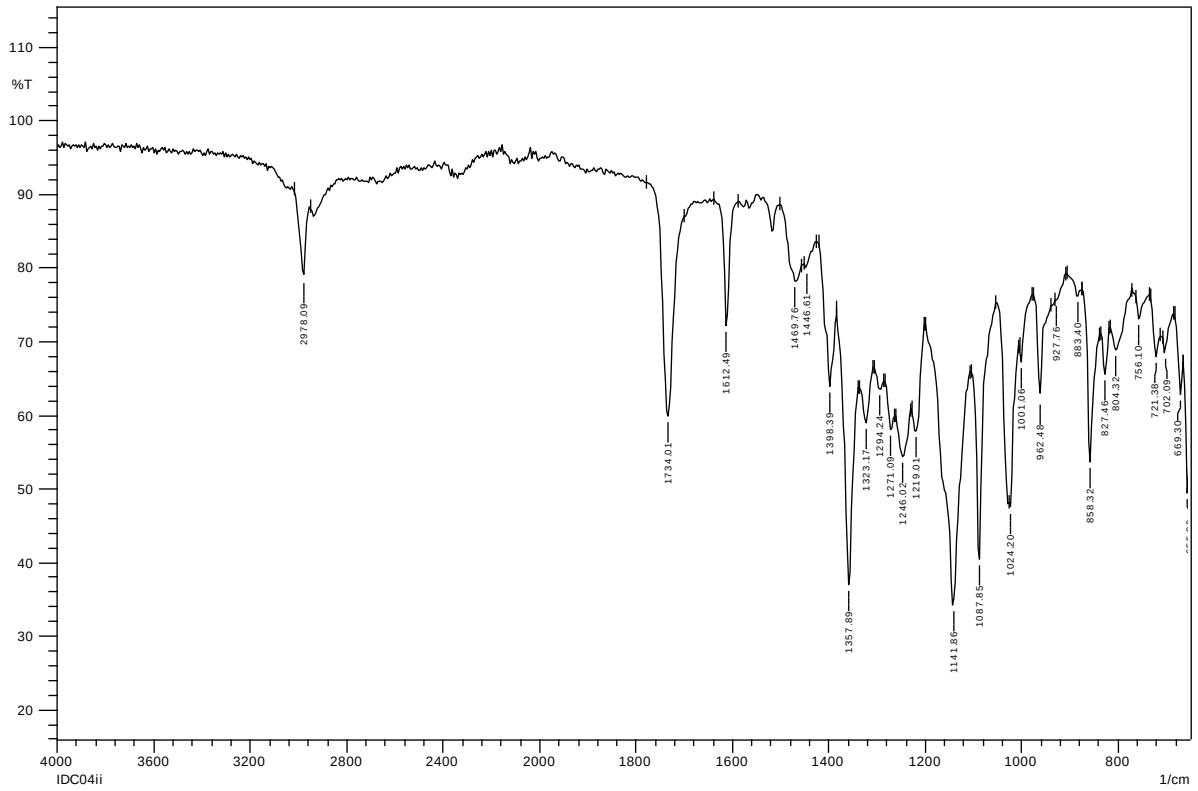
^{1}H NMR



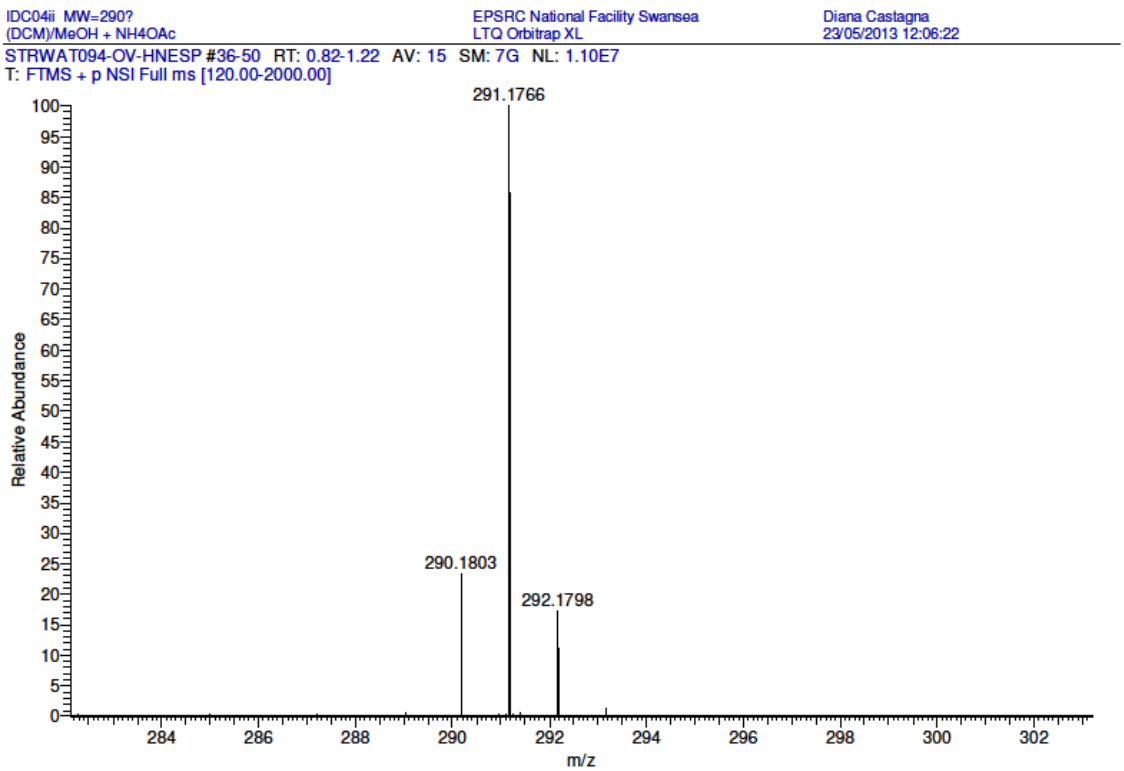
^{13}C NMR of 40



IR of 40

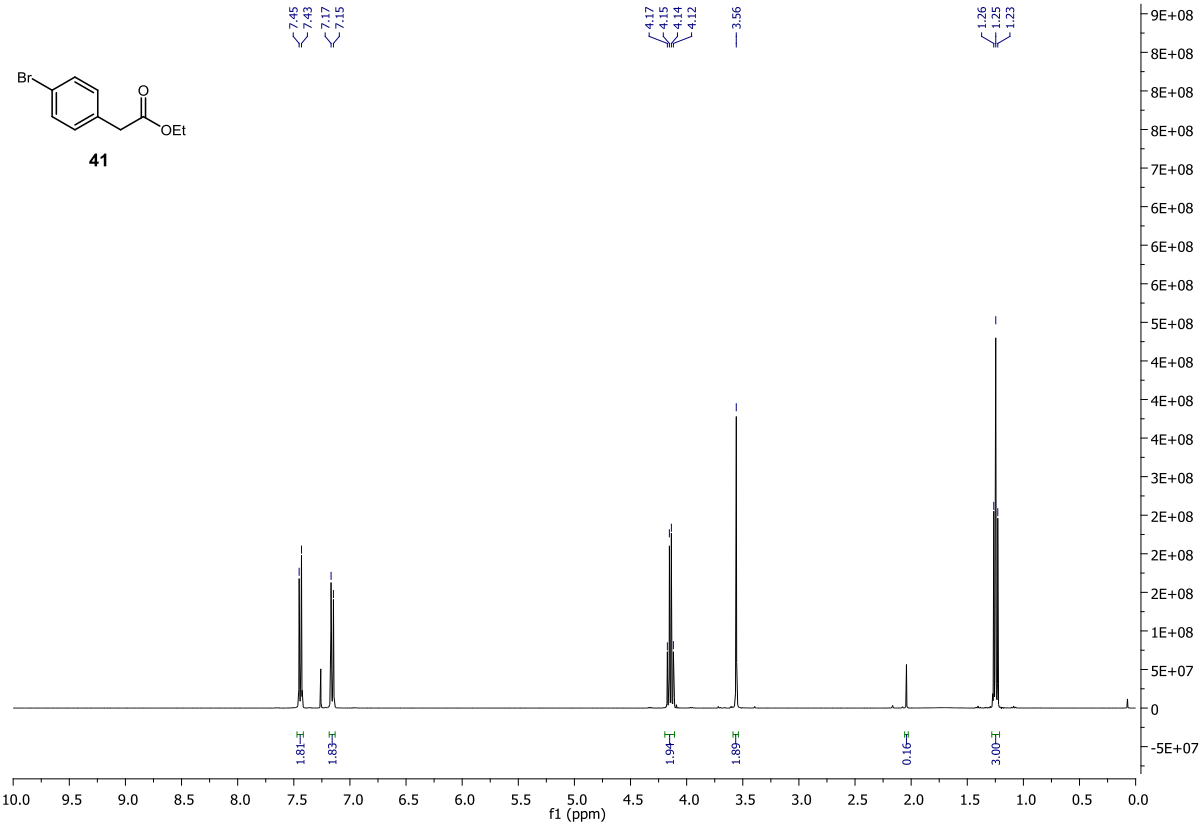


HRMS of 40

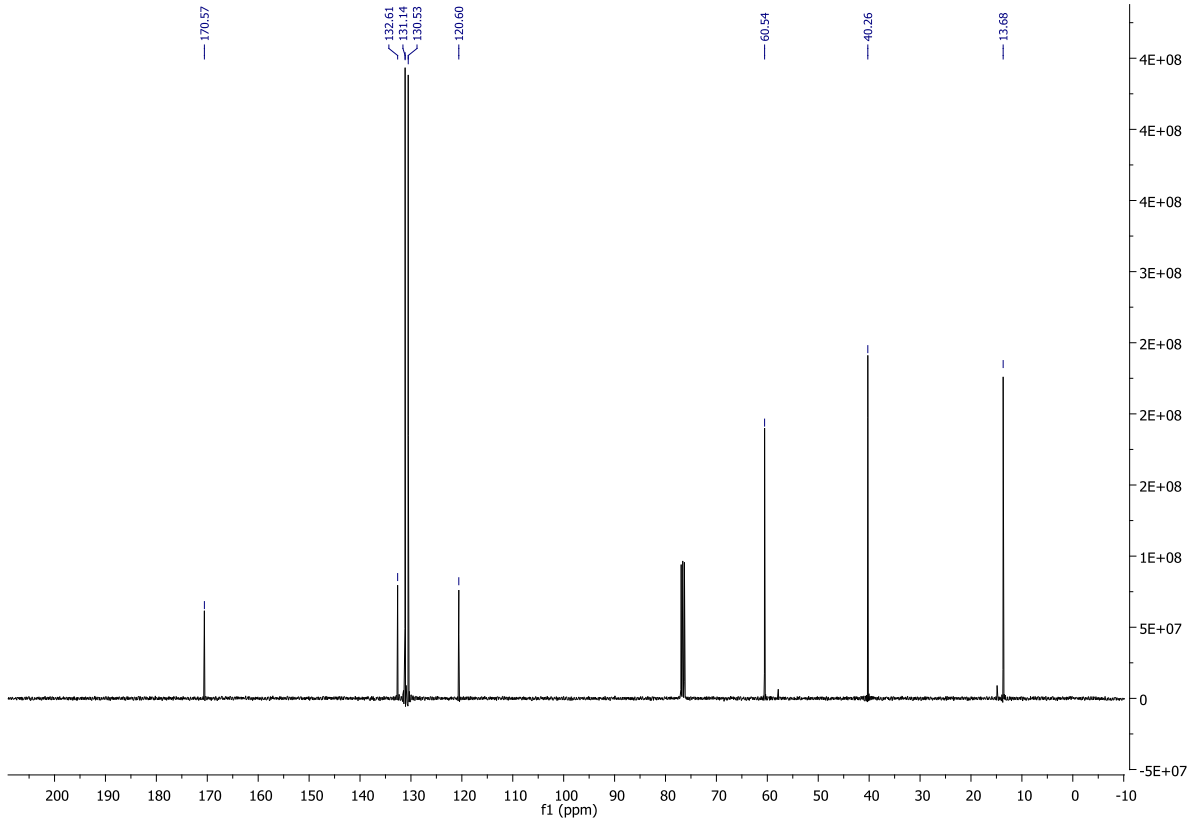


Compound 41

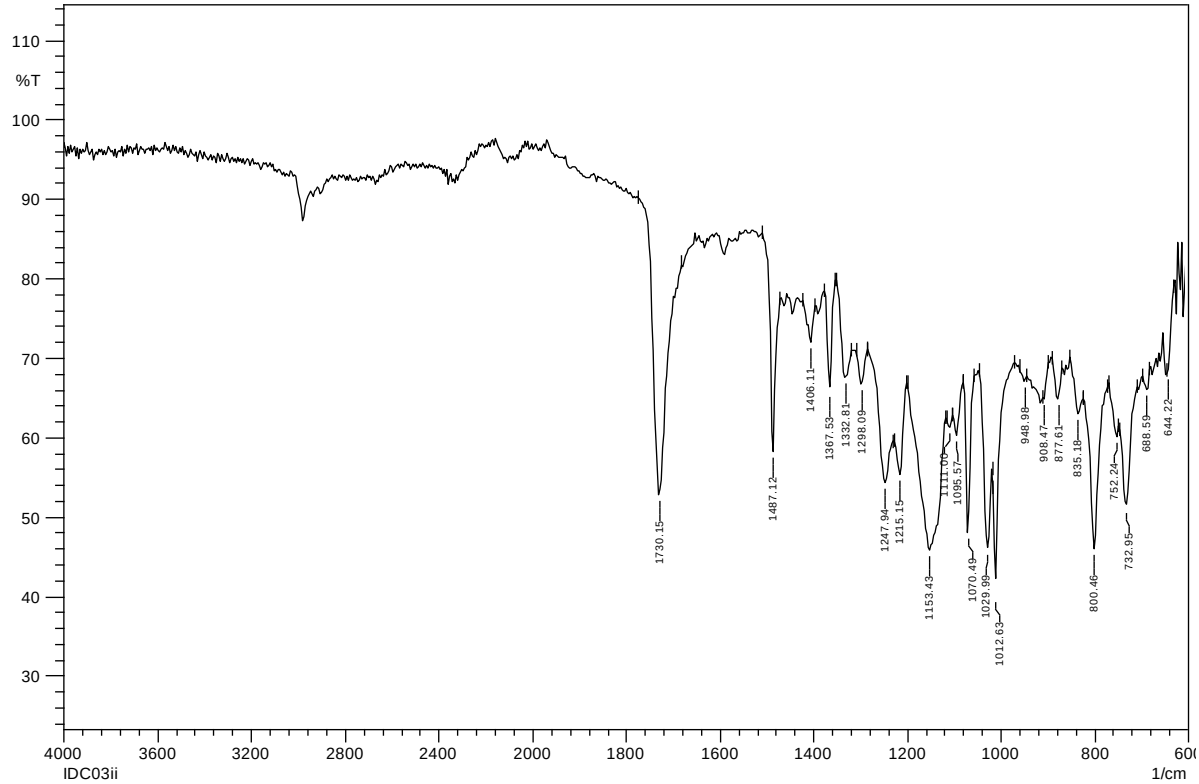
^{1}H NMR



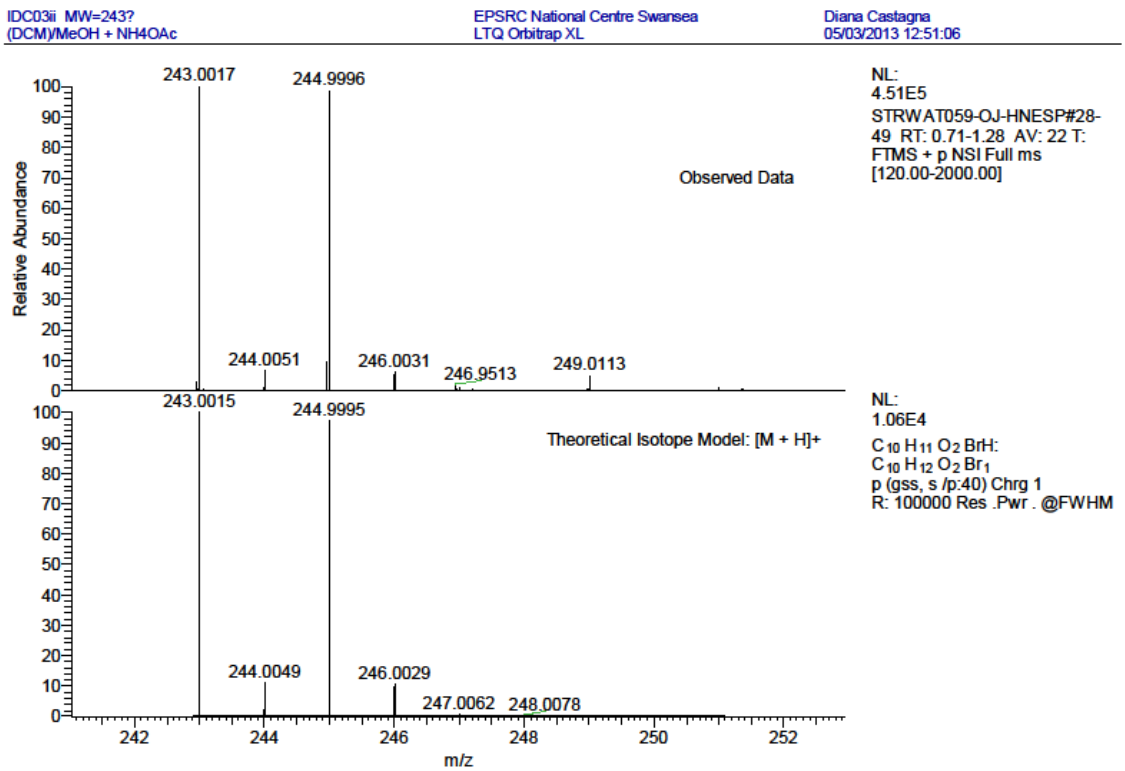
^{13}C NMR of 41



IR of 41

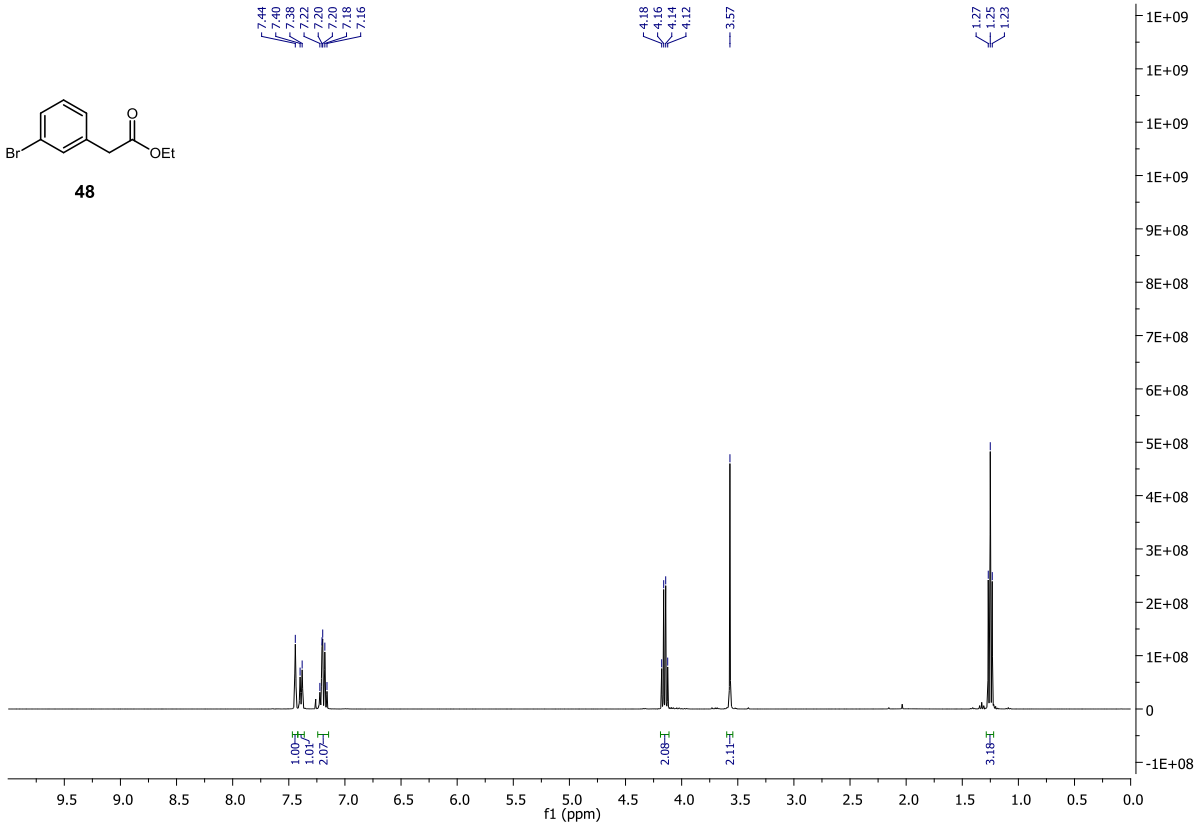


HRMS of 41

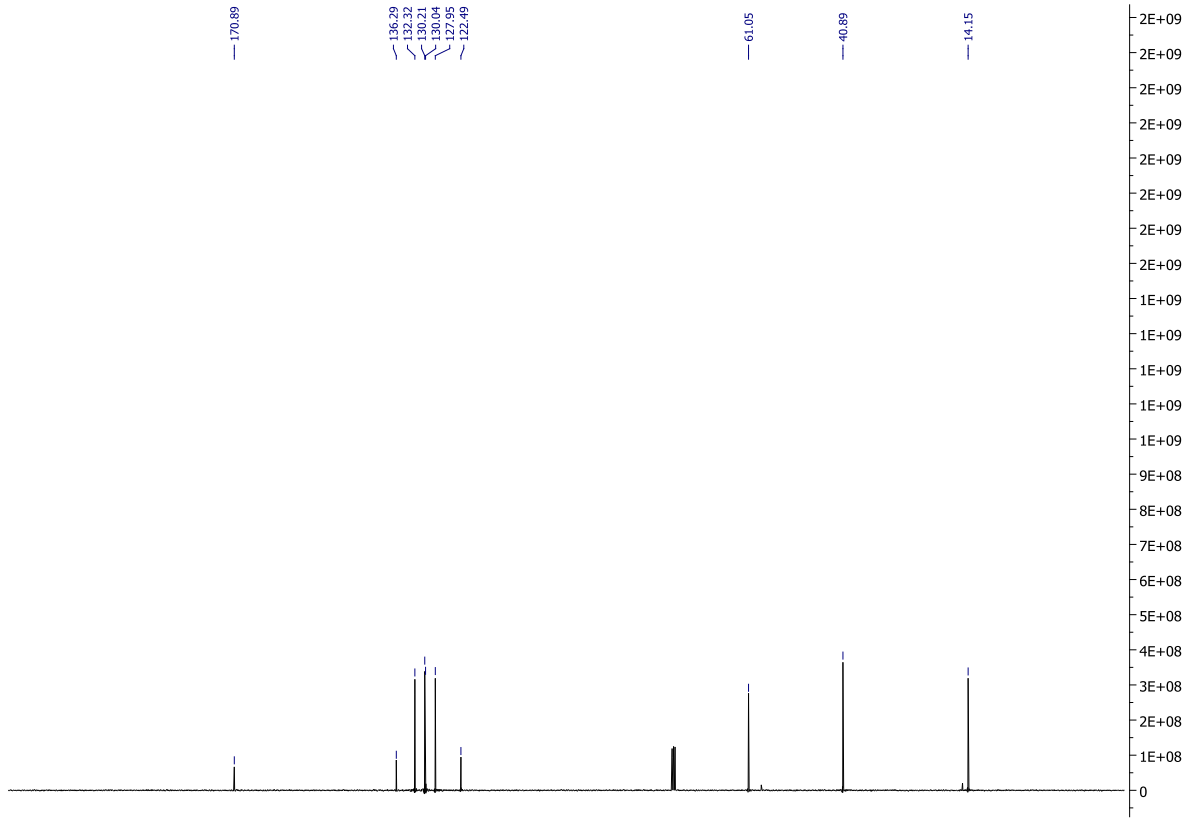


Compound 48

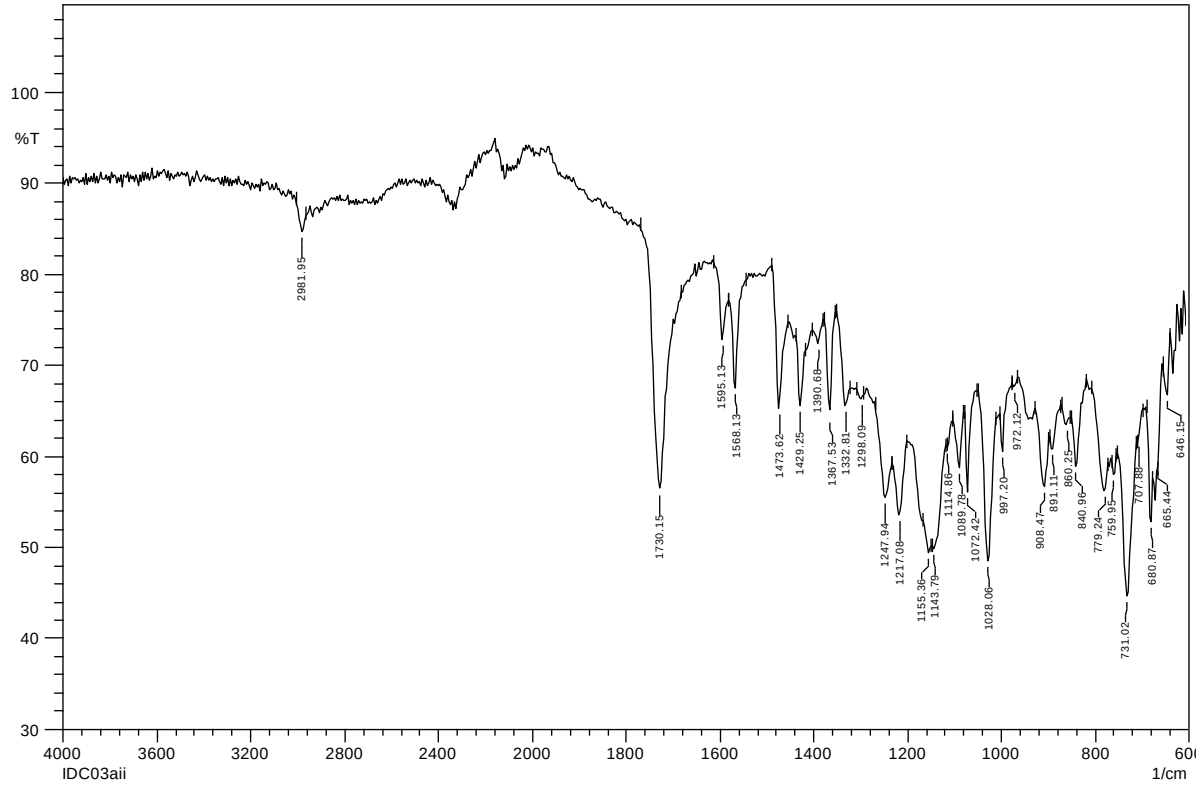
^{1}H NMR



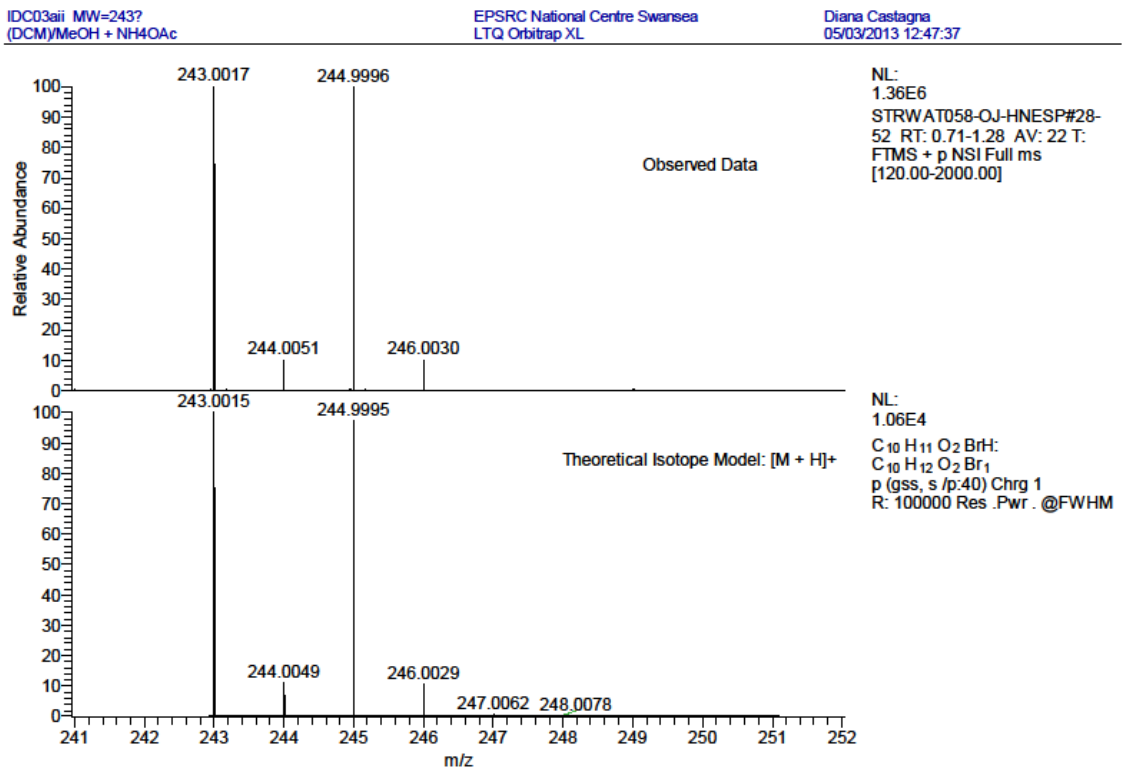
^{13}C NMR of 48



IR of 48

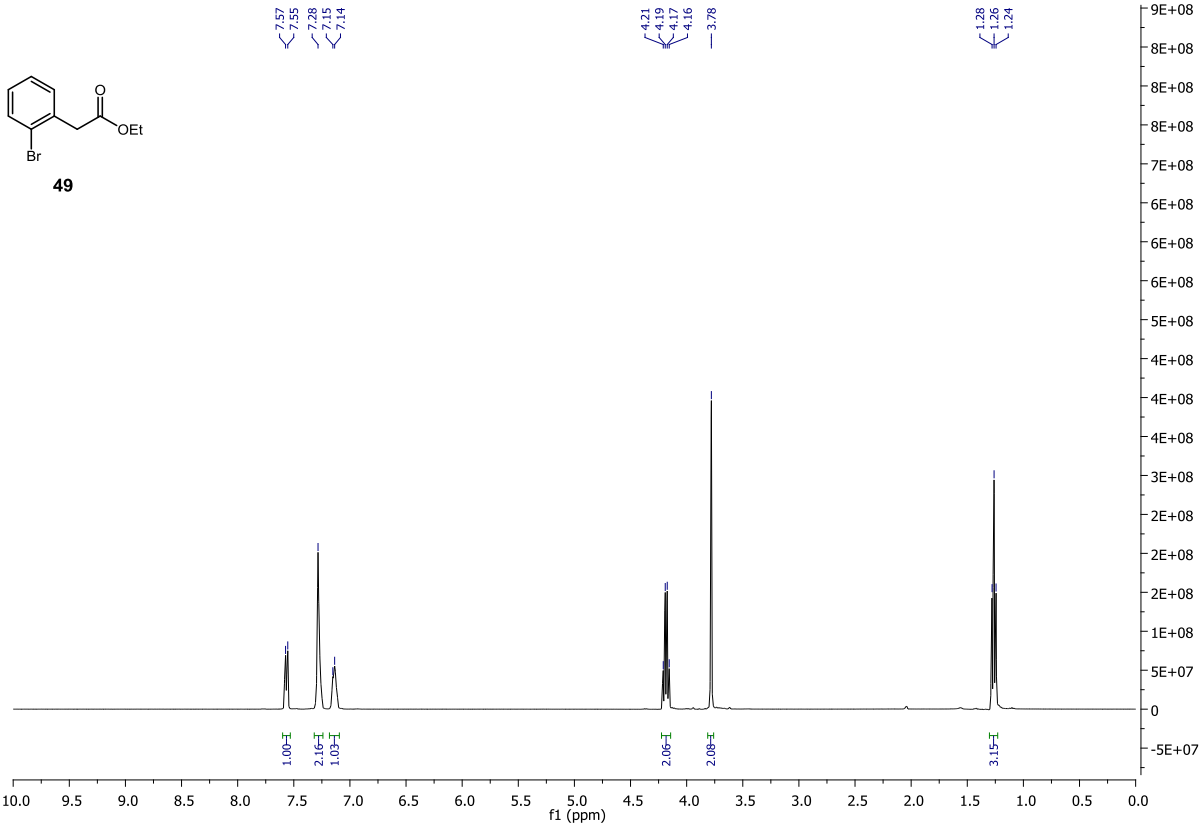


HRMS of 48

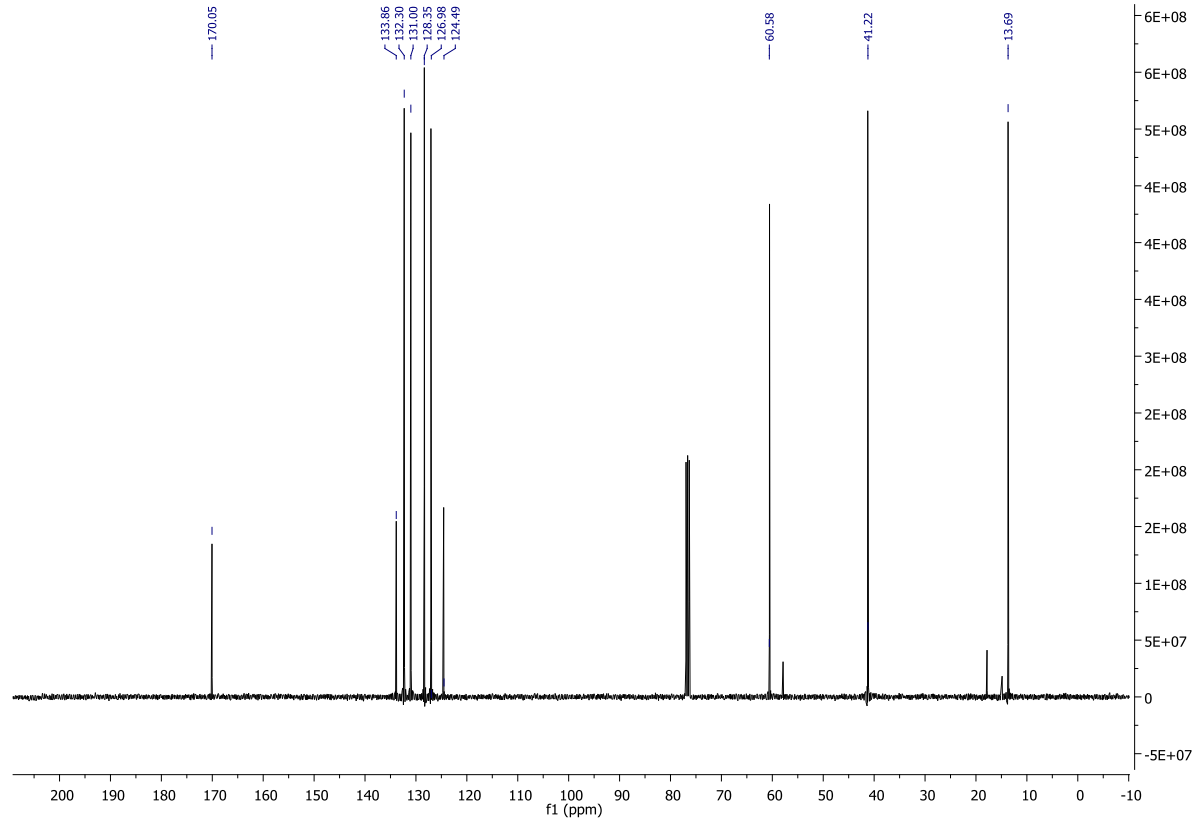


Compound 49

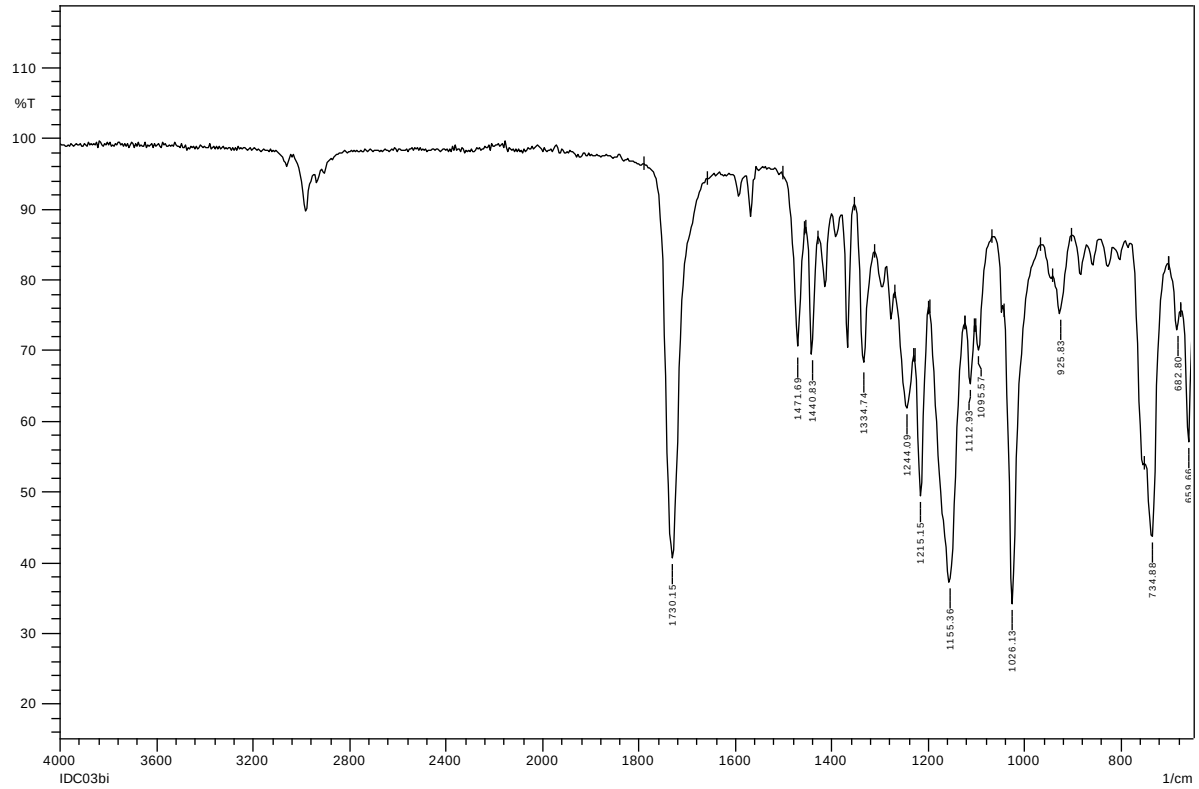
^{1}H NMR



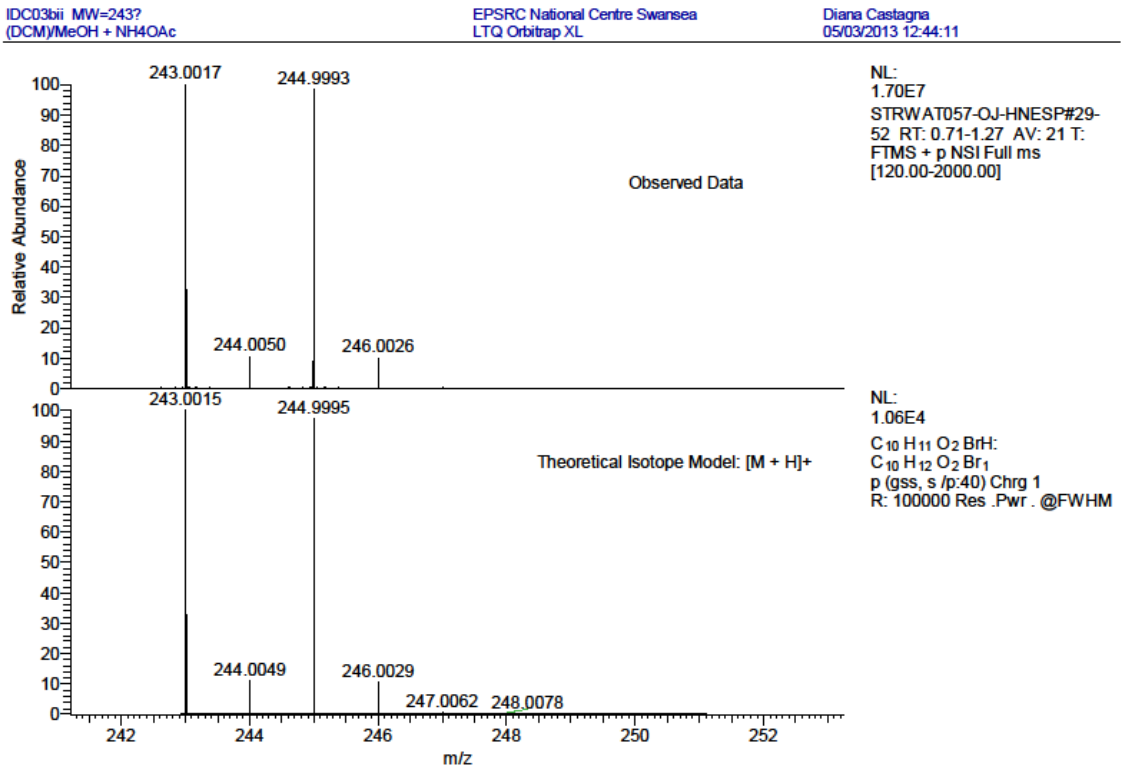
^{13}C NMR of 49



IR of 49

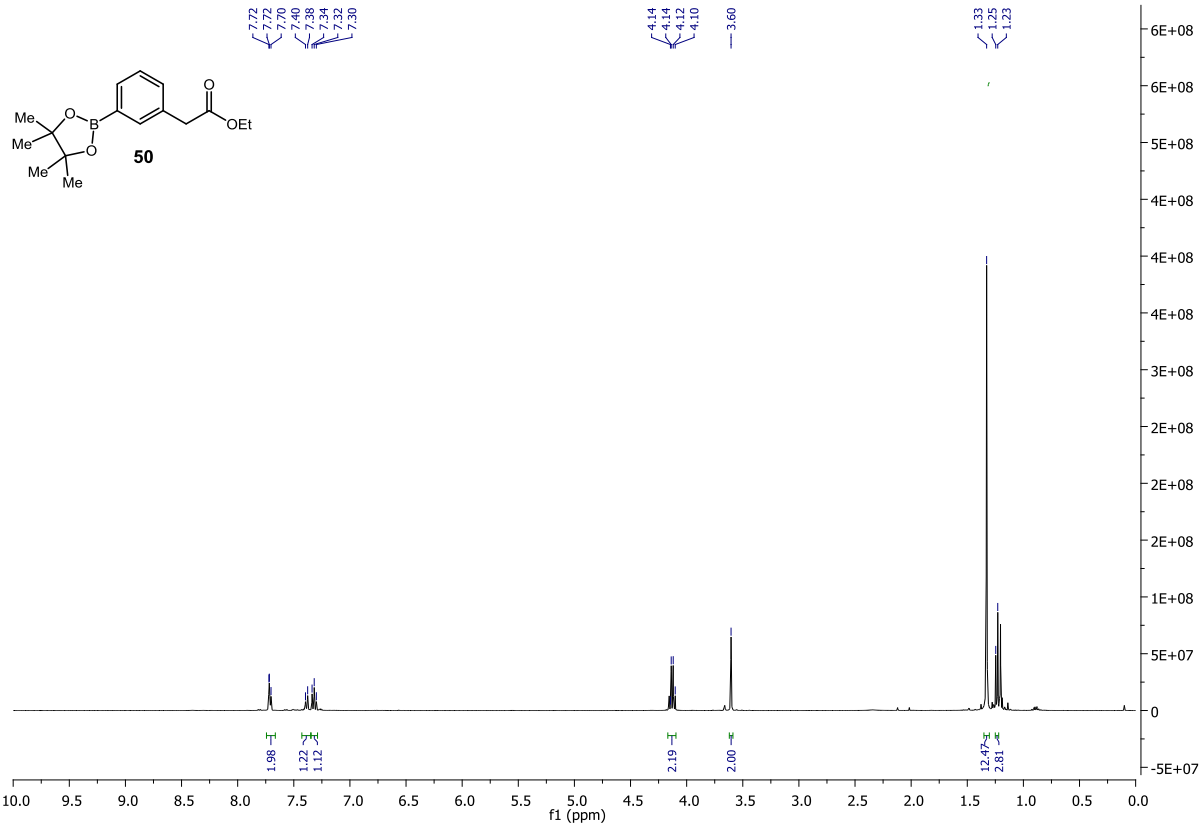


HRMS of 49

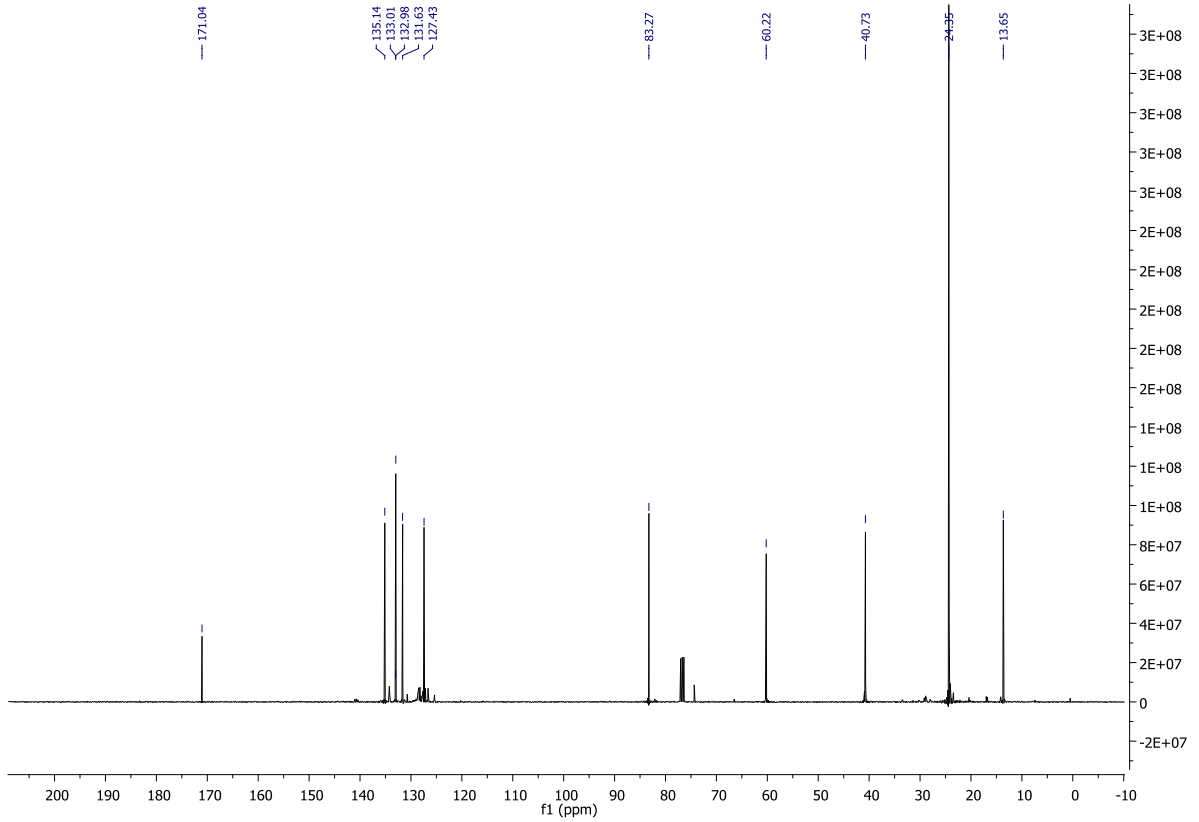


Compound 50

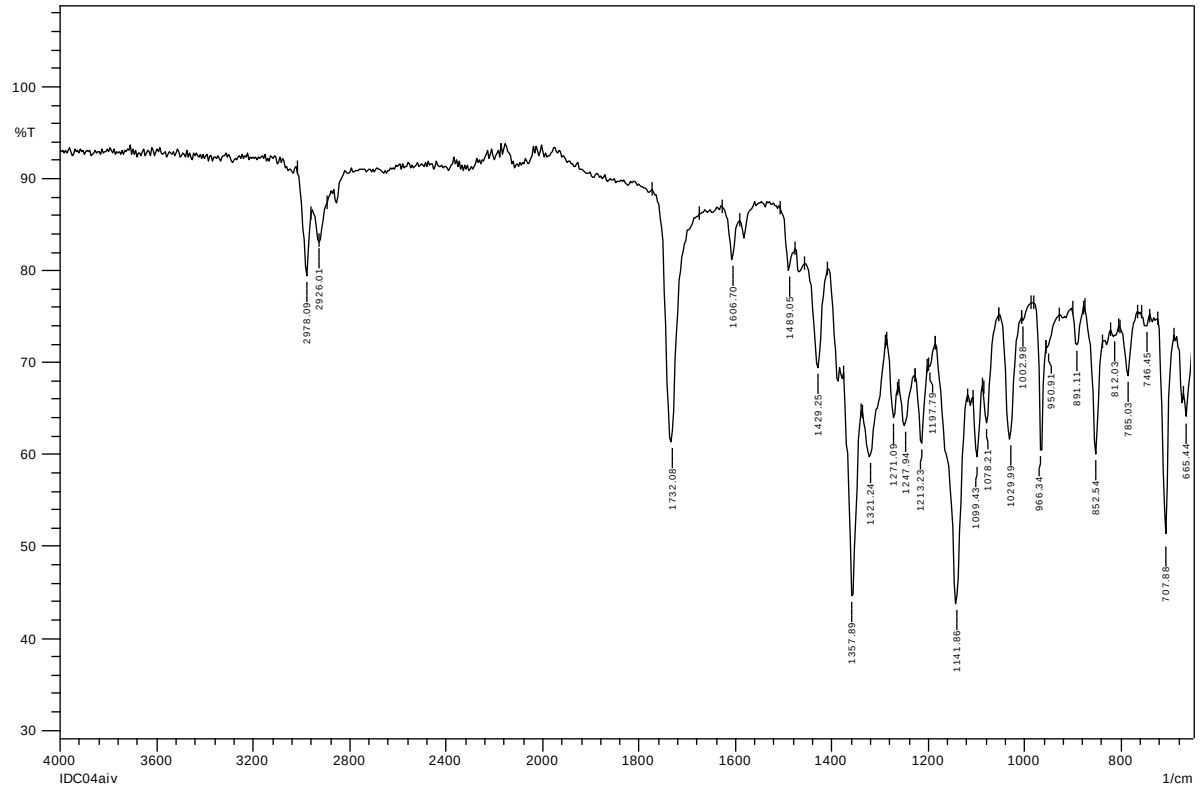
^{1}H NMR



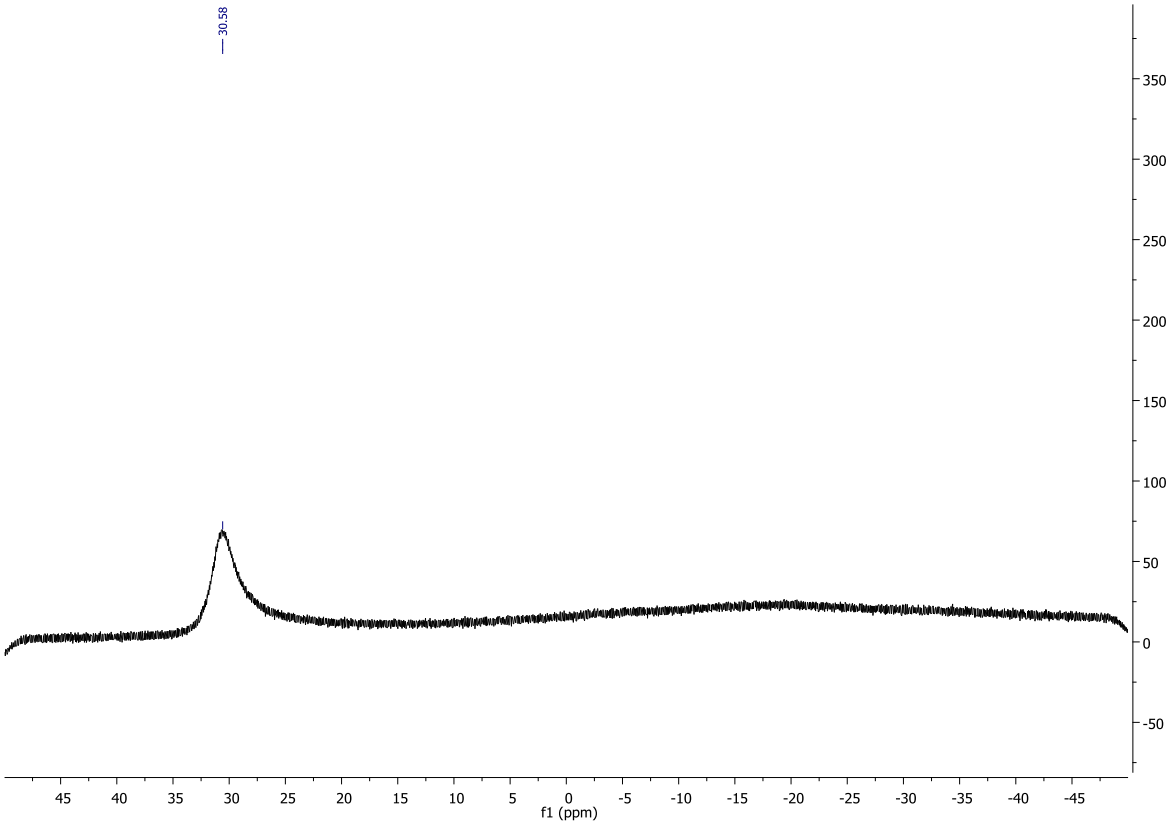
^{13}C NMR of 50



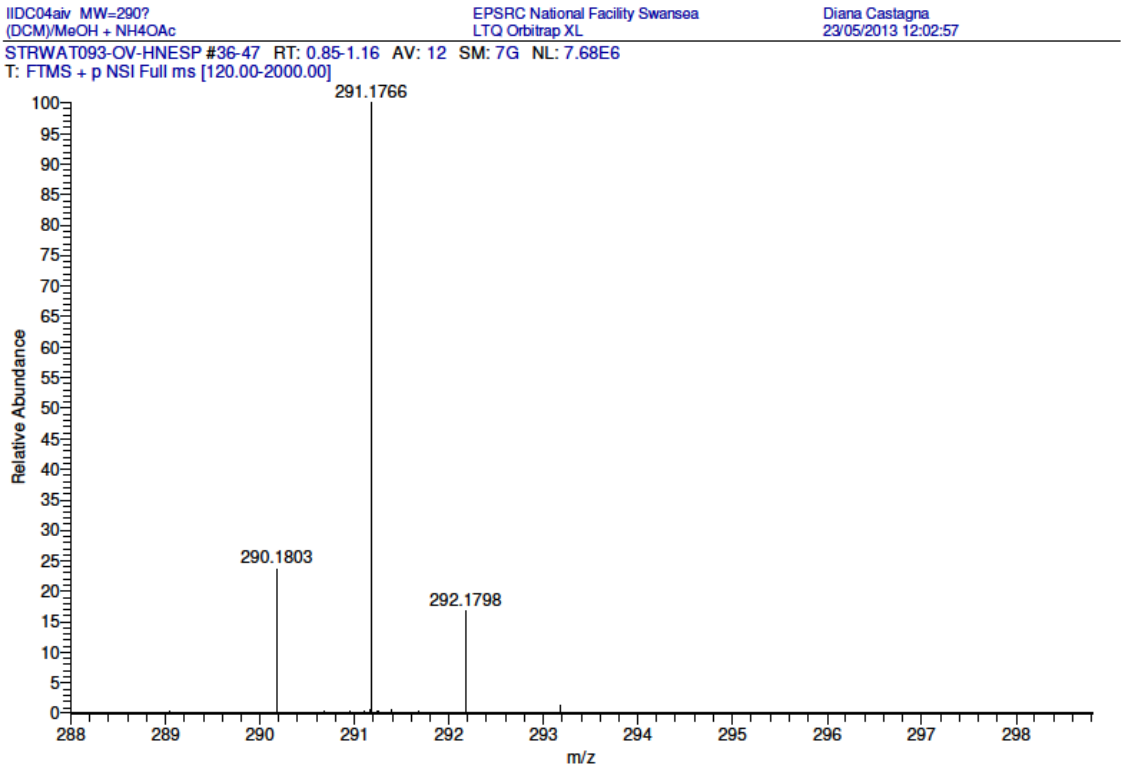
IR of 50



^{1}B NMR of 50

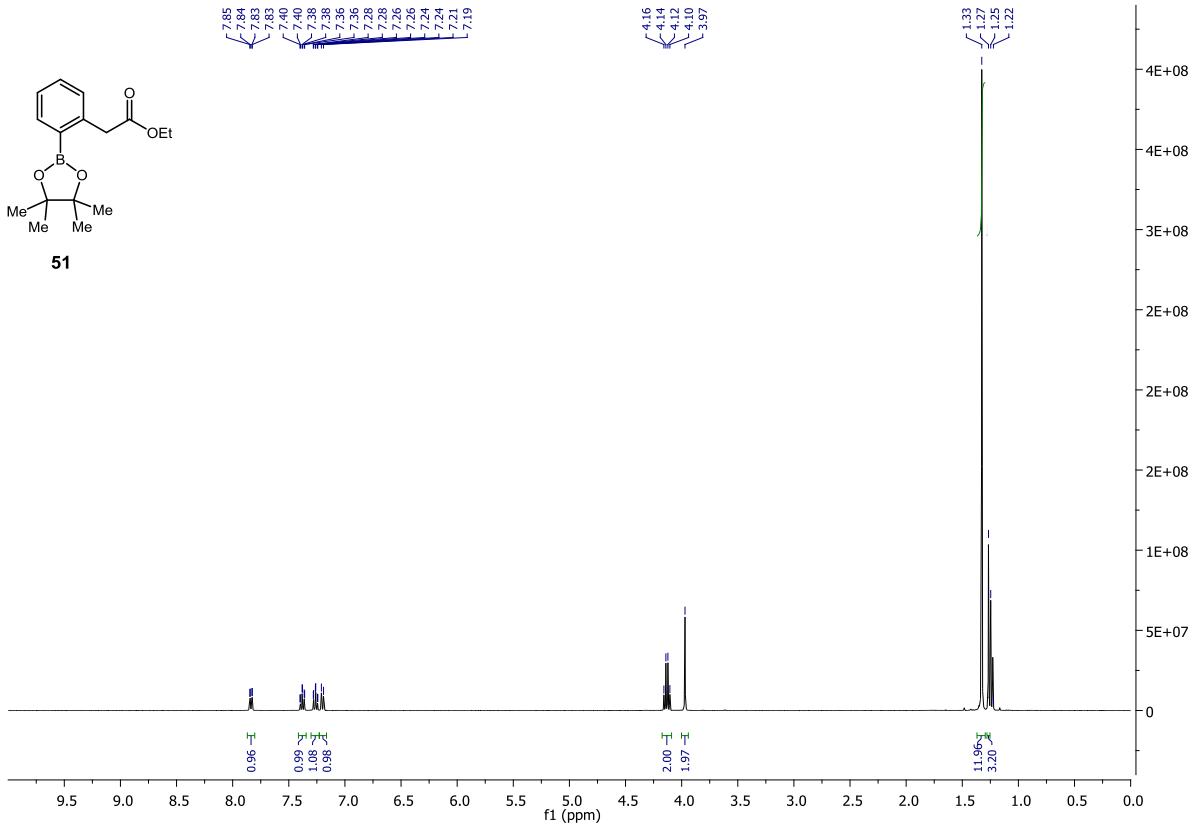


HRMS of 50

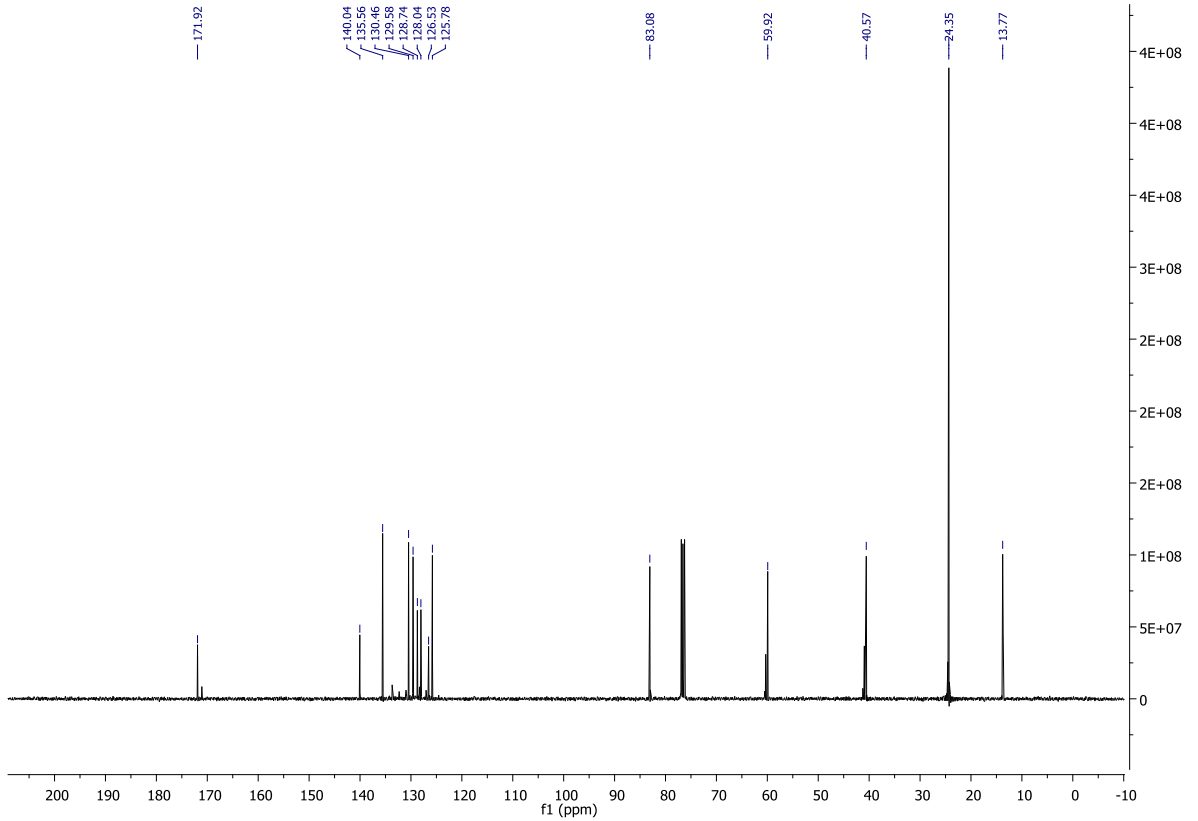

IIDC04aiv MW=290?
(DCM)/MeOH + NH4OAc
EPSRC National Facility Swansea
LTQ Orbitrap XL
Diana Castagna
23/05/2013 12:02:57
STRWAT093-OV-HNESP #36-47 RT: 0.85-1.16 AV: 12 SM: 7G NL: 7.68E6
T: FTMS + p NSI Full ms [120.00-2000.00]
291.1766
290.1803
292.1798
Relative Abundance
m/z

Compound 51

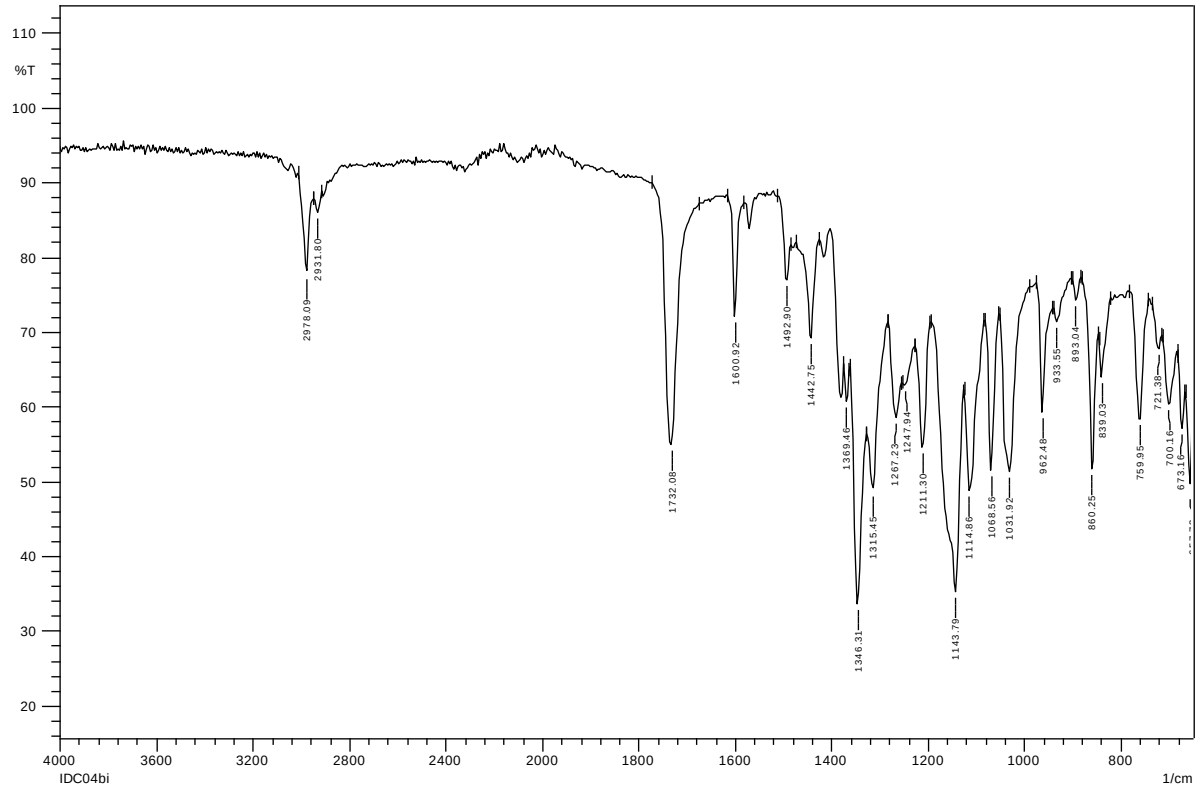
^{1}H NMR



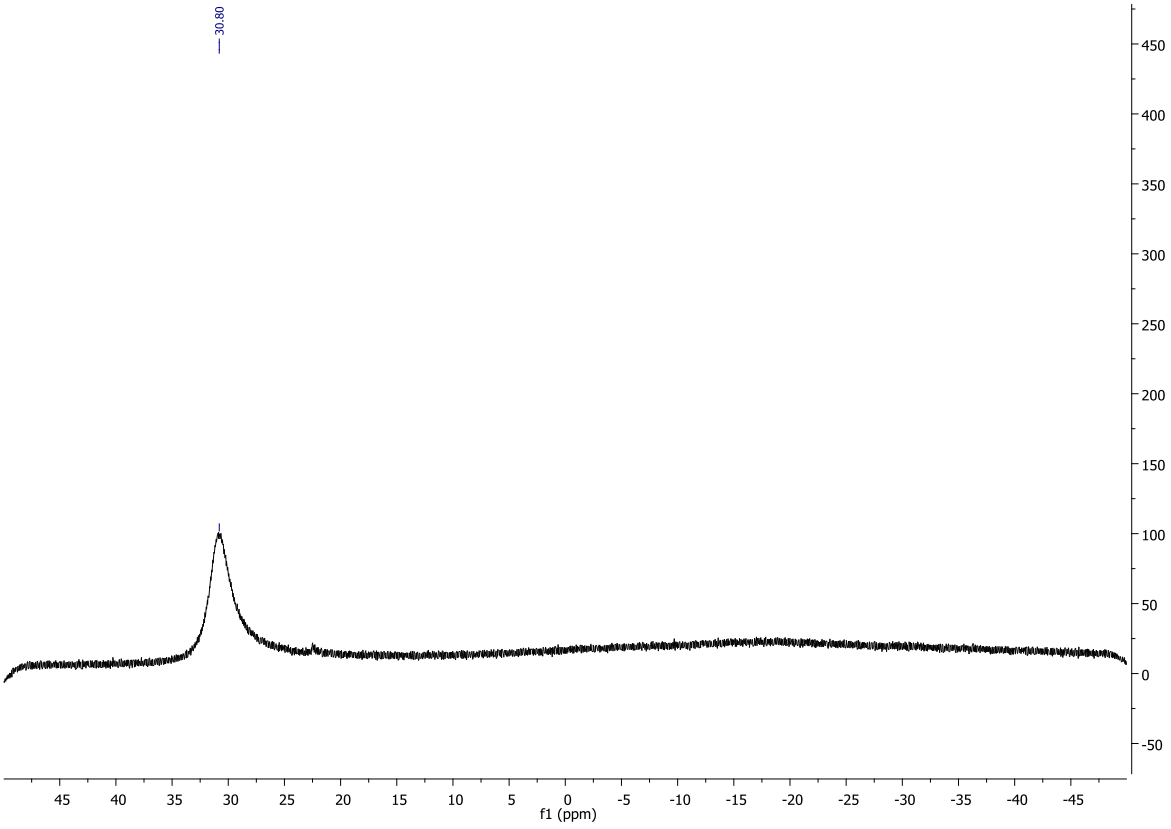
^{13}C NMR of 51



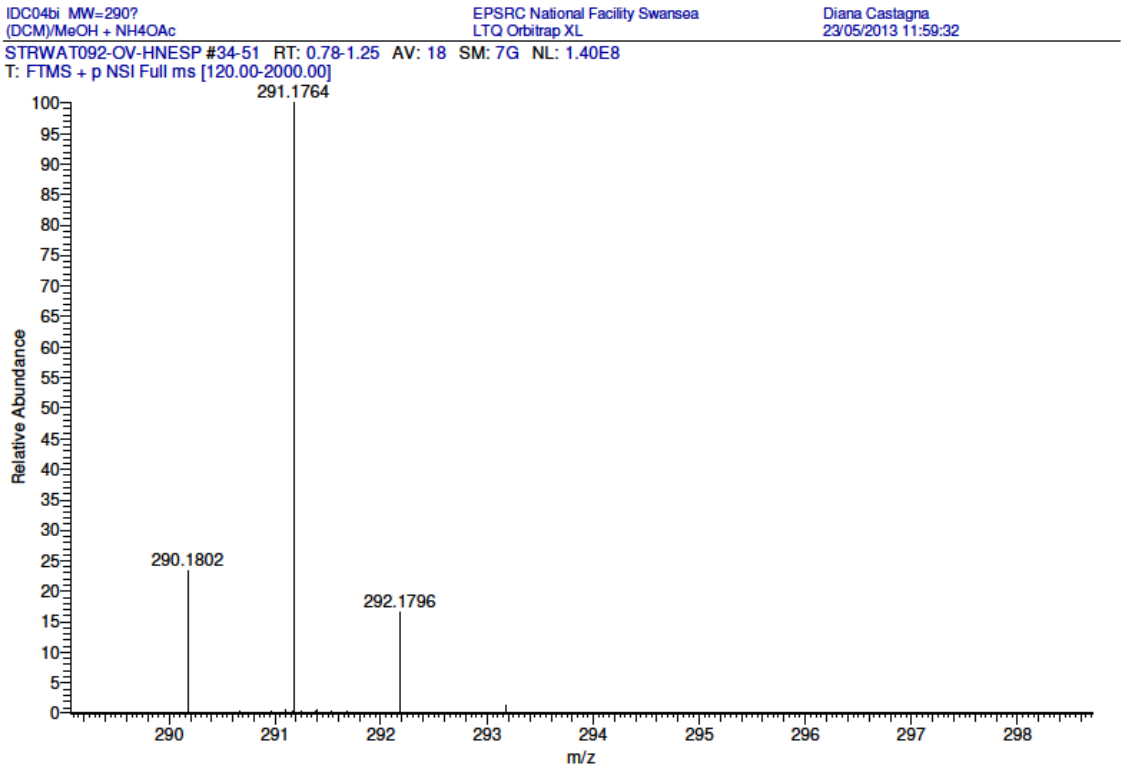
IR of 51



^{1}B NMR of 51

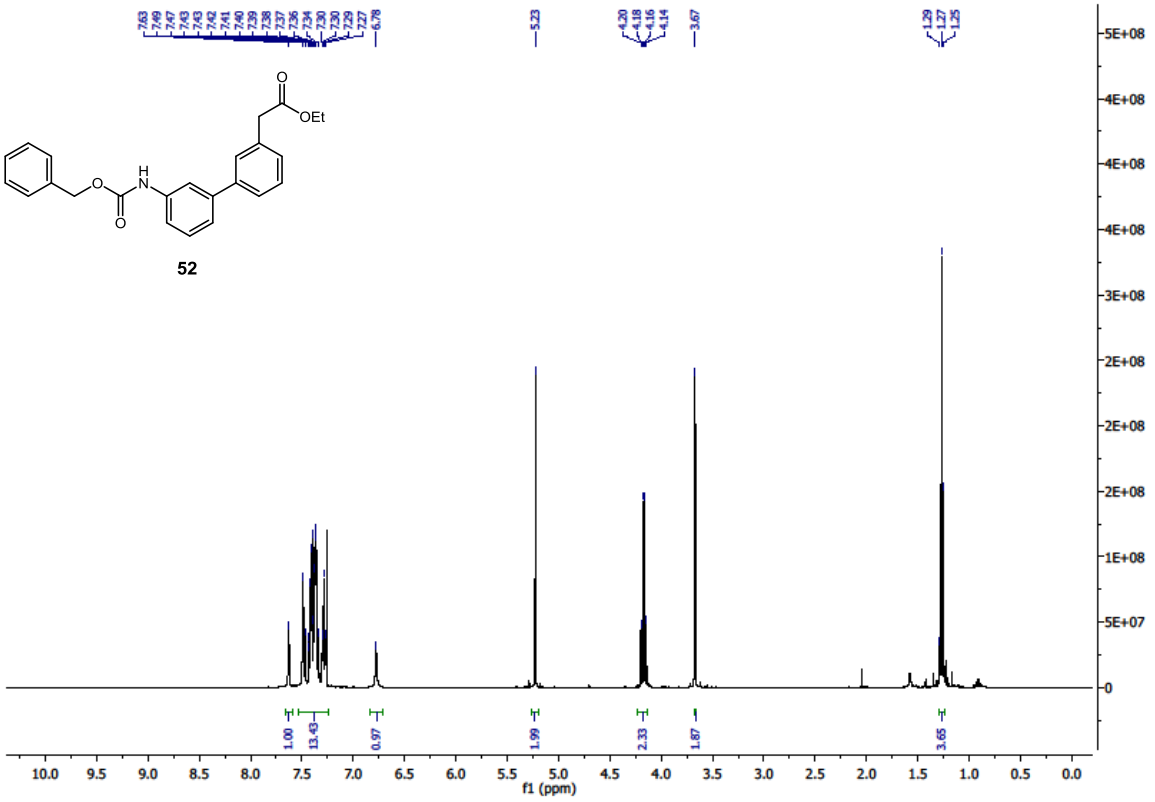


HRMS of 51

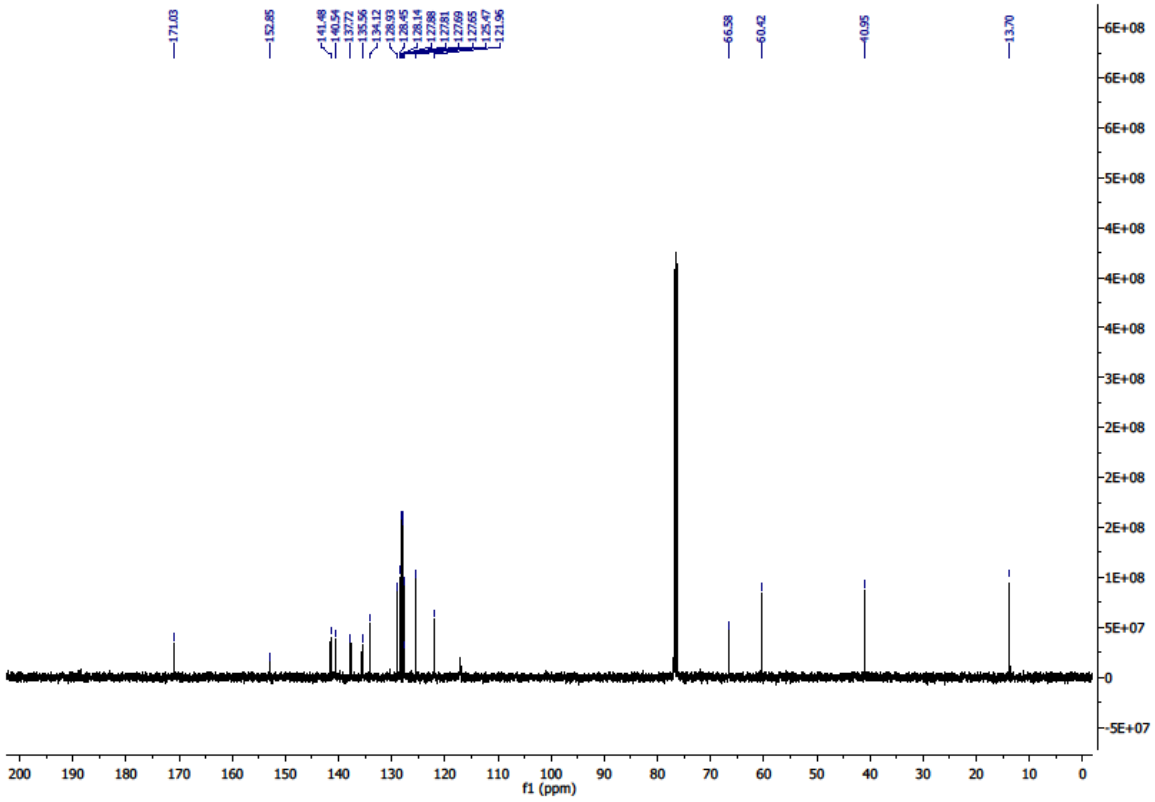

IDC04bi MW=290?
(DCM)/MeOH + NH4OAc
EPSRC National Facility Swansea
LTQ Orbitrap XL
Diana Castagna
23/05/2013 11:59:32
STRWAT092-OV-HNESP #34-51 RT: 0.78-1.25 AV: 18 SM: 7G NL: 1.40E8
T: FTMS + p NSI Full ms [120.00-2000.00]
291.1764
290.1802
292.1796
Relative Abundance
m/z

Compound 52

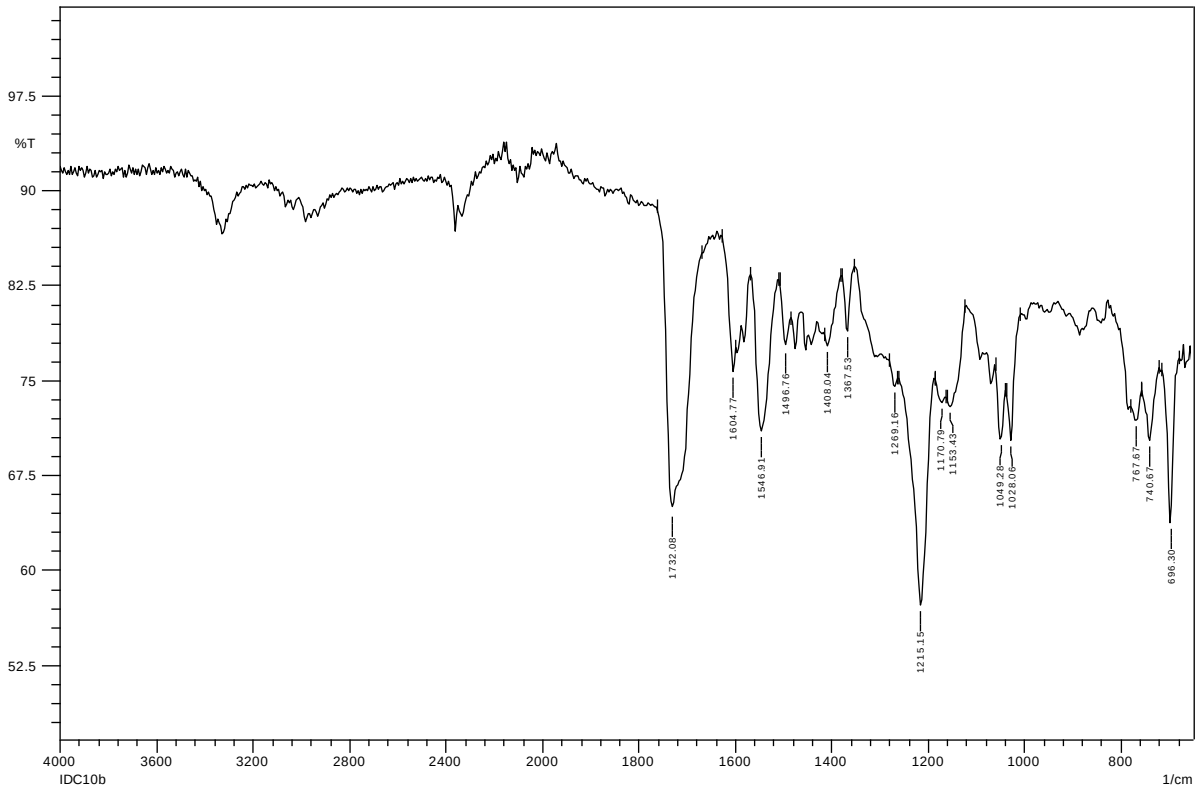
^{1}H NMR



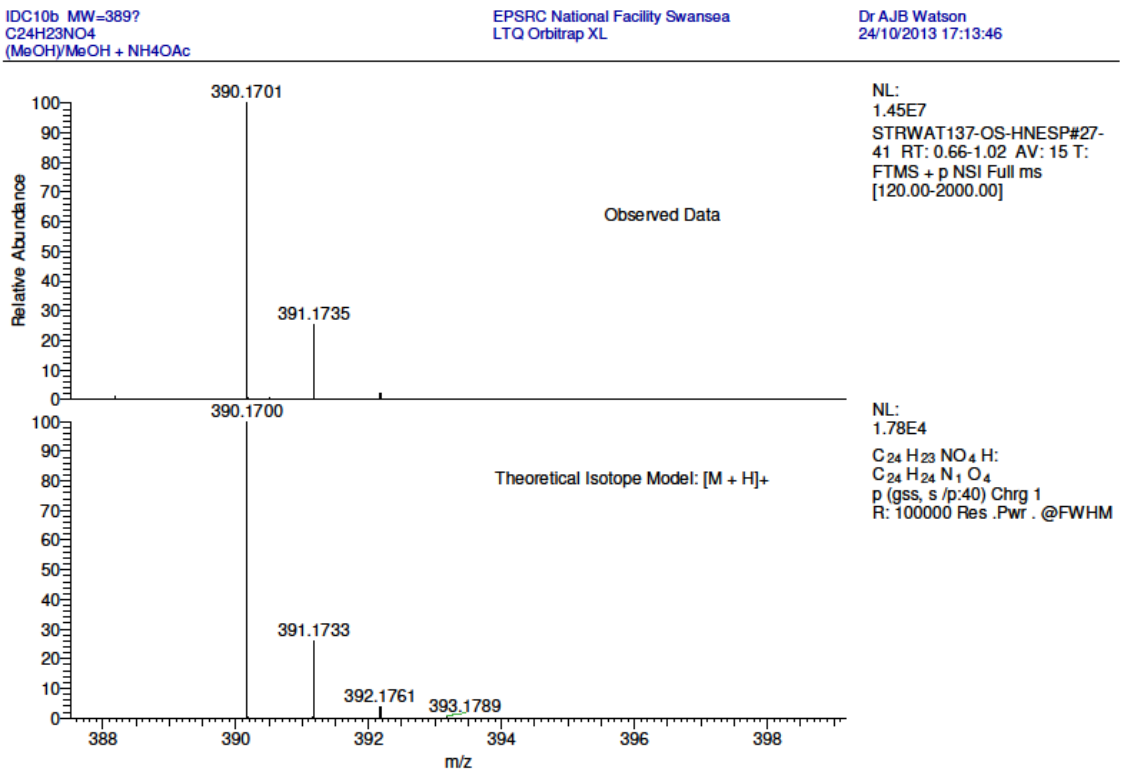
^{13}C NMR of 52



IR of 52

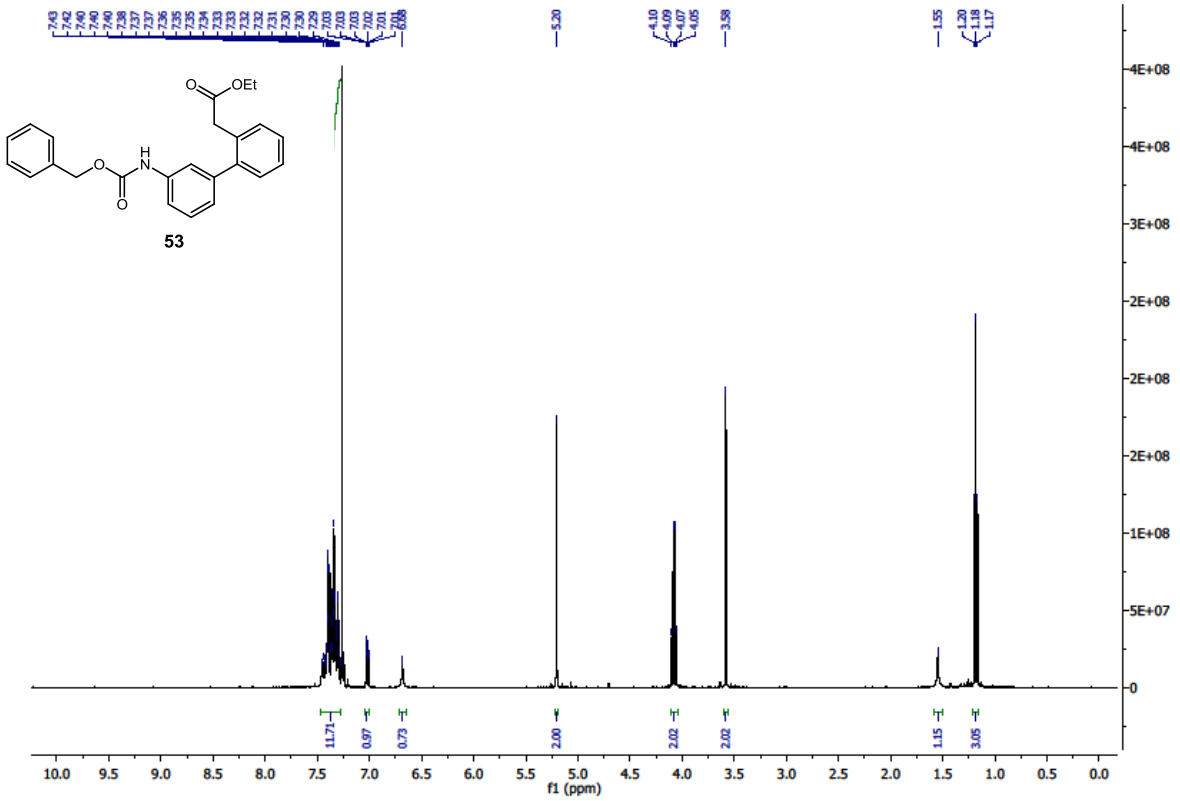


HRMS of 52

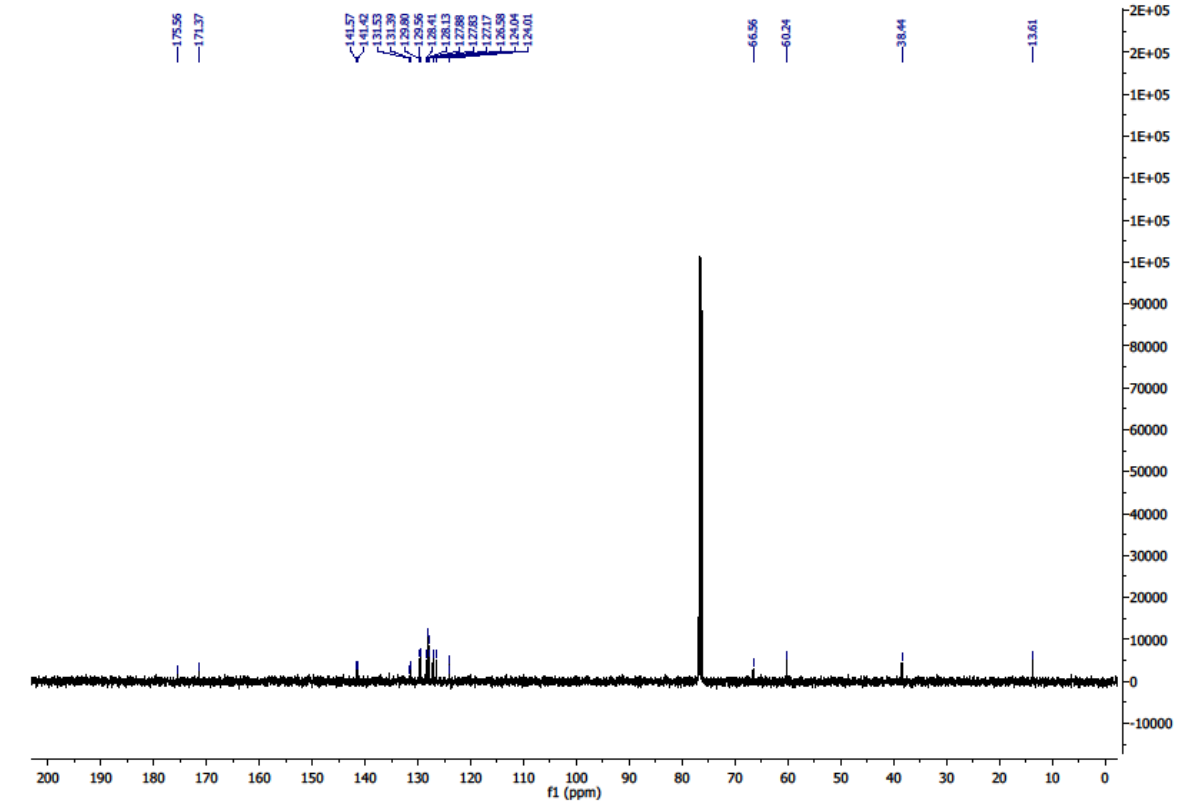


Compound 53

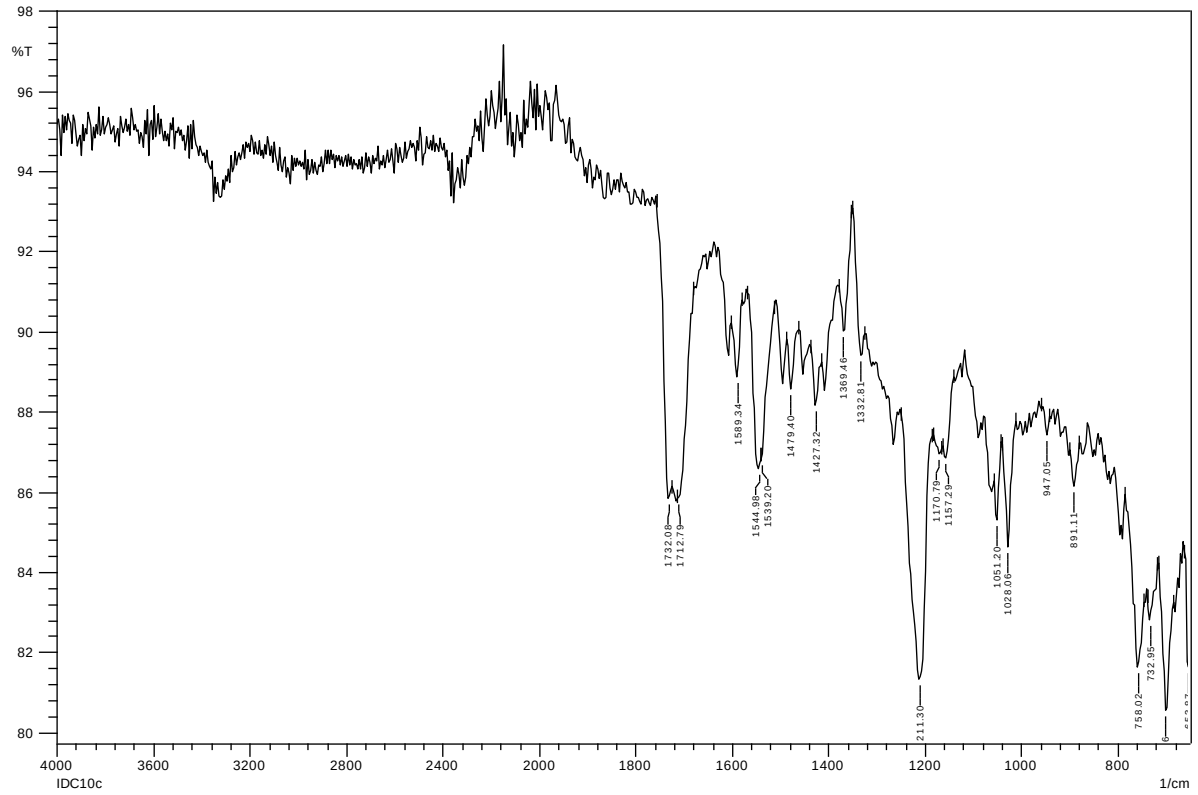
^{1}H NMR



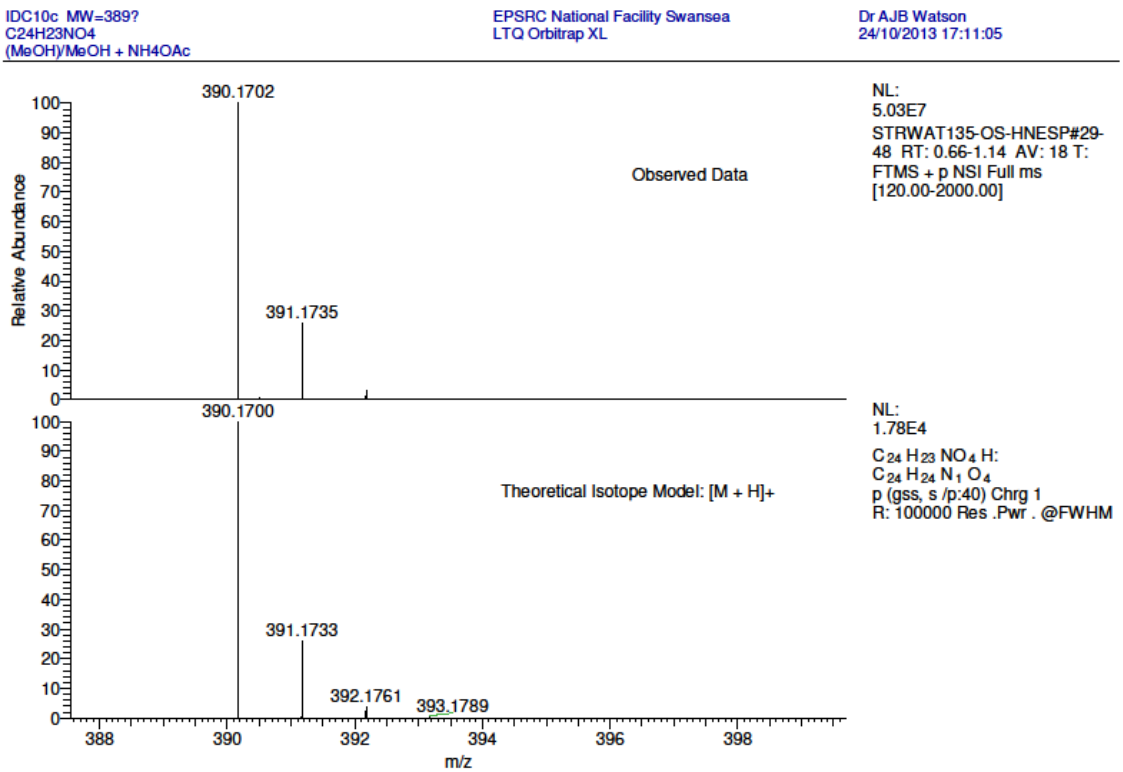
^{13}C NMR of 53



IR of 53

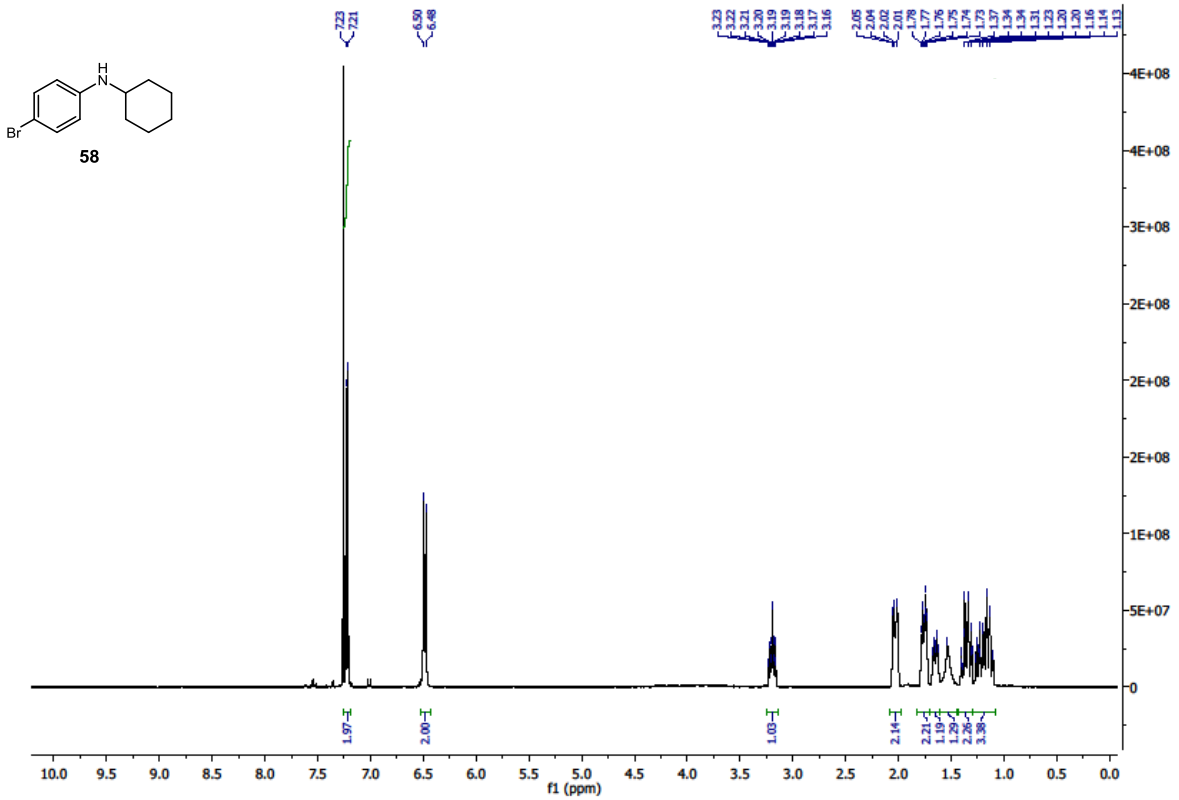


HRMS of 53

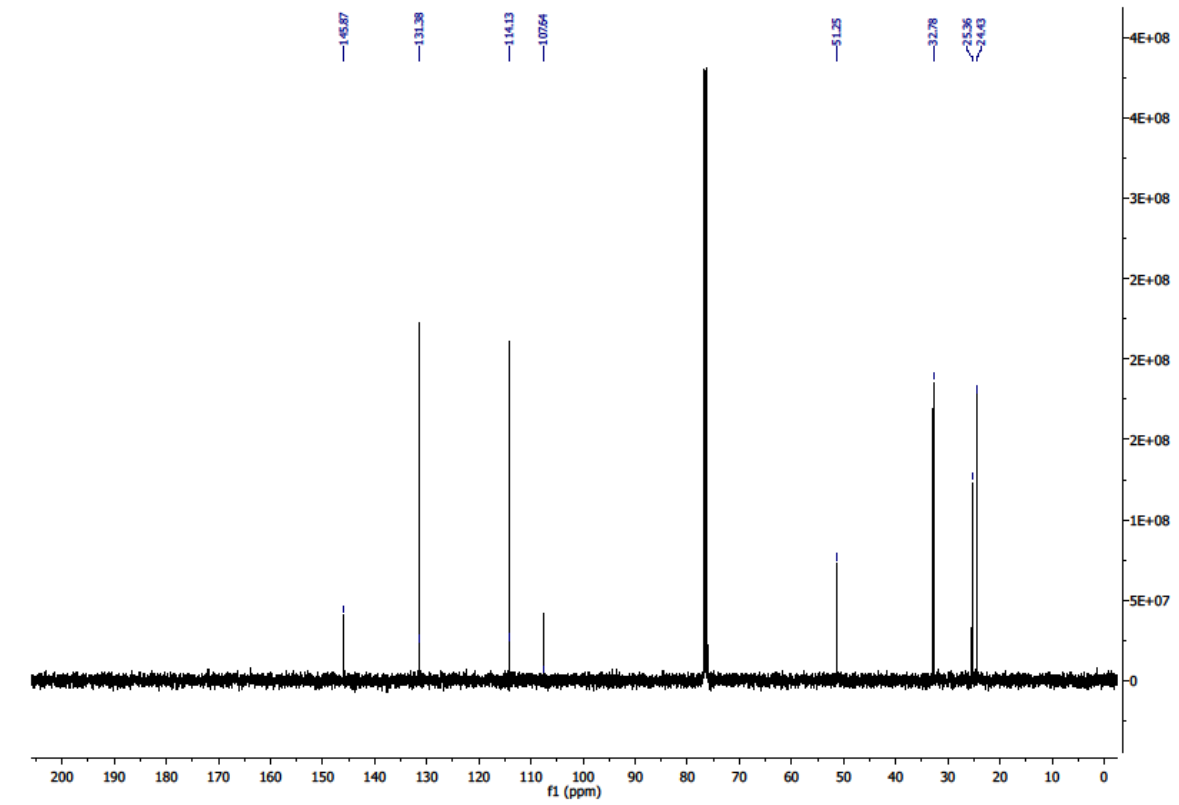


Compound 58

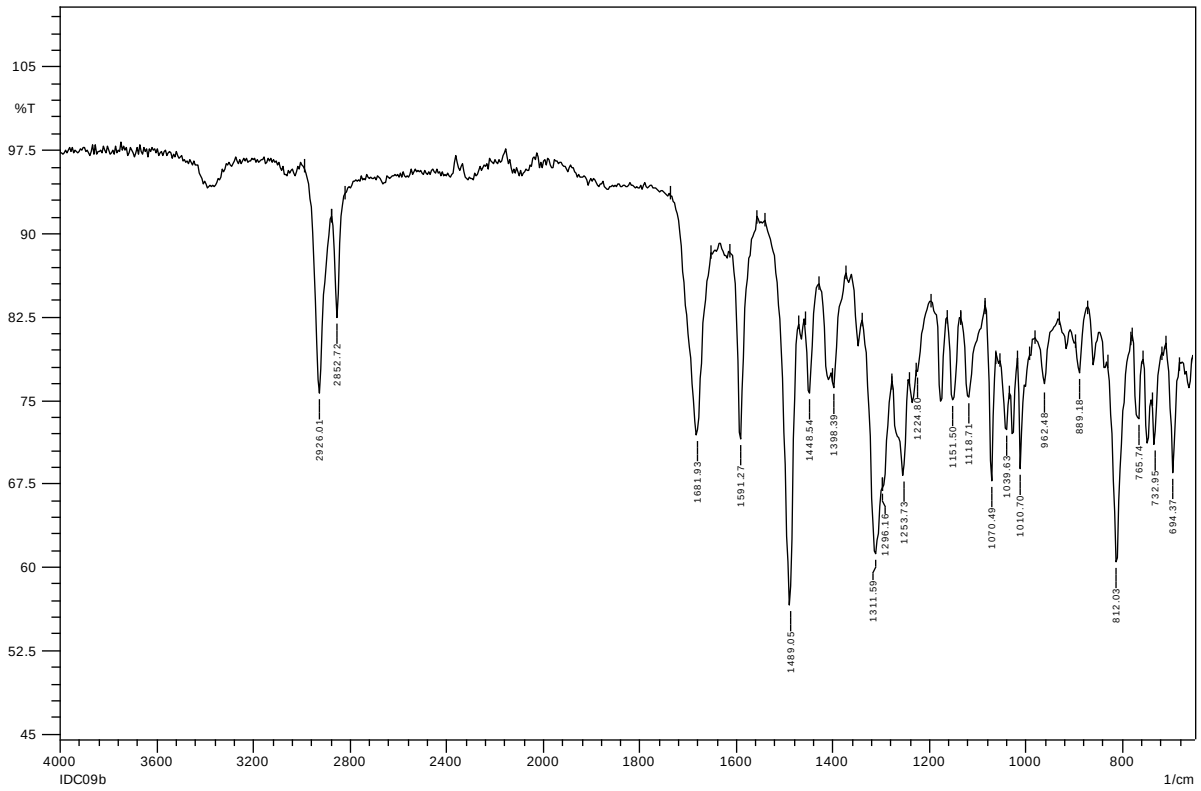
^{1}H NMR



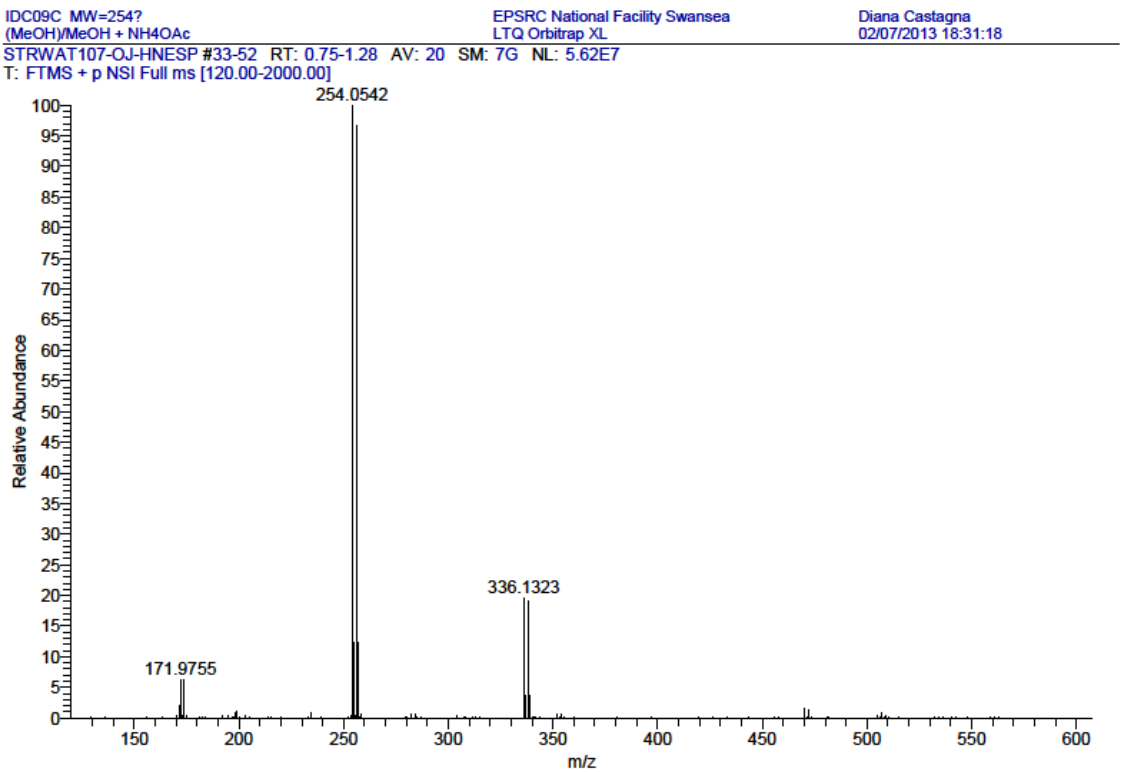
^{13}C NMR of 58



IR of 58

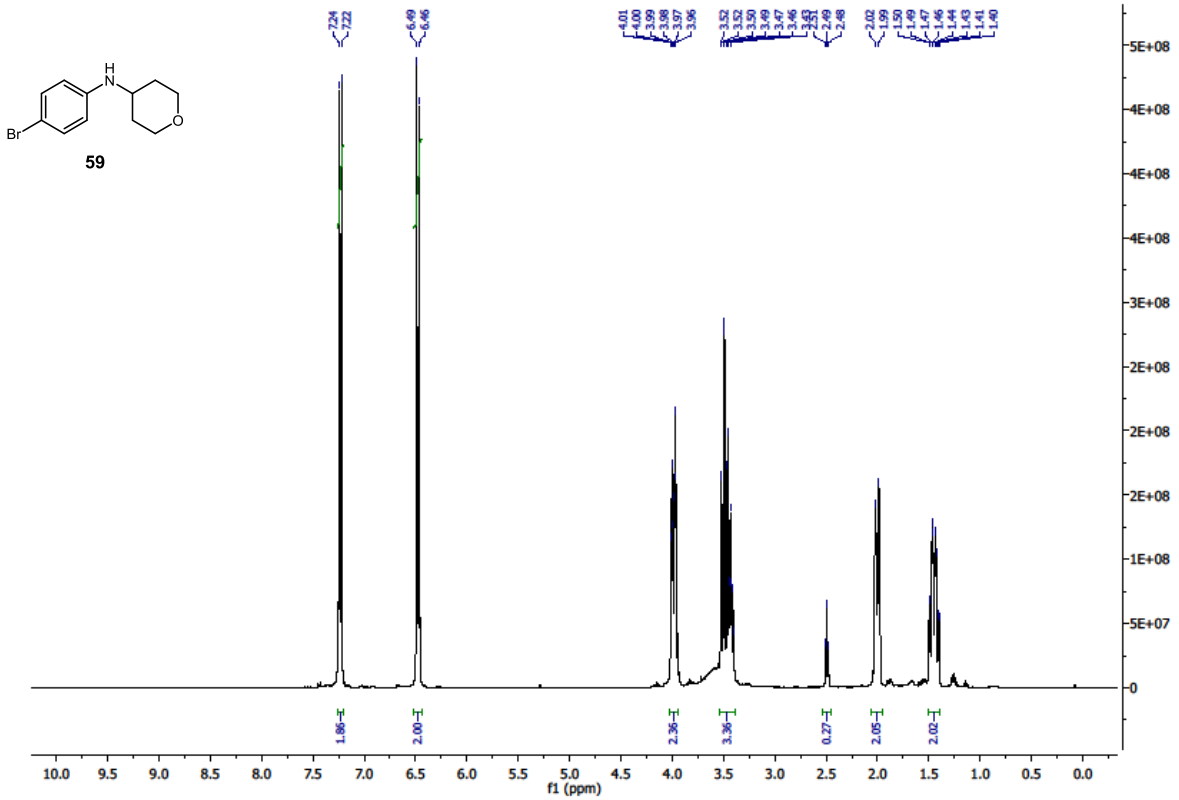


HRMS of 58

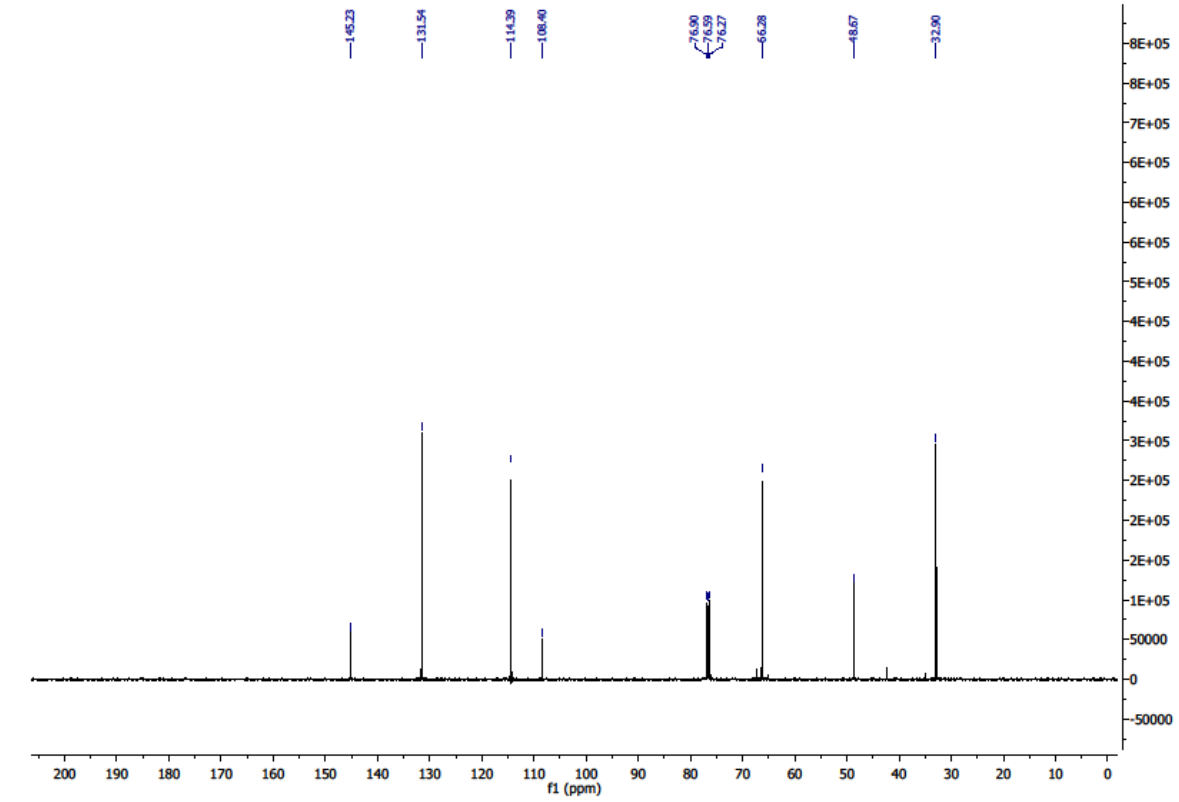


Compound 59

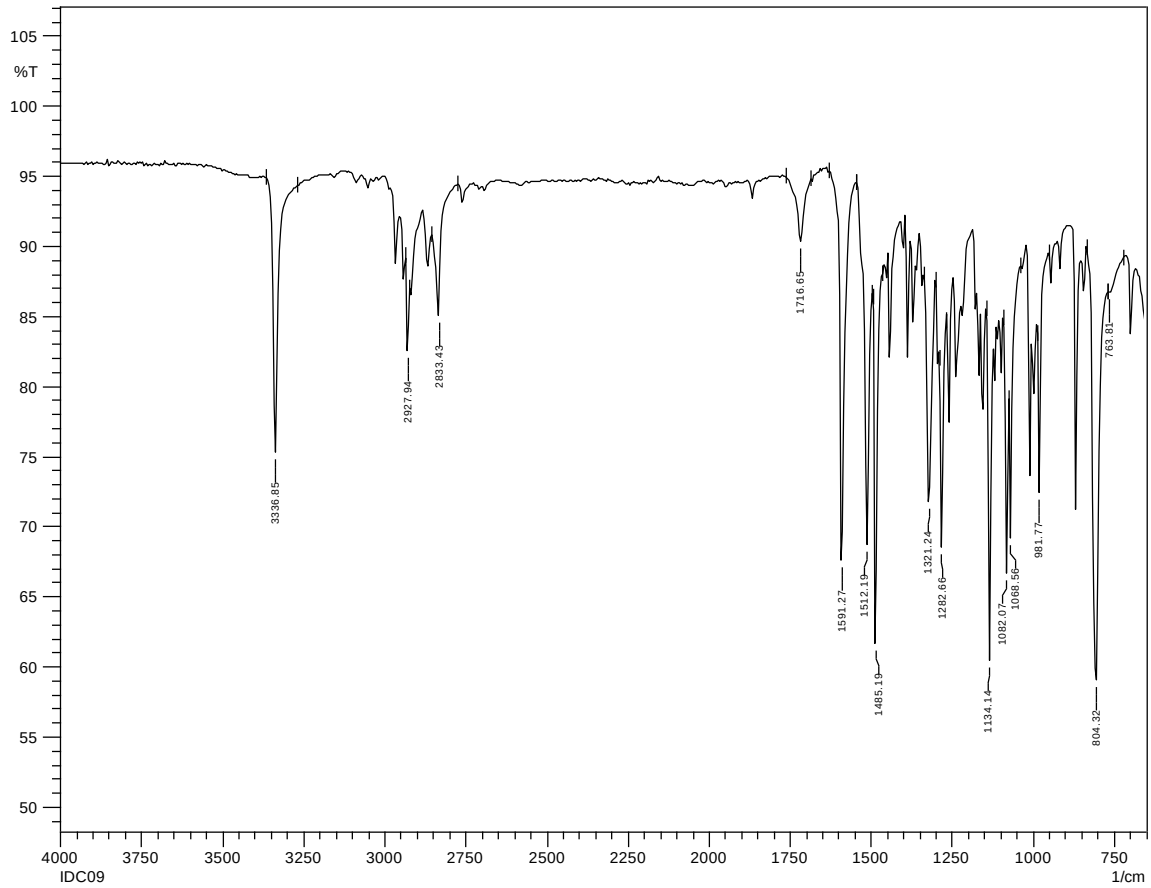
^{1}H NMR



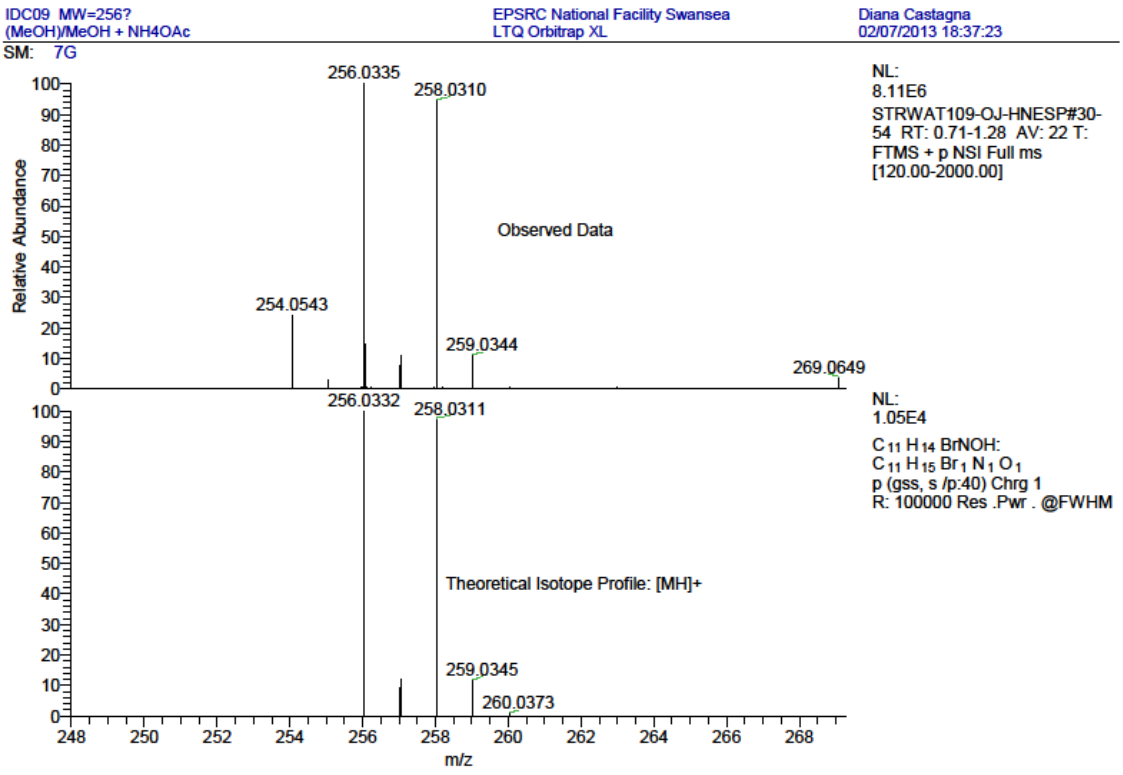
^{13}C NMR of 59



IR of 59

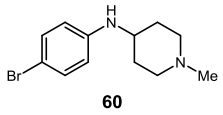


HRMS of 59



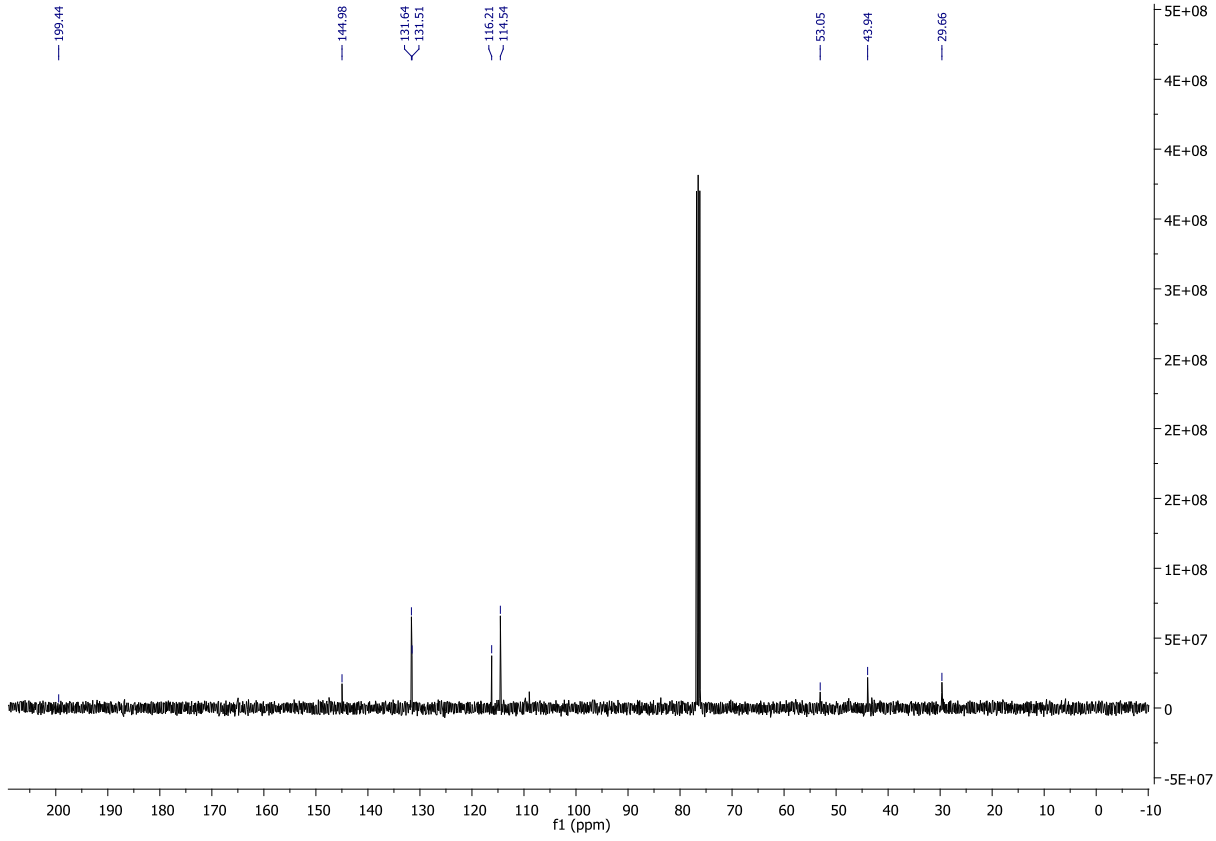
Compound 60

^{1}H NMR

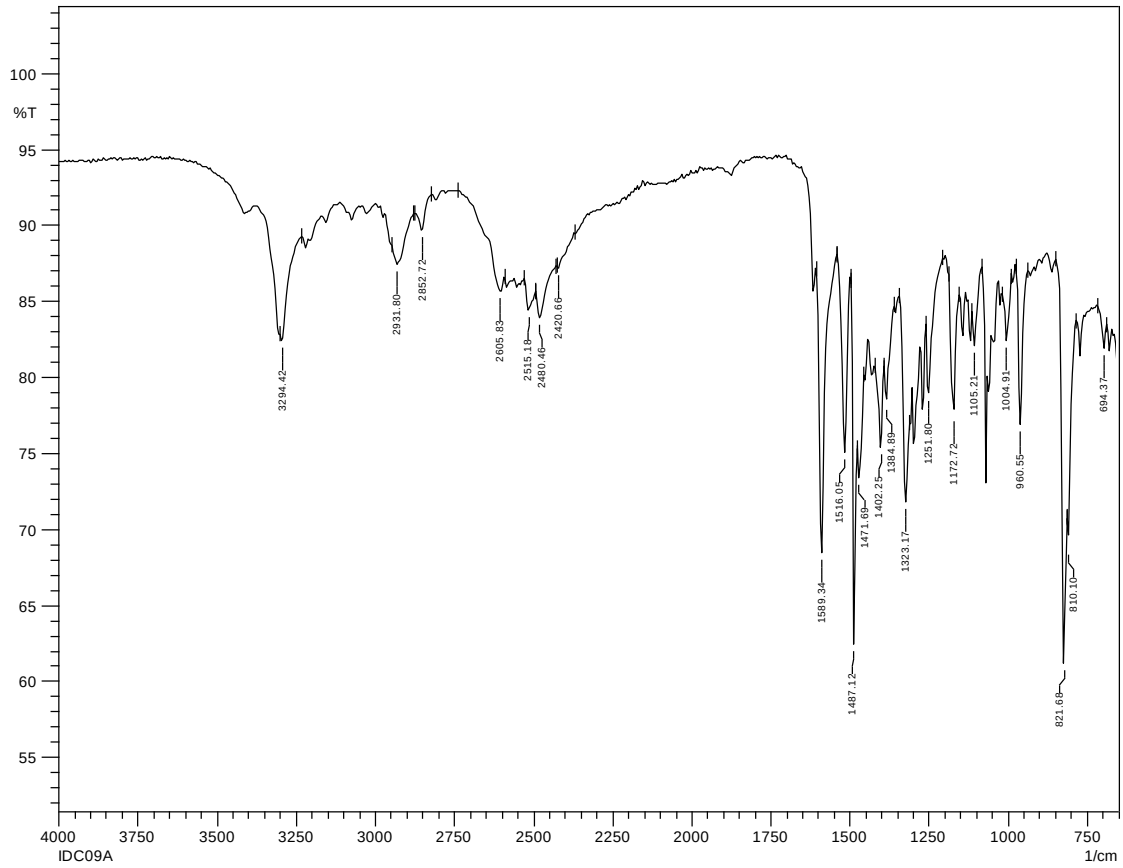


60

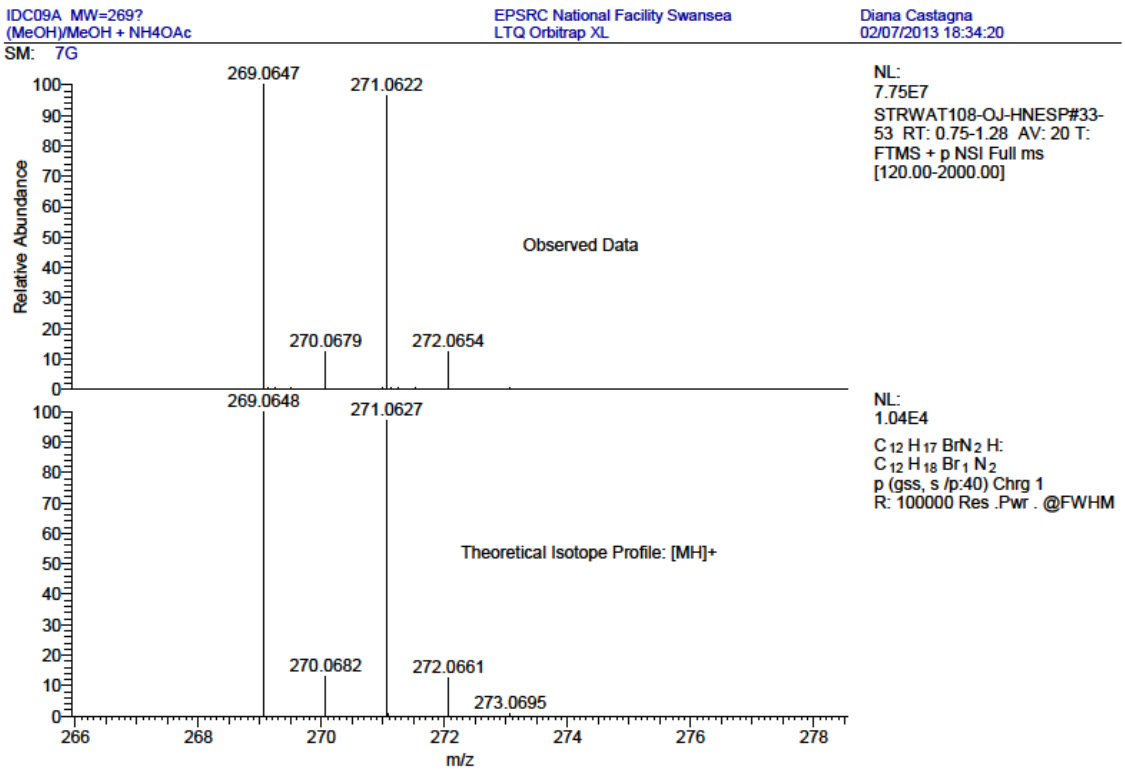
^{13}C NMR of 60



IR of 60

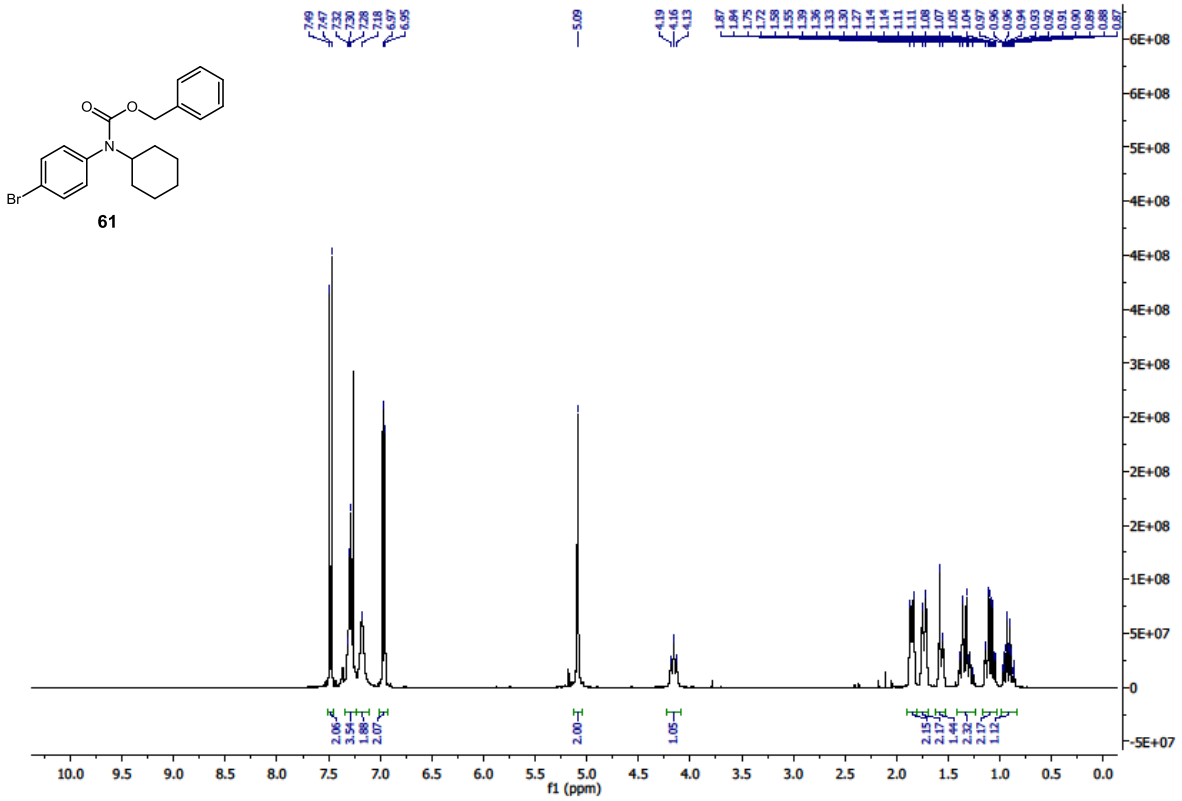


HRMS of 60

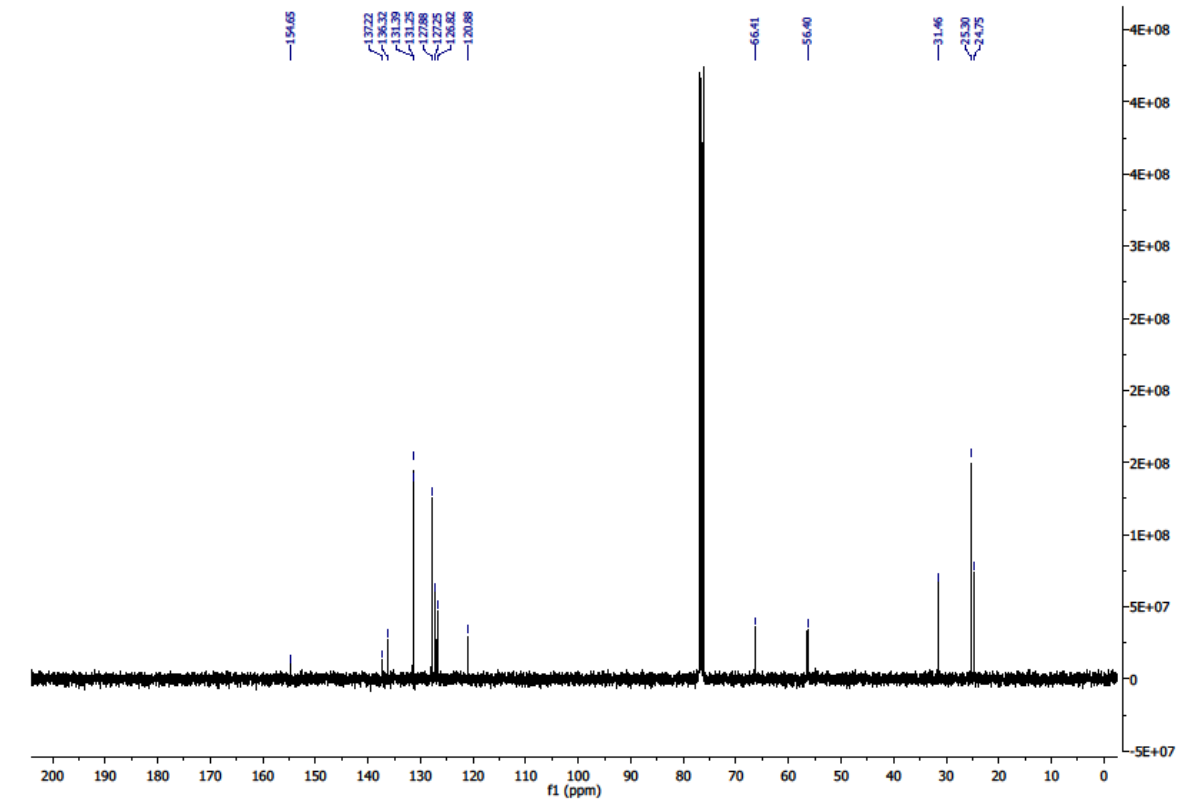


Compound 61

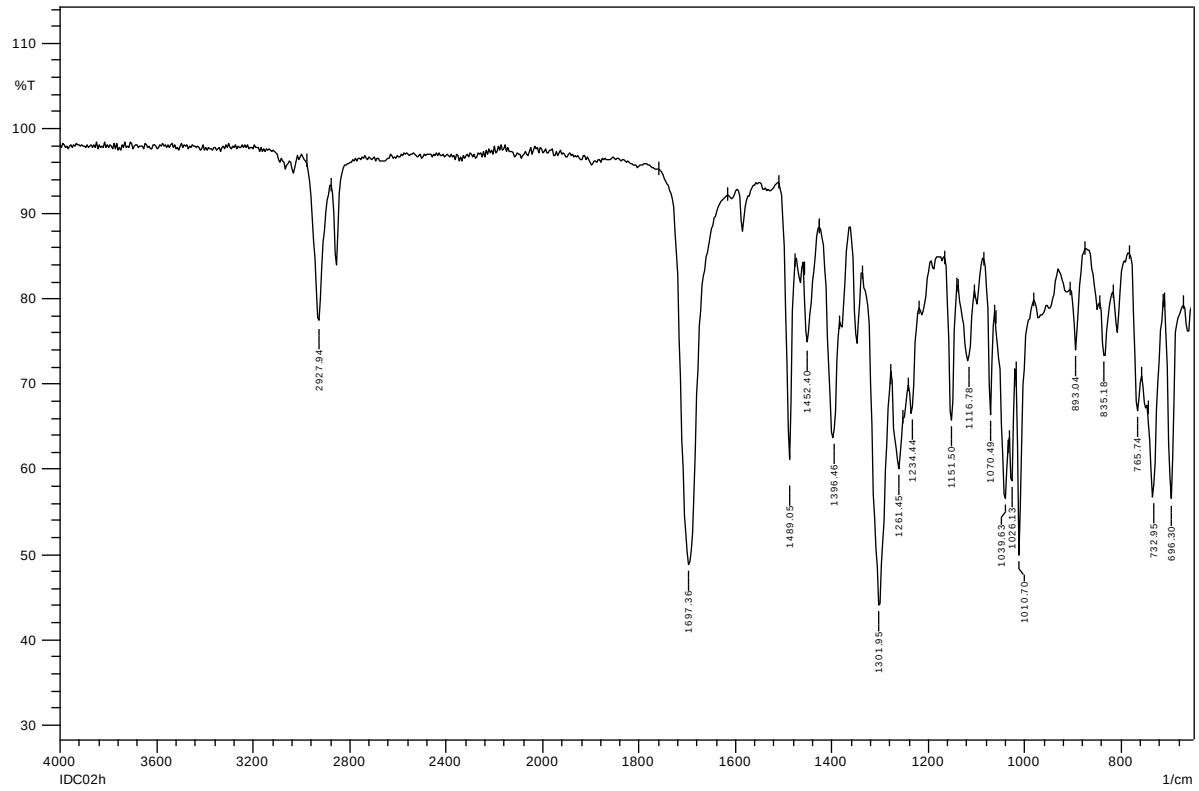
^{1}H NMR



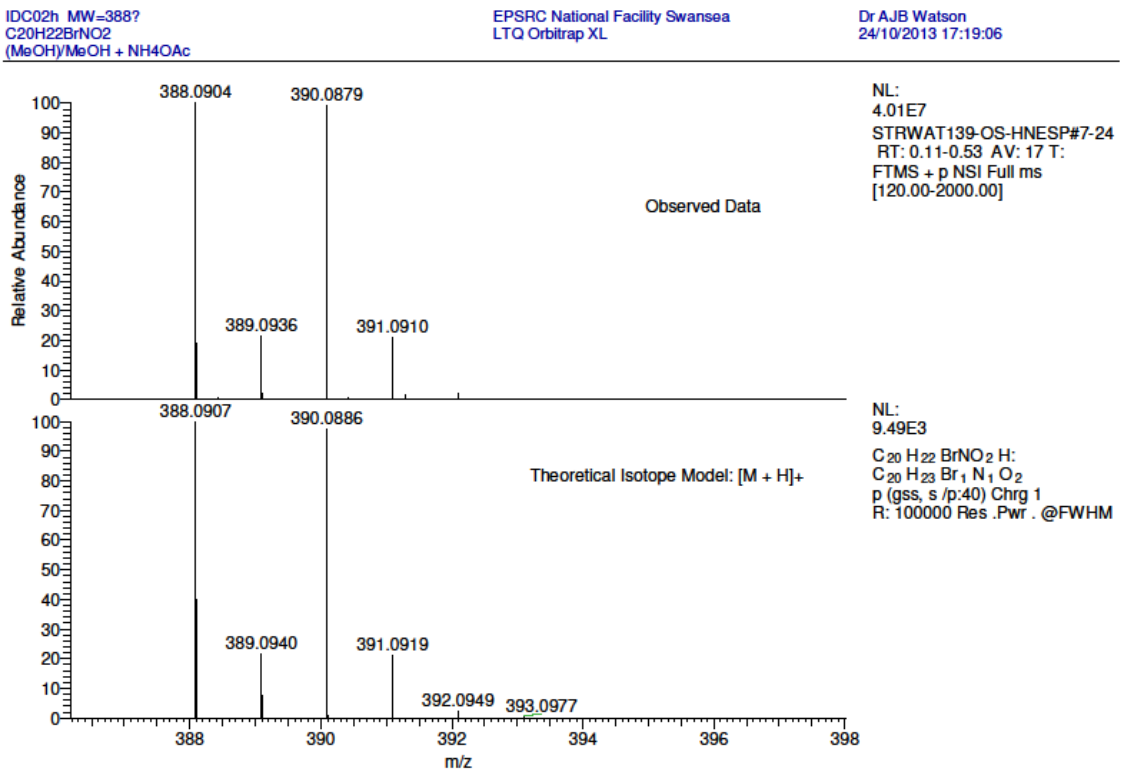
^{13}C NMR of 61



IR of 61

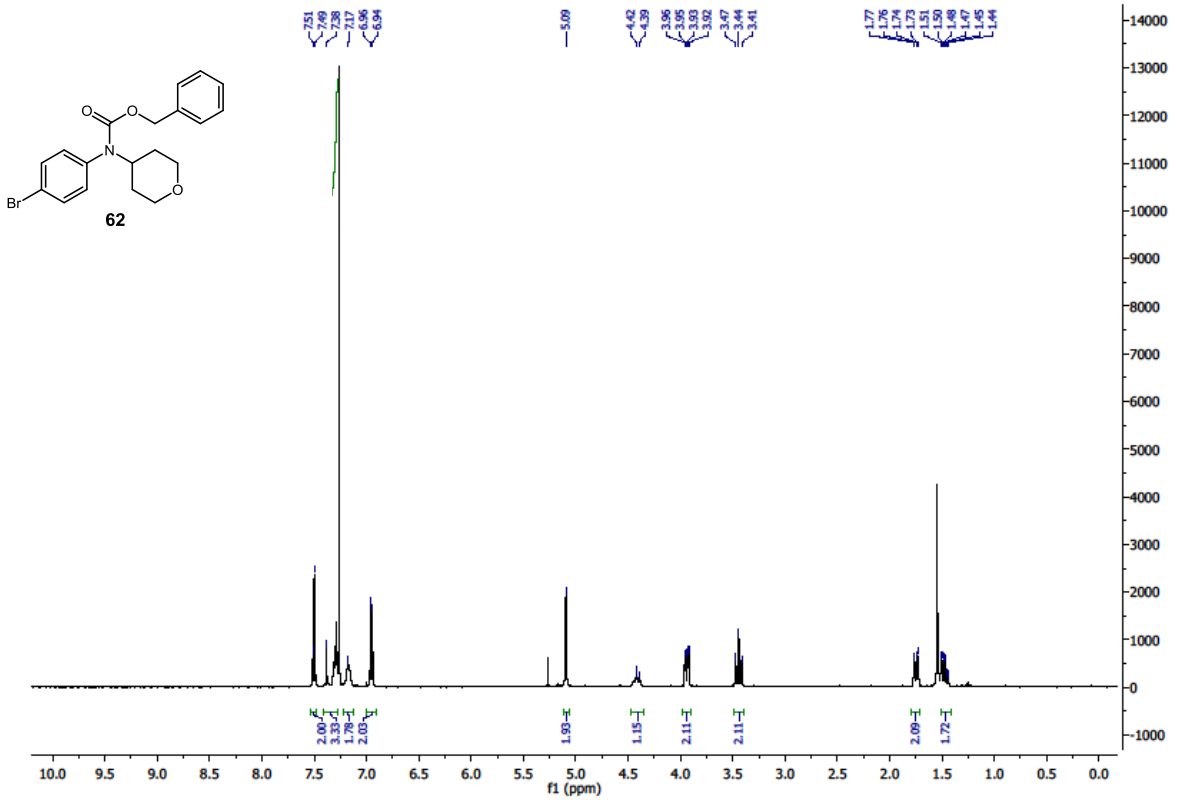


HRMS of 61

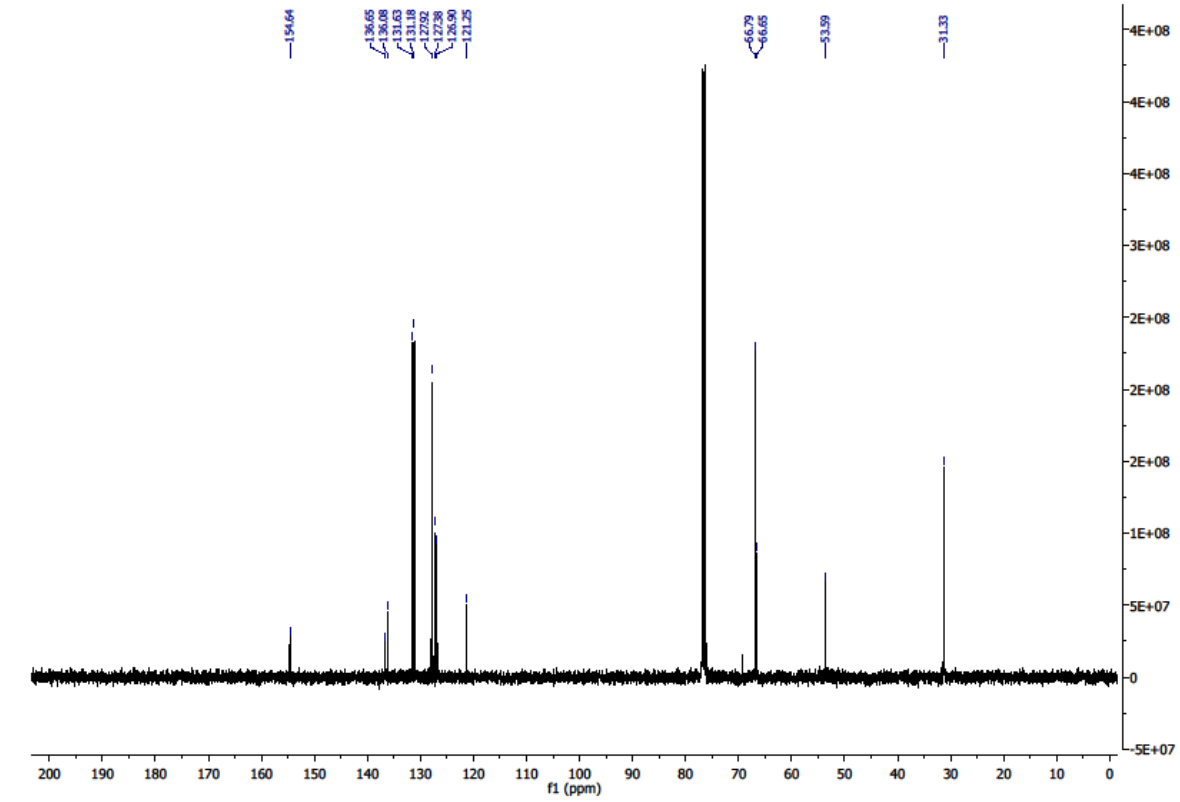


Compound 62

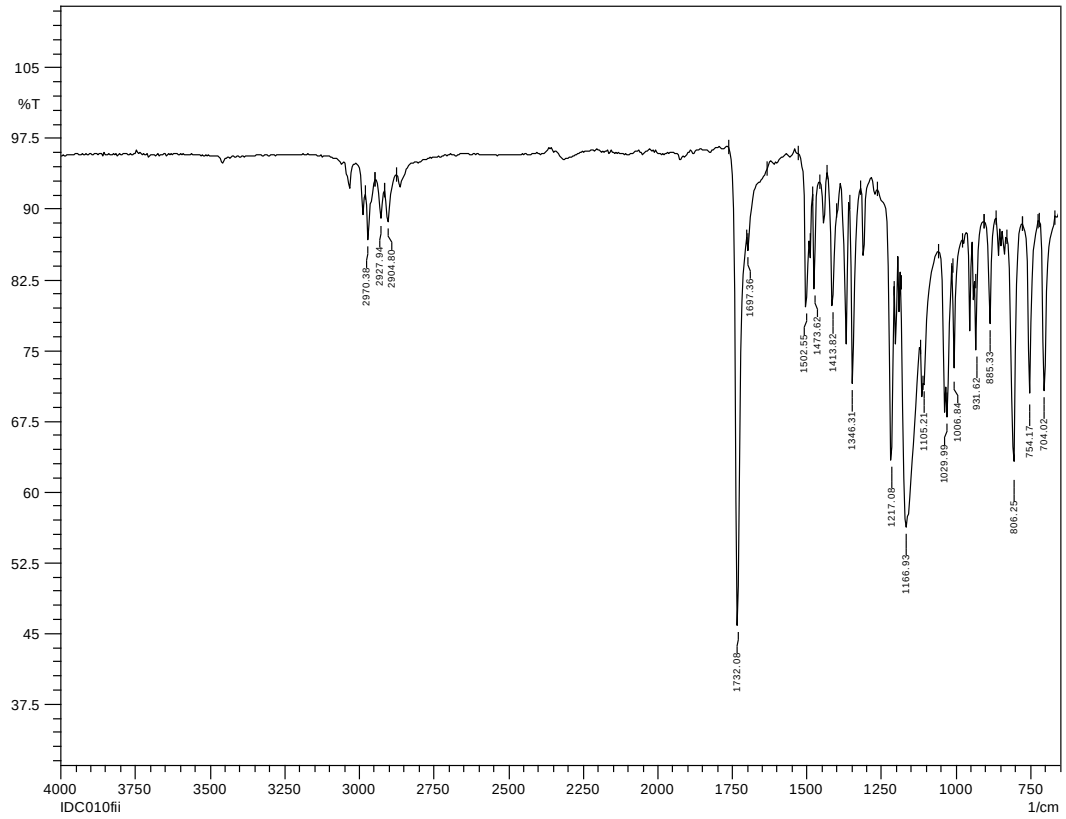
^{1}H NMR



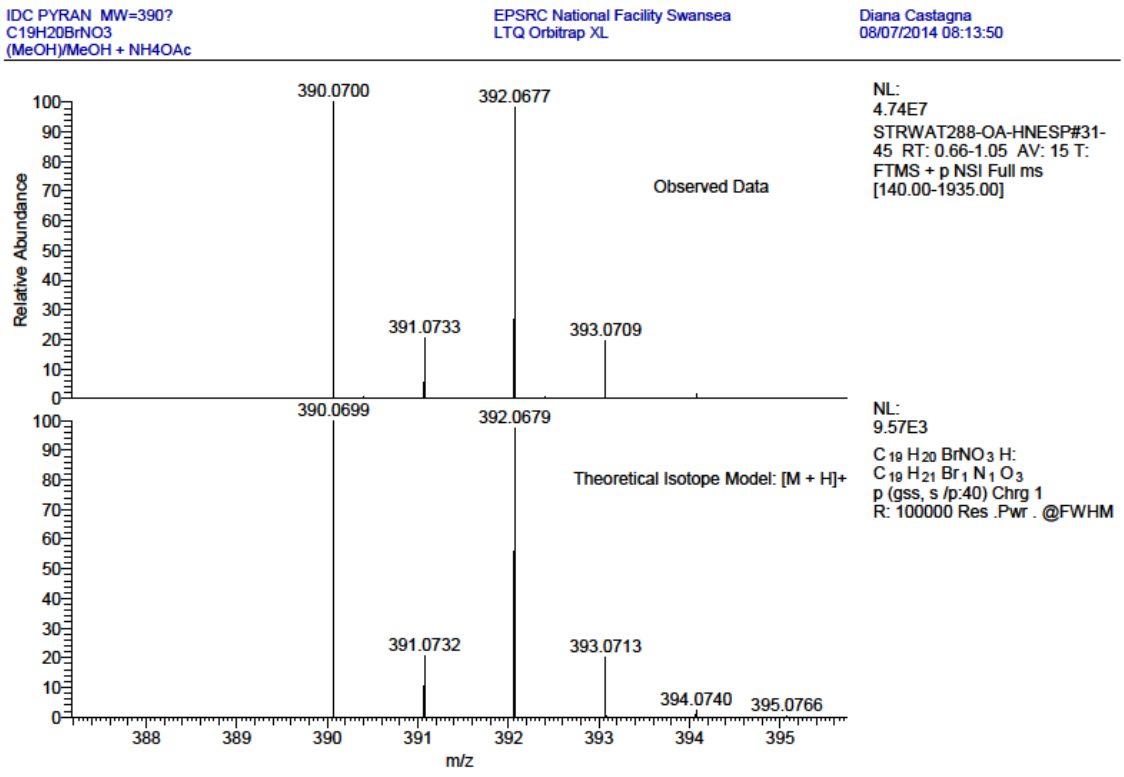
^{13}C NMR of 62



IR of 62

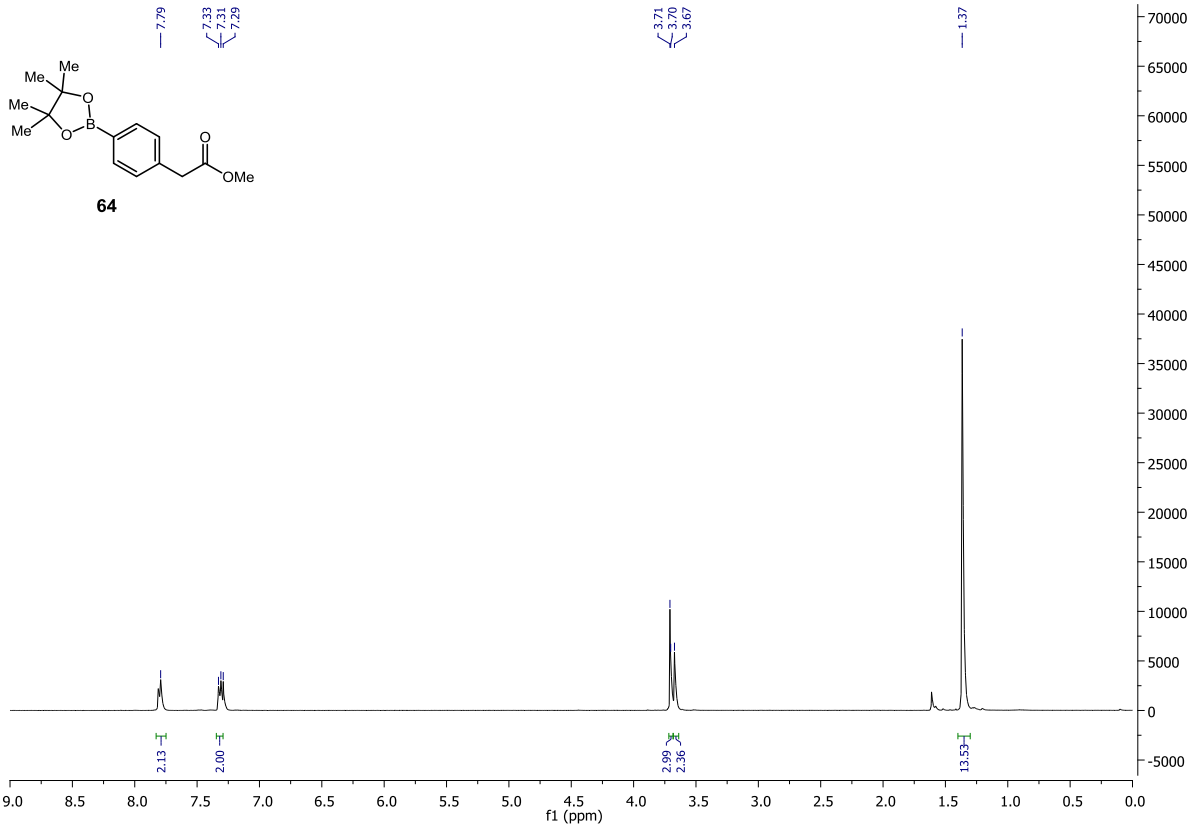


HRMS of 62

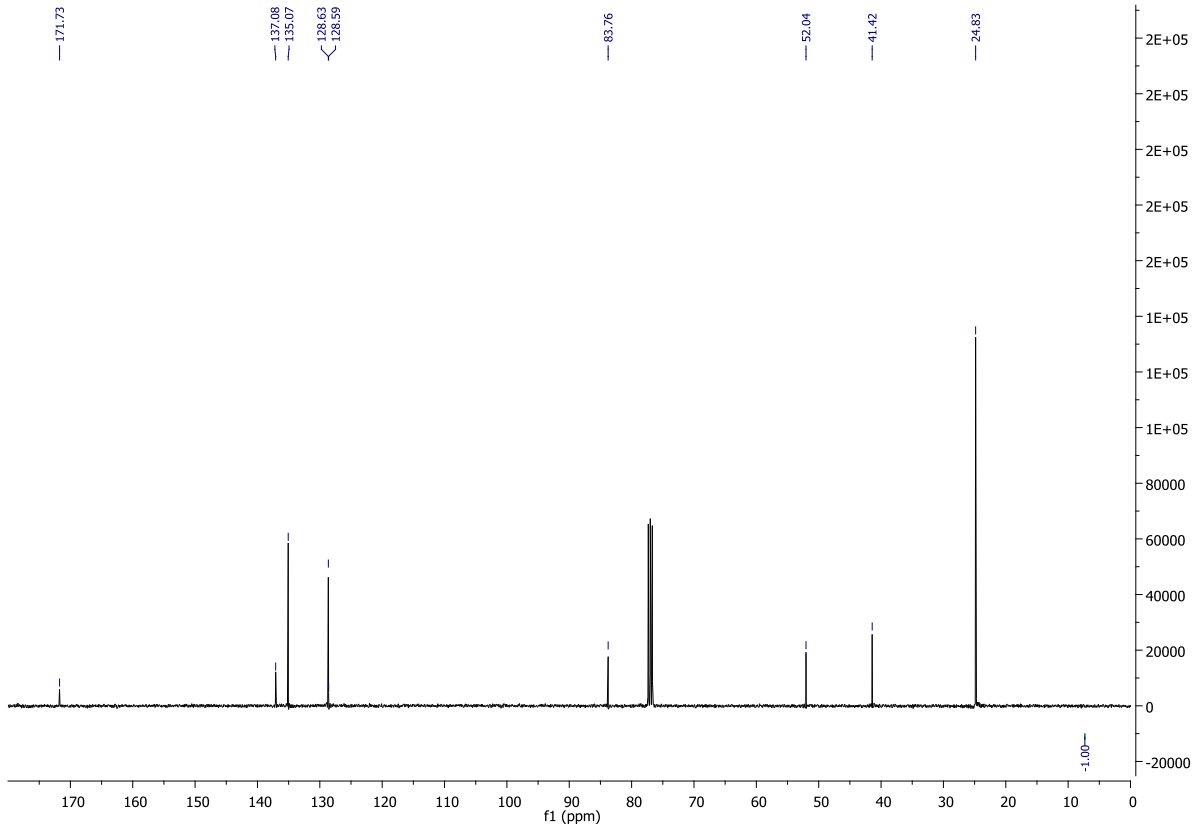


Compound 64

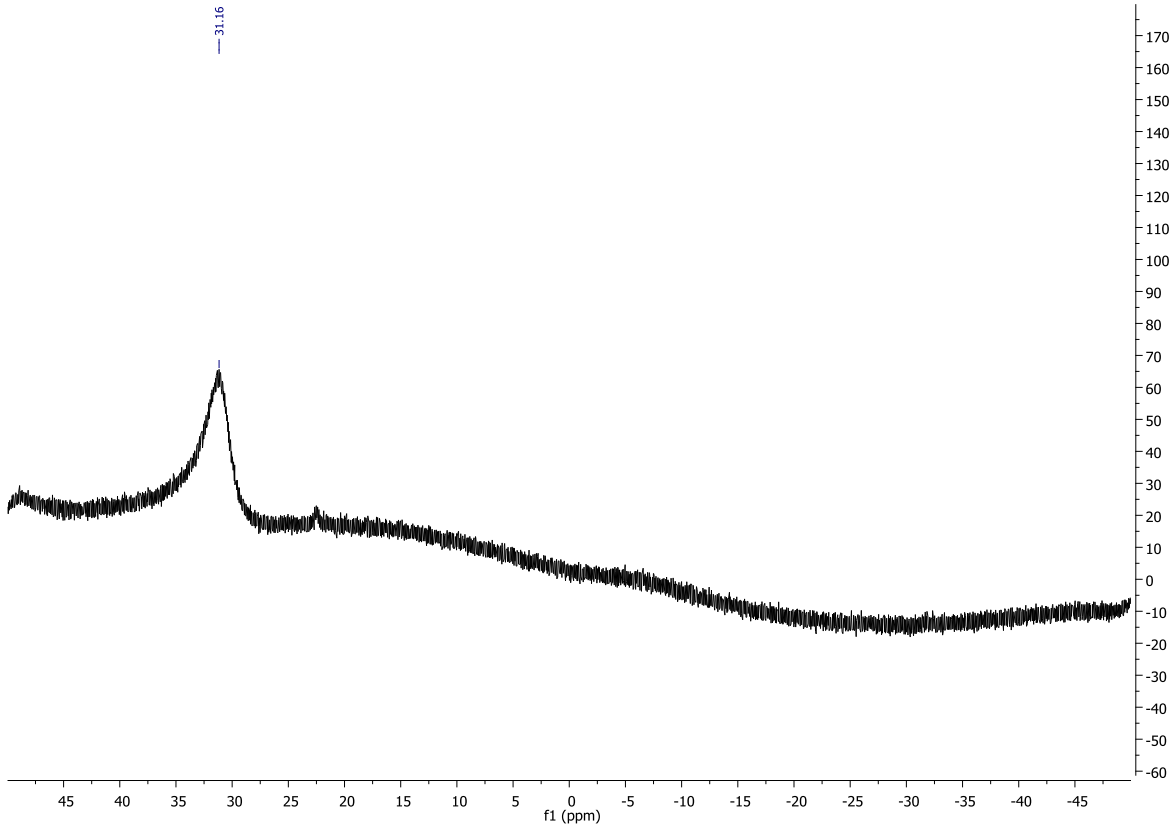
^{1}H NMR



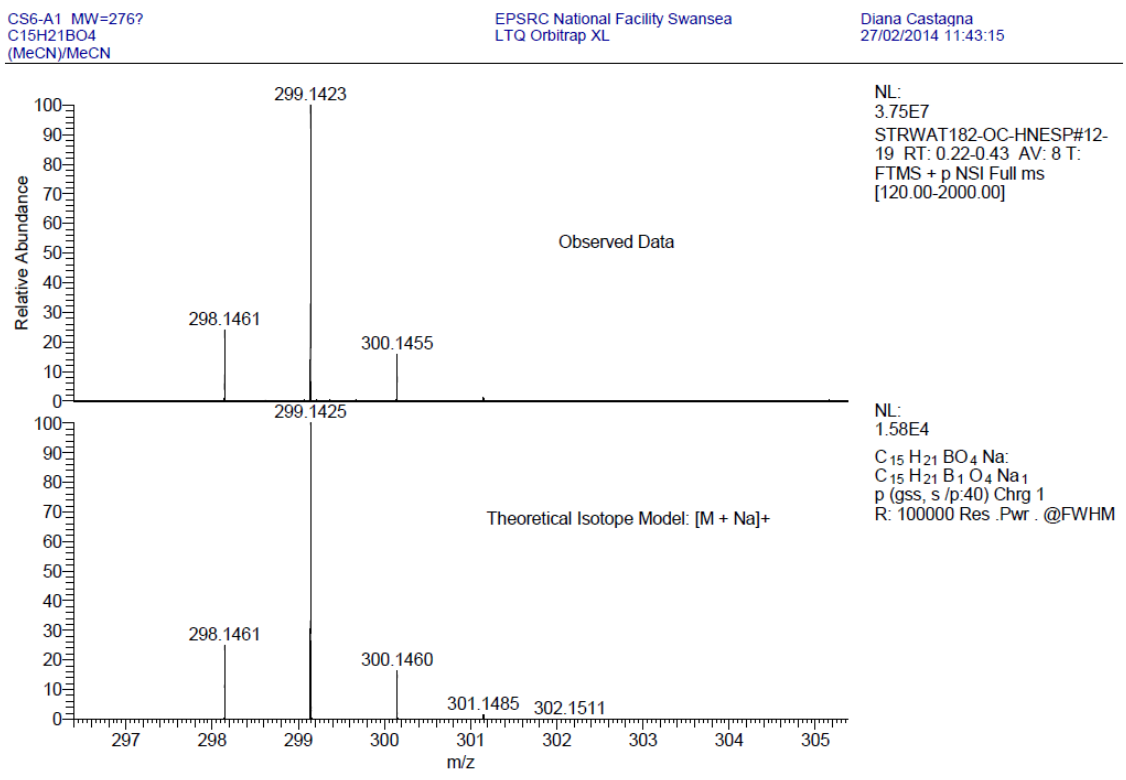
^{13}C NMR of 64



^{1}B NMR of 64

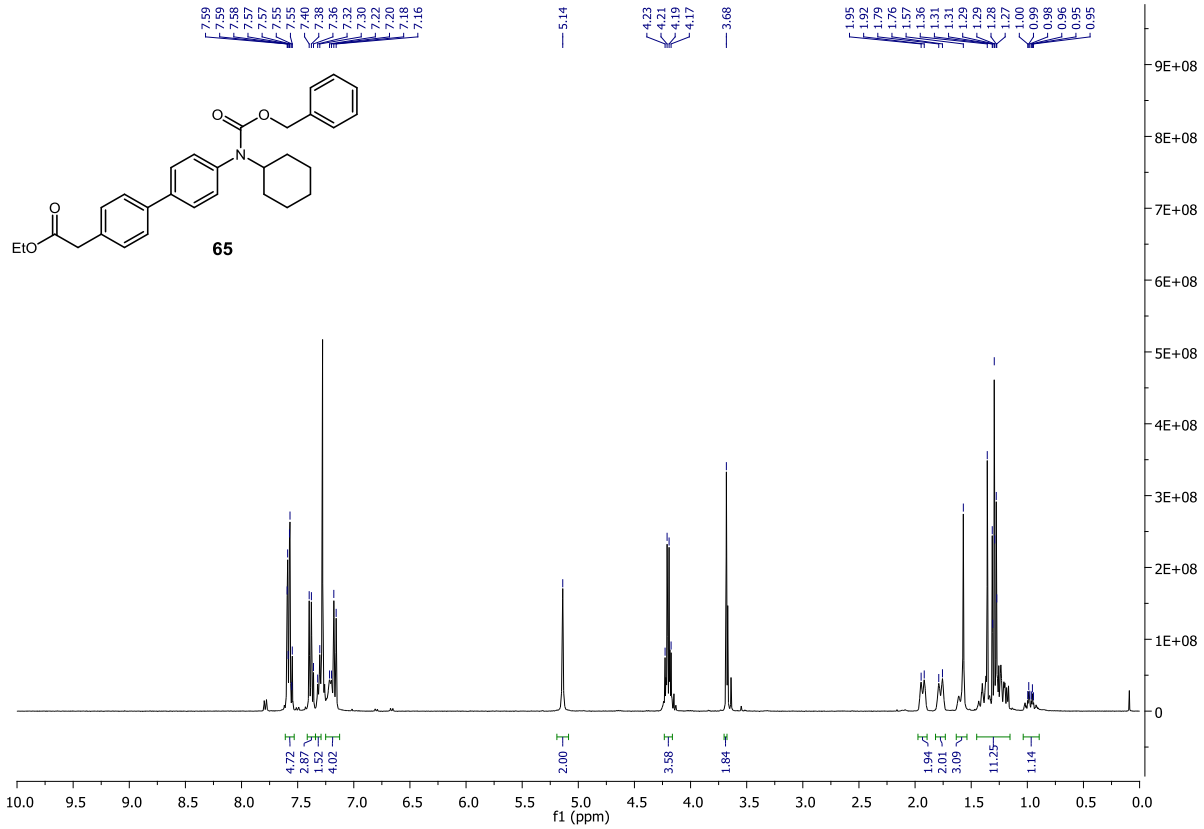


HRMS of 64

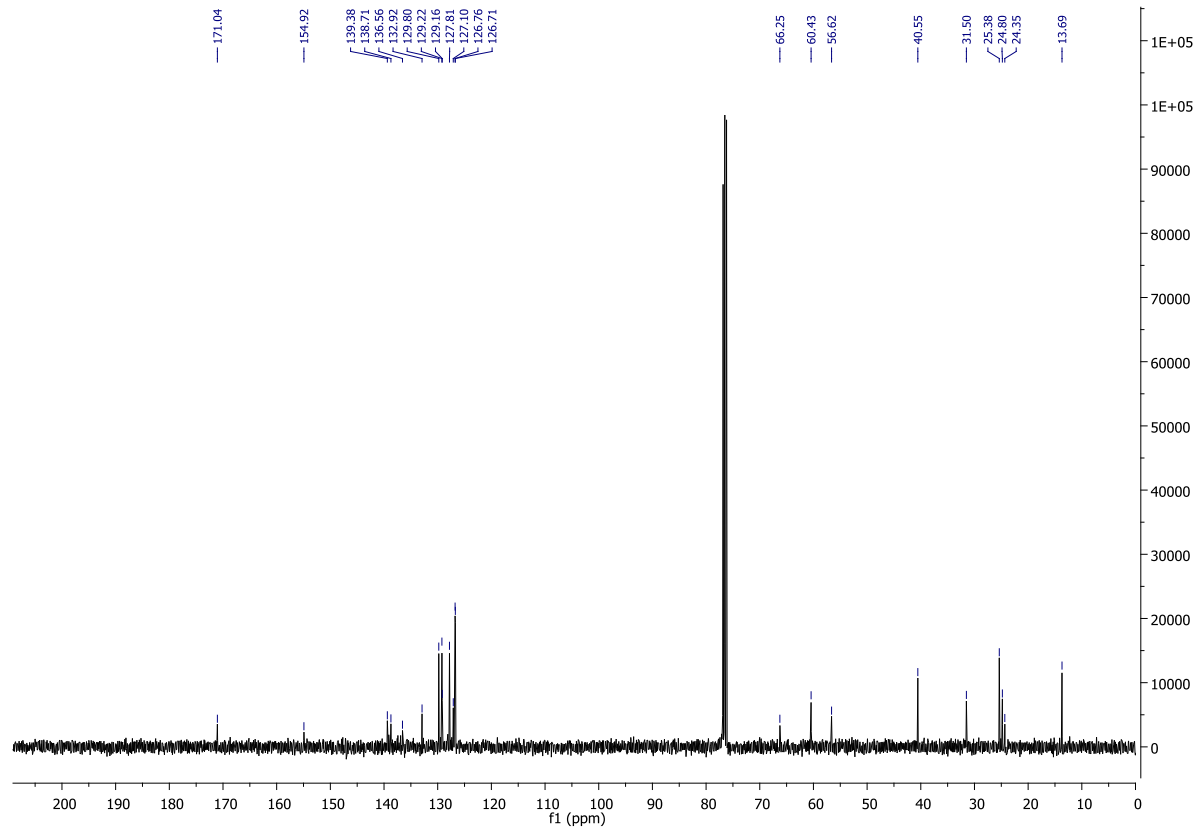


Compound 65

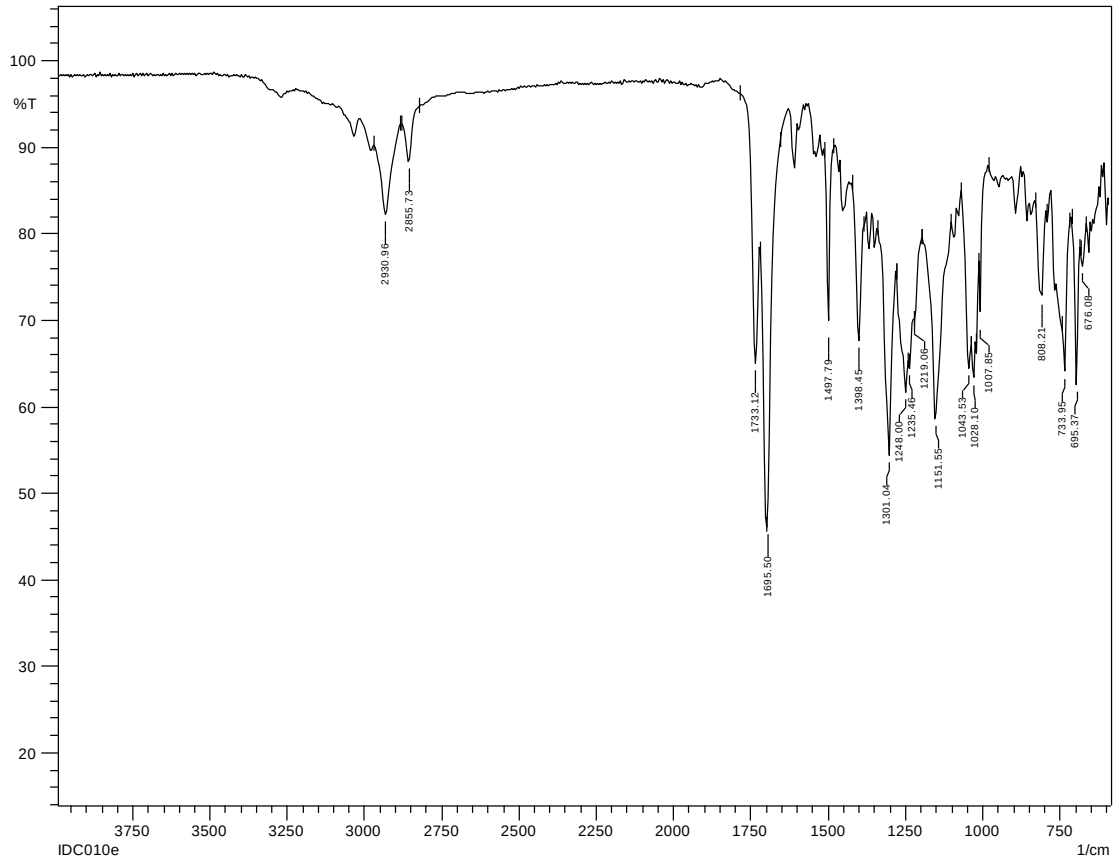
^{1}H NMR



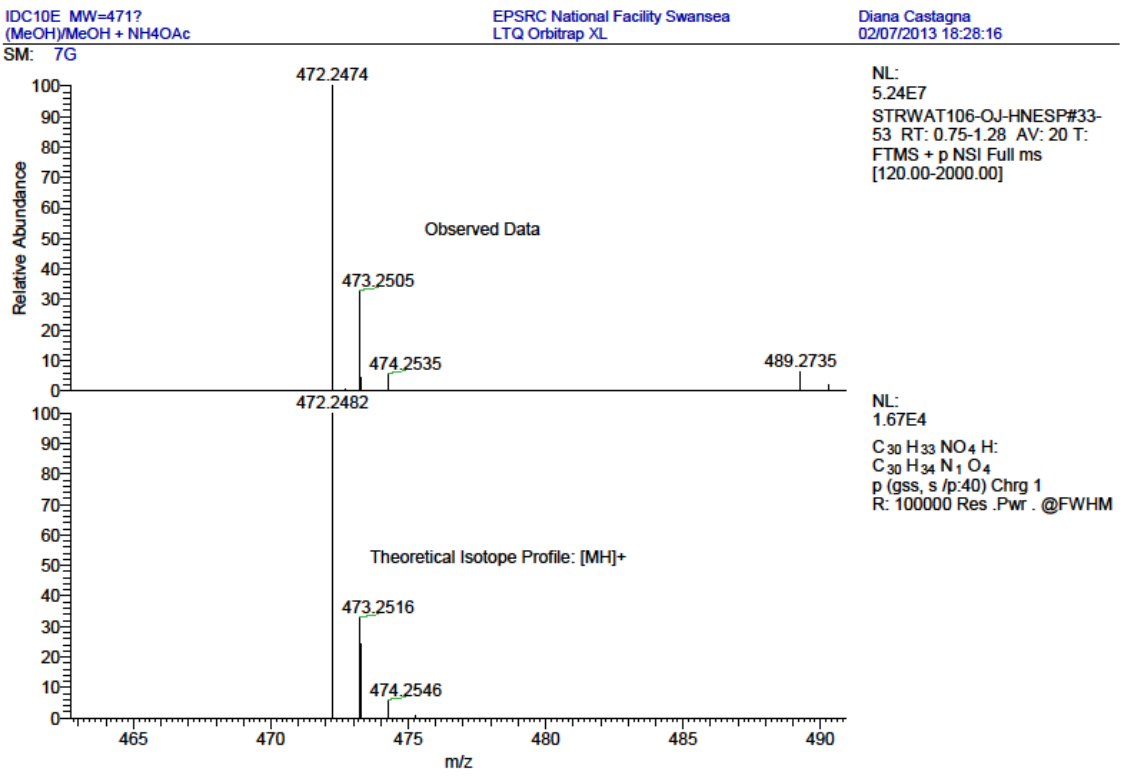
^{13}C NMR of 65



IR of 65

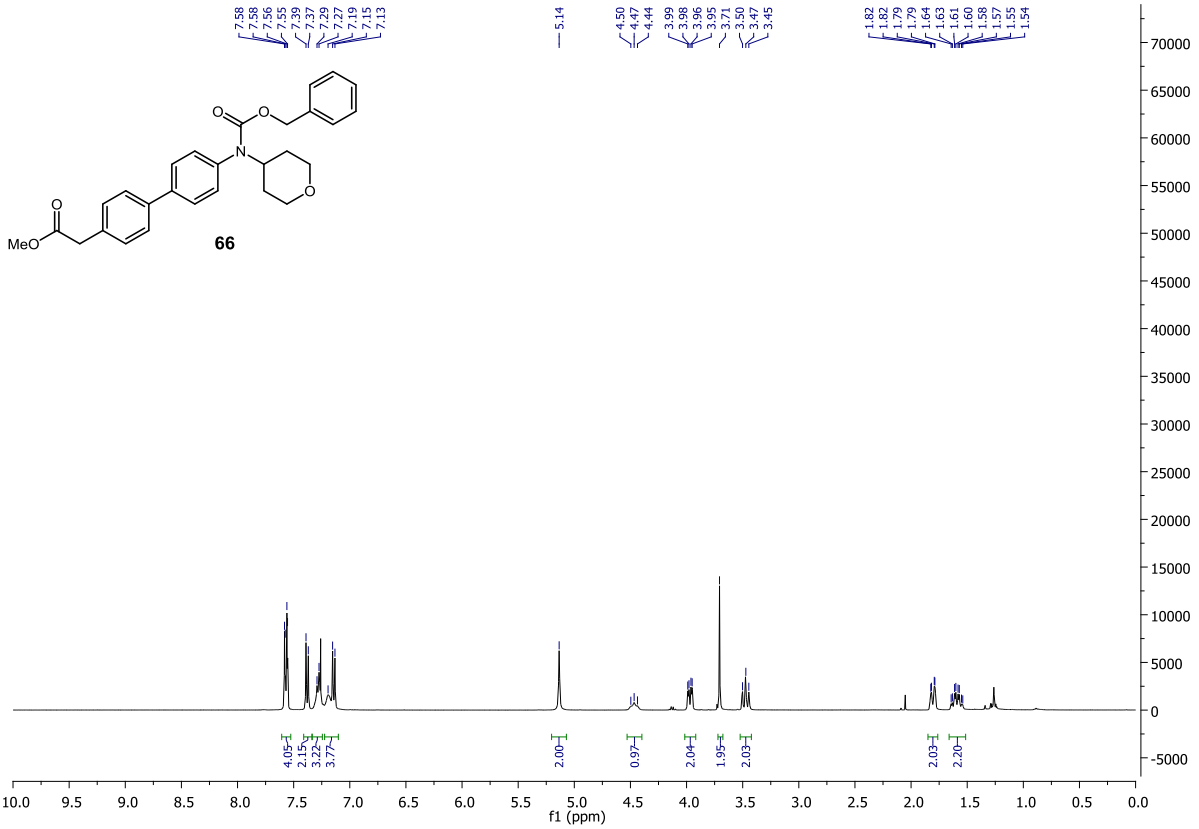


HRMS of 65

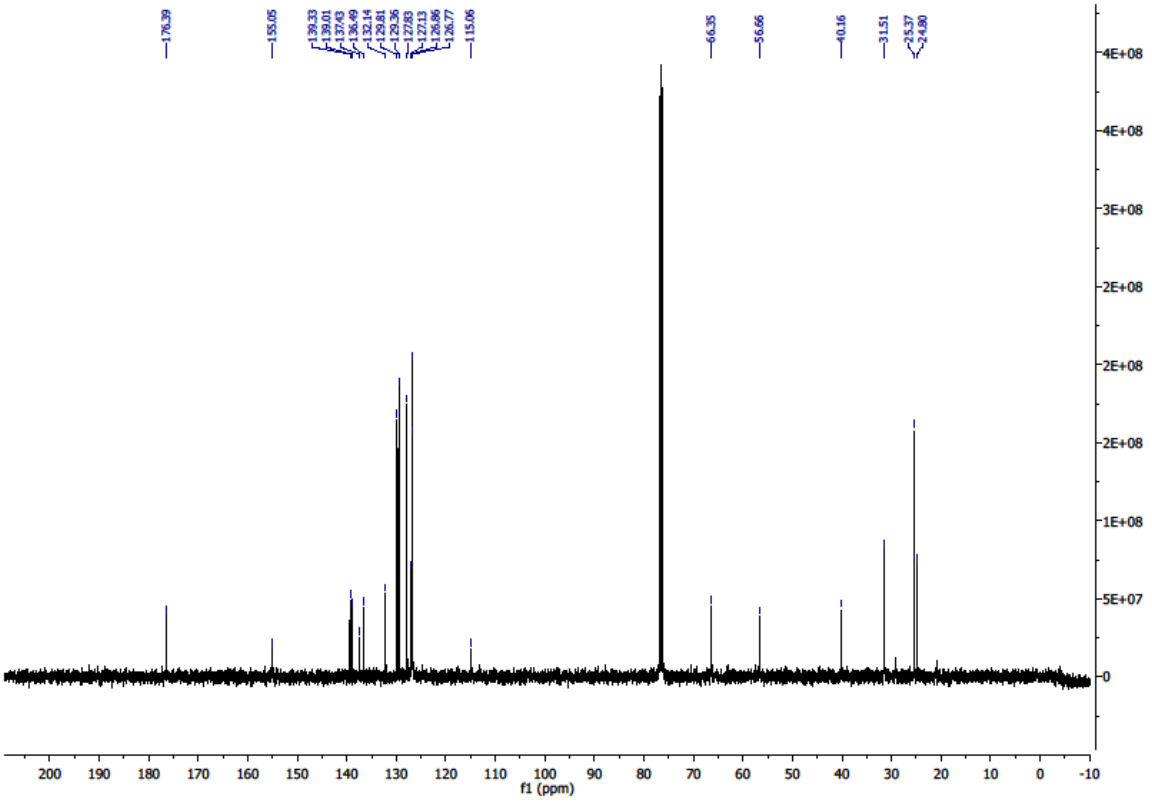


Compound 66

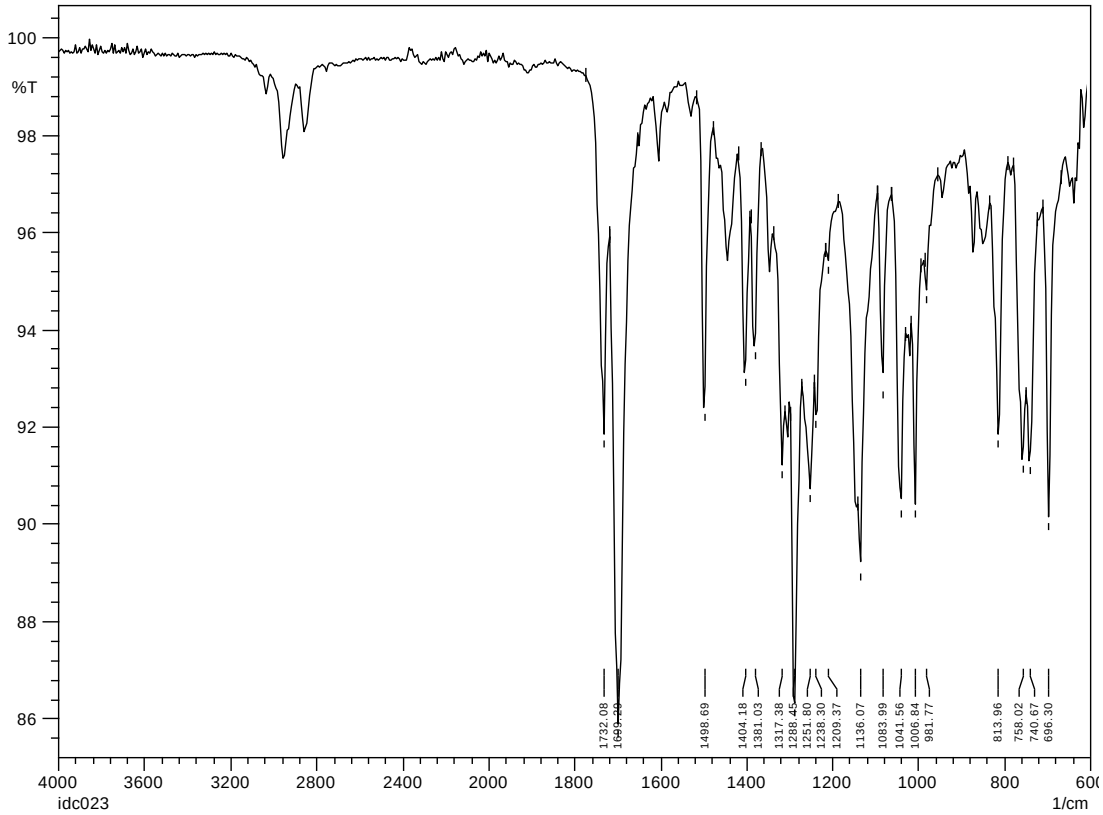
^{1}H NMR



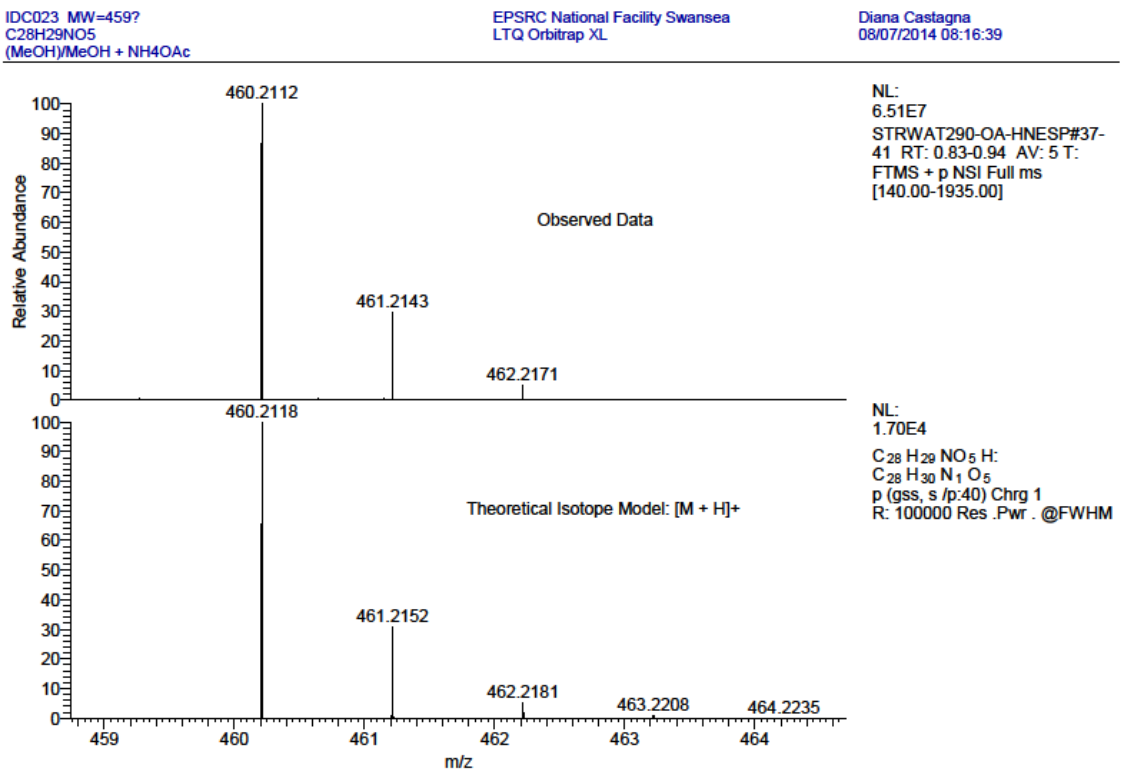
^{13}C NMR of 66



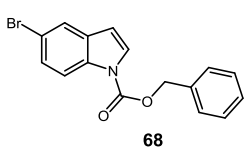
IR of 66



HRMS of 66

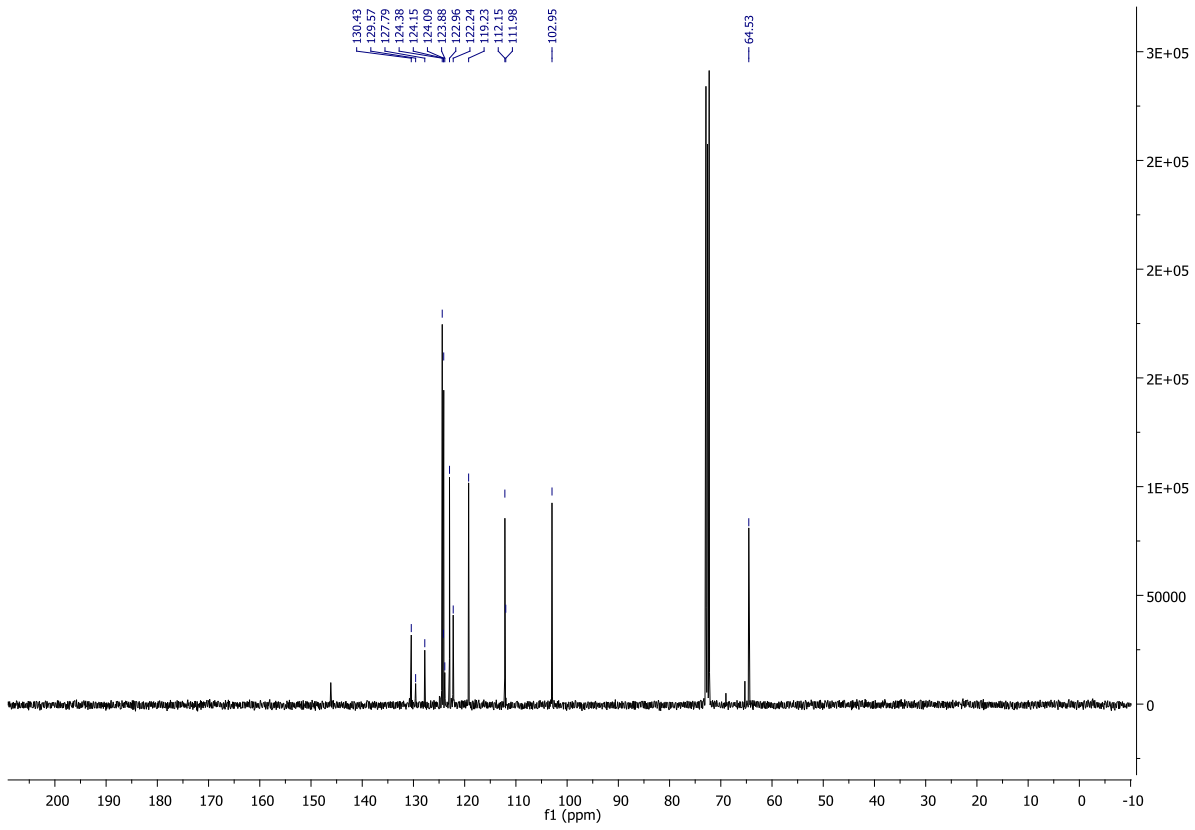


Compound 68
^{1}H NMR

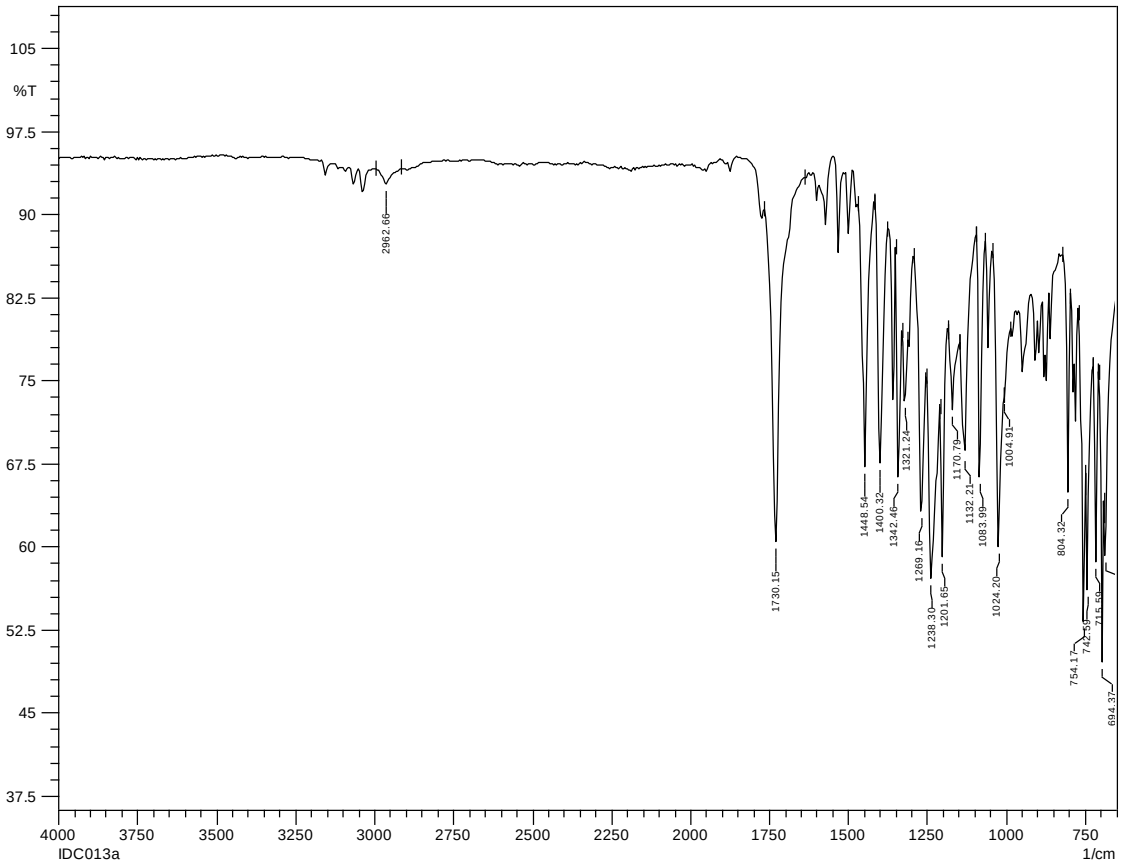


68

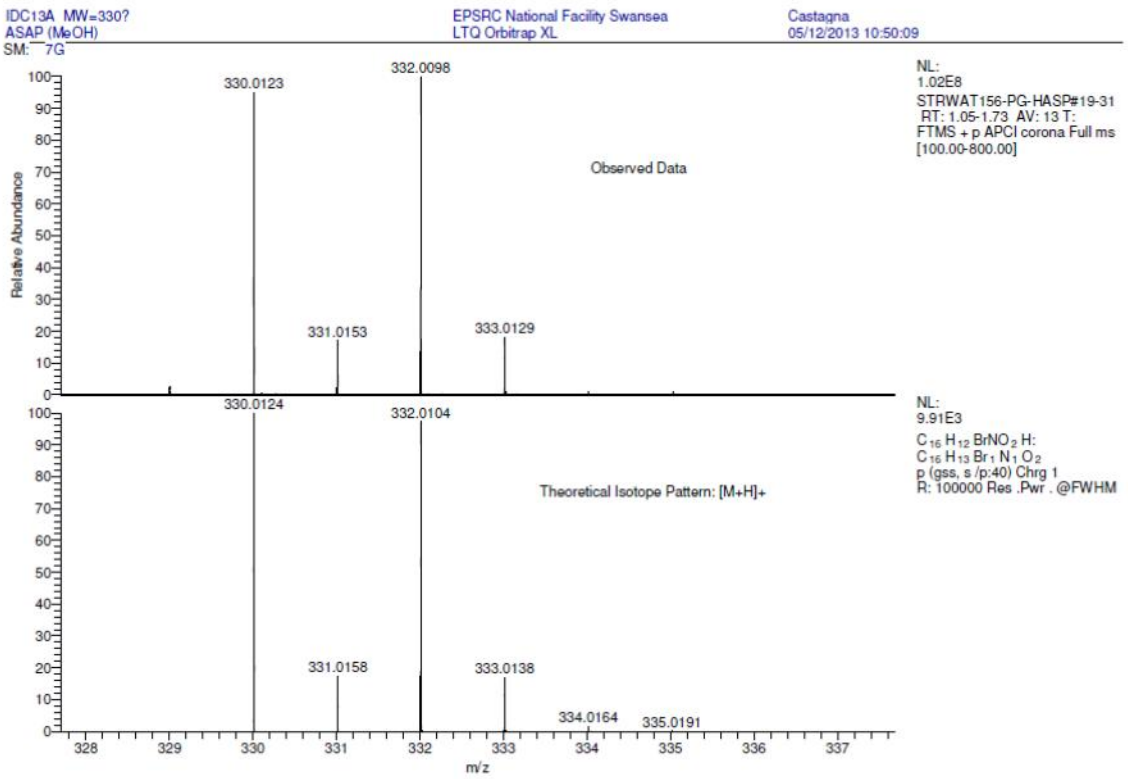
^{13}C NMR of 68



IR of 68

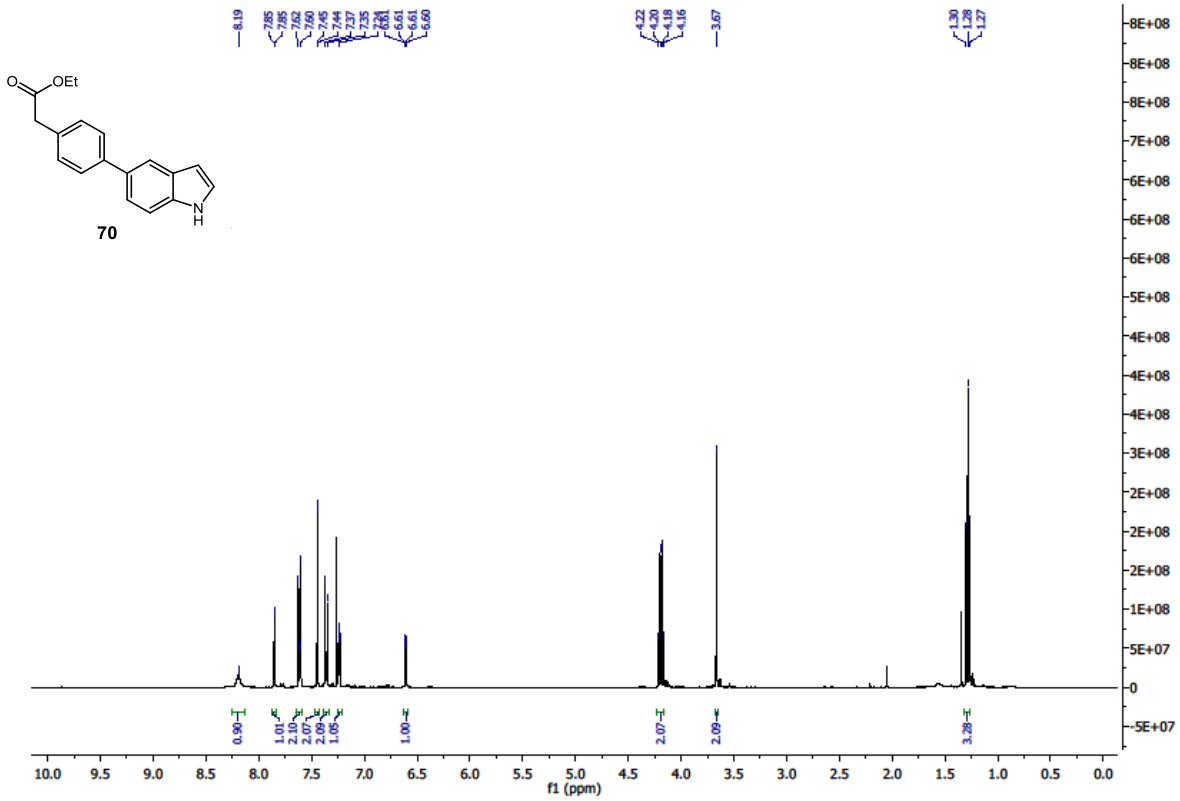


HRMS of 68

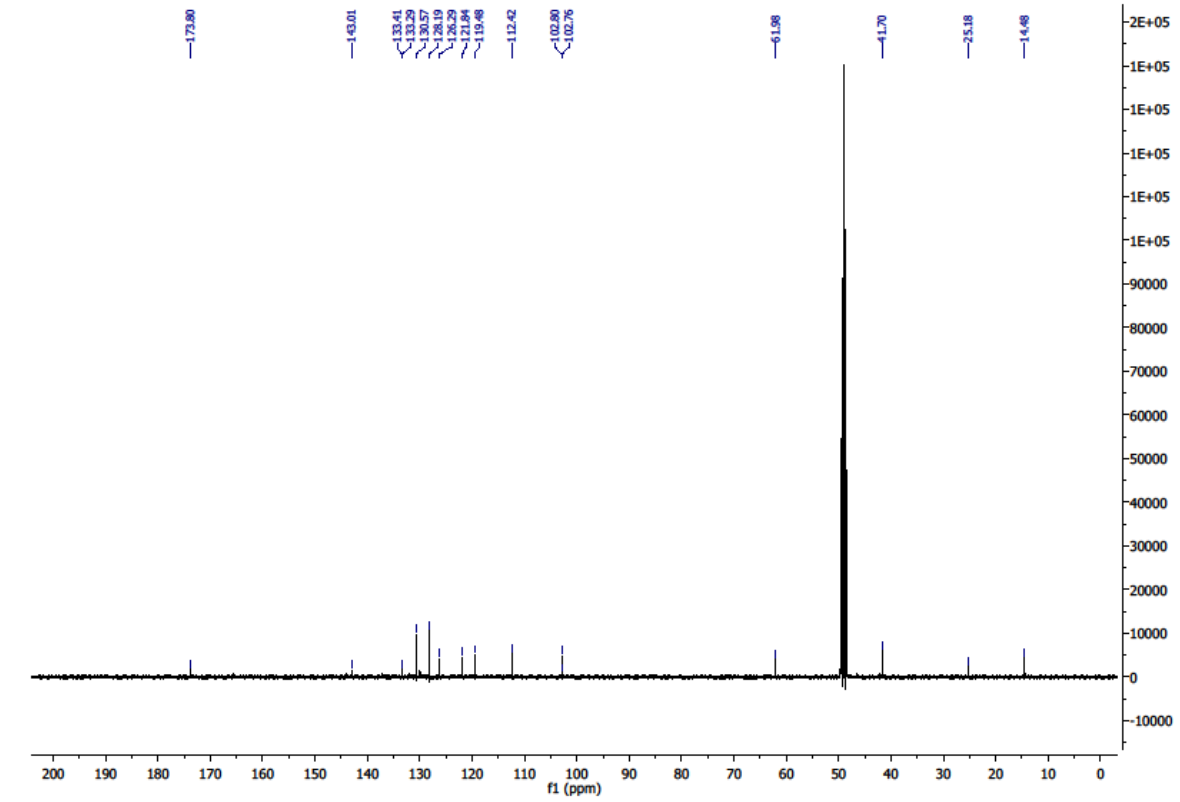


Compound 70

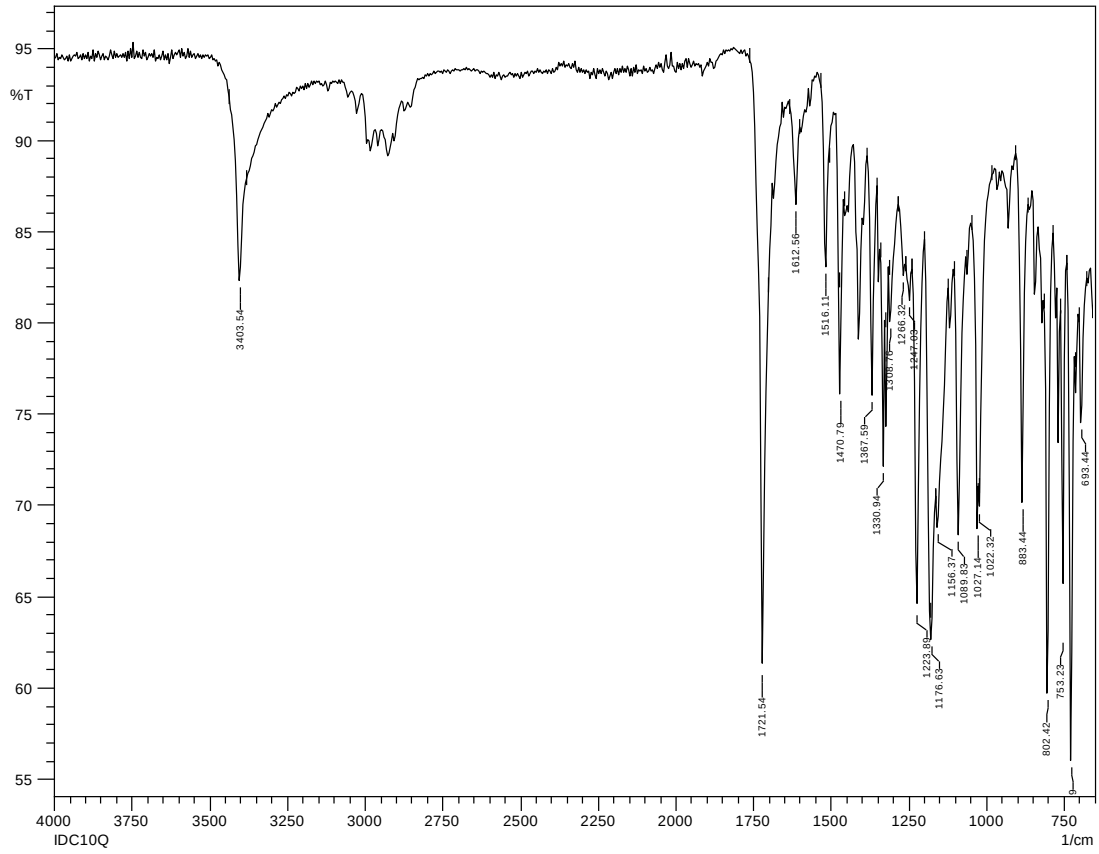
^{1}H NMR



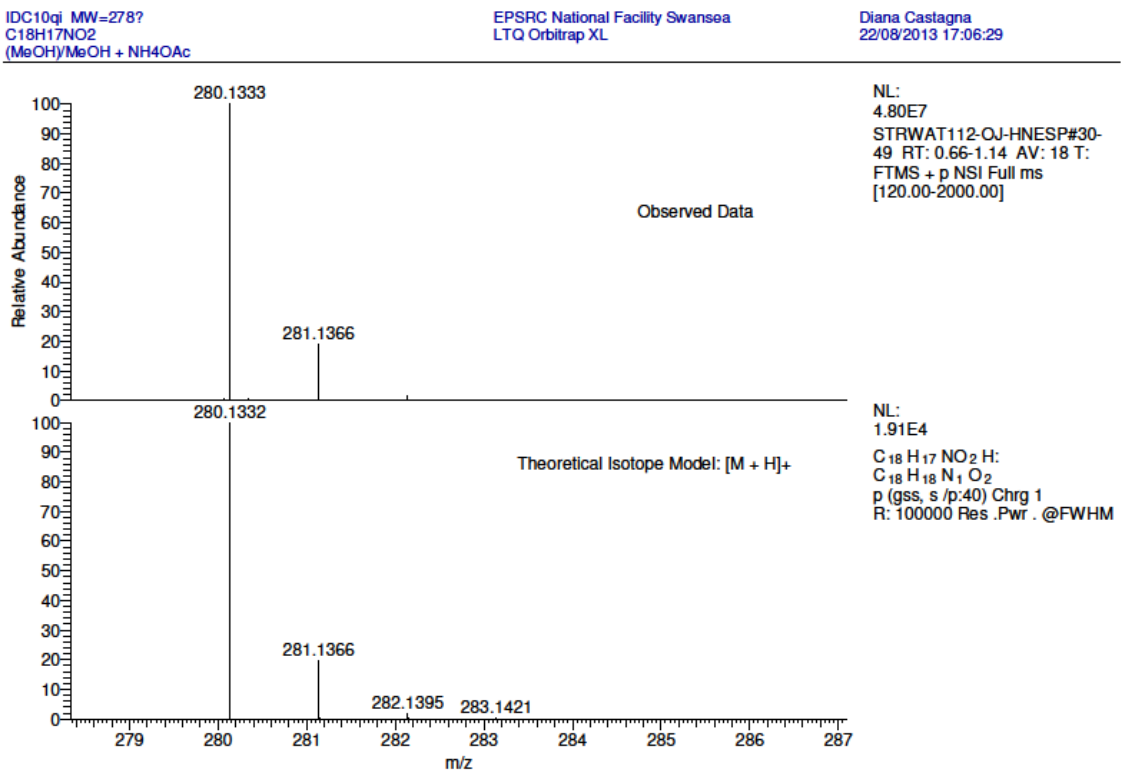
^{13}C NMR of 70



IR of 70

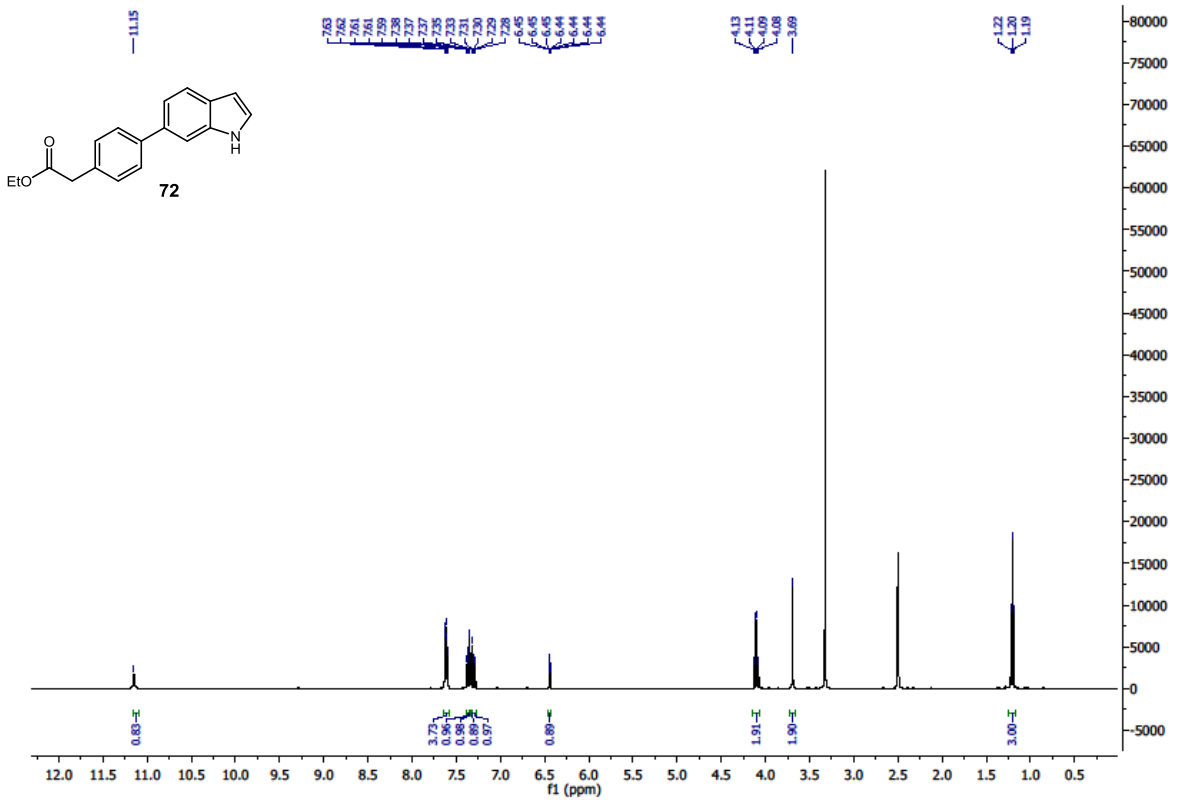


HRMS of 70

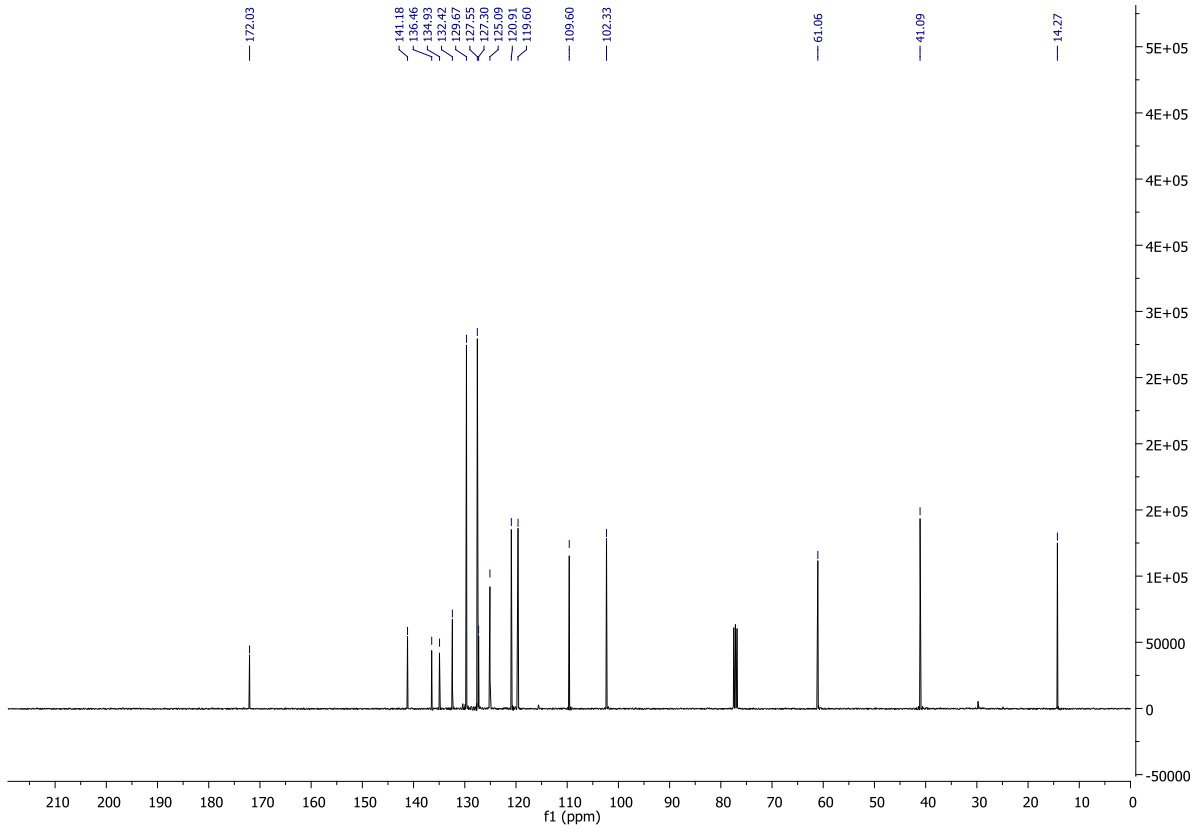


Compound 72

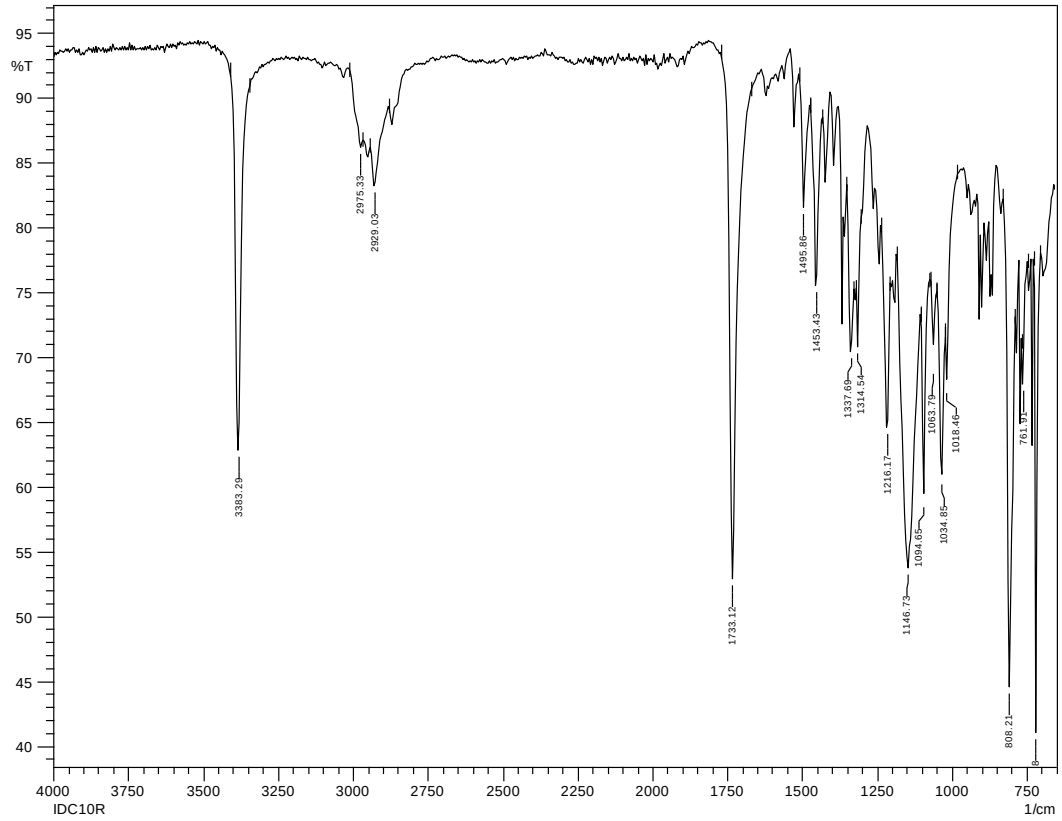
^{1}H NMR



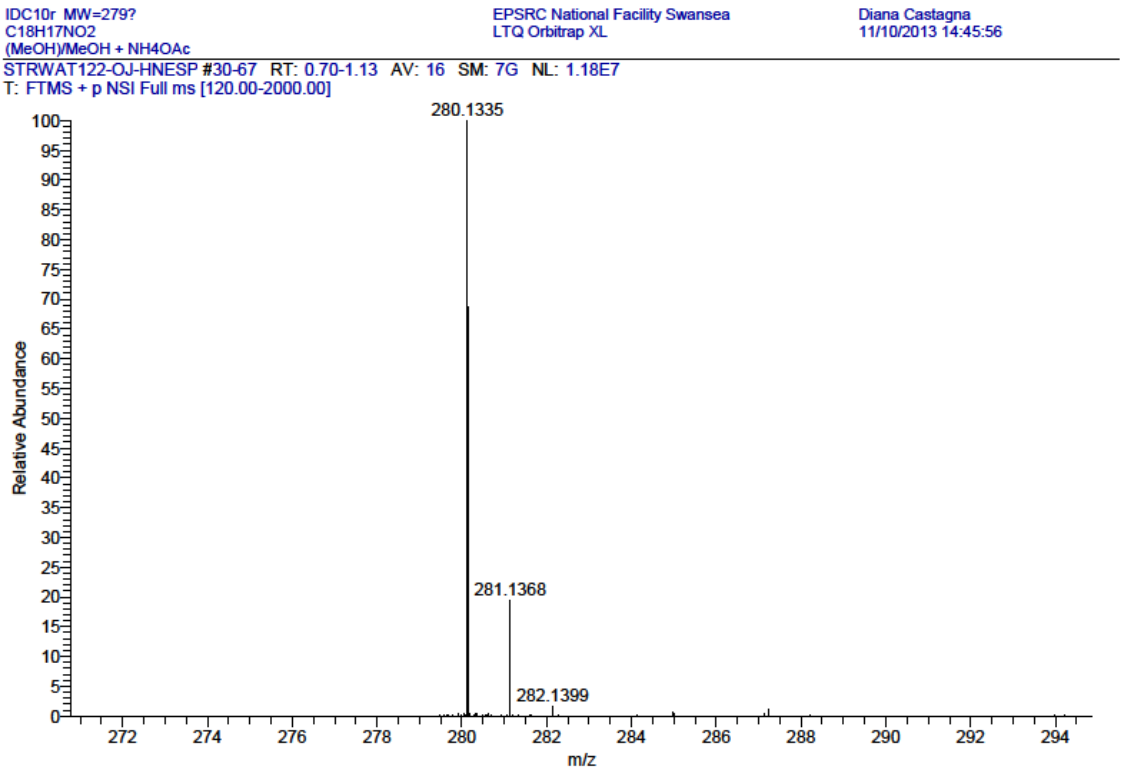
^{13}C NMR of 72



IR of 72

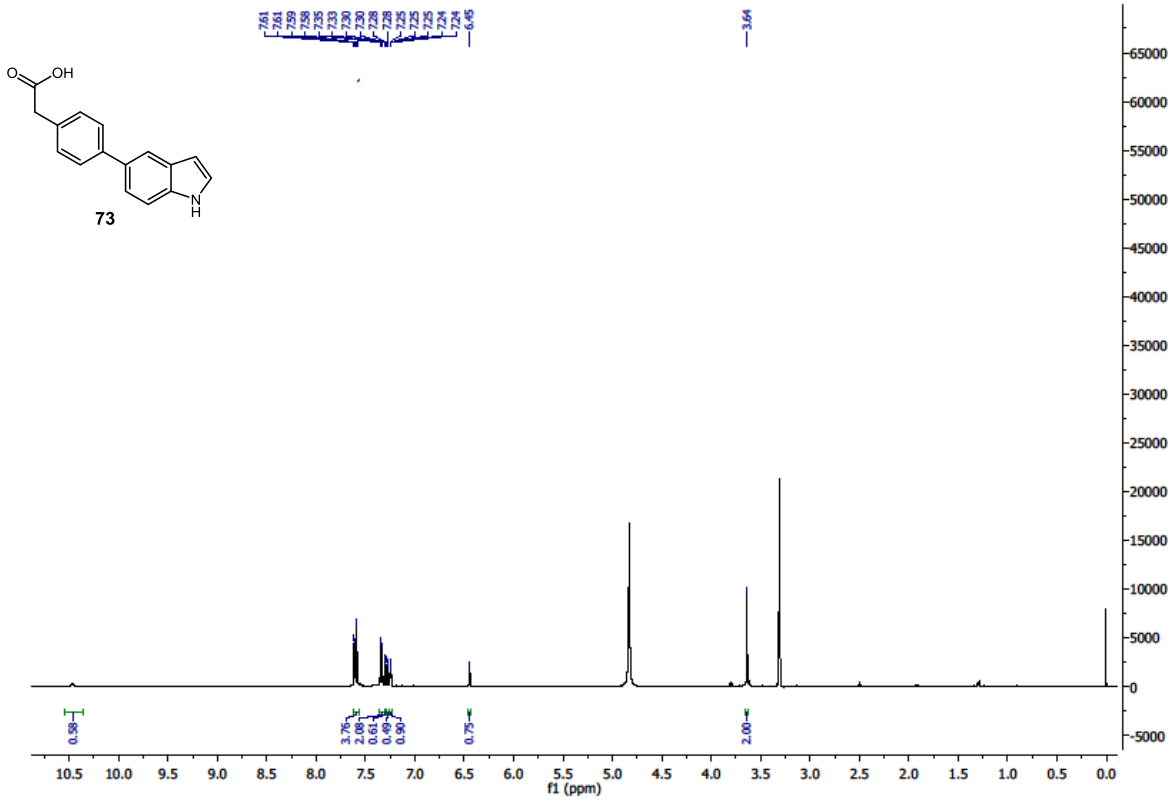


HRMS of 72

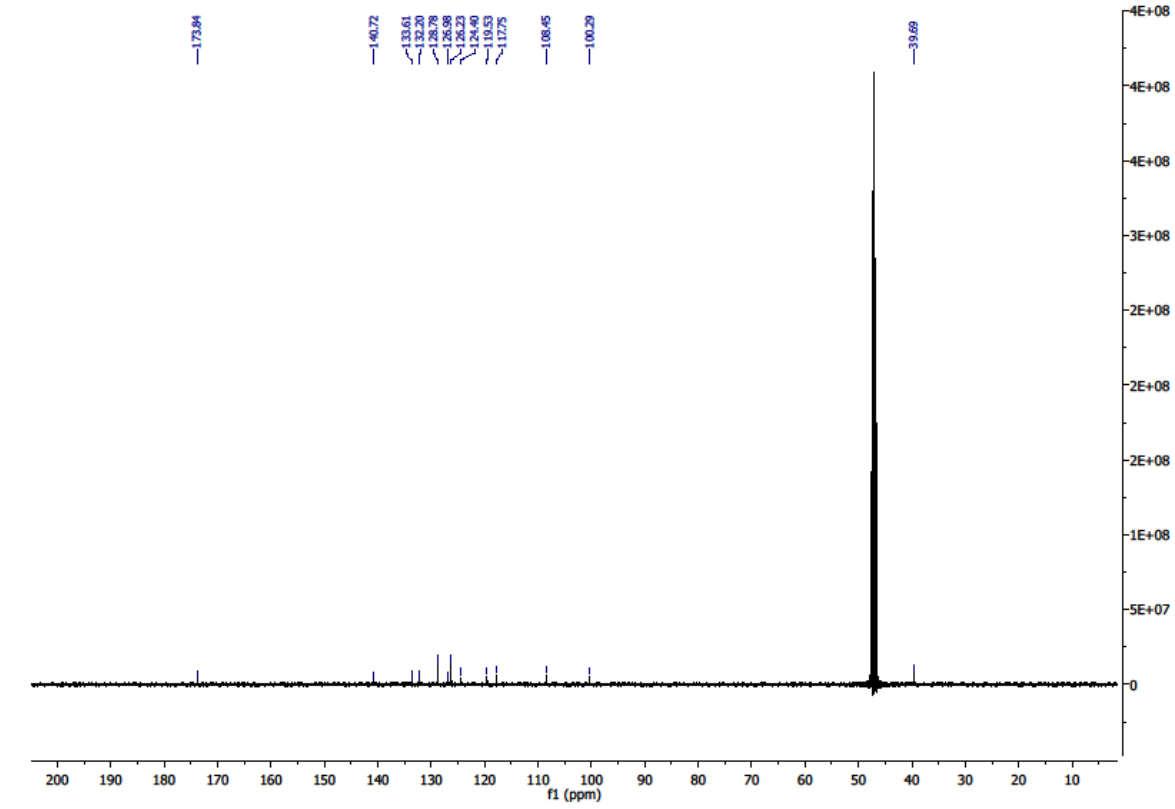


Compound 73

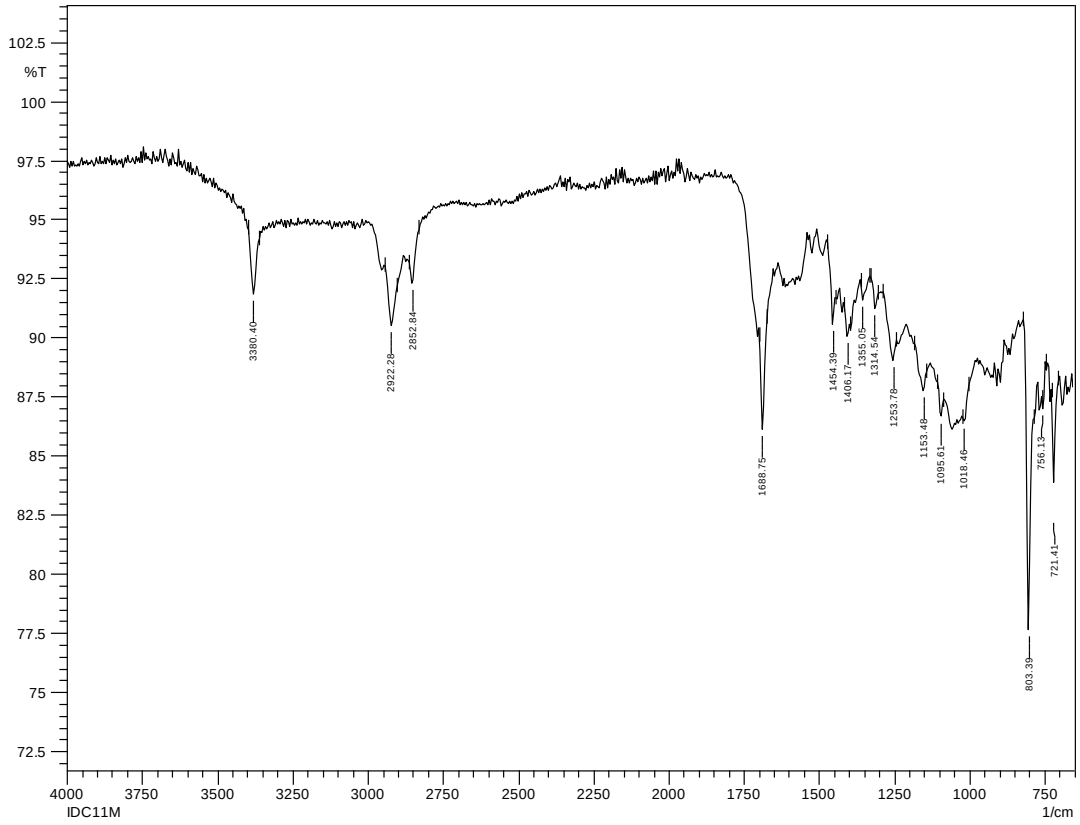
^{1}H NMR



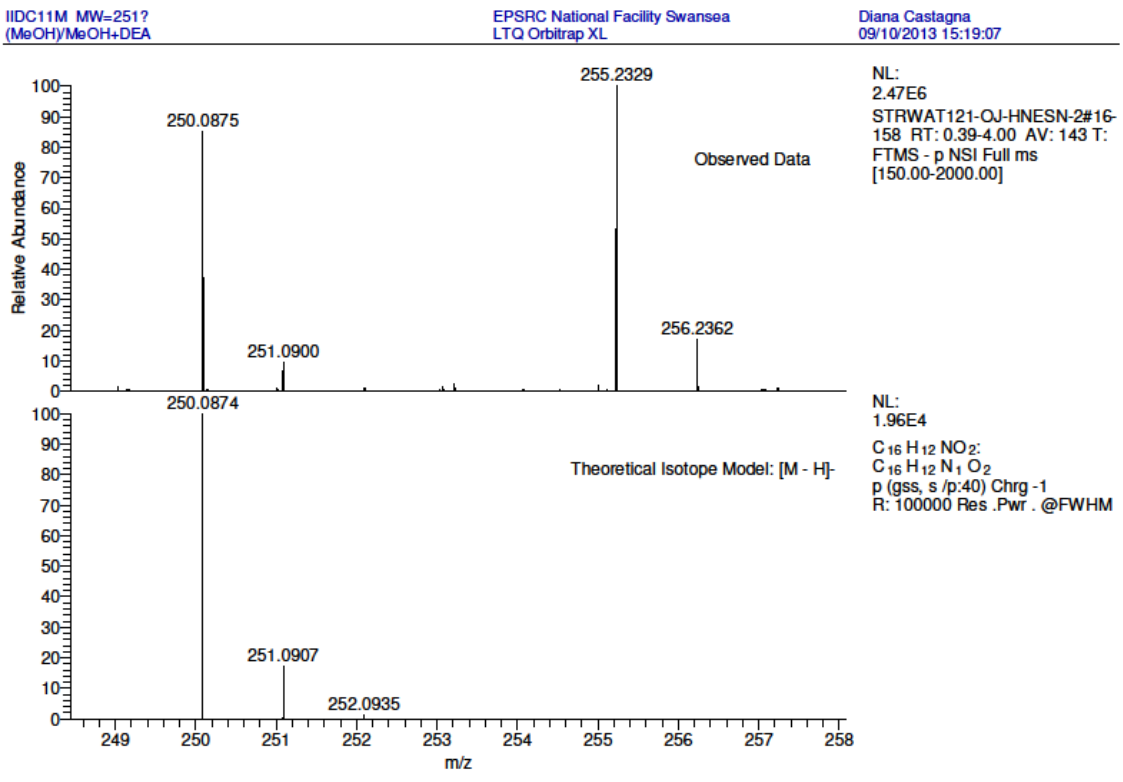
^{13}C NMR of 73



IR of 73

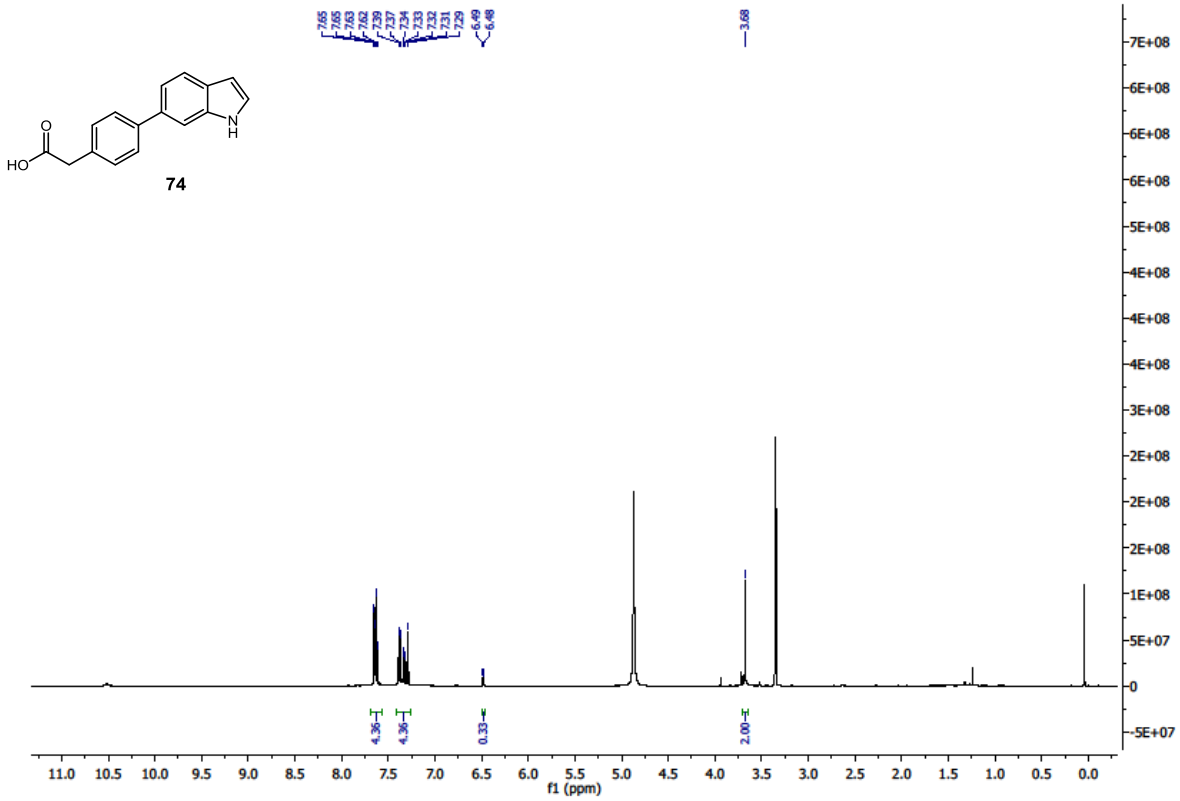


HRMS of 73

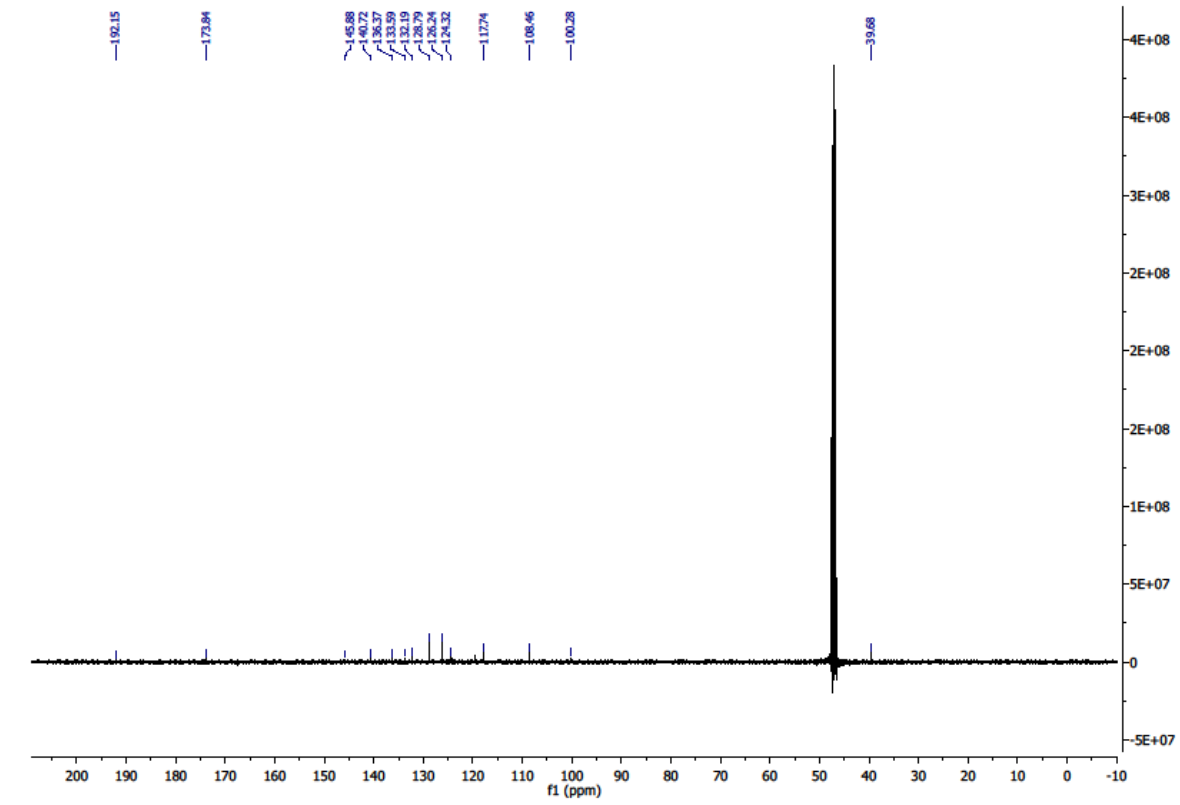


Compound 74

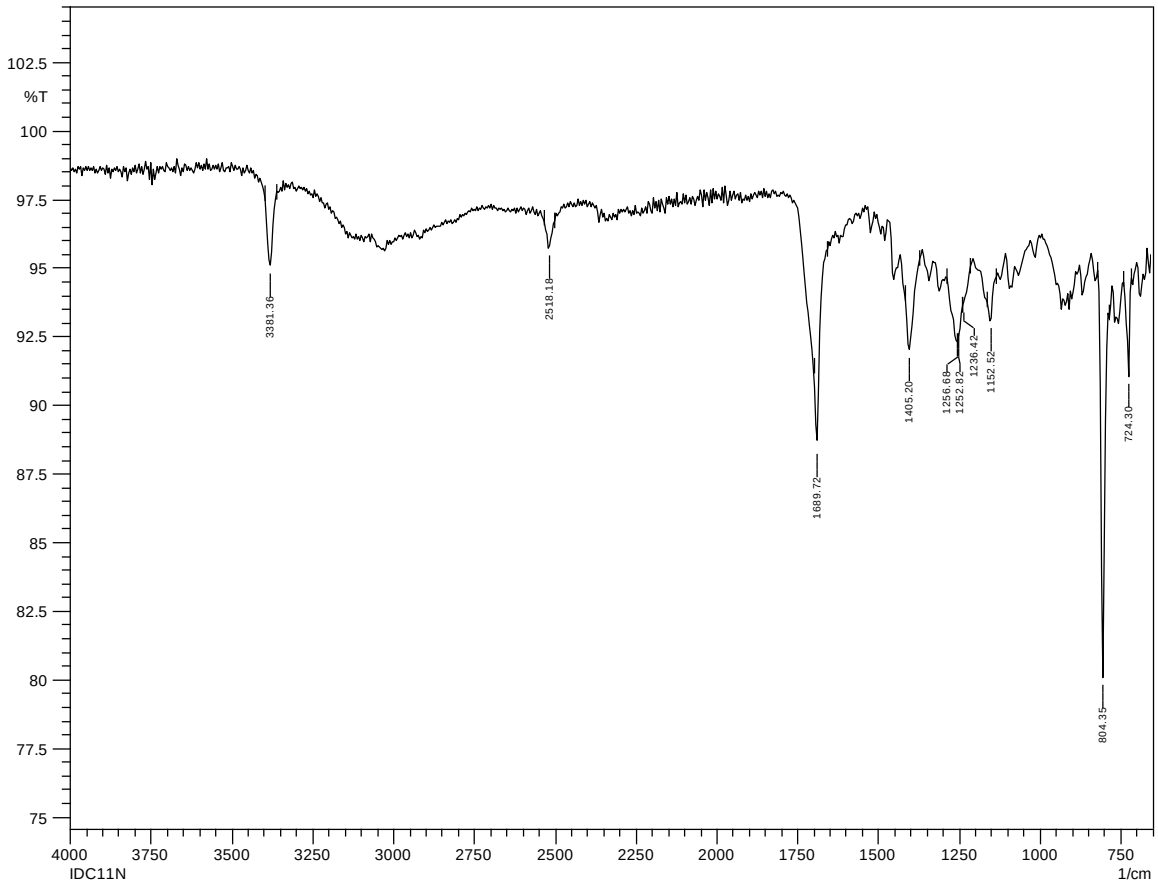
^{1}H NMR



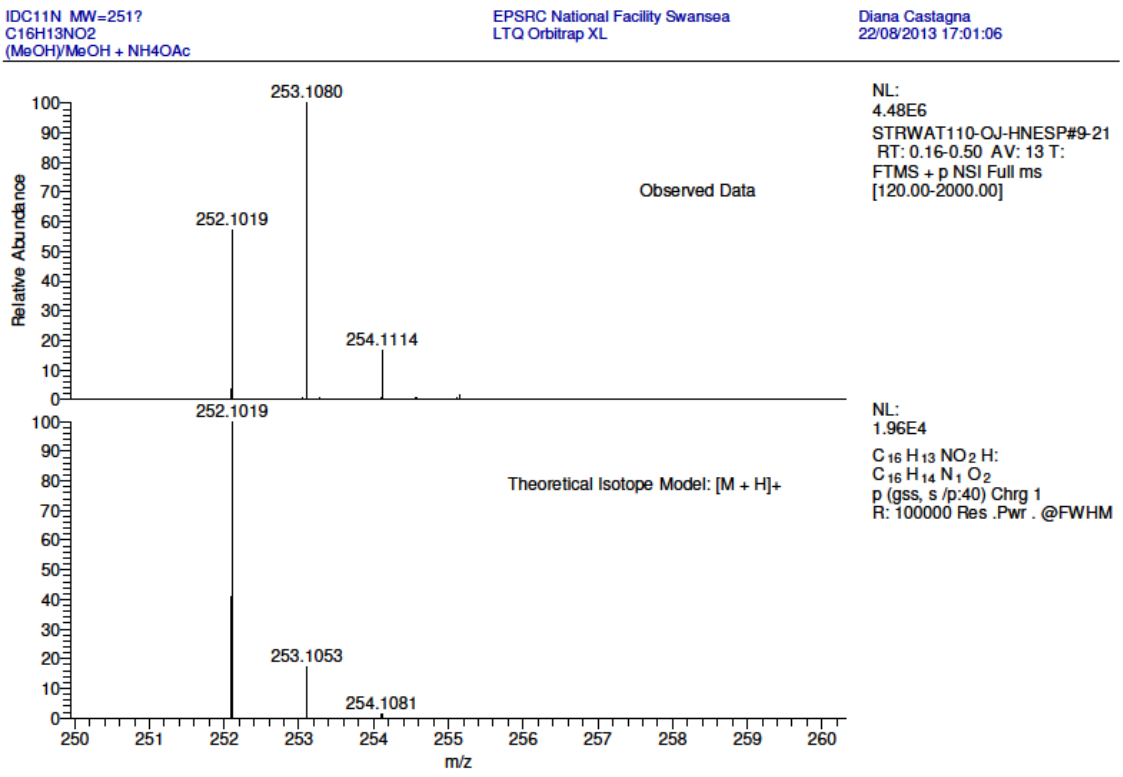
^{13}C NMR of 74



IR of 74

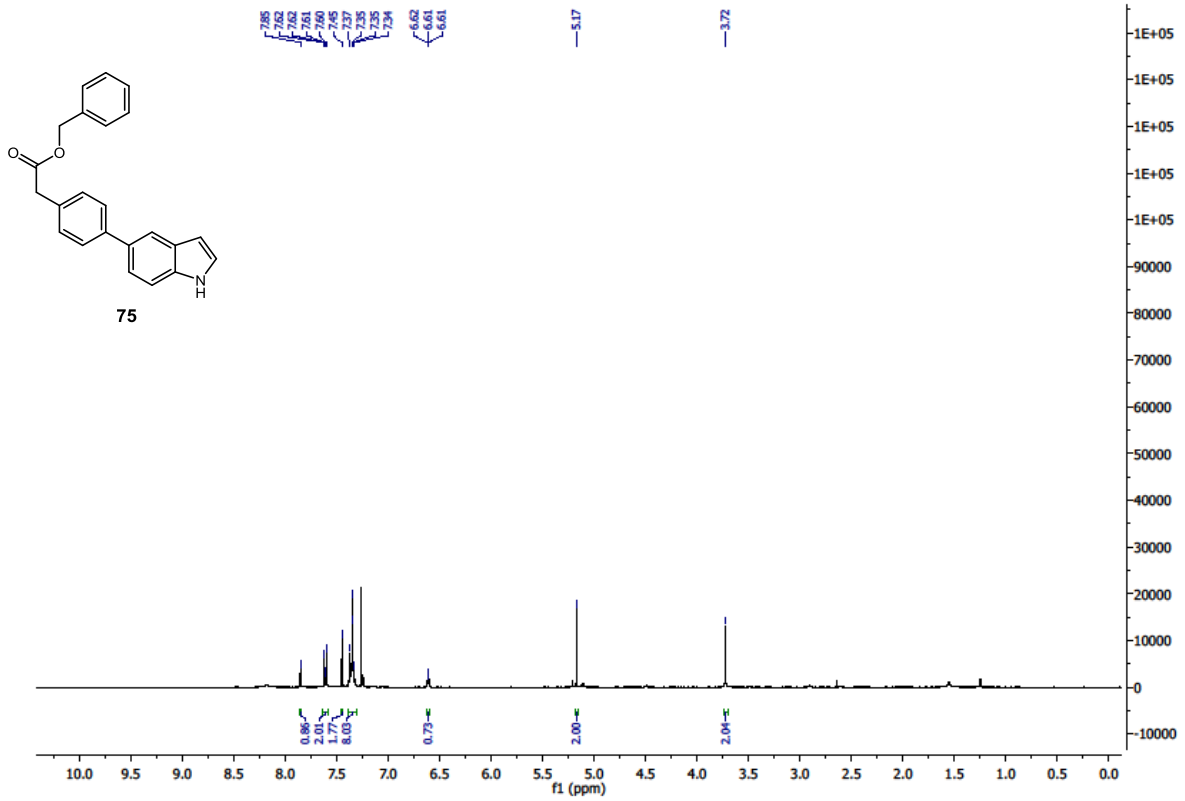


HRMS of 74

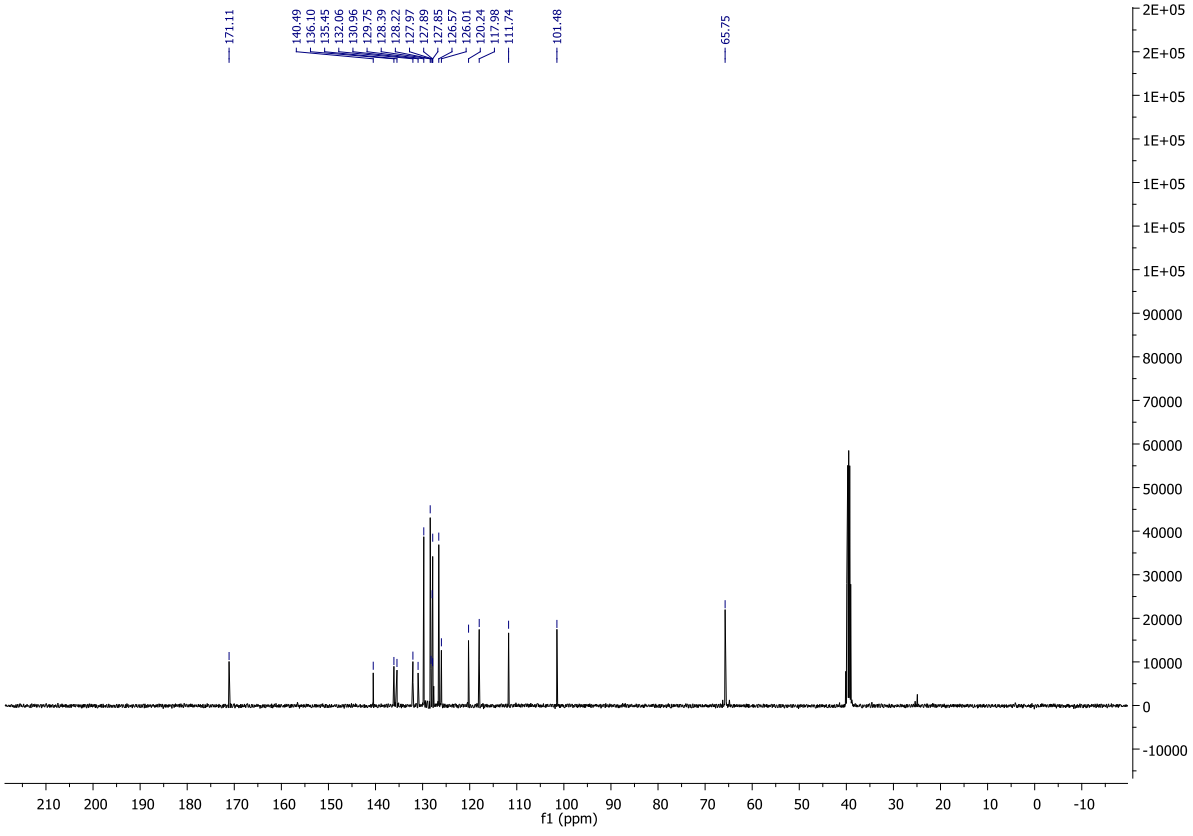


Compound 75

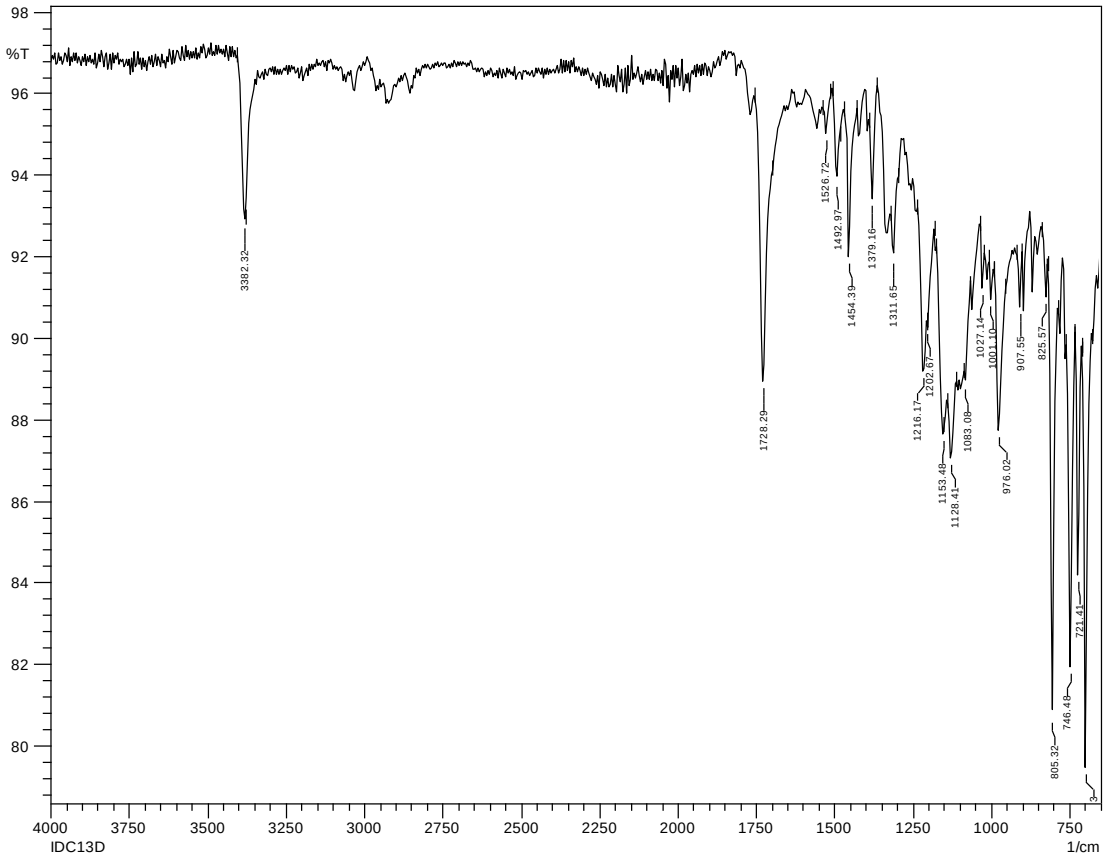
^{1}H NMR



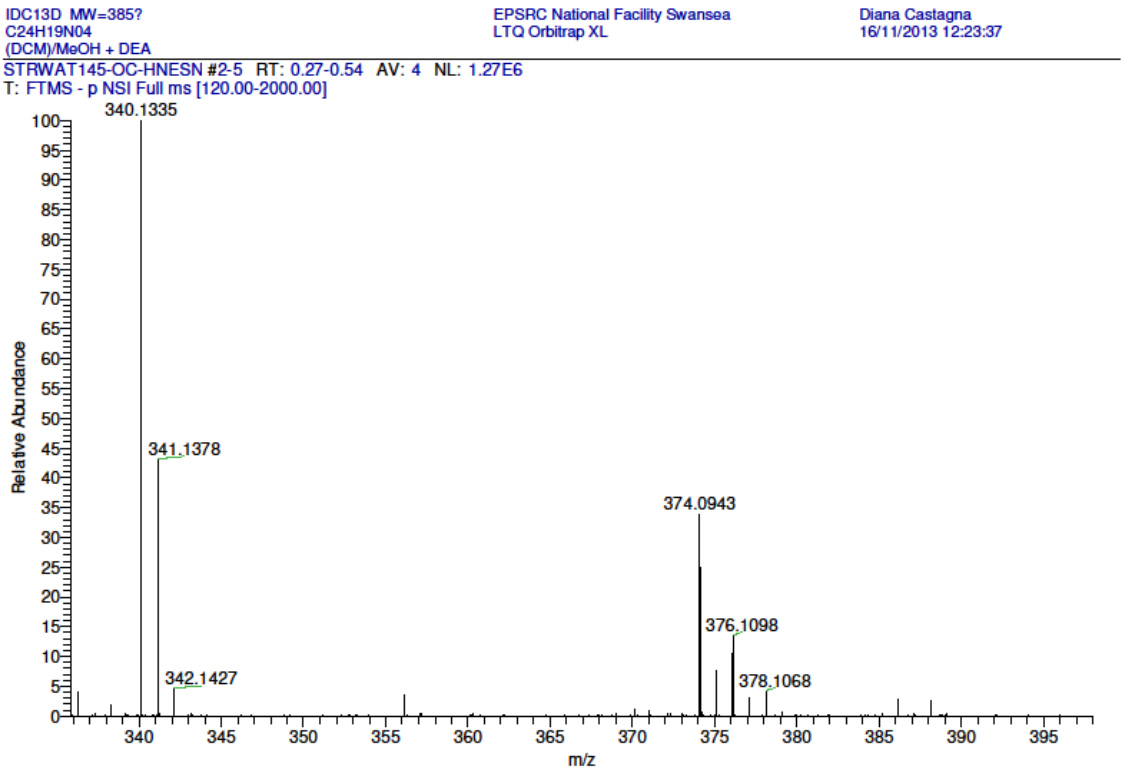
^{13}C NMR of 75



IR of 75

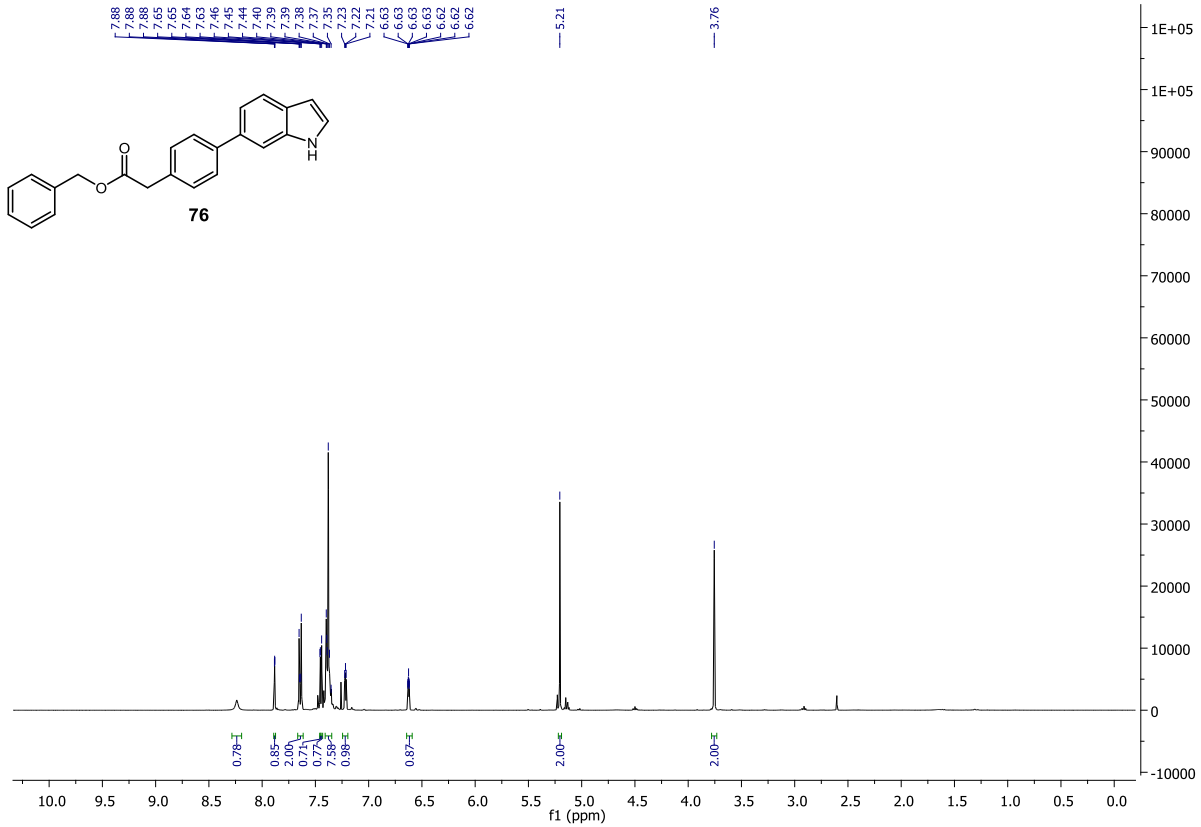


HRMS of 75

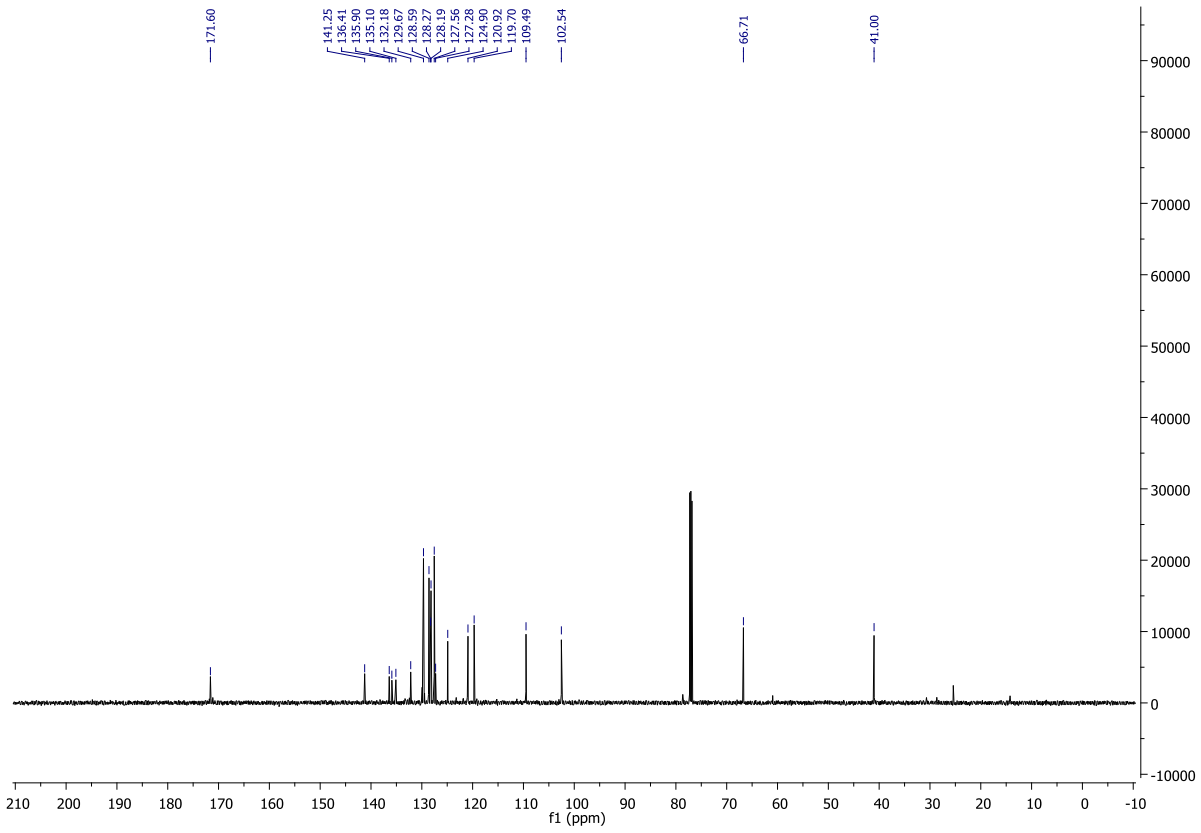


Compound 76

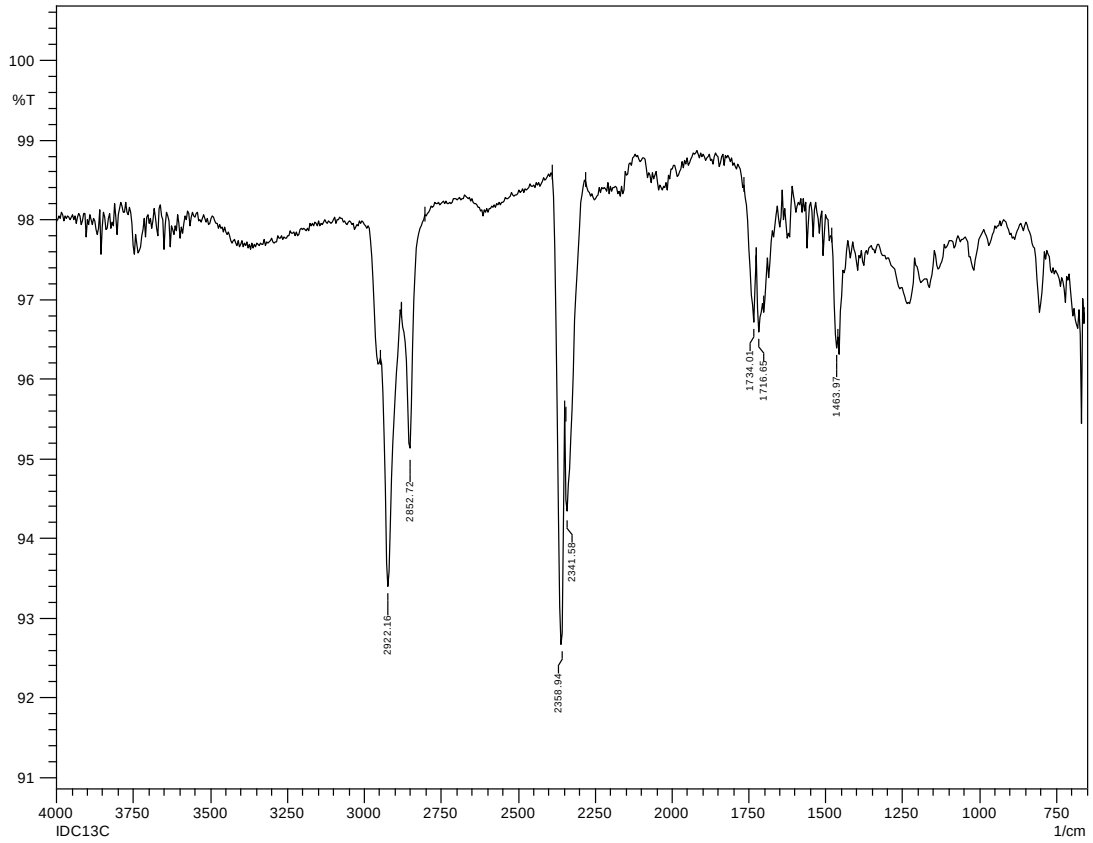
^{1}H NMR



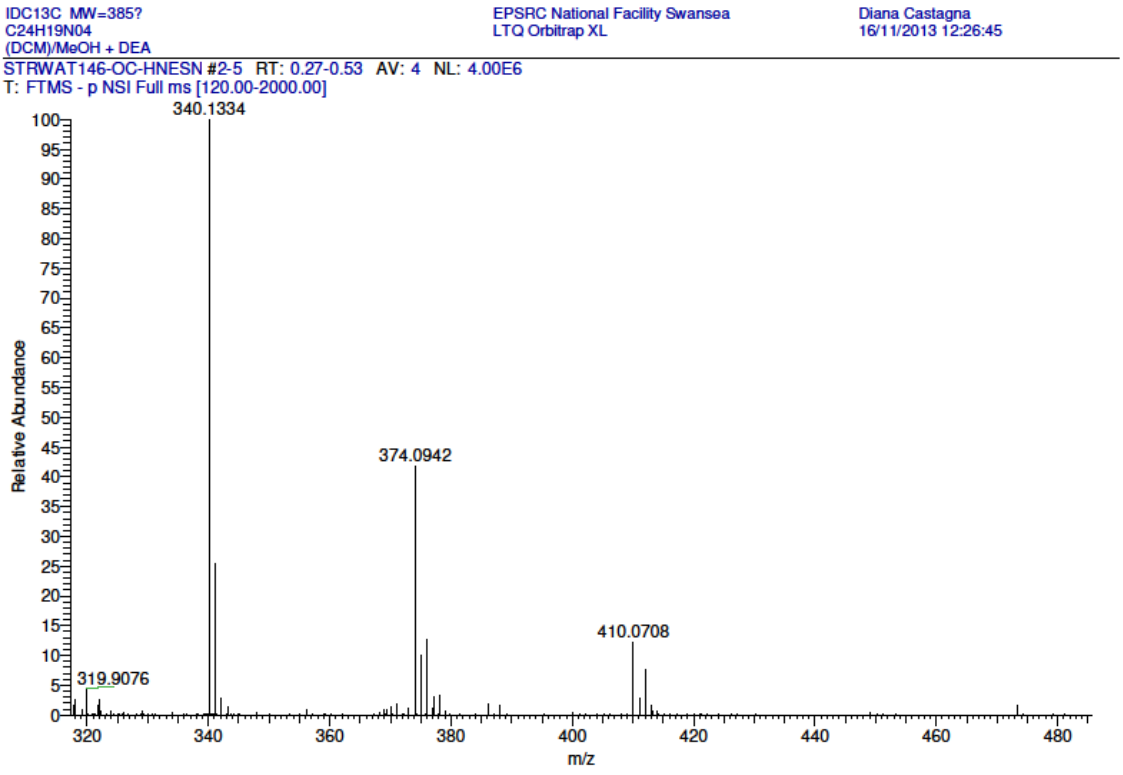
^{13}C NMR of 76



IR of 76

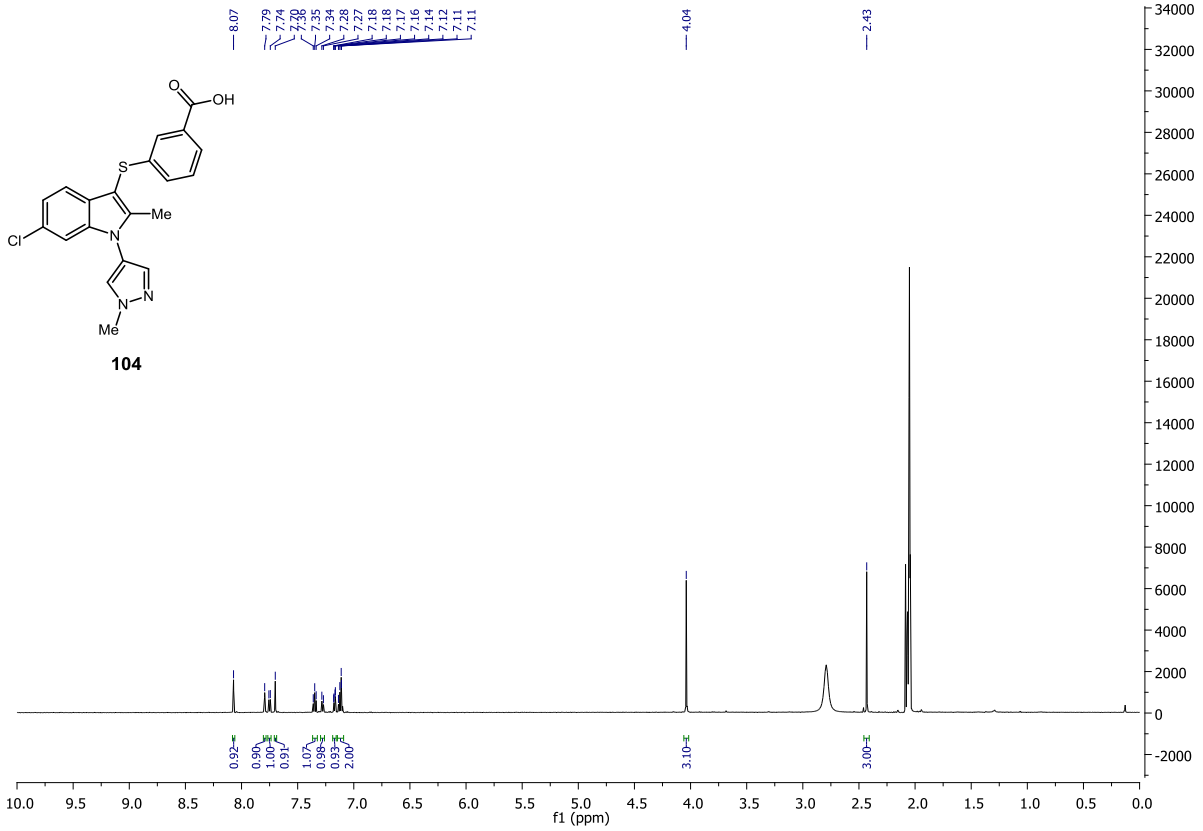


HRMS of 76

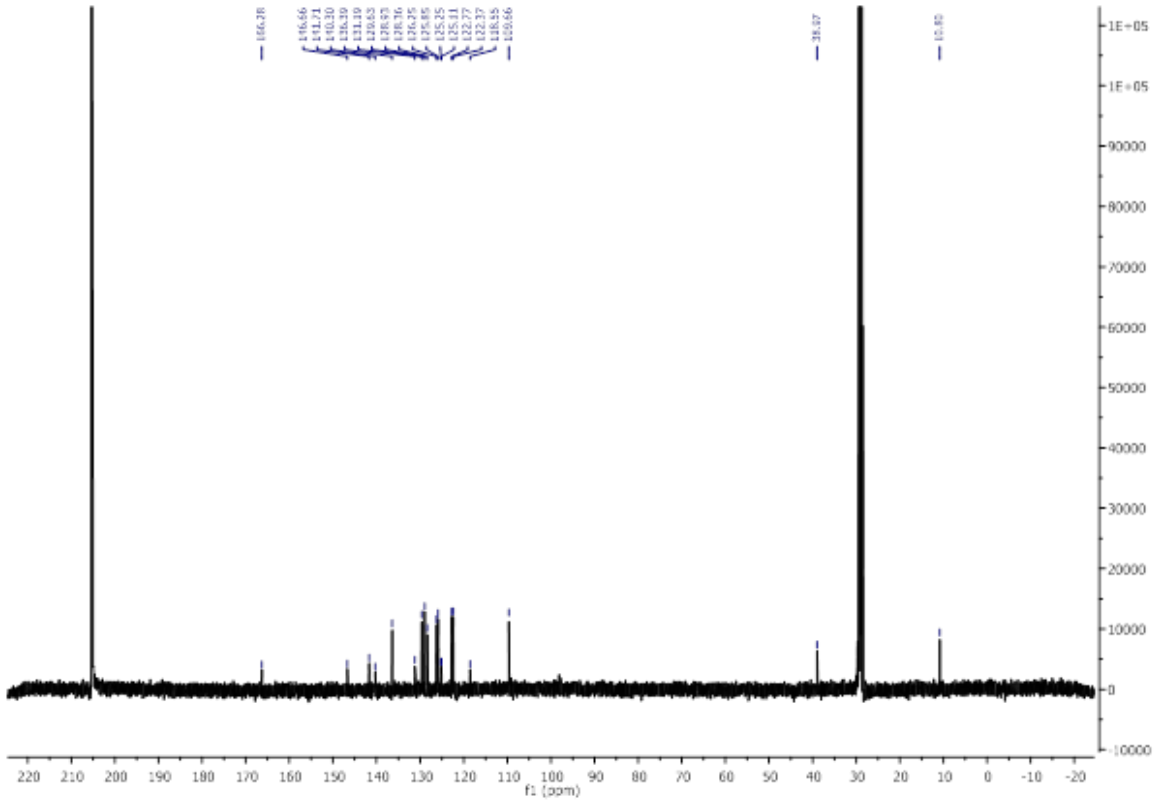


Compound 104

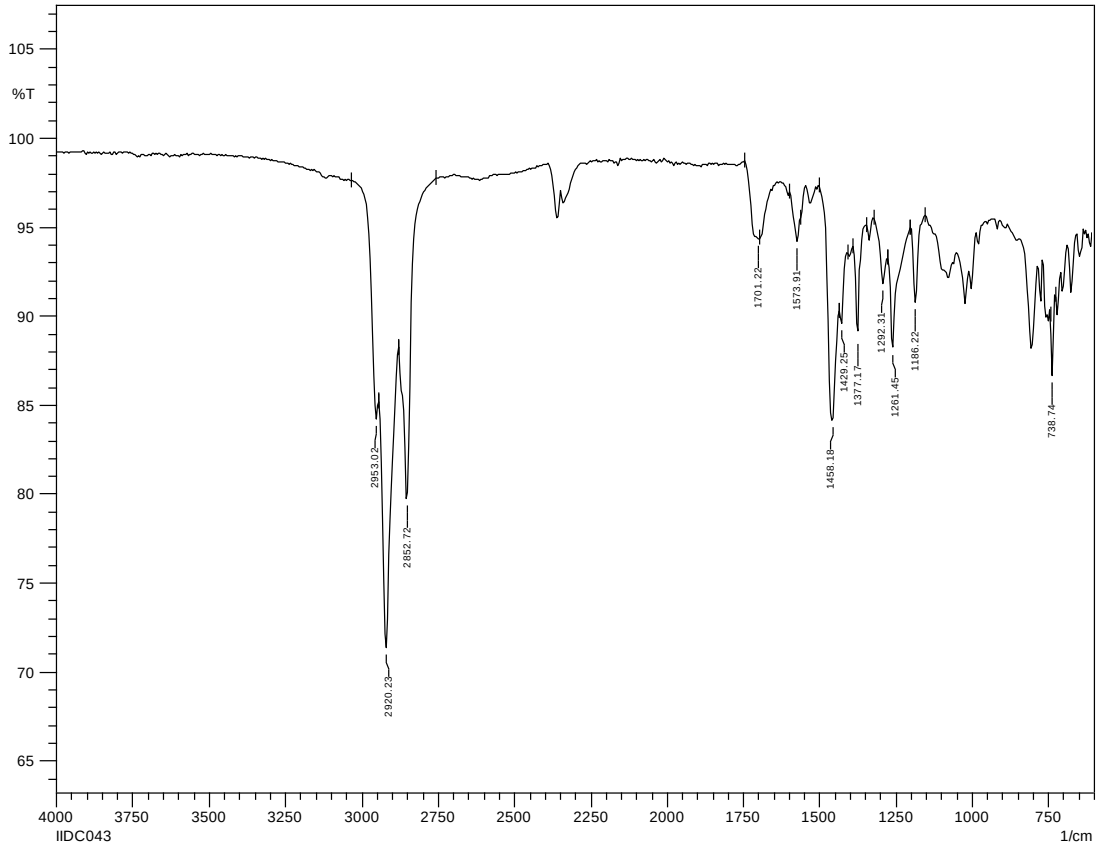
^{1}H NMR



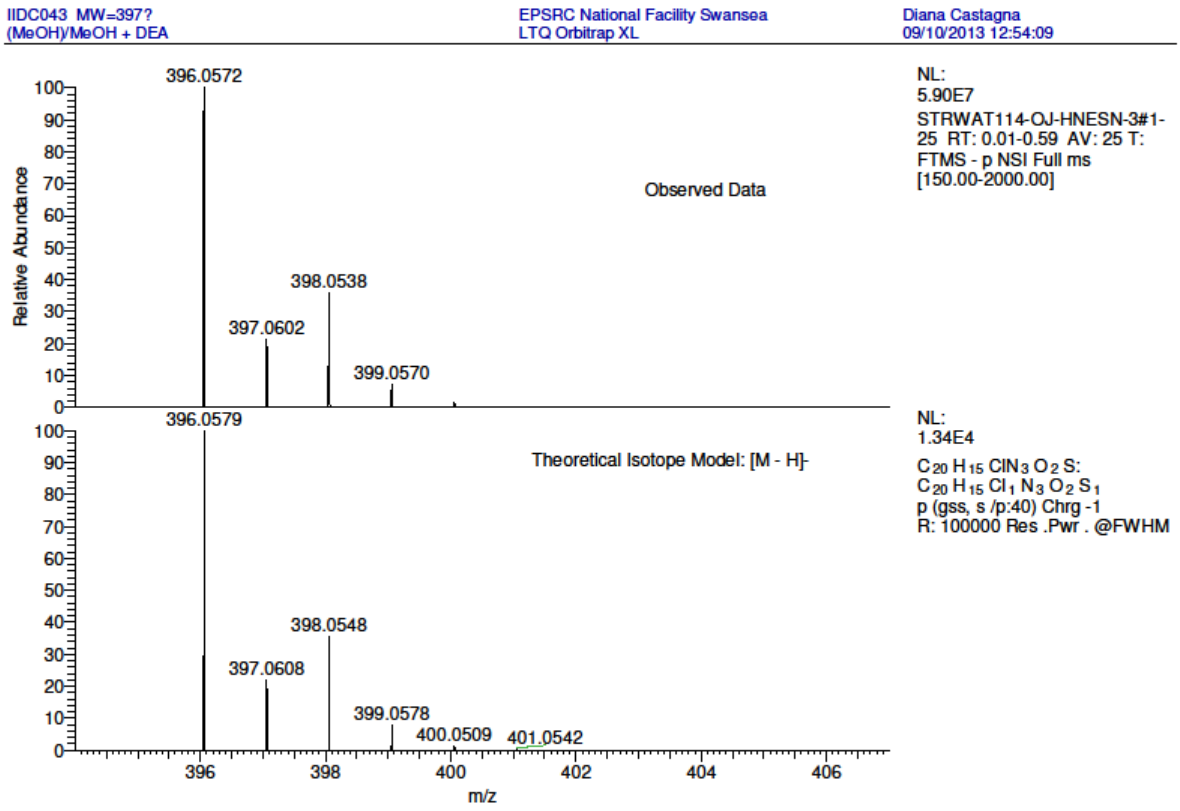
^{13}C NMR of 104



IR of 104

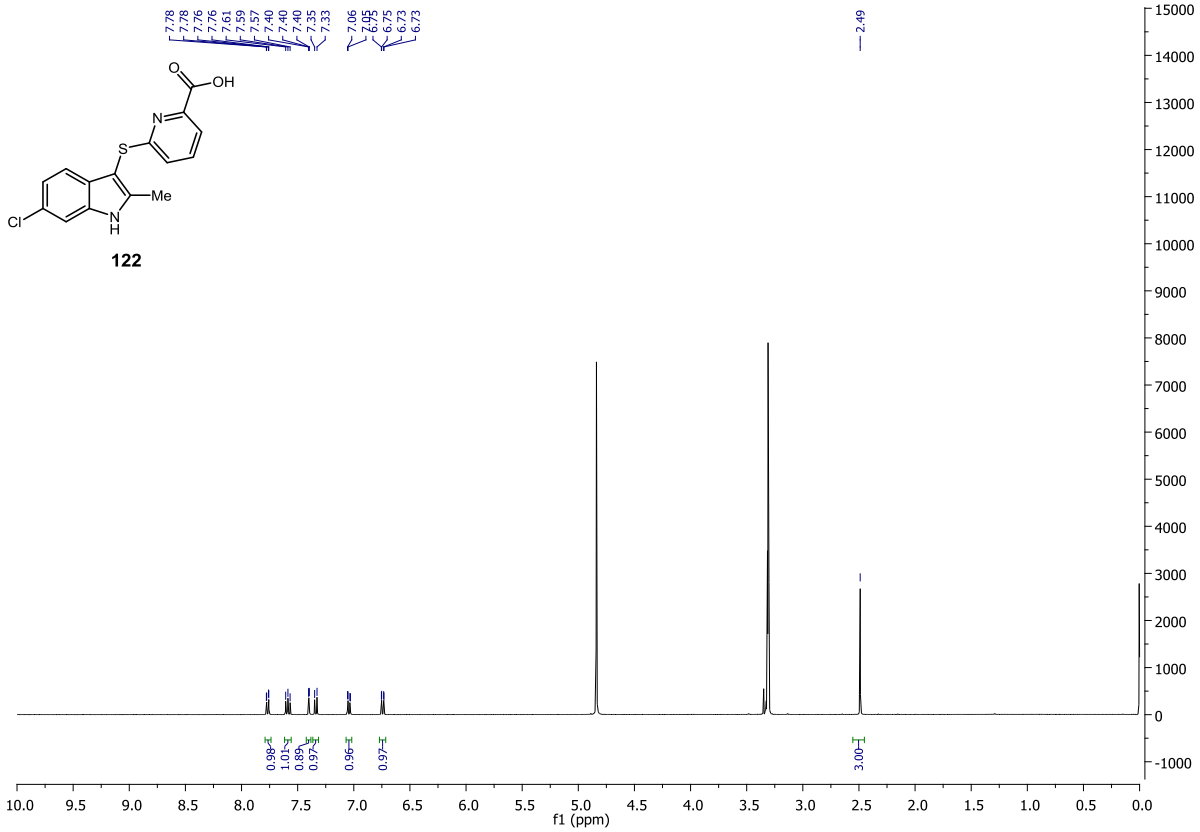


HRMS of 104

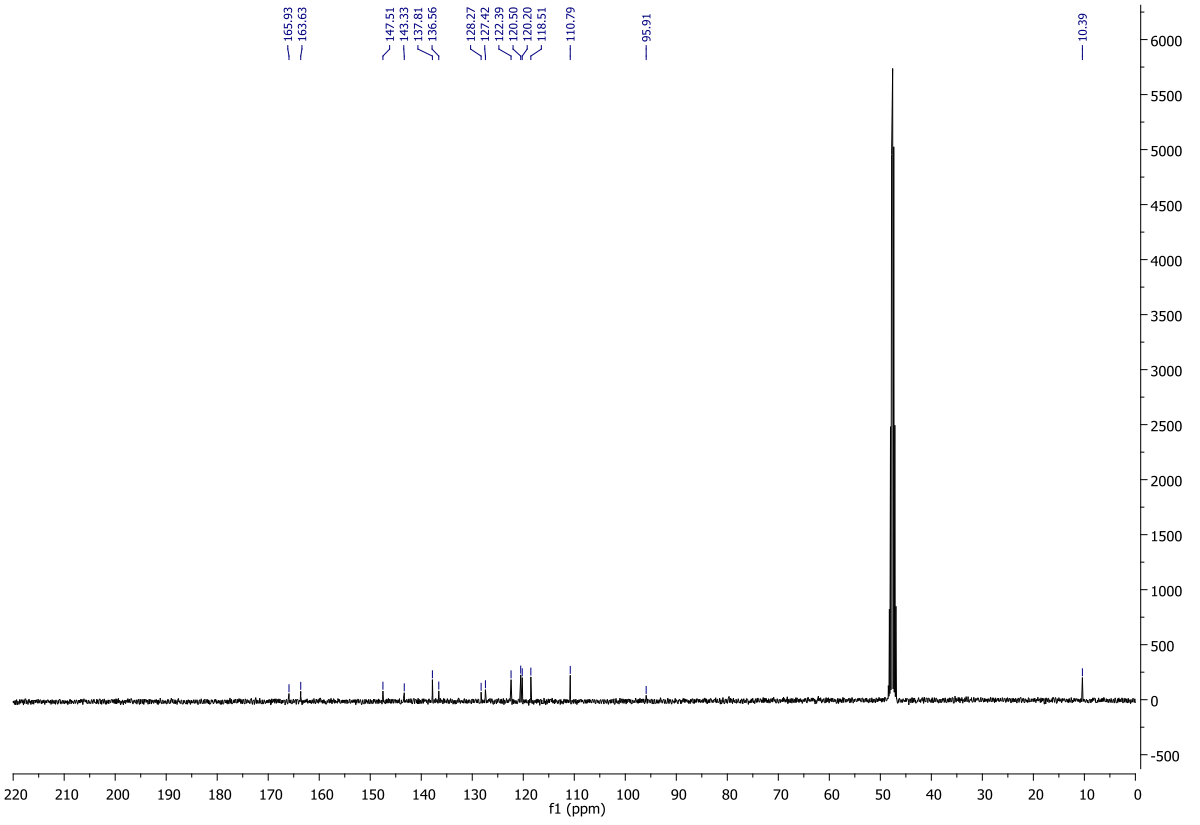


Compound 122

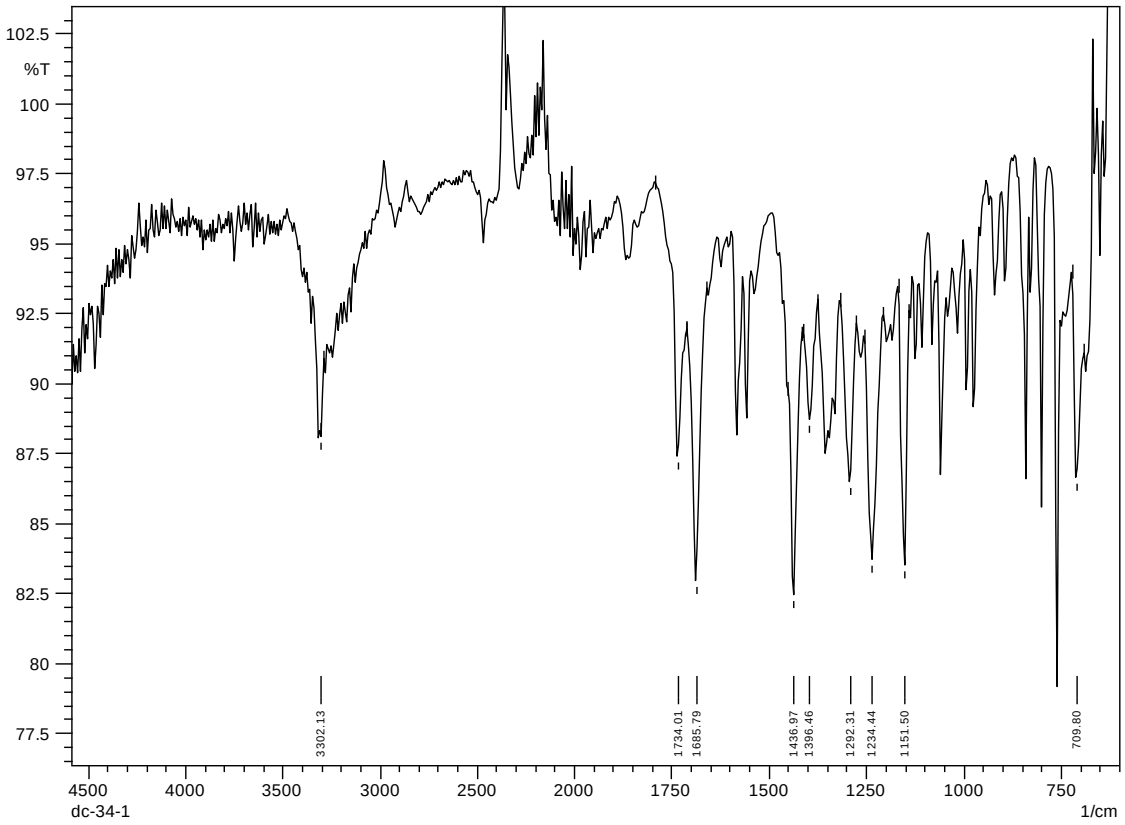
^{1}H NMR



^{13}C NMR of 122



IR of 122



HRMS of 122

Bruker maXis Impact: LC-MS SmartFormula Report

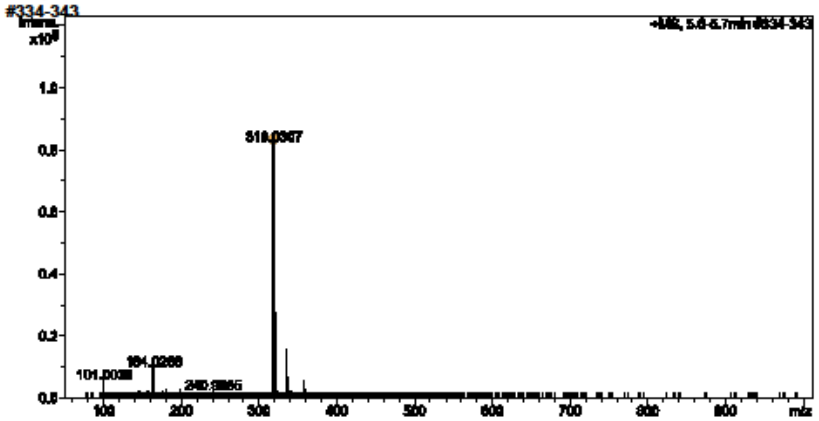
Analysis Info

Analysis Name	C:\Data\Data\N34272-34-1_1-A,3_01_961.d	Acquisition Date	07/10/2014 06:24:35
Method	lcms pos 50-1000.m	Operator	Spectroscopy
Sample Name	N34272-34-1	Instrument / Ser	maXis impact 282001.0 0101
Comment			

Acquisition Parameter

Source Type	ESI	Scan Begin	50 m/z
Ion Polarity	Positive	Scan End	1000 m/z

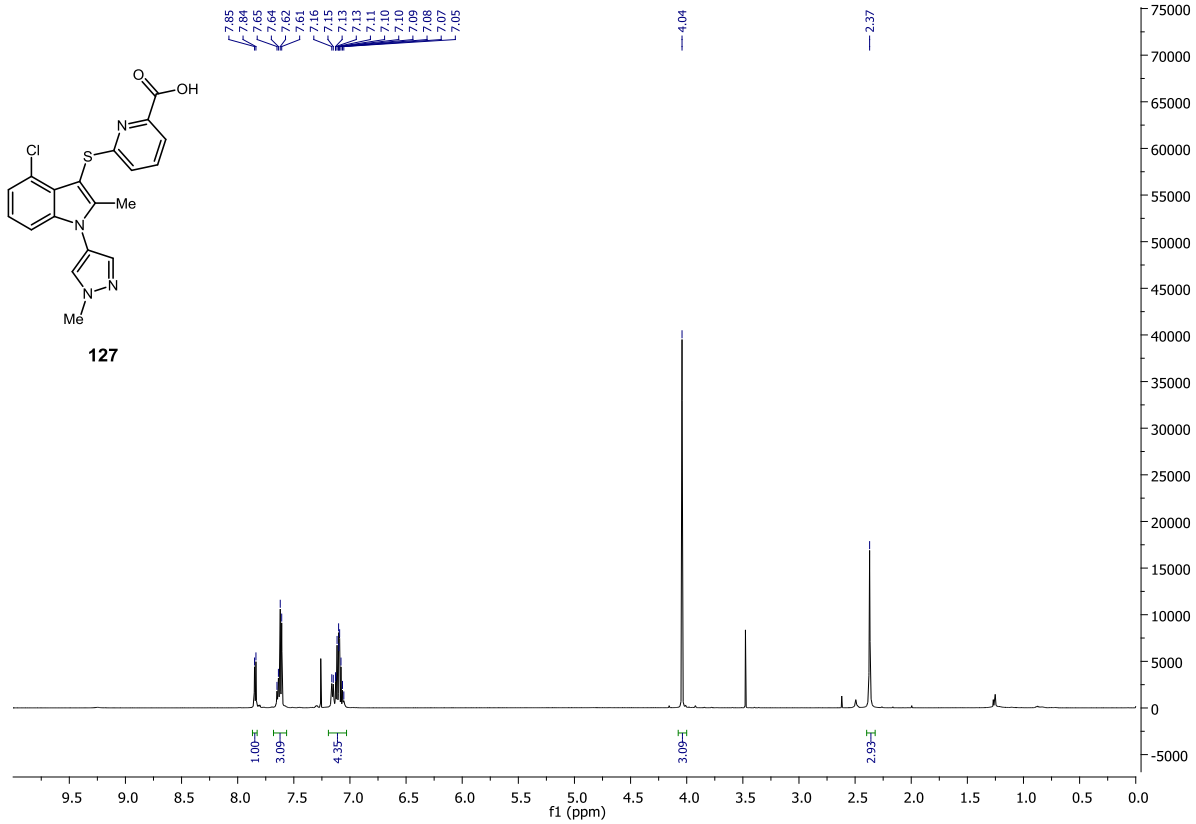
+MS, 5.6-5.7min
#334-343



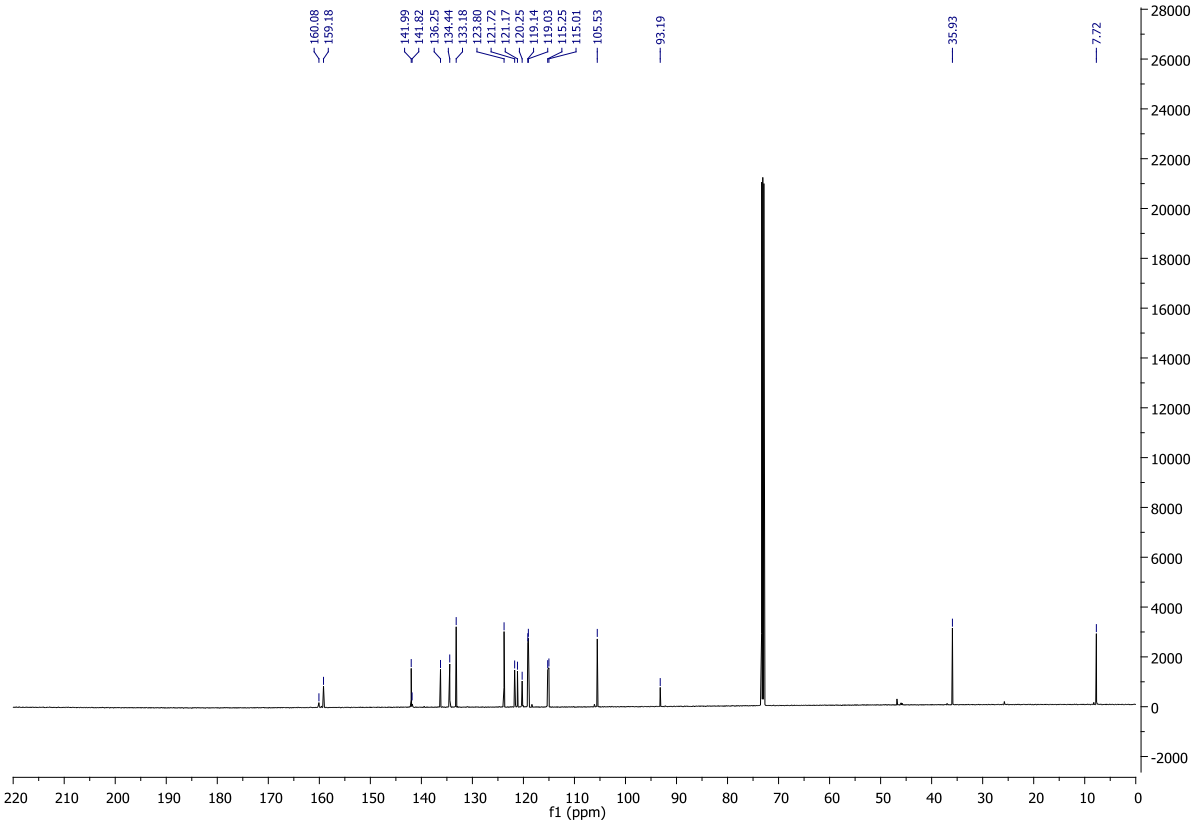
Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
319.0307	1	C15H12ClN2O2S	319.0303	-1.5	36.6	1	100.00	10.5	even	ok

Compound 127

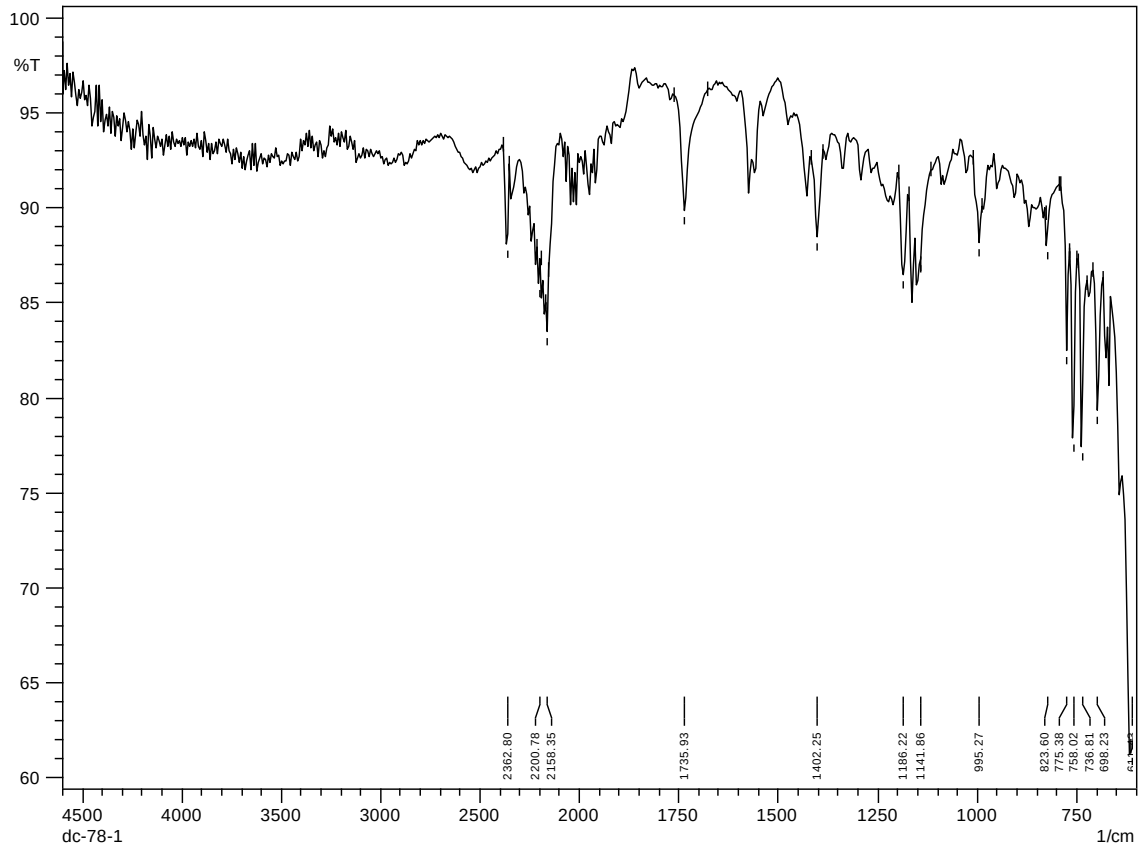
^{1}H NMR



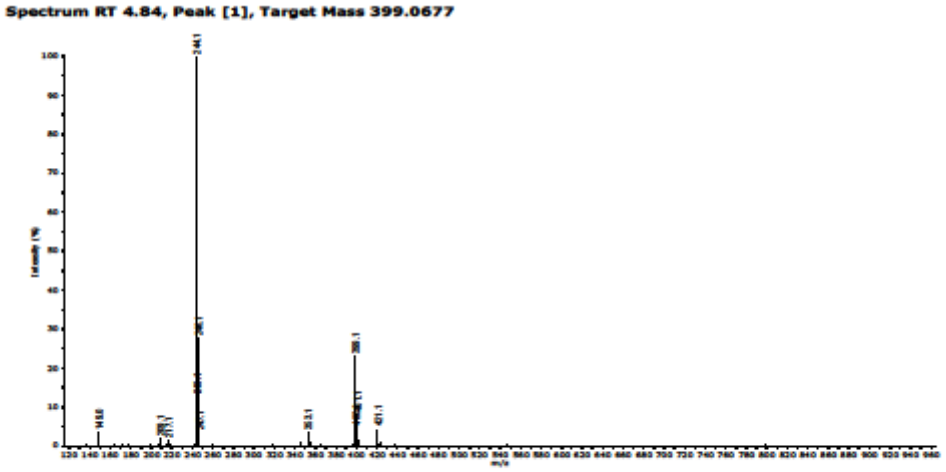
^{13}C NMR of 127

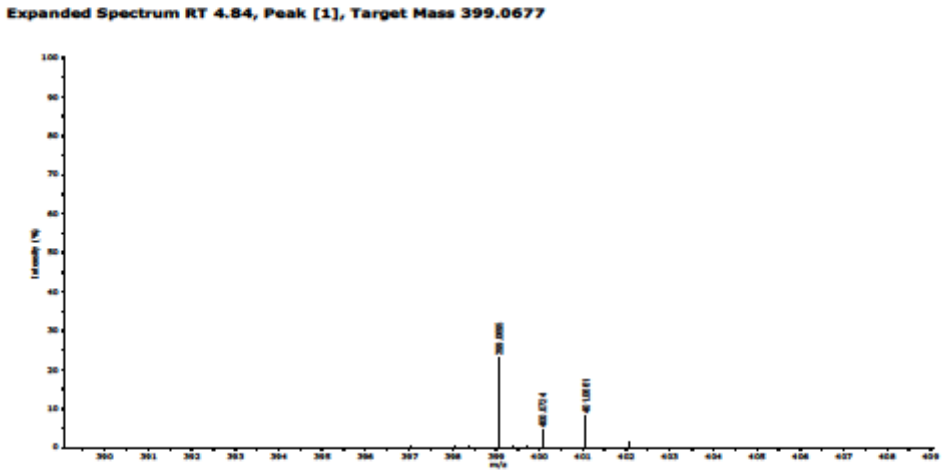


IR of 127


100
%T
95
90
85
80
75
70
65
60
2362.80
2200.78
2158.35
1735.93
1402.25
1186.22
1141.86
995.27
823.60
775.38
758.02
736.81
698.23
4500
4000
3500
3000
2500
2000
1750
1500
1250
1000
750
dc-78-1
1/cm

HRMS of 127

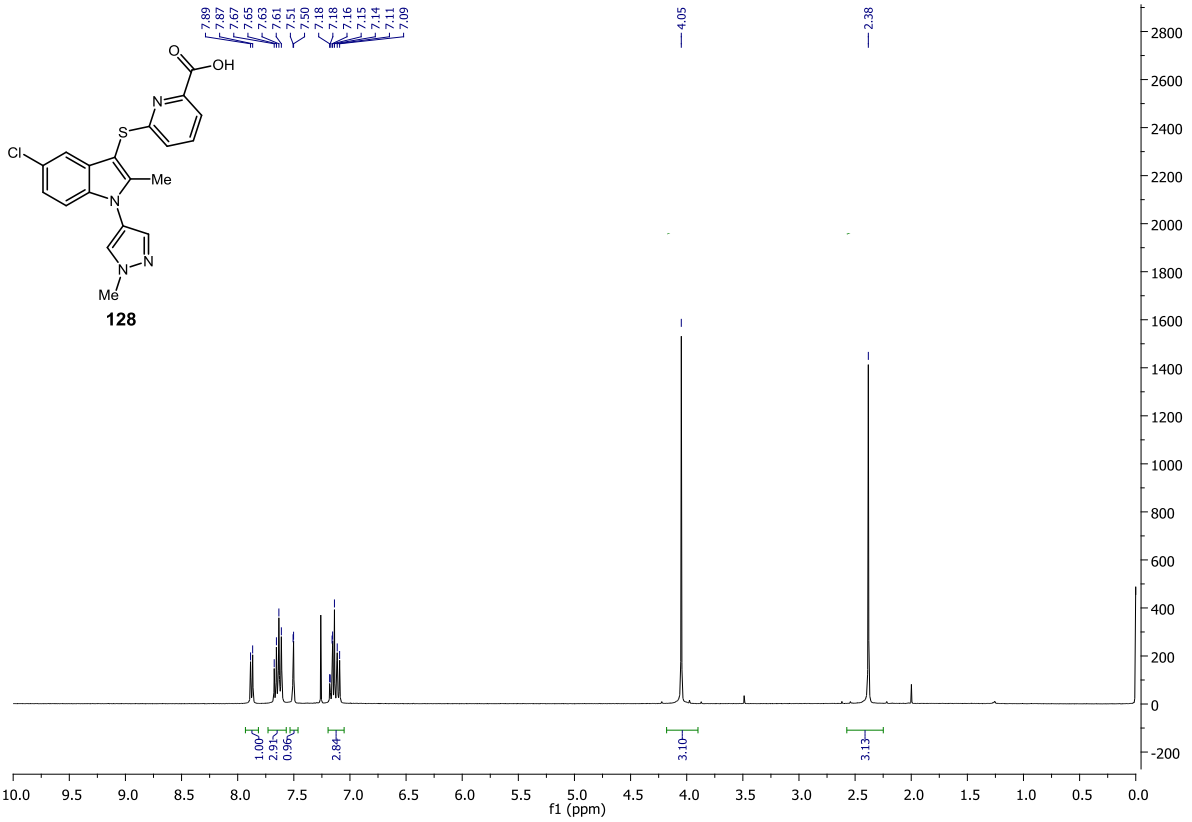




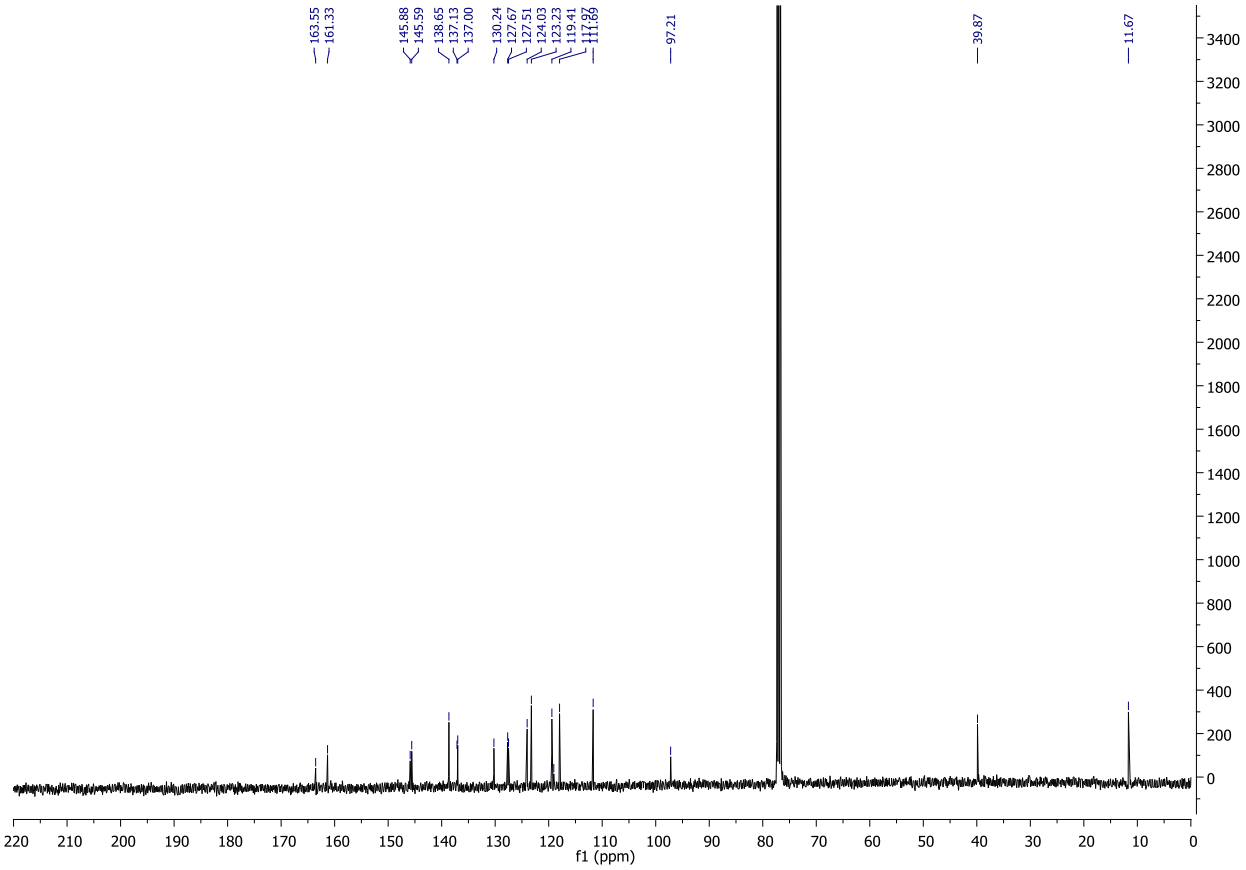
Measured Mass	Calculated Mass	Error (mDa)	Error (ppm)	Formula $[M+H]^+$
399.0680	399.0677	0.3	0.8	$C_{19}H_{16}ClN_4O_2S$

Compound 128

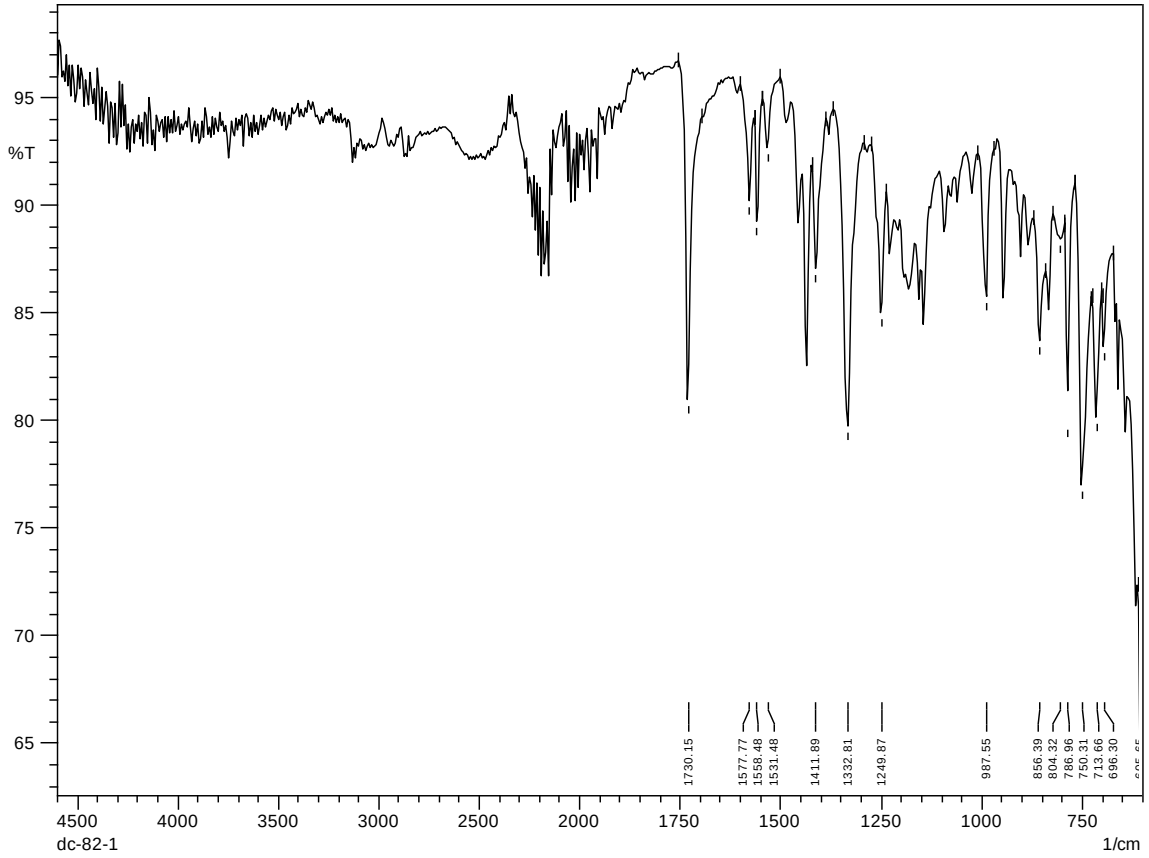
^{1}H NMR



^{13}C NMR of 128

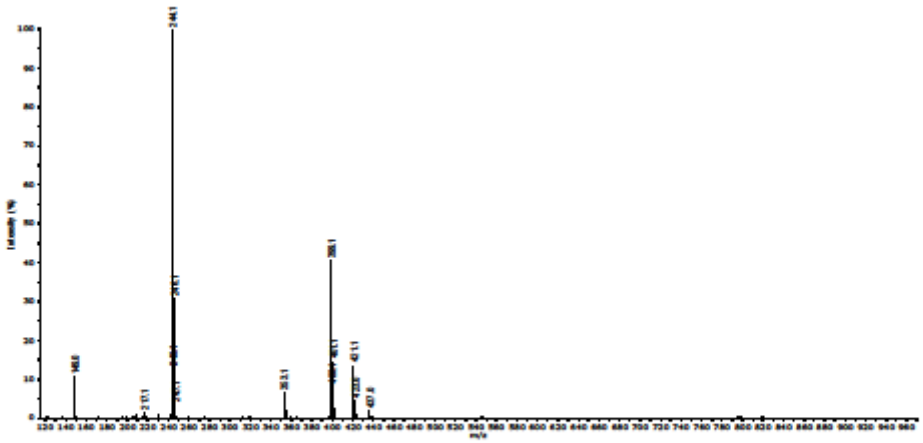


IR of 128

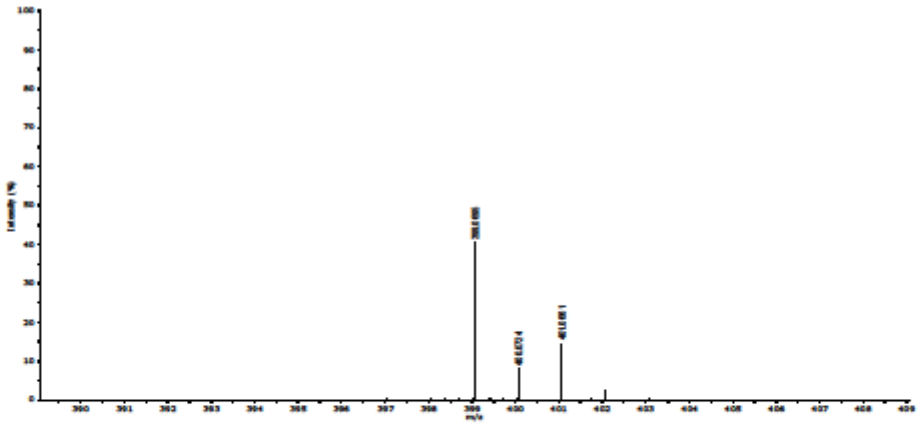

%T
95
90
85
80
75
70
65
1730.15
1577.77
1558.48
1531.48
1411.89
1332.81
1249.87
987.55
856.39
804.32
786.96
750.31
713.66
696.30
4500
4000
3500
3000
2500
2000
1750
1500
1250
1000
750
dc-82-1
1/cm

HRMS of 128

Spectrum RT 5.09, Peak [1], Target Mass 399.0677



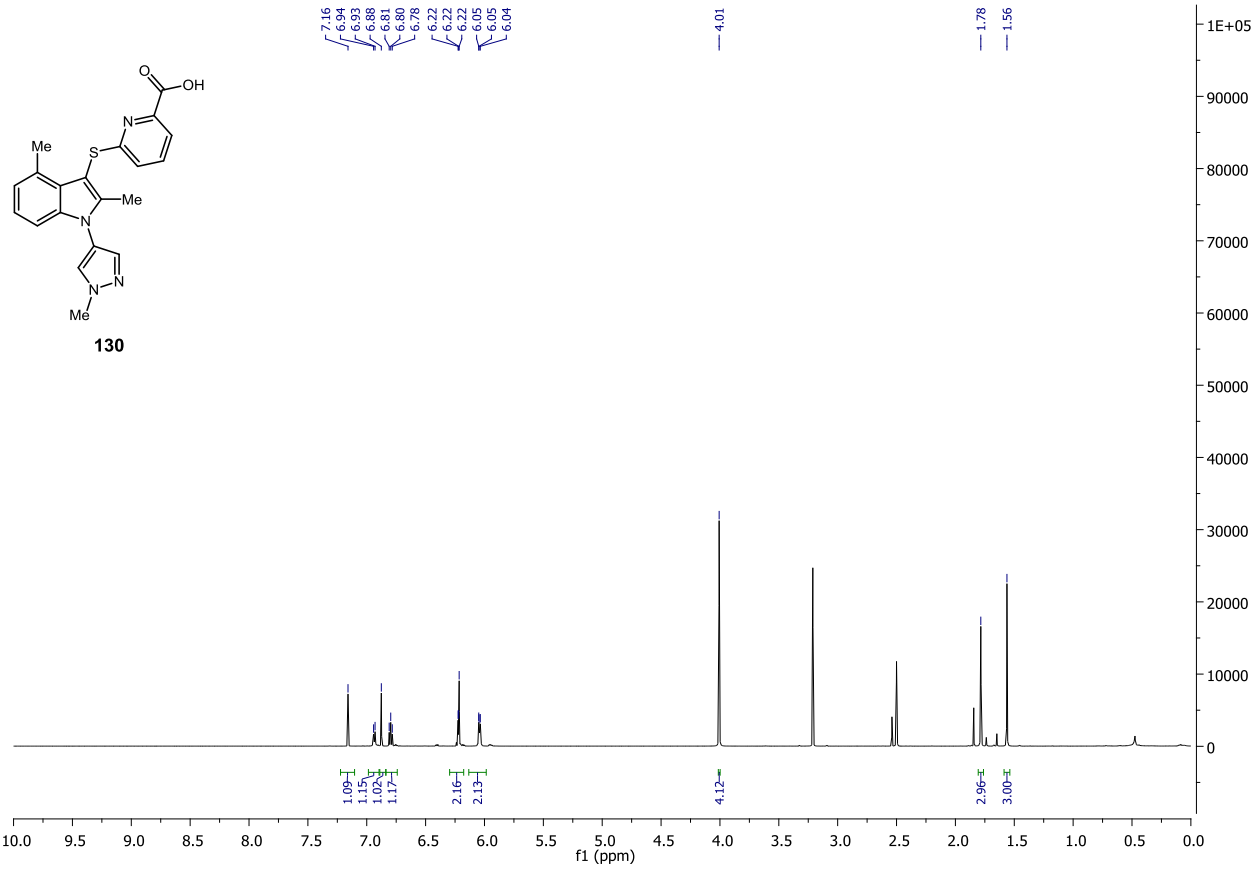
Expanded Spectrum RT 5.09, Peak [1], Target Mass 399.0677



Measured Mass	Calculated Mass	Error (mDa)	Error (ppm)	Formula $[M+H]^+$
399.0680	399.0677	0.3	0.8	$C_{19}H_{16}ClN_4O_2S$

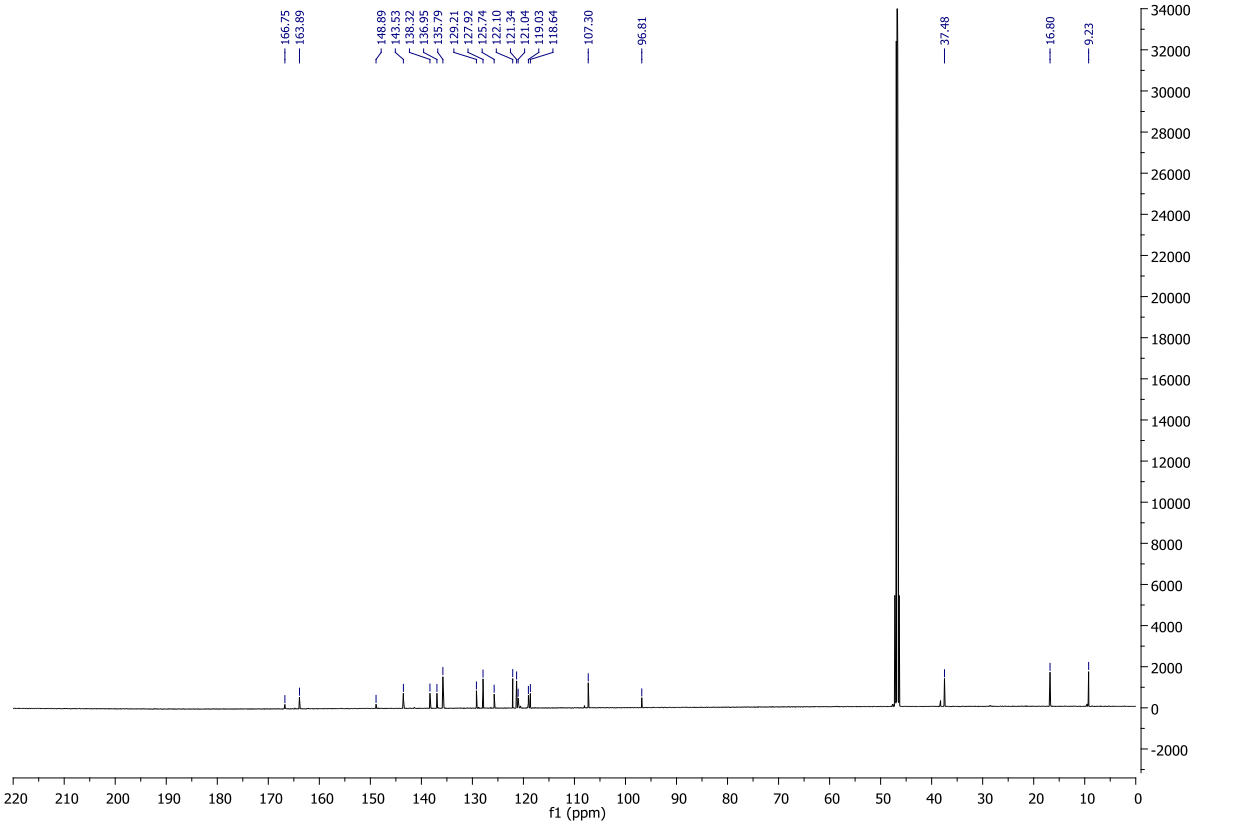
Compound 130

^{1}H NMR

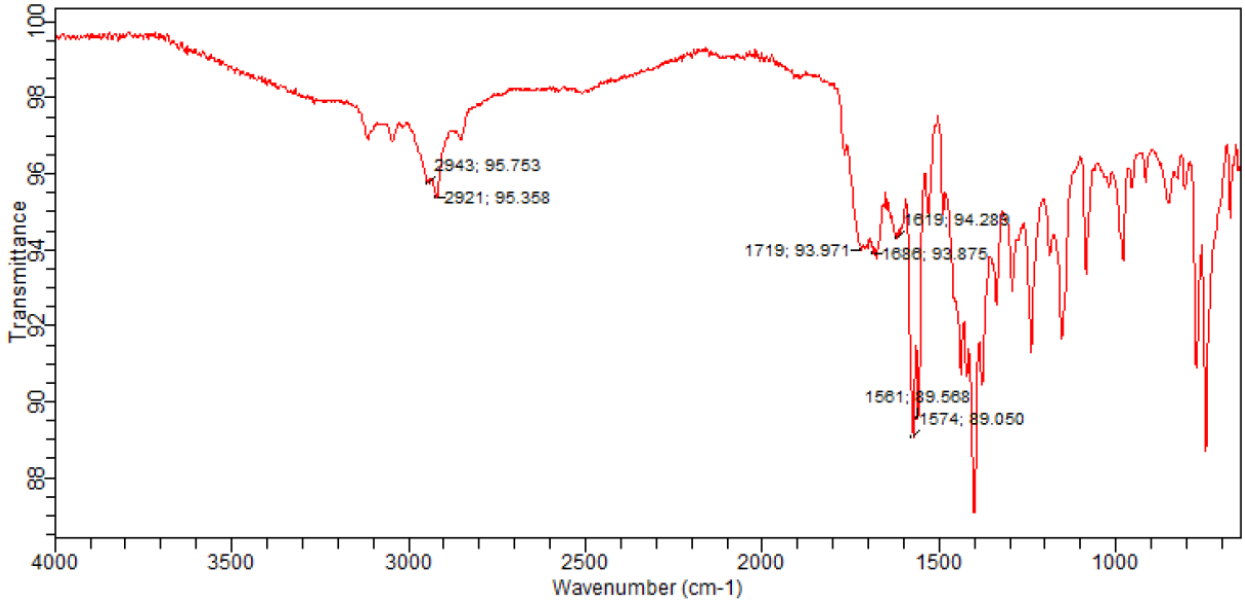


130

^{13}C NMR of 130

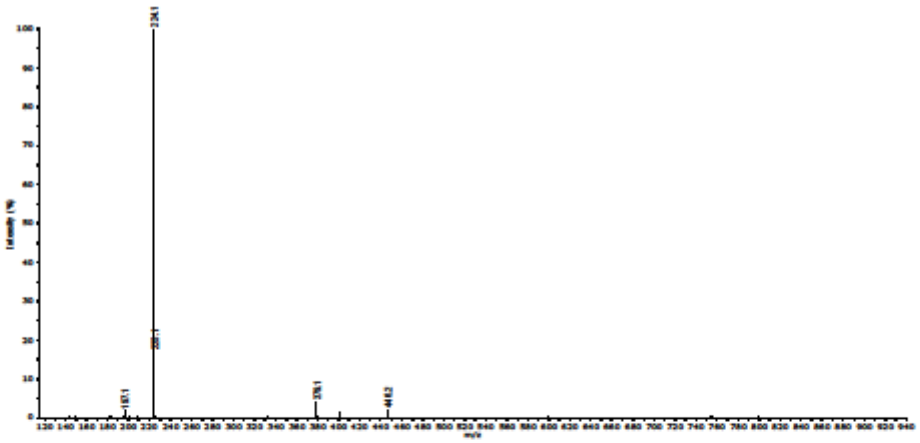


IR of 130

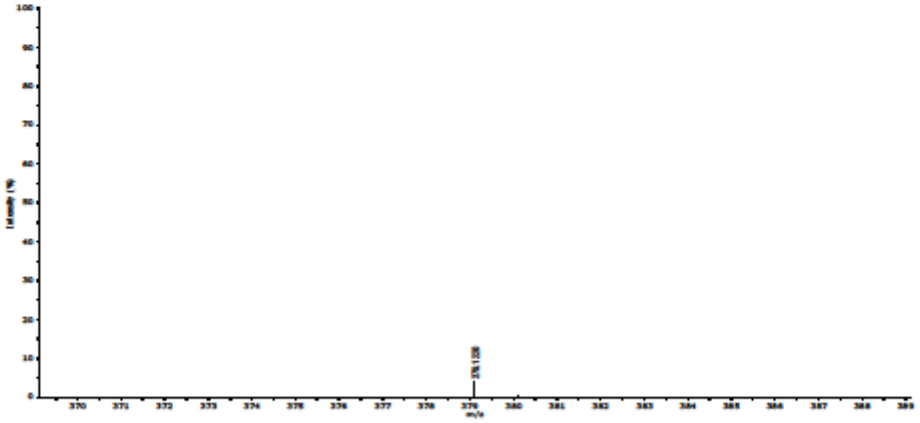

Transmittance
100
98
96
94
92
90
88
2943; 95.753
2921; 95.358
1719; 93.971
1619; 94.289
1686; 93.875
1561; 89.568
1574; 89.050
4000
3500
3000
2500
2000
1500
1000
Wavenumber (cm-1)

HRMS of 130

Spectrum RT 4.87, Peak [1], Target Mass 379.1223



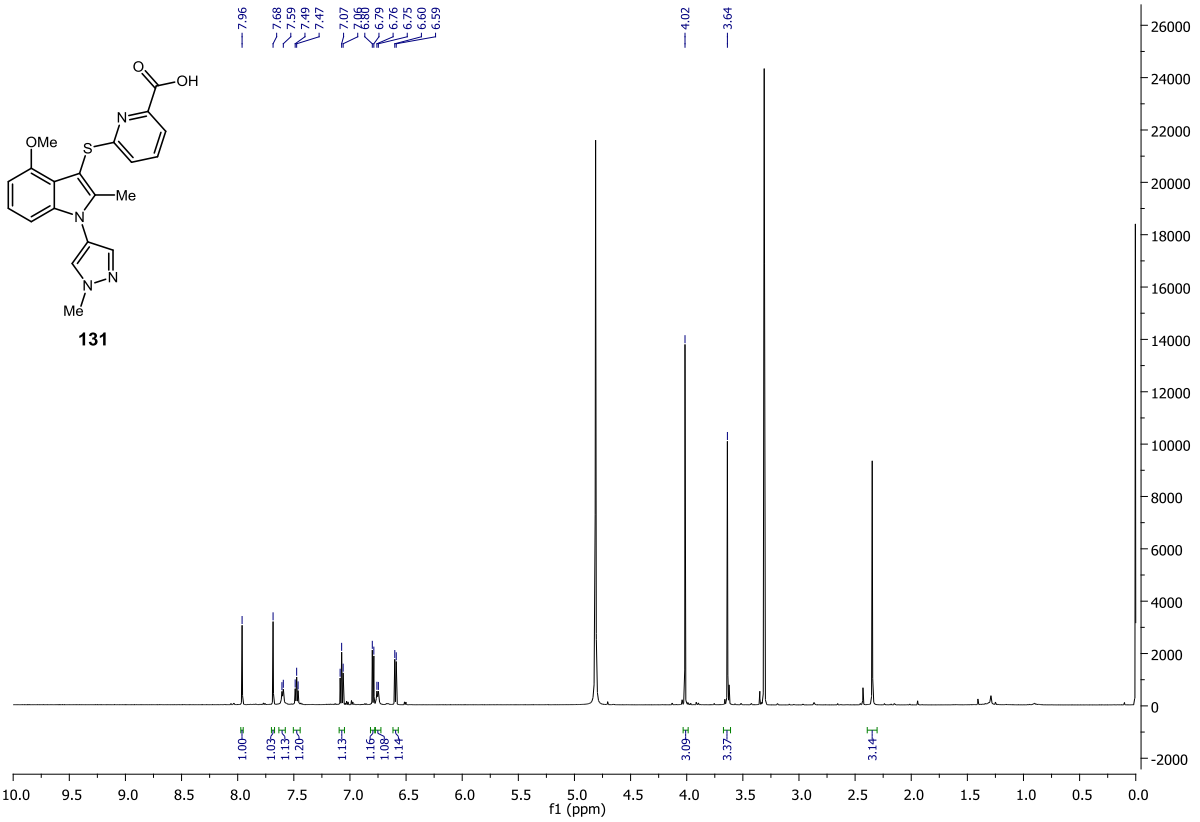
Expanded Spectrum RT 4.87, Peak [1], Target Mass 379.1223



Measured Mass	Calculated Mass	Error (mDa)	Error (ppm)	Formula $[M+H]^+$
379.1220	379.1223	-0.3	-0.8	$C_{20}H_{19}N_4O_2S$

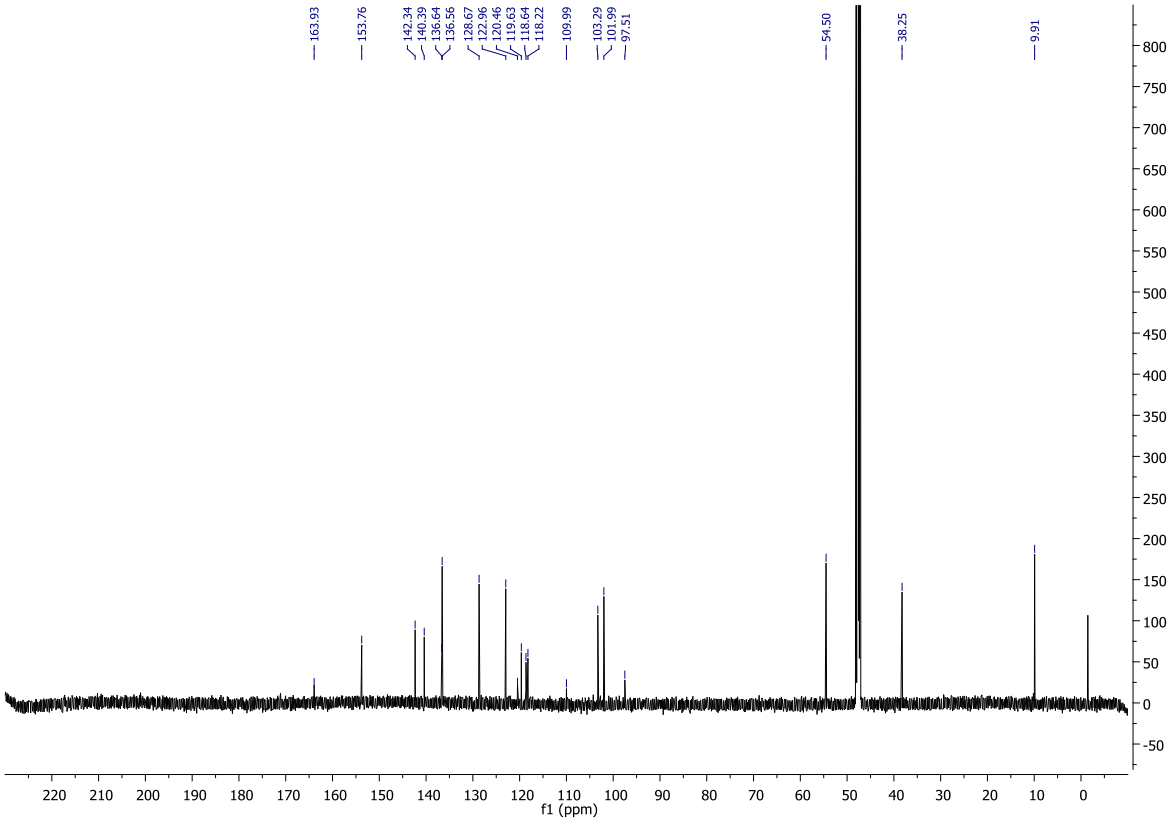
Compound 131

^{1}H NMR

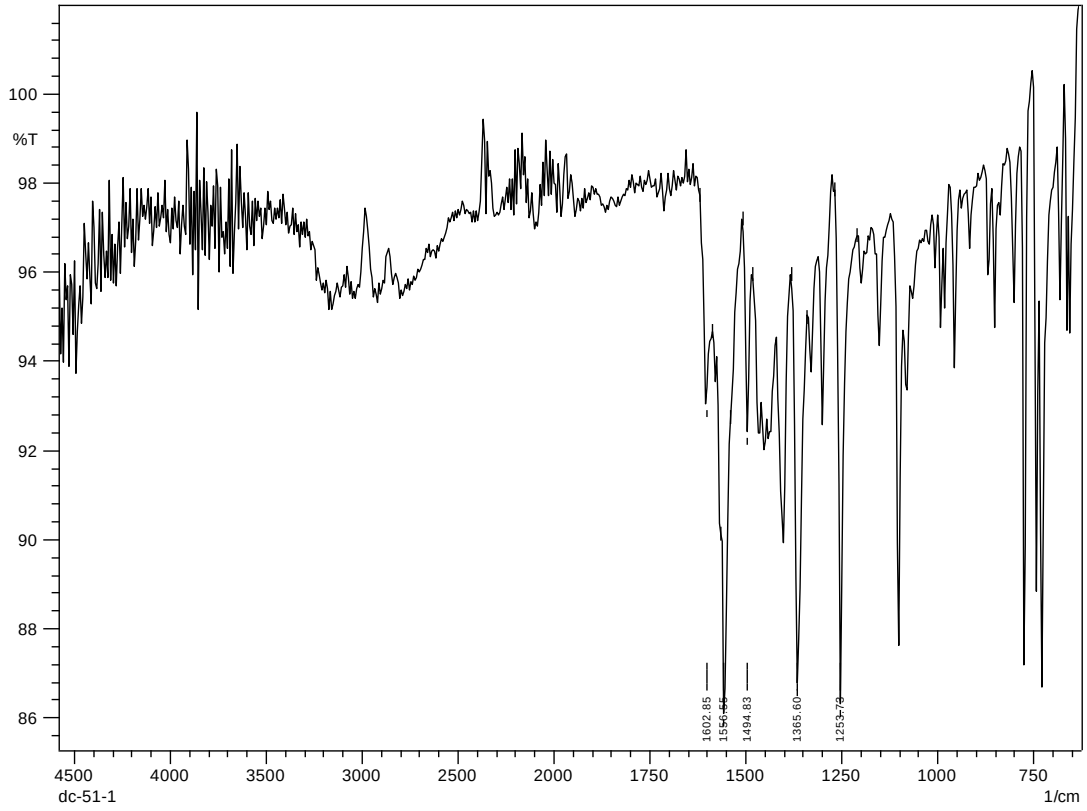


131

^{13}C NMR of 131



IR of 131



HRMS of 131

Bruker maXis Impact: LC-MS SmartFormula Report

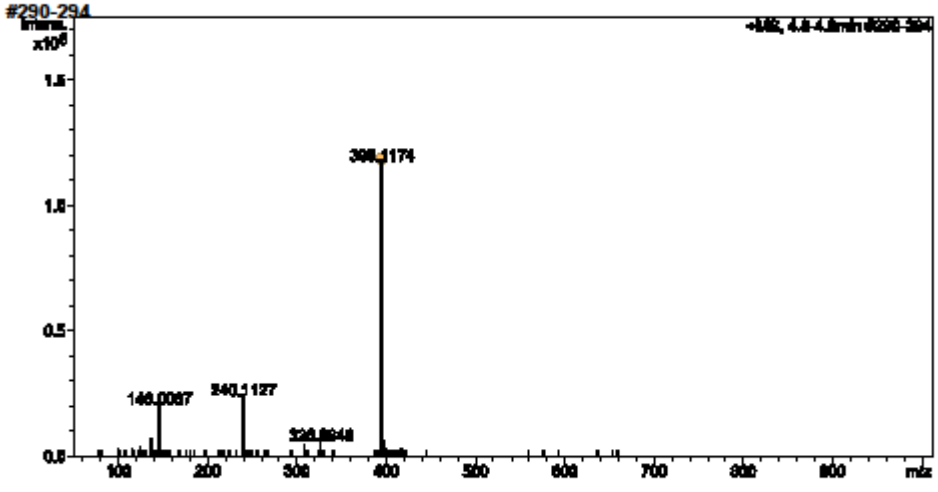
Analysis Info

Analysis Name	C:\Data\Data\N34272-64-8_1-A,9_01_1123.d	Acquisition Date	24/10/2014 16:01:28
Method	lcms pos 50-1000.m	Operator	Spectroscopy
Sample Name	N34272-64-8	Instrument / Ser	maXis impact 282001.0 0101
Comment			

Acquisition Parameter

Source Type	ESI	Scan Begin	50 m/z
Ion Polarity	Positive	Scan End	1000 m/z

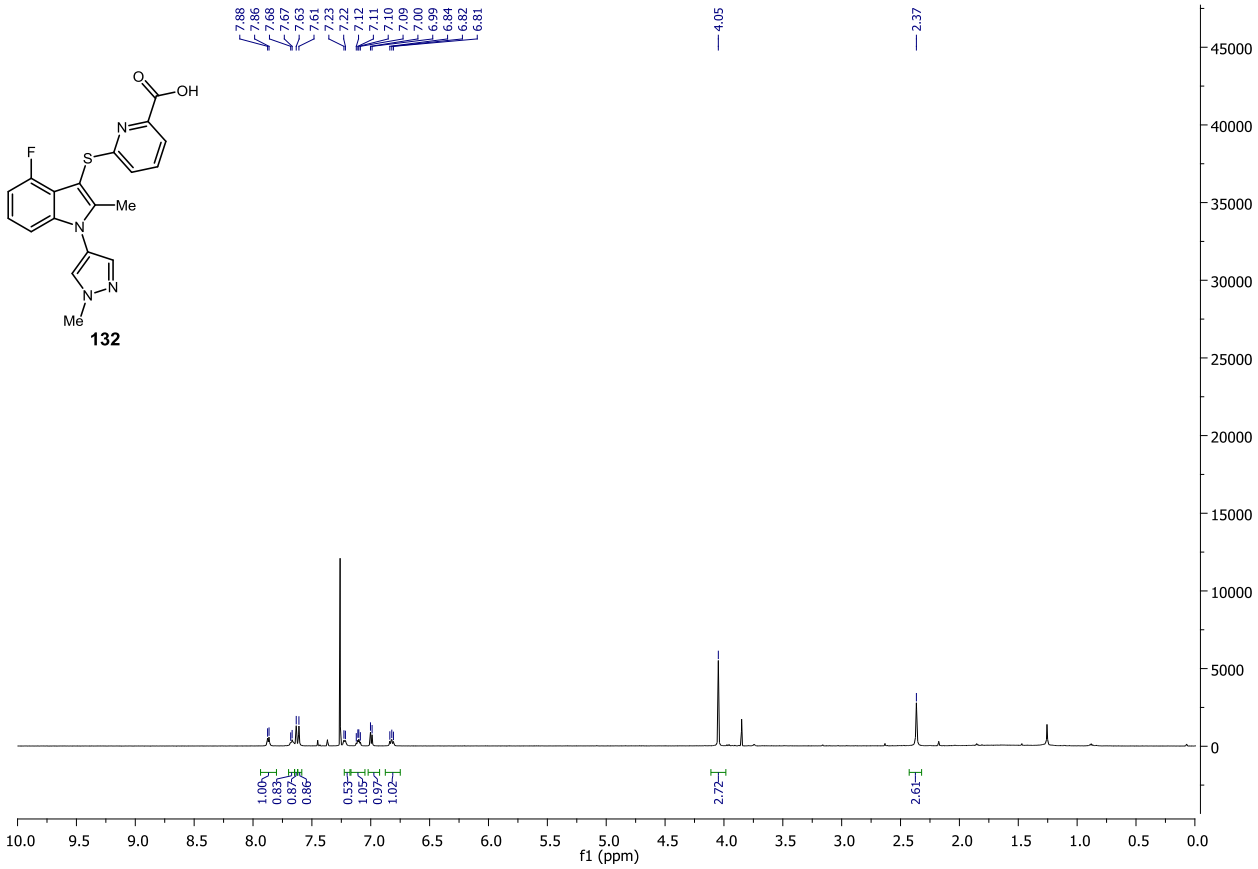
+MS, 4.8-4.9min
#290-294



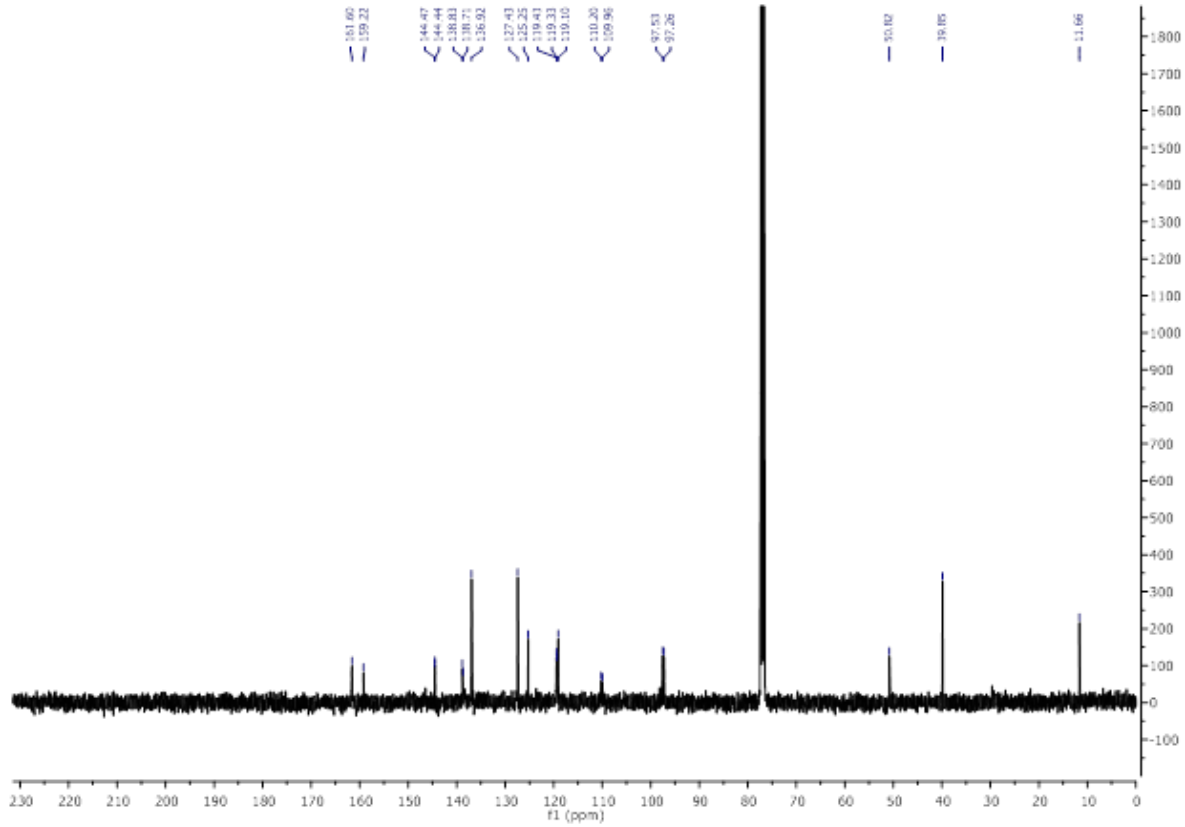
Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
395.1174	1	C20H19N4O3S	395.1172	0.3	27.1	1	100.00	13.5	even	ok

Compound 132

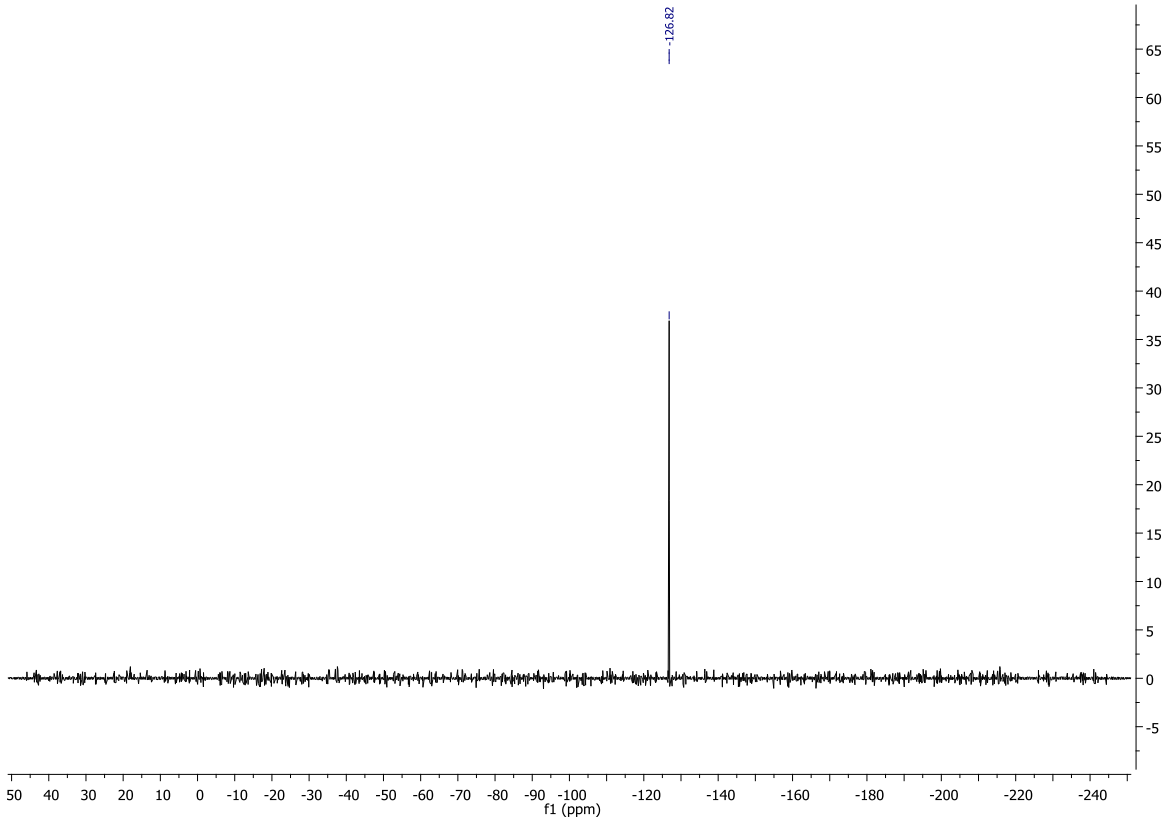
^{1}H NMR



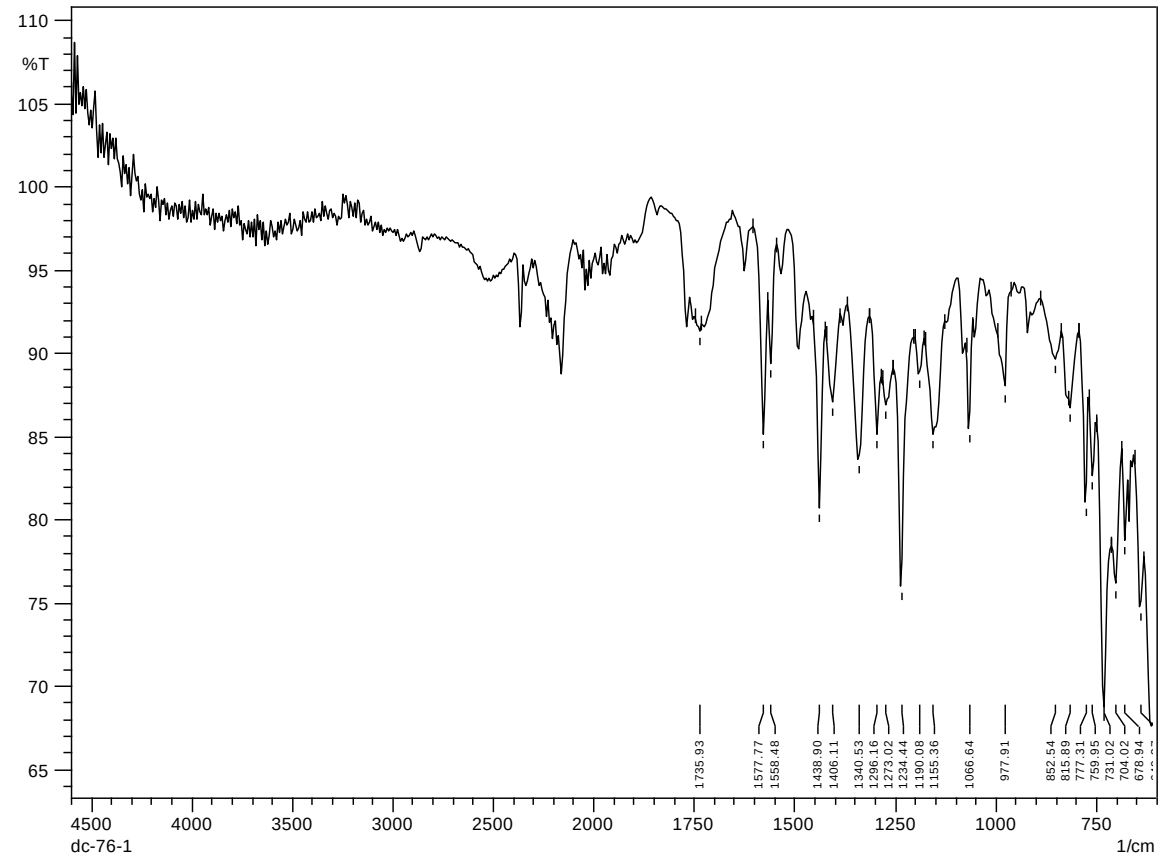
^{13}C NMR of 132



^{19}F NMR of 132

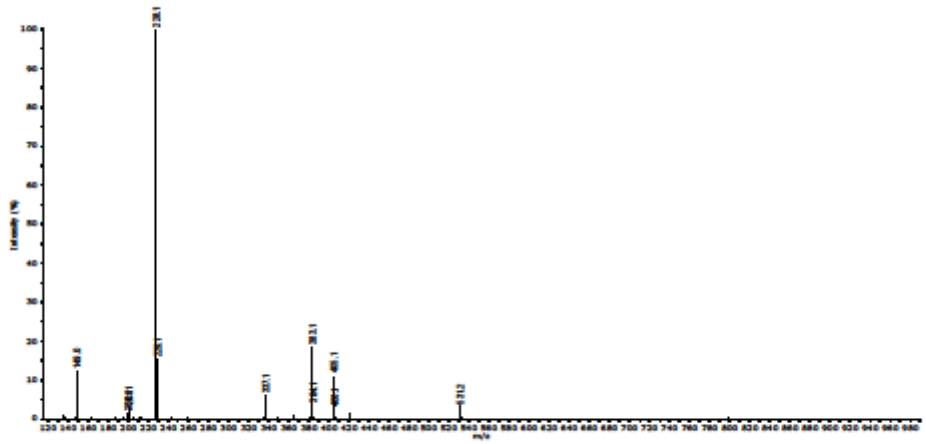


IR of 132

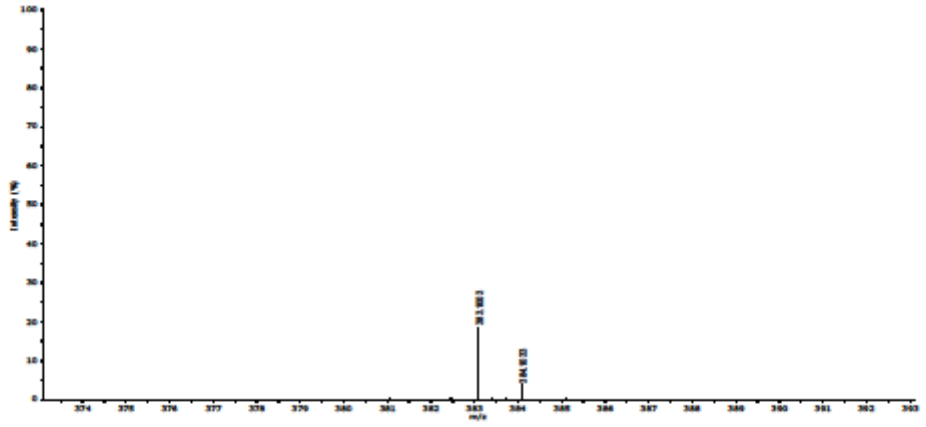


HRMS of 132

Spectrum RT 4.61, Peak [1], Target Mass 383.0973



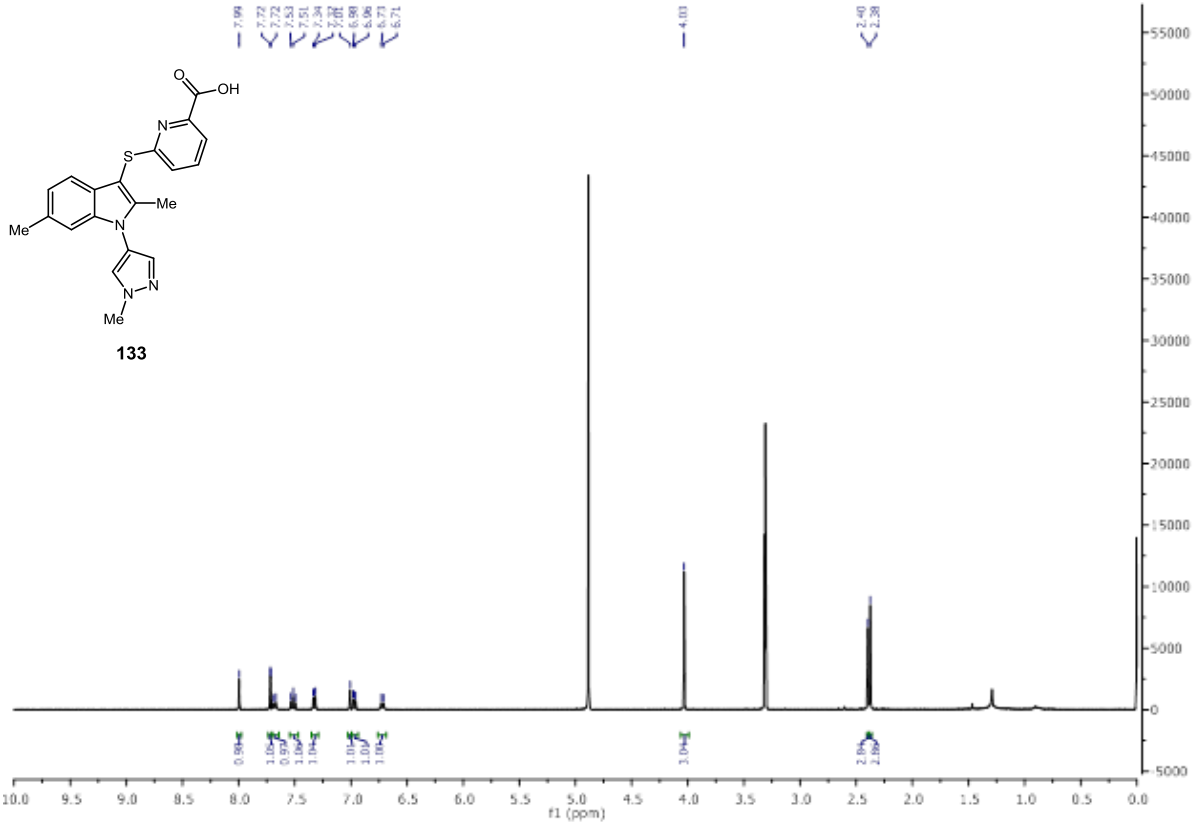
Expanded Spectrum RT 4.61, Peak [1], Target Mass 383.0973



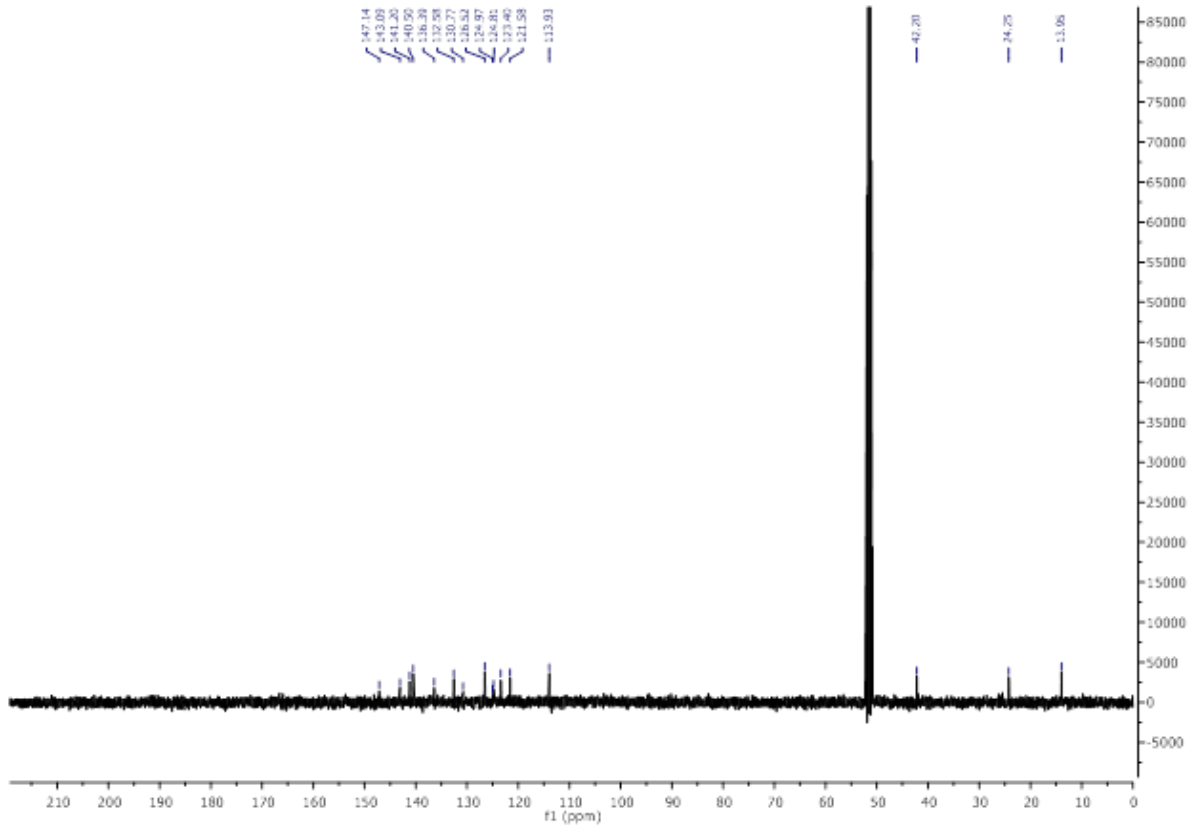
Measured Mass	Calculated Mass	Error (mDa)	Error (ppm)	Formula $[M+H]^+$
383.0975	383.0973	0.2	0.6	$C_{19}H_{16}FN_4O_2S$

Compound 133

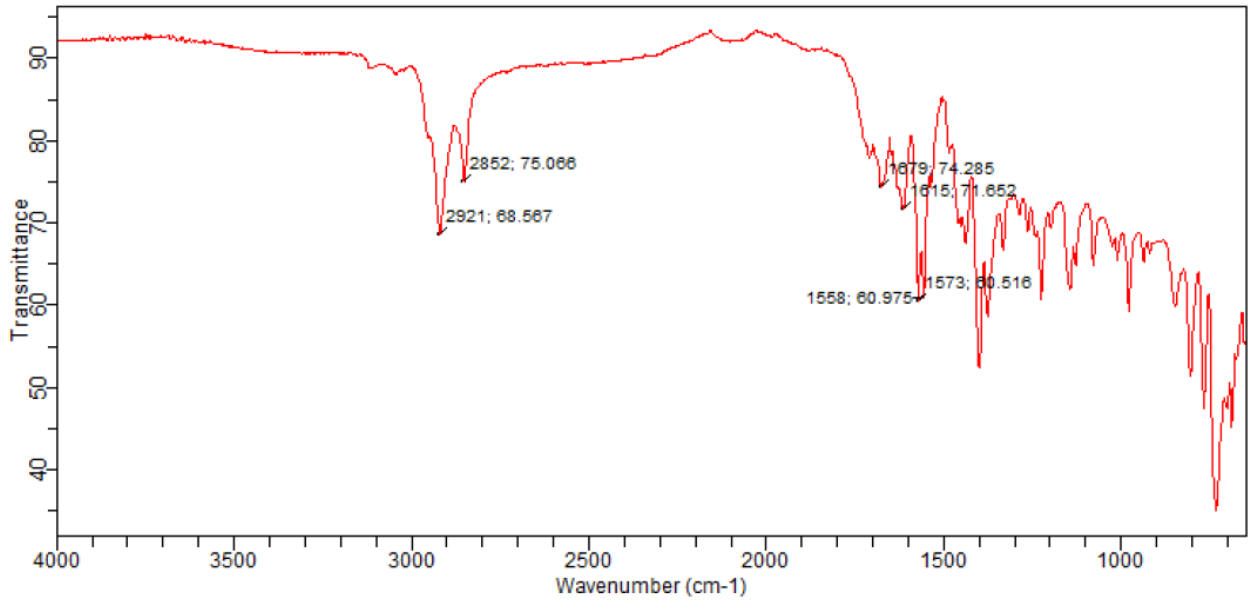
^{1}H NMR



^{13}C NMR of 133

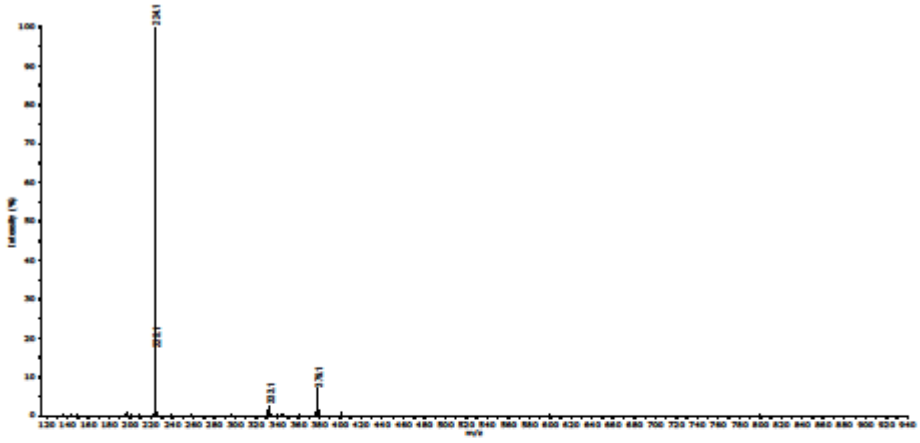


IR of 133

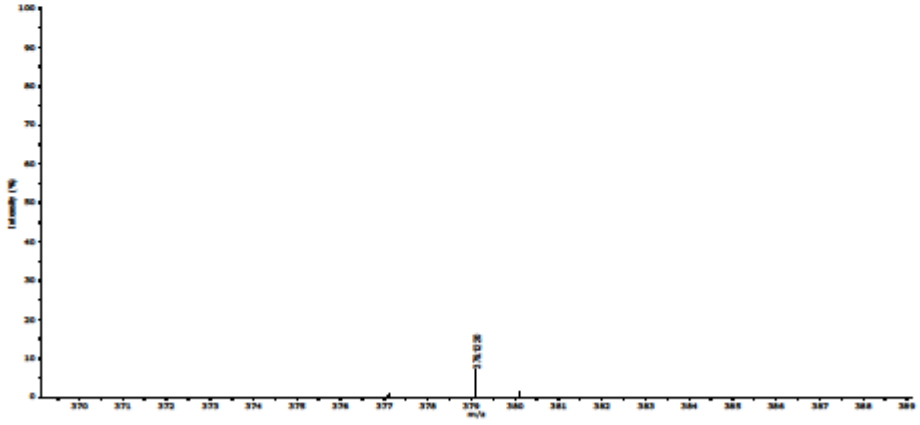

Transmittance
90
80
70
60
50
40
2852; 75.066
2921; 68.567
1679; 74.285
1615; 71.652
1573; 60.516
1558; 60.975
4000
3500
3000
2500
2000
1500
1000
Wavenumber (cm-1)

HRMS of 133

Spectrum RT 4.95, Peak [1], Target Mass 379.1223



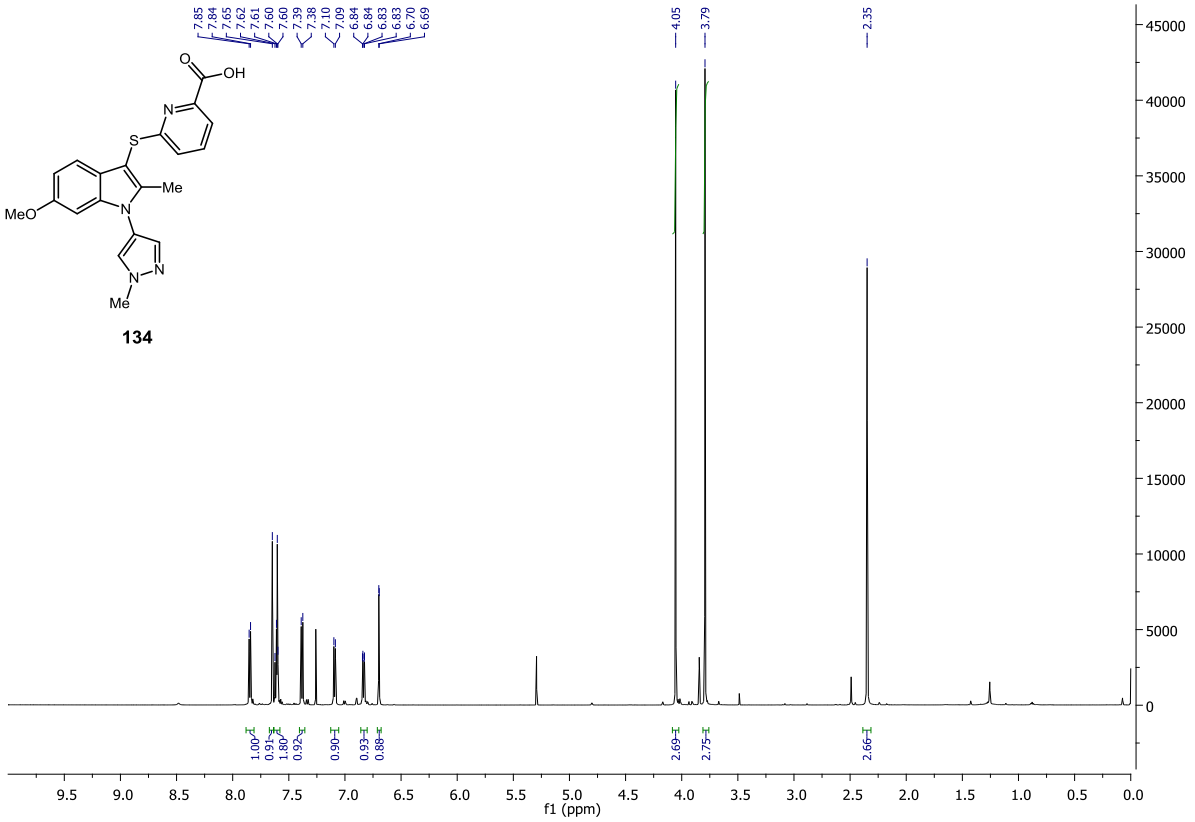
Expanded Spectrum RT 4.95, Peak [1], Target Mass 379.1223



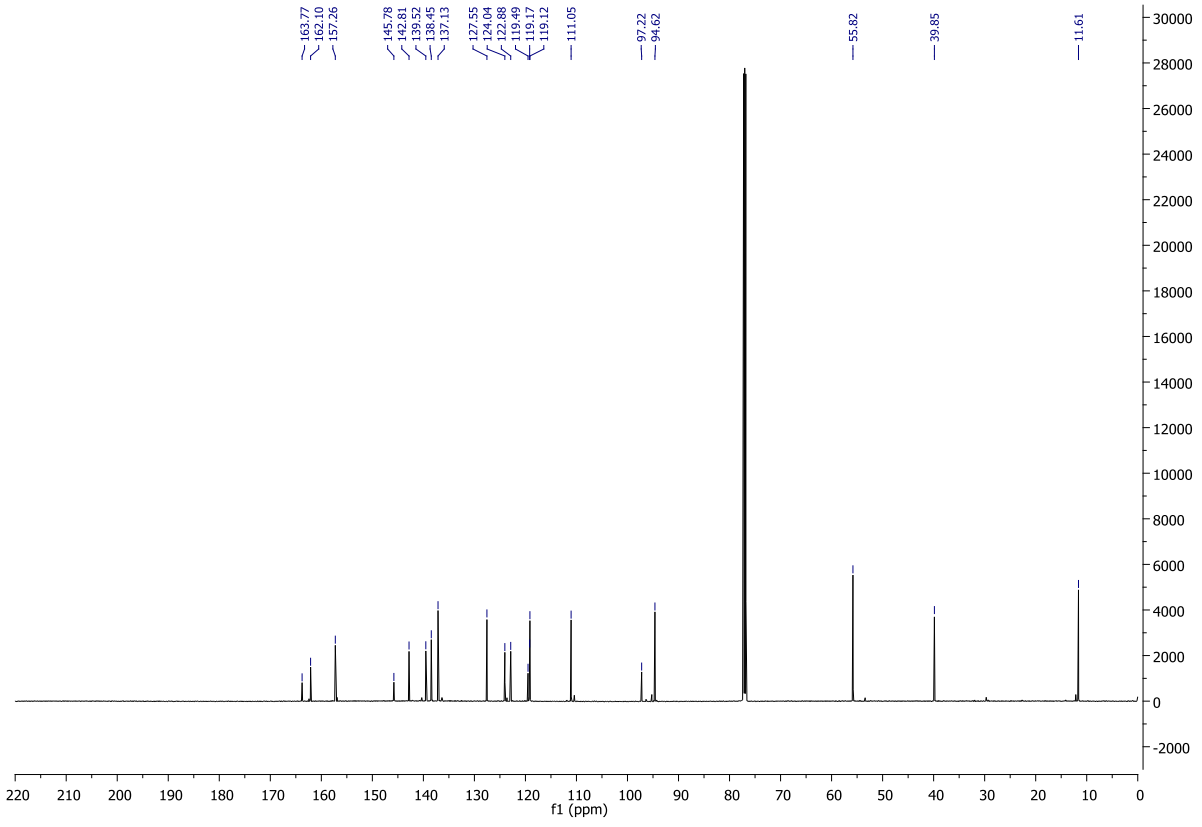
Measured Mass	Calculated Mass	Error (mDa)	Error (ppm)	Formula $[M+H]^+$
379.1220	379.1223	-0.3	-0.8	$C_{20}H_{19}N_4O_2S$

Compound 134

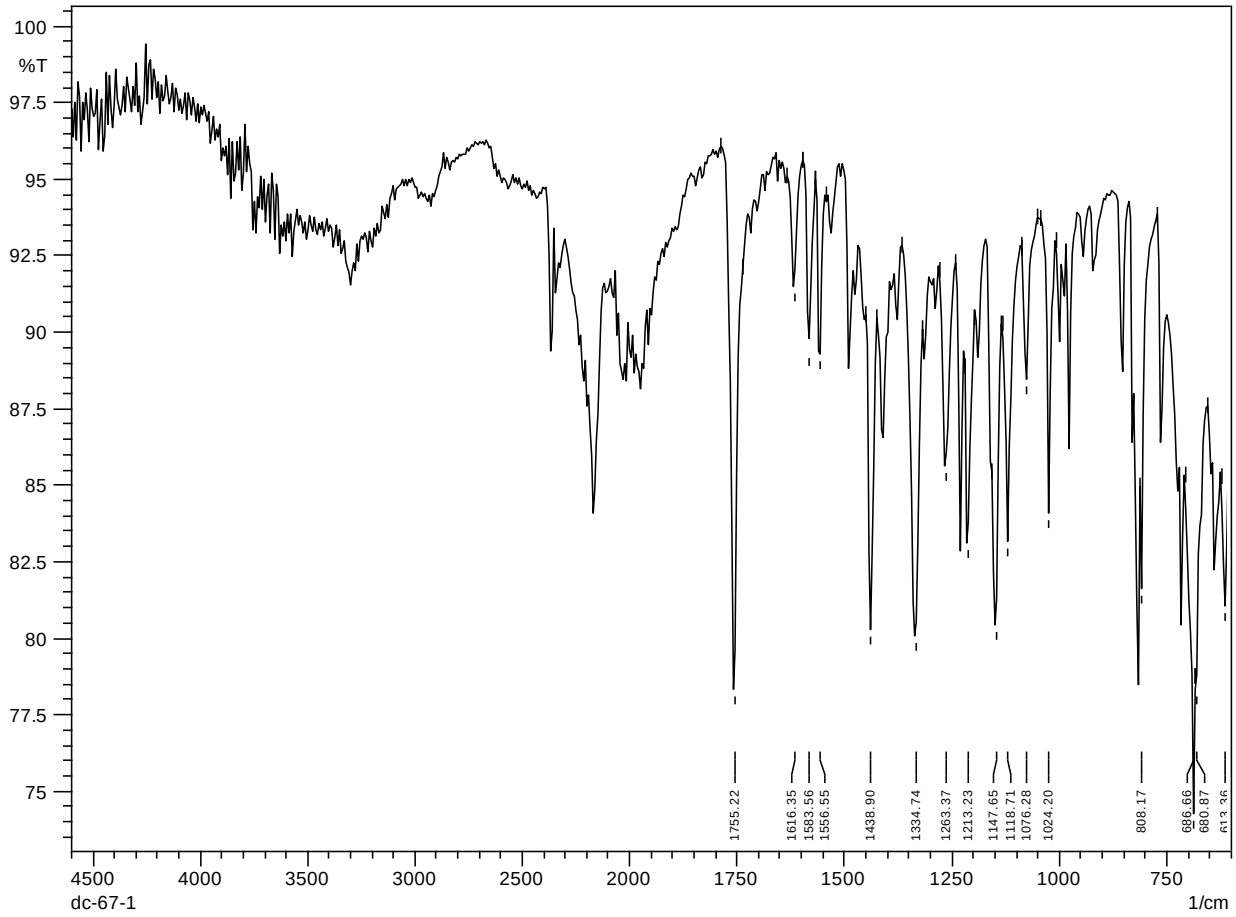
^{1}H NMR



^{13}C NMR of 134

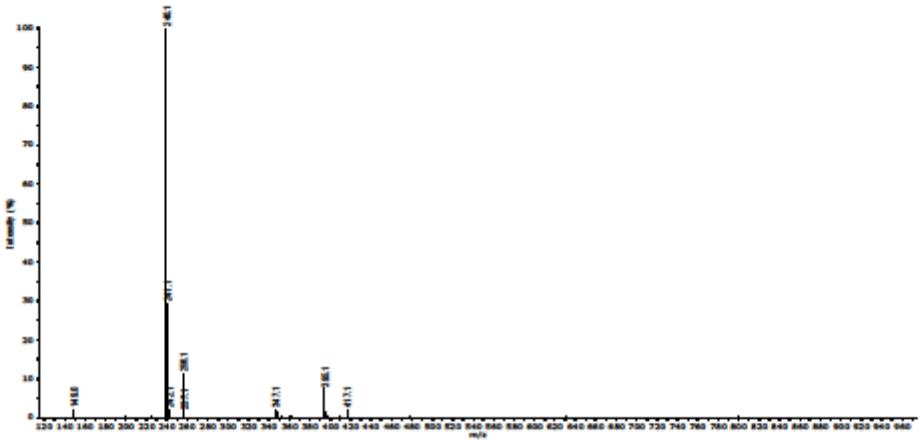


IR of 134

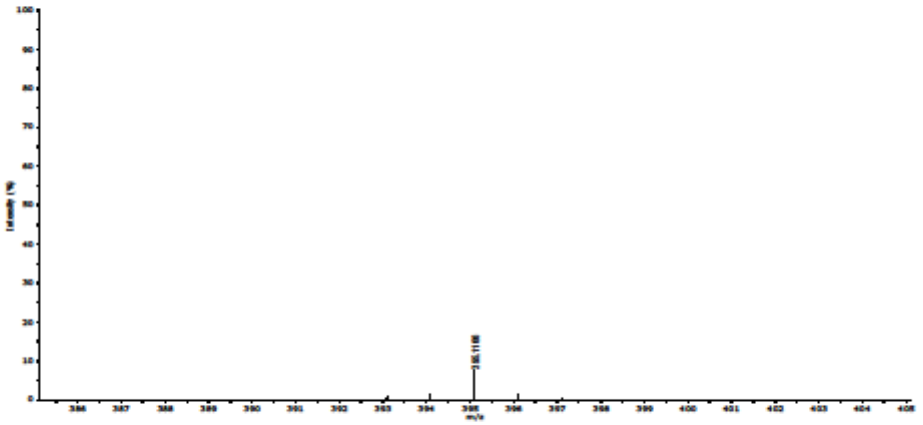

100
%T
97.5
95
92.5
90
87.5
85
82.5
80
77.5
75
1755.22
1616.35
1583.56
1556.55
1438.90
1334.74
1263.37
1213.23
1147.65
1118.71
1076.28
1024.20
808.17
686.66
680.87
4500
4000
3500
3000
2500
2000
1750
1500
1250
1000
750
dc-67-1
1/cm

HRMS of 134

Spectrum RT 4.59, Peak [1], Target Mass 395.1172



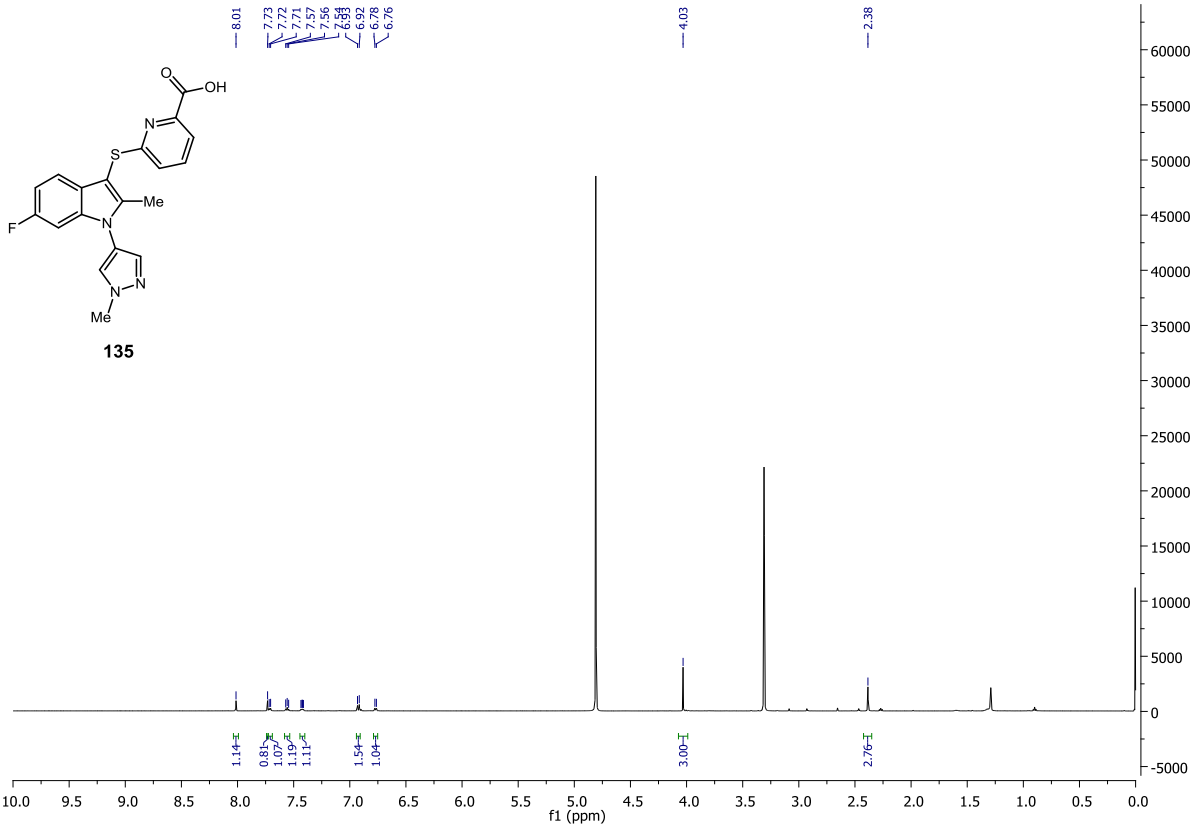
Expanded Spectrum RT 4.59, Peak [1], Target Mass 395.1172



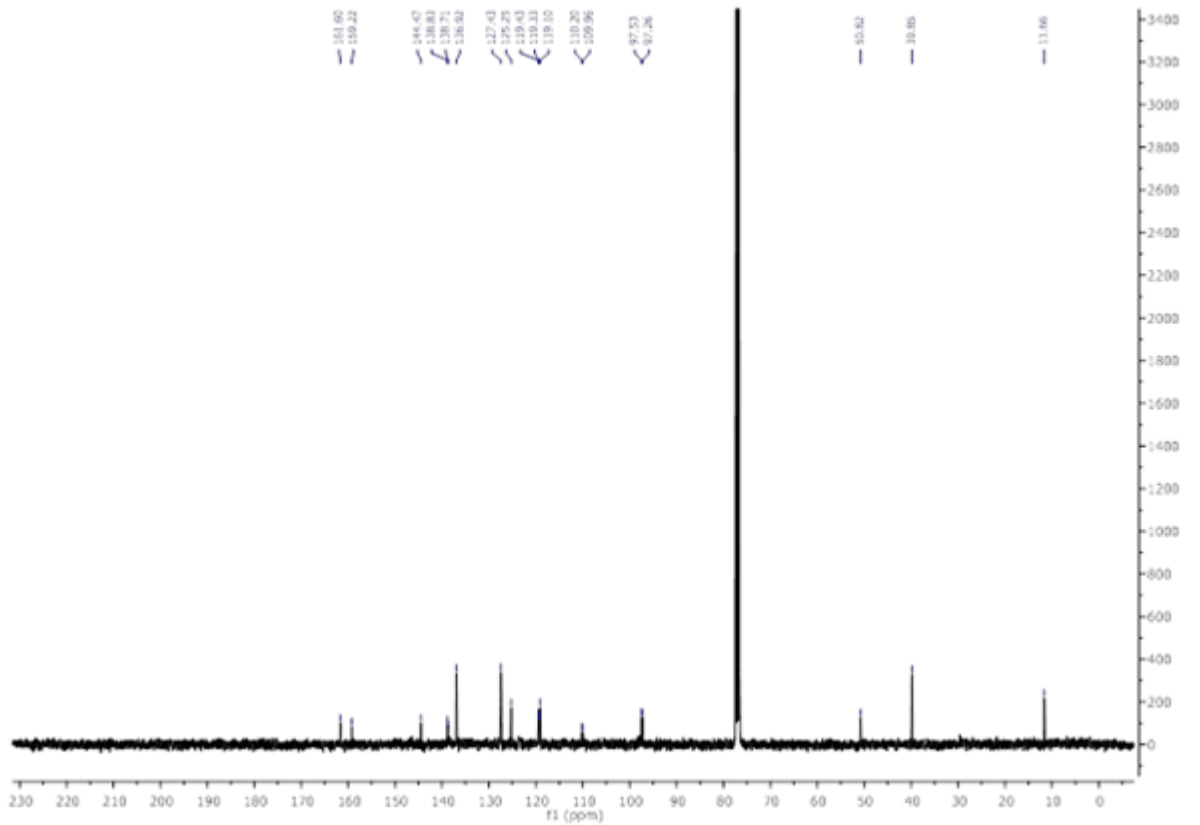
Measured Mass	Calculated Mass	Error (mDa)	Error (ppm)	Formula $[M+H]^+$
395.1173	395.1172	0.1	0.2	$C_{20}H_{19}N_4O_3S$

Compound 135

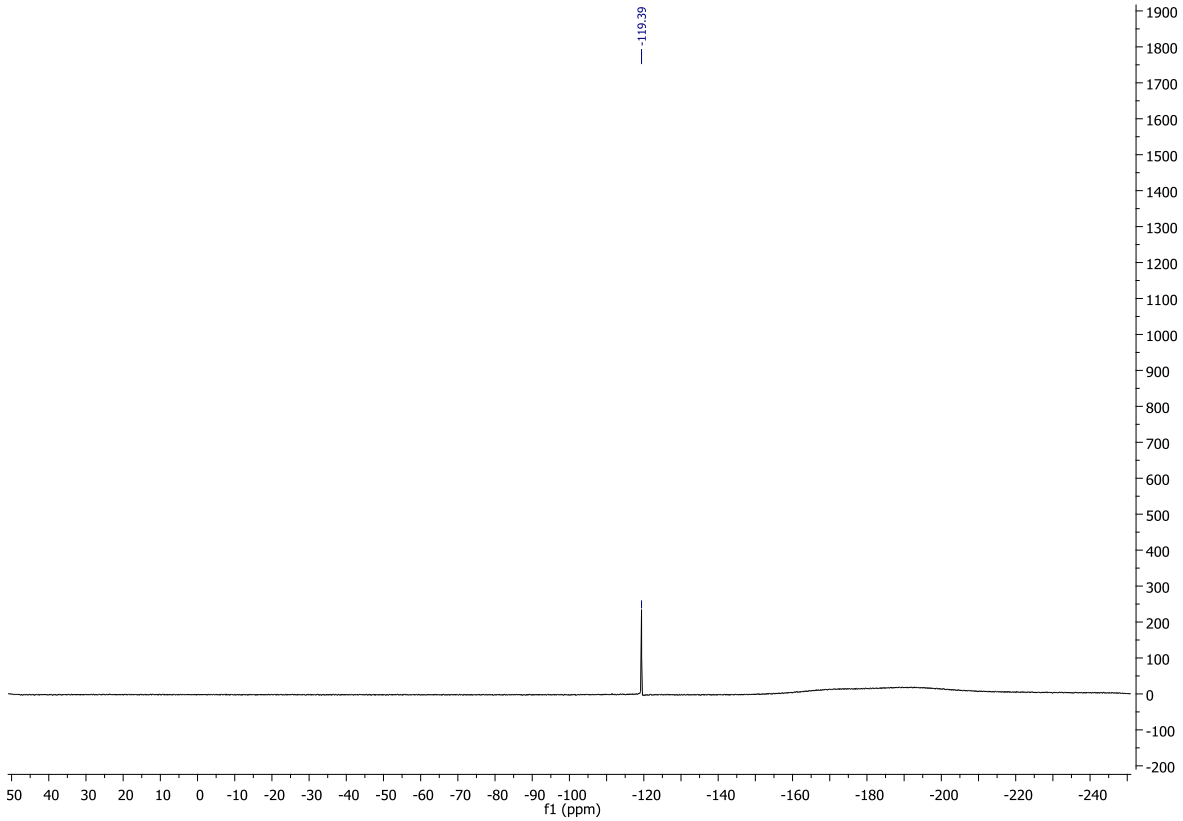
^{1}H NMR



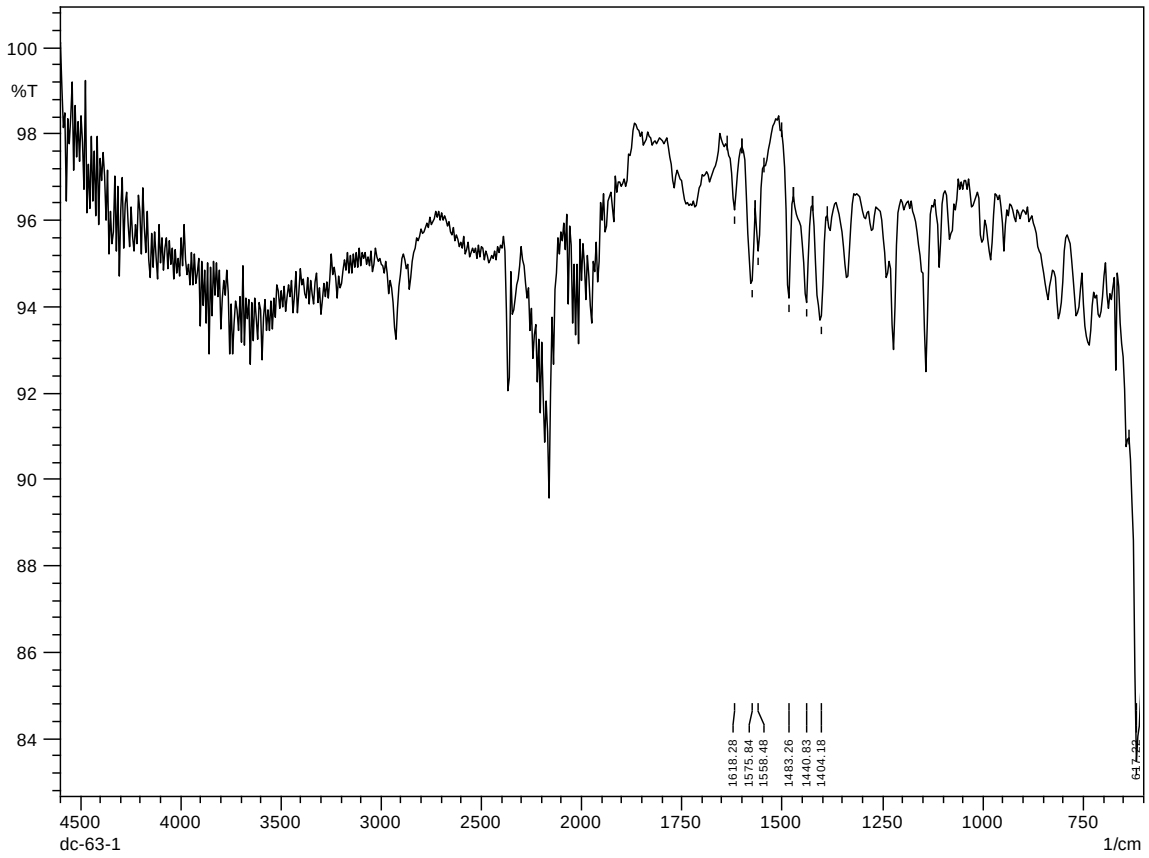
^{13}C NMR of 135



^{19}F NMR of 135



IR of 135



HRMS of 135

Bruker maXis Impact: LC-MS SmartFormula Report

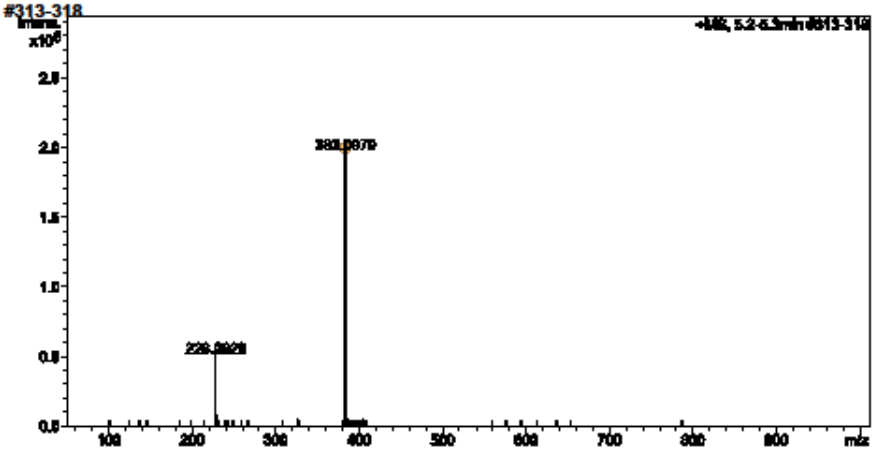
Analysis Info

Analysis Name	C:\Data\Data\N34272-64-2_1-A,3_01_1117.d	Acquisition Date	24/10/2014 14:56:54
Method	lcms pos 50-1000.m	Operator	Spectroscopy
Sample Name	N34272-64-2	Instrument / Ser	maXis impact 282001.00101
Comment			

Acquisition Parameter

Source Type	ESI	Scan Begin	50 m/z
Ion Polarity	Positive	Scan End	1000 m/z

+MS, 5.2-5.3min
#313-318

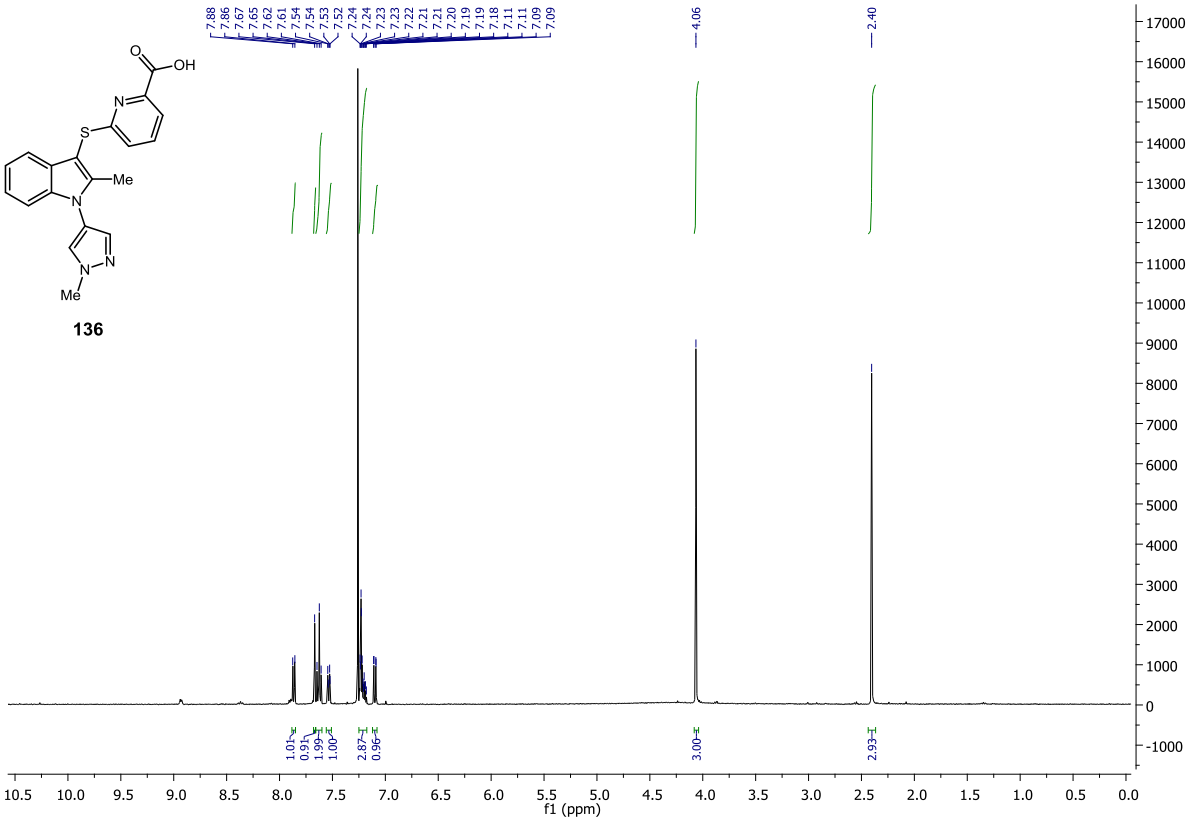


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
383.0979	1	C19H16FN4O2S	383.0973	1.6	19.3	1	100.00	13.5	even	ok

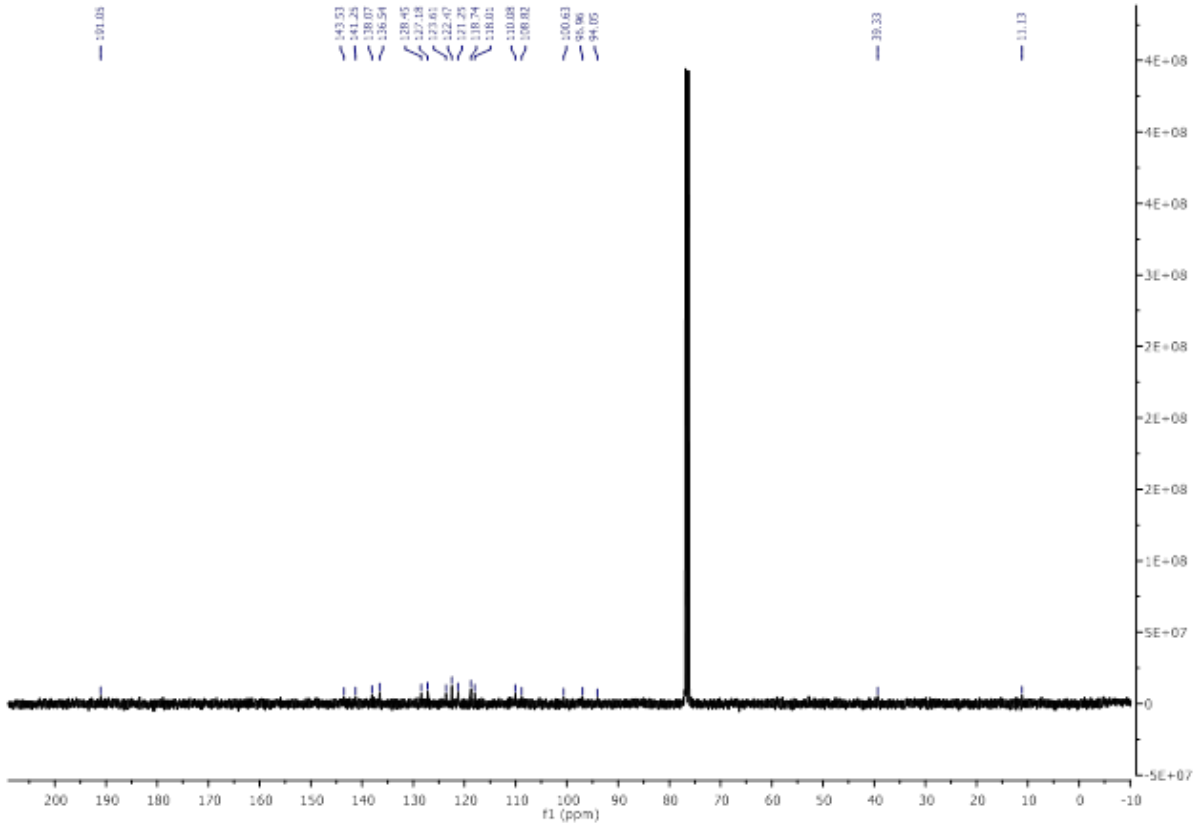
Measured mass should be within ±5 ppm of target mass

Compound 136

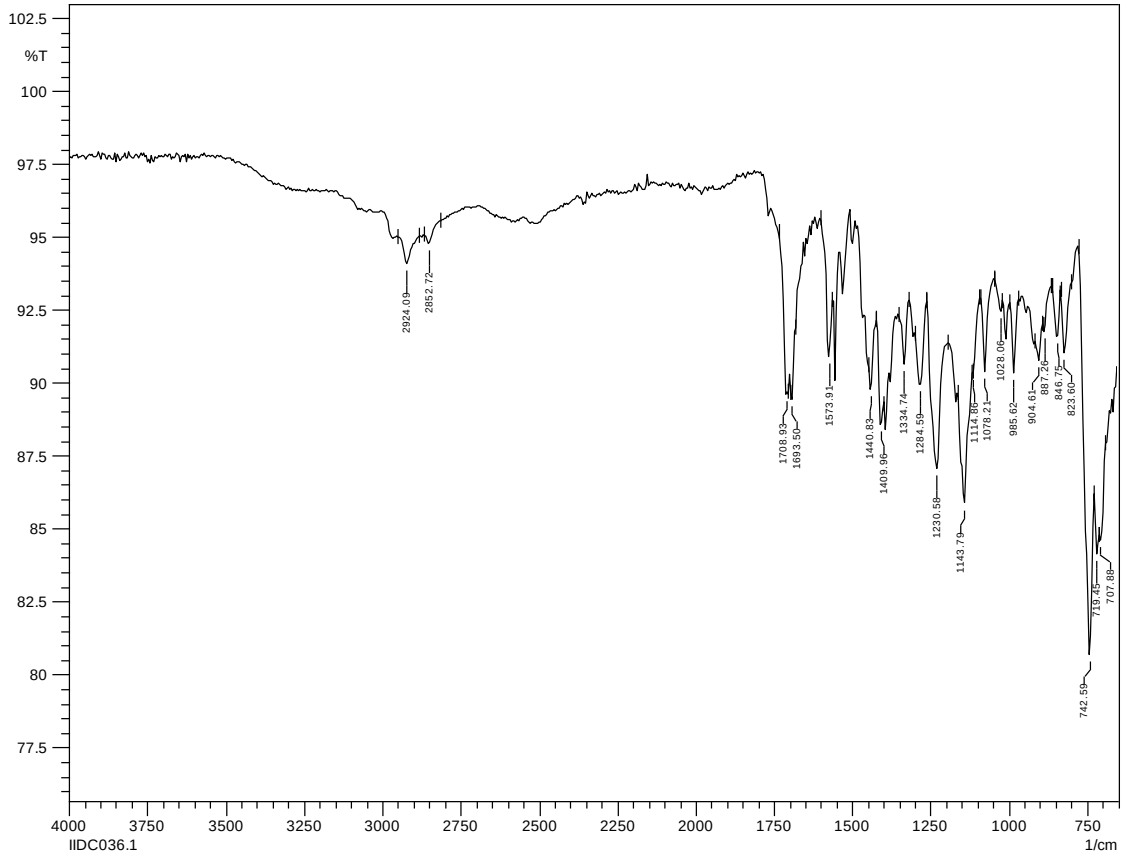
^{1}H NMR



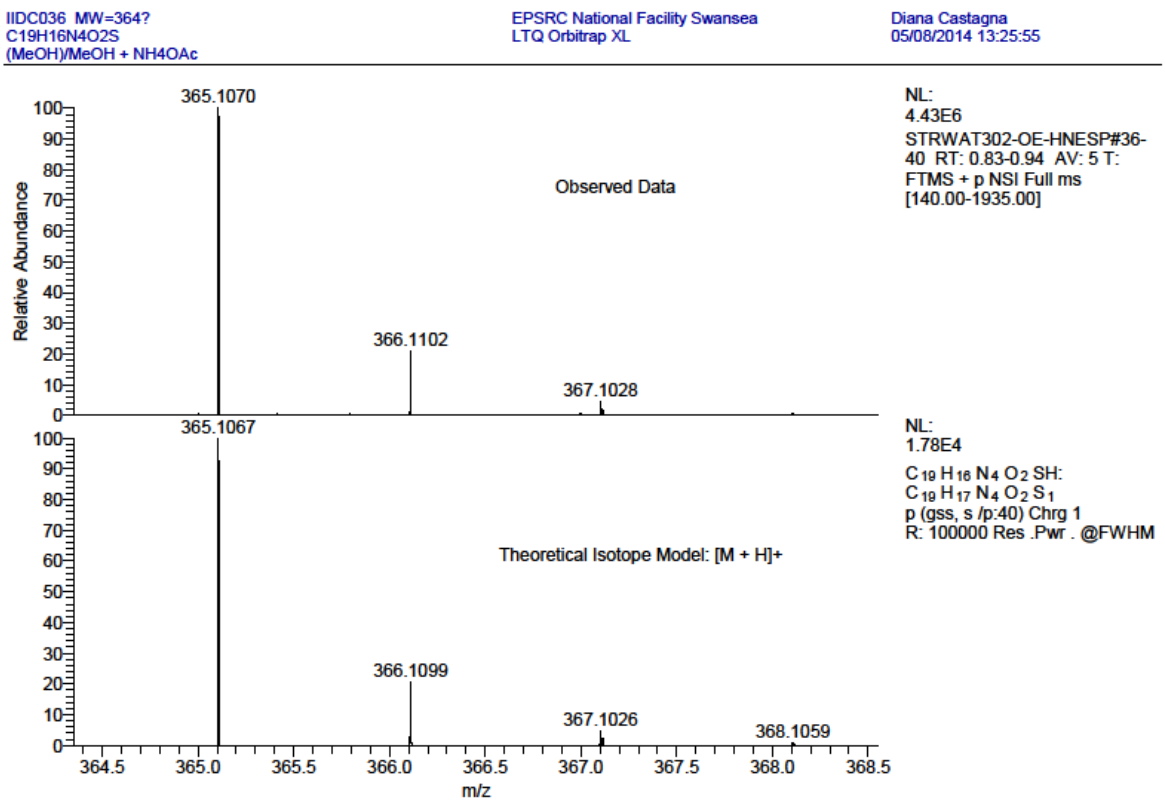
^{13}C NMR of 136



IR of 136

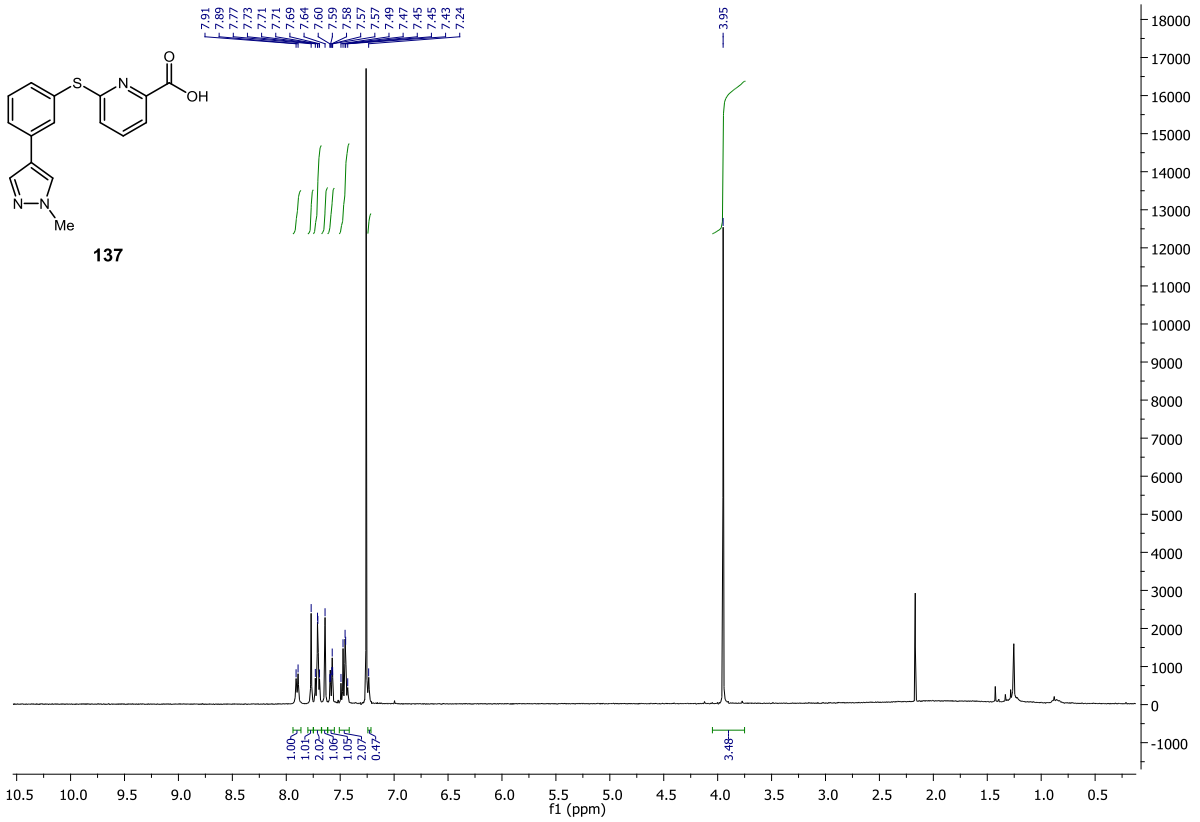


HRMS of 136

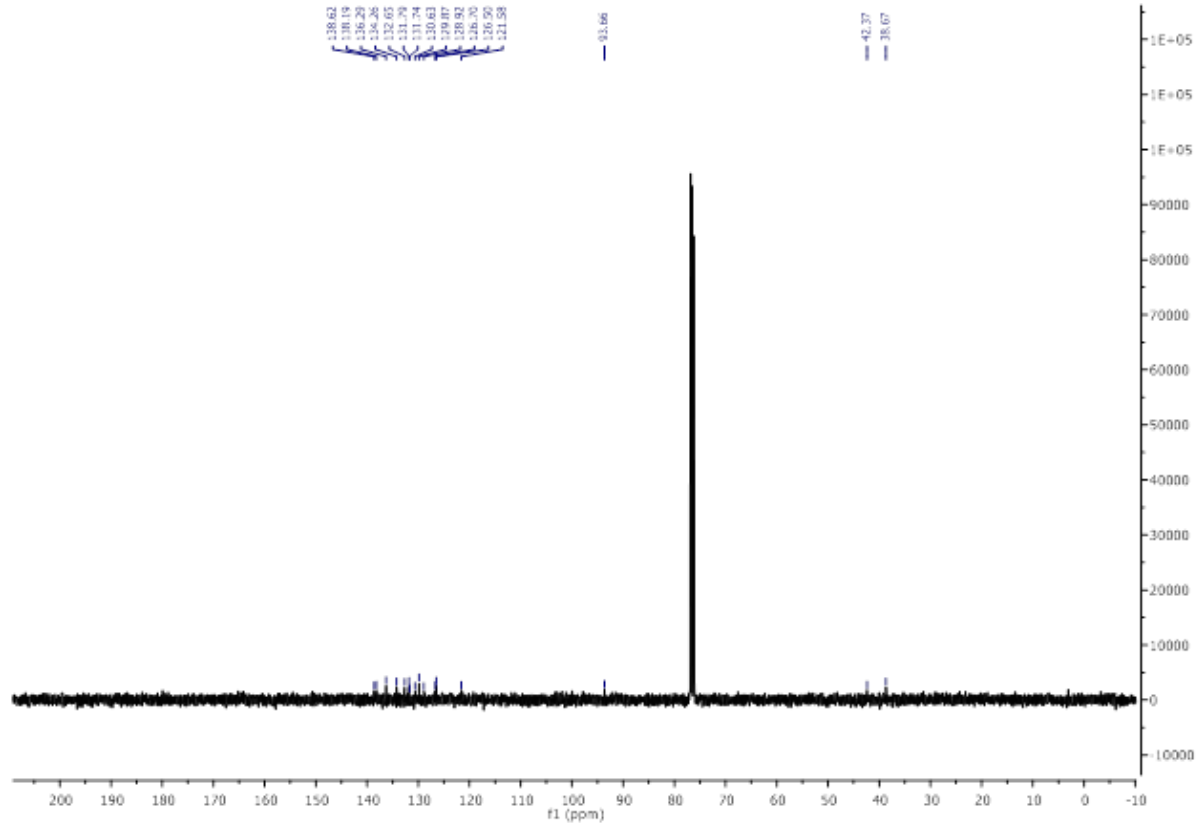


Compound 137

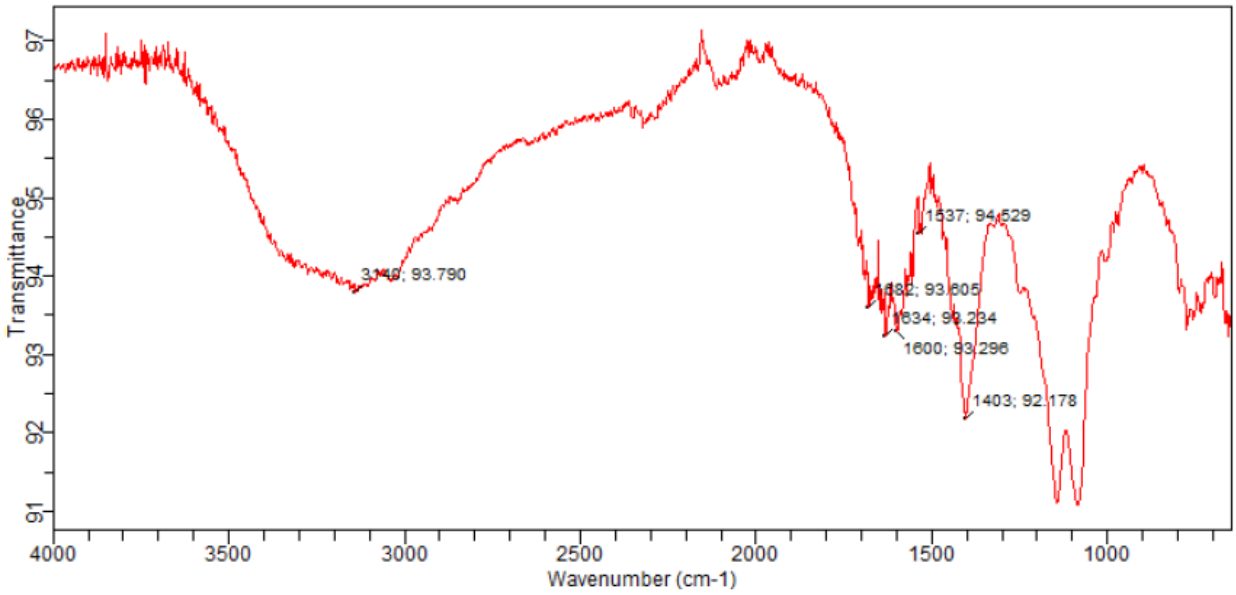
^{1}H NMR



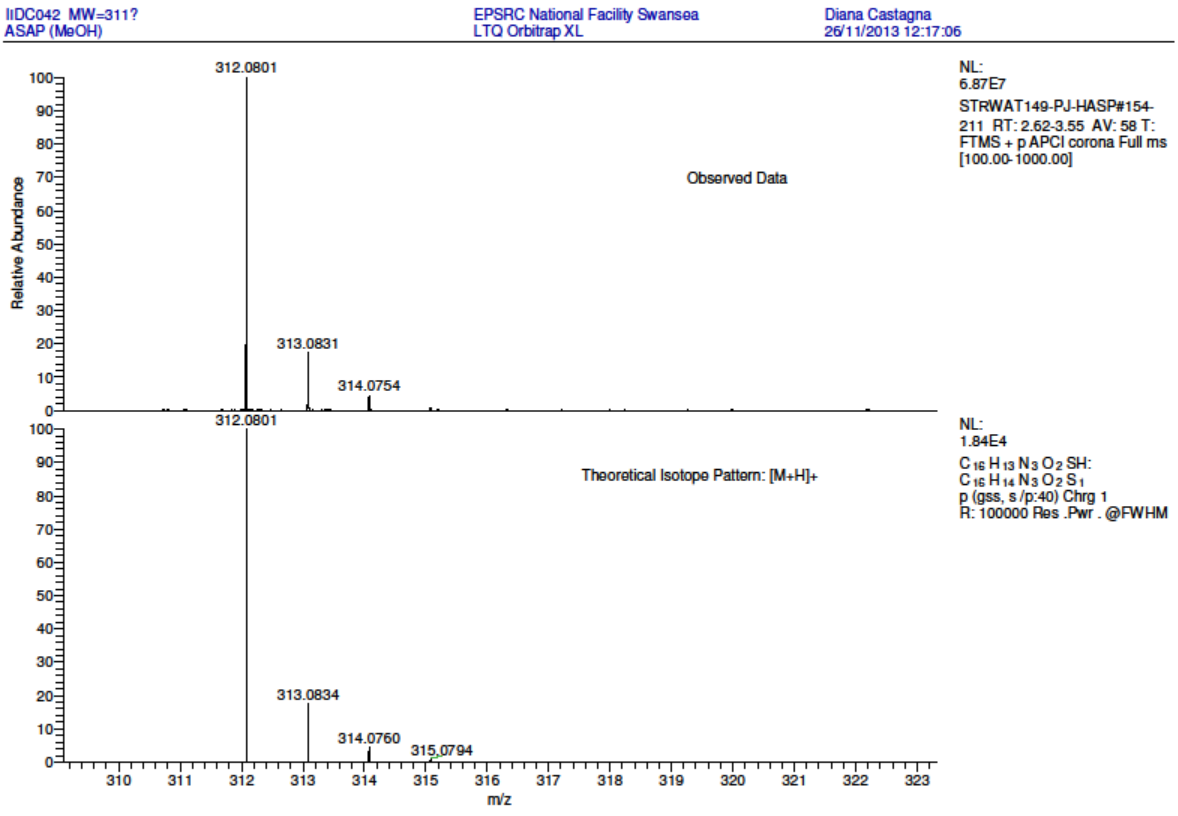
^{13}C NMR of 137



IR of 137

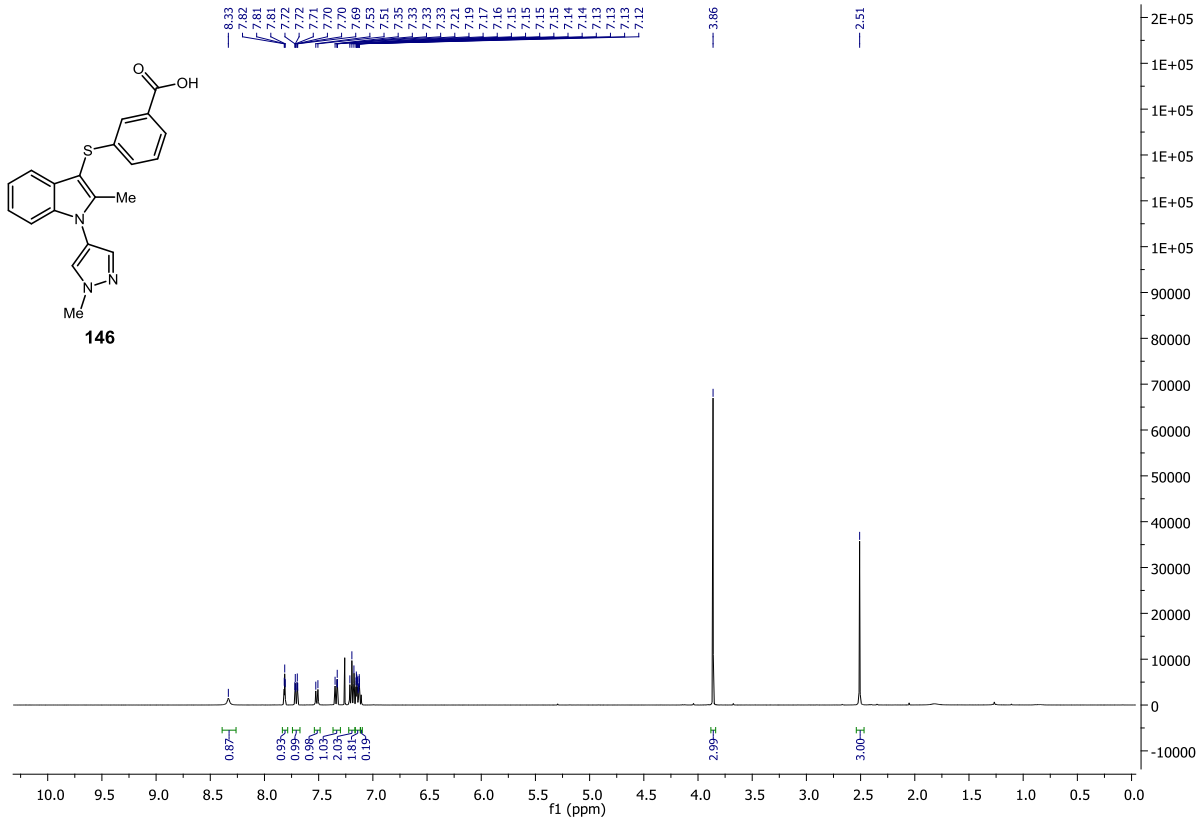


HRMS of 137

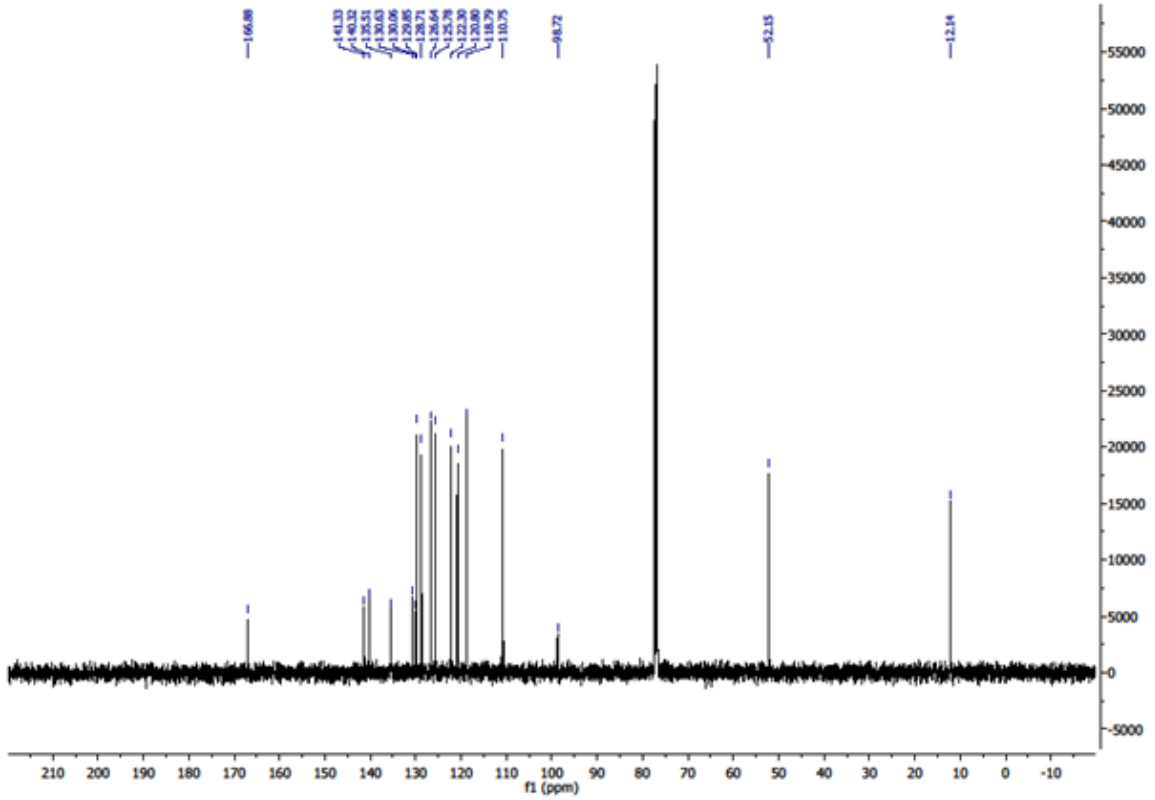


Compound 146

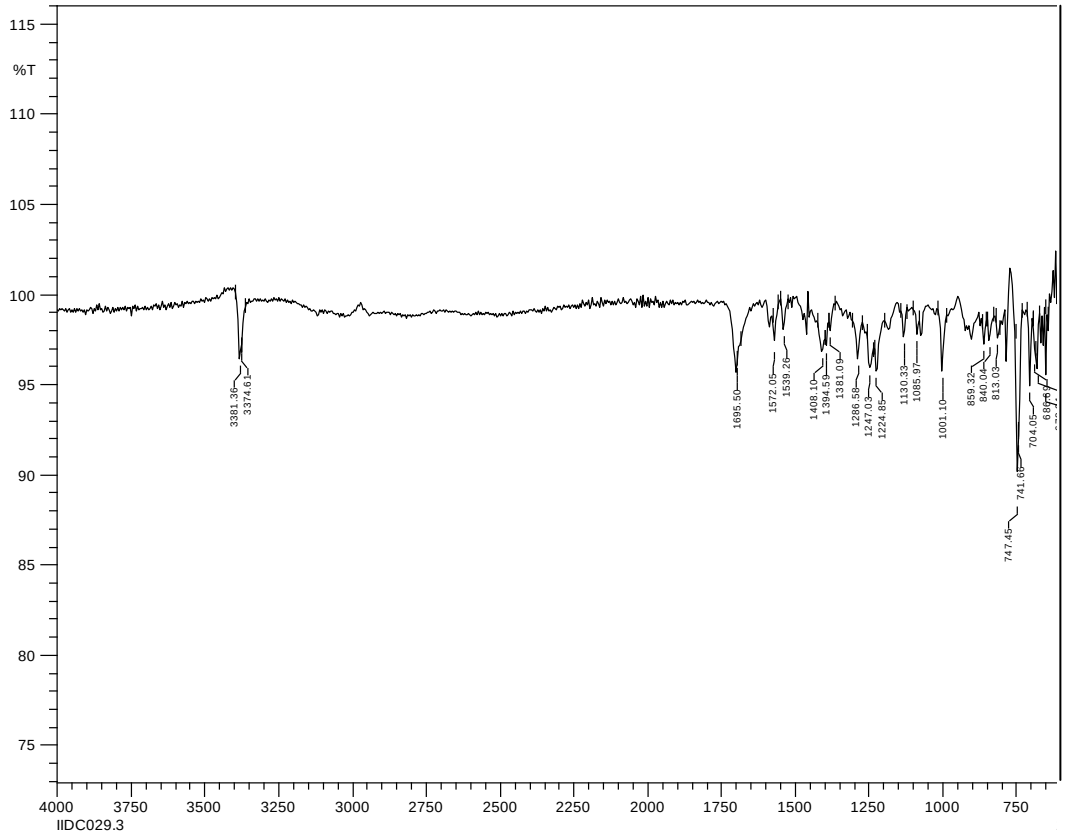
^{1}H NMR



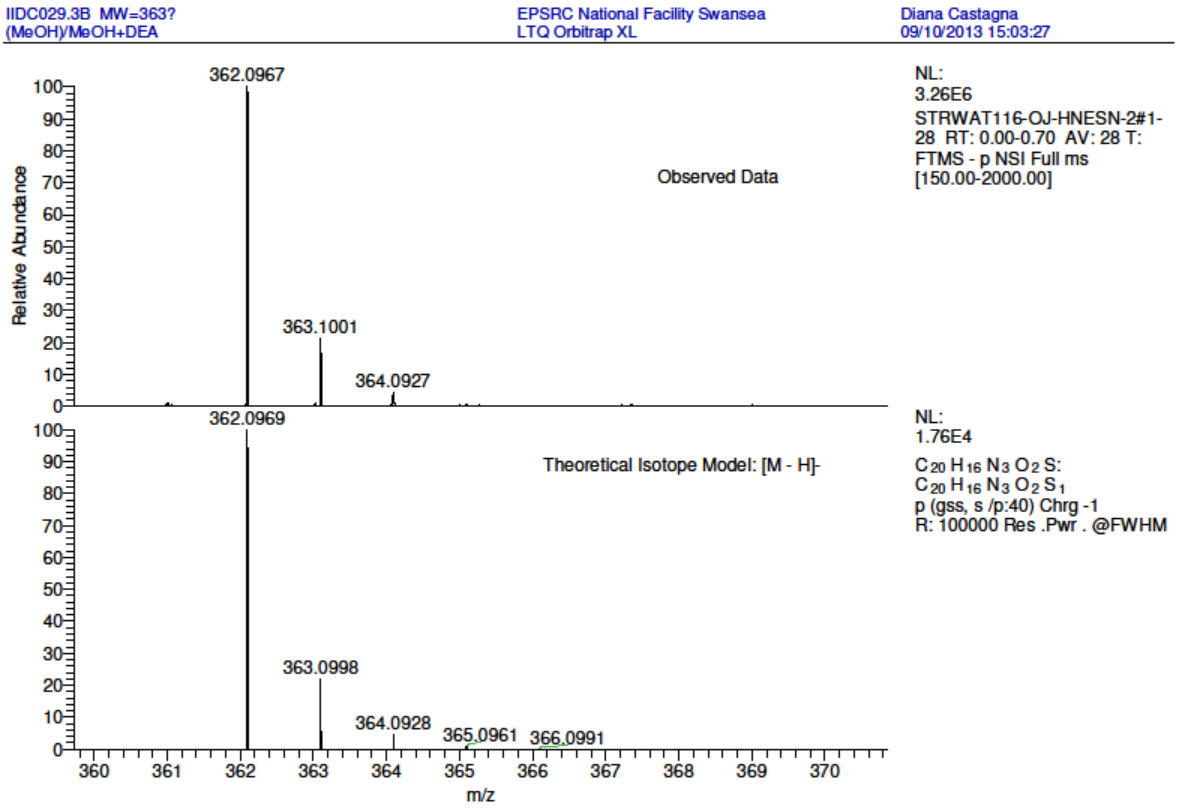
^{13}C NMR of 146



IR of 146

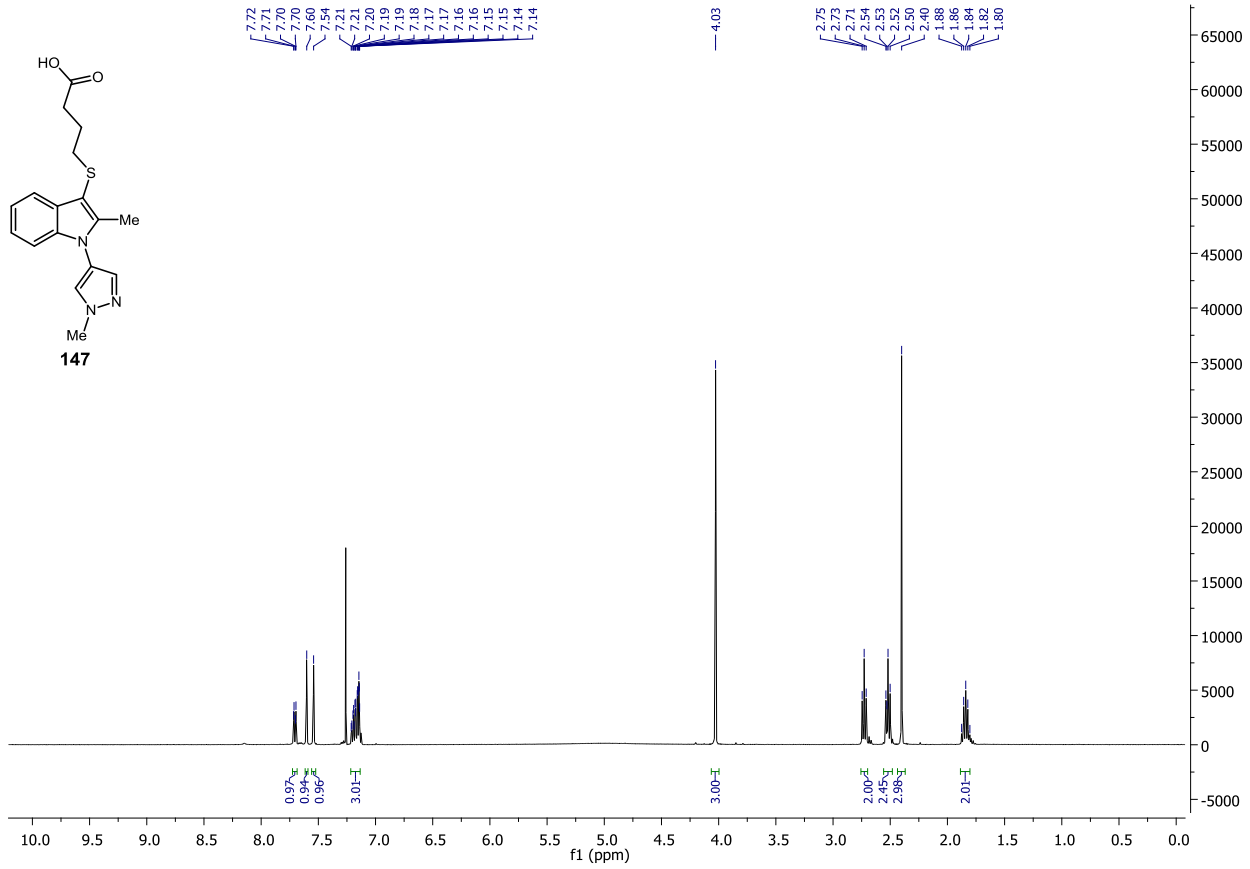


HRMS of 146

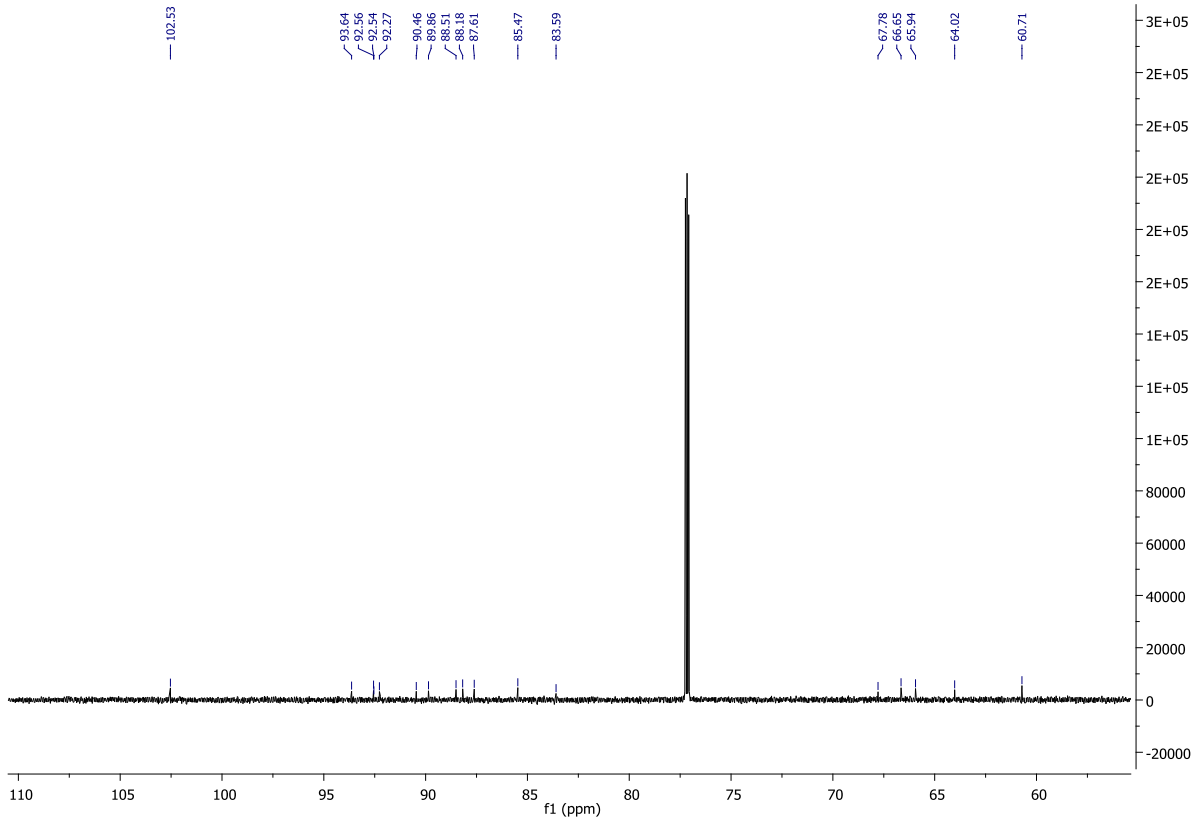


Compound 147

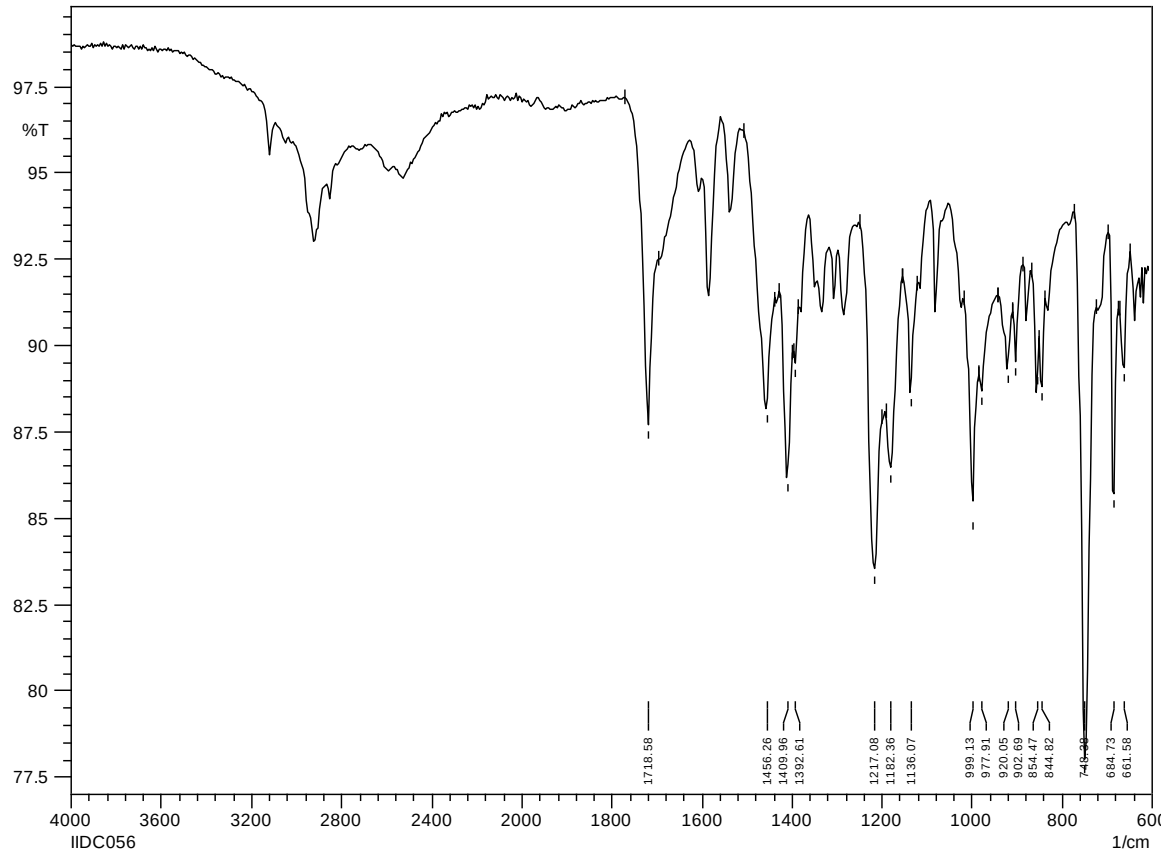
^{1}H NMR



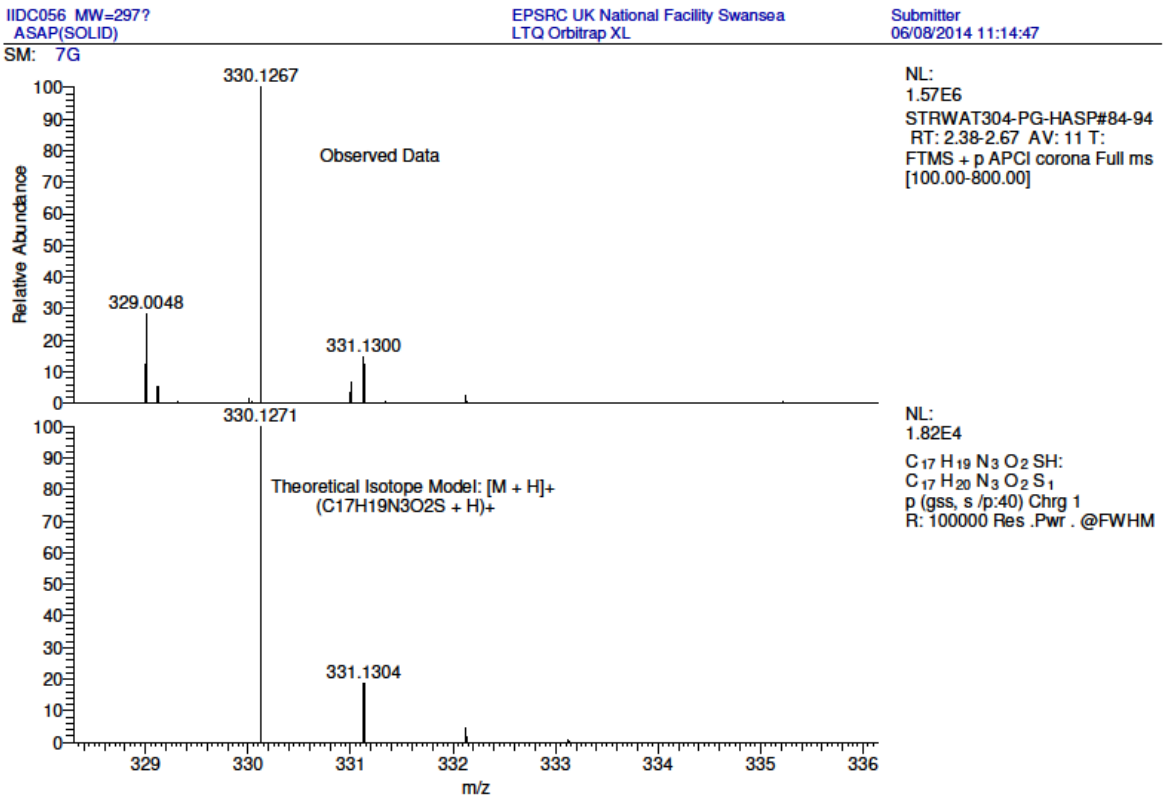
^{13}C NMR of 147



IR of 147

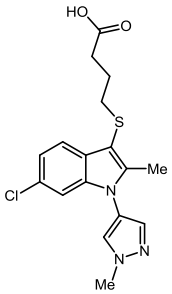


HRMS of 147



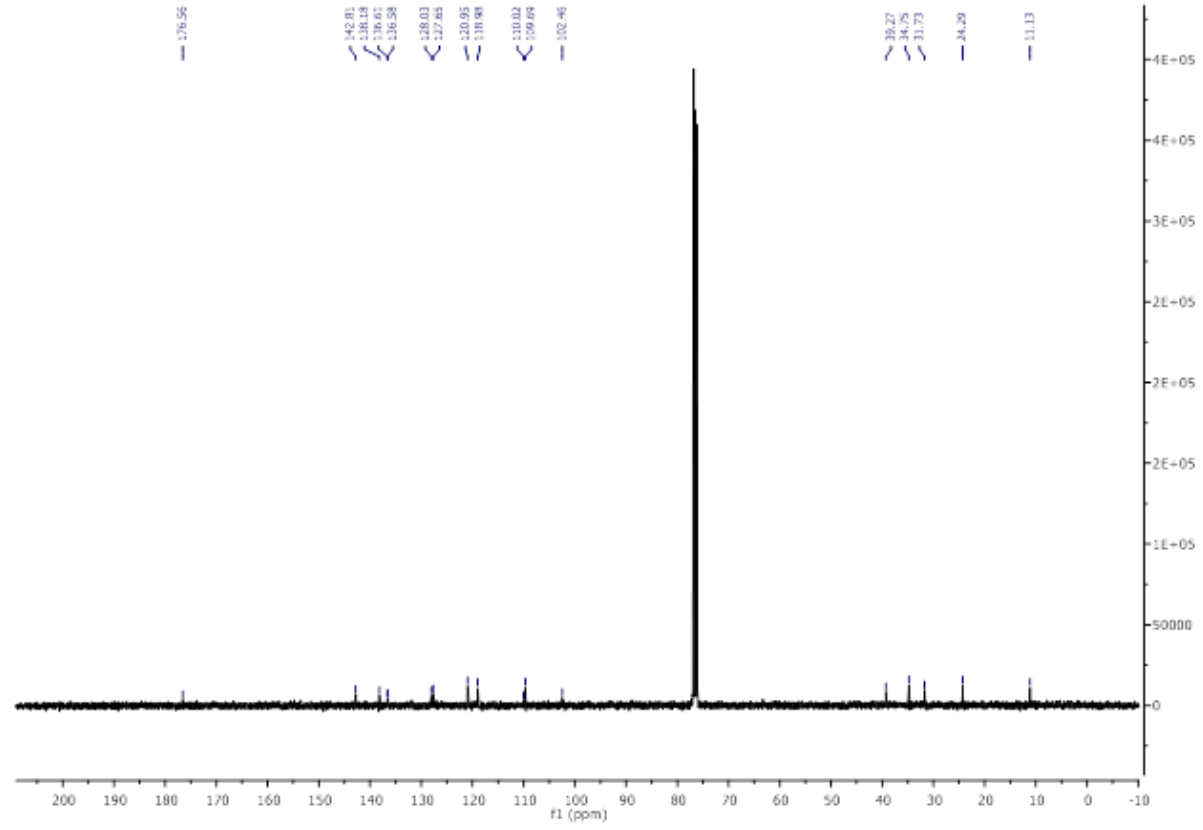
Compound 148

^{1}H NMR

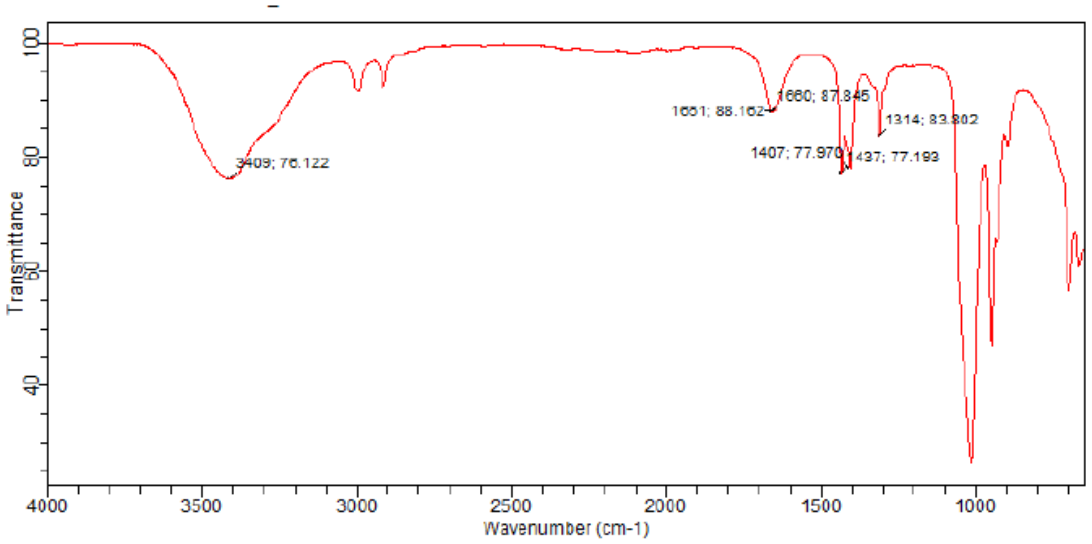


148

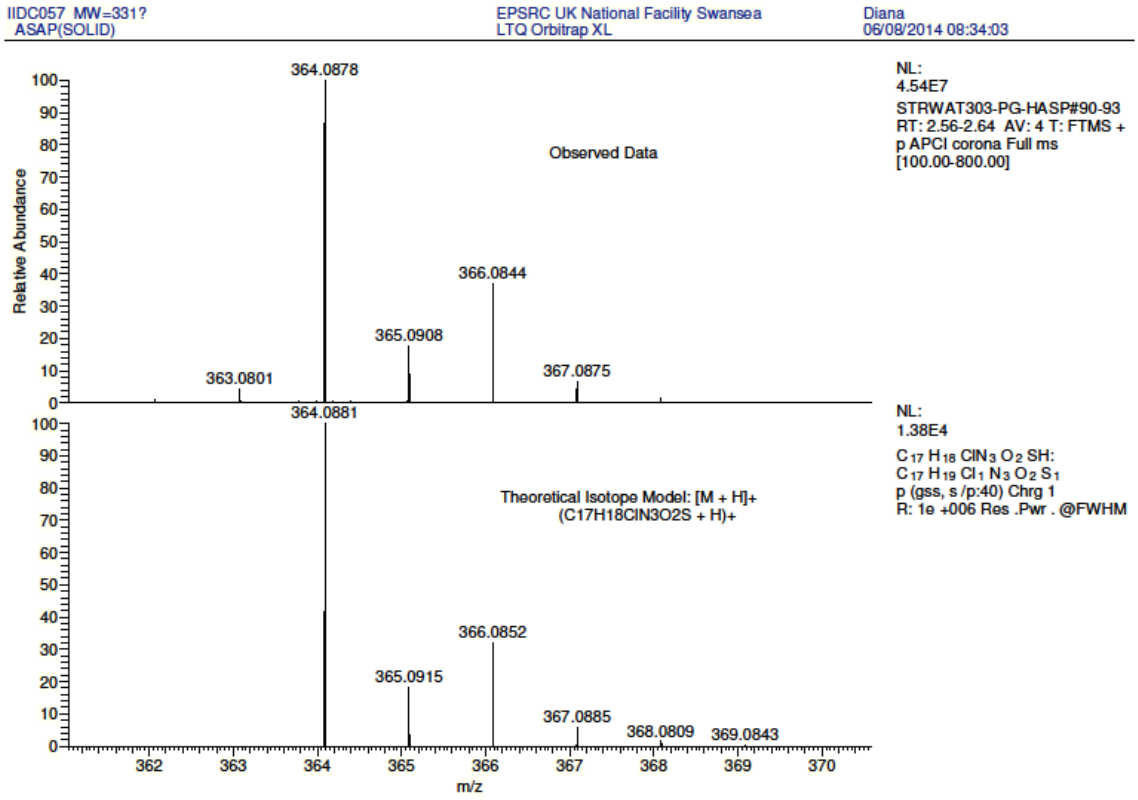
^{13}C NMR of 148



IR of 148

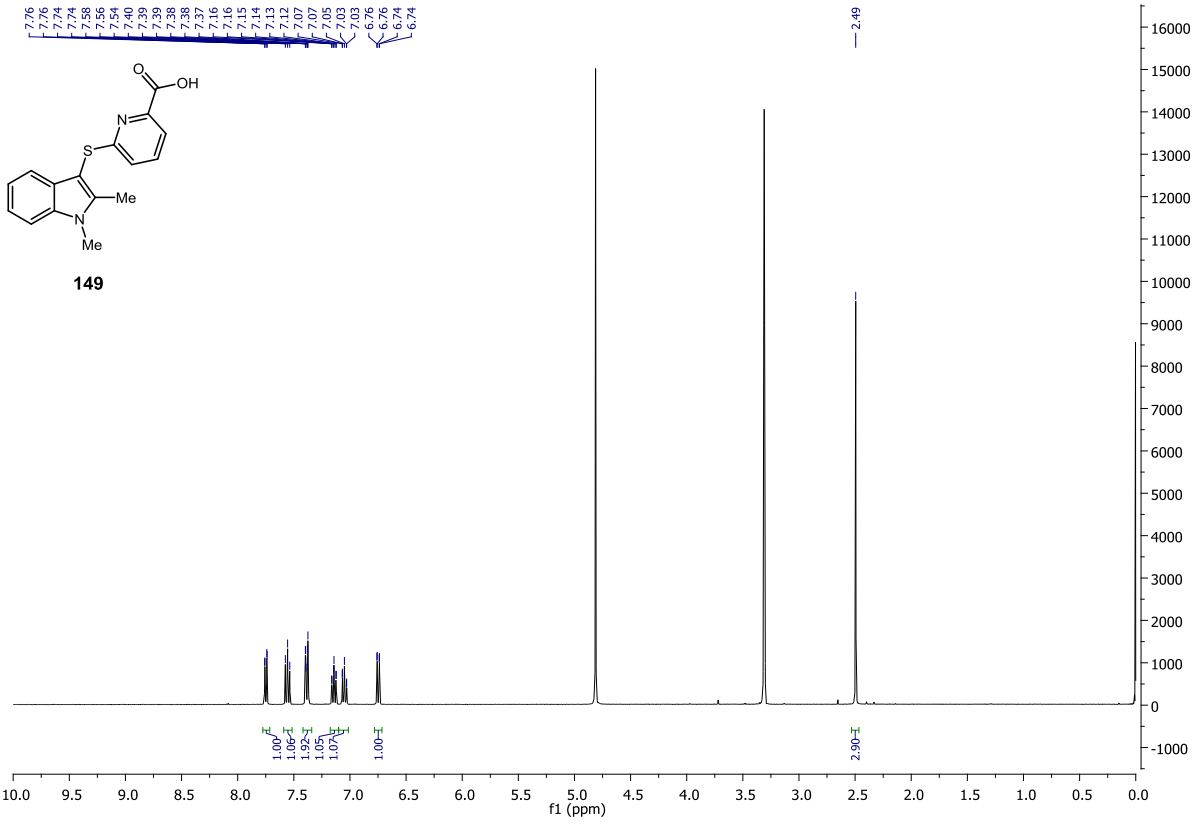


HRMS of 148

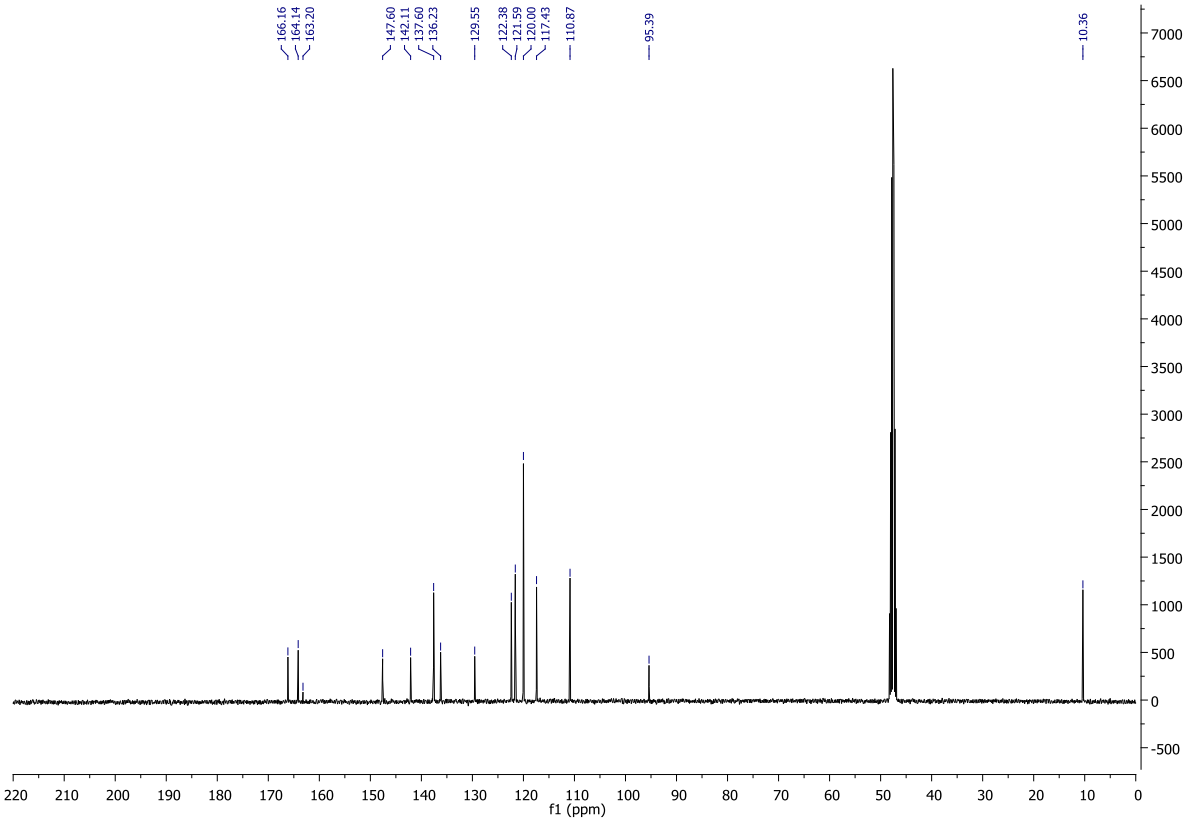


Compound 149

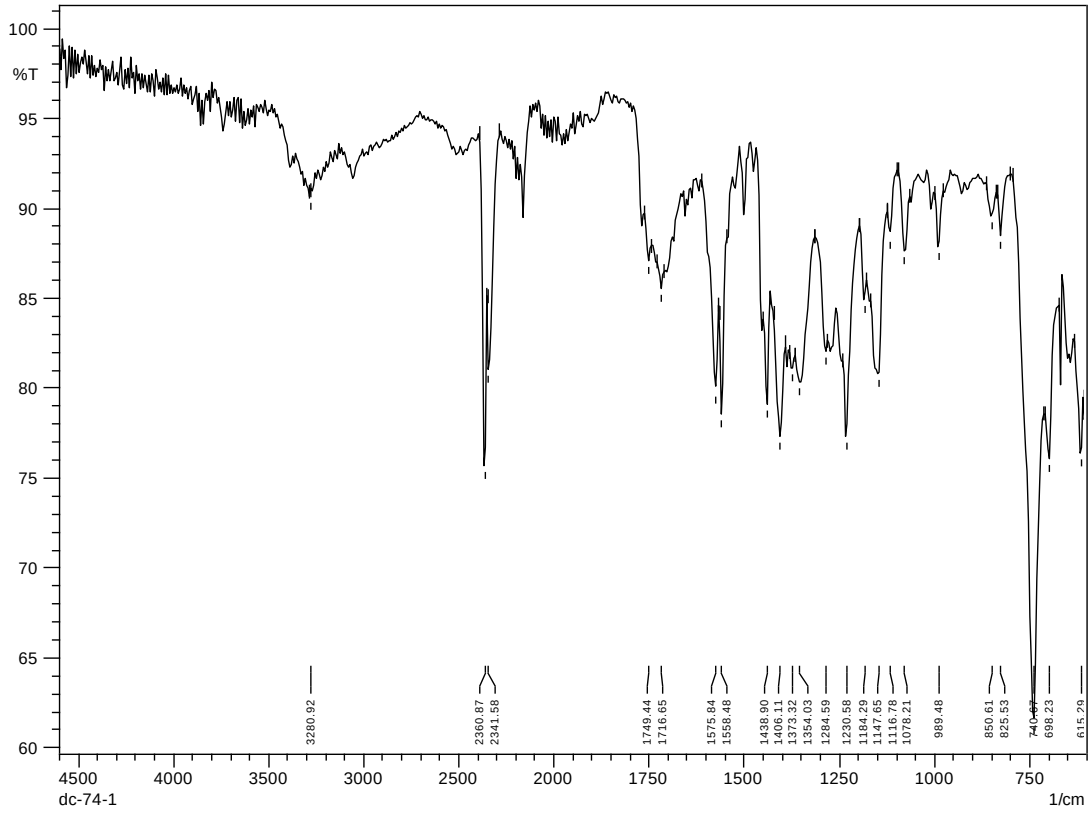
^{1}H NMR



^{13}C NMR of 149

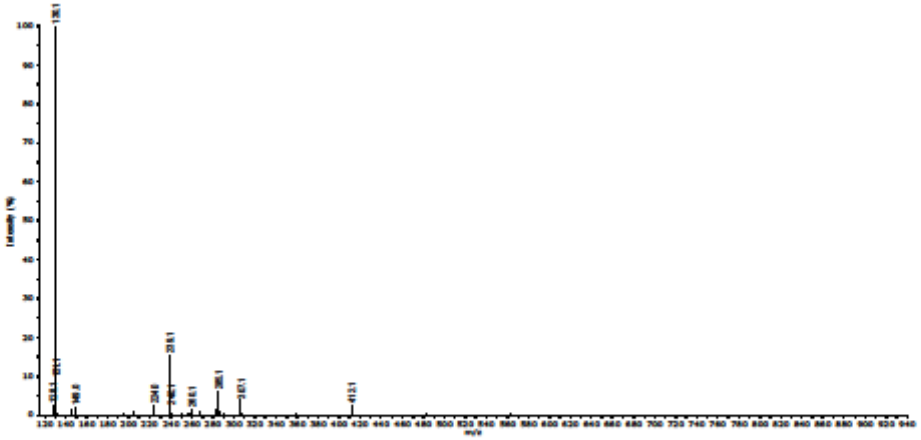


IR of 149

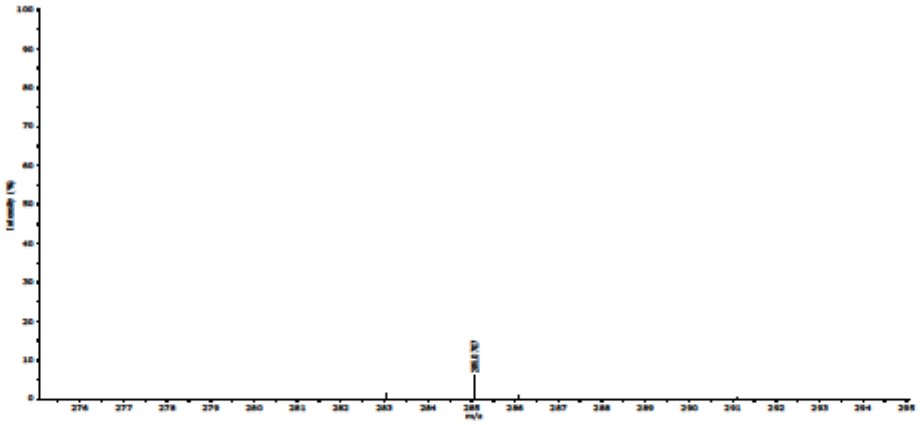

100
%T
95
90
85
80
75
70
65
60
3280.92
2360.87
2341.58
1749.44
1716.65
1575.84
1558.48
1438.90
1406.11
1373.32
1354.03
1284.59
1230.58
1184.29
1147.65
1116.78
1078.21
989.48
850.61
825.53
740.67
698.23
615.29
4500
4000
3500
3000
2500
2000
1750
1500
1250
1000
750
dc-74-1
1/cm

HRMS of 149

Spectrum RT 4.19, Peak [1], Target Mass 285.0692



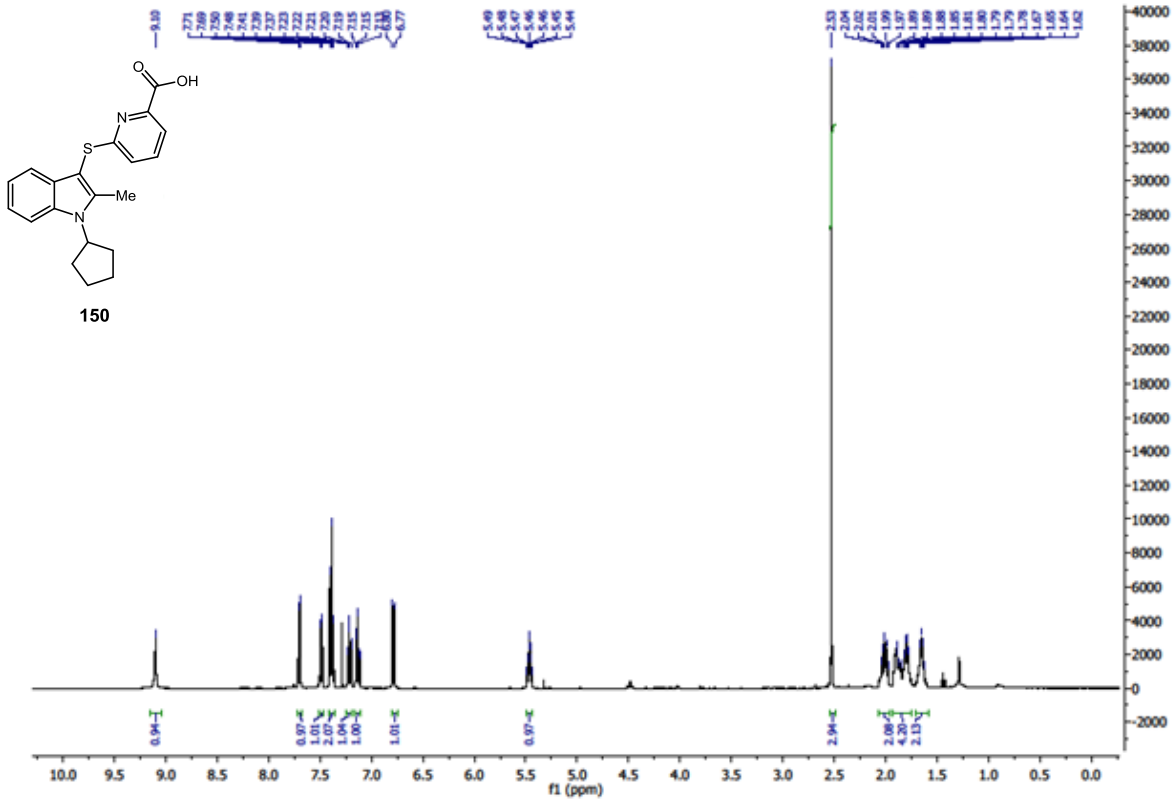
Expanded Spectrum RT 4.19, Peak [1], Target Mass 285.0692



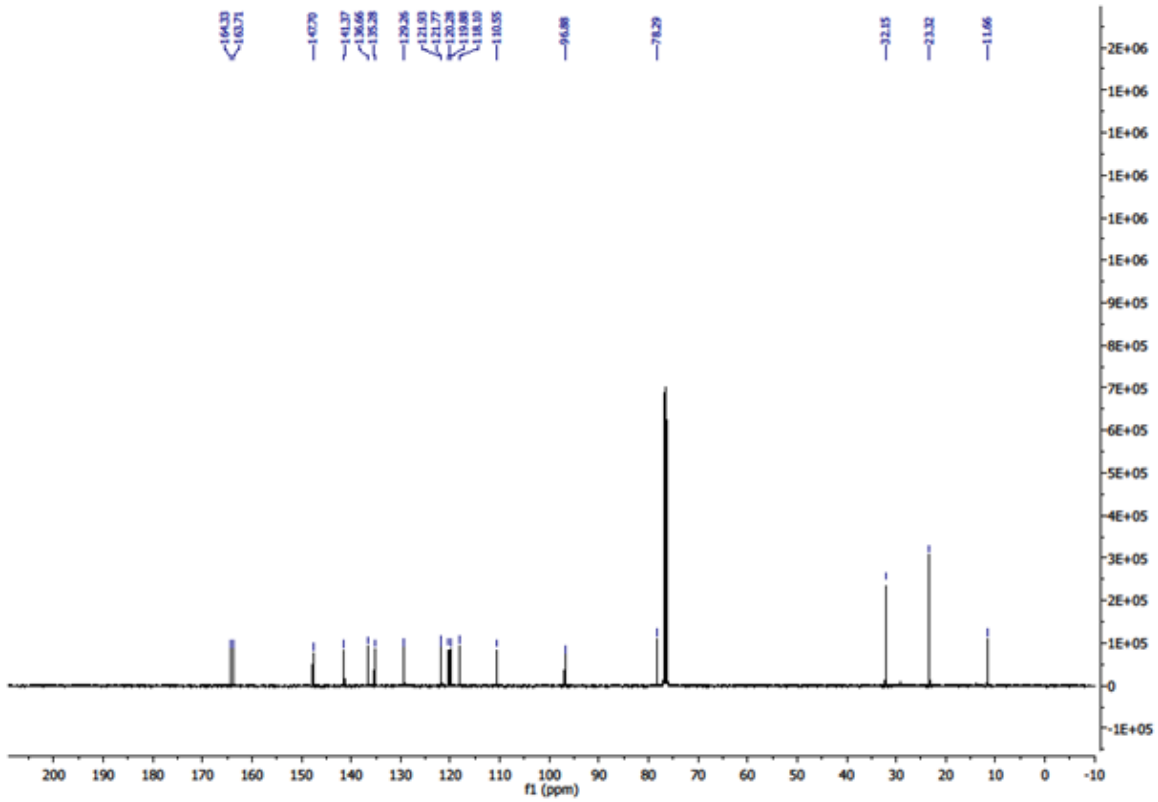
Measured Mass	Calculated Mass	Error (mDa)	Error (ppm)	Formula $[M+H]^+$
285.0693	285.0692	0.1	0.2	$C_{15}H_{13}N_2O_2S$

Compound 150

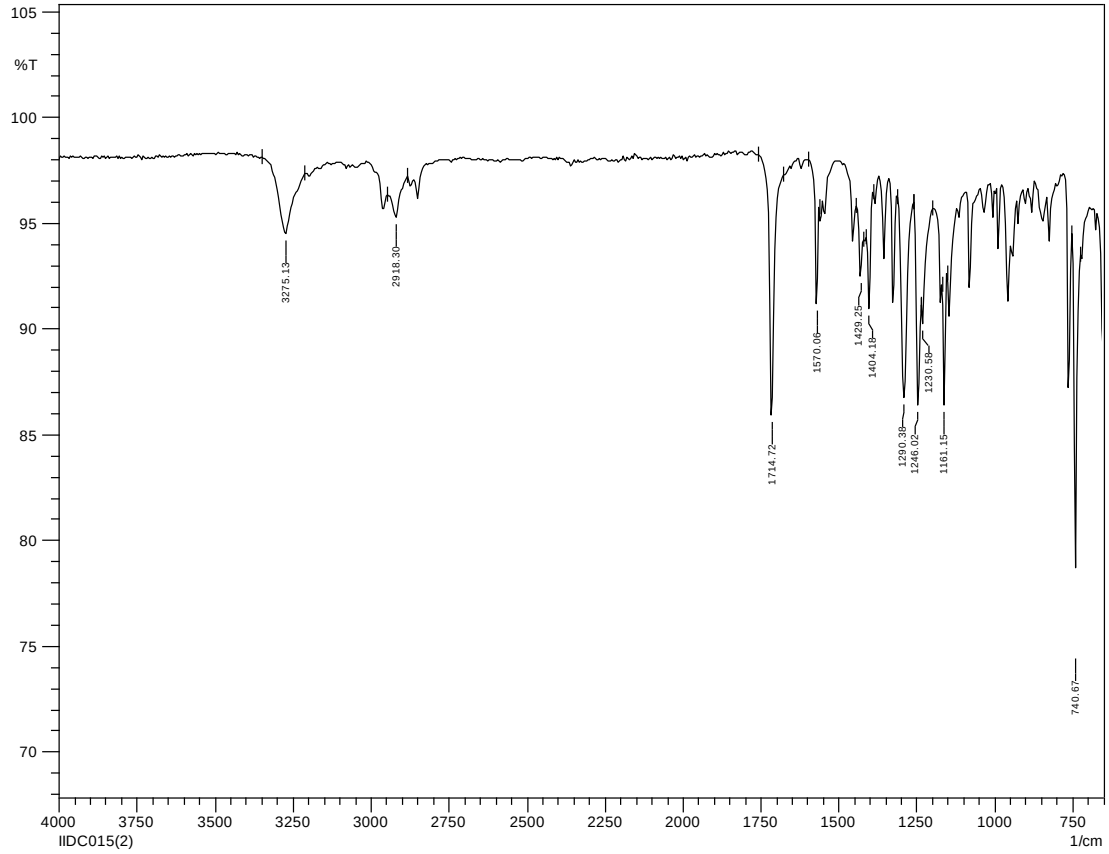
^{1}H NMR



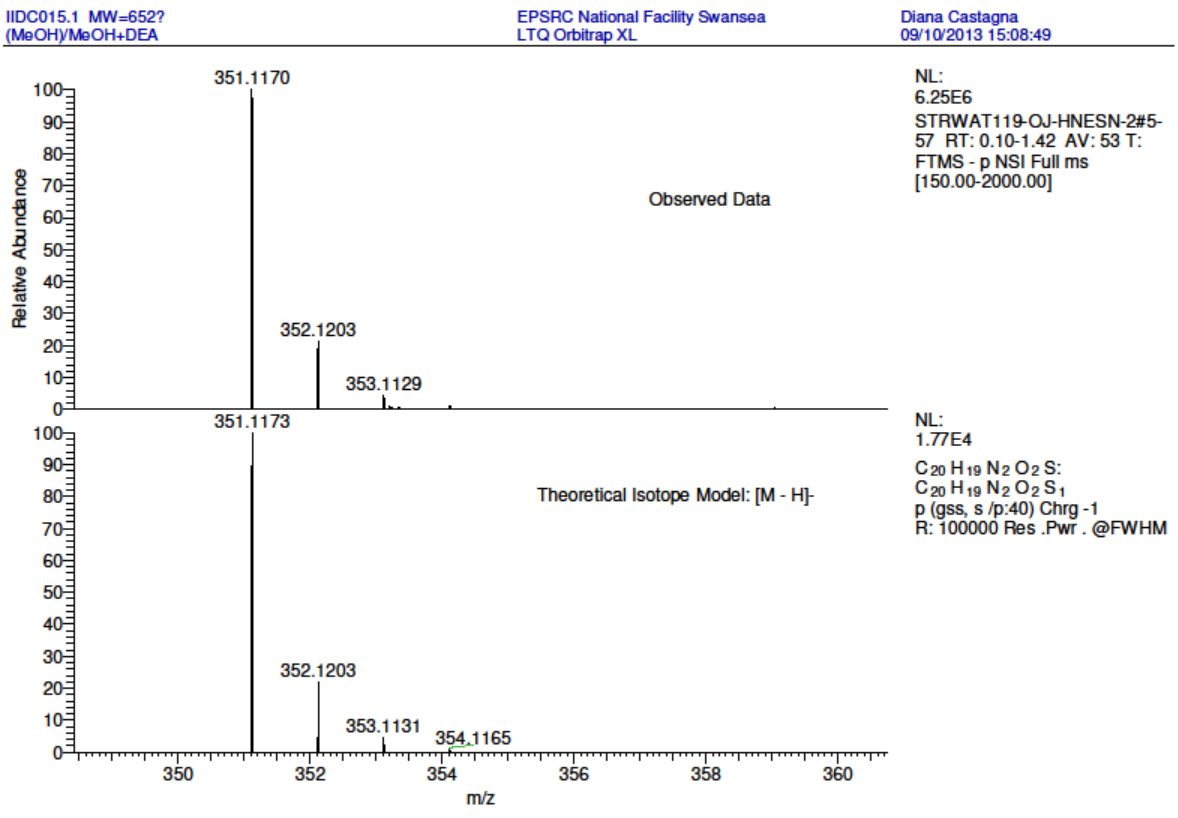
^{13}C NMR of 150



IR of 150

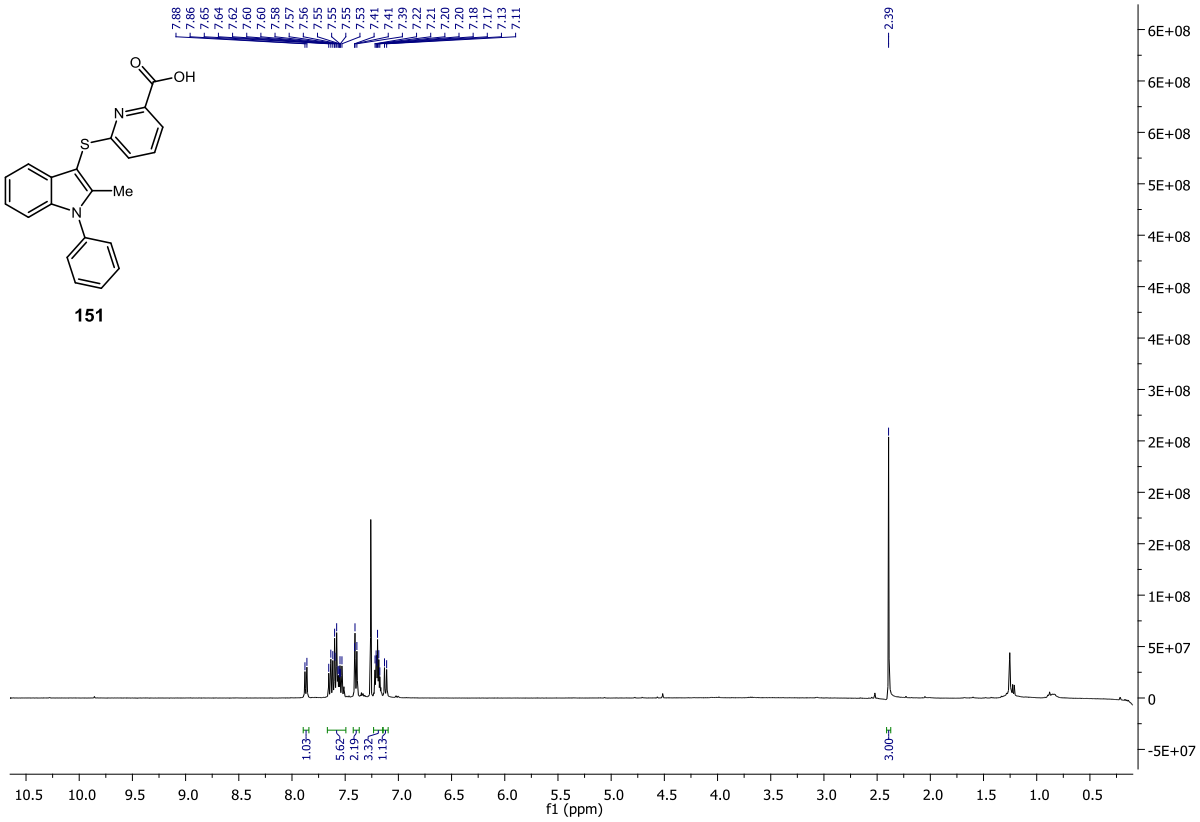


HRMS of 150

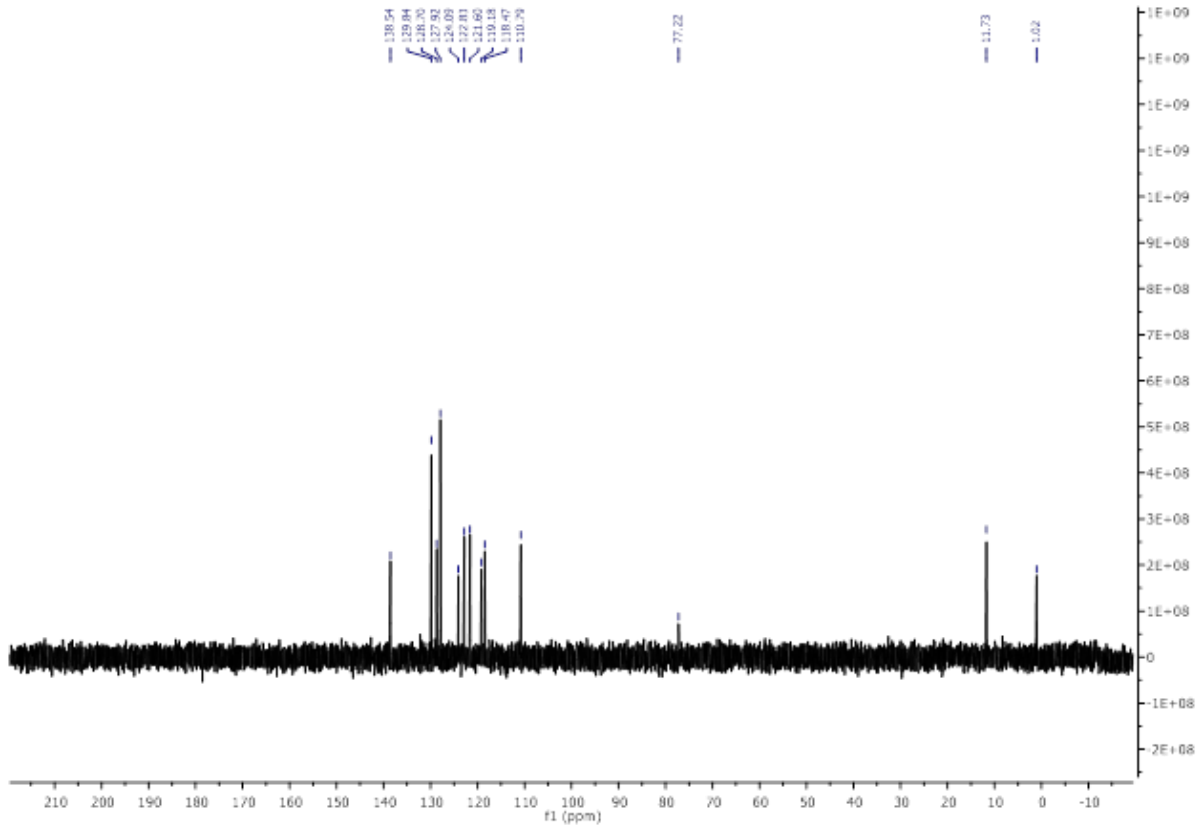


Compound 151

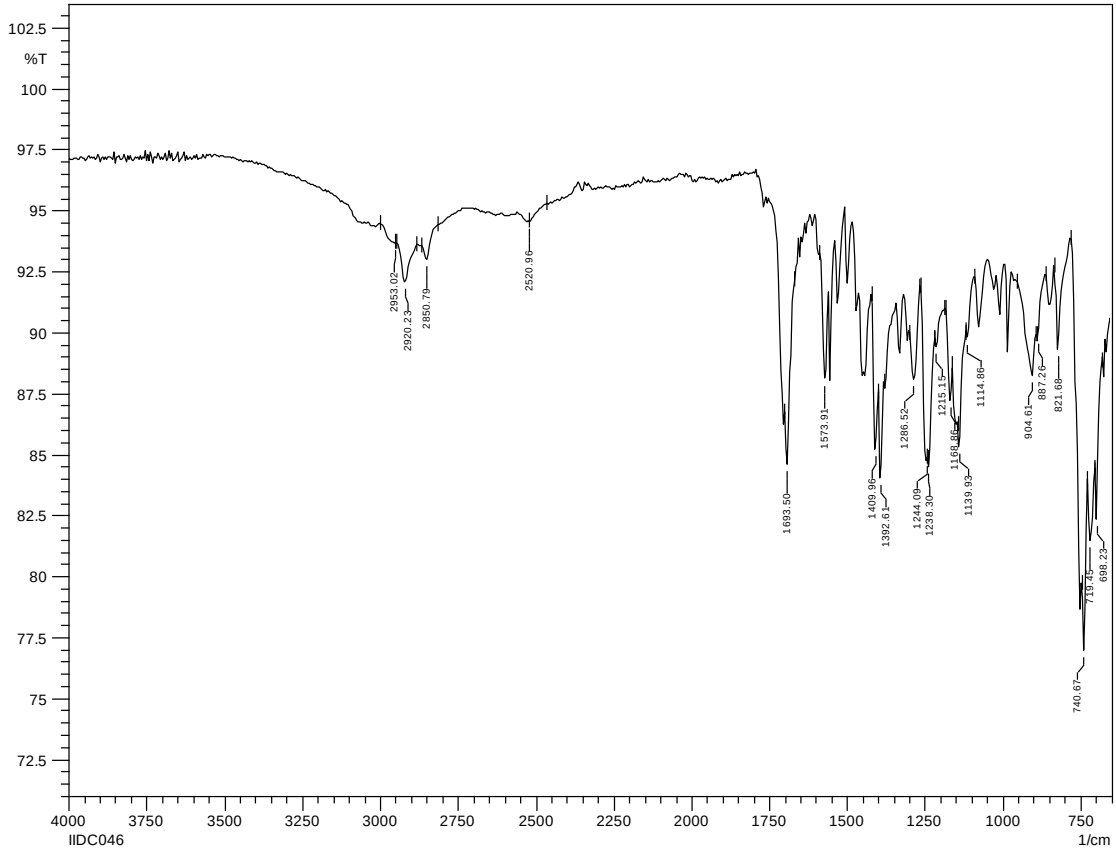
^{1}H NMR



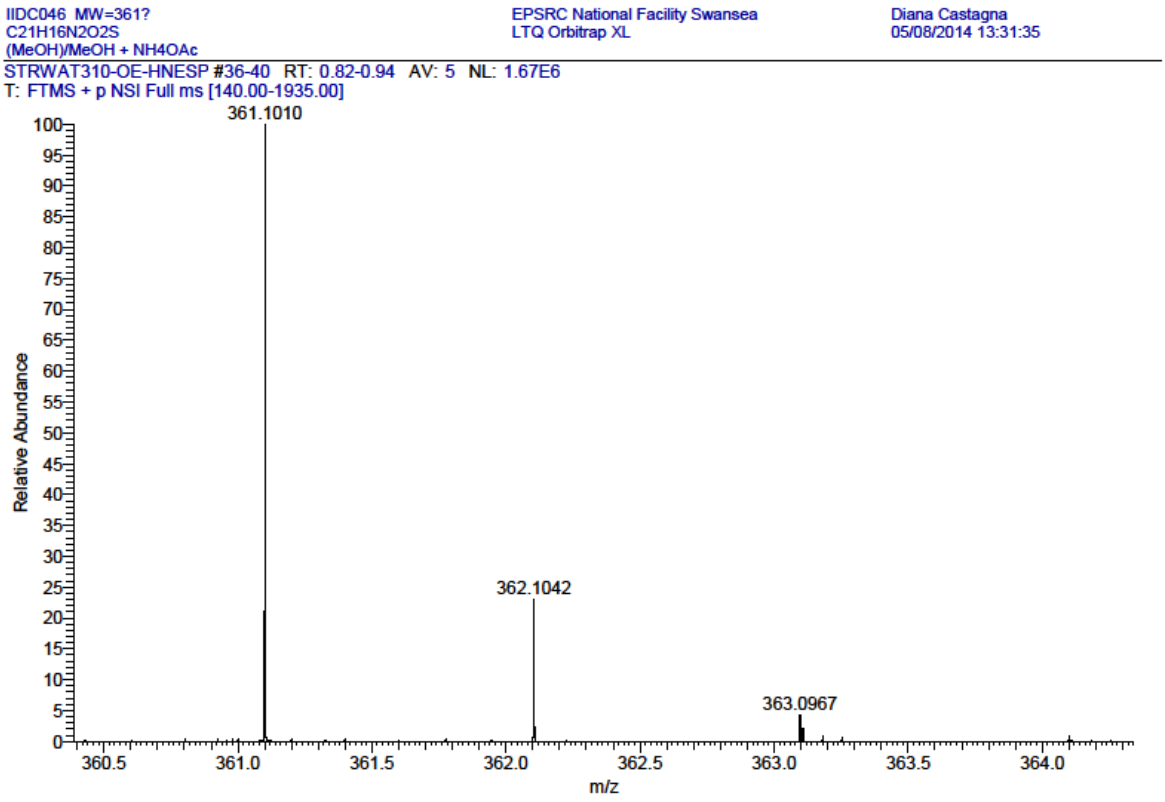
^{13}C NMR of 151



IR of 151

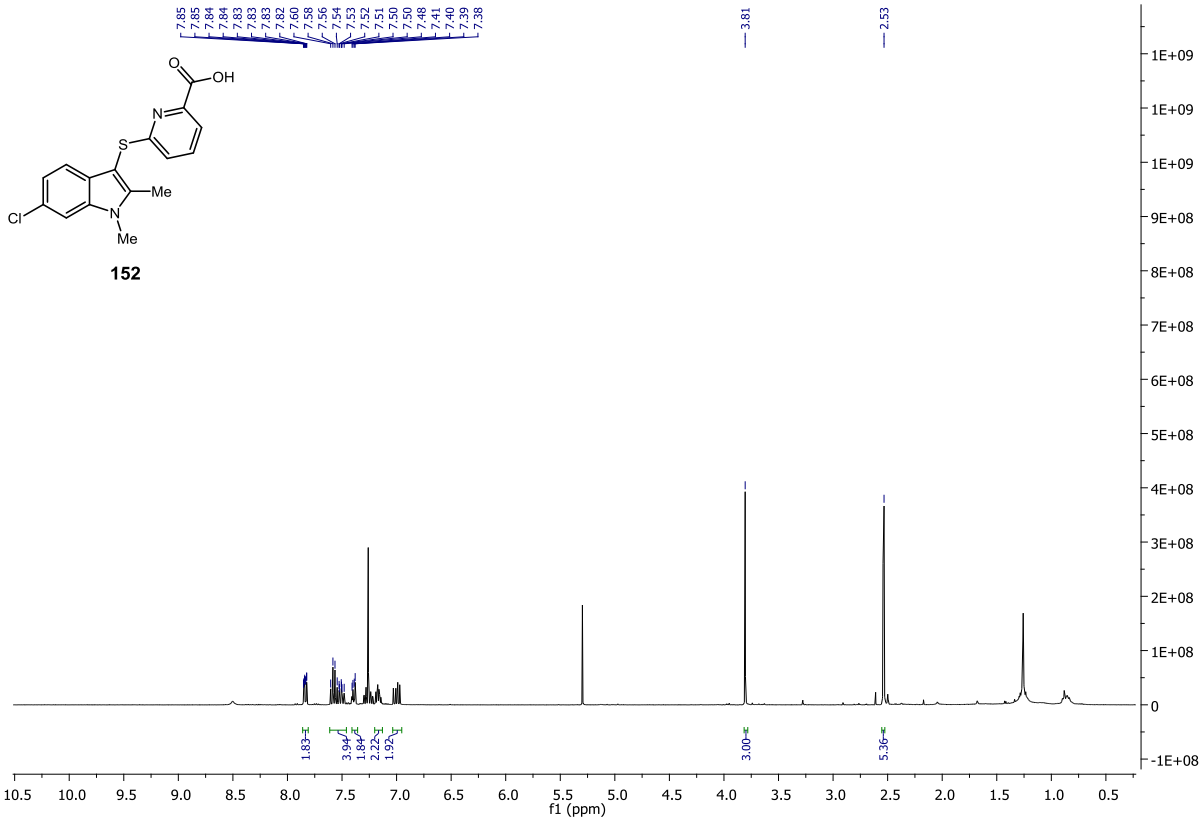


HRMS of 151

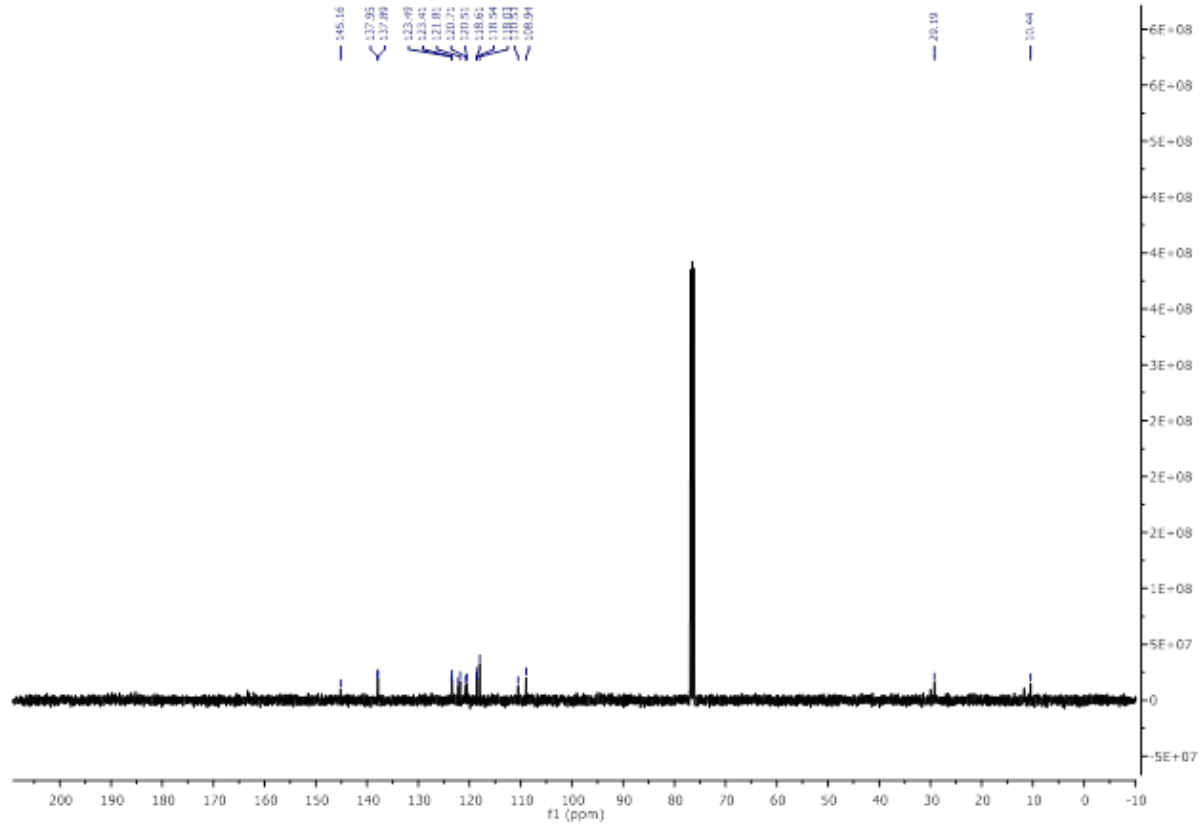


Compound 152

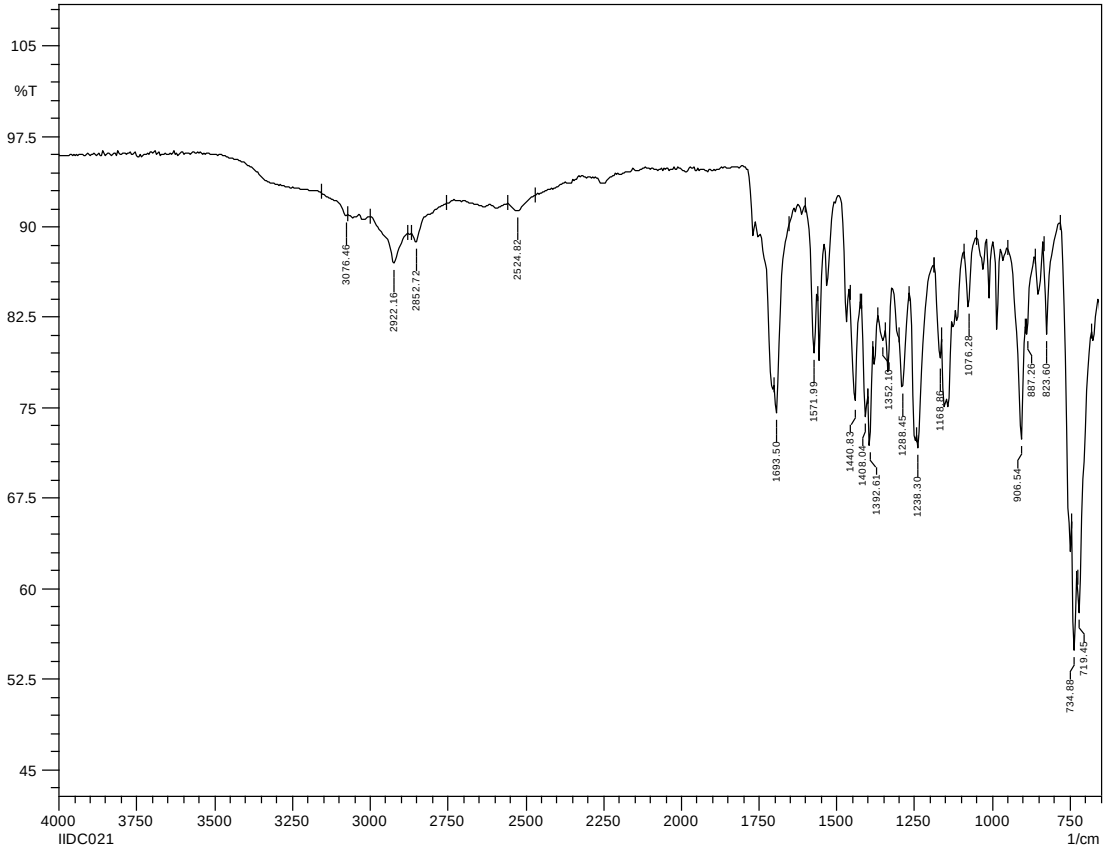
^{1}H NMR



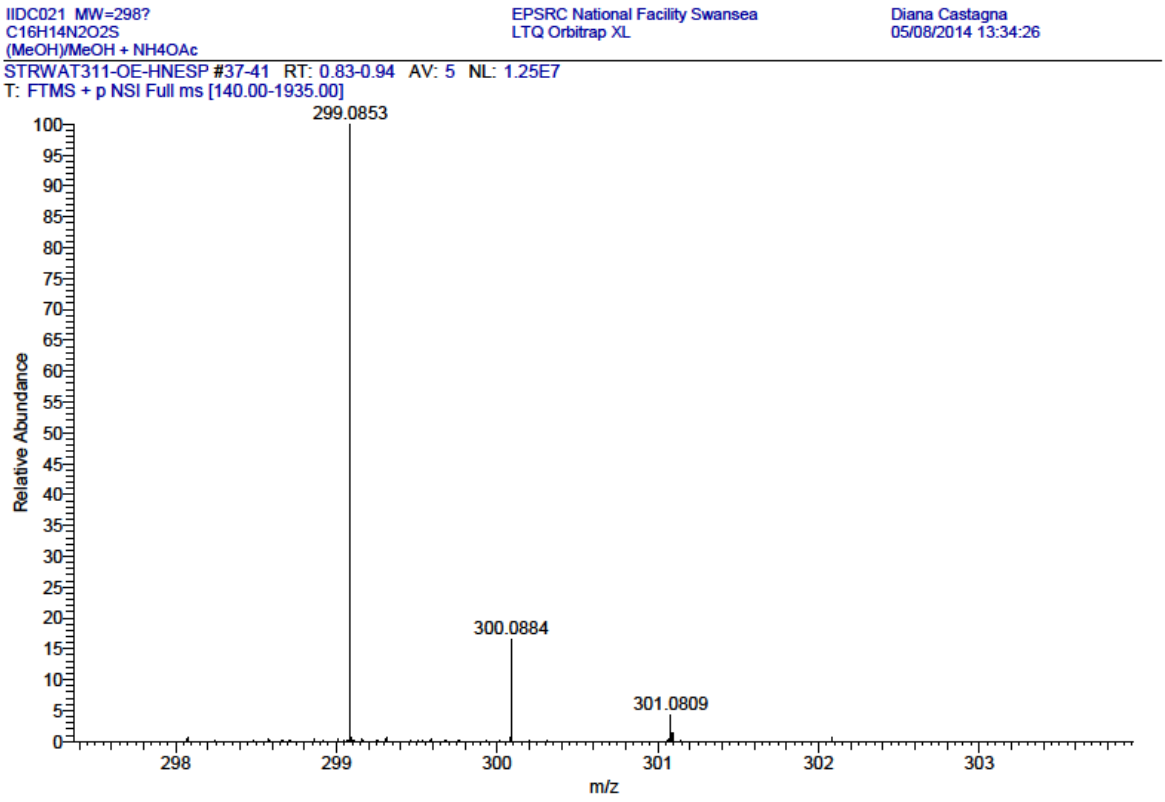
^{13}C NMR of 152



IR of 152

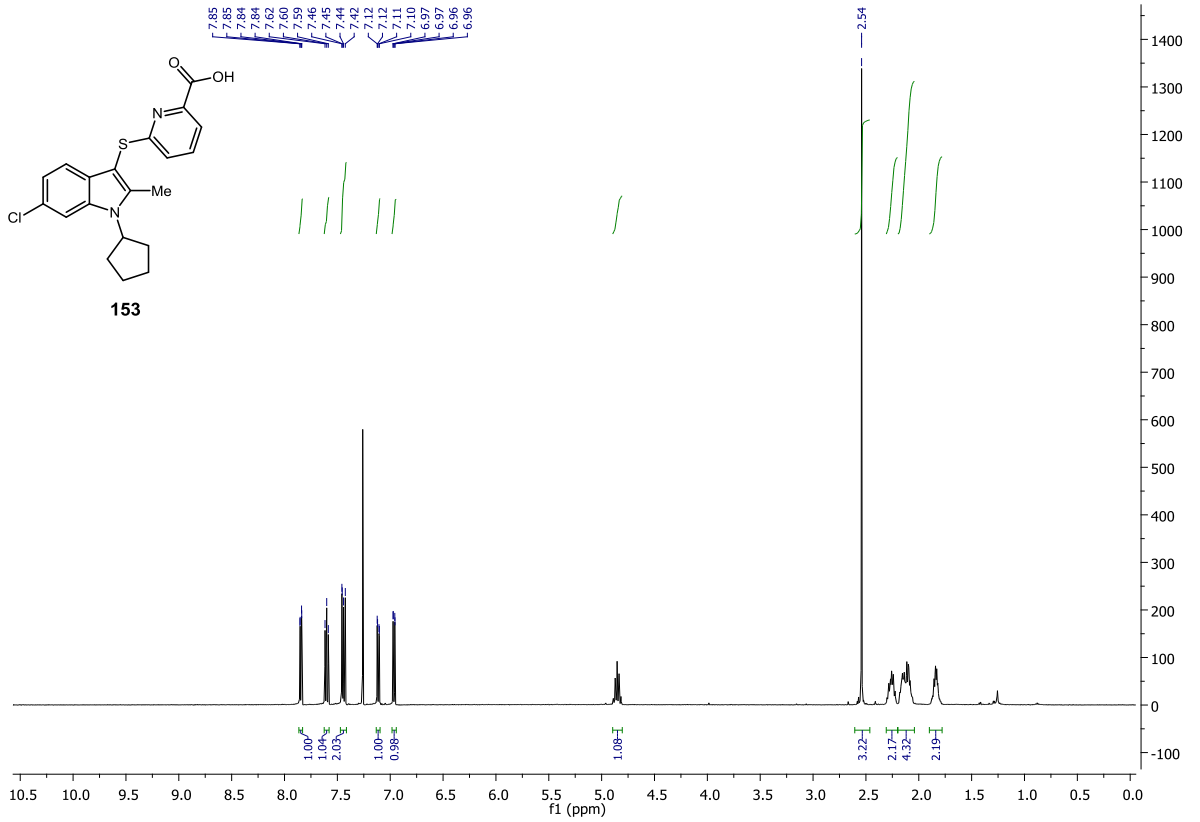


HRMS of 152

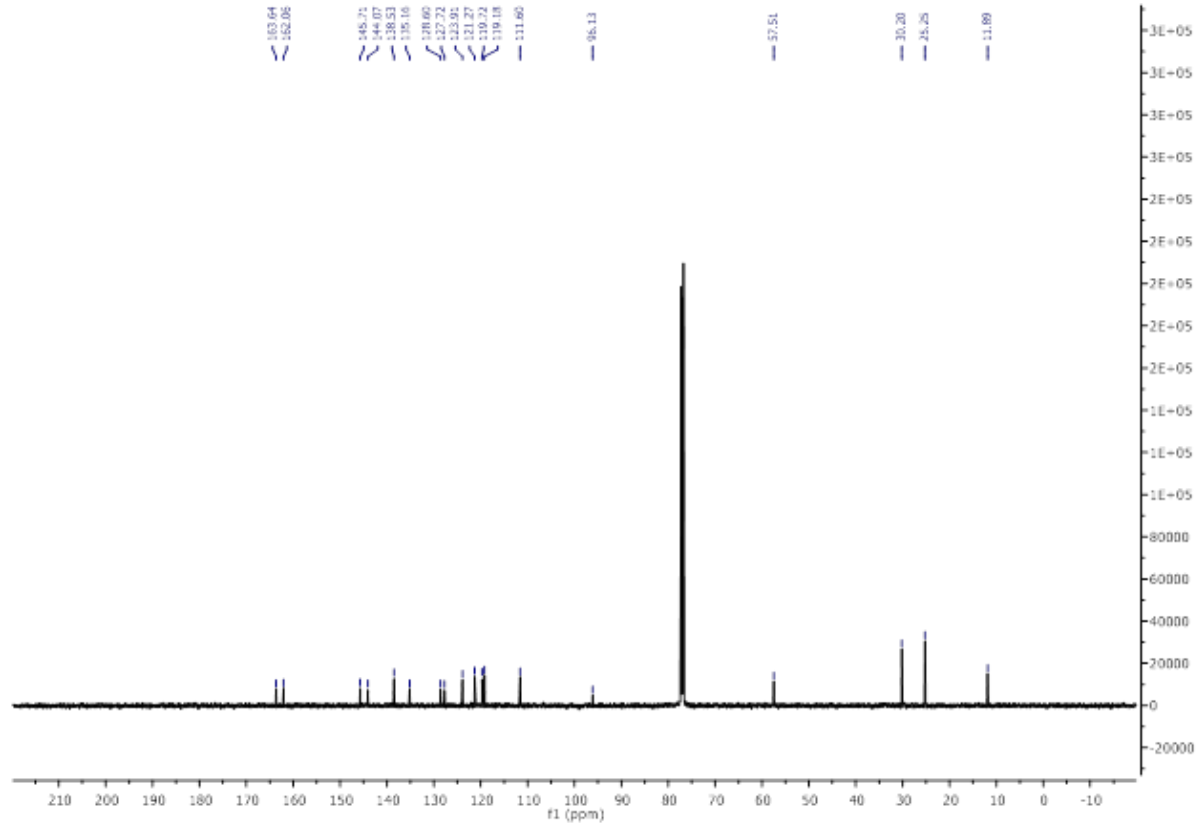


Compound 153

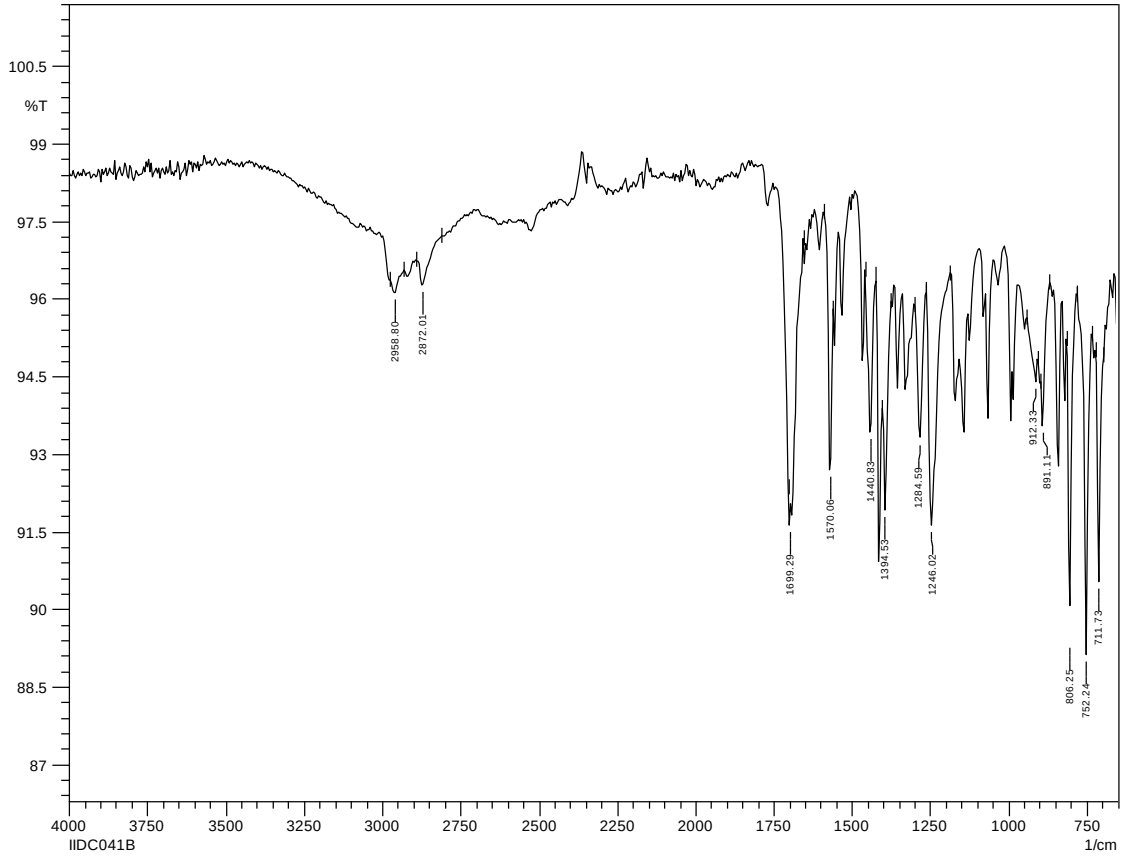
^{1}H NMR



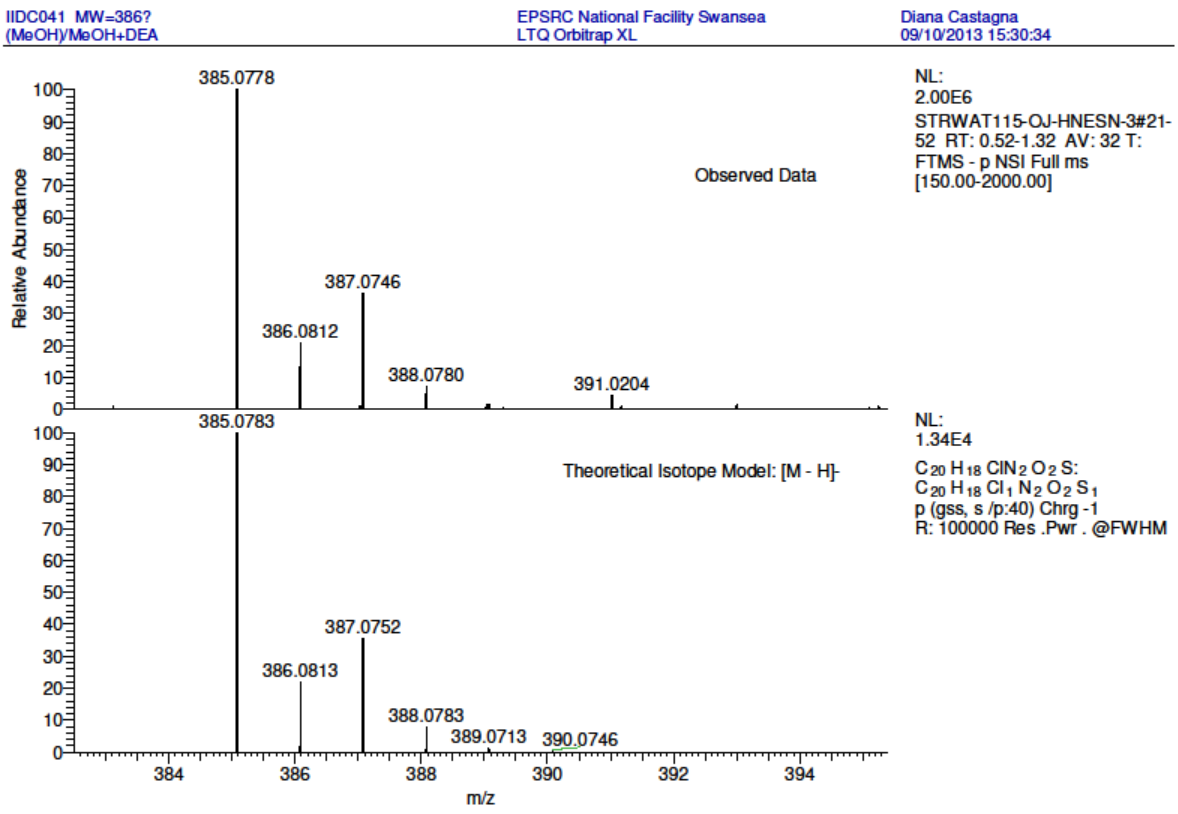
^{13}C NMR of 153



IR of 153

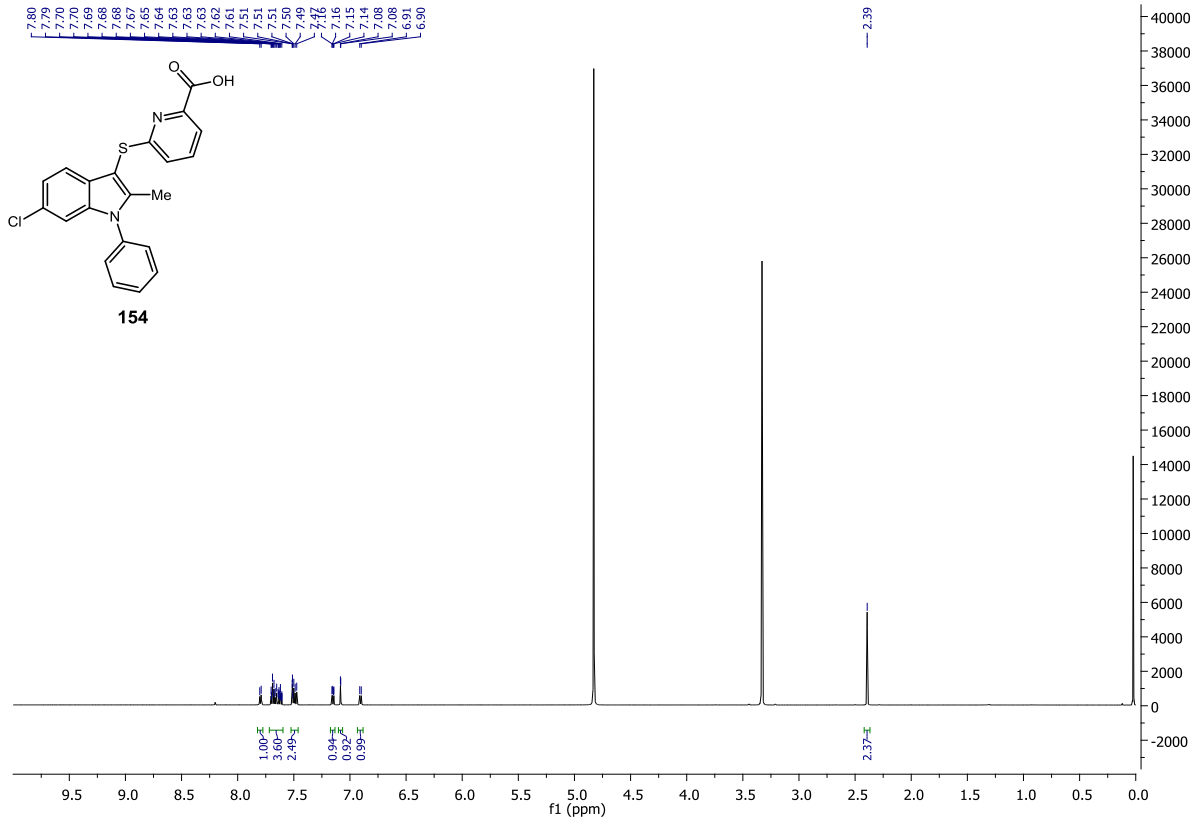


HRMS of 153

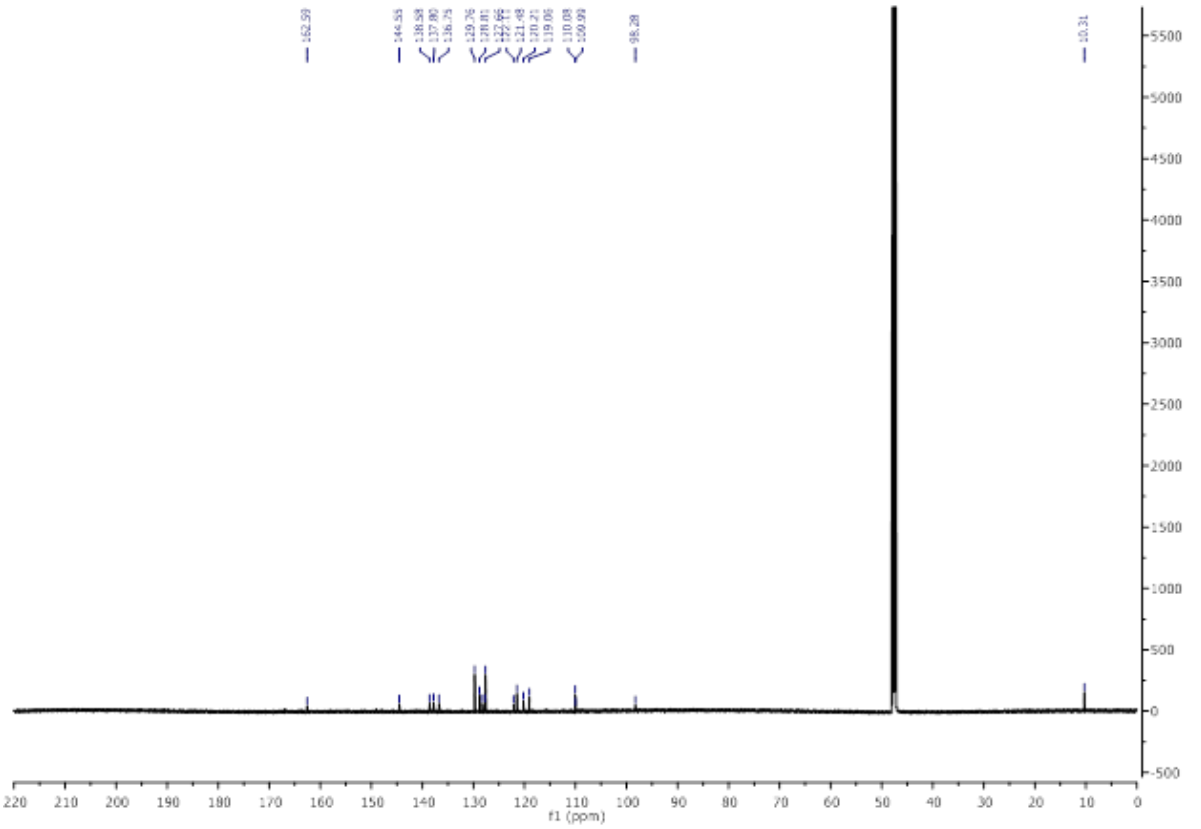


Compound 154

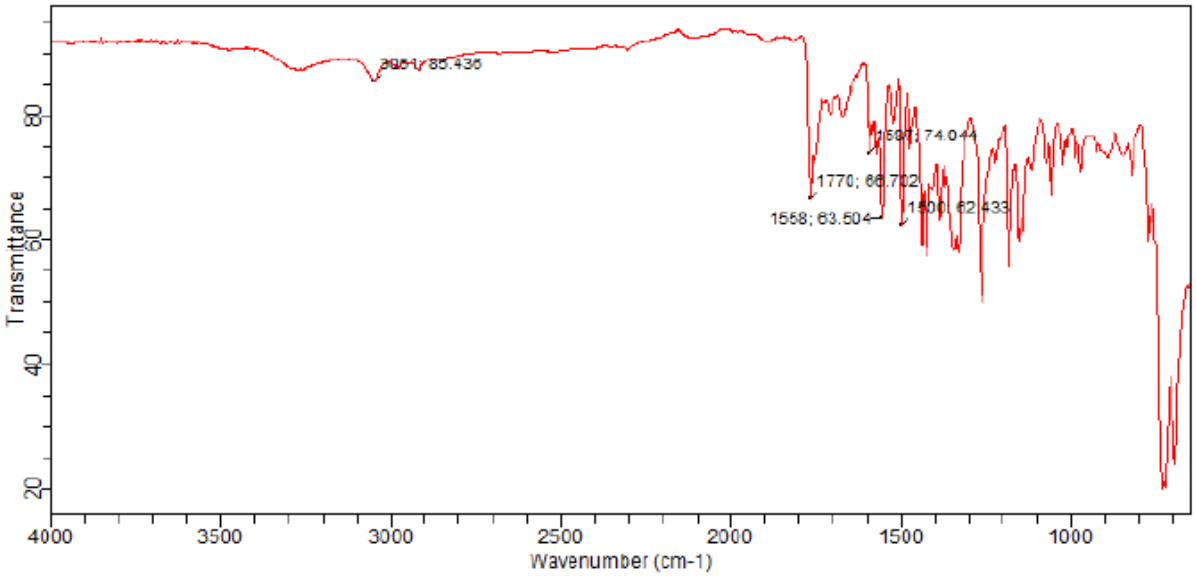
^{1}H NMR



^{13}C NMR of 154

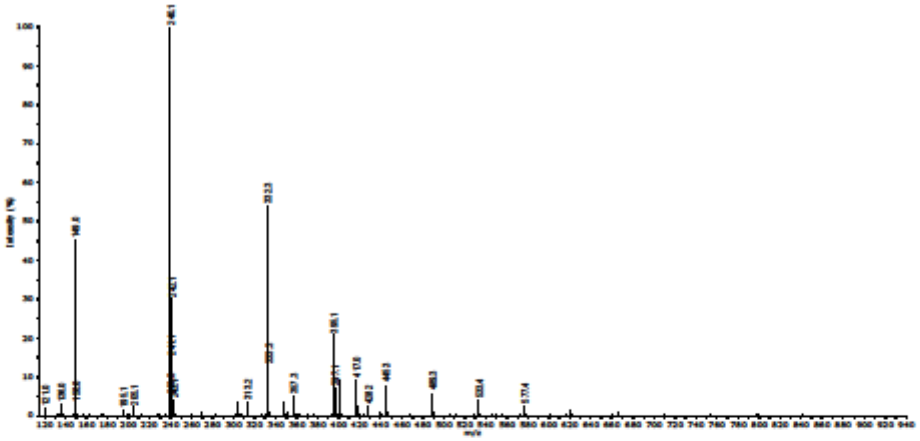


IR of 154

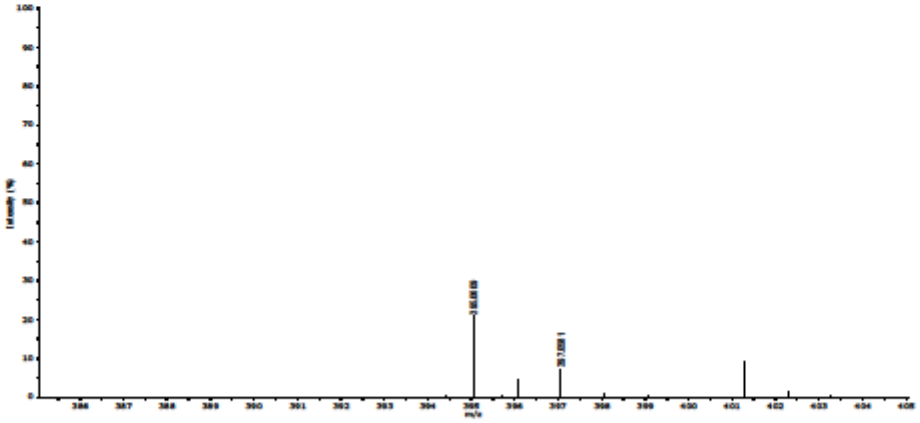

Transmittance
80
60
40
20
4000
3500
3000
2500
2000
1500
1000
Wavenumber (cm-1)
1770; 66.702
1558; 63.504
1500; 62.433

HRMS of 154

Spectrum RT 6.11, Peak [1], Target Mass 395.0616



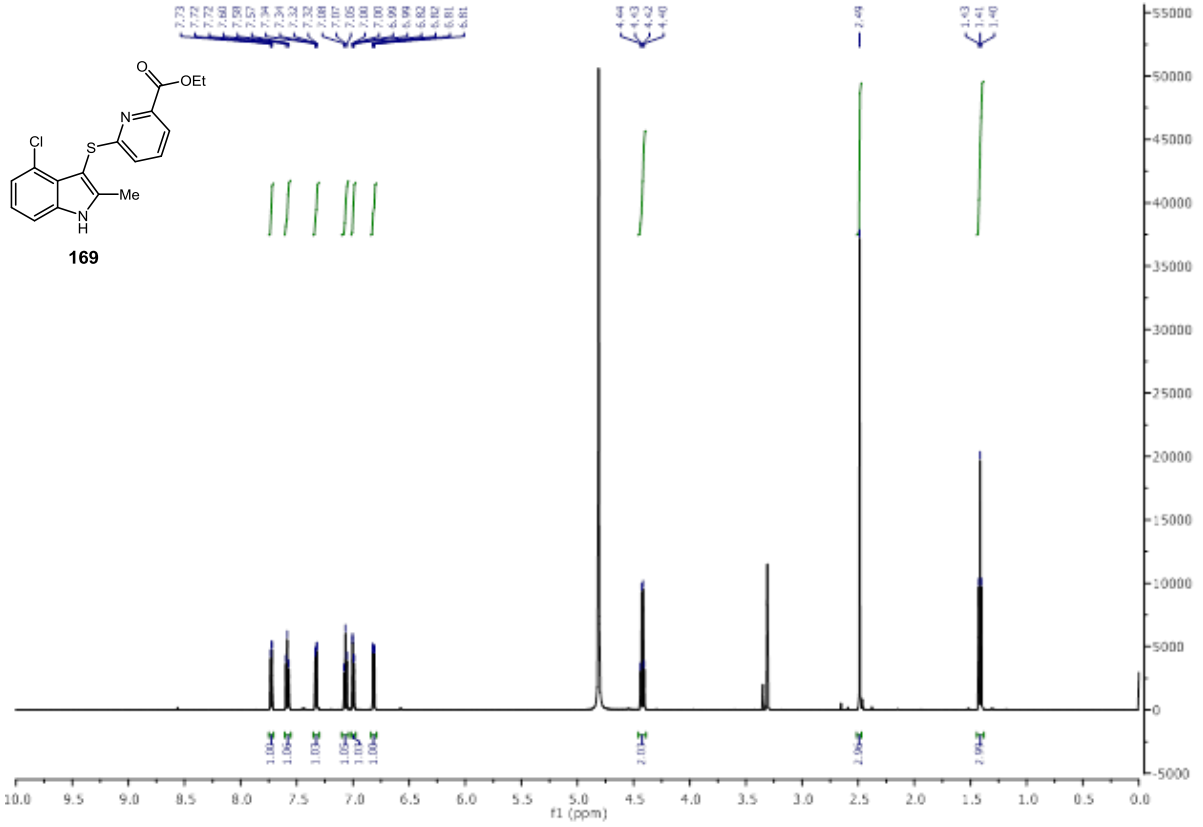
Expanded Spectrum RT 6.11, Peak [1], Target Mass 395.0616



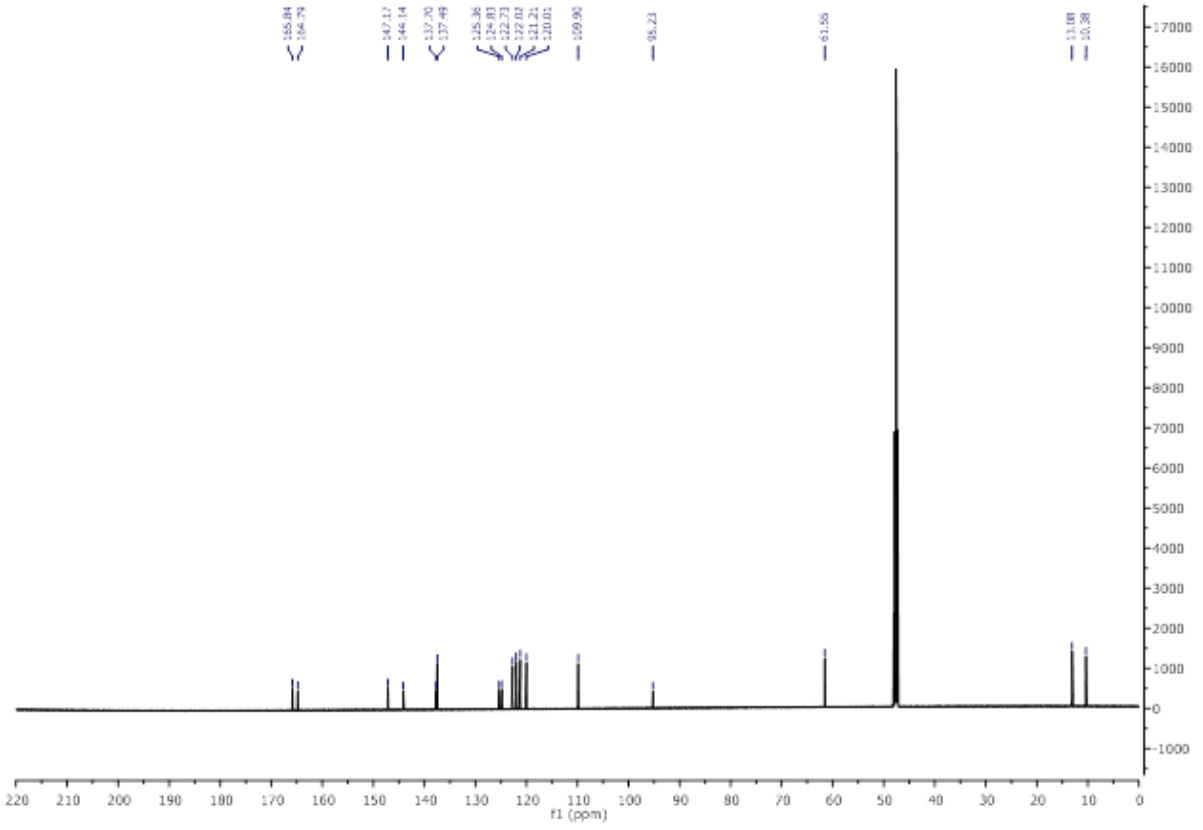
Measured Mass	Calculated Mass	Error (mDa)	Error (ppm)	Formula $[M+H]^+$
395.0617	395.0616	0.1	0.3	$C_{21}H_{16}ClN_2O_2S$

Compound 169

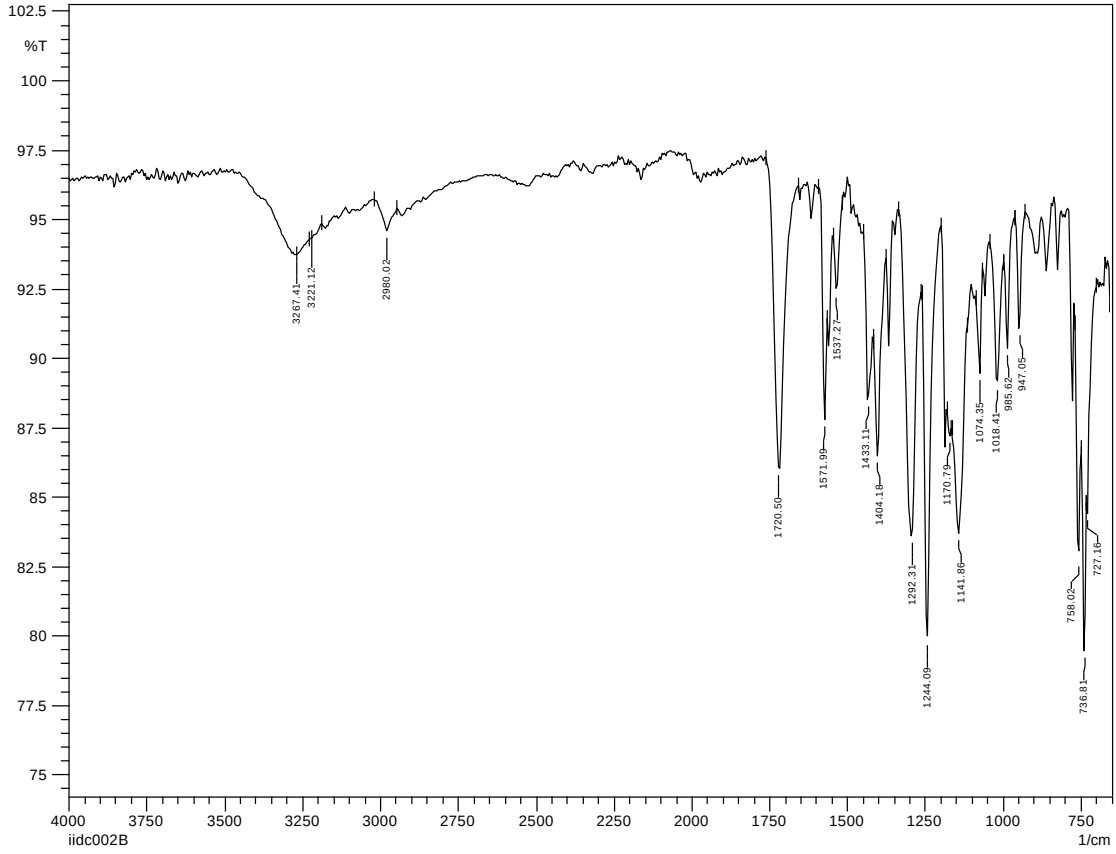
^{1}H NMR



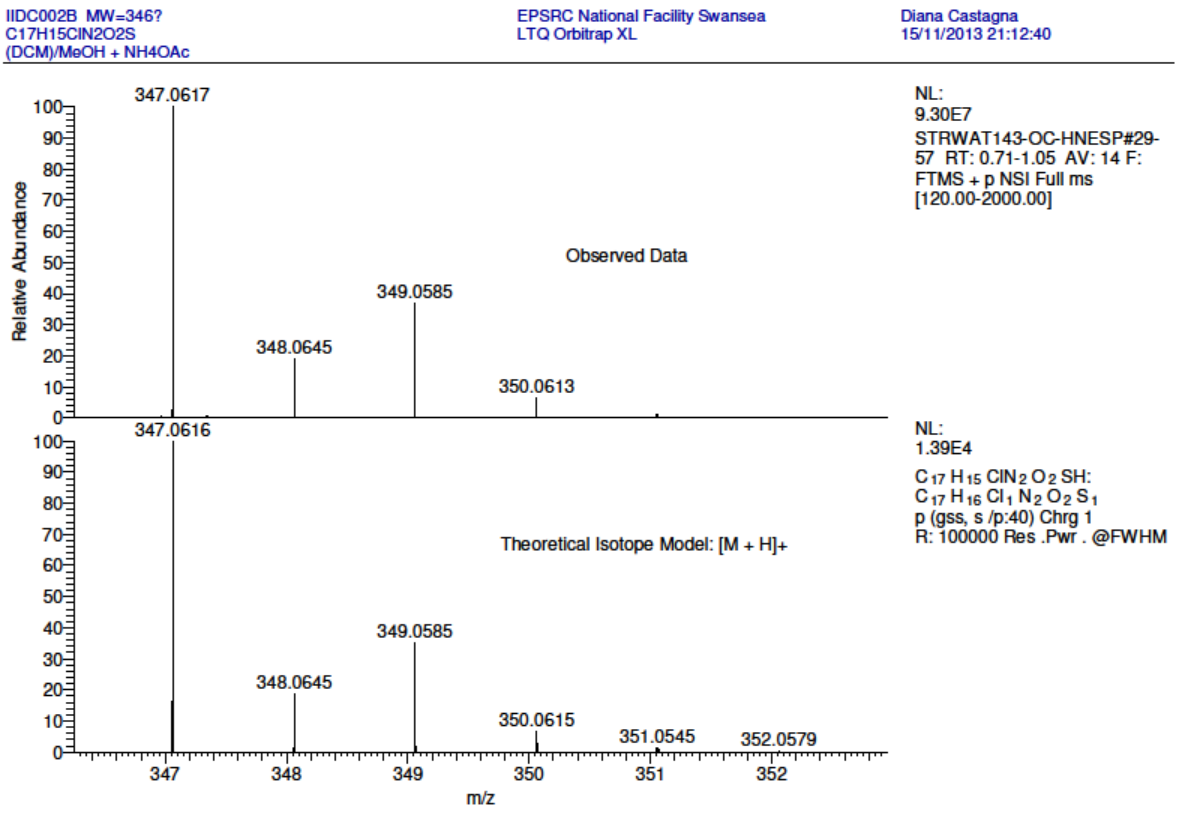
^{13}C NMR of 169



IR of 169

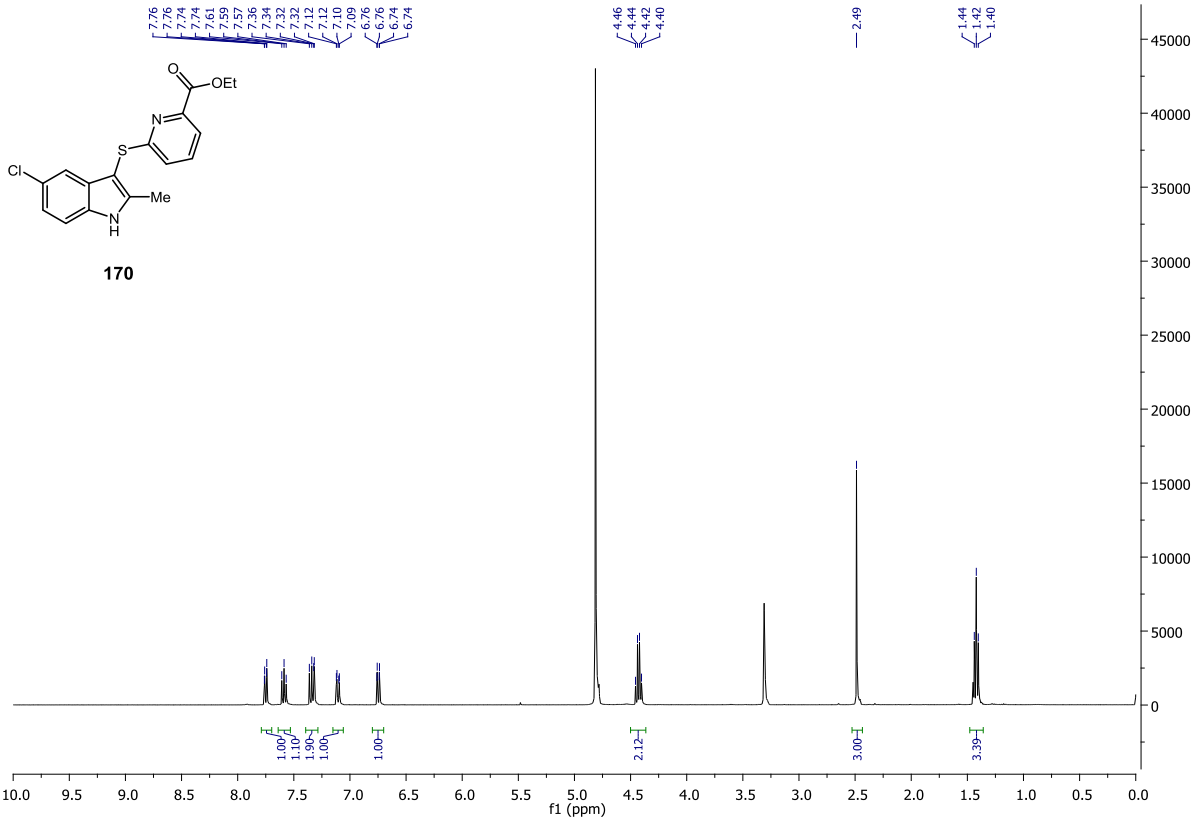


HRMS of 169

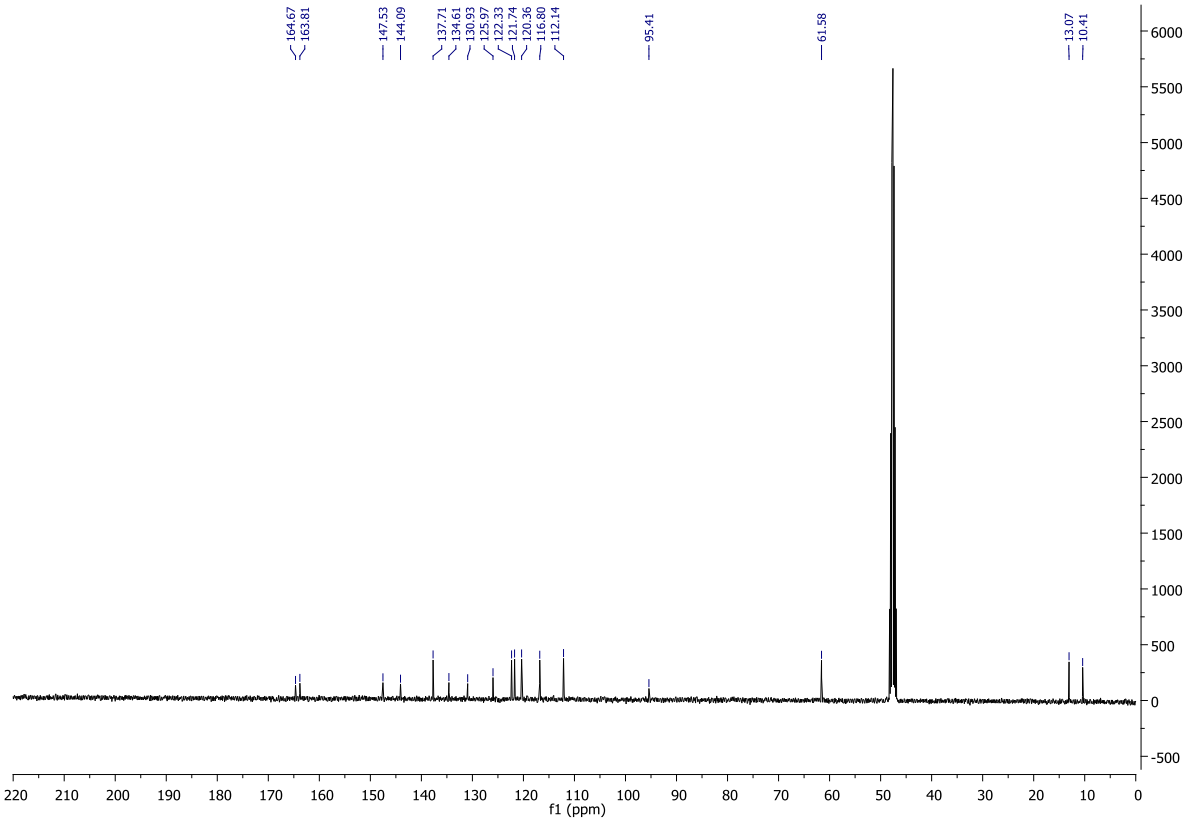


Compound 170

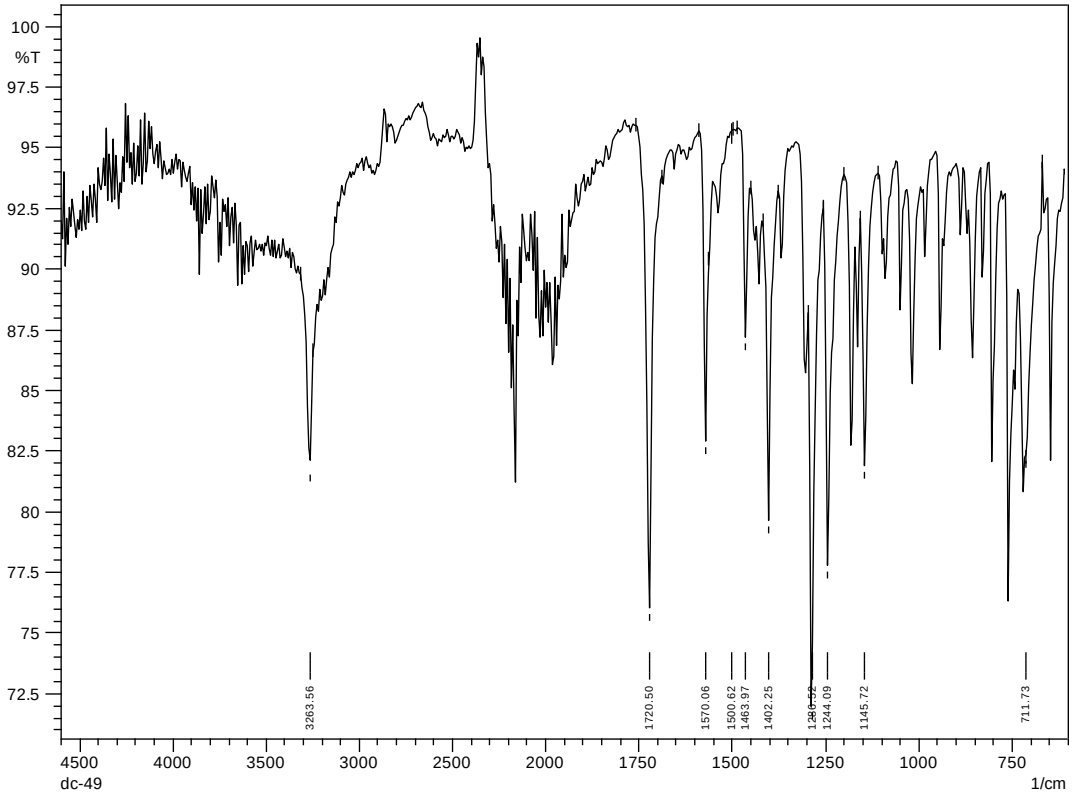
^{1}H NMR



^{13}C NMR of 170



IR of 170


100
%T
97.5
95
92.5
90
87.5
85
82.5
80
77.5
75
72.5
3263.56
1720.50
1570.06
1500.62
1463.97
1402.25
1244.09
1145.72
711.73
4500
4000
3500
3000
2500
2000
1750
1500
1250
1000
750
dc-49
1/cm

HRMS of 170

Bruker maXis Impact: LC-MS SmartFormula Report

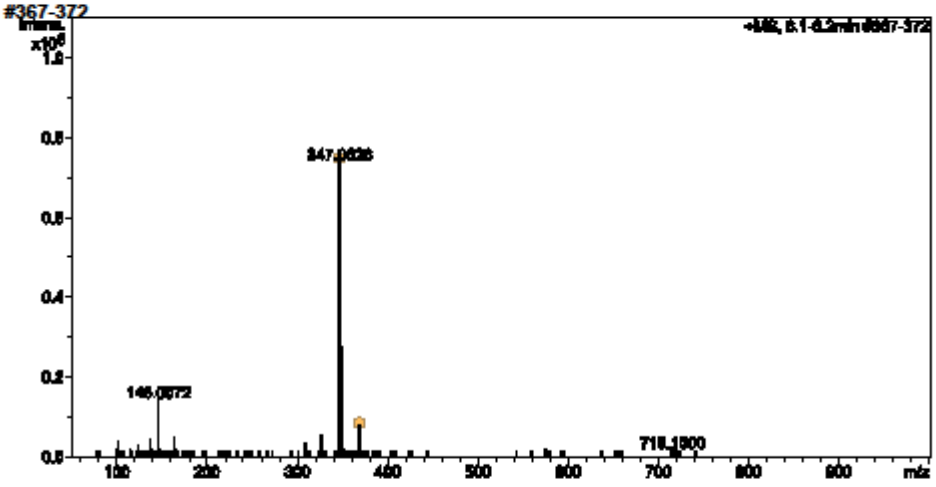
Analysis Info

Analysis Name	C:\Data\Data\N34272-59-5_1-A,8_01_1070.d	Acquisition Date	22/10/2014 09:19:10
Method	lcms pos 50-1000.m	Operator	Spectroscopy
Sample Name	N34272-59-5	Instrument / Ser	maXis impact 282001.0 0101
Comment			

Acquisition Parameter

Source Type	ESI	Scan Begin	50 m/z
Ion Polarity	Positive	Scan End	1000 m/z

+MS, 6.1-6.2min
#367-372

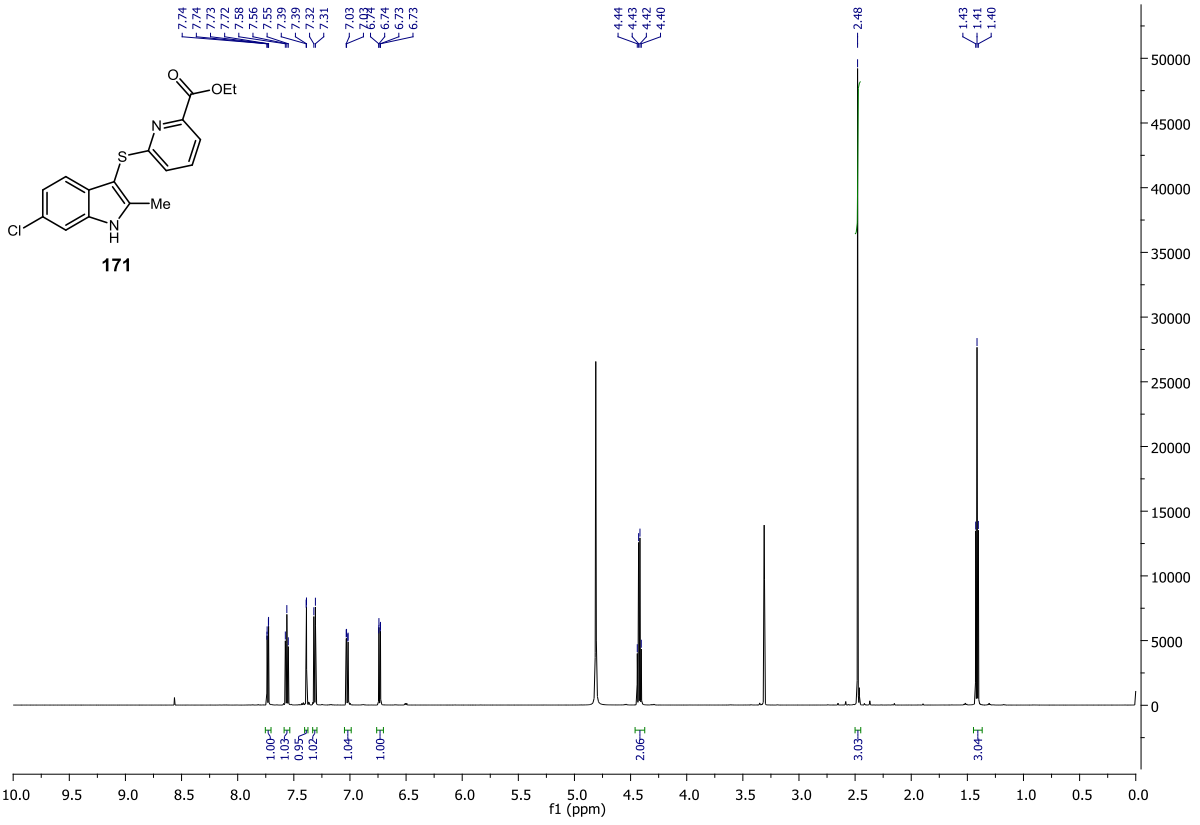


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
347.0626	1	C17H16ClN2O2S	347.0616	2.9	24.9	1	100.00	10.5	even	ok
369.0440	1	C17H15ClN2NaO2S	369.0435	1.5	61.9	1	100.00	10.5	even	ok

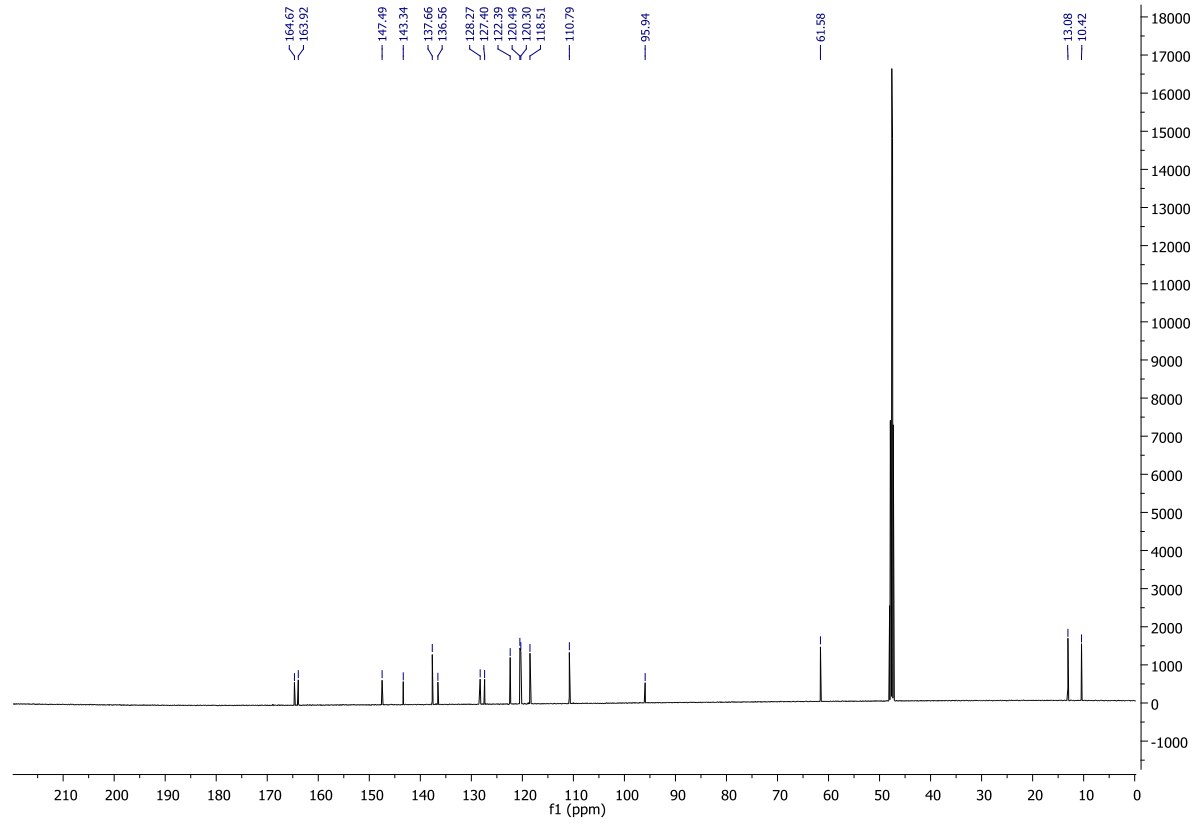
Measured mass should be within ±5 ppm of target mass

Compound 171

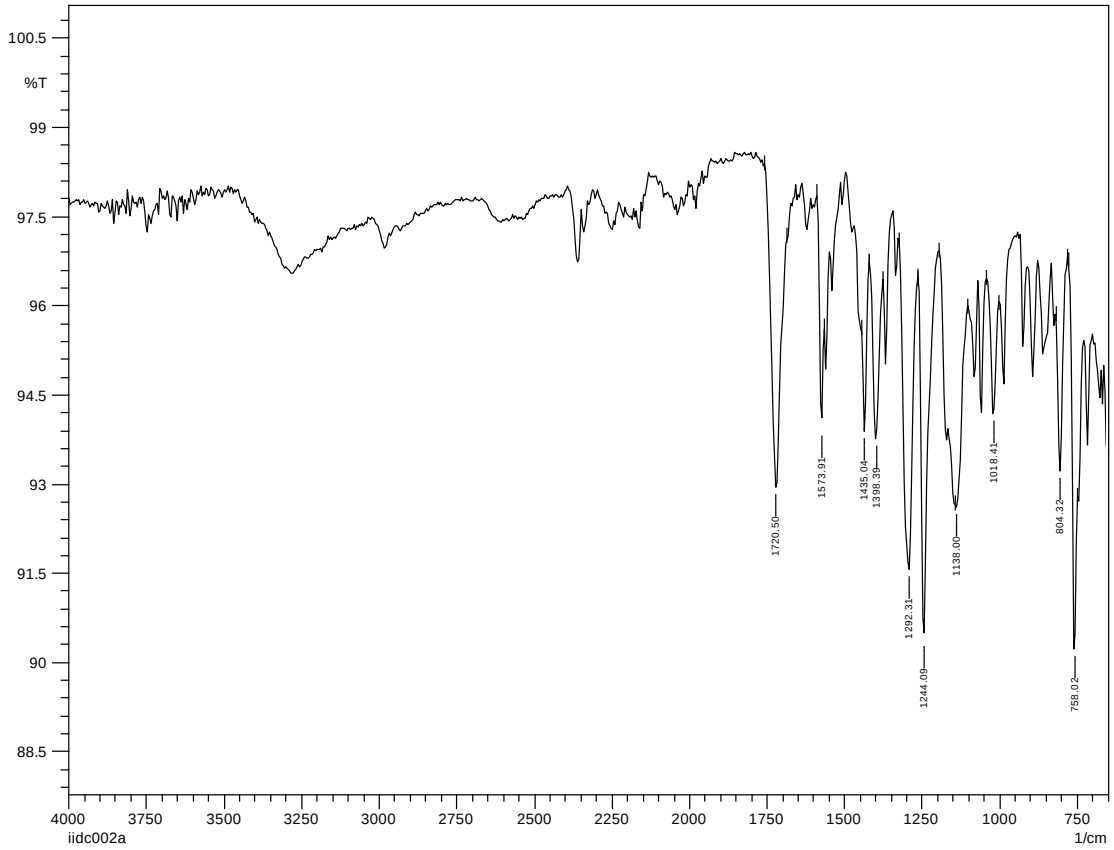
^{1}H NMR



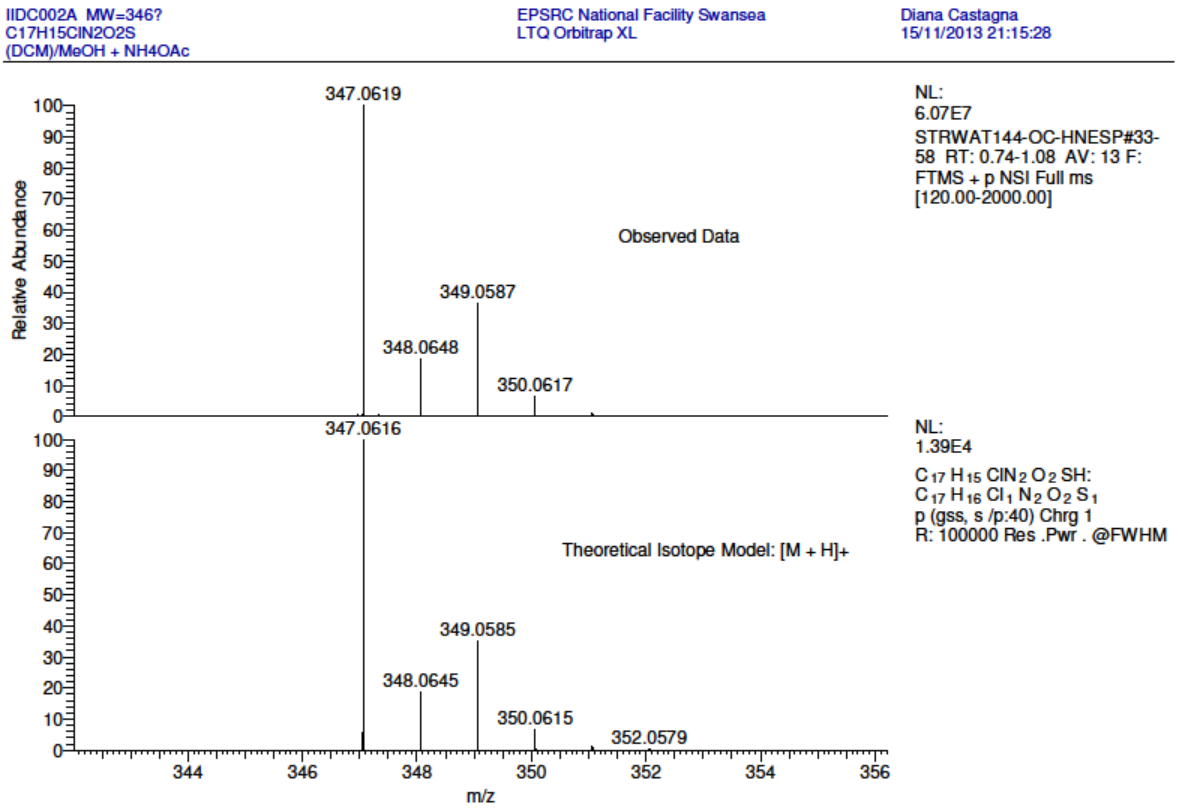
^{13}C NMR of 171



IR of 171

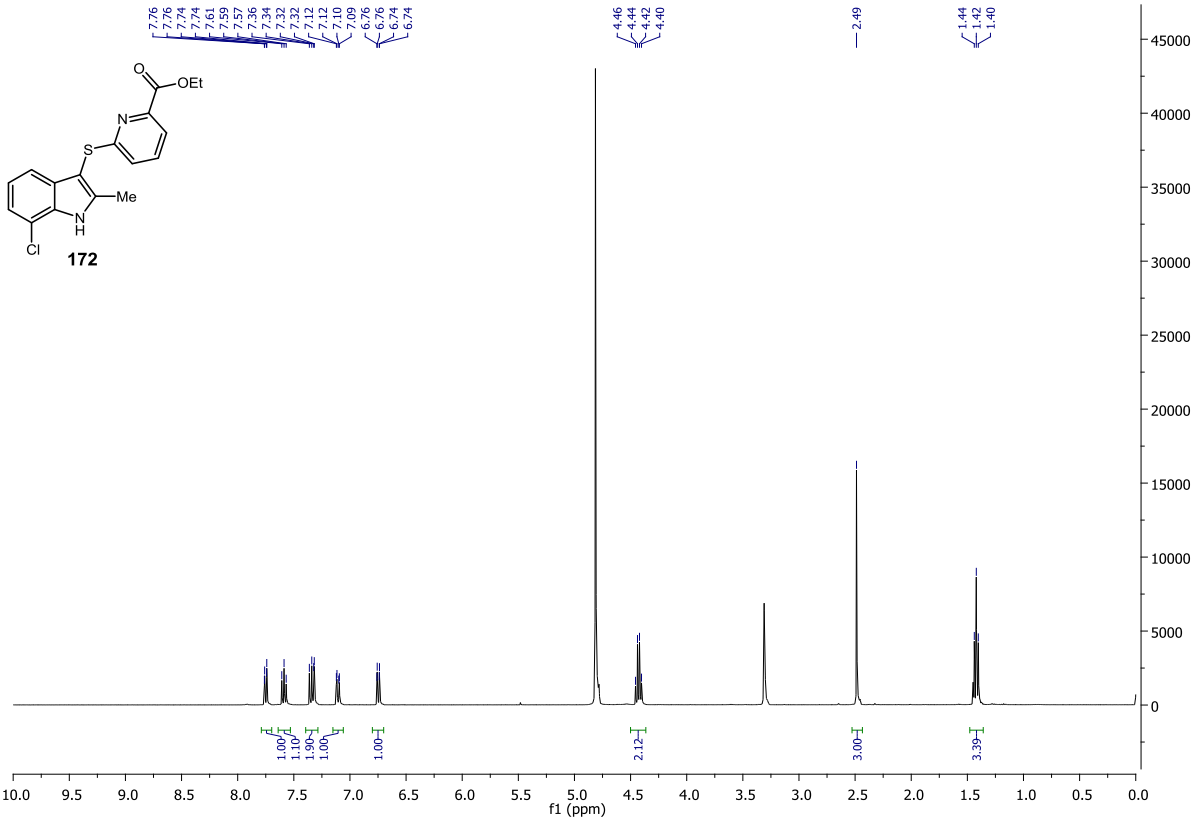


HRMS of 171

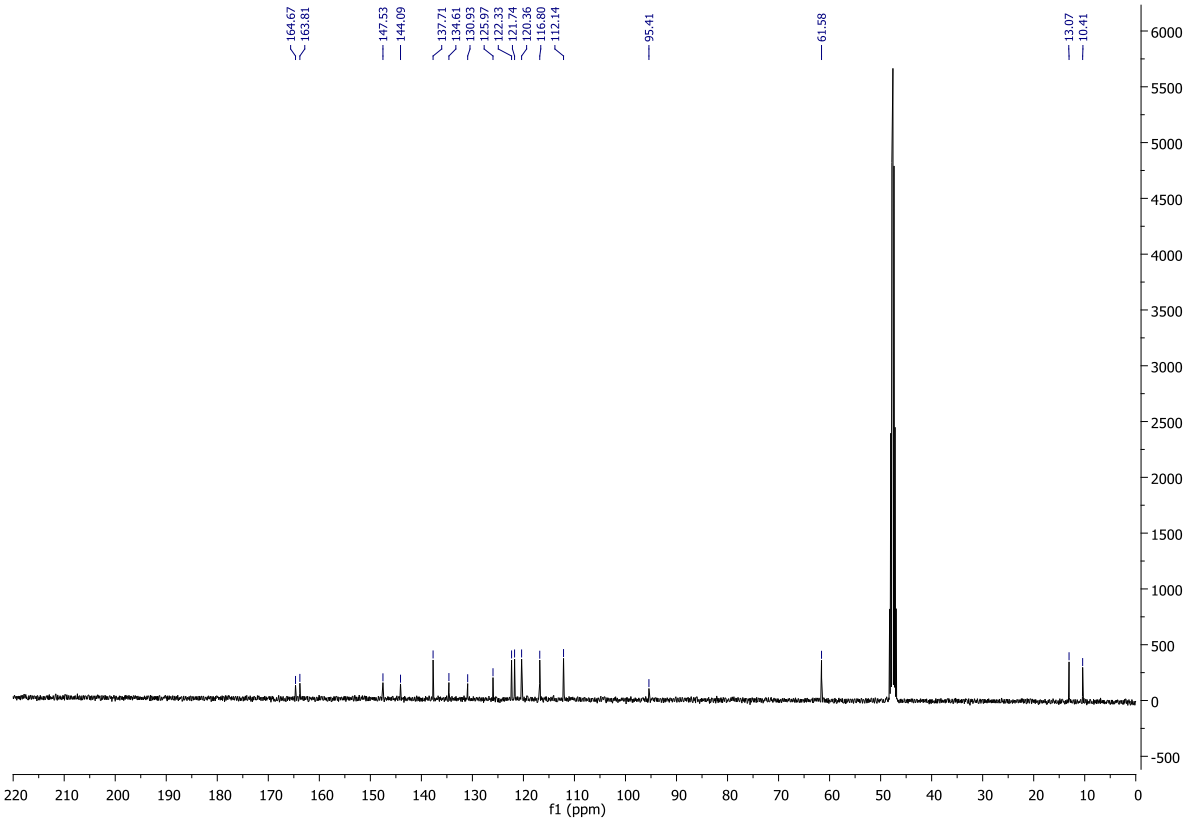


Compound 172

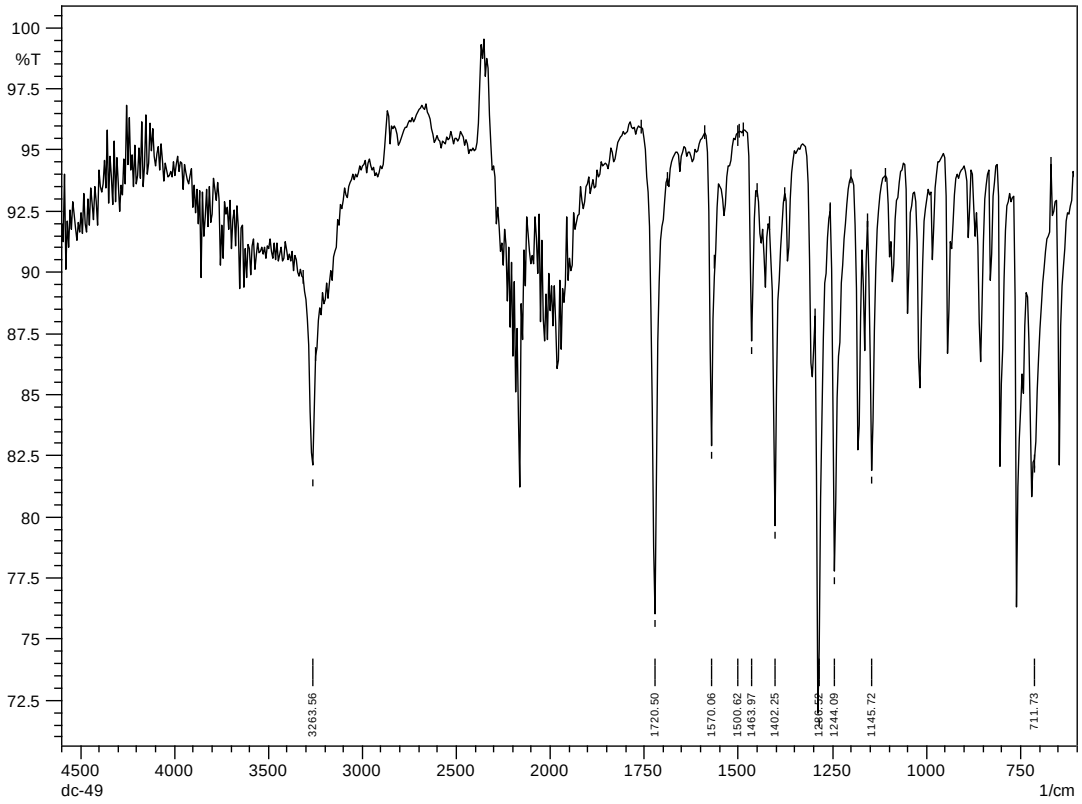
^{1}H NMR



^{13}C NMR of 172



IR of 172


100
%T
97.5
95
92.5
90
87.5
85
82.5
80
77.5
75
72.5
3263.56
1720.50
1570.06
1500.62
1463.97
1402.25
1244.09
1145.72
711.73
4500
4000
3500
3000
2500
2000
1750
1500
1250
1000
750
dc-49
1/cm

HRMS of 172

Bruker maXis Impact: LC-MS SmartFormula Report

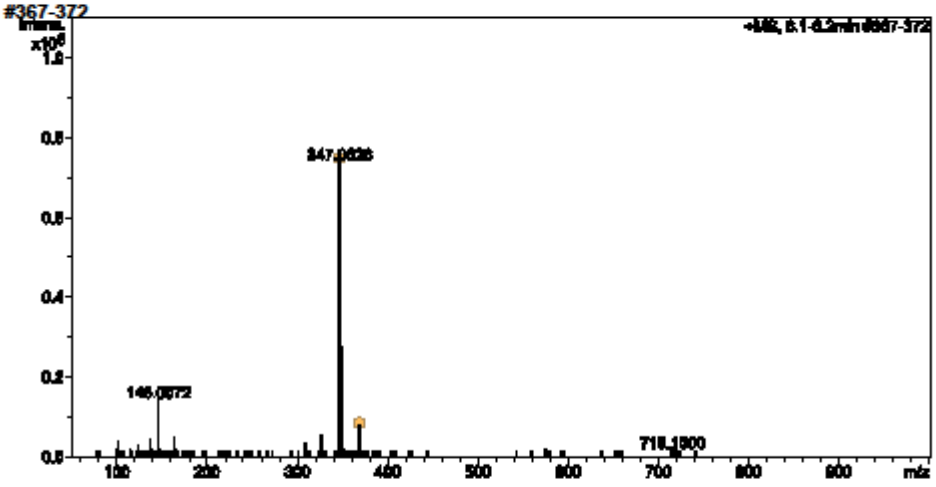
Analysis Info

Analysis Name	C:\Data\Data\N34272-59-5_1-A,8_01_1070.d	Acquisition Date	22/10/2014 09:19:10
Method	lcms pos 50-1000.m	Operator	Spectroscopy
Sample Name	N34272-59-5	Instrument / Ser	maXis impact 282001.0 0101
Comment			

Acquisition Parameter

Source Type	ESI	Scan Begin	50 m/z
Ion Polarity	Positive	Scan End	1000 m/z

+MS, 6.1-6.2min
#367-372

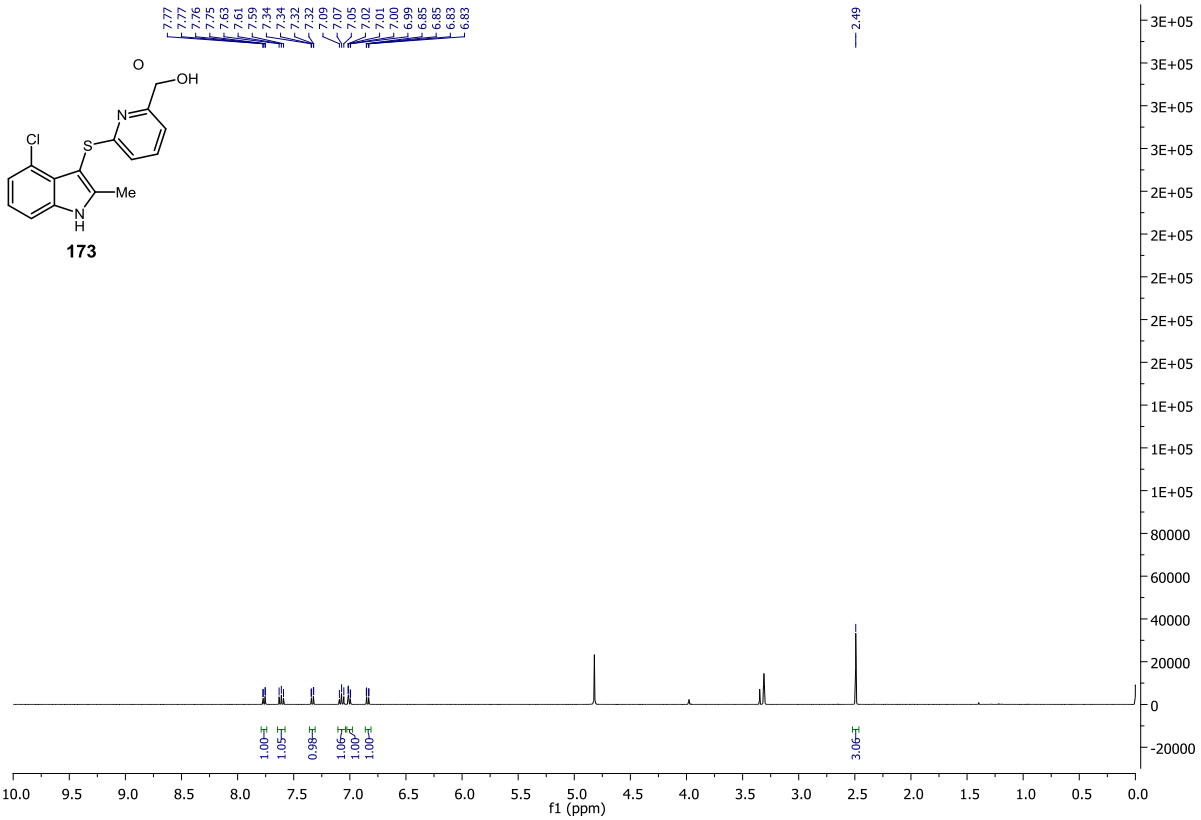


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
347.0626	1	C17H16ClN2O2S	347.0616	2.9	24.9	1	100.00	10.5	even	ok
369.0440	1	C17H15ClN2NaO2S	369.0435	1.5	61.9	1	100.00	10.5	even	ok

Measured mass should be within ±5 ppm of target mass

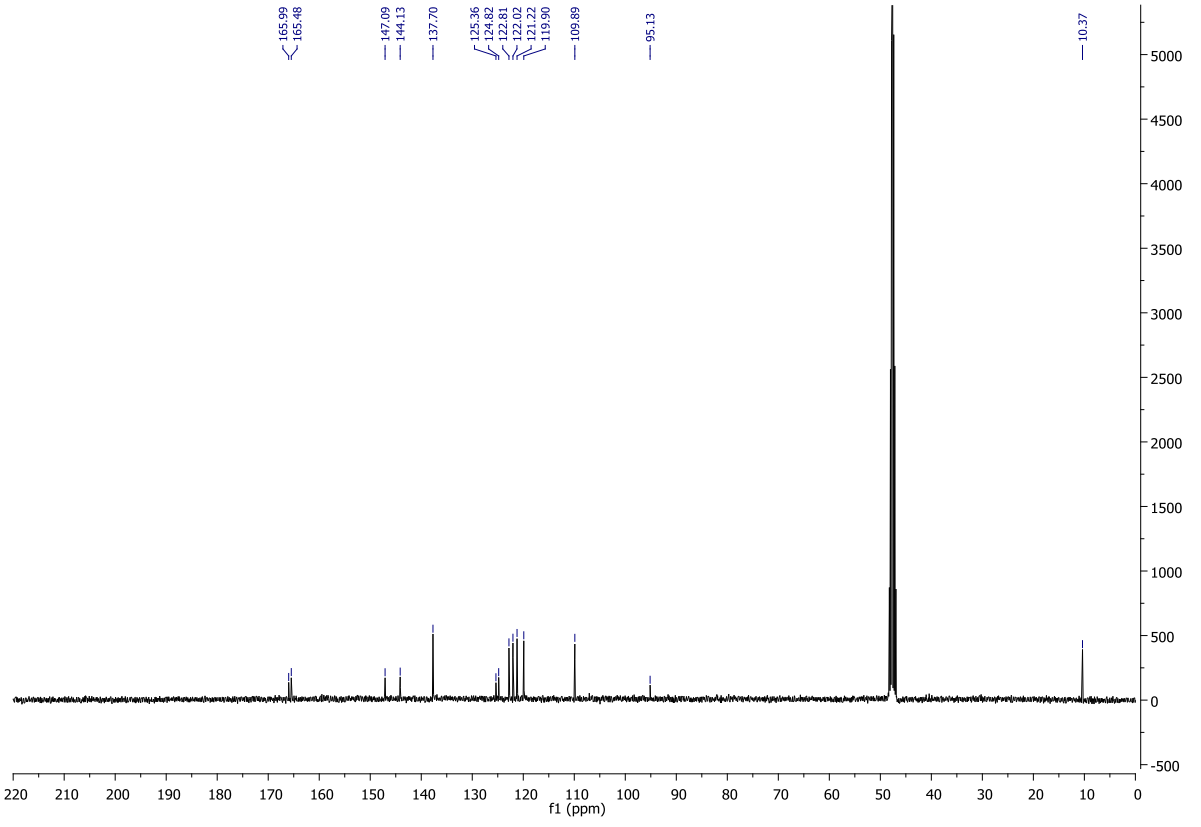
Compound 173

^{1}H NMR

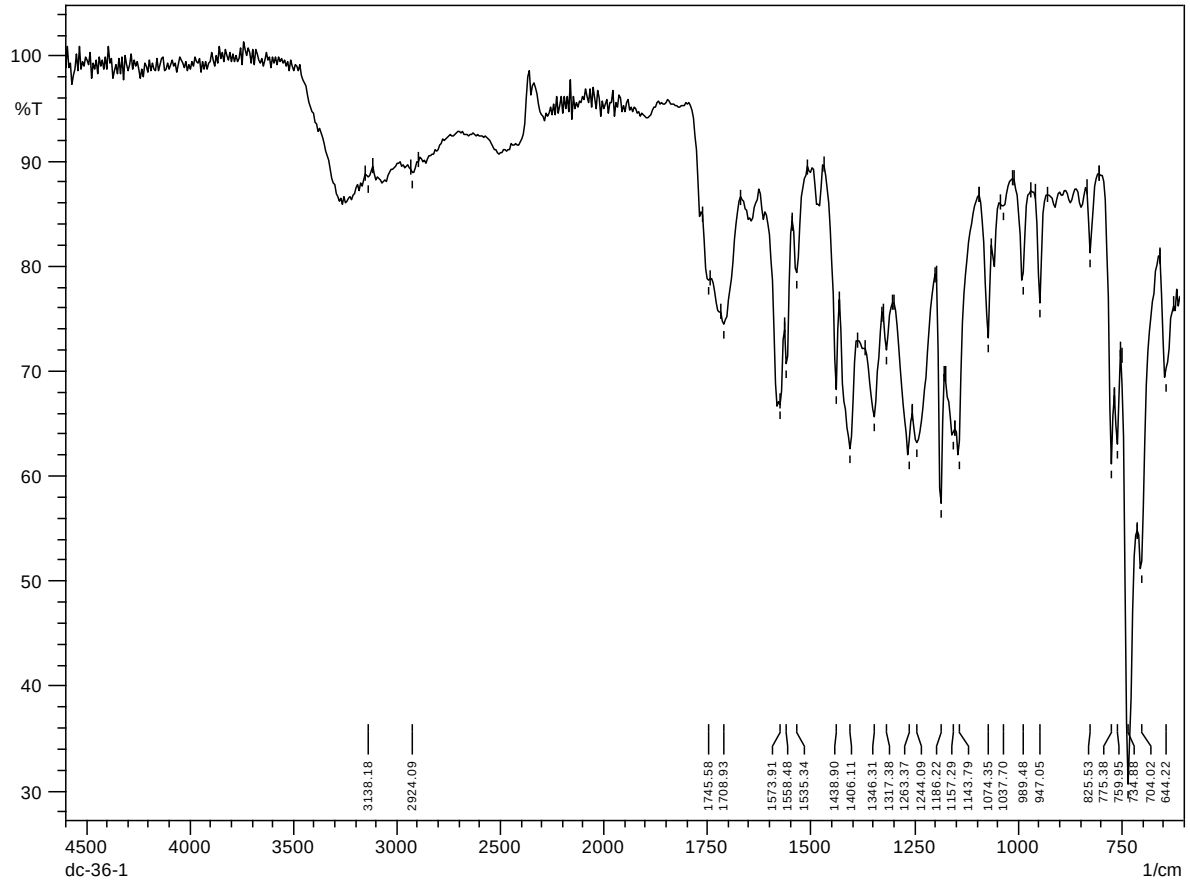


173

^{13}C NMR of 173



IR of 173


100
%T
90
80
70
60
50
40
30
3138.18
2924.09
1745.58
1708.93
1573.91
1558.48
1535.34
1438.90
1406.11
1346.31
1317.38
1263.37
1244.09
1186.22
1157.29
1143.79
1074.35
1037.70
989.48
947.05
825.53
775.38
759.95
734.88
704.02
644.22
4500
4000
3500
3000
2500
2000
1750
1500
1250
1000
750
dc-36-1
1/cm

HRMS of 173

Bruker maXis Impact: LC-MS SmartFormula Report

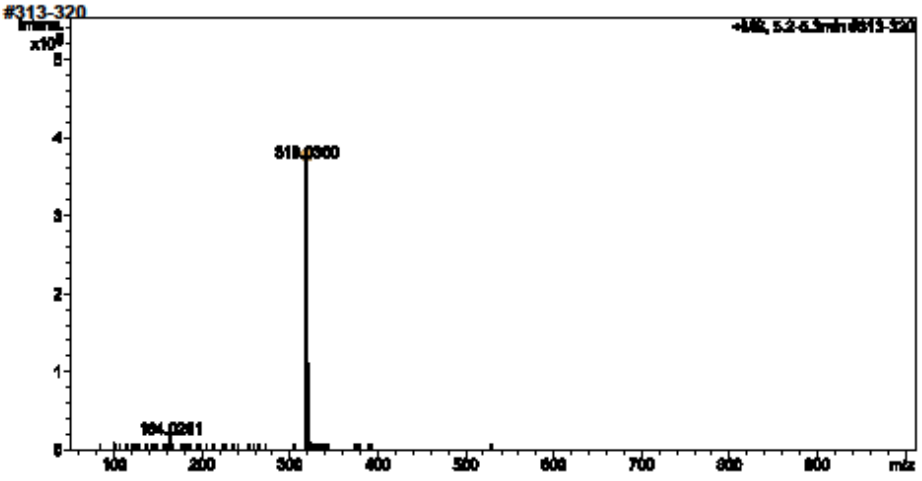
Analysis Info

Analysis Name	C:\Data\Data\N34272-36-1_1-A,4_01_962.d	Acquisition Date	07/10/2014 06:35:20
Method	lcms pos 50-1000.m	Operator	Spectroscopy
Sample Name	N34272-36-1	Instrument / Ser	maXis impact 282001.0 0101
Comment			

Acquisition Parameter

Source Type	ESI	Scan Begin	50 m/z
Ion Polarity	Positive	Scan End	1000 m/z

+MS, 5.2-5.3min
#313-320

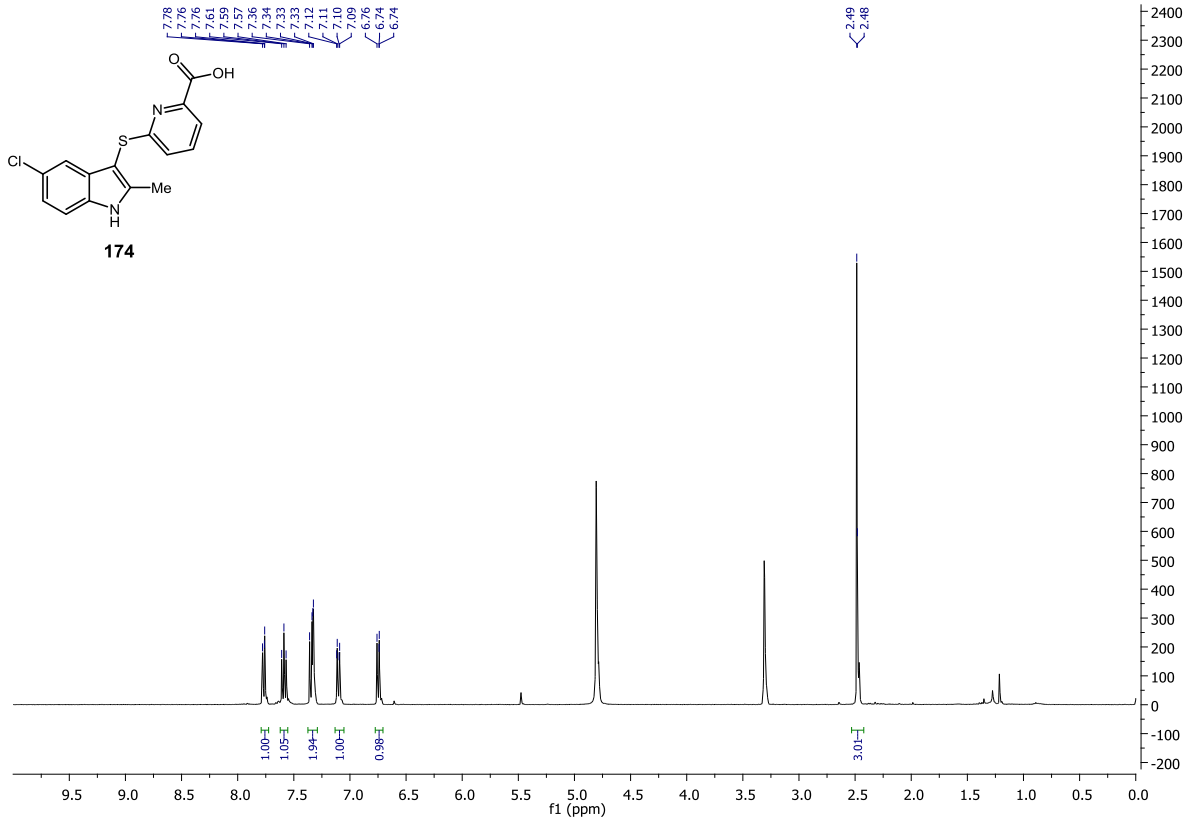


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
319.0300	1	C15H12ClN2O2S	319.0303	-0.7	53.6	1	100.00	10.5	even	ok

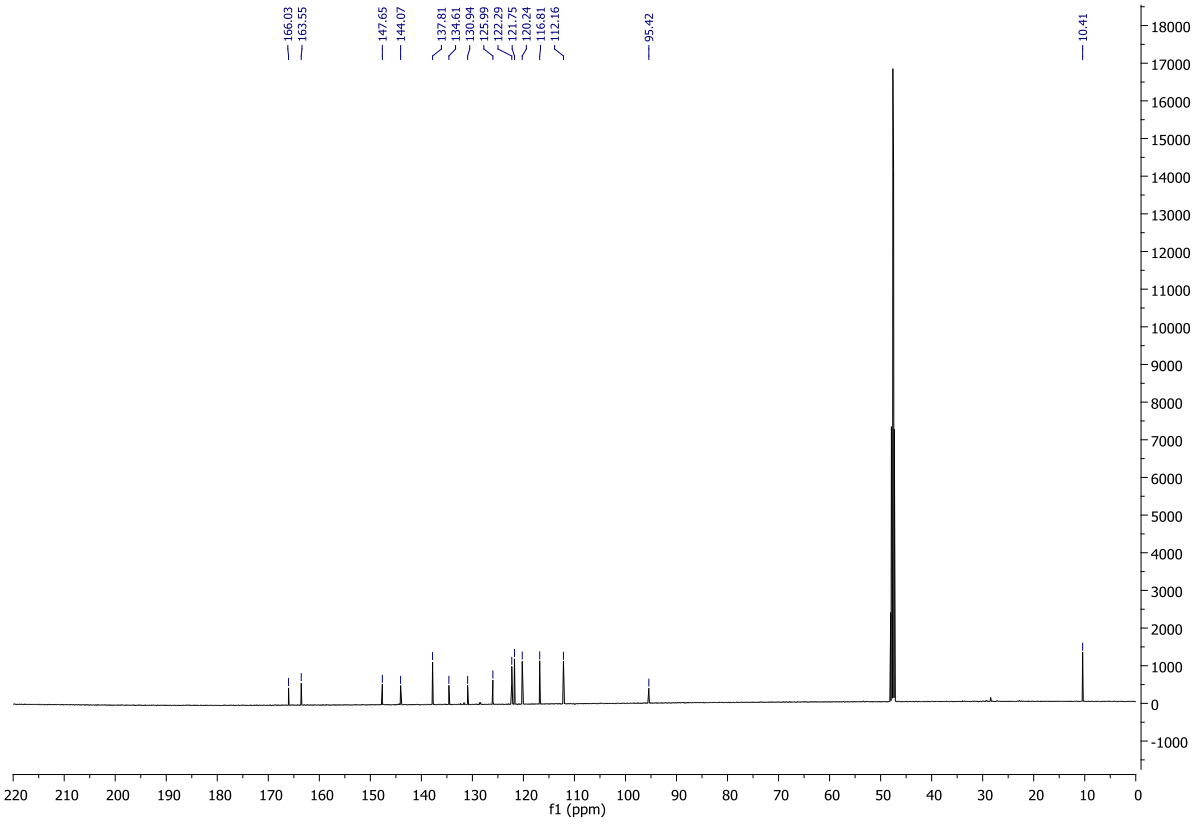
Measured mass should be within ±5 ppm of target mass

Compound 174

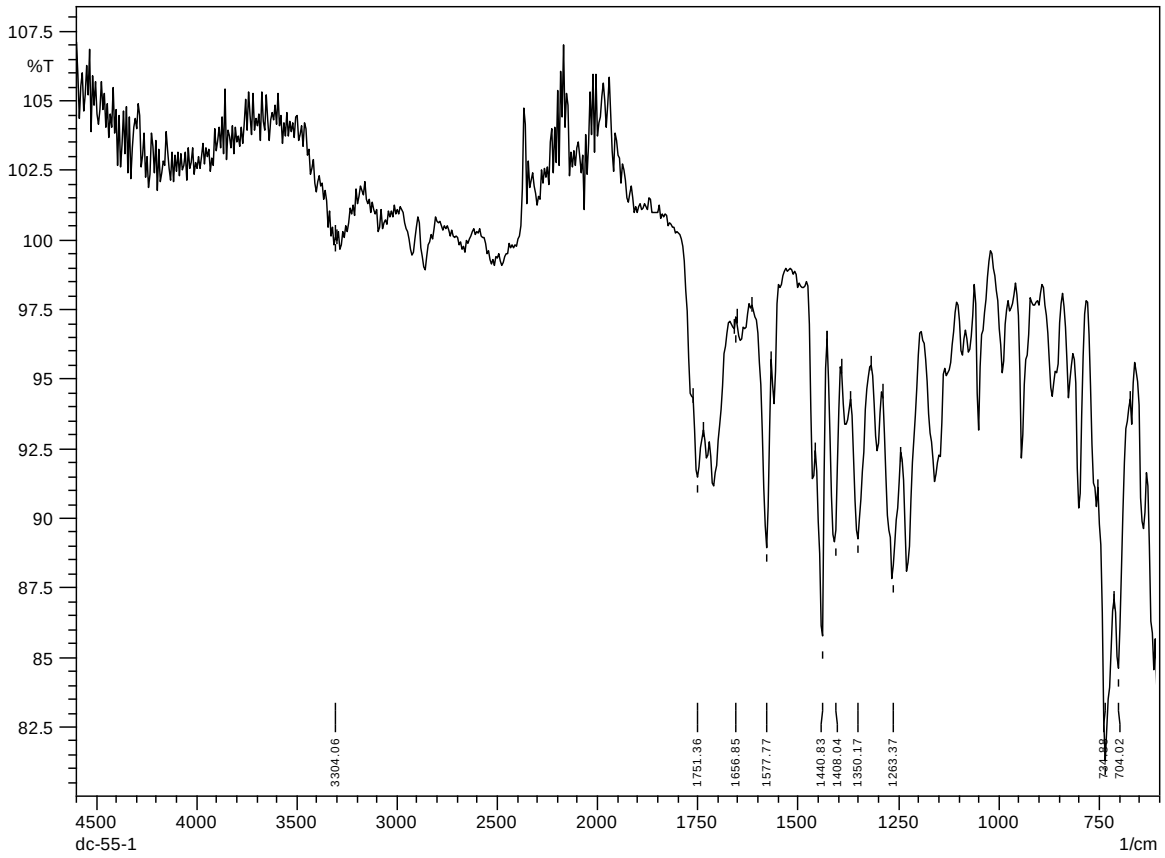
^{1}H NMR



^{13}C NMR of 174



IR of 174


107.5
%T
105
102.5
100
97.5
95
92.5
90
87.5
85
82.5
3304.06
1751.36
1656.85
1577.77
1440.83
1408.04
1350.17
1263.37
704.02
4500
4000
3500
3000
2500
2000
1750
1500
1250
1000
750
dc-55-1
1/cm

HRMS of 174

Bruker maXis Impact: LC-MS SmartFormula Report

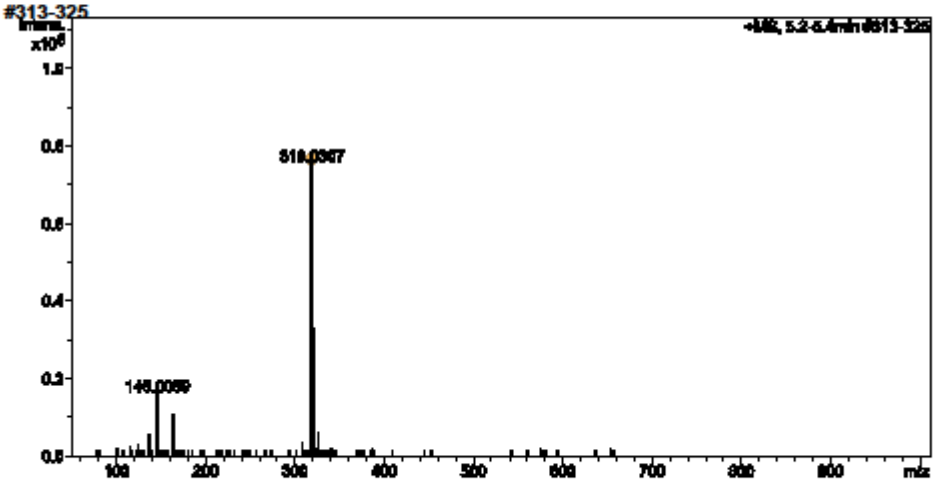
Analysis Info

Analysis Name	C:\Data\Data\N34272-64-7_1-A,8_01_1122.d	Acquisition Date	24/10/2014 15:50:43
Method	lcms pos 50-1000.m	Operator	Spectroscopy
Sample Name	N34272-64-7	Instrument / Ser	maXis impact 282001.0 0101
Comment			

Acquisition Parameter

Source Type	ESI	Scan Begin	50 m/z
Ion Polarity	Positive	Scan End	1000 m/z

+MS, 5.2-5.4min
#313-325

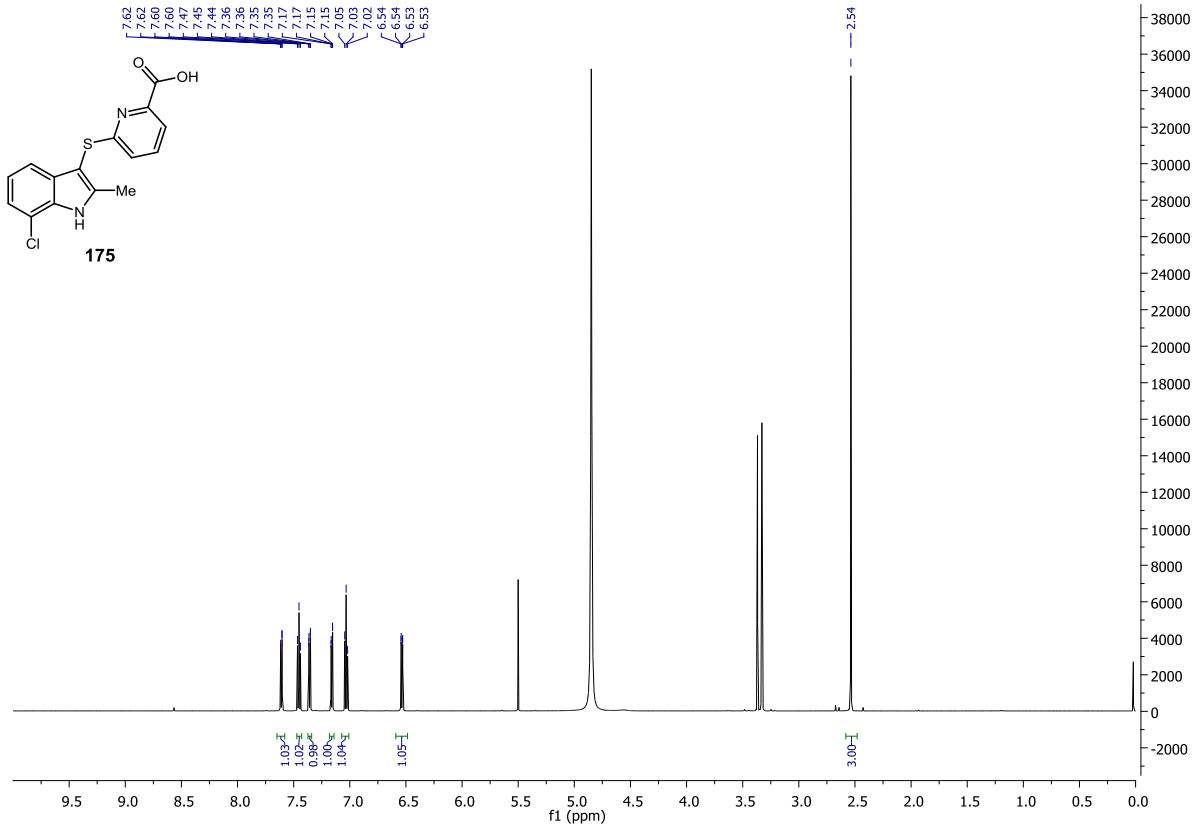


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
319.0307	1	C15H12ClN2O2S	319.0303	1.5	24.3	1	100.00	10.5	even	ok

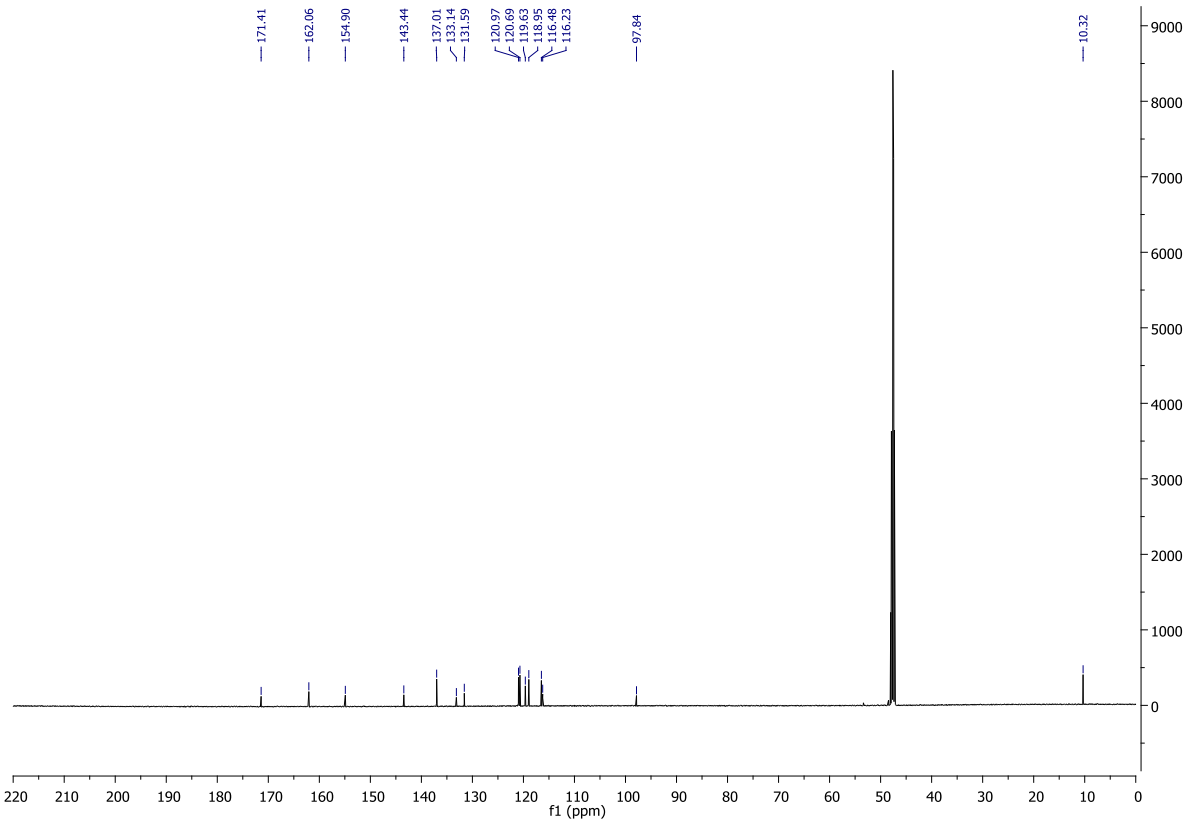
Measured mass should be within ±5 ppm of target mass

Compound 175

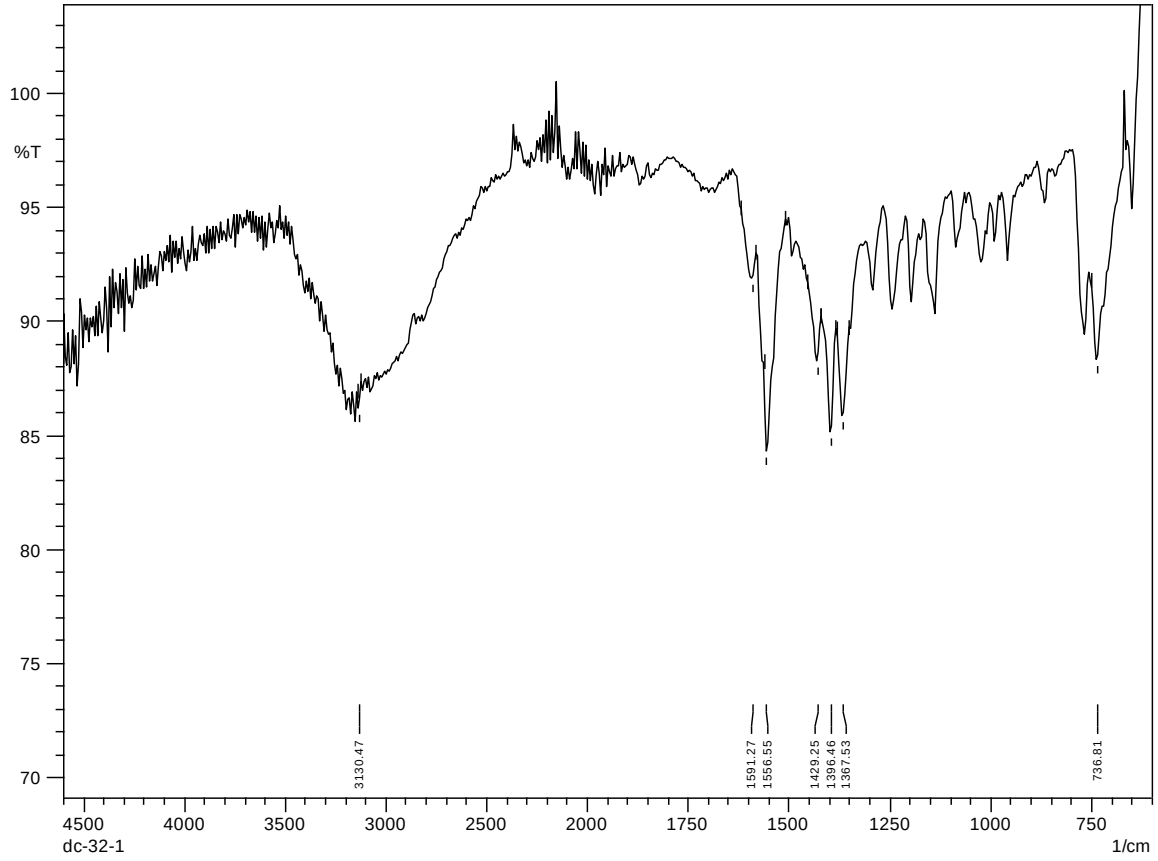
^{1}H NMR



^{13}C NMR of 175



IR of 175


100
%T
95
90
85
80
75
70
3130.47
1591.27
1556.55
1429.25
1396.46
1367.53
736.81
4500
4000
3500
3000
2500
2000
1750
1500
1250
1000
750
dc-32-1
1/cm

HRMS of 175

Bruker maXis Impact: LC-MS SmartFormula Report

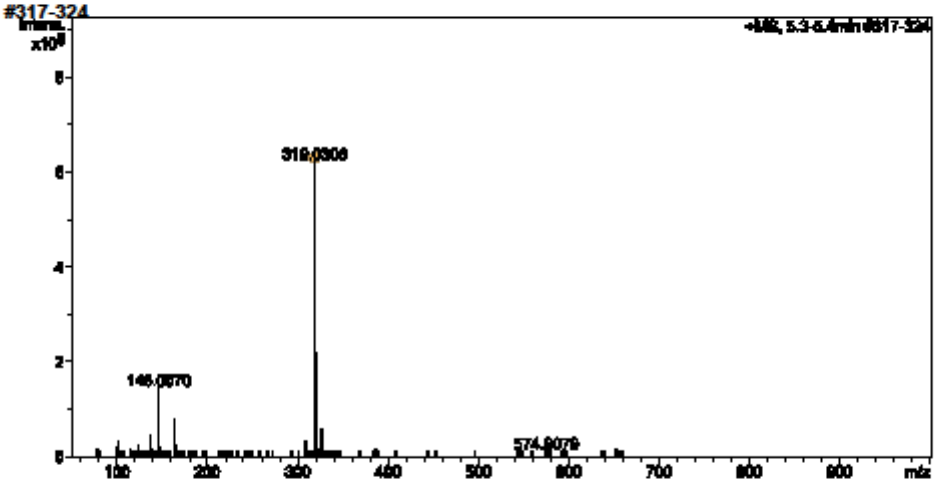
Analysis Info

Analysis Name	C:\Data\Data\N34272-59-3_1-A,6_01_1068.d	Acquisition Date	22/10/2014 08:57:38
Method	lcms pos 50-1000.m	Operator	Spectroscopy
Sample Name	N34272-59-3	Instrument / Ser	maXis impact 282001.0 0101
Comment			

Acquisition Parameter

Source Type	ESI	Scan Begin	50 m/z
Ion Polarity	Positive	Scan End	1000 m/z

+MS, 5.3-5.4min
#317-324

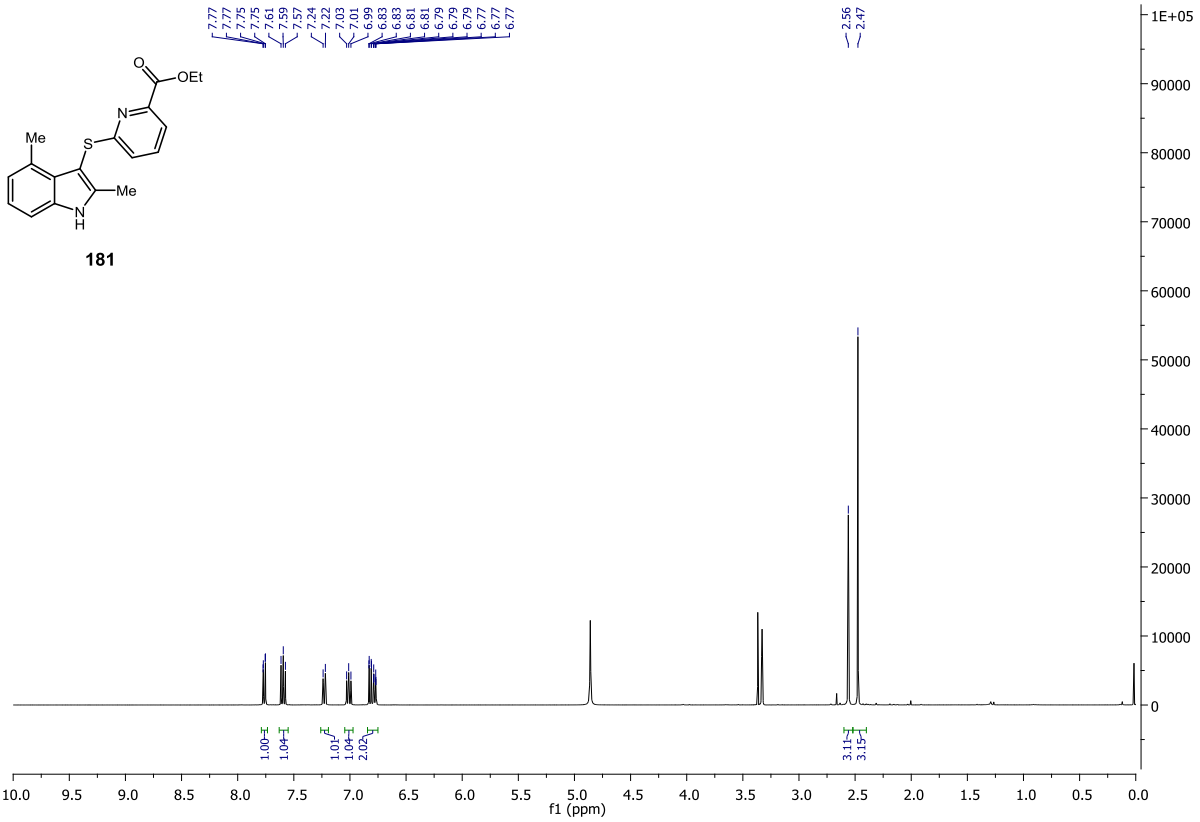


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
319.0306	1	C15H12ClN2O2S	319.0303	1.1	36.4	1	100.00	10.5	even	ok

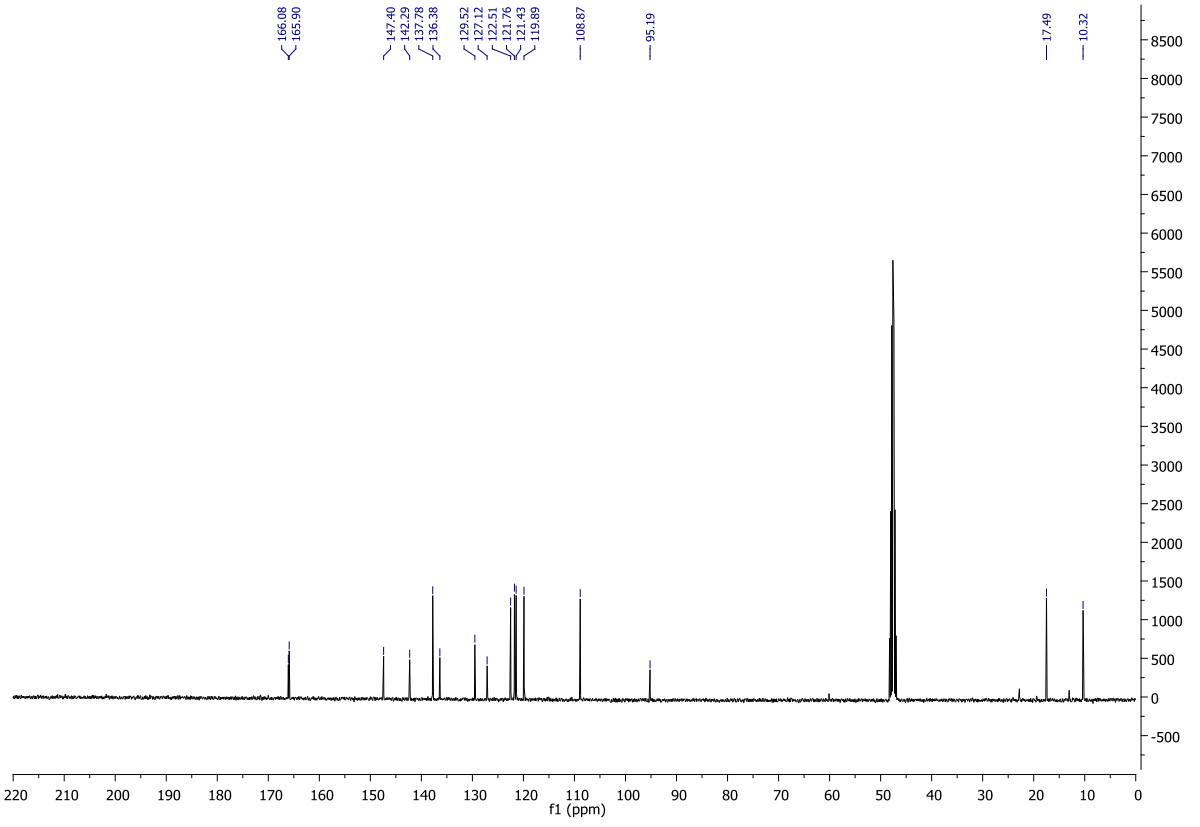
Measured mass should be within ±5 ppm of target mass

Compound 181

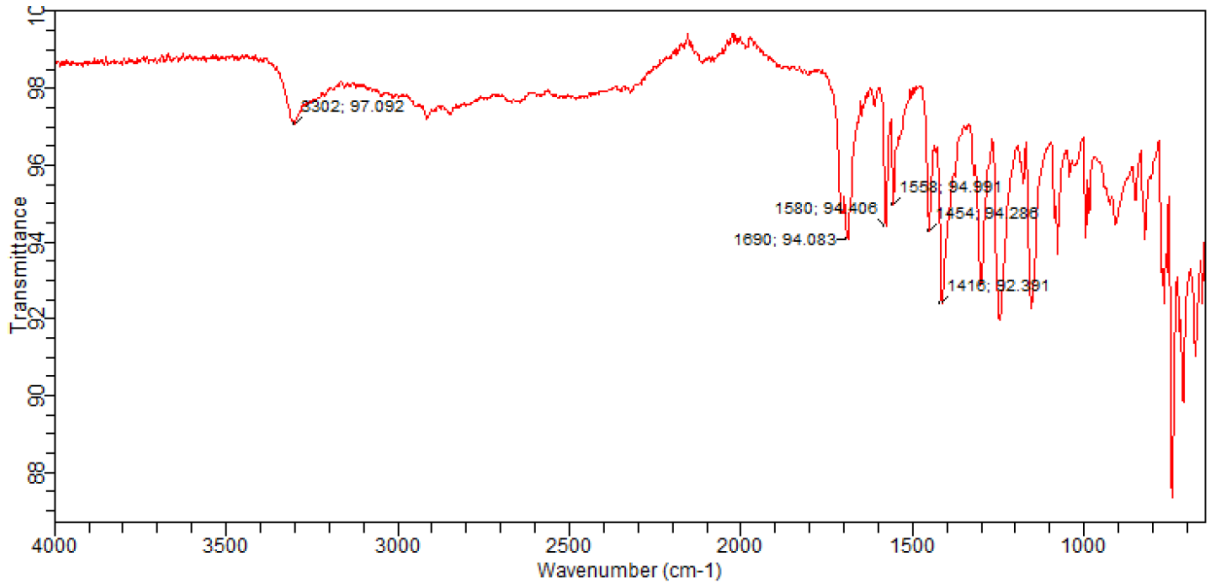
^{1}H NMR



^{13}C NMR of 181



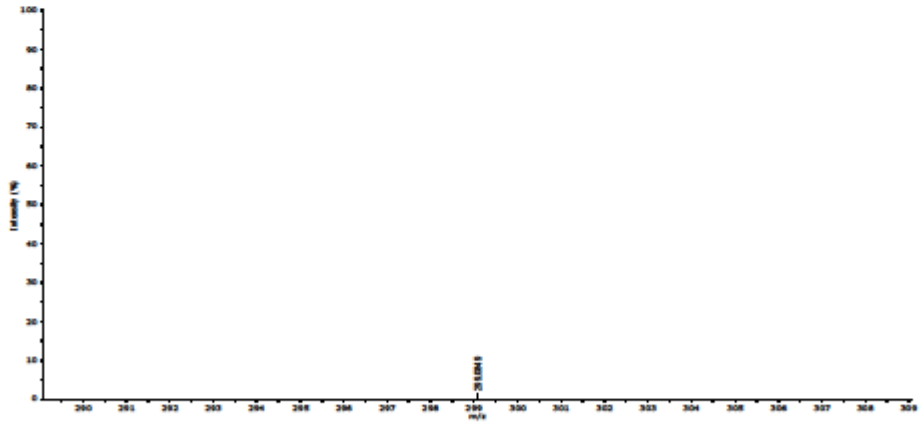
IR of 181


3302; 97.092
1690; 94.083
1580; 94.406
1558; 94.991
1454; 94.286
1416; 92.391
Transmittance
Wavenumber (cm-1)
4000
3500
3000
2500
2000
1500
1000
98
96
94
92
90
88

HRMS of 181

Spectrum RT 4.45, Peak [1], Target Mass 299.0849

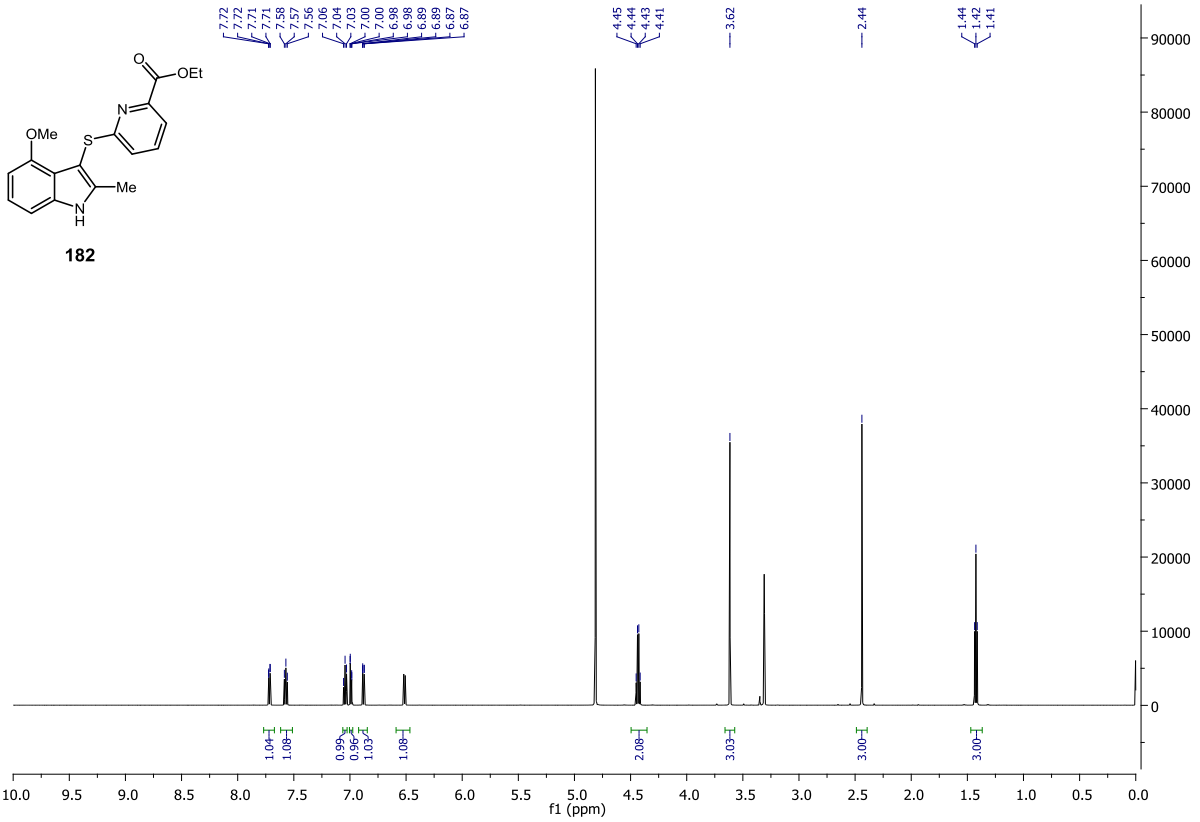
Expanded Spectrum RT 4.45, Peak [1], Target Mass 299.0849



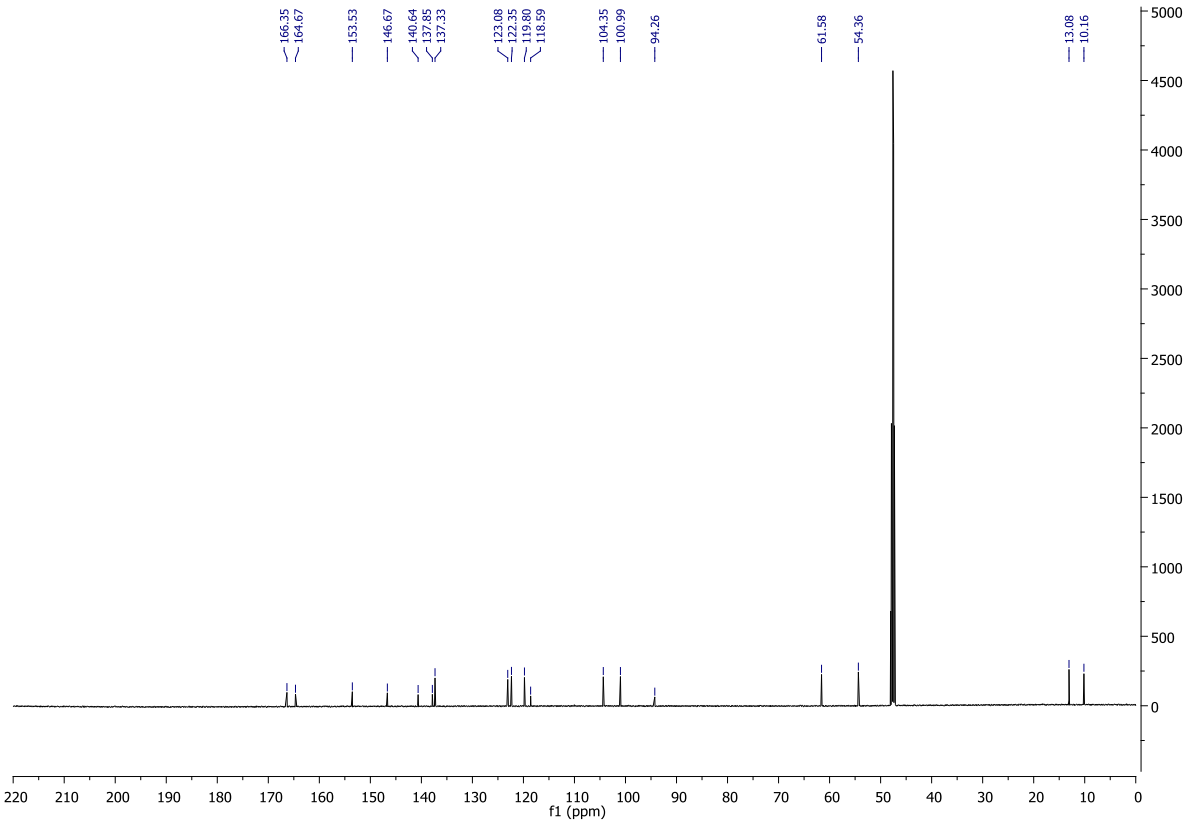
Measured Mass	Calculated Mass	Error (mDa)	Error (ppm)	Formula $[M+H]^+$
299.0849	299.0849	0.0	0.0	$C_{16}H_{15}N_2O_2S$

Compound 182

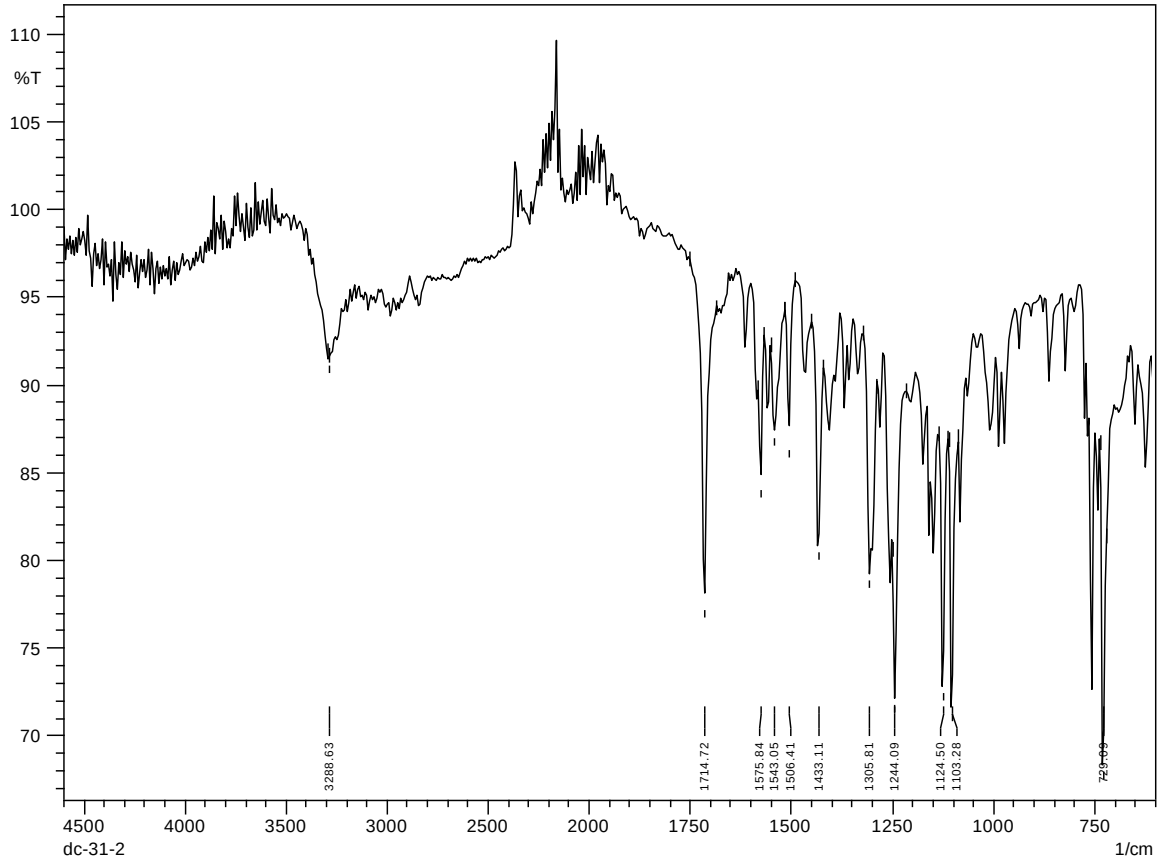
^{1}H NMR



^{13}C NMR of 182



IR of 182


110
%T
105
100
95
90
85
80
75
70
3288.63
1714.72
1575.84
1543.05
1506.41
1433.11
1305.81
1244.09
1124.50
1103.28
729.09
4500
4000
3500
3000
2500
2000
1750
1500
1250
1000
750
dc-31-2
1/cm

HRMS of 182

Bruker maXis Impact: LC-MS SmartFormula Report

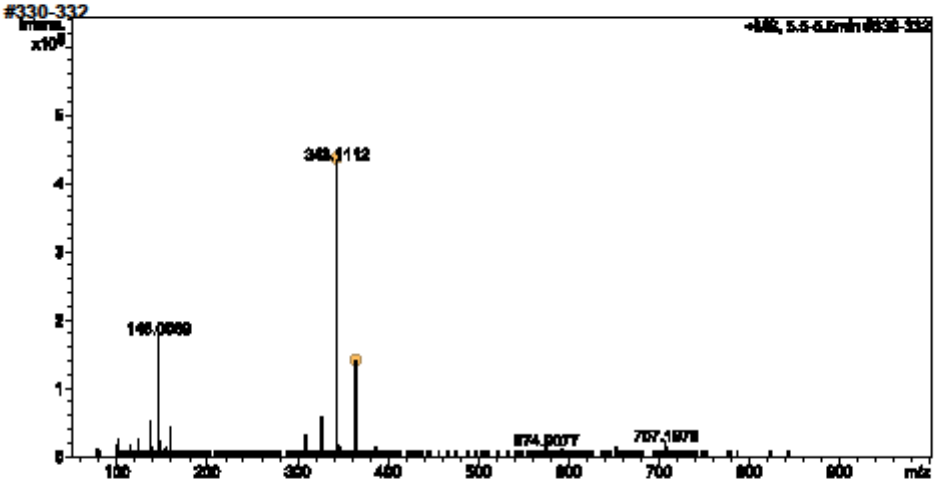
Analysis Info

Analysis Name	C:\Data\Data\N34272-64-4_1-A,5_01_1119.d	Acquisition Date	24/10/2014 15:18:25
Method	lcms pos 50-1000.m	Operator	Spectroscopy
Sample Name	N34272-64-4	Instrument / Ser	maXis impact 282001.00101
Comment			

Acquisition Parameter

Source Type	ESI	Scan Begin	50 m/z
Ion Polarity	Positive	Scan End	1000 m/z

+MS, 5.5-5.5min
#330-332

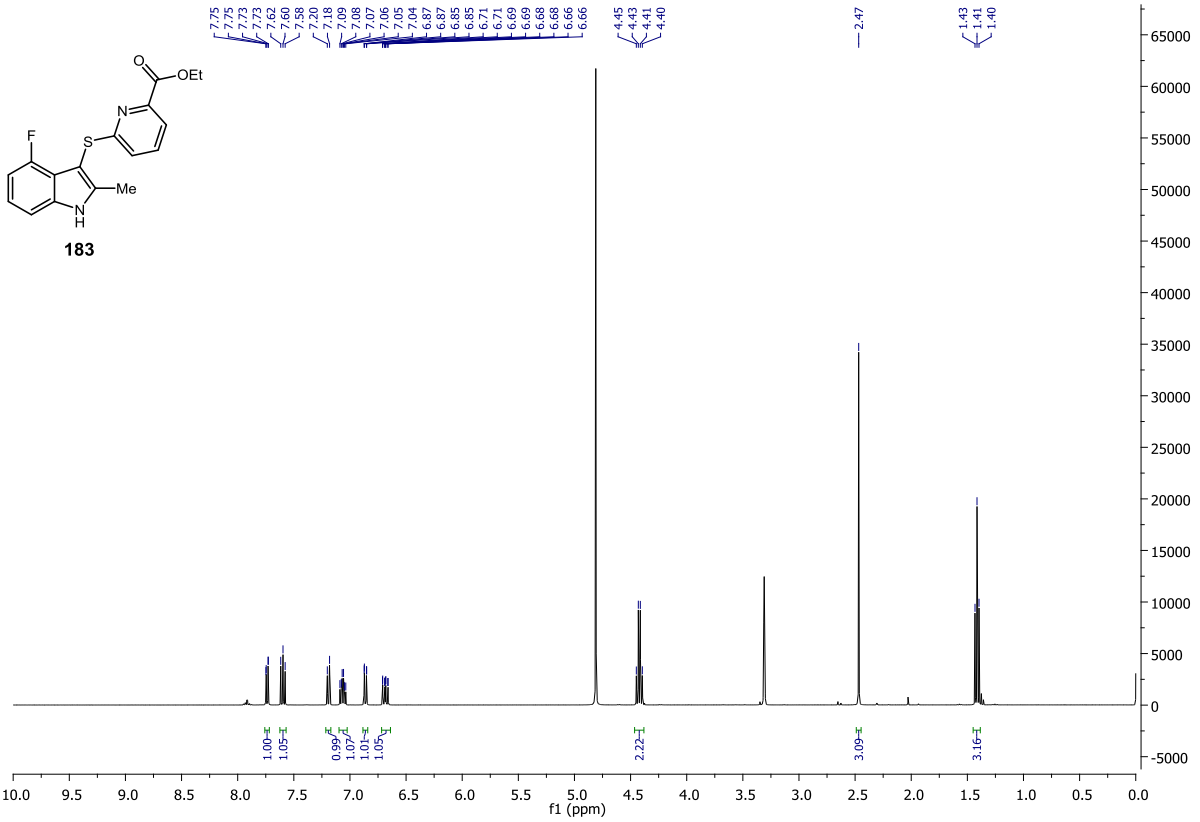


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
343.1112	1	C18H19N2O3S	343.1111	-0.2	52.9	1	100.00	10.5	even	ok
365.0929	1	C18H18N2NaO3S	365.0930	0.3	59.2	1	100.00	10.5	even	ok

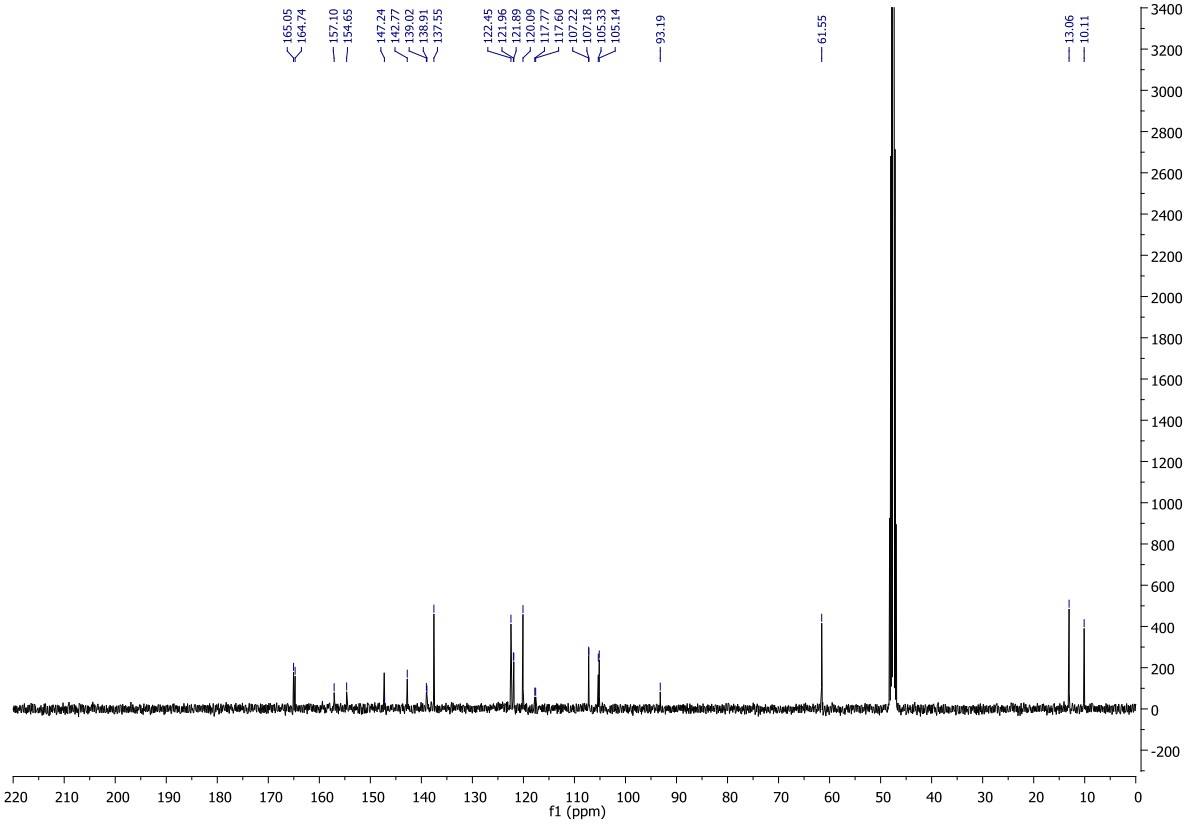
Measured mass should be within ±5 ppm of target mass

Compound 183

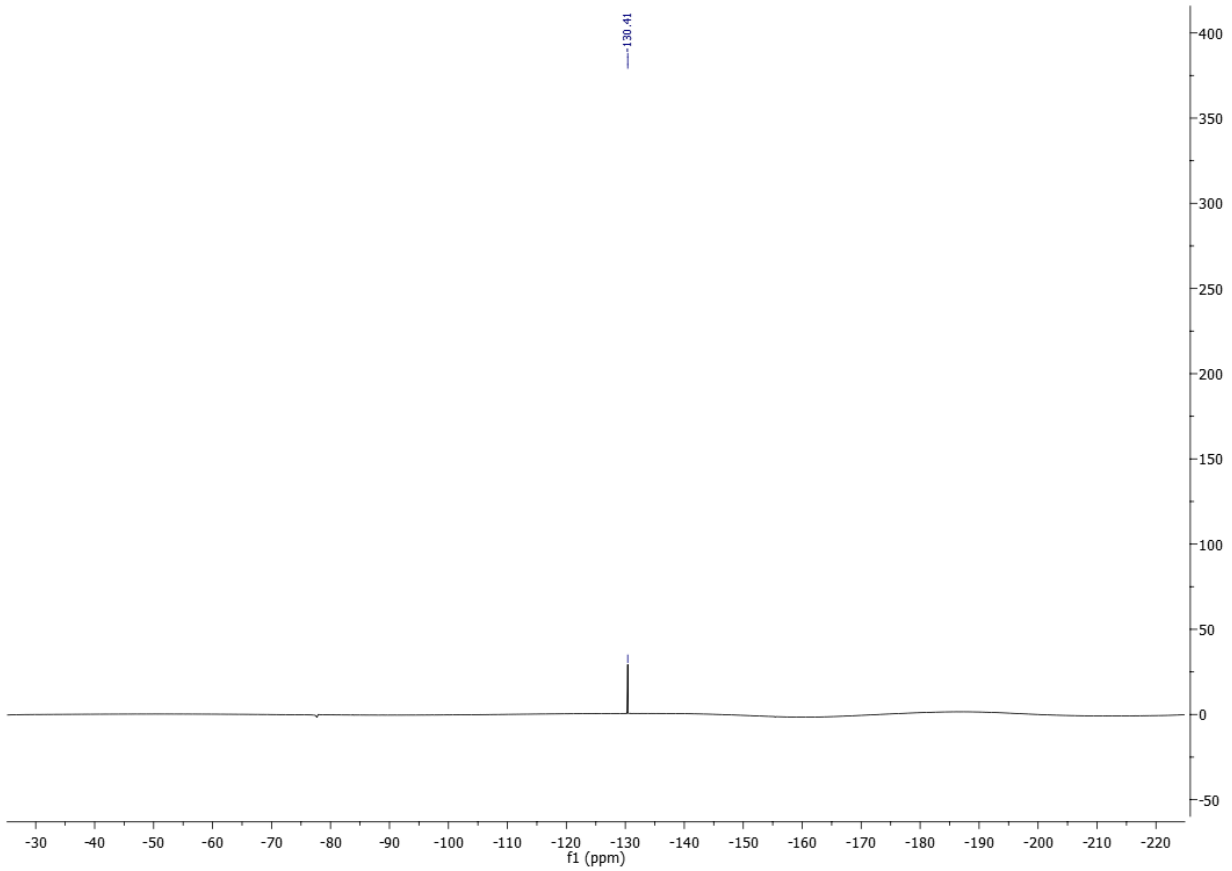
^{1}H NMR



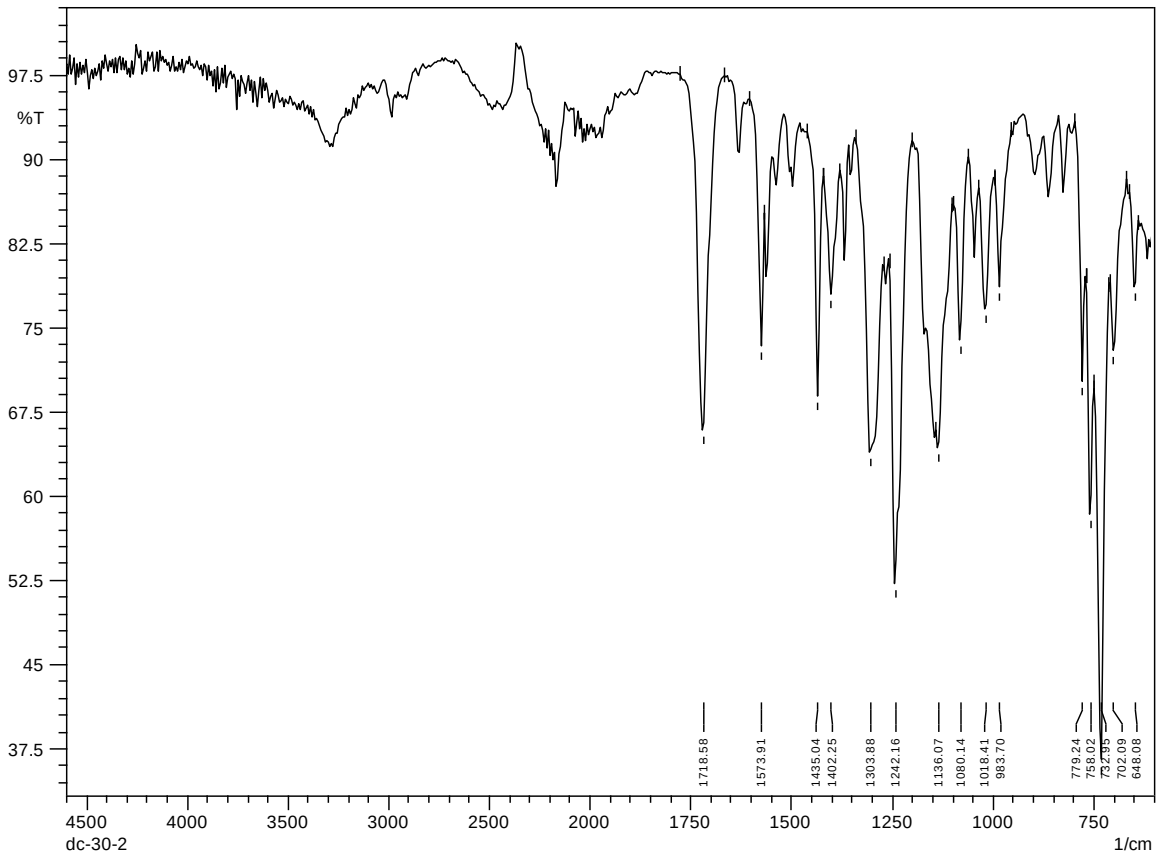
^{13}C NMR of 183



^{19}F NMR of 183



IR of 183



HRMS of 183

Bruker maXis Impact: LC-MS SmartFormula Report

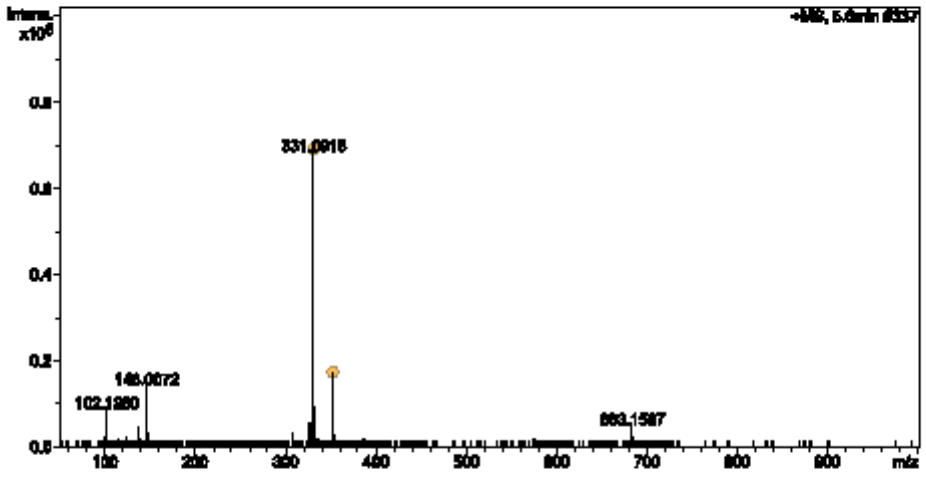
Analysis Info

Analysis Name	C:\Data\Data\N34272-59-2_1-A,5_01_1067.d	Acquisition Date	22/10/2014 08:46:53
Method	lcms pos 50-1000.m	Operator	Spectroscopy
Sample Name	N34272-59-2	Instrument / Ser	maXis impact 282001.0 0101
Comment			

Acquisition Parameter

Source Type	ESI	Scan Begin	50 m/z
Ion Polarity	Positive	Scan End	1000 m/z

+MS, 5.6min #337

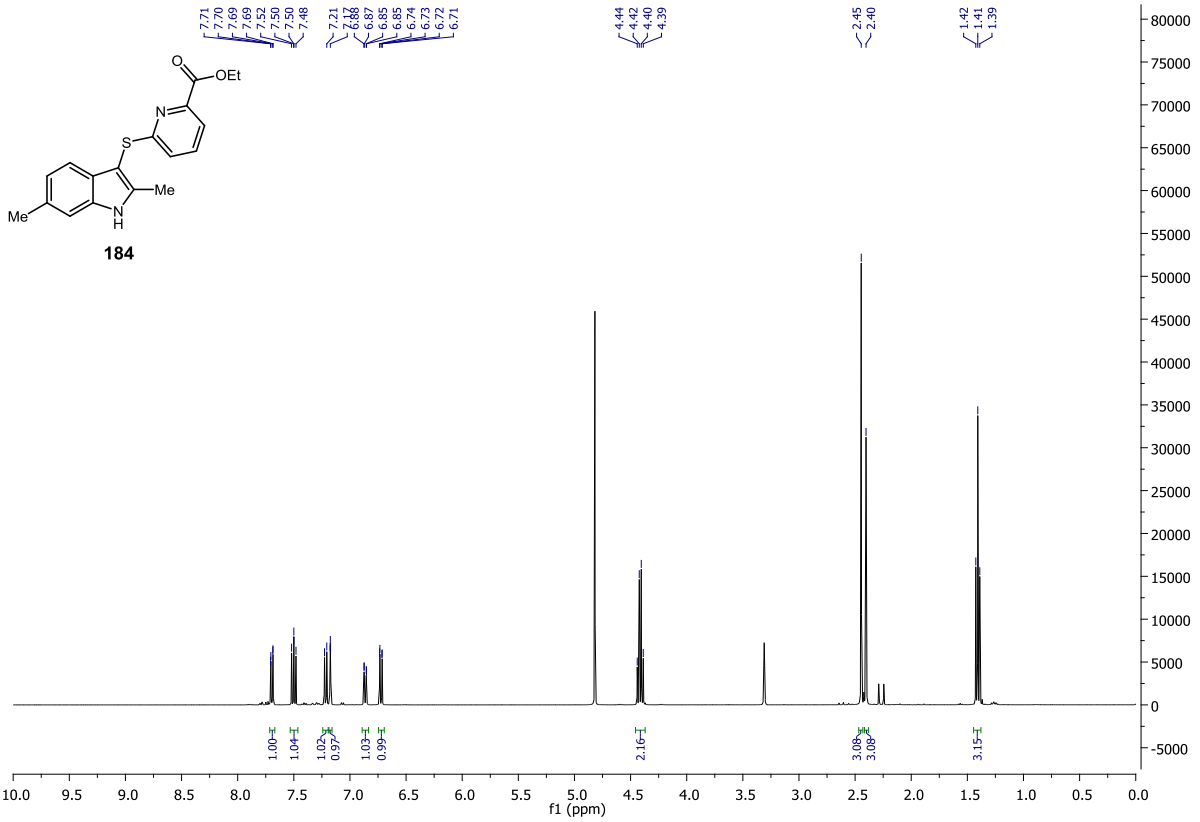


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
331.0918	1	C17H16FN2O2S	331.0911	2.1	45.0	1	100.00	10.5	even	ok
353.0735	1	C17H15FN2NaO2S	353.0730	1.3	53.1	1	100.00	10.5	even	ok

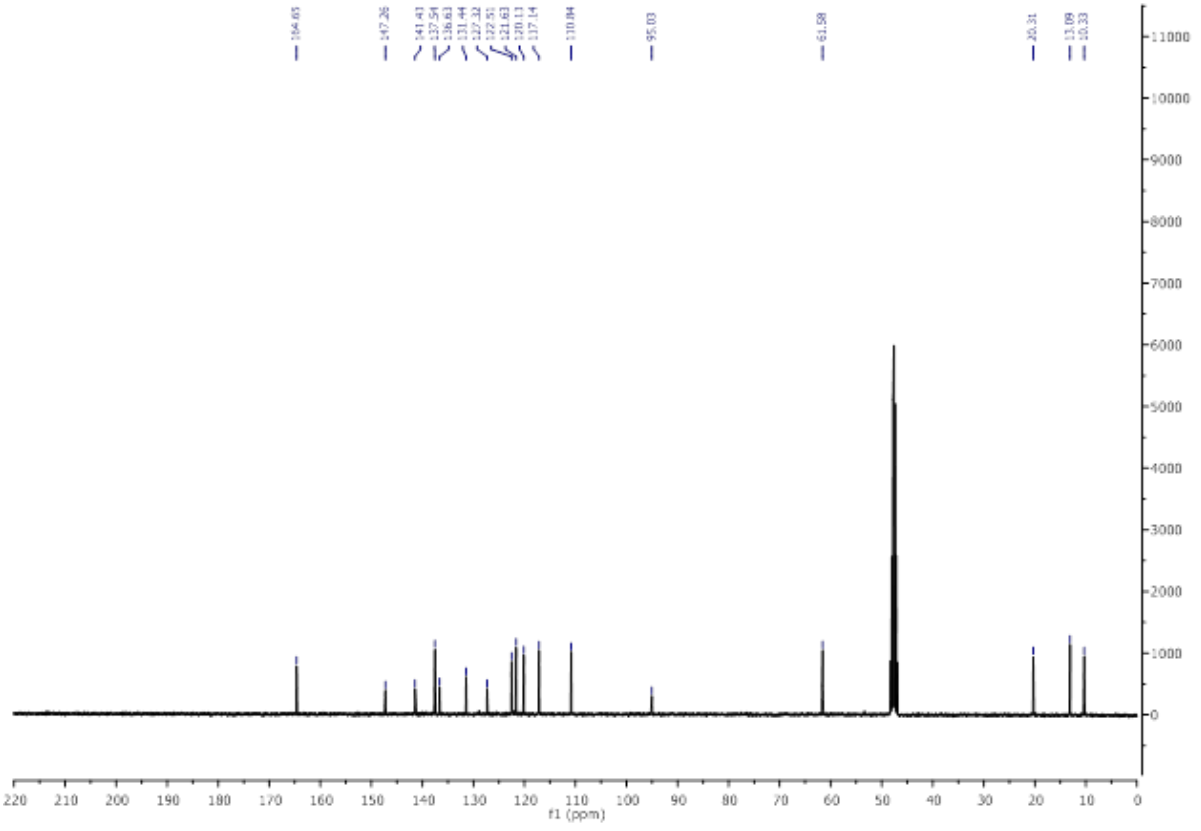
Measured mass should be within ±5 ppm of target mass

Compound 184

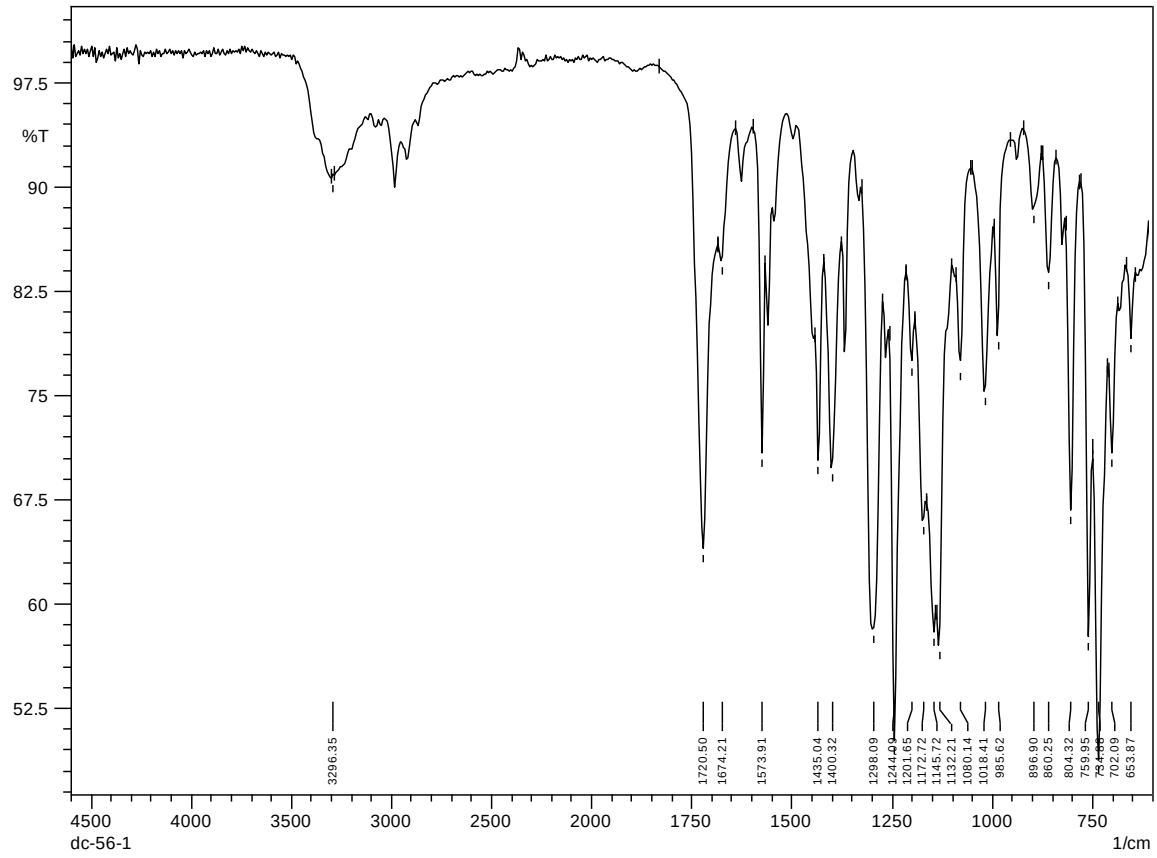
^{1}H NMR



^{13}C NMR of 184

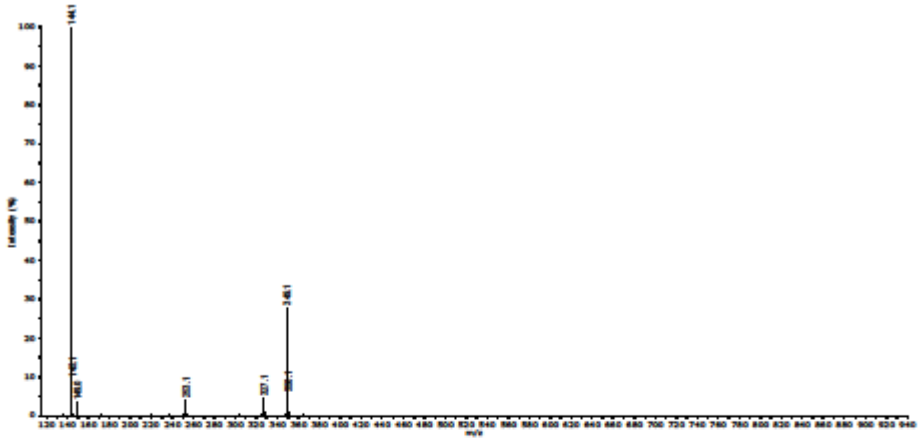


IR of 184

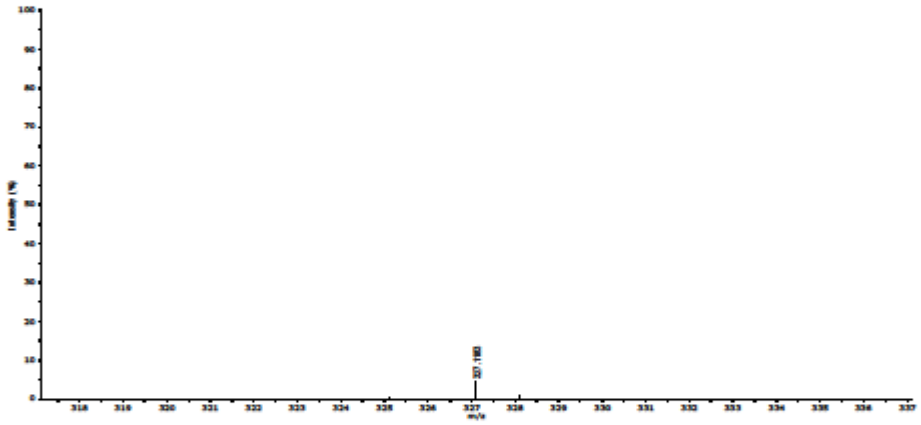

97.5
%T
90
82.5
75
67.5
60
52.5
3296.35
1720.50
1674.21
1573.91
1435.04
1400.32
1298.09
1244.09
1201.65
1172.72
1145.72
1132.21
1080.14
1018.41
985.62
896.90
860.25
804.32
759.95
734.86
702.09
653.87
4500
4000
3500
3000
2500
2000
1750
1500
1250
1000
750
dc-56-1
1/cm

HRMS of 184

Spectrum RT 5.47, Peak [1], Target Mass 327.1162



Expanded Spectrum RT 5.47, Peak [1], Target Mass 327.1162



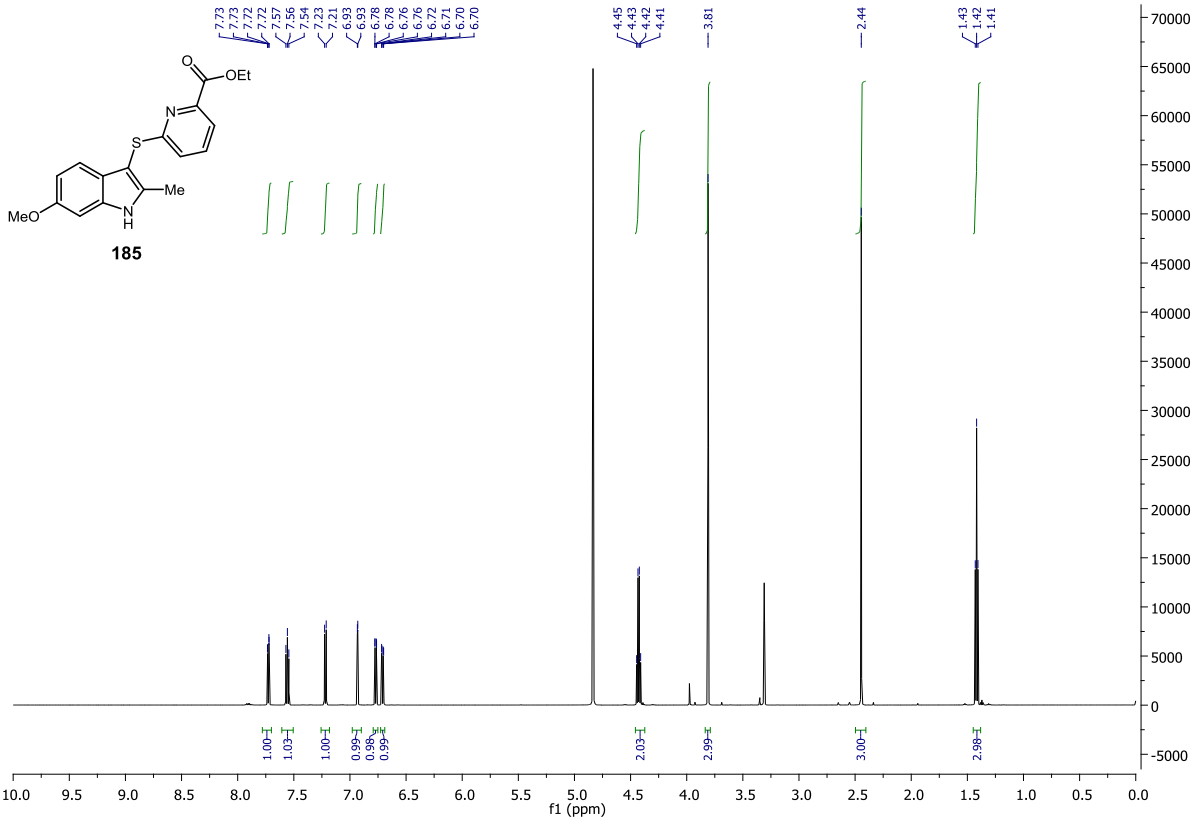
Measured Mass	Calculated Mass	Error (mDa)	Error (ppm)	Formula $[M+H]^+$
327.1161	327.1162	-0.1	-0.2	$C_{18}H_{19}N_2O_2S$

An error of < 5ppm indicates that the measured mass is consistent with the proposed formula.

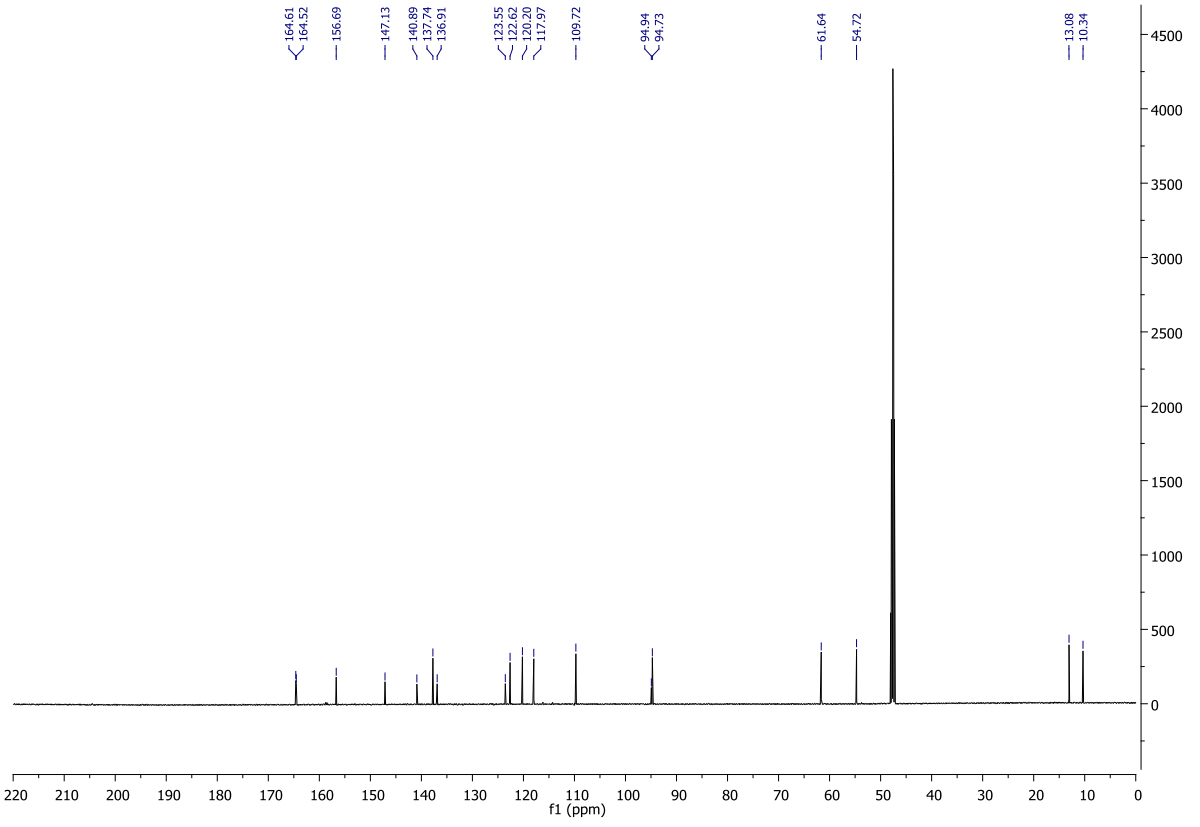
Contacts: Marco Smith #3727 or Alec Simpson #3732

Compound 185

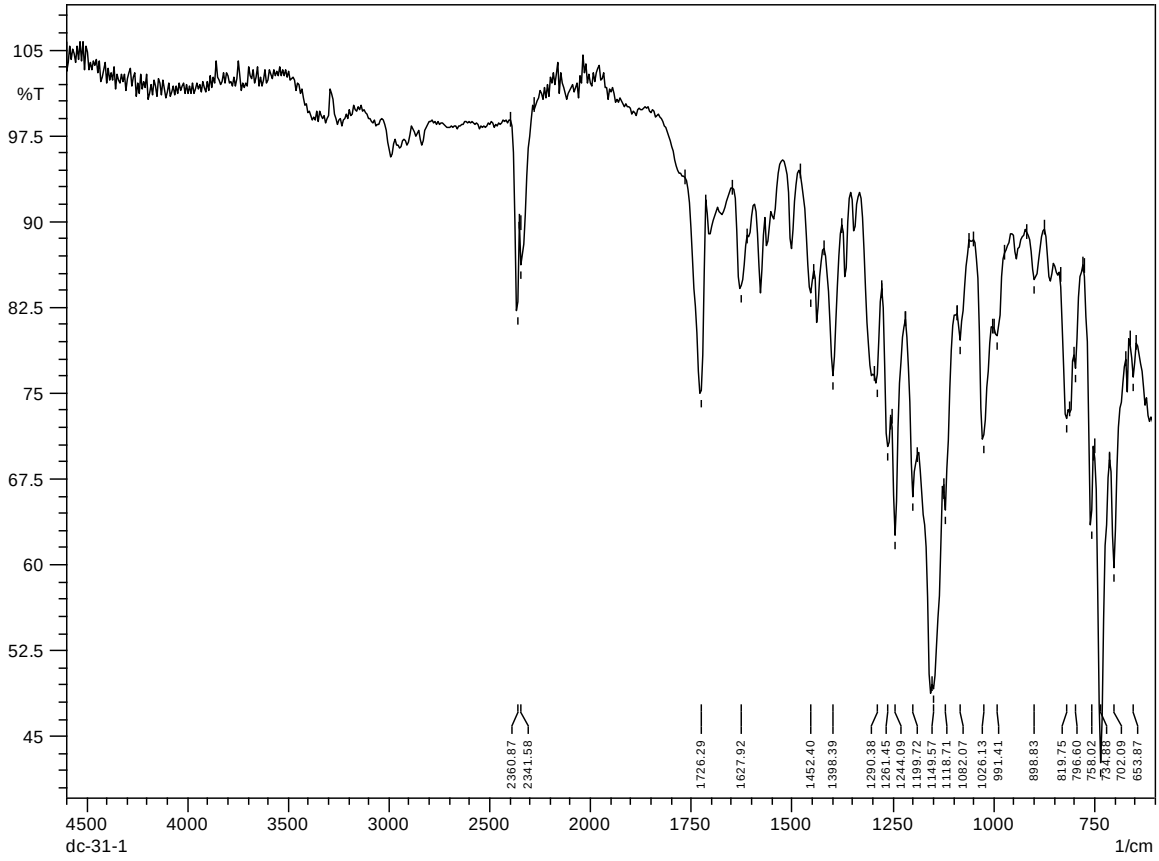
^{1}H NMR



^{13}C NMR of 185



IR of 185


105
%T
97.5
90
82.5
75
67.5
60
52.5
45
2360.87
2341.58
1726.29
1627.92
1452.40
1398.39
1290.38
1261.45
1244.09
1199.72
1149.57
1118.71
1082.07
1026.13
991.41
898.83
819.75
796.60
758.02
734.88
702.09
653.87
4500
4000
3500
3000
2500
2000
1750
1500
1250
1000
750
dc-31-1
1/cm

HRMS of 185

Bruker maXis Impact: LC-MS SmartFormula Report

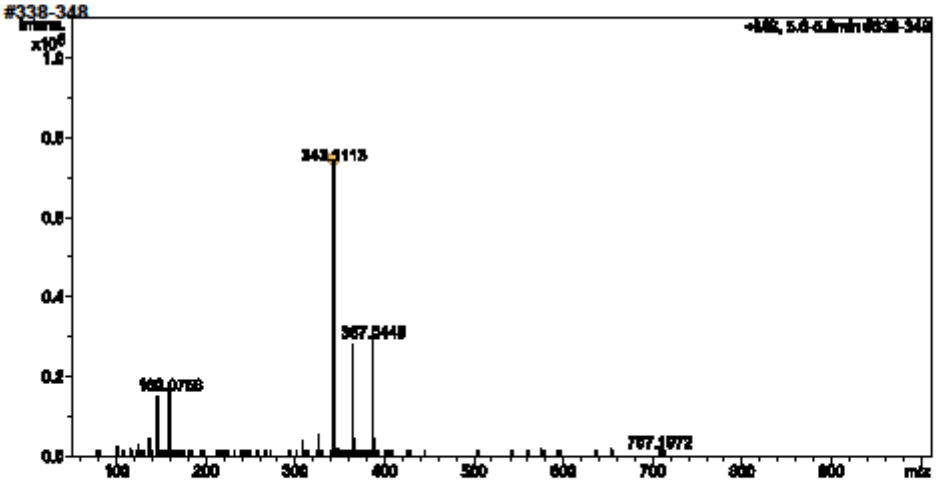
Analysis Info

Analysis Name	C:\Data\Data\N34272-64-3_1-A,4_01_1118.d	Acquisition Date	24/10/2014 15:07:39
Method	lcms pos 50-1000.m	Operator	Spectroscopy
Sample Name	N34272-64-3	Instrument / Ser	maXis impact 282001.0 0101
Comment			

Acquisition Parameter

Source Type	ESI	Scan Begin	50 m/z
Ion Polarity	Positive	Scan End	1000 m/z

+MS, 5.6-5.8min
#338-348

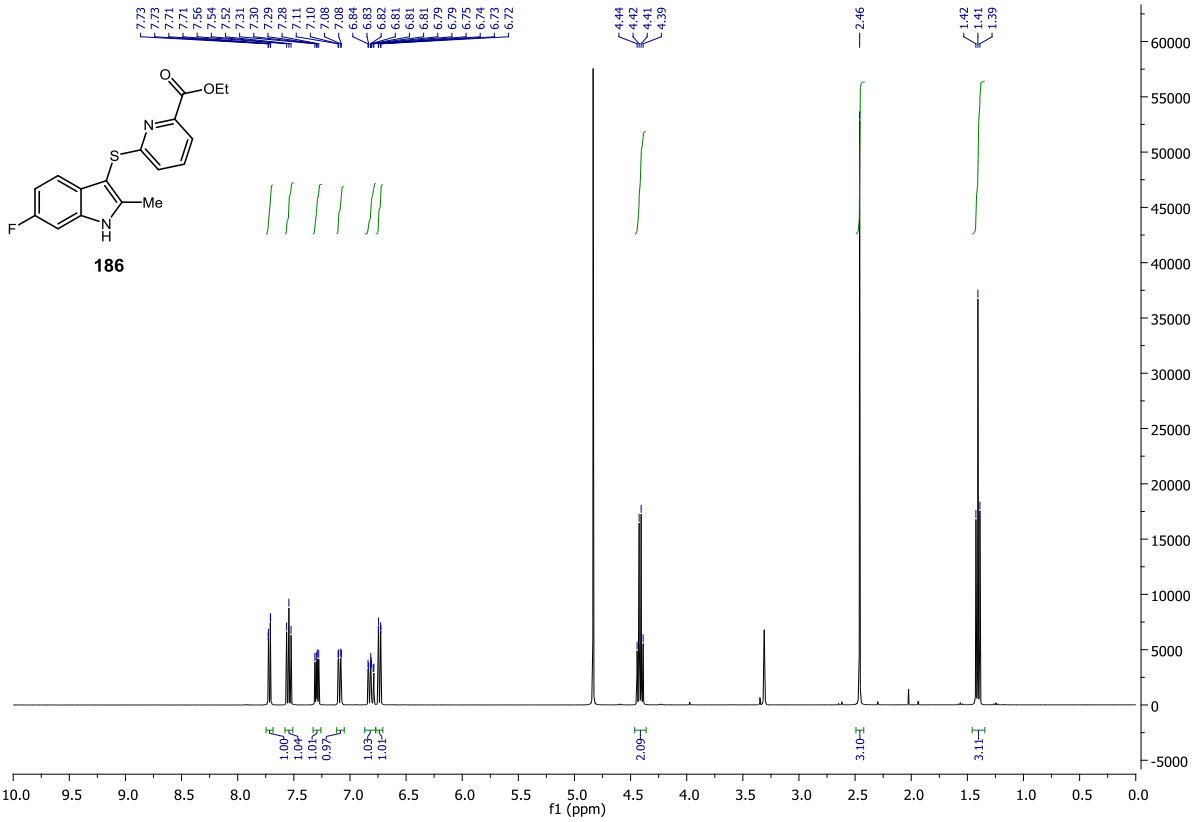


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
343.1113	1	C18H19N2O3S	343.1111	-0.6	35.3	1	100.00	10.5	even	ok

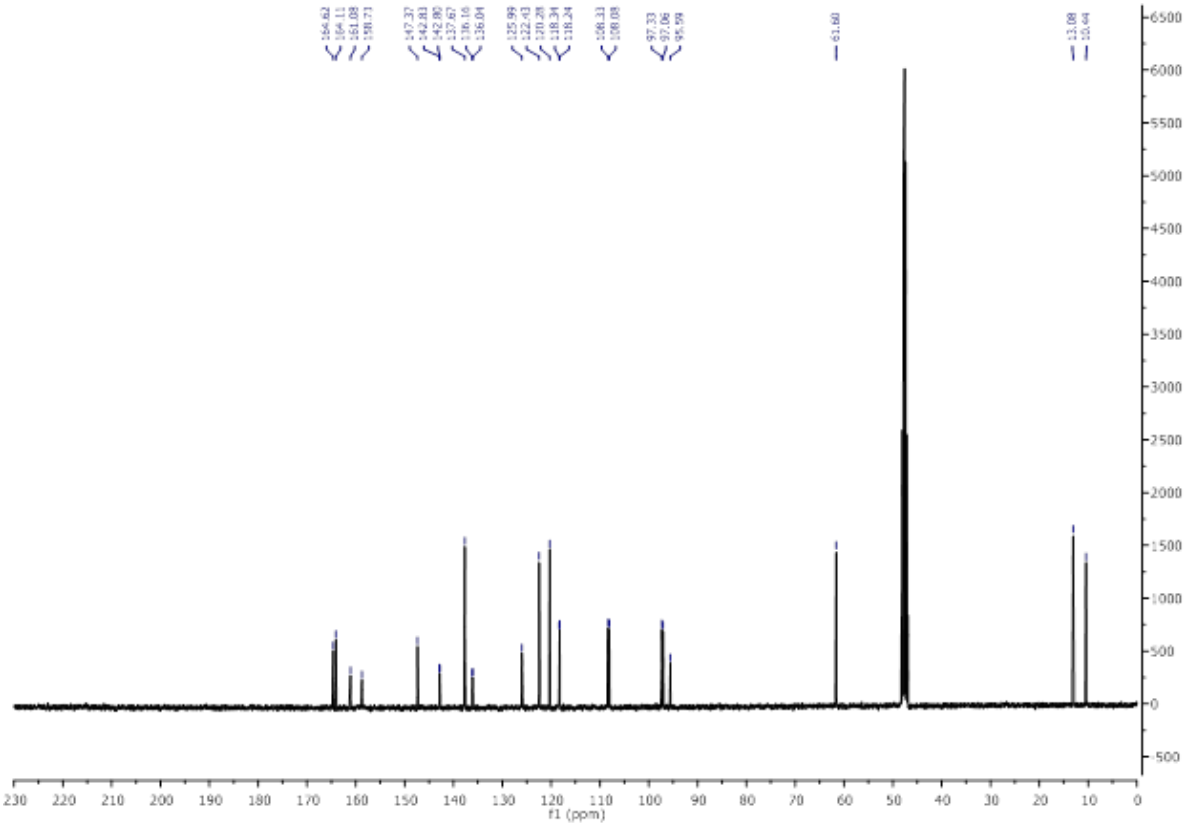
Measured mass should be within ±5 ppm of target mass

Compound 186

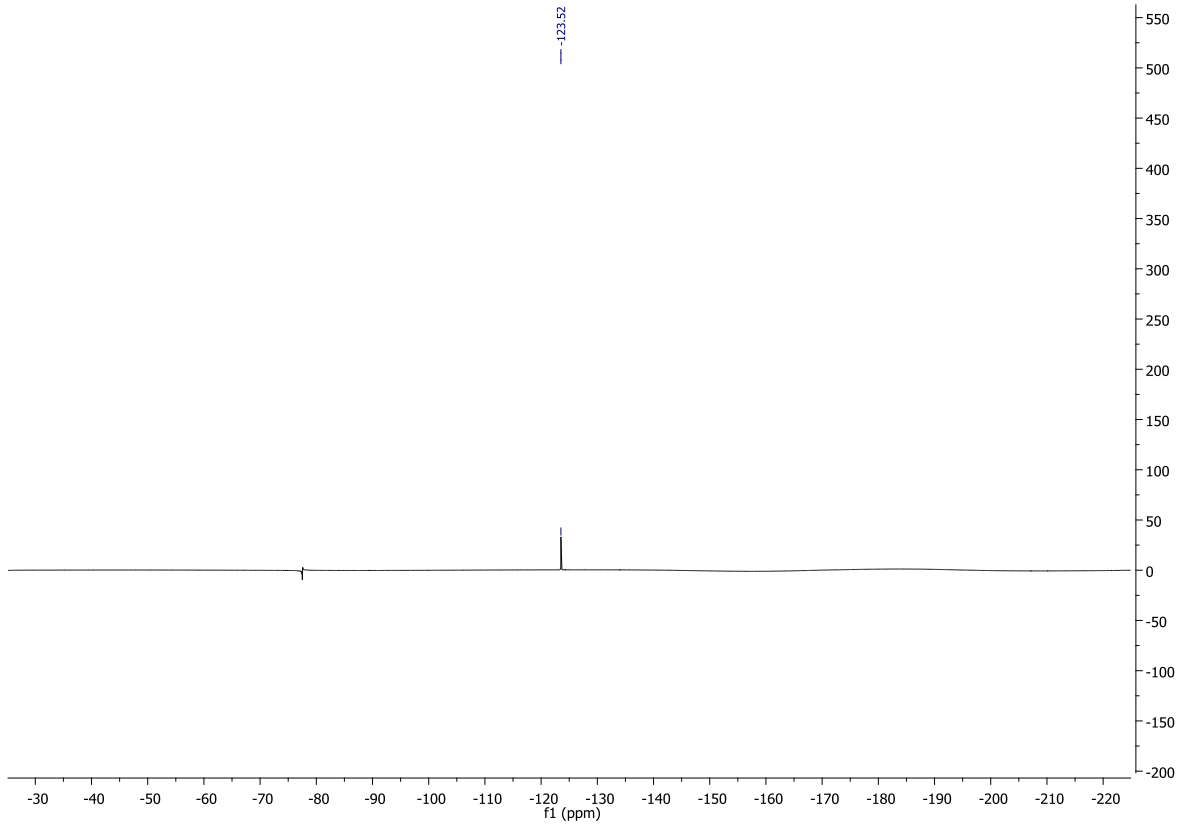
^{1}H NMR



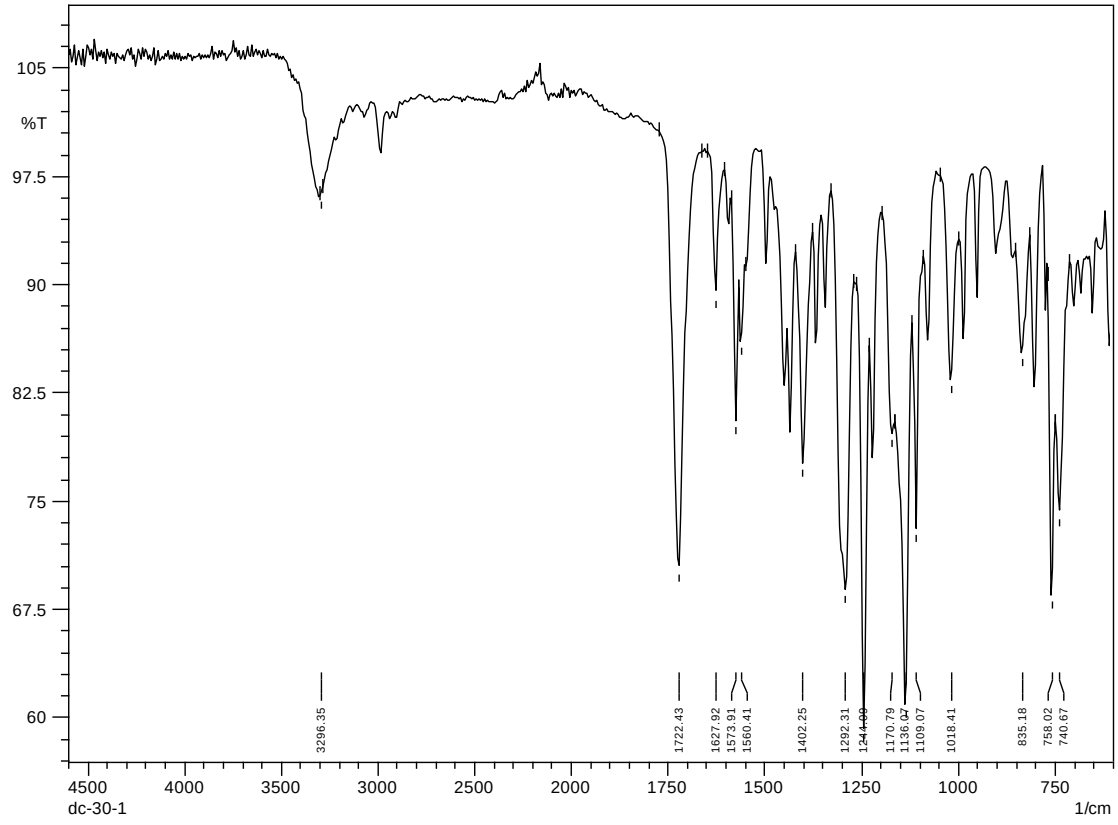
^{13}C NMR of 186



^{19}F NMR of 186



IR of 186



HRMS of 186

Bruker maXis Impact: LC-MS SmartFormula Report

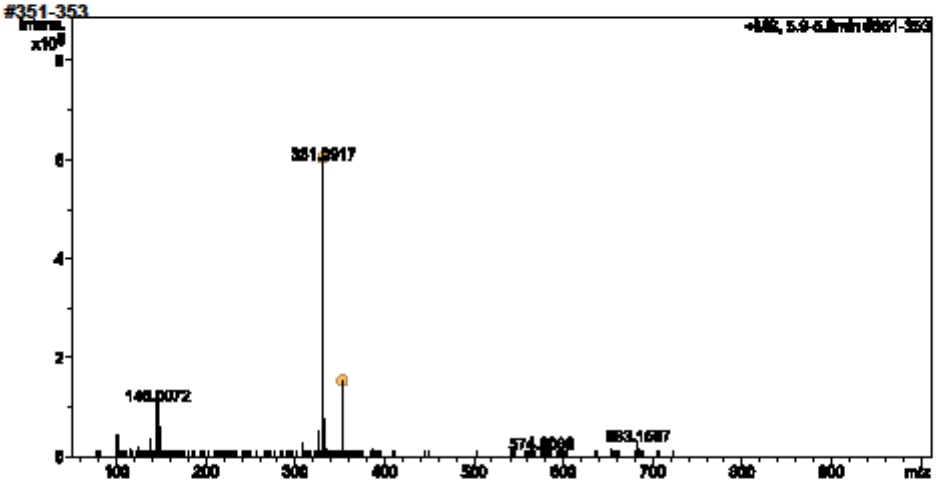
Analysis Info

Analysis Name	C:\Data\Data\N34272-59-1_1-A,4_01_1066.d	Acquisition Date	22/10/2014 08:36:06
Method	lcms pos 50-1000.m	Operator	Spectroscopy
Sample Name	N34272-59-1	Instrument / Ser	maXis impact 282001.0 0101
Comment			

Acquisition Parameter

Source Type	ESI	Scan Begin	50 m/z
Ion Polarity	Positive	Scan End	1000 m/z

+MS, 5.9-5.9min
#351-353

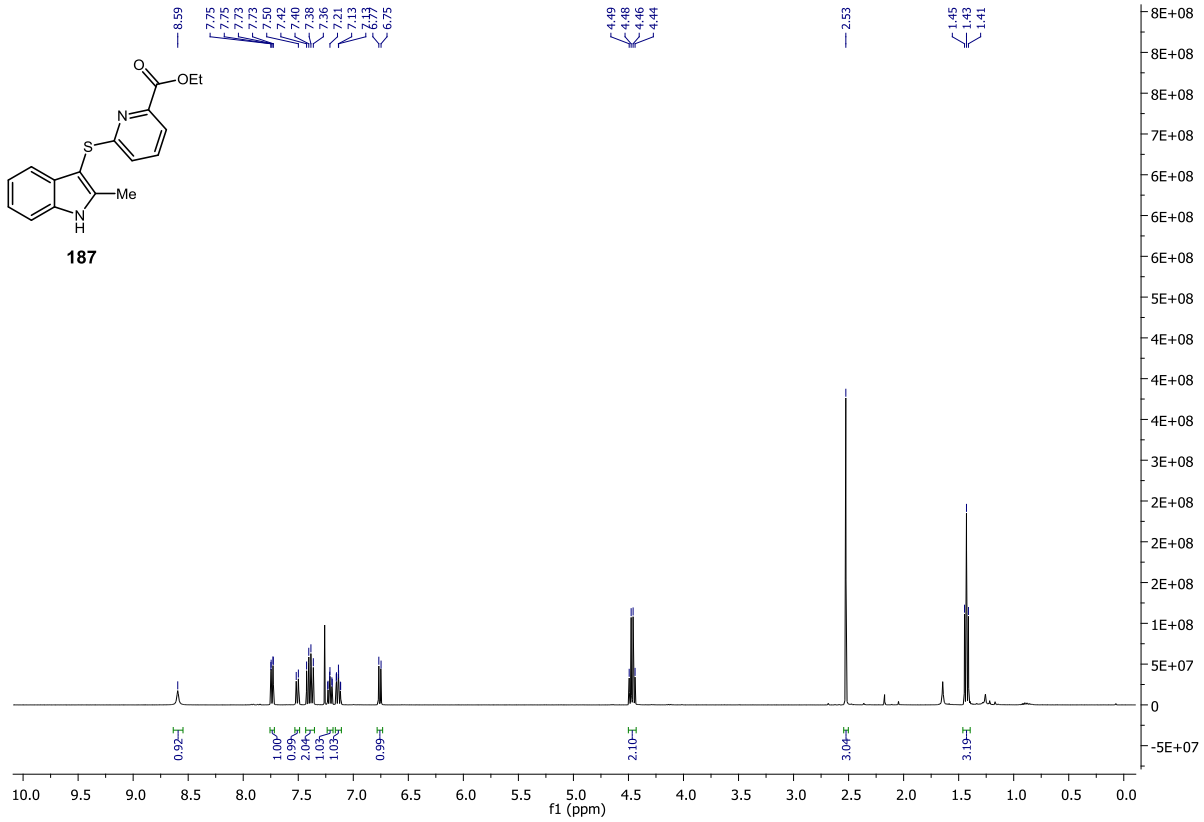


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
331.0917	1	C17H16FN2O2S	331.0911	1.9	51.2	1	100.00	10.5	even	ok
353.0734	1	C17H15FN2NaO2S	353.0730	1.1	55.2	1	100.00	10.5	even	ok

Measured mass should be within ±5 ppm of target mass

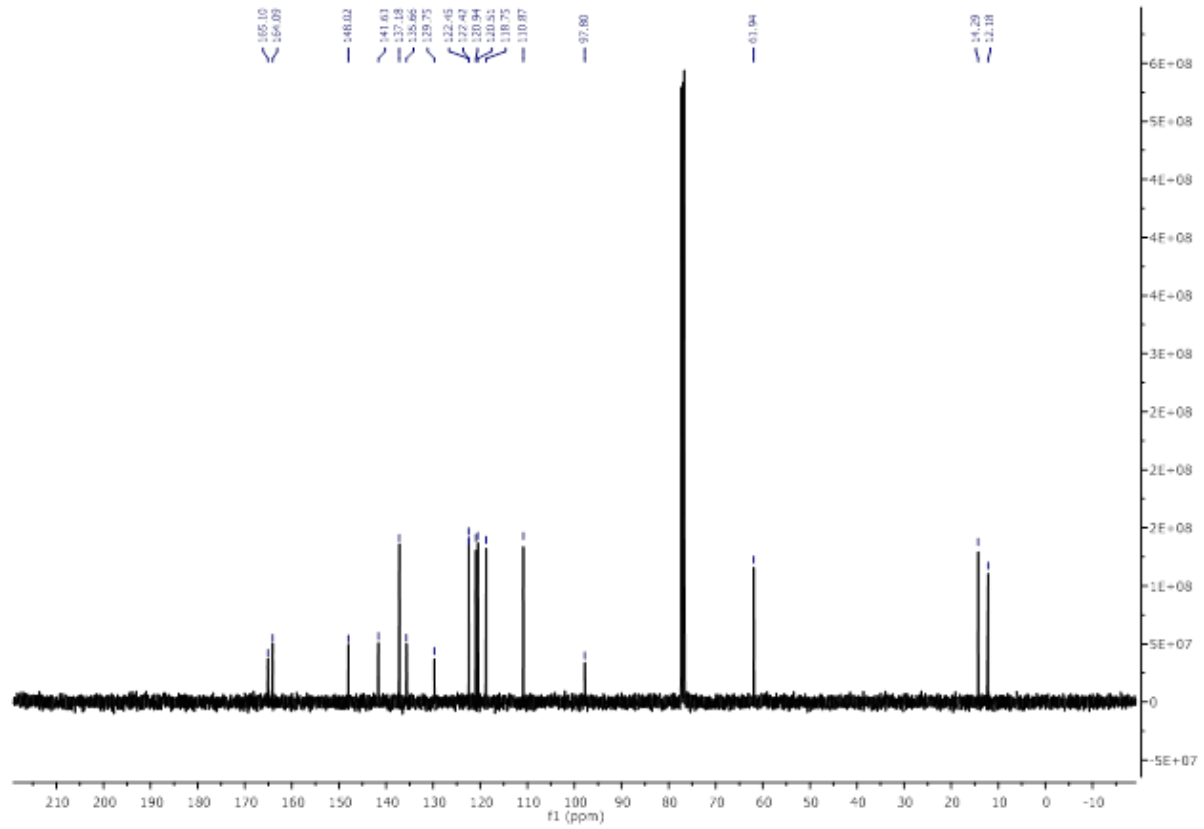
Compound 187

^{1}H NMR

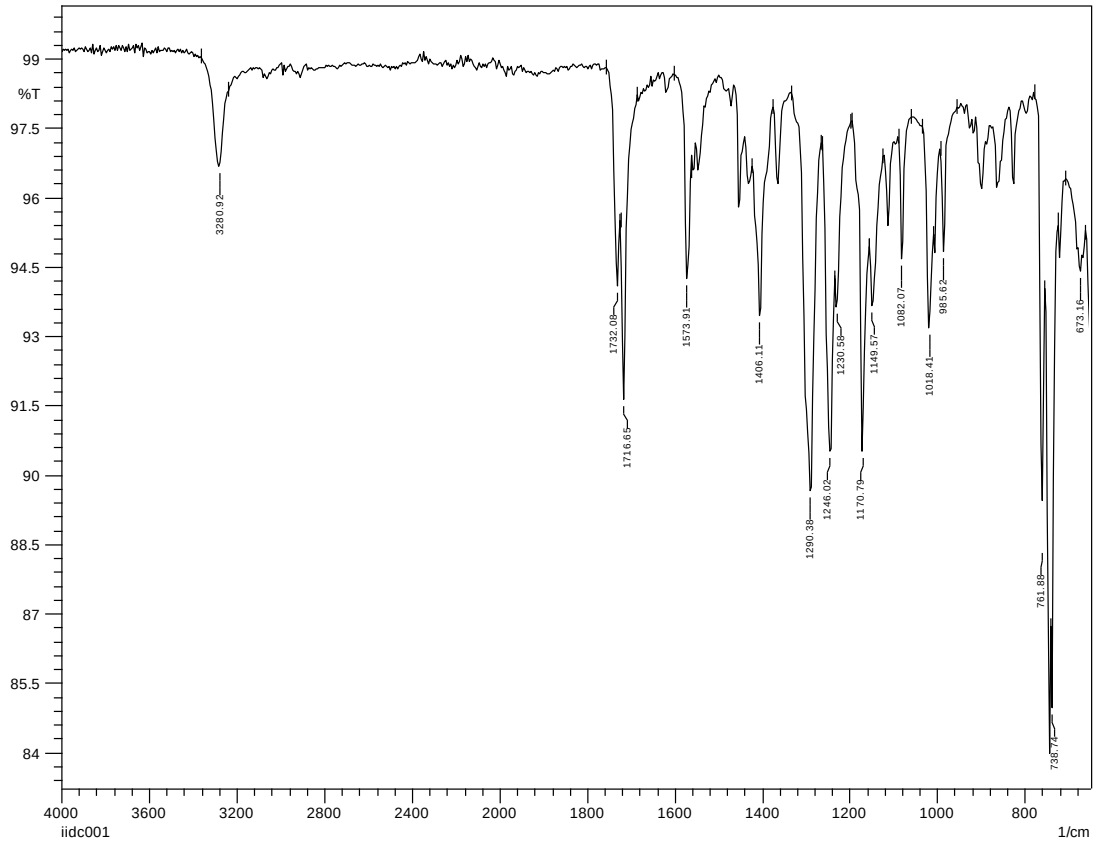


187

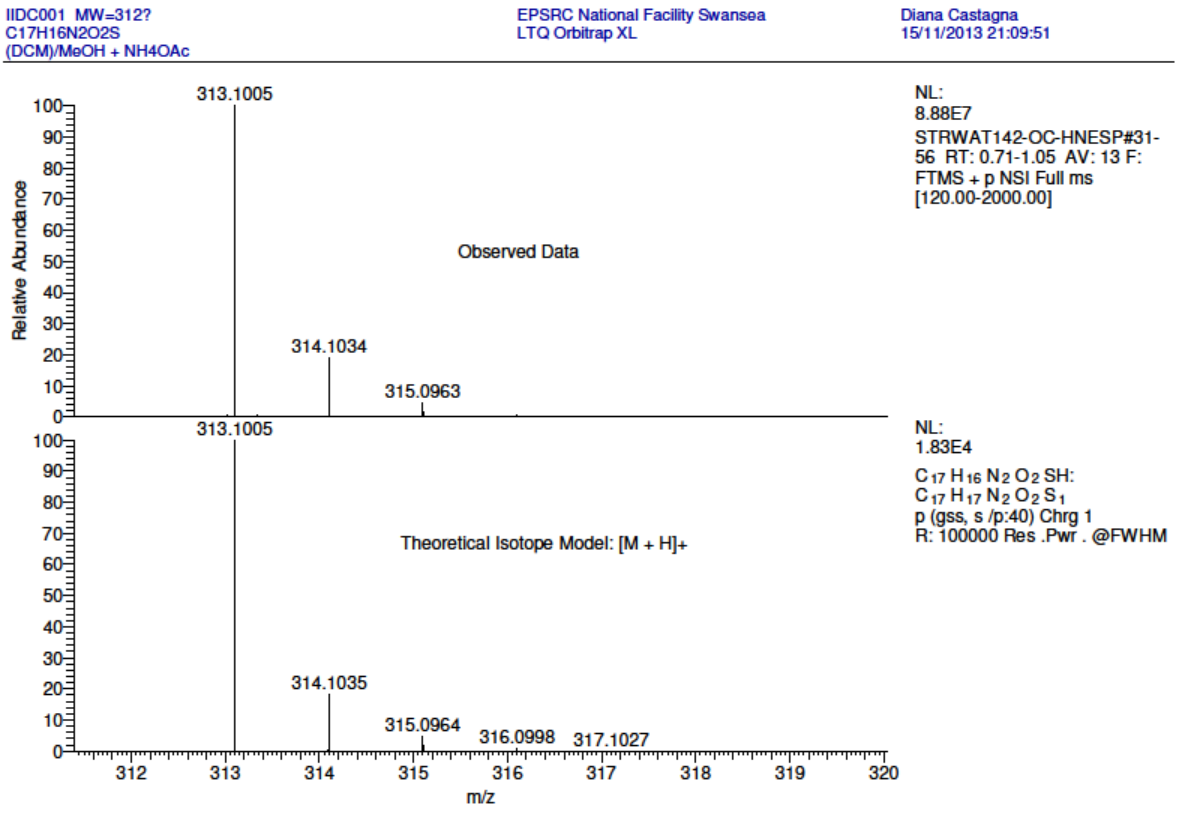
^{13}C NMR of 187



IR of 187

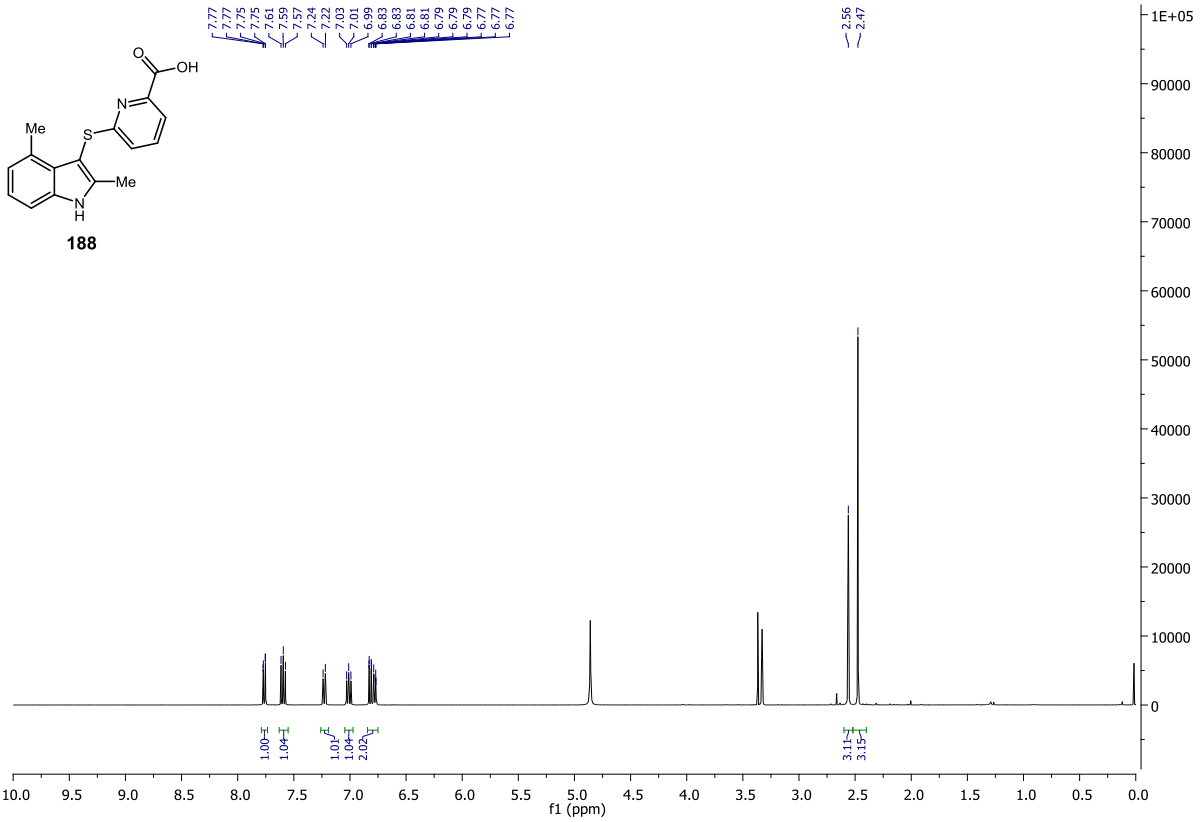


HRMS of 187



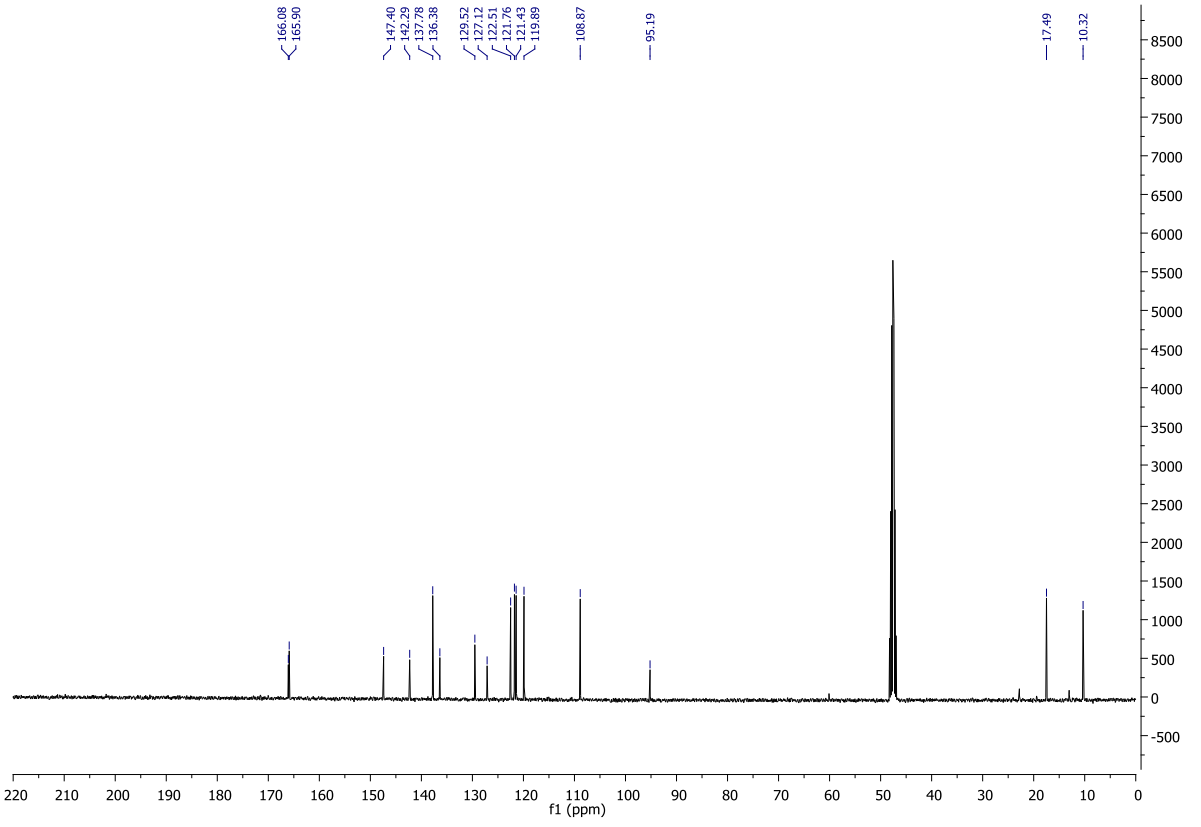
Compound 188

^{1}H NMR

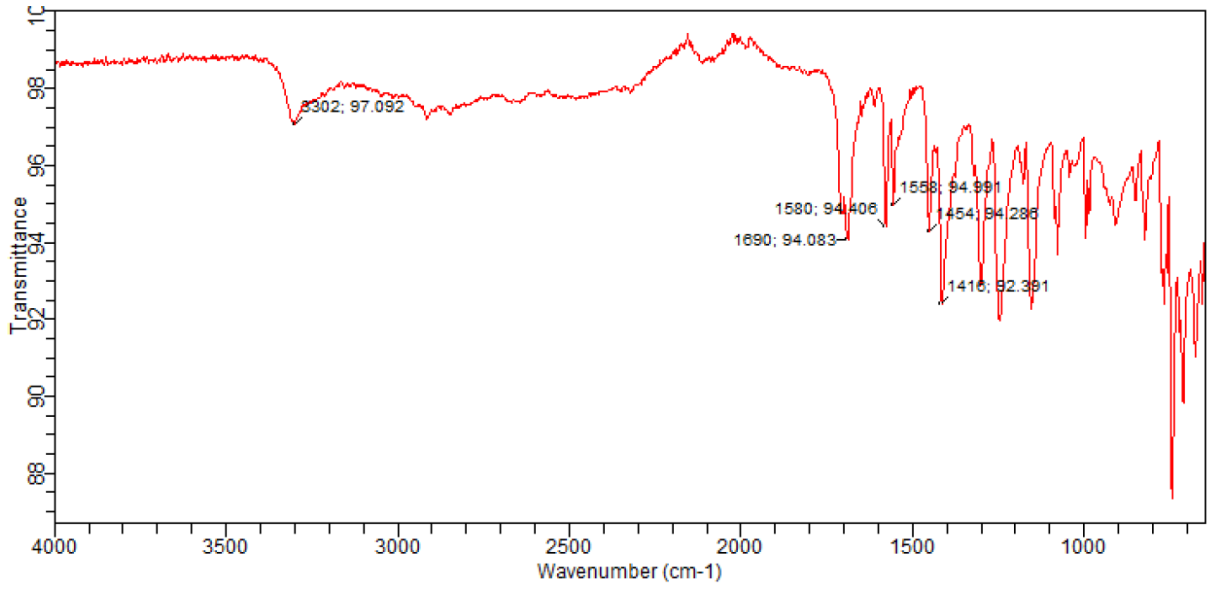


188

^{13}C NMR of 188



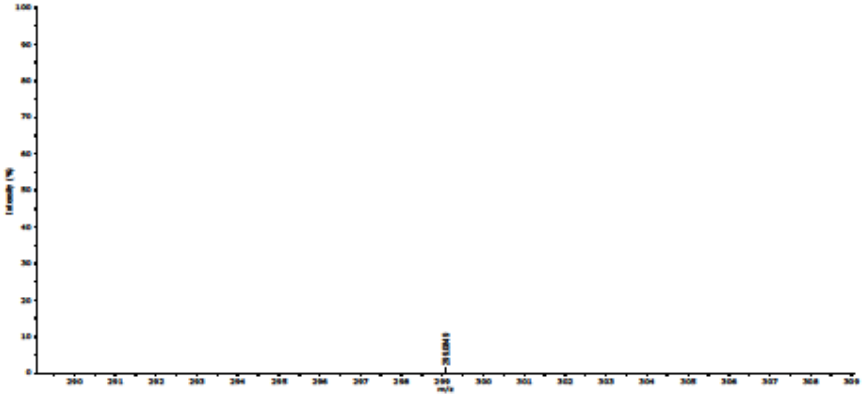
IR of 188



HRMS of 188

Spectrum RT 4.45, Peak [1], Target Mass 299.0849

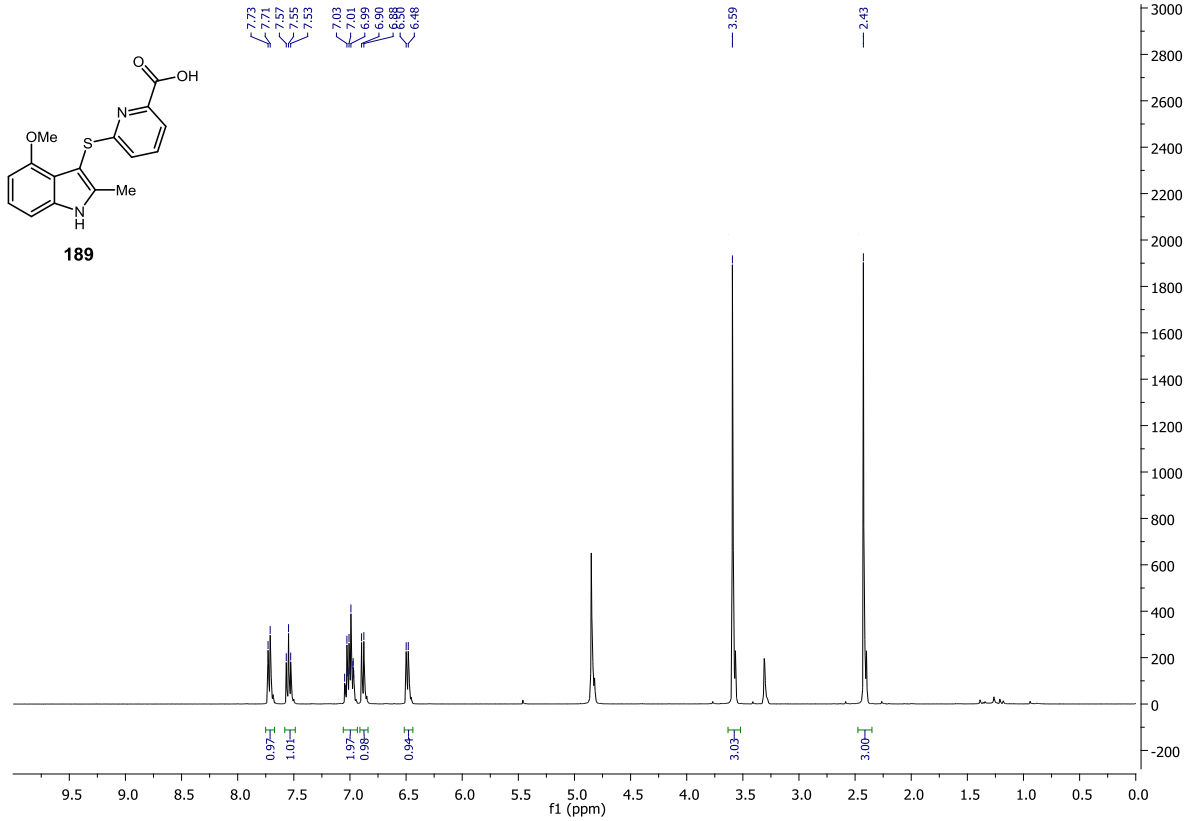
Expanded Spectrum RT 4.45, Peak [1], Target Mass 299.0849



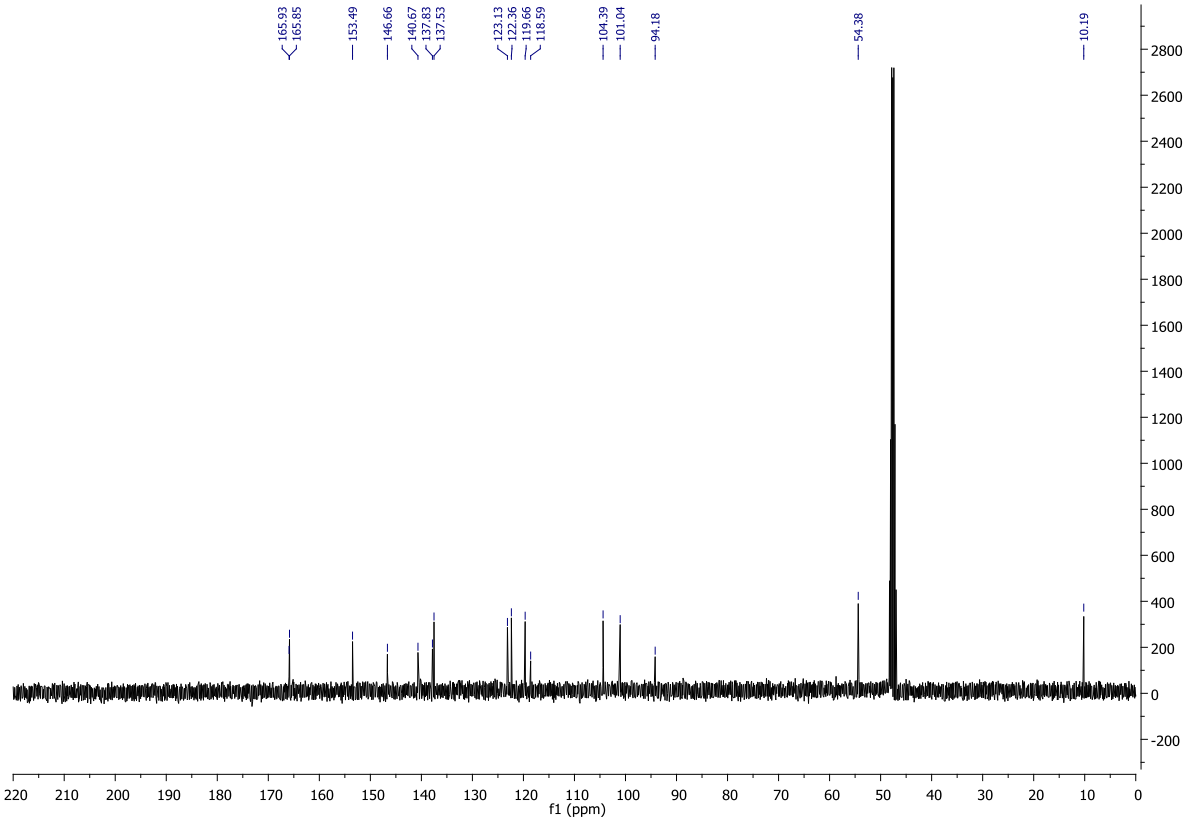
Measured Mass	Calculated Mass	Error (mDa)	Error (ppm)	Formula $[M+H]^+$
299.0849	299.0849	0.0	0.0	$C_{16}H_{15}N_2O_2S$

Compound 189

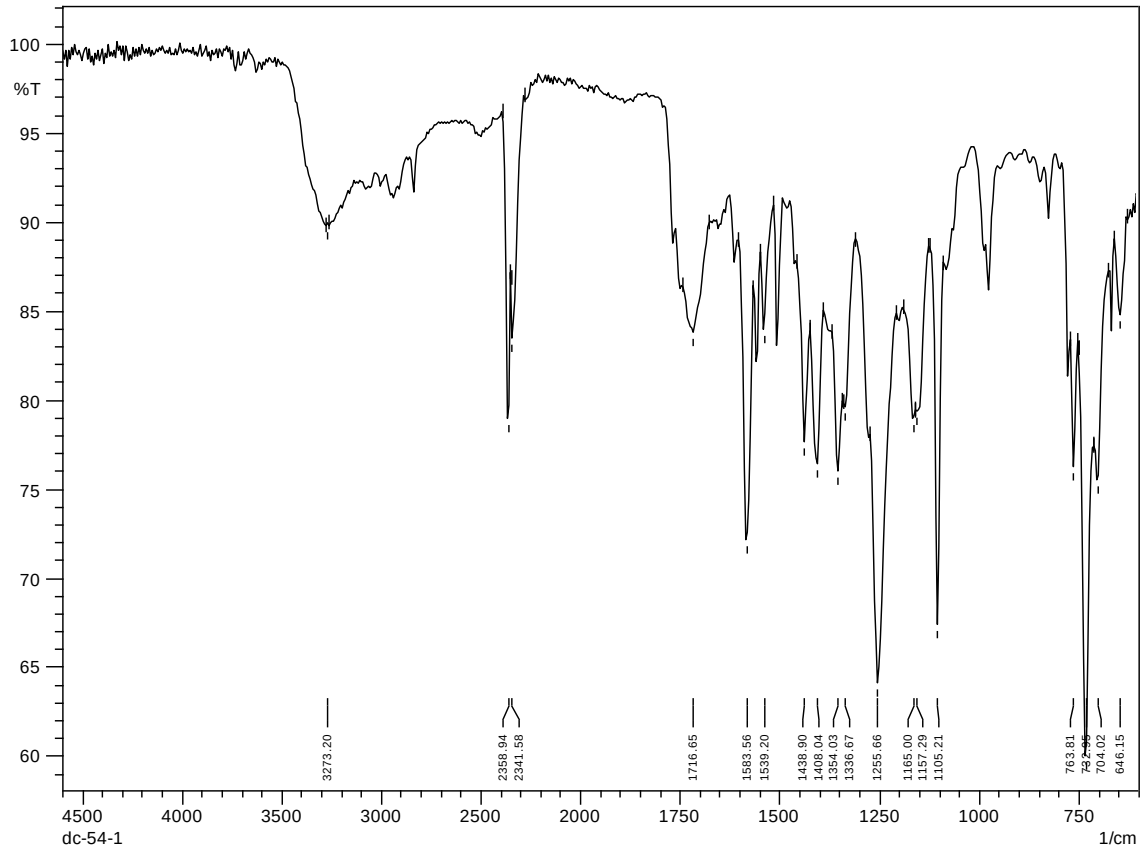
^{1}H NMR



^{13}C NMR of 189



IR of 189


100
%T
95
90
85
80
75
70
65
60
3273.20
2358.94
2341.58
1716.65
1583.56
1539.20
1438.90
1408.04
1354.03
1336.67
1255.66
1165.00
1157.29
1105.21
763.81
742.66
704.02
646.15
4500
4000
3500
3000
2500
2000
1750
1500
1250
1000
750
dc-54-1
1/cm

HRMS of 189

Bruker maXis Impact: LC-MS SmartFormula Report

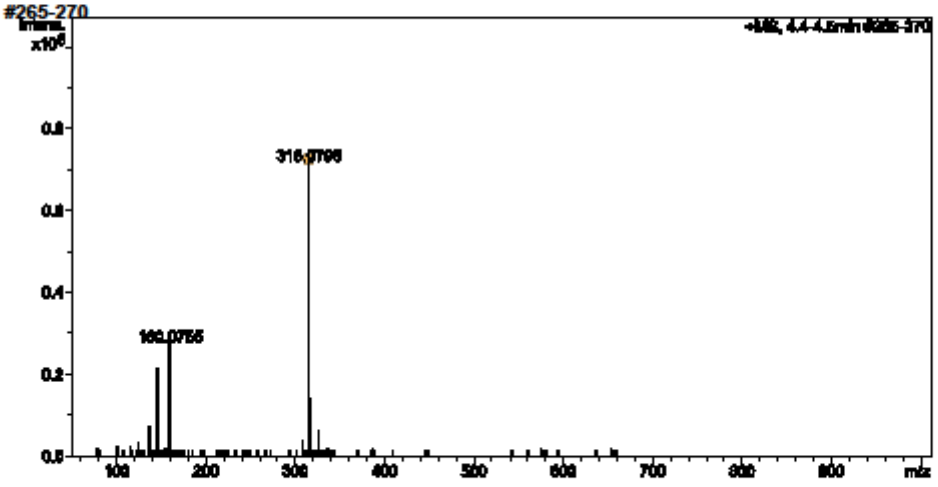
Analysis Info

Analysis Name	C:\Data\Data\N34272-64-6_1-A,7_01_1121.d	Acquisition Date	24/10/2014 15:39:57
Method	lcms pos 50-1000.m	Operator	Spectroscopy
Sample Name	N34272-64-6	Instrument / Ser	maXis impact 282001.0 0101
Comment			

Acquisition Parameter

Source Type	ESI	Scan Begin	50 m/z
Ion Polarity	Positive	Scan End	1000 m/z

+MS, 4.4-4.5min
#265-270

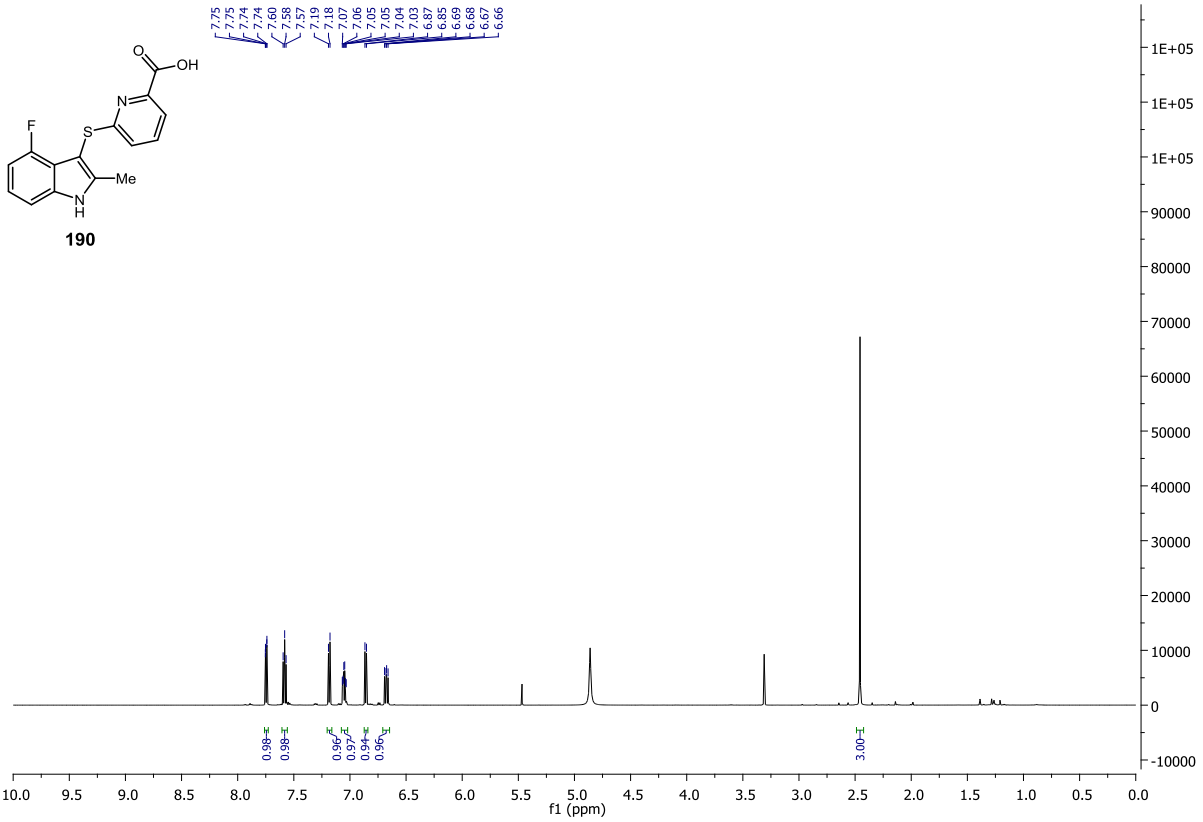


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
315.0798	1	C16H15N2O3S	315.0798	0.1	20.5	1	100.00	10.5	even	ok

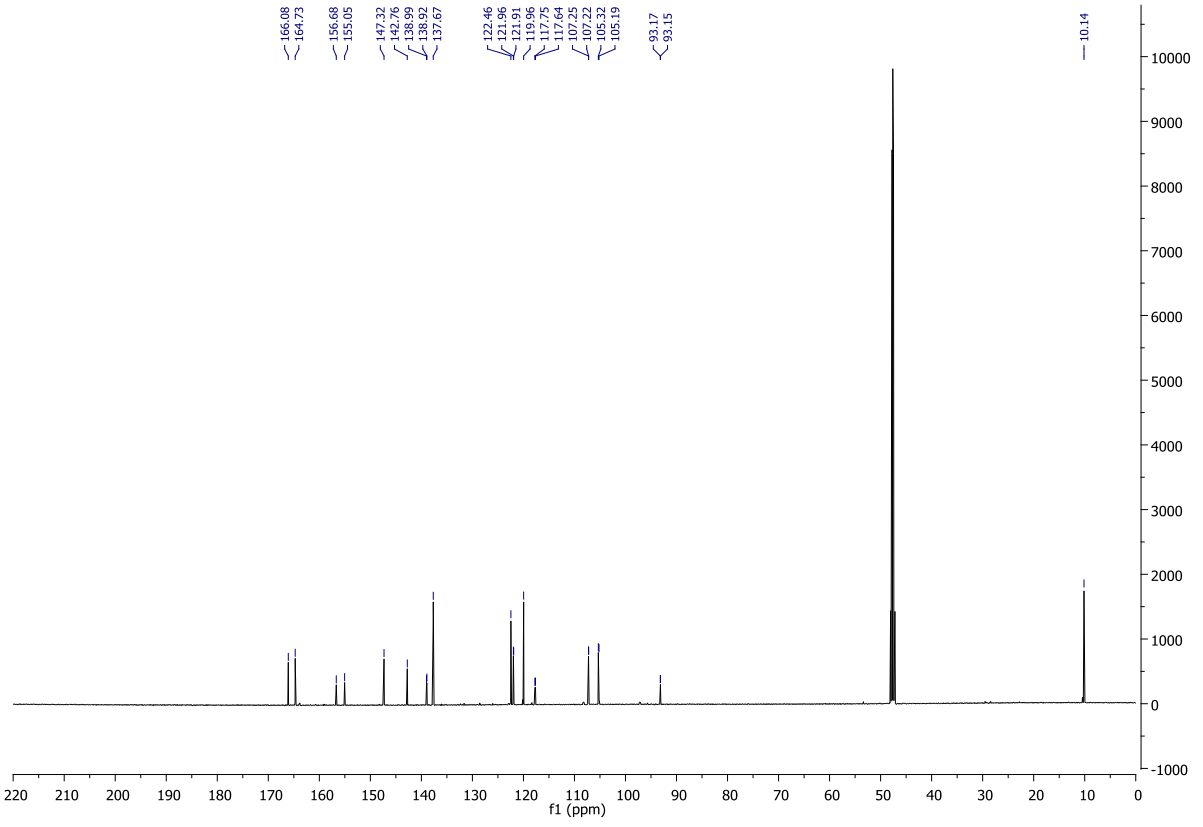
Measured mass should be within ±5 ppm of target mass

Compound 190

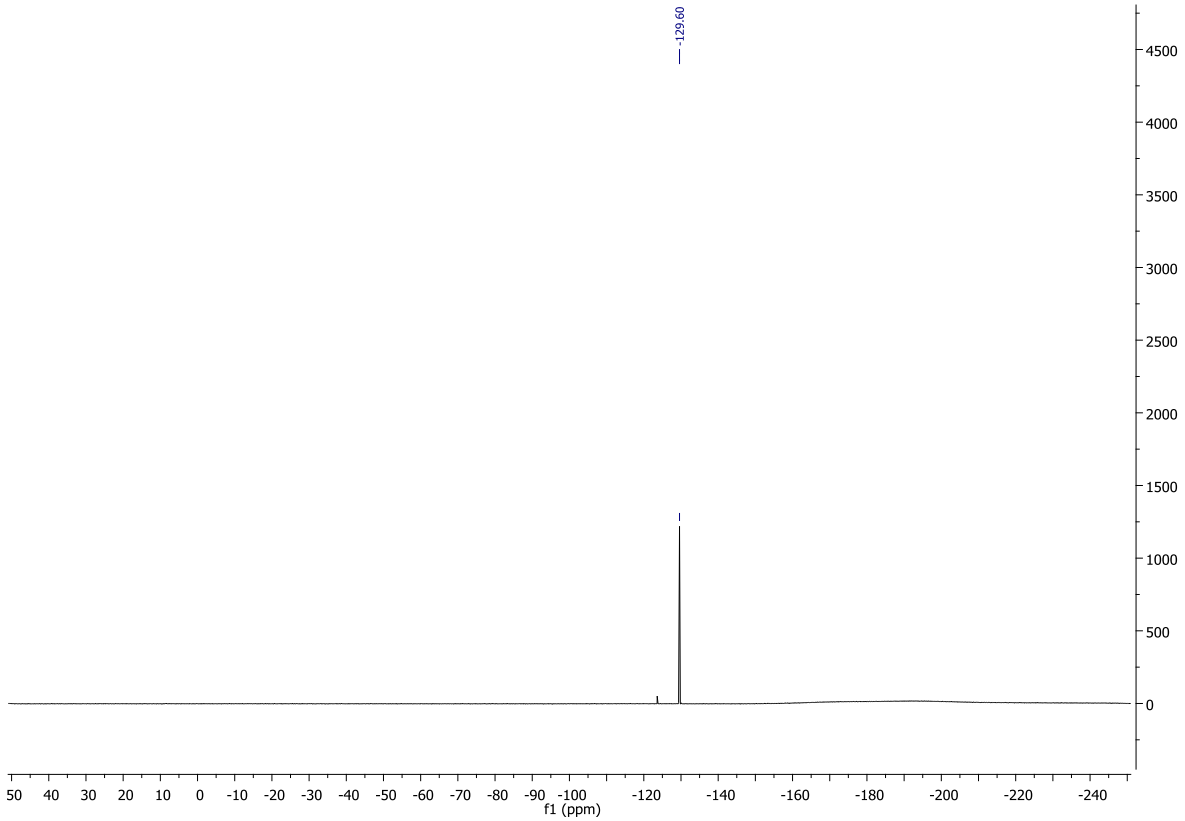
^{1}H NMR



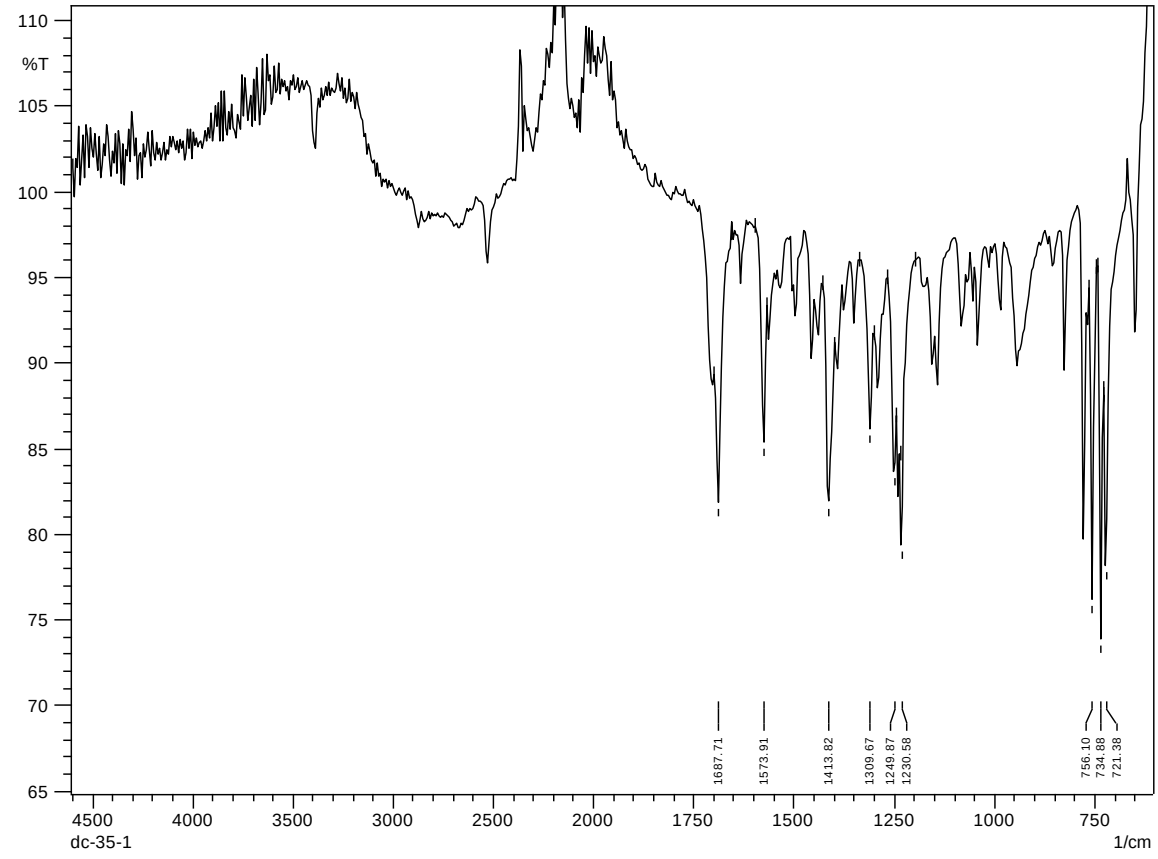
^{13}C NMR of 190



^{19}F NMR of 190

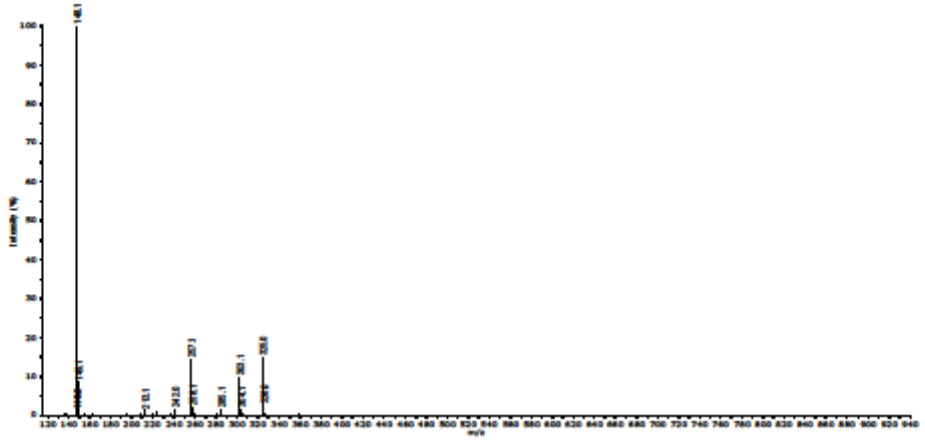


IR of 190

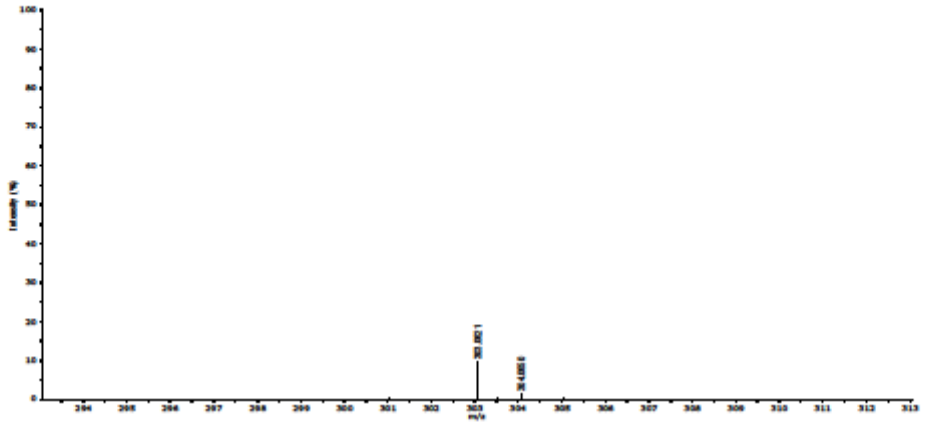


HRMS of 190

Spectrum RT 4.22, Peak [1], Target Mass 303.0598



Expanded Spectrum RT 4.22, Peak [1], Target Mass 303.0598



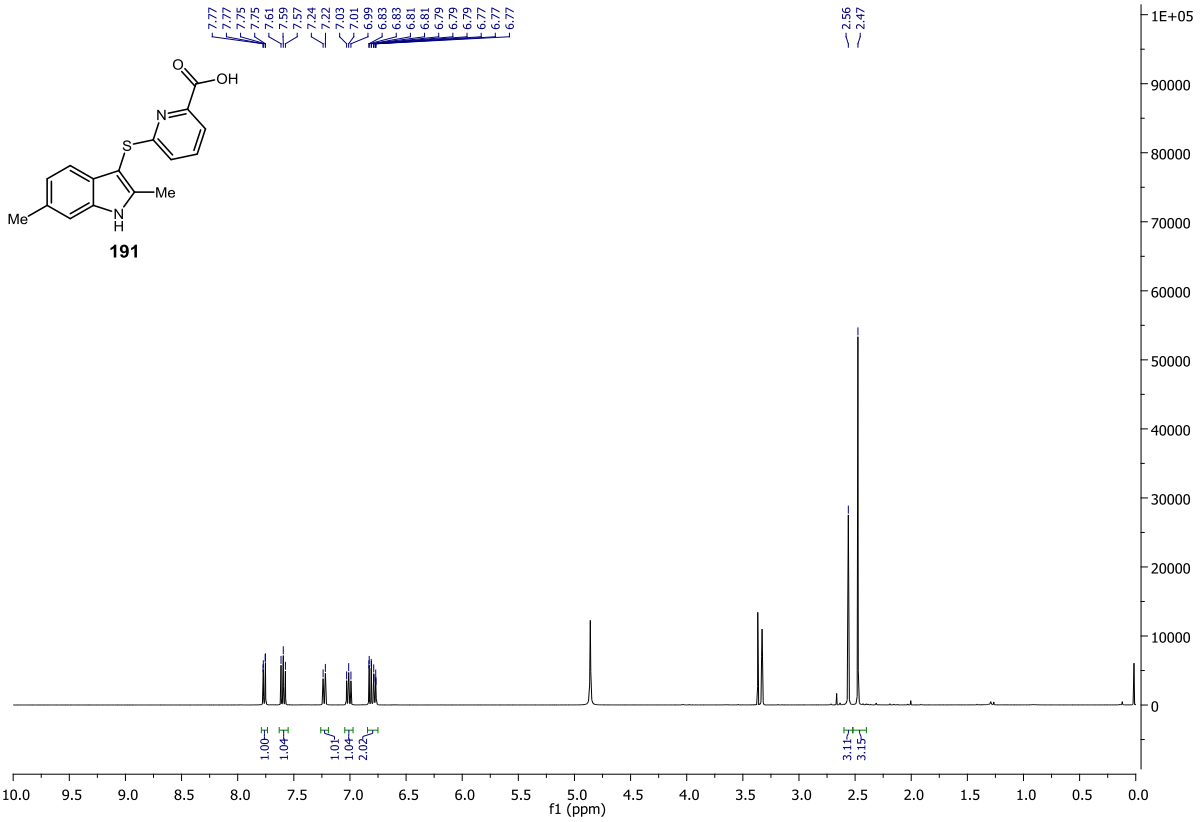
Measured Mass	Calculated Mass	Error (mDa)	Error (ppm)	Formula $[M+H]^+$
303.0596	303.0598	-0.2	-0.7	$C_{15}H_{12}FN_2O_2S$

An error of < 5ppm indicates that the measured mass is consistent with the proposed formula.

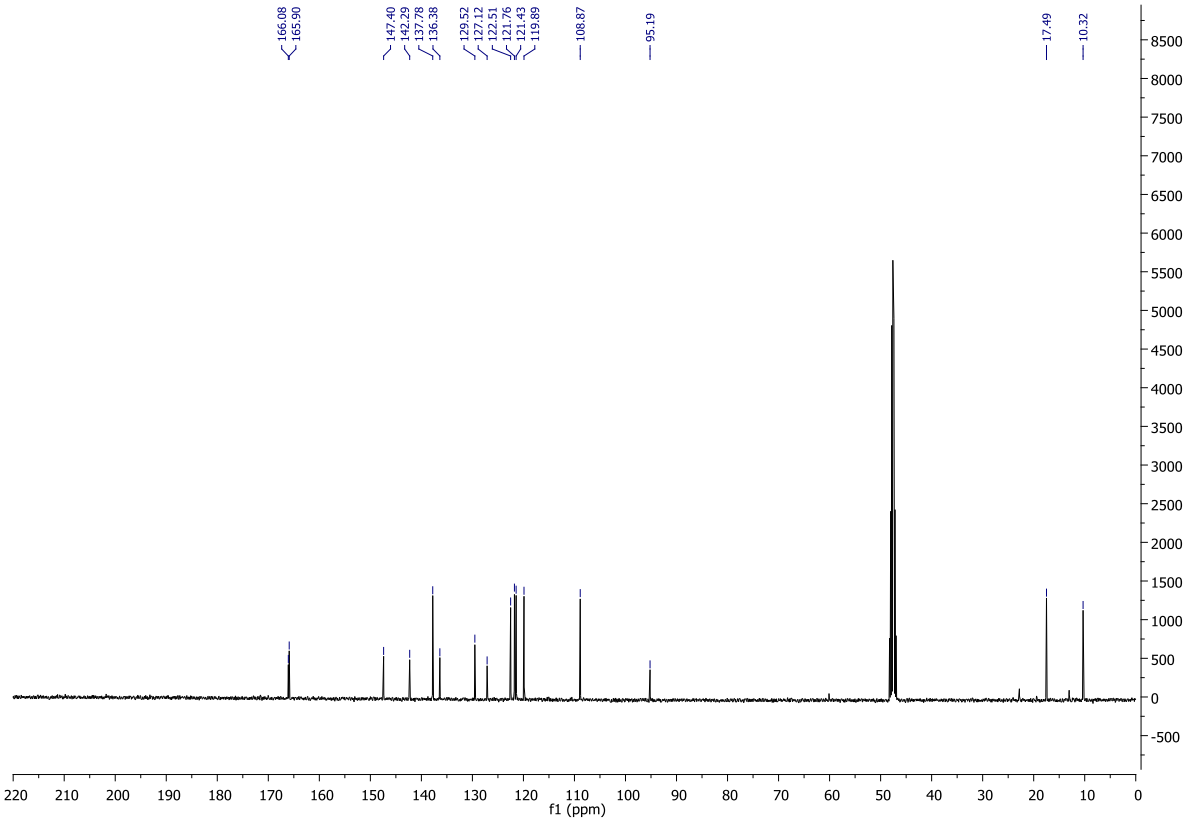
Contacts: Marco Smith #3727 or Alec Simpson #3732

Compound 191

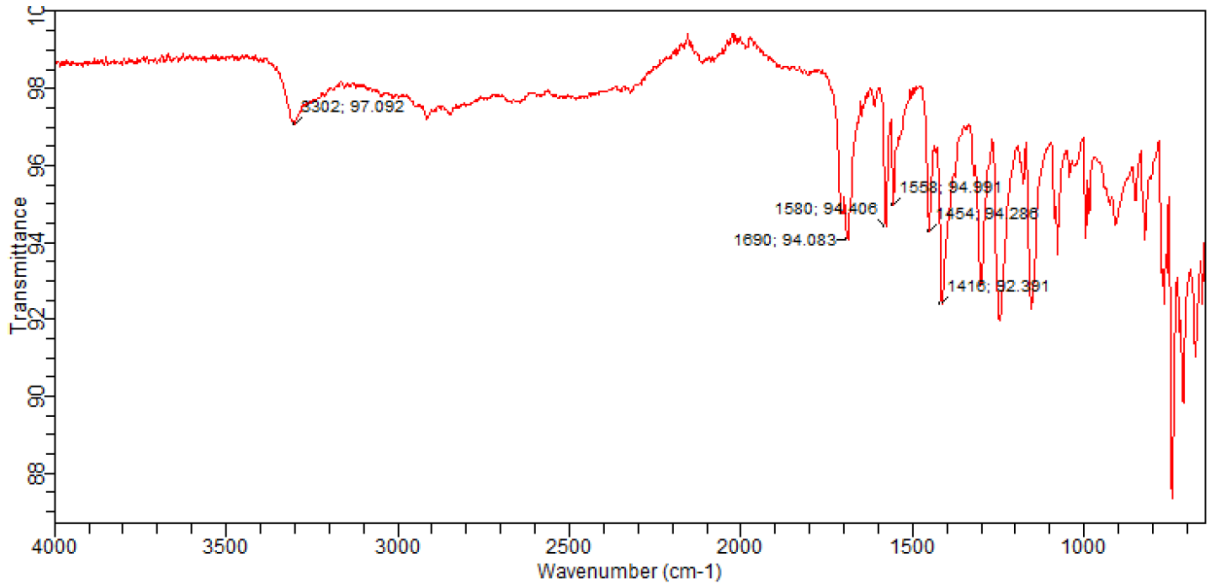
^{1}H NMR



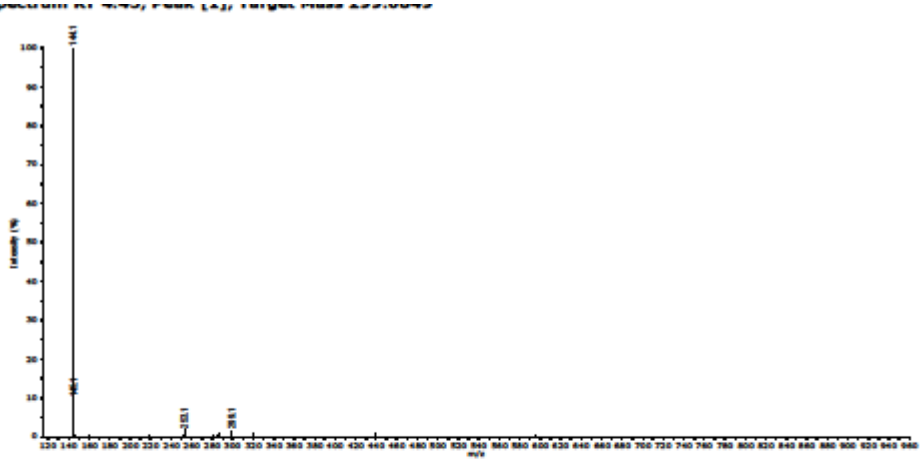
^{13}C NMR of 191



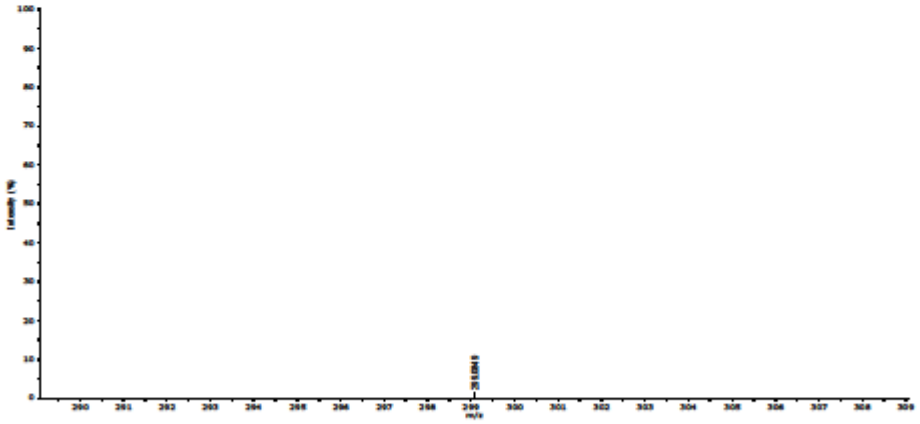
IR of 191


Transmittance
Wavenumber (cm-1)
4000
3500
3000
2500
2000
1500
1000
98
96
94
92
90
88
3302; 97.092
1690; 94.083
1580; 94.406
1558; 94.991
1454; 94.286
1416; 92.391

HRMS of 191



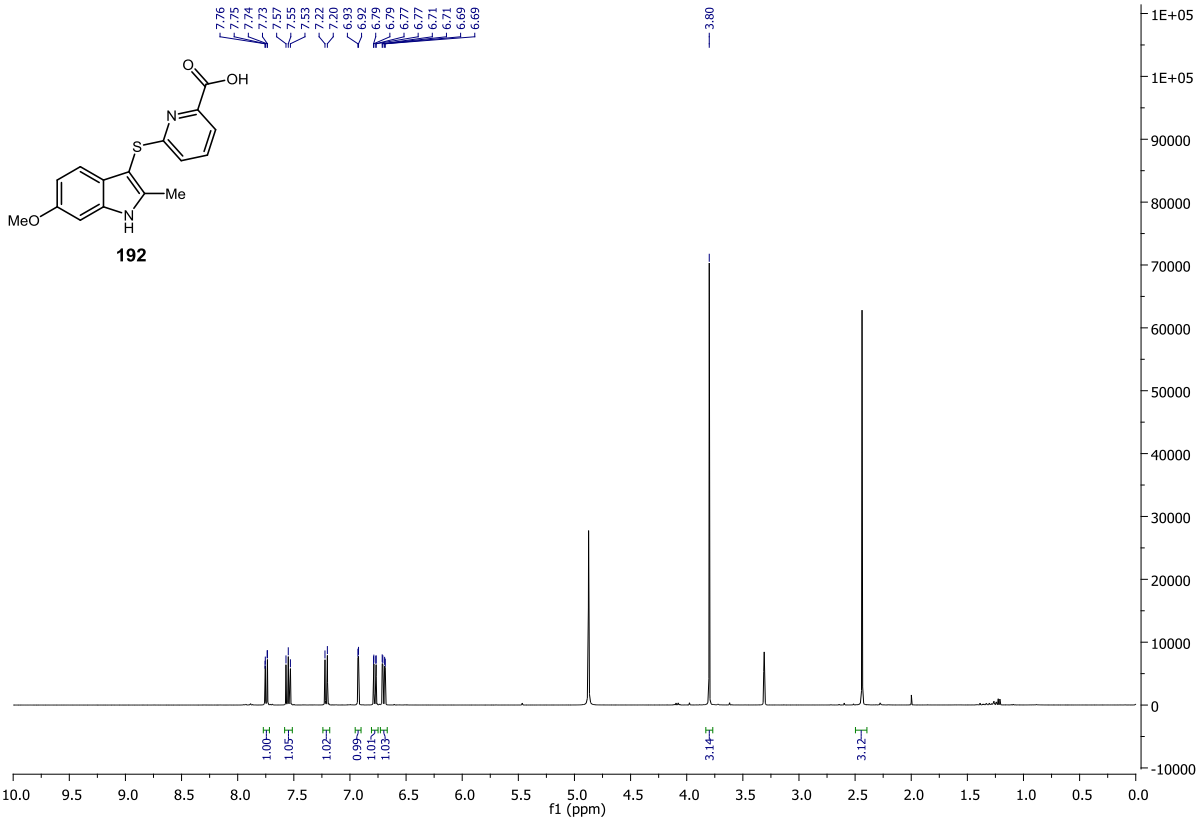
Expanded Spectrum RT 4.45, Peak [1], Target Mass 299.0849



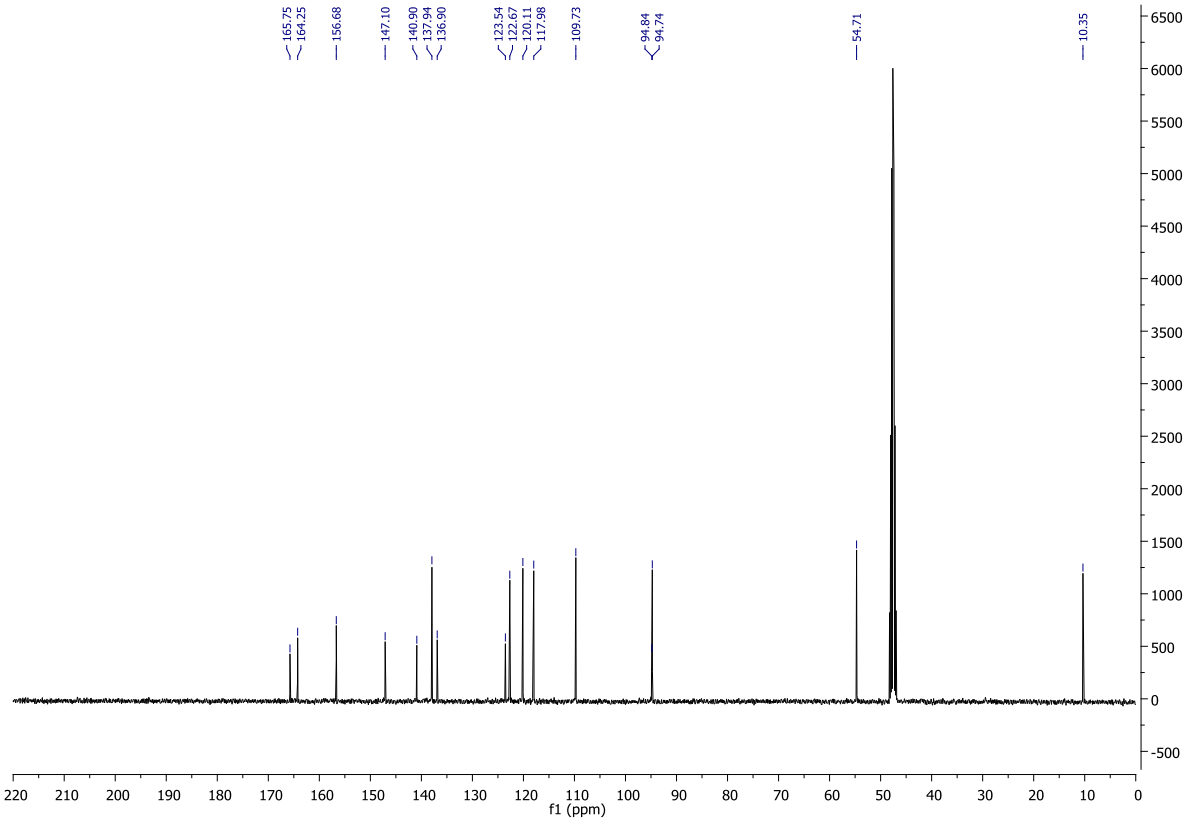
Measured Mass	Calculated Mass	Error (mDa)	Error (ppm)	Formula $[M+H]^+$
299.0849	299.0849	0.0	0.0	$C_{16}H_{15}N_2O_2S$

Compound 192

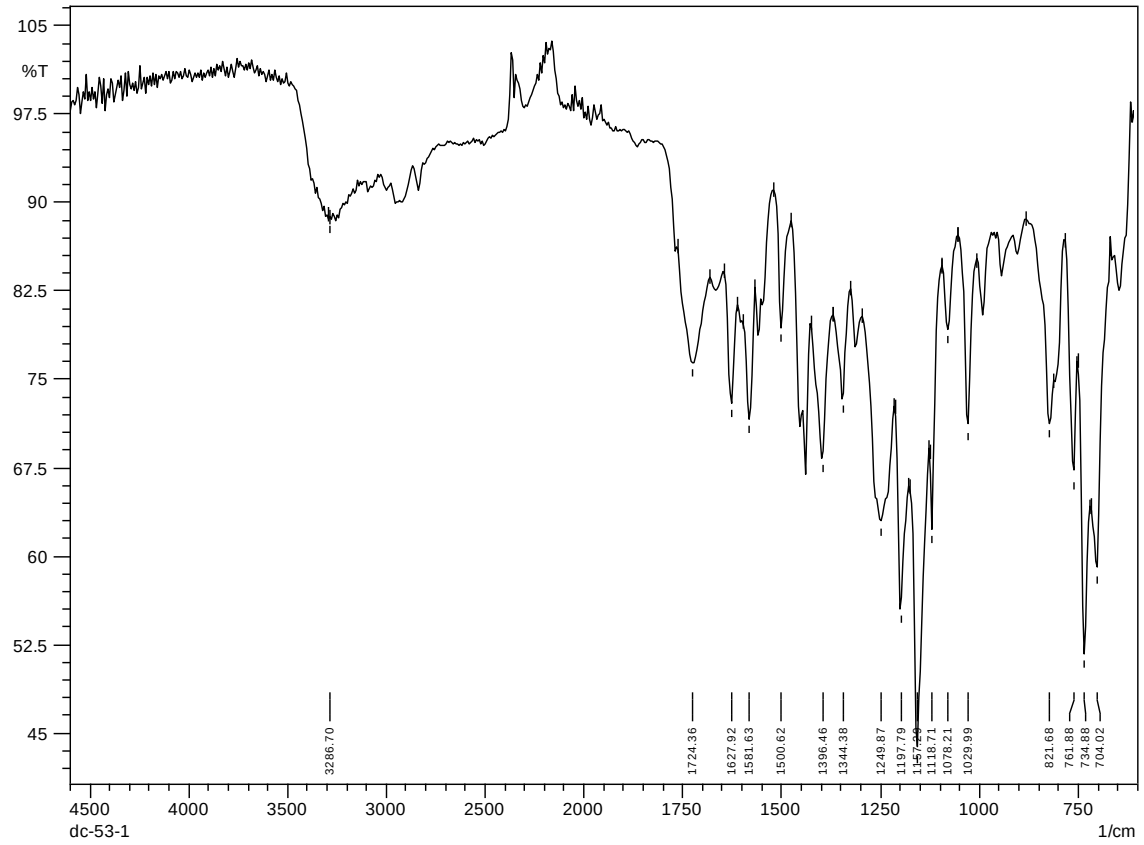
^{1}H NMR



^{13}C NMR of 192



IR of 192


105
%T
97.5
90
82.5
75
67.5
60
52.5
45
3286.70
1724.36
1627.92
1581.63
1500.62
1396.46
1344.38
1249.87
1197.79
1157.29
1118.71
1078.21
1029.99
821.68
761.88
734.88
704.02
4500
4000
3500
3000
2500
2000
1750
1500
1250
1000
750
dc-53-1
1/cm

HRMS of 192

Bruker maXis Impact: LC-MS SmartFormula Report

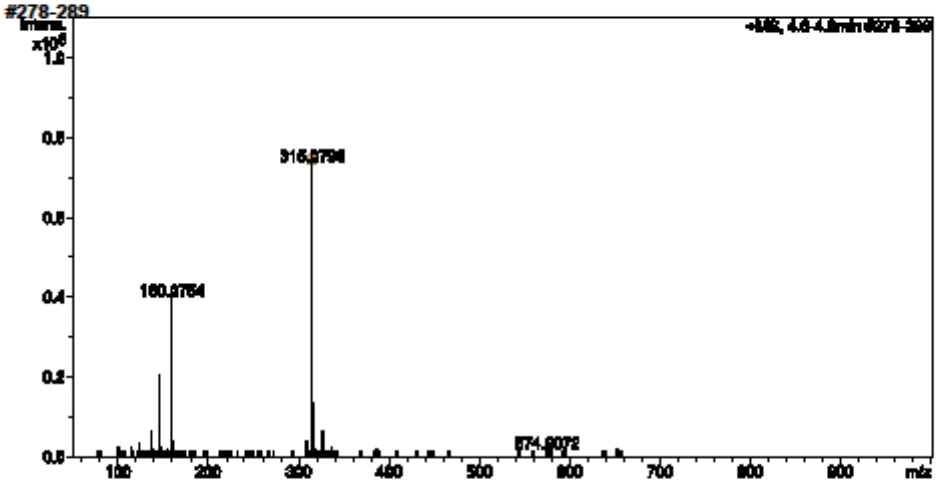
Analysis Info

Analysis Name	C:\Data\Data\N34272-64-5_1-A,6_01_1120.d	Acquisition Date	24/10/2014 15:29:12
Method	lcms pos 50-1000.m	Operator	Spectroscopy
Sample Name	N34272-64-5	Instrument / Ser	maXis impact 282001.00101
Comment			

Acquisition Parameter

Source Type	ESI	Scan Begin	50 m/z
Ion Polarity	Positive	Scan End	1000 m/z

+MS, 4.6-4.8min
#278-289

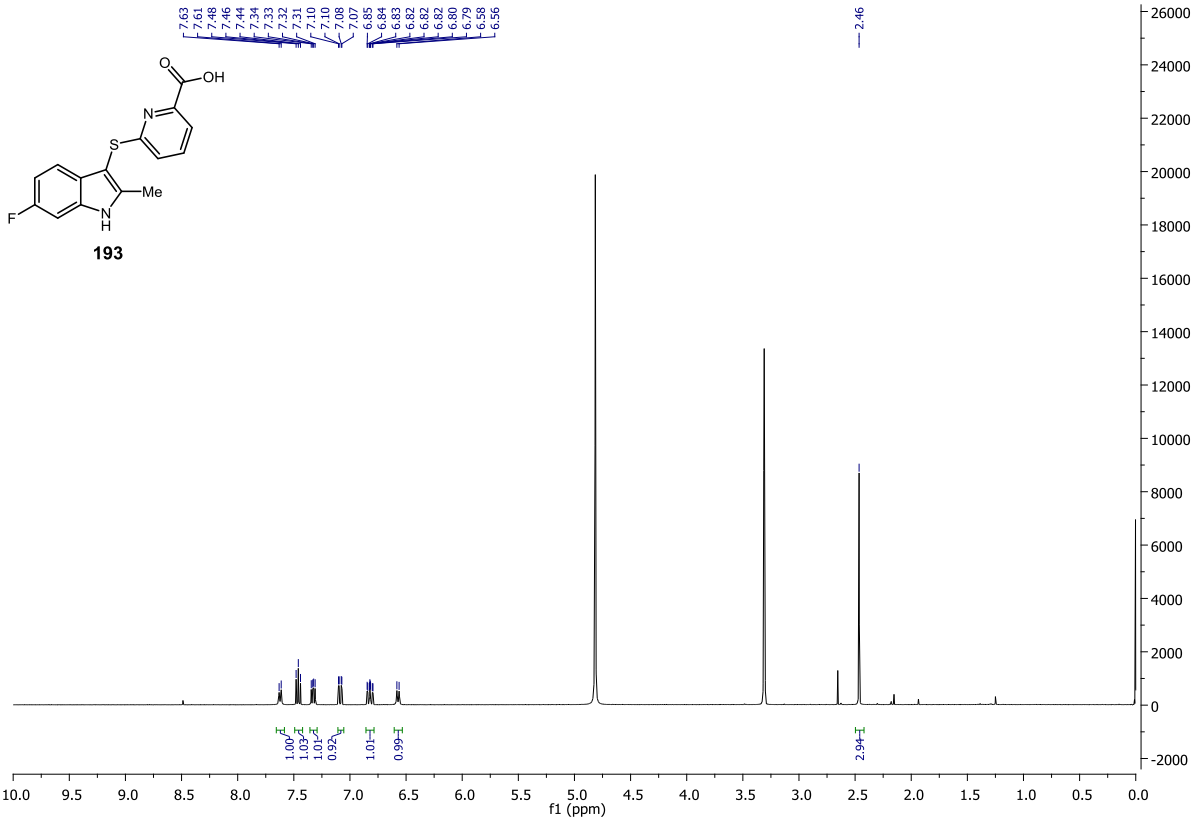


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
315.0798	1	C16H15N2O3S	315.0798	-0.1	21.8	1	100.00	10.5	even	ok

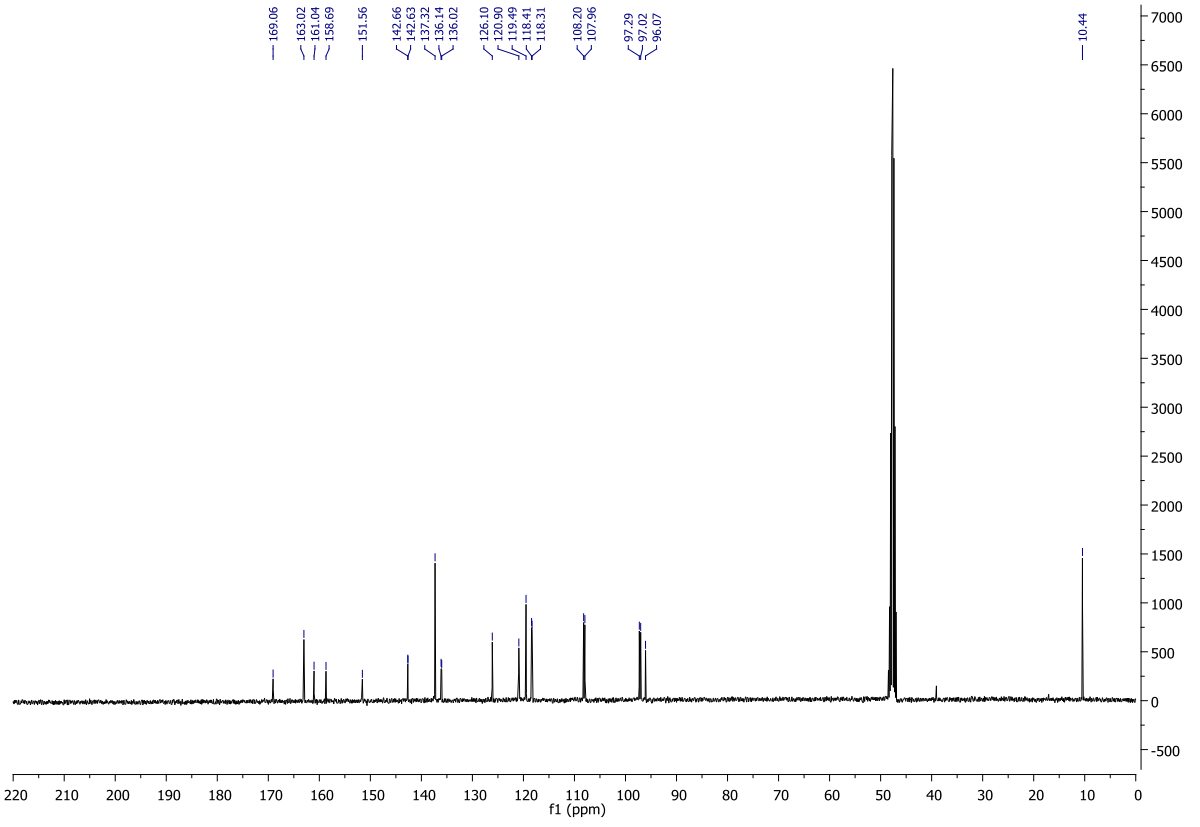
Measured mass should be within ±5 ppm of target mass

Compound 193

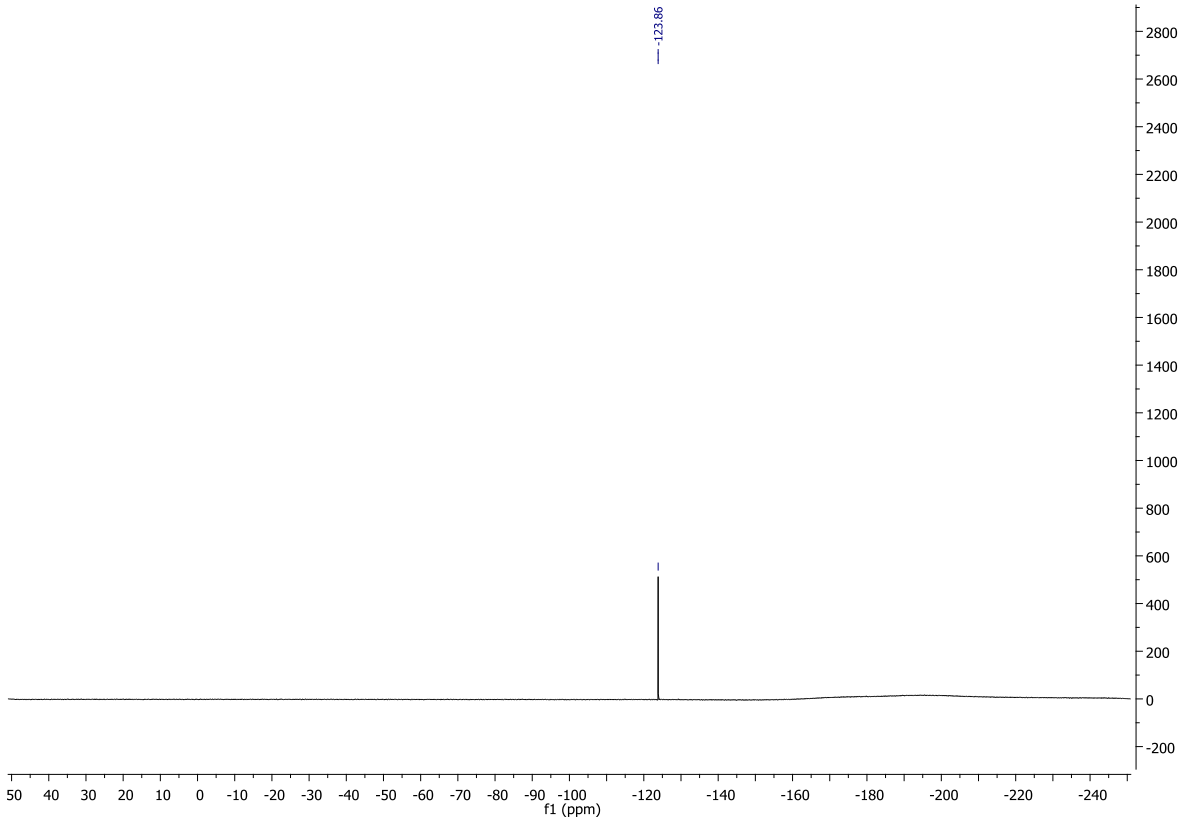
^{1}H NMR



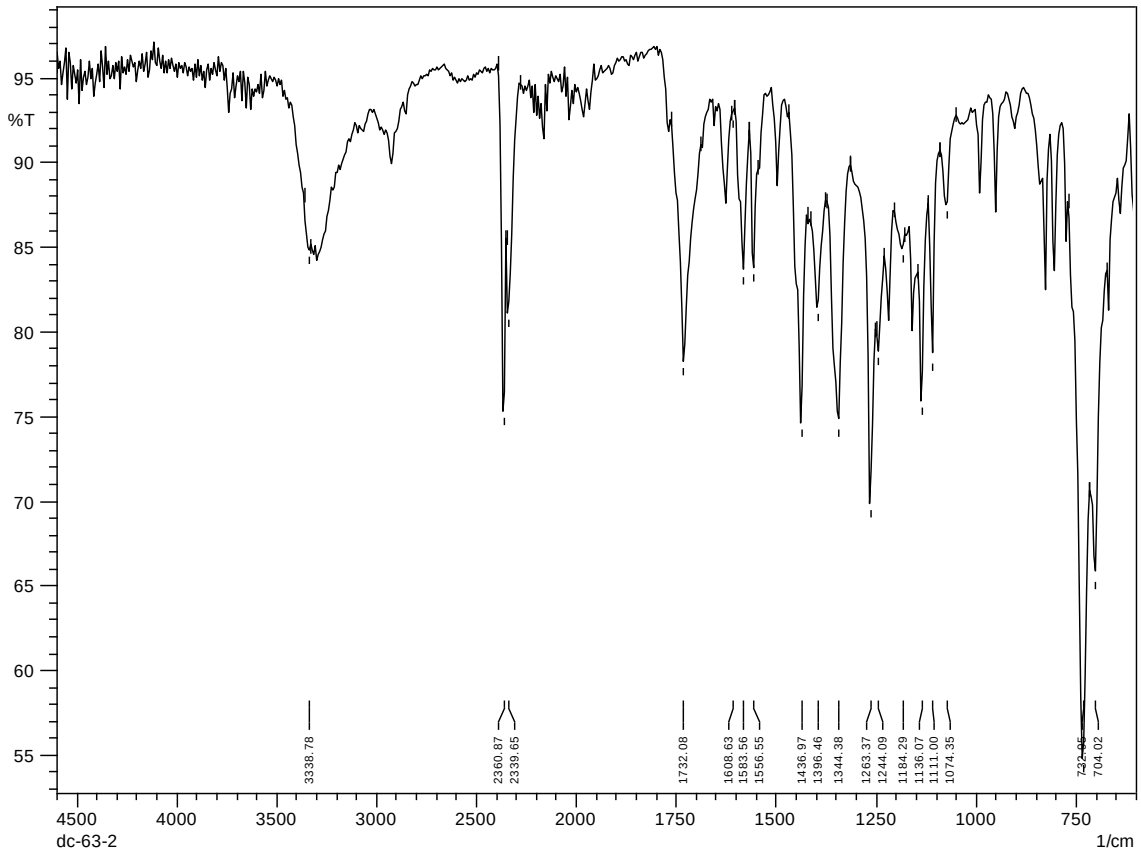
^{13}C NMR of 193



^{19}F NMR of 193



IR of 193



HRMS of 193

Bruker maXis Impact: LC-MS SmartFormula Report

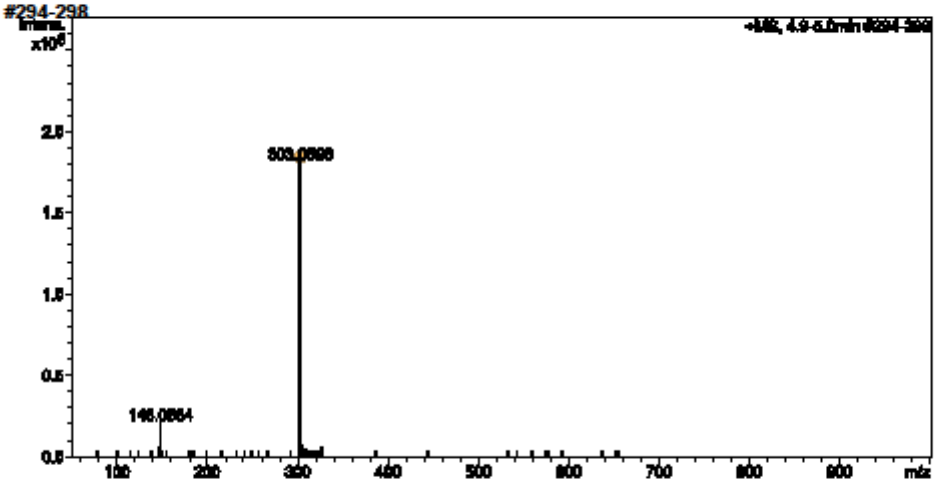
Analysis Info

Analysis Name	C:\Data\Data\N34272-64-1_1-A,2_01_1116.d	Acquisition Date	24/10/2014 14:46:10
Method	lcms pos 50-1000.m	Operator	Spectroscopy
Sample Name	N34272-64-1	Instrument / Ser	maXis impact 282001.0 0101
Comment			

Acquisition Parameter

Source Type	ESI	Scan Begin	50 m/z
Ion Polarity	Positive	Scan End	1000 m/z

+MS, 4.9-5.0min
#294-298

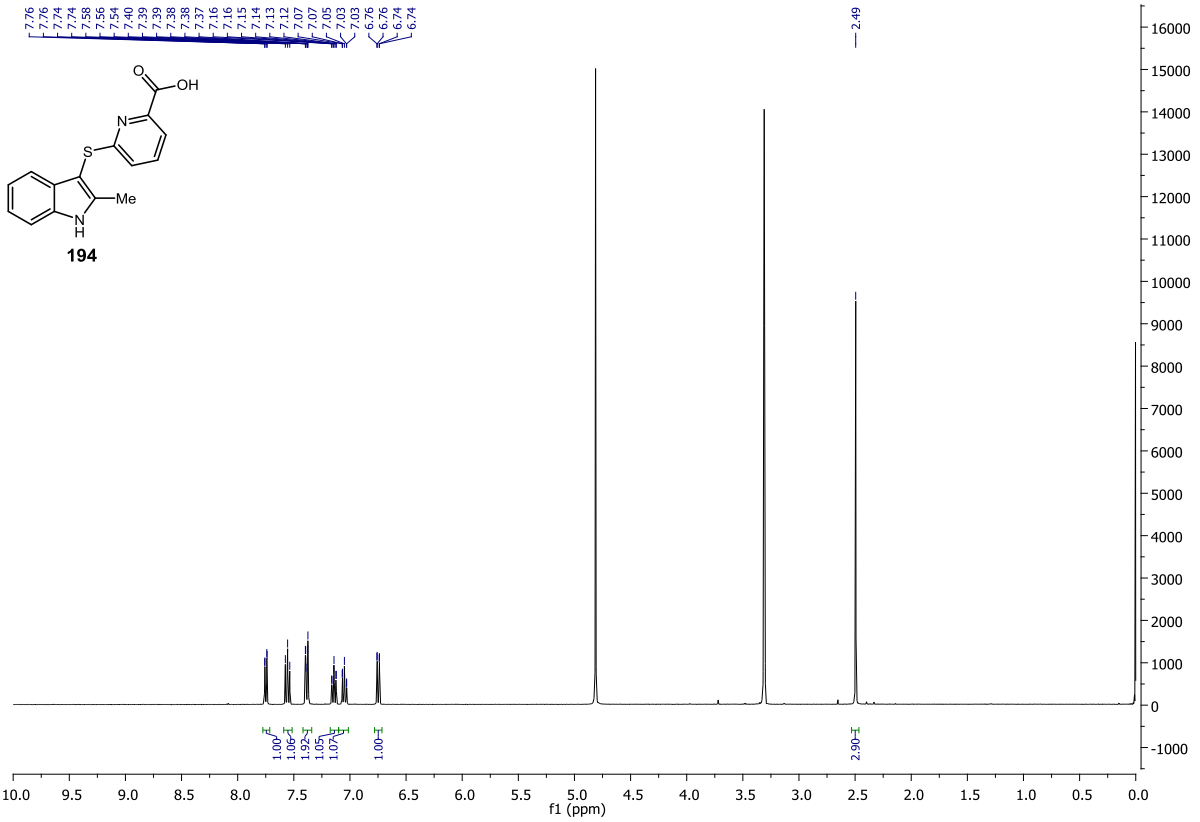


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
303.0596	1	C15H12FN2O2S	303.0598	-0.6	37.6	1	100.00	10.5	even	ok

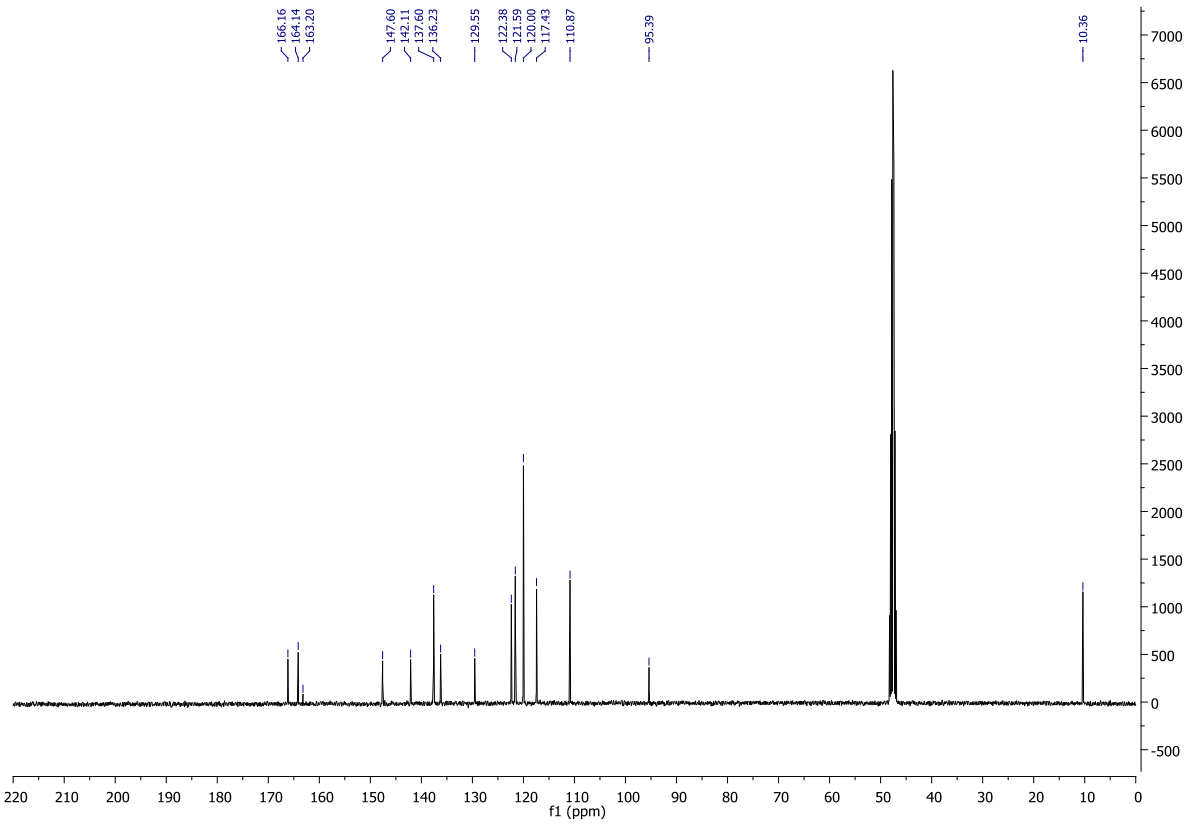
Measured mass should be within ±5 ppm of target mass

Compound 194

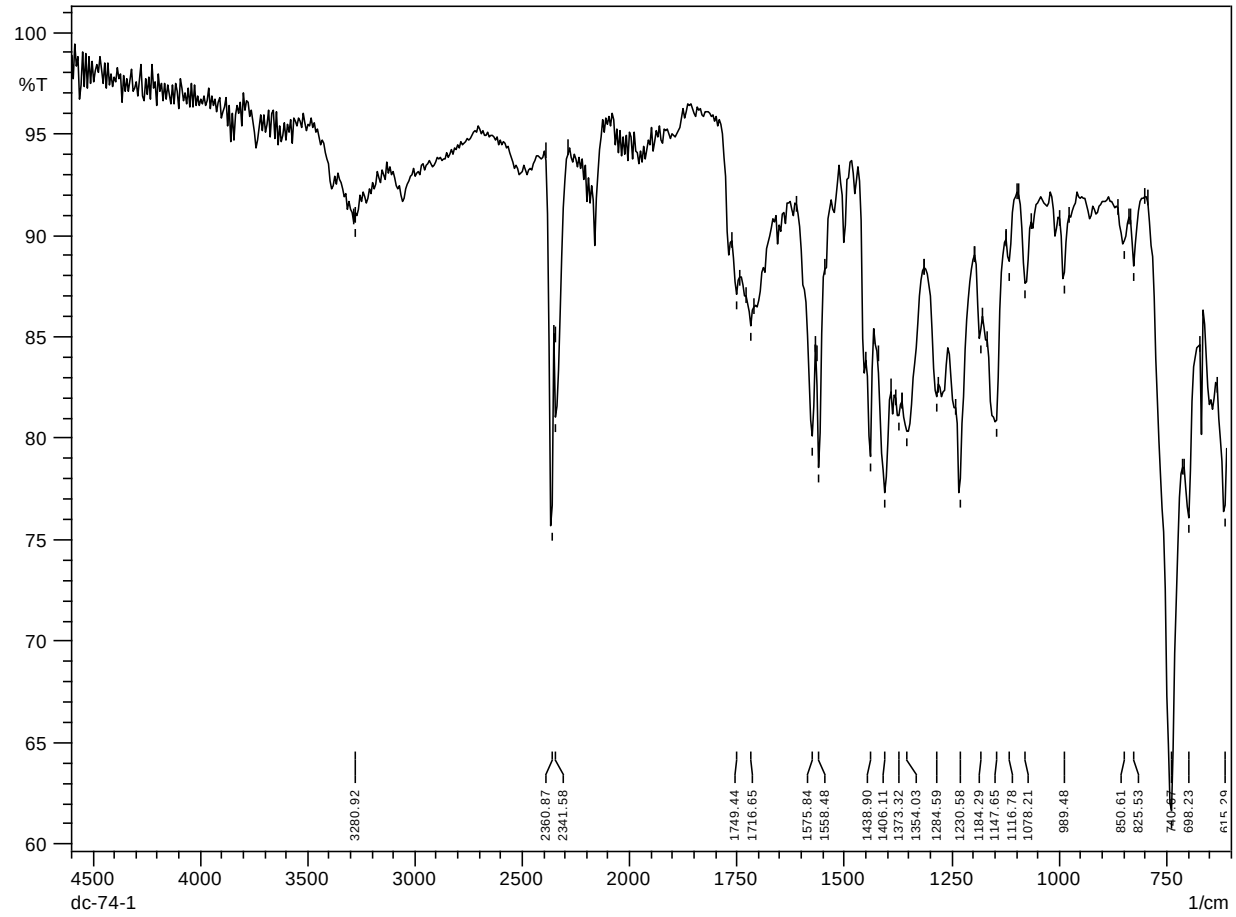
^{1}H NMR



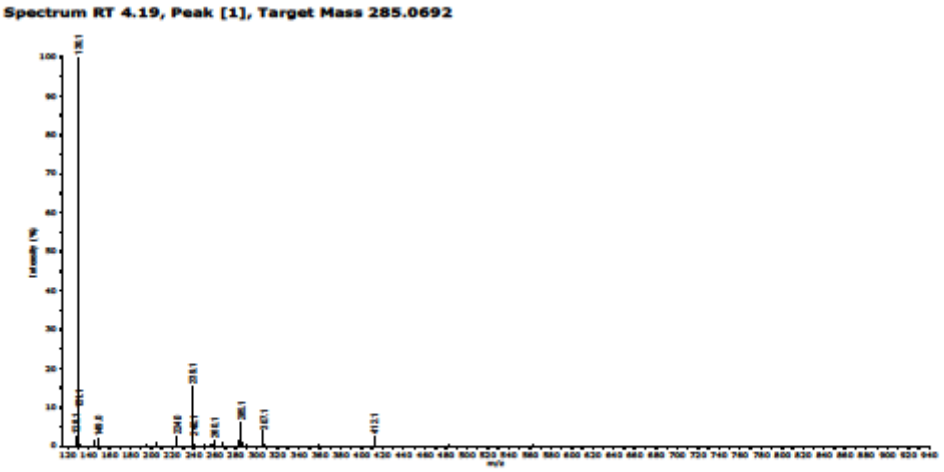
^{13}C NMR of 194

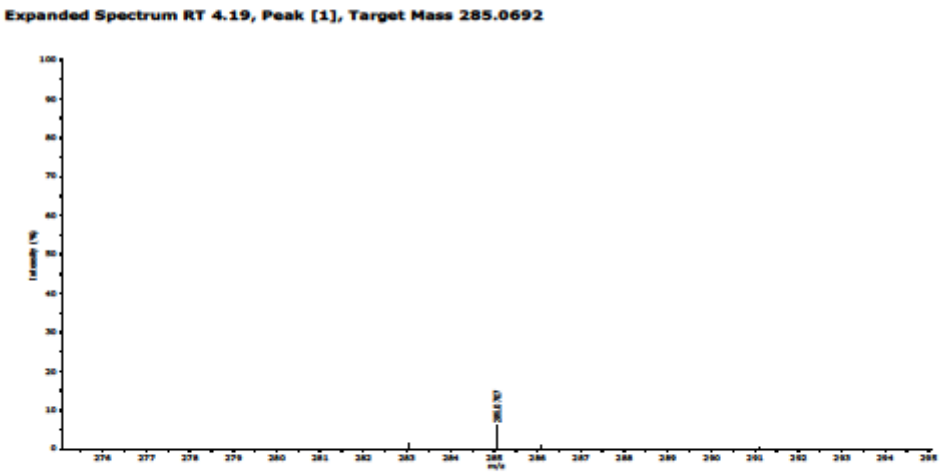


IR of 194


100
%T
95
90
85
80
75
70
65
60
3280.92
2360.87
2341.58
1749.44
1716.65
1575.84
1558.48
1438.90
1406.11
1373.32
1354.03
1284.59
1230.58
1184.29
1147.65
1116.78
1078.21
989.48
850.61
825.53
698.23
4500
4000
3500
3000
2500
2000
1750
1500
1250
1000
750
dc-74-1
1/cm

HRMS of 194

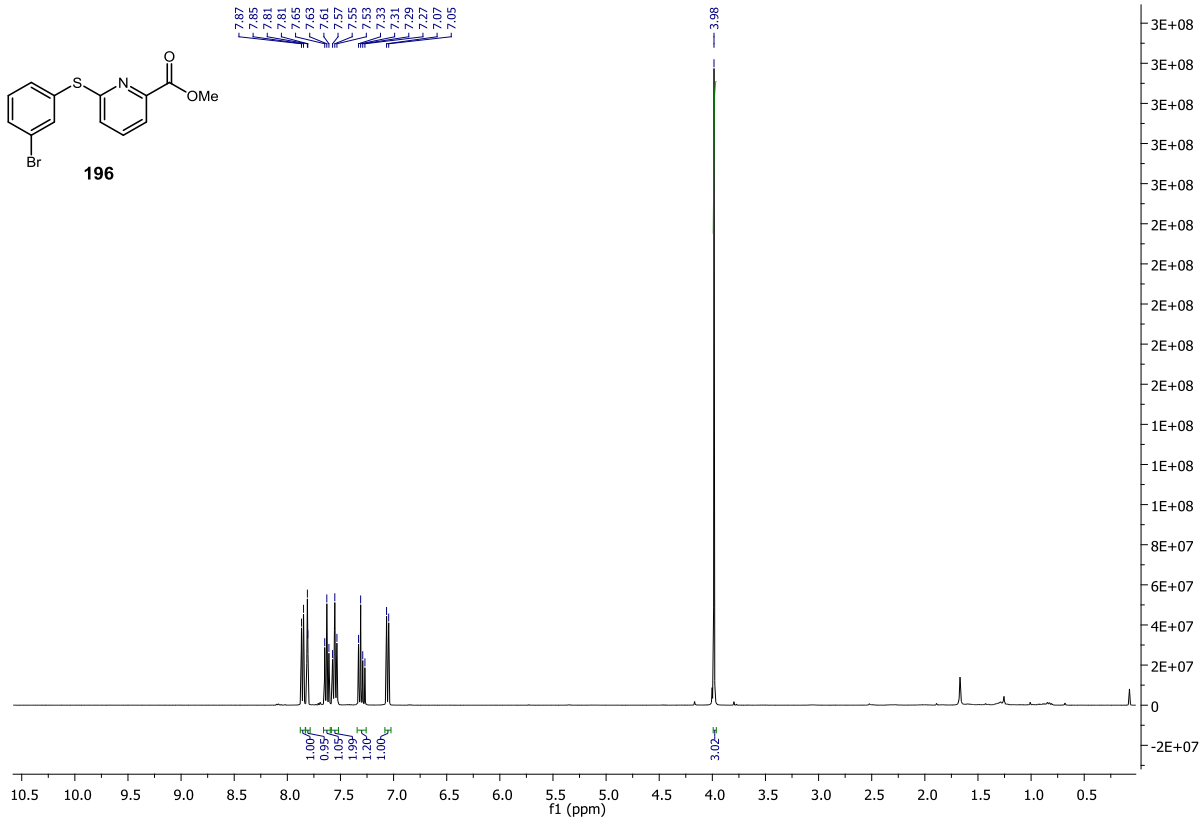




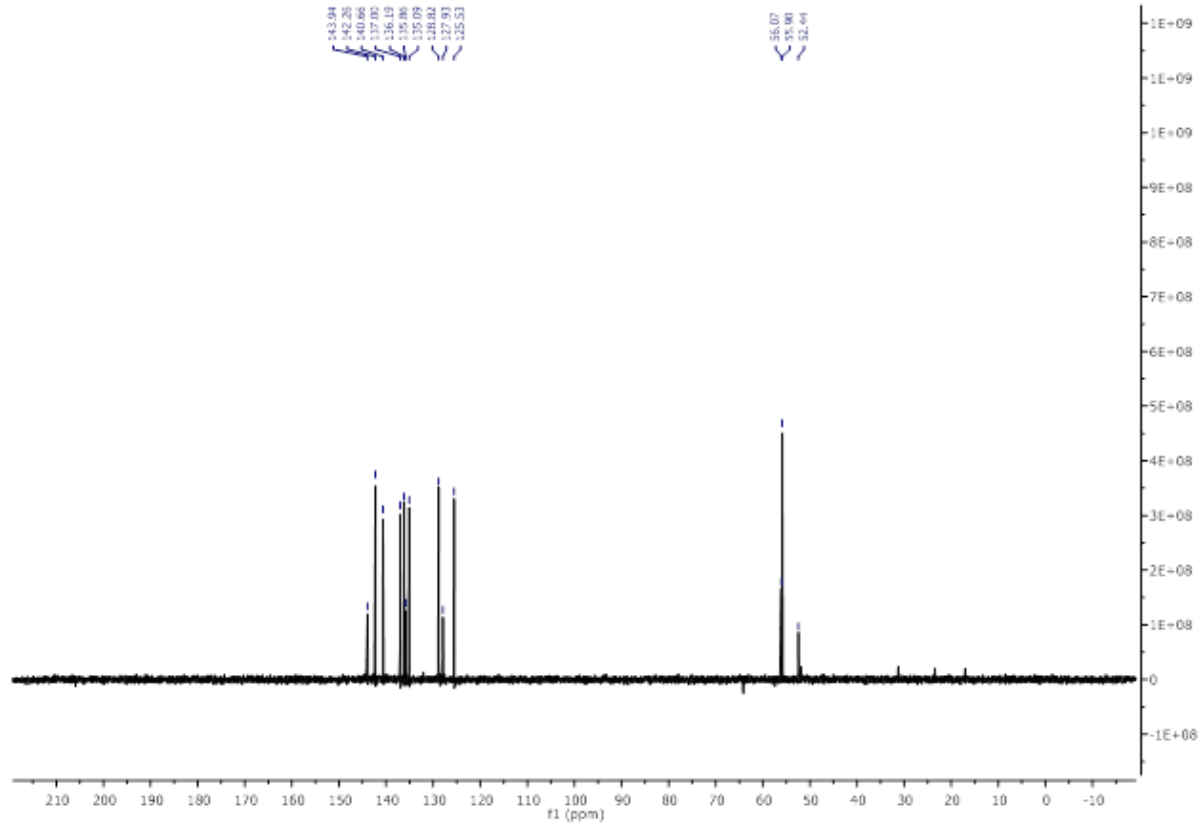
Measured Mass	Calculated Mass	Error (mDa)	Error (ppm)	Formula $[M+H]^+$
285.0693	285.0692	0.1	0.2	$C_{15}H_{13}N_2O_2S$

Compound 196

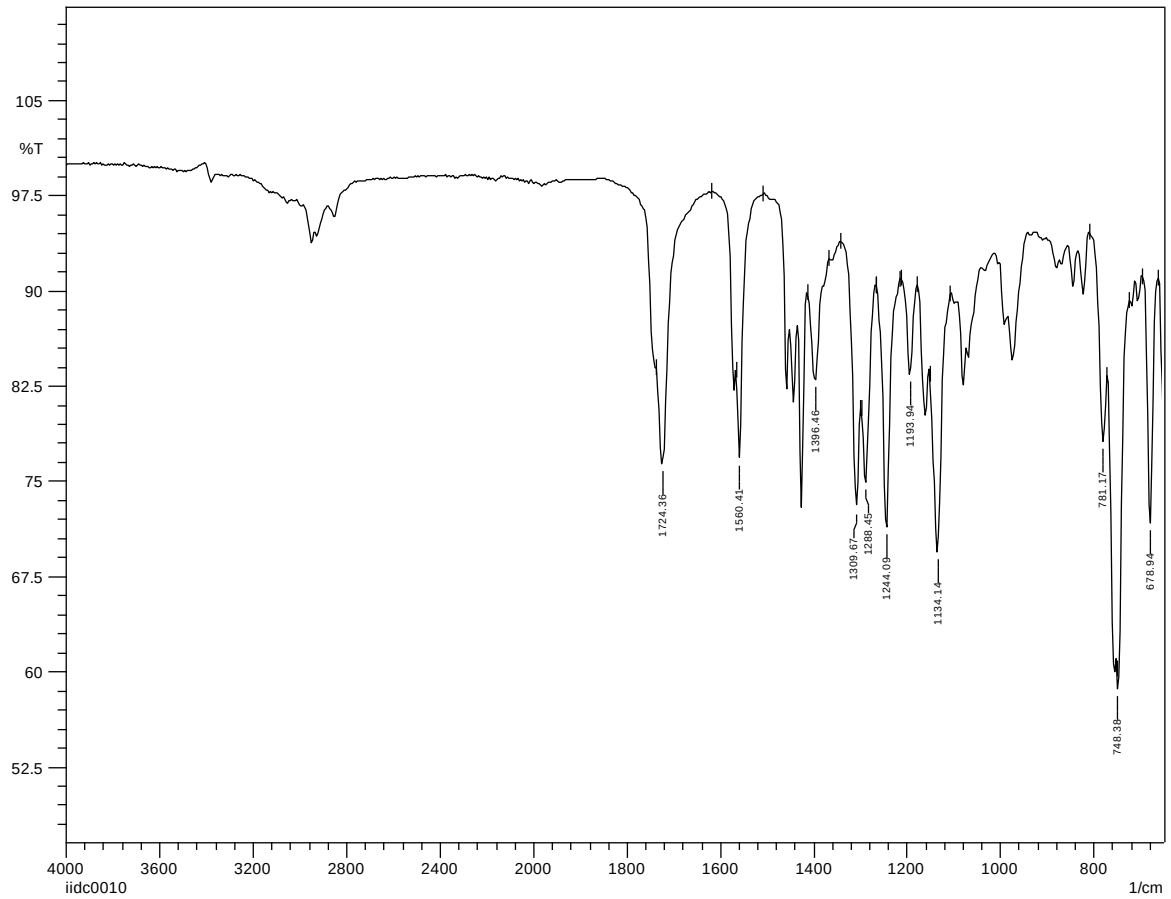
^{1}H NMR



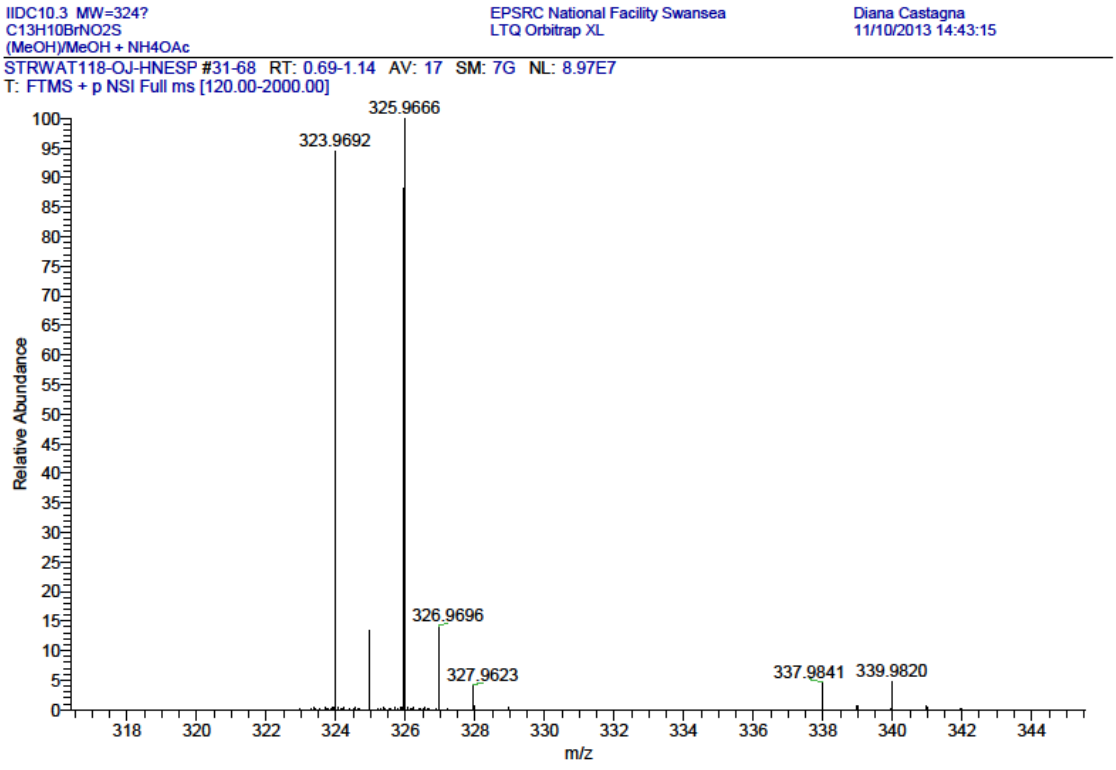
^{13}C NMR of 196



IR of 196

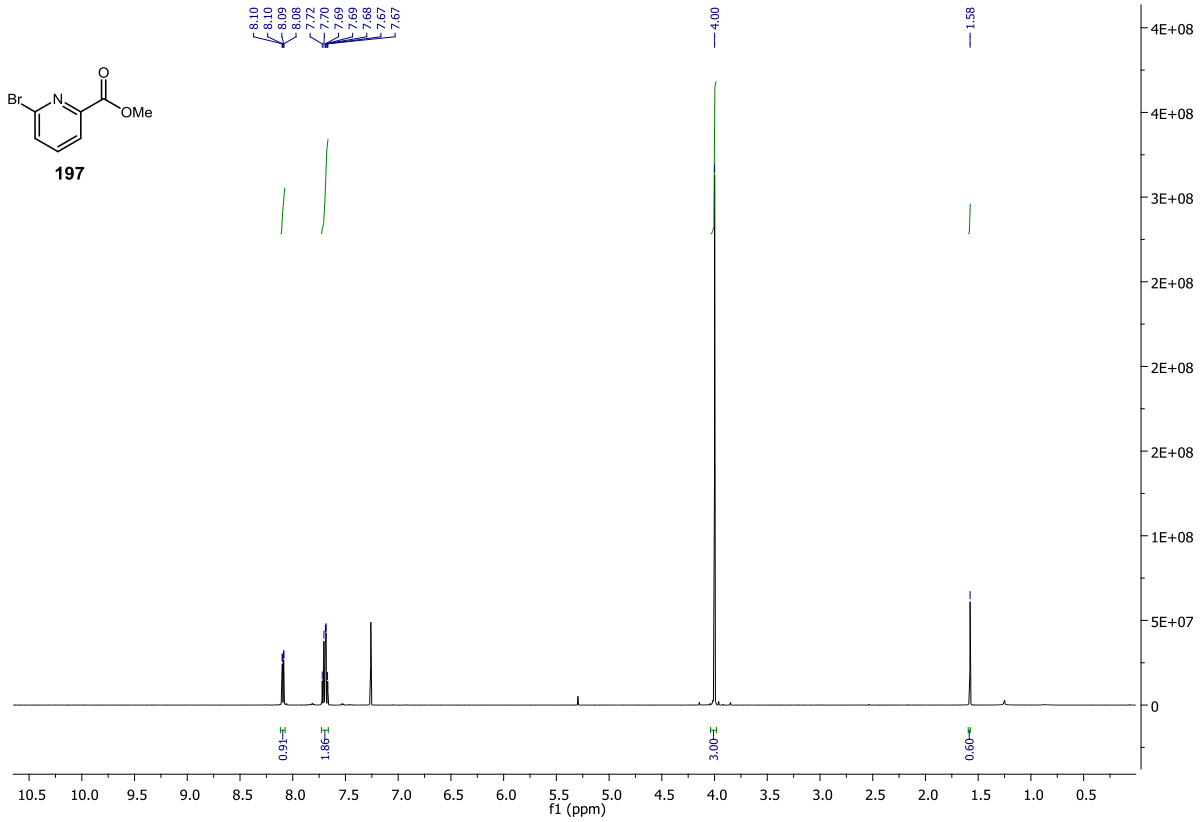


HRMS of 196

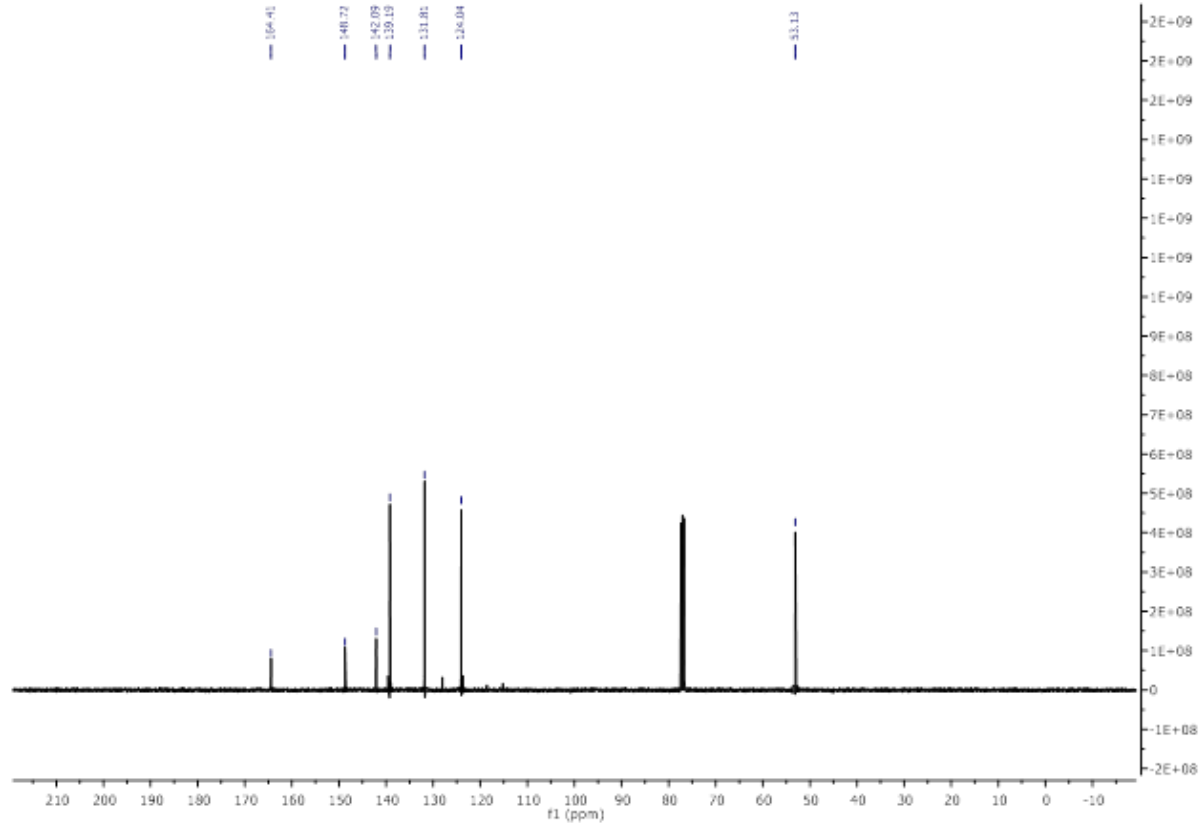


Compound 197

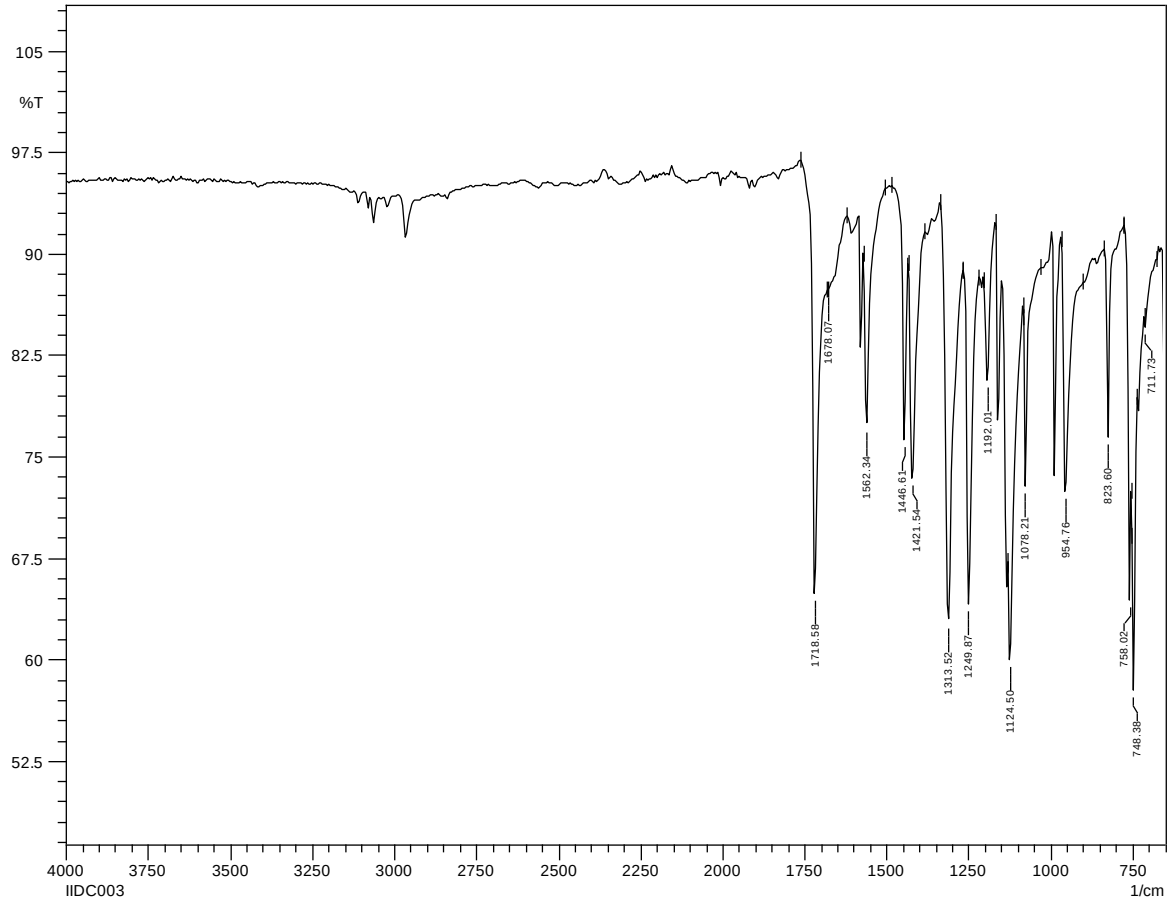
^{1}H NMR



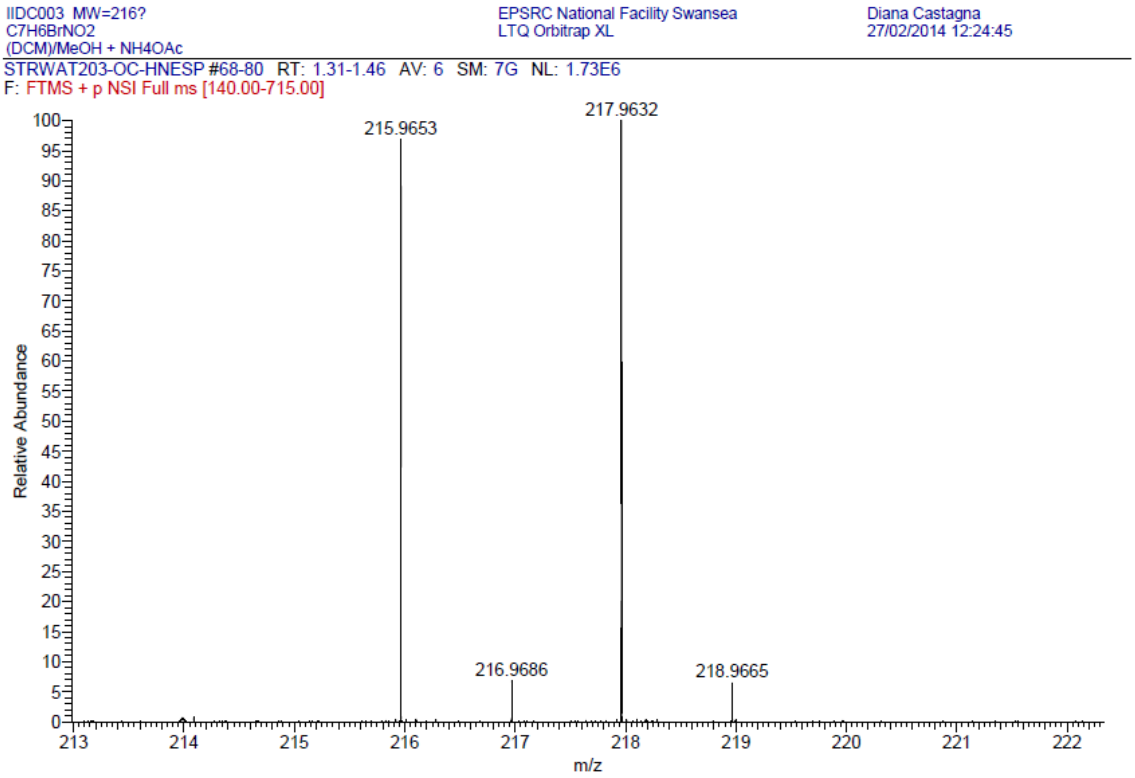
^{13}C NMR of 197



IR of 197

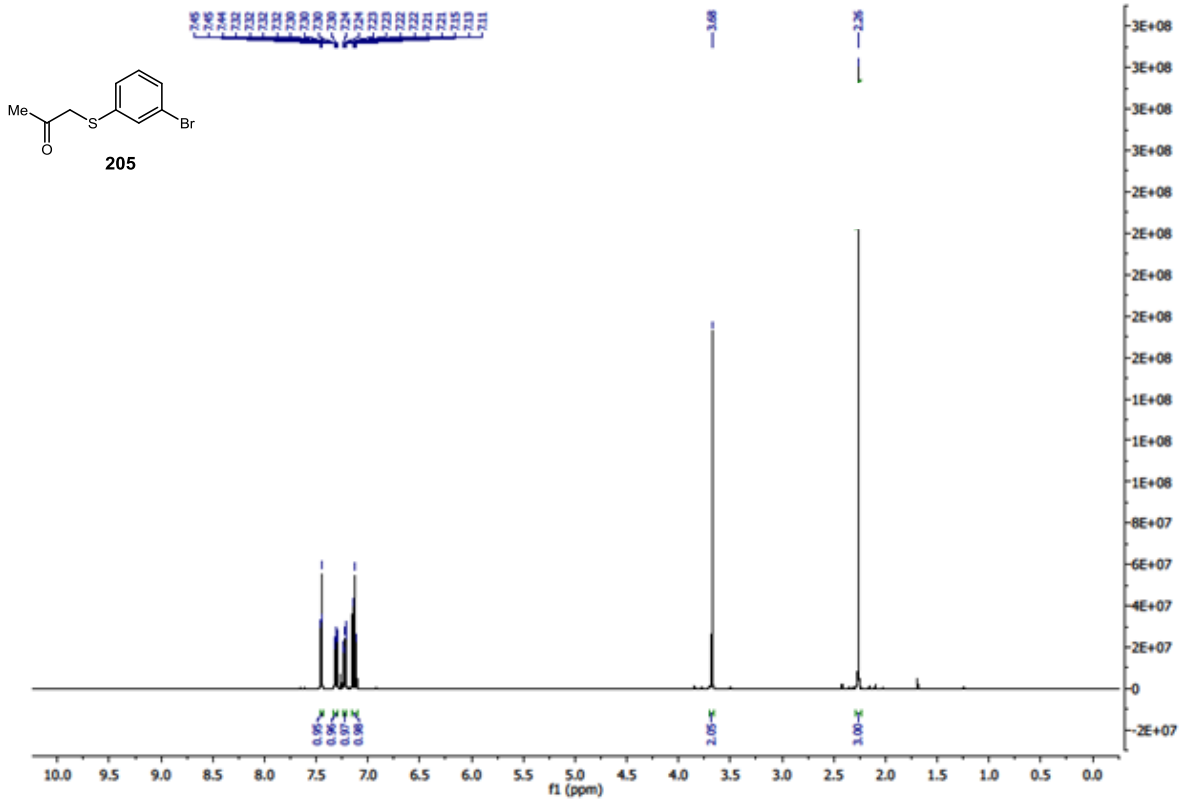


HRMS of 197

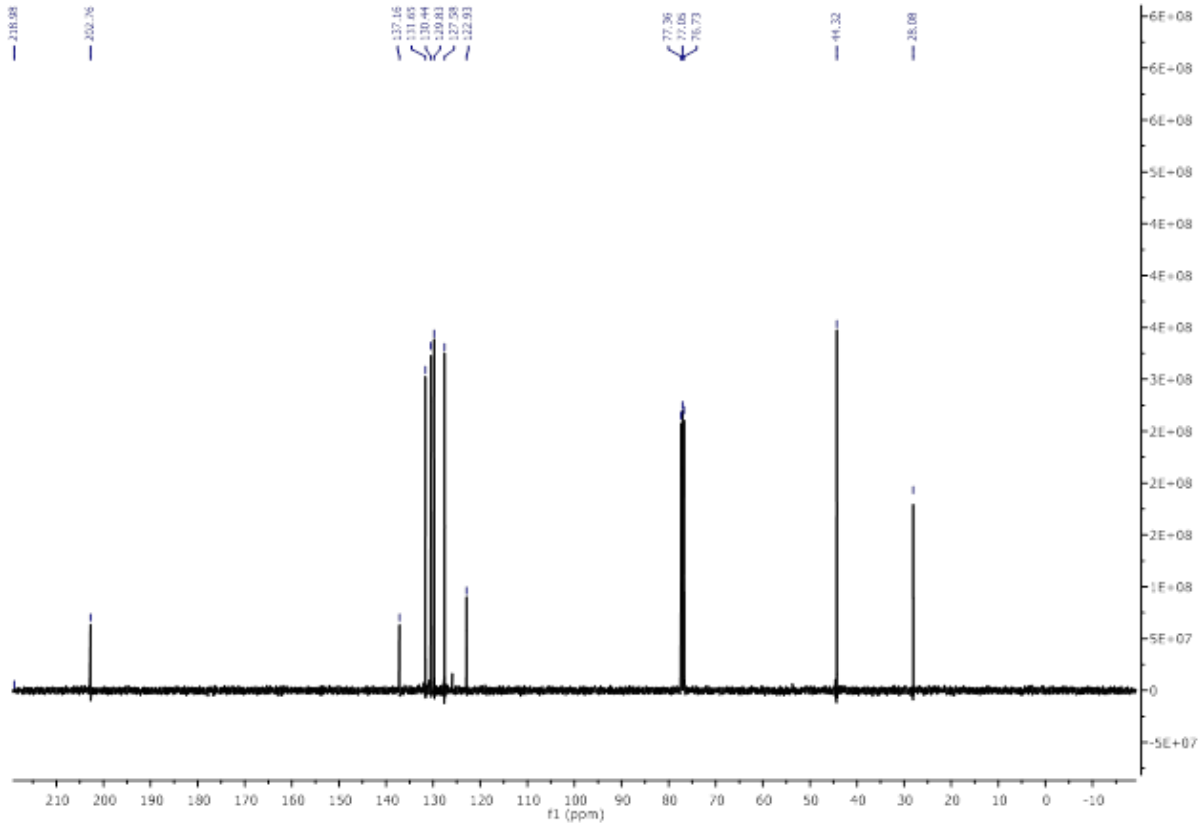


Compound 205

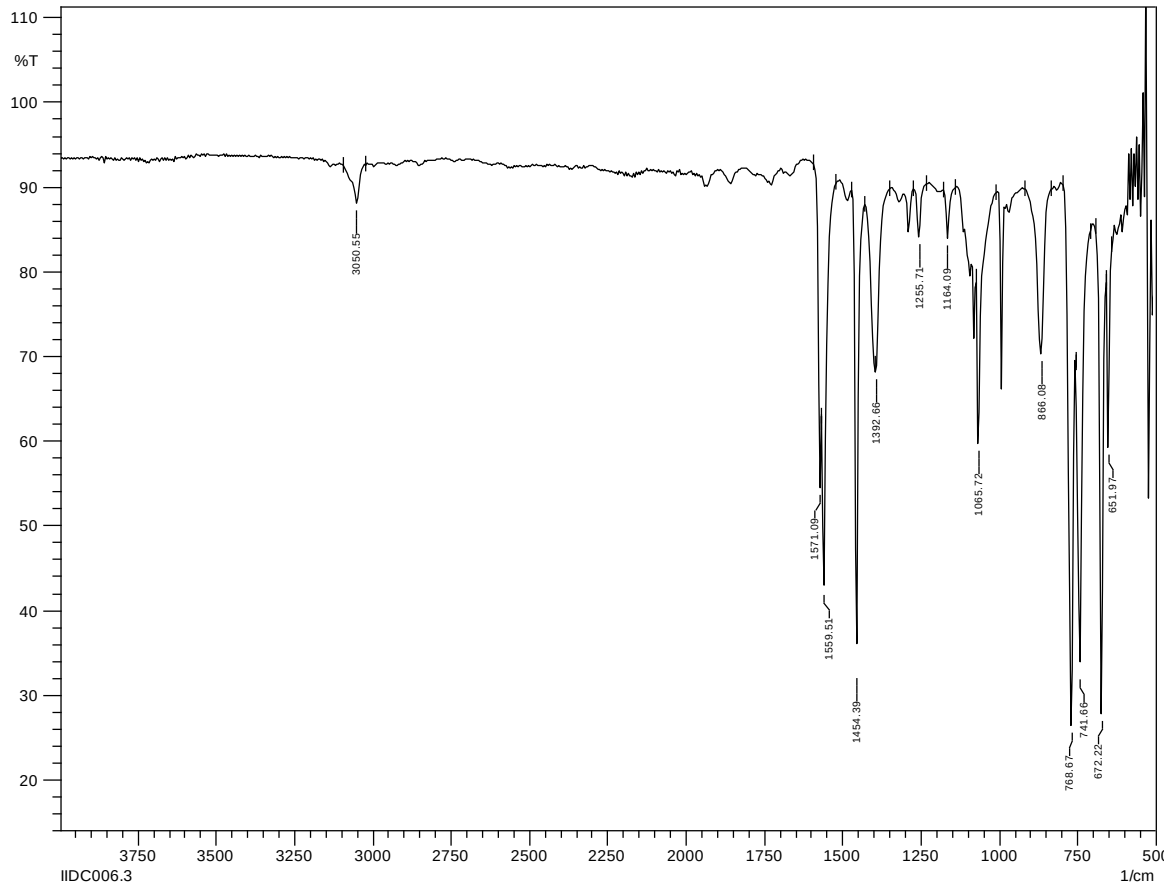
^{1}H NMR



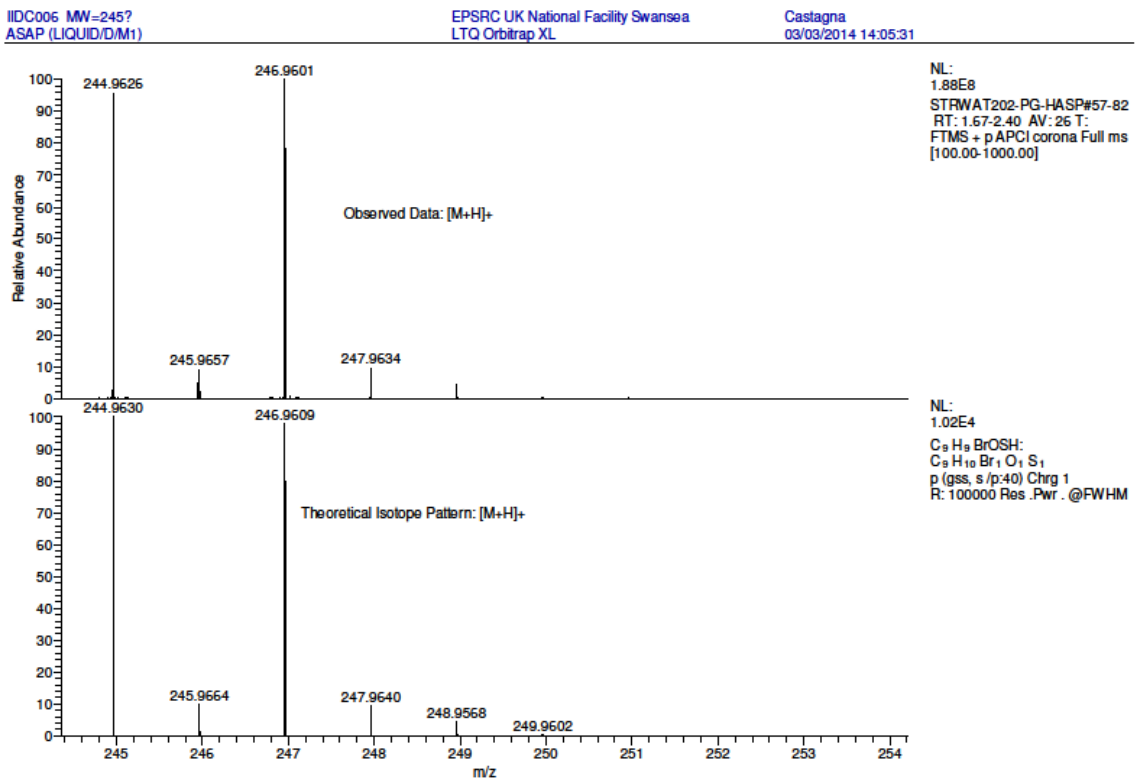
^{13}C NMR of 205



IR of 205

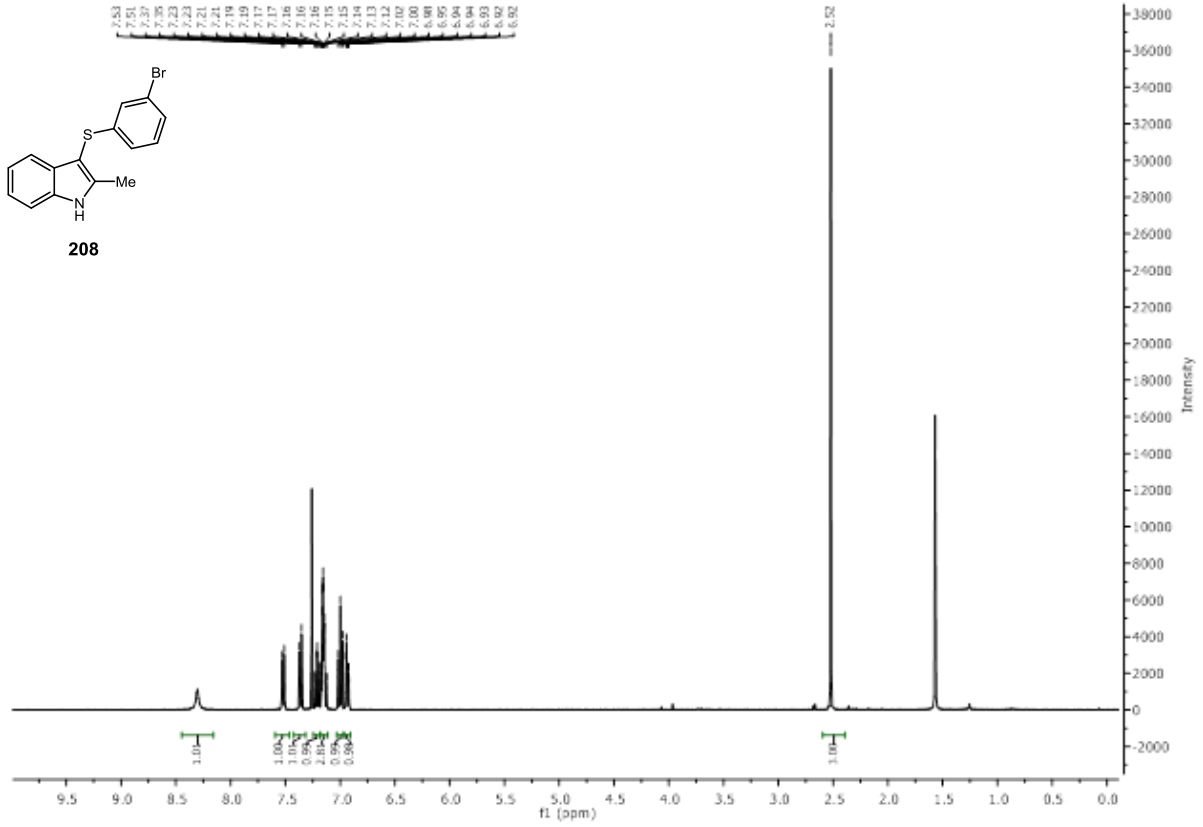


HRMS of 205

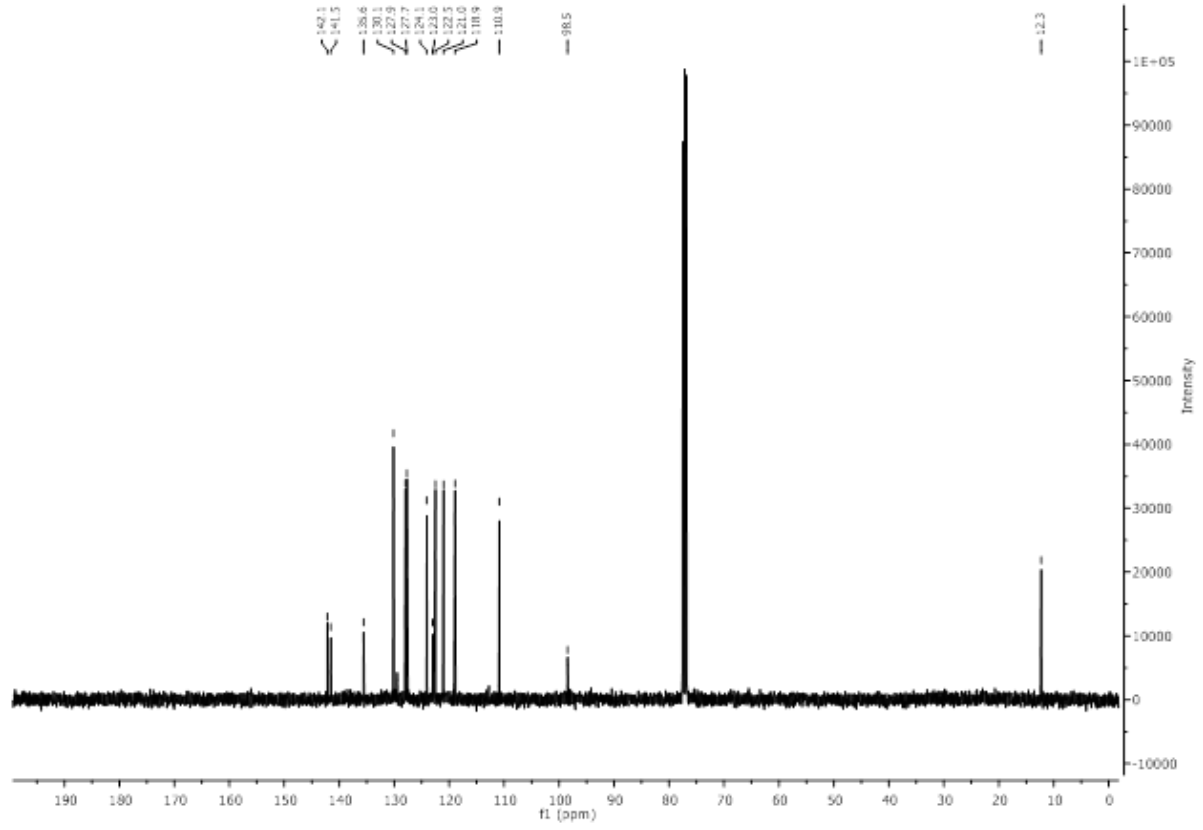


Compound 208

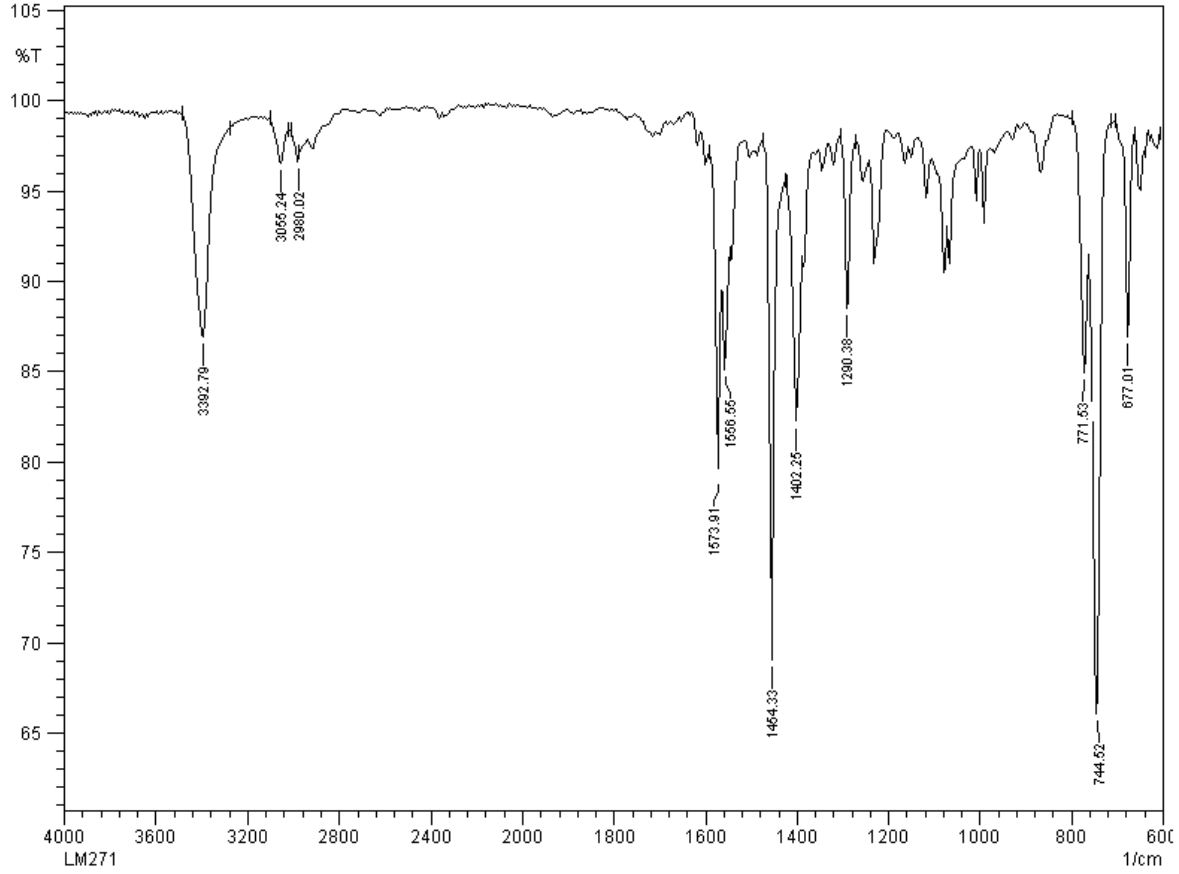
^{1}H NMR



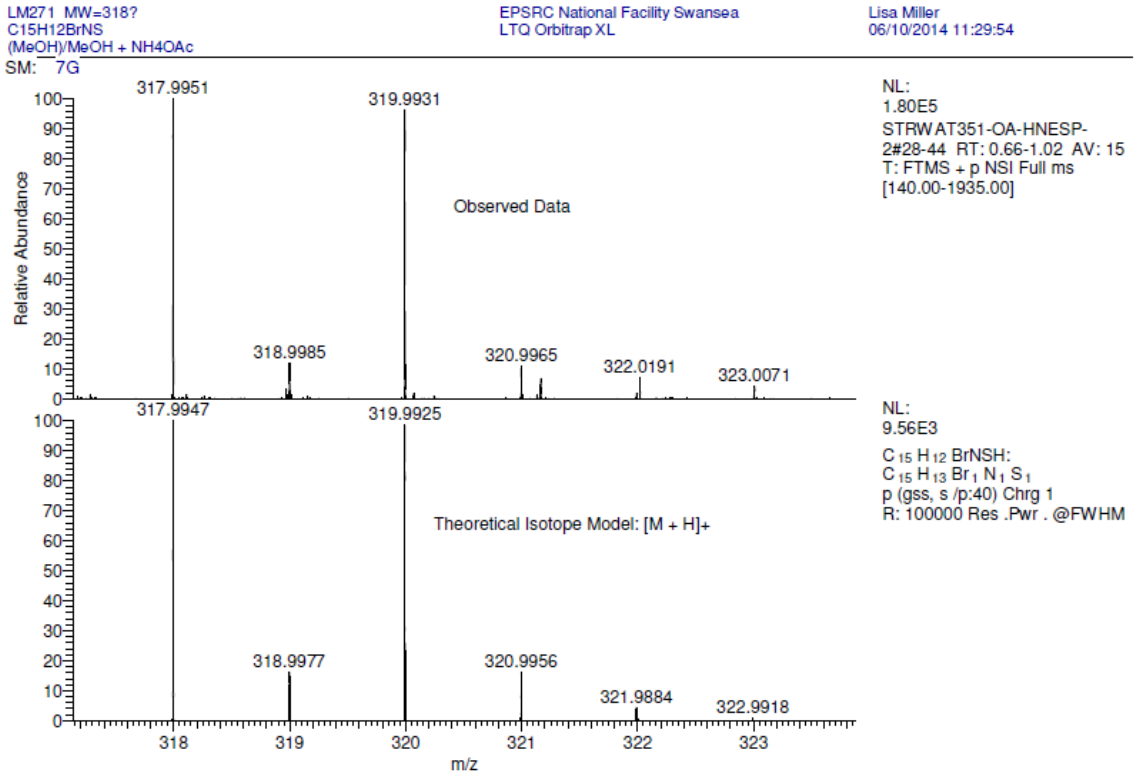
^{13}C NMR of 208



IR of 208

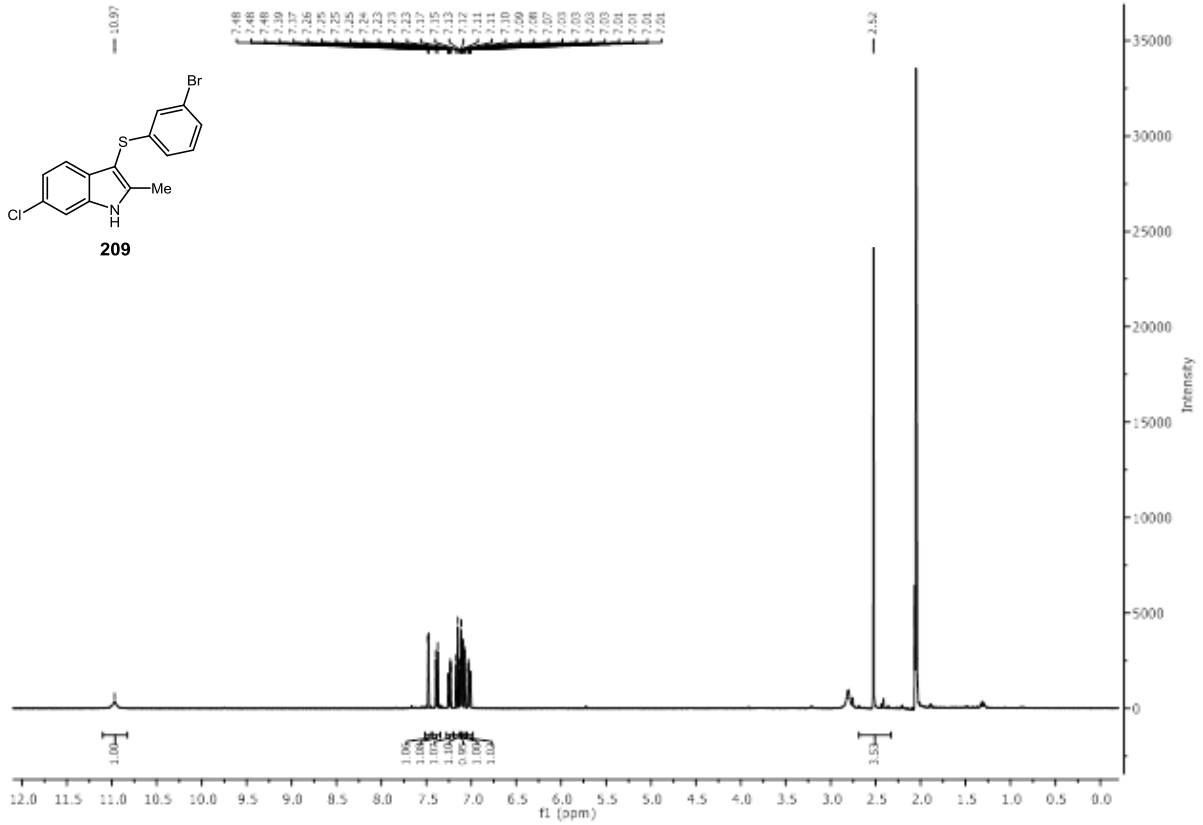


HRMS of 208

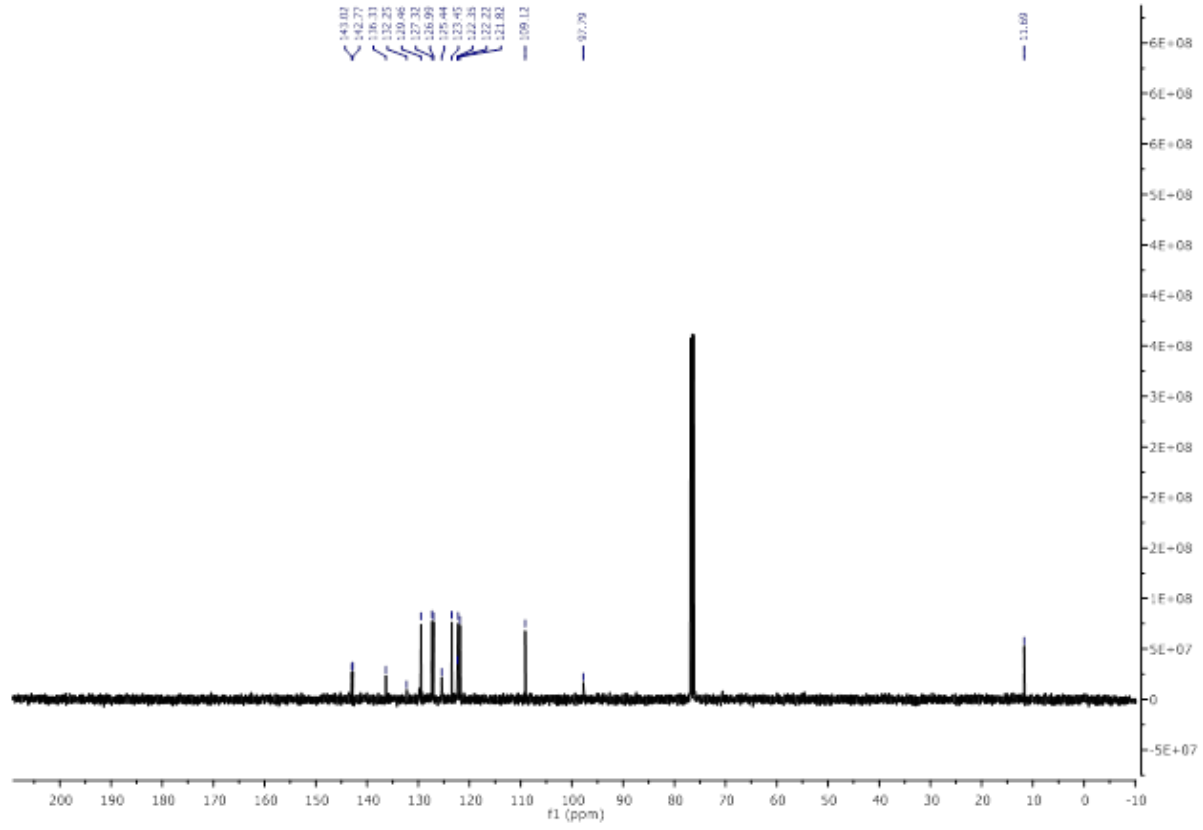


Compound 209

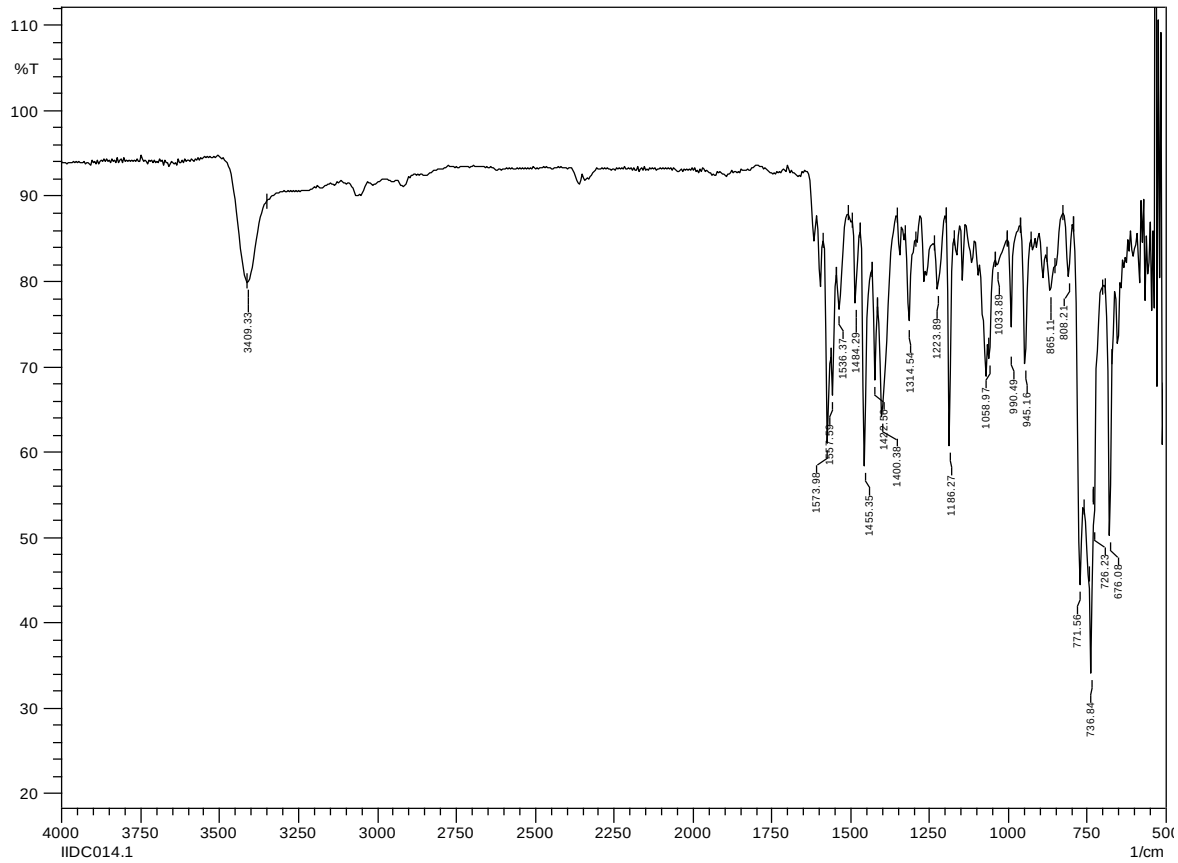
^{1}H NMR



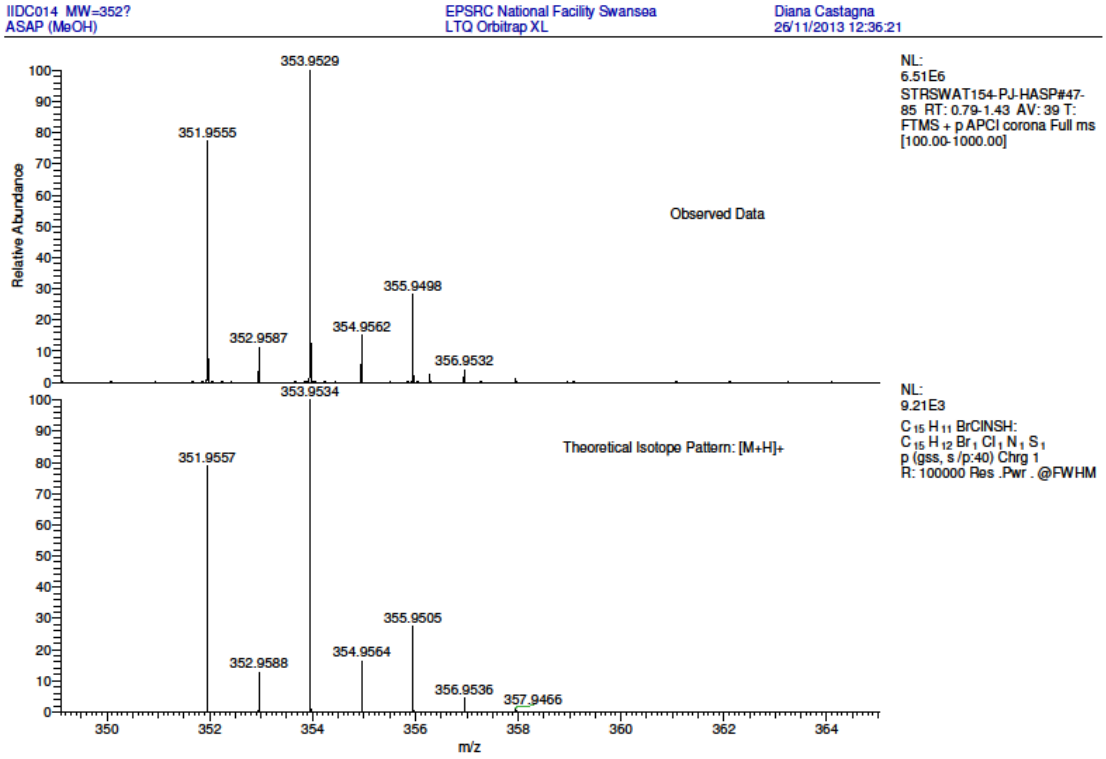
^{13}C NMR of 209



IR of 209

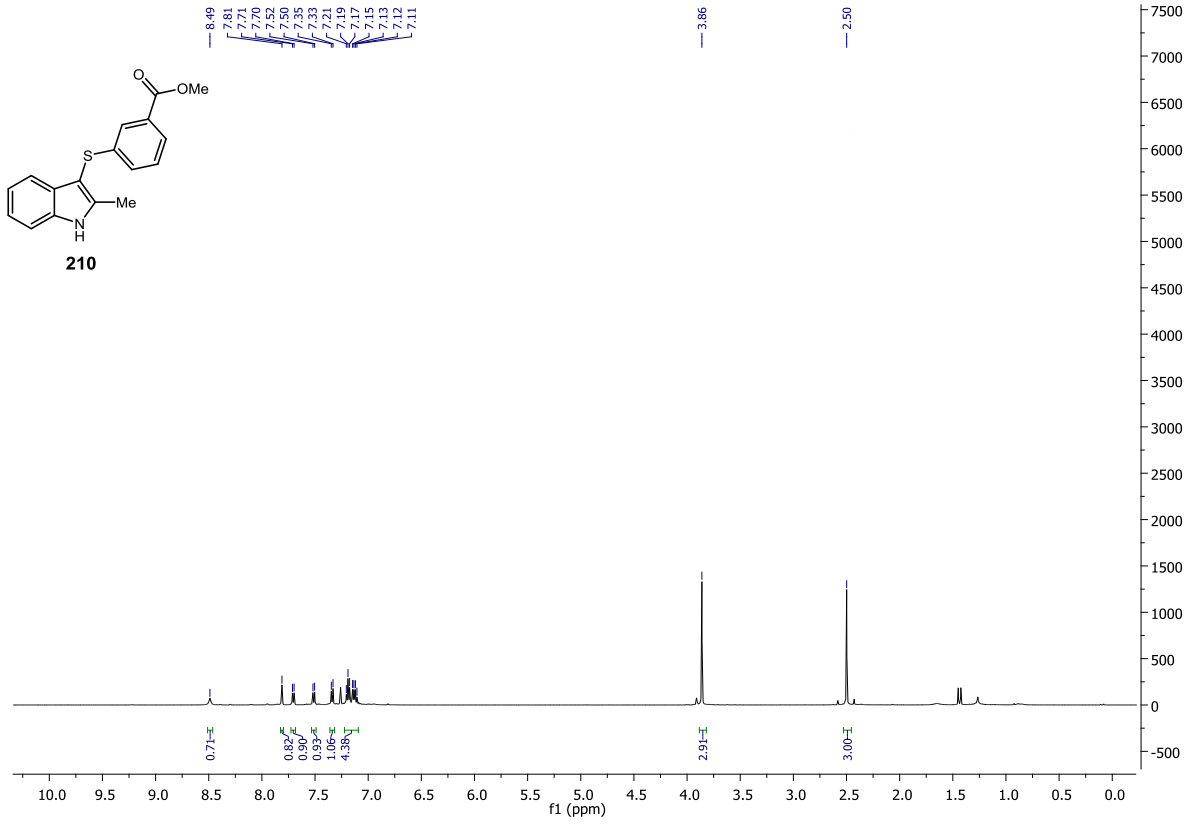


HRMS of 209



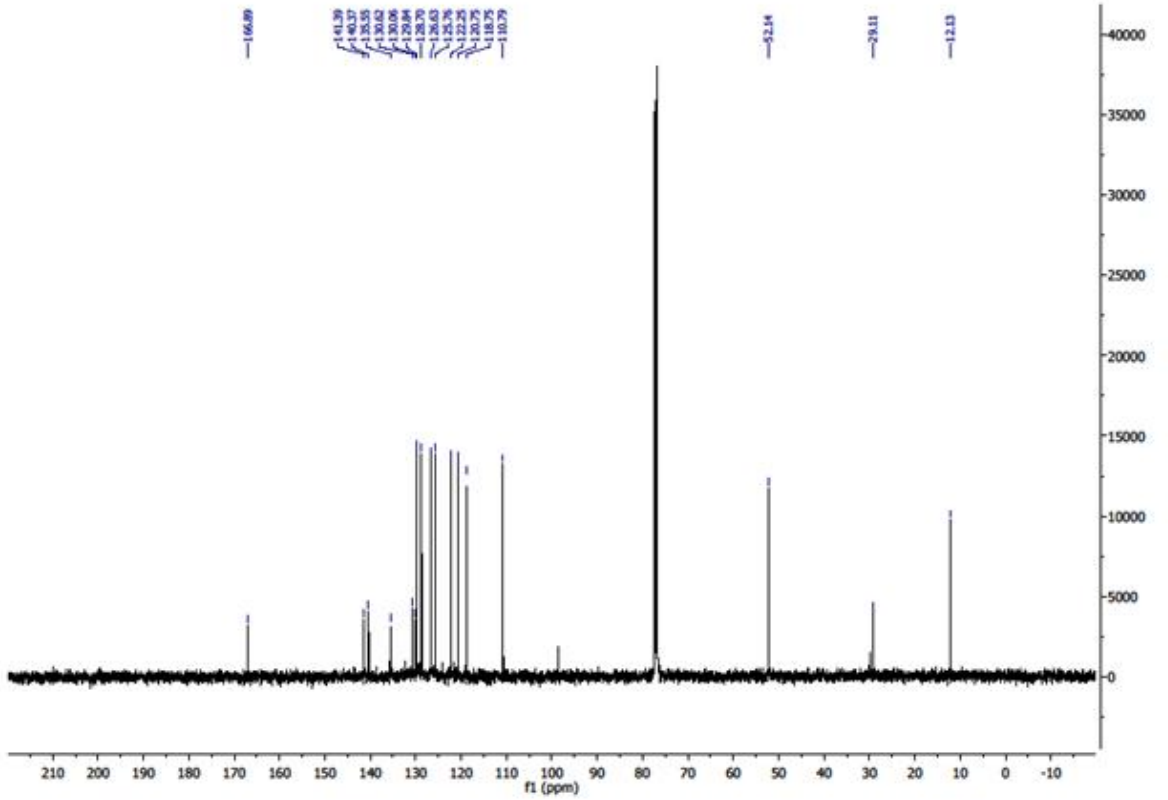
Compound 210

^{1}H NMR

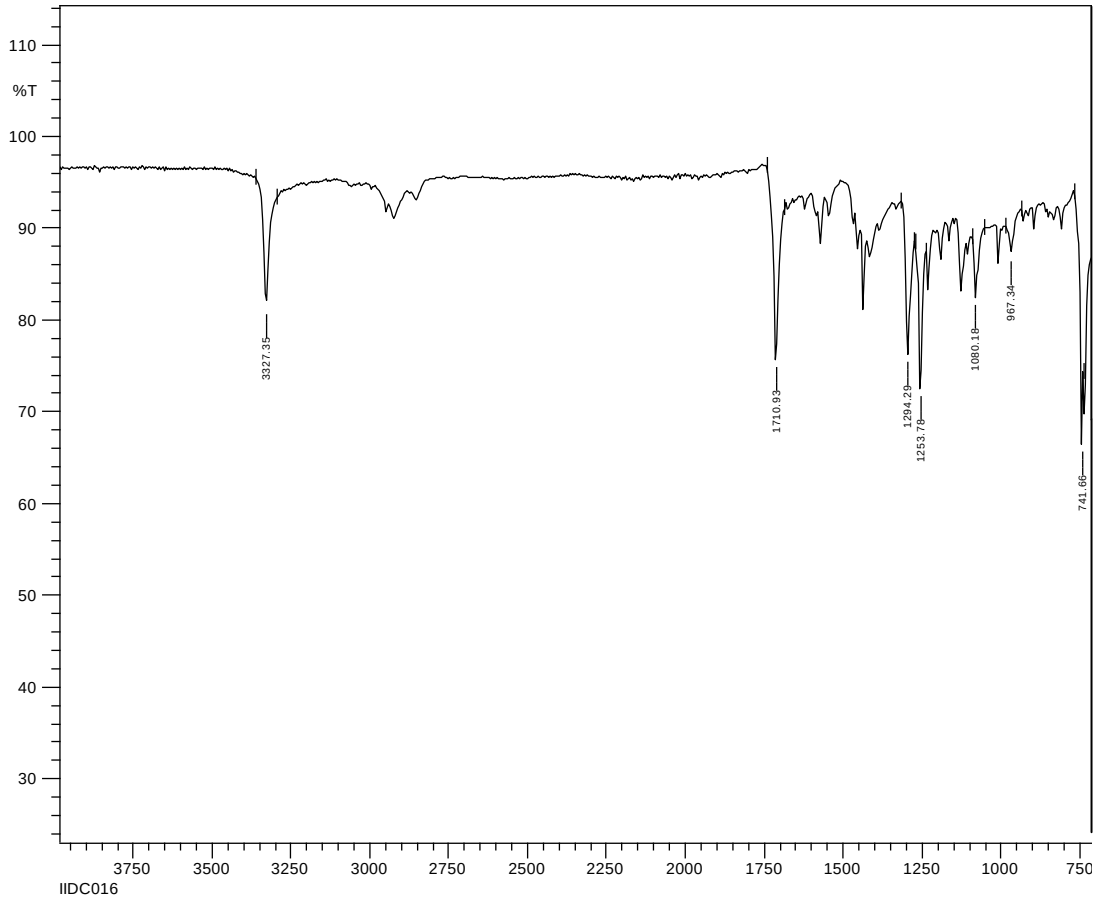


210

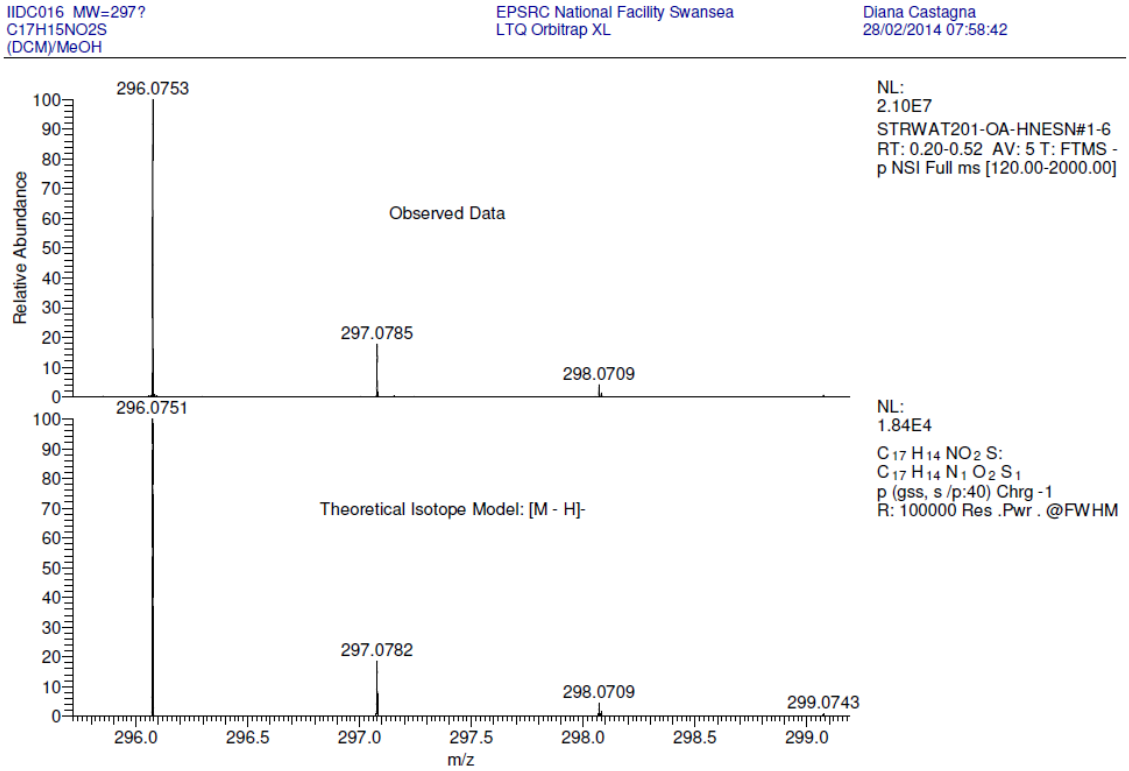
^{13}C NMR of 210



IR of 210

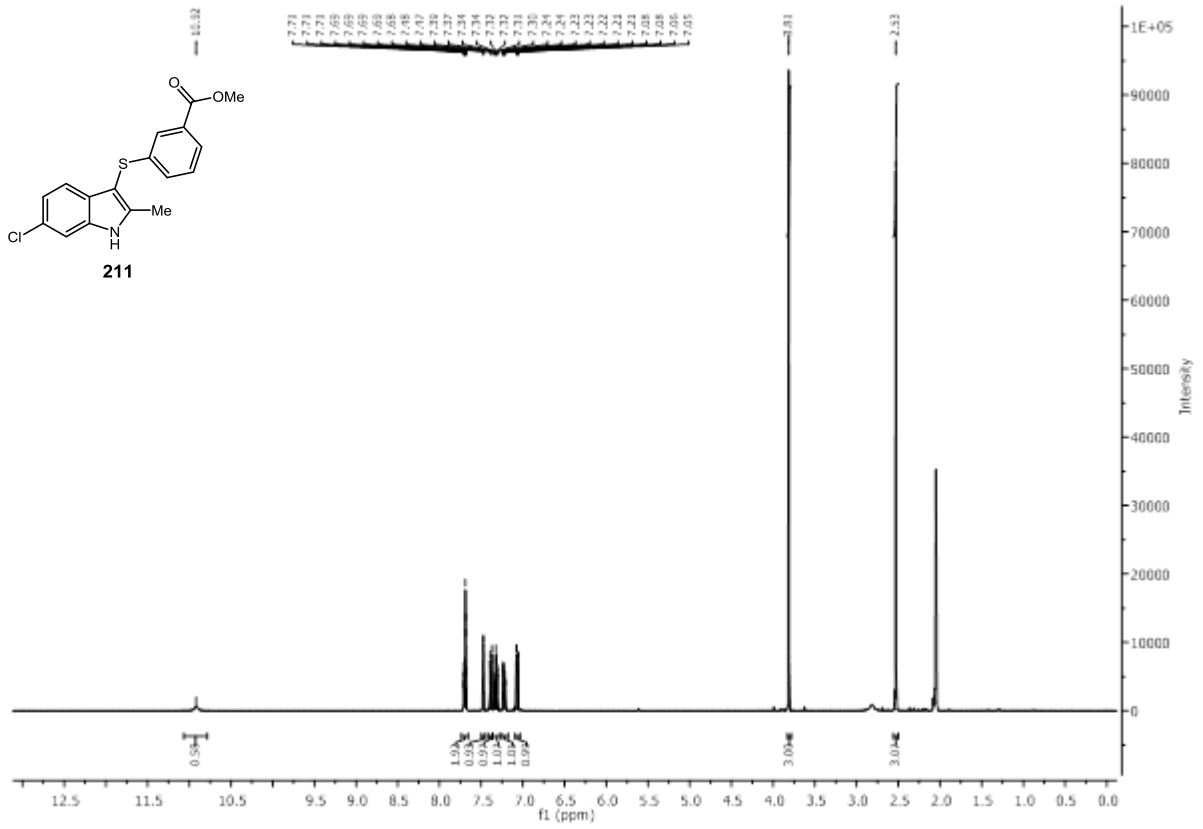


HRMS of 210

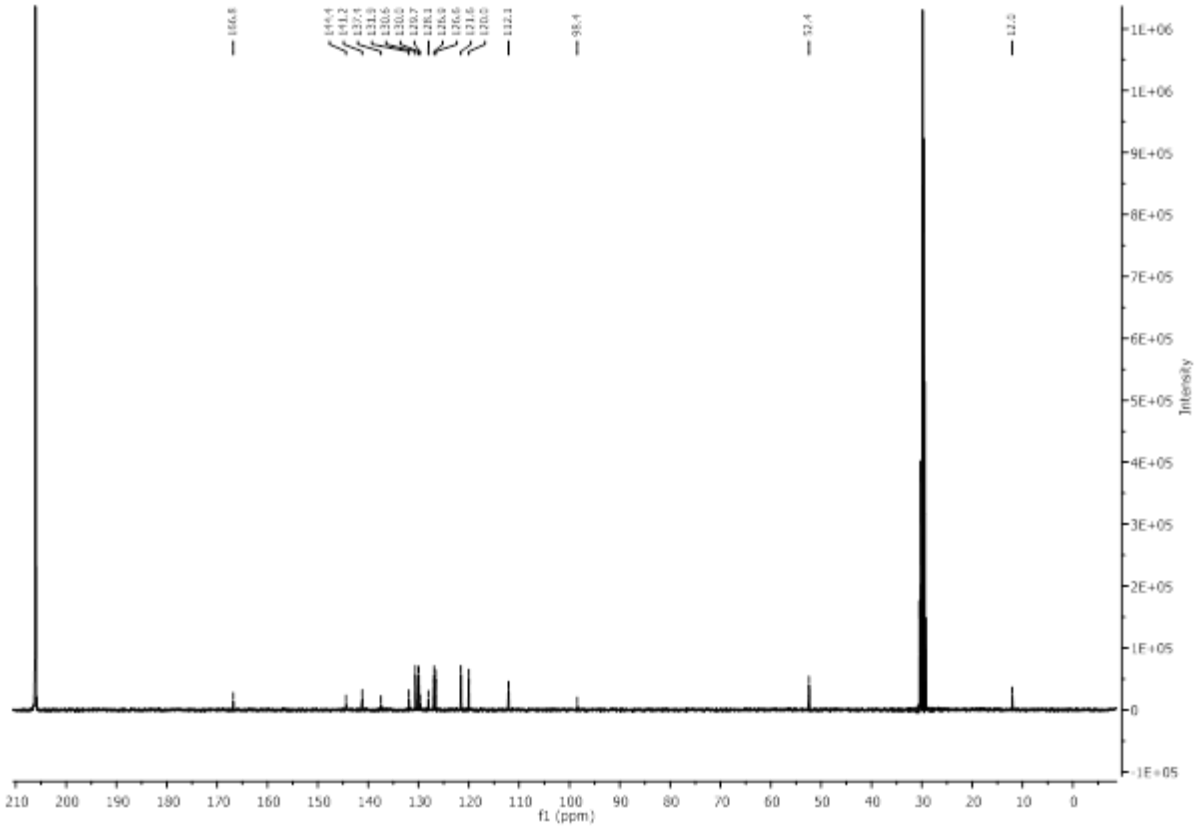


Compound 211

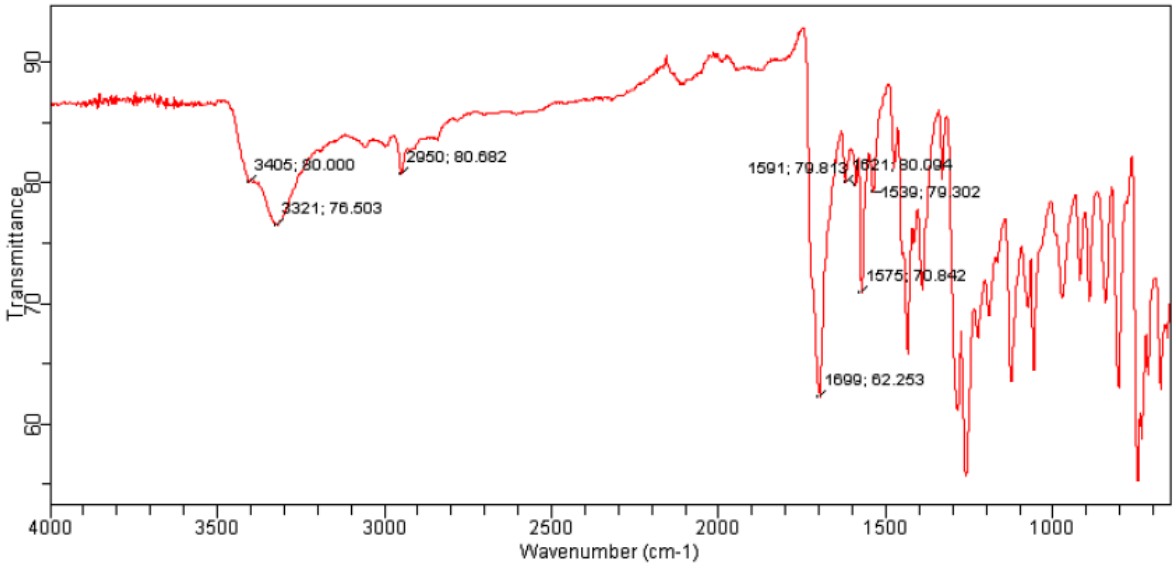
^{1}H NMR



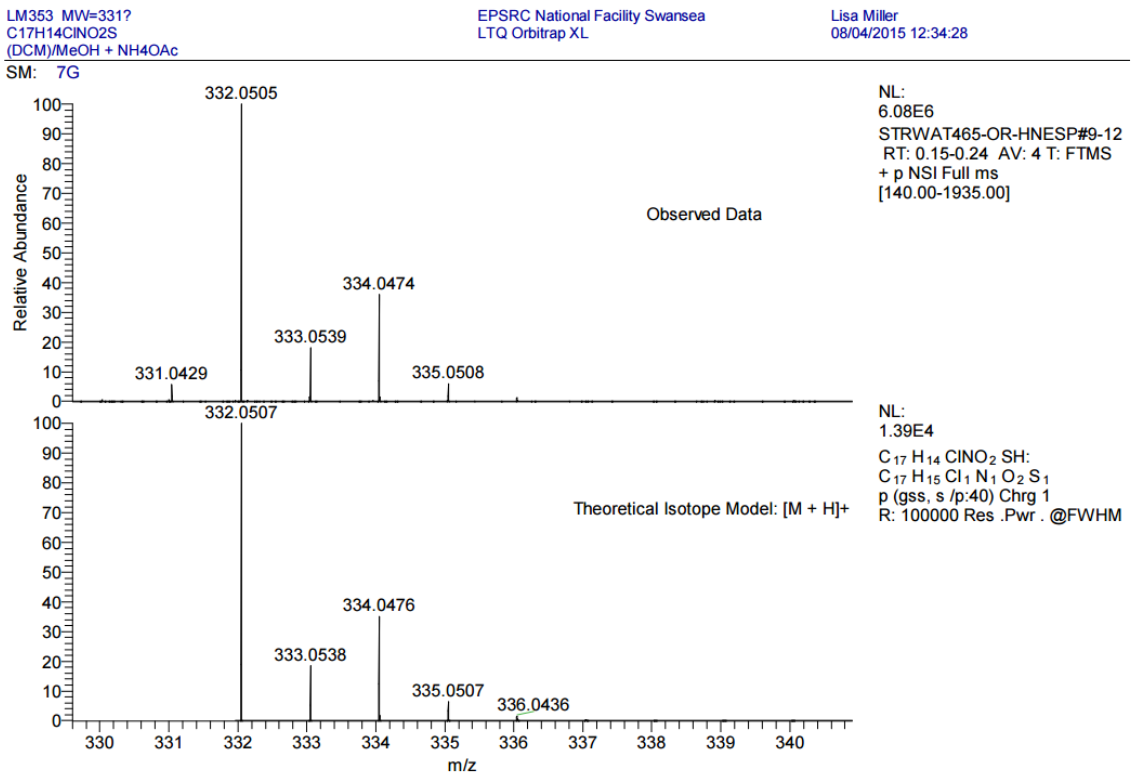
^{13}C NMR of 211



IR of 211

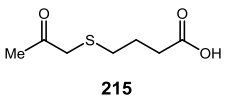


HRMS of 211



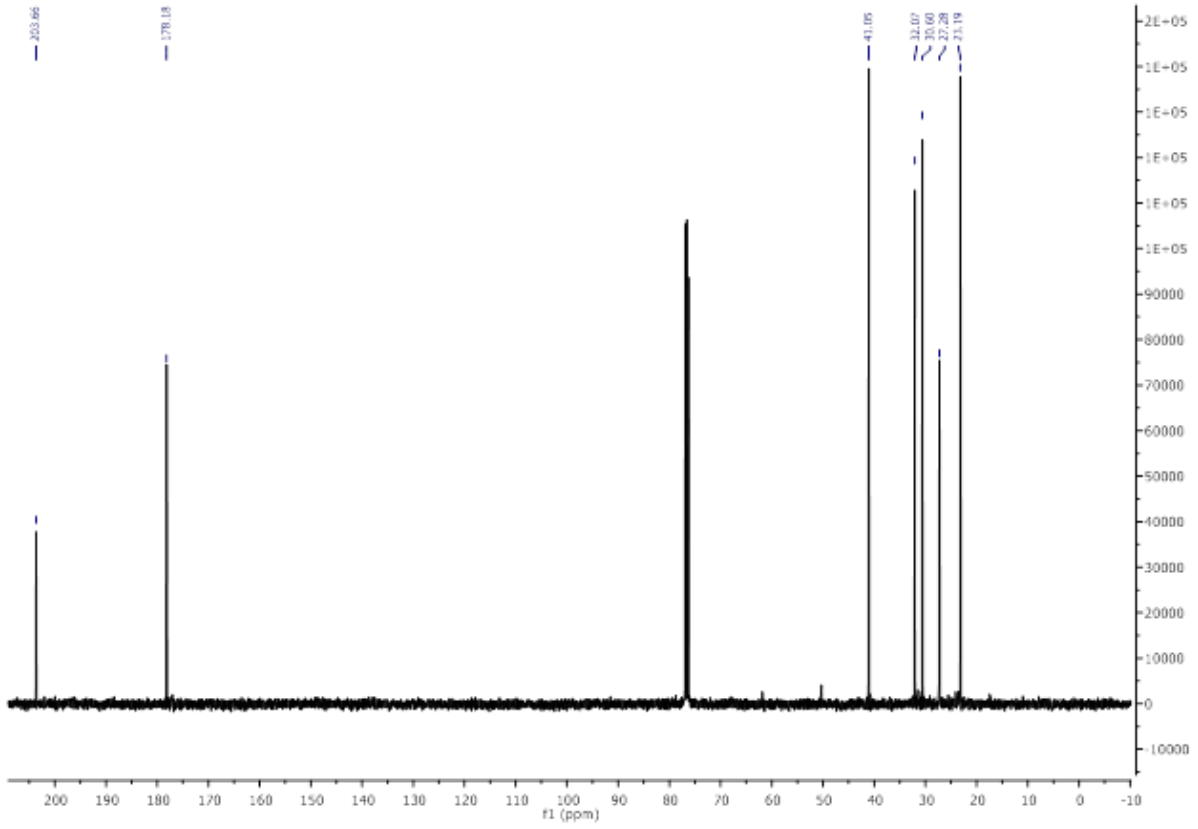
Compound 215

^{1}H NMR

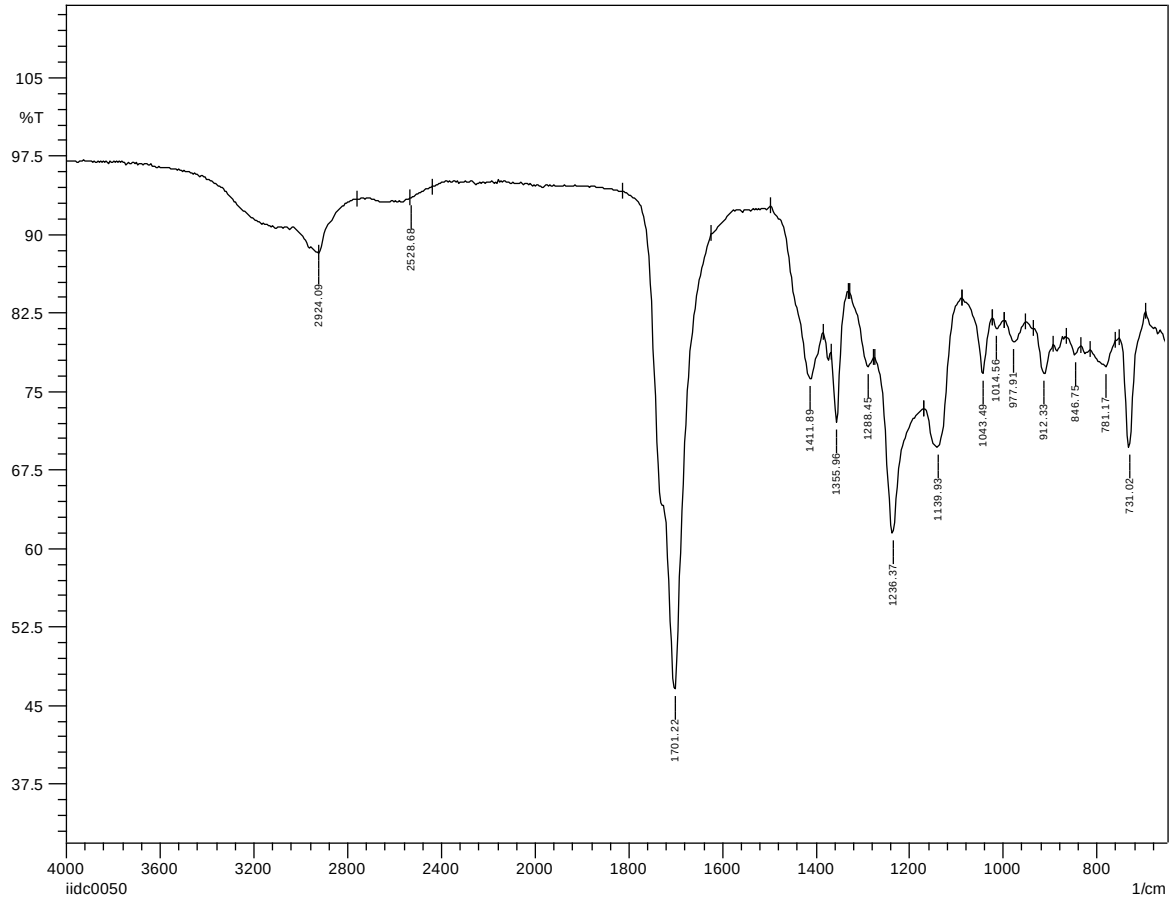


215

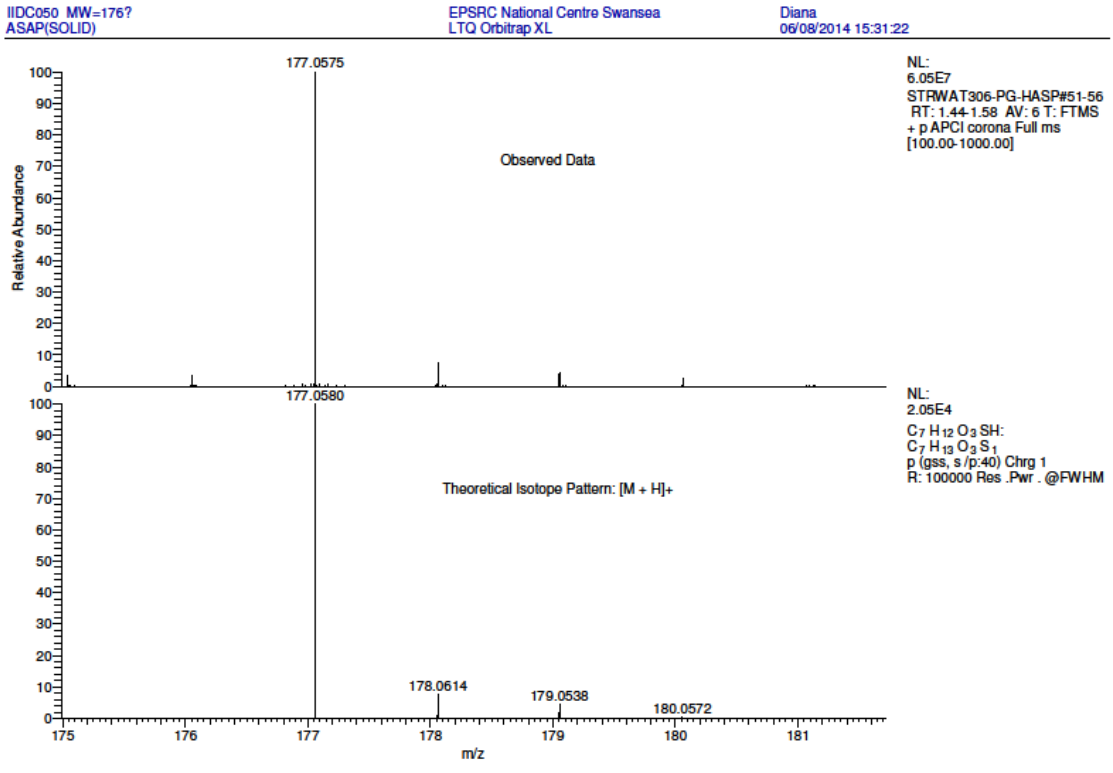
^{13}C NMR of 215



IR of 215

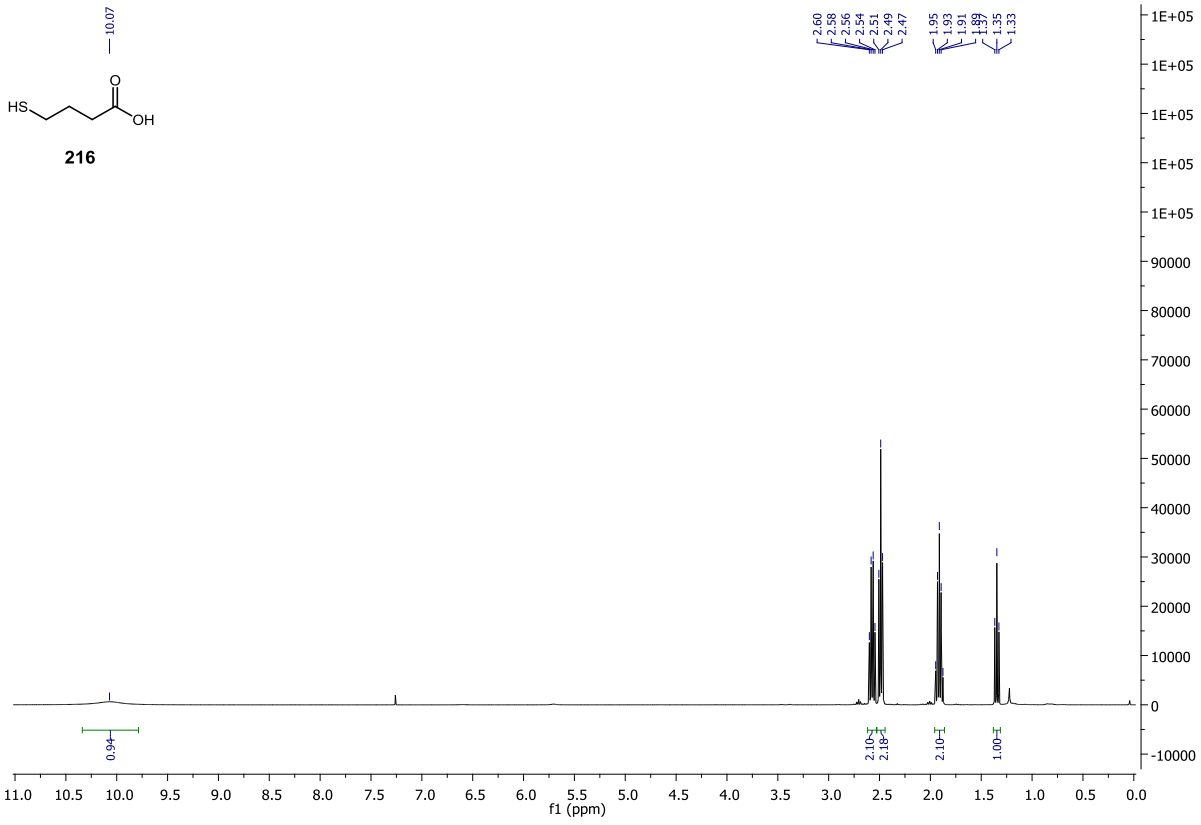


HRMS of 215

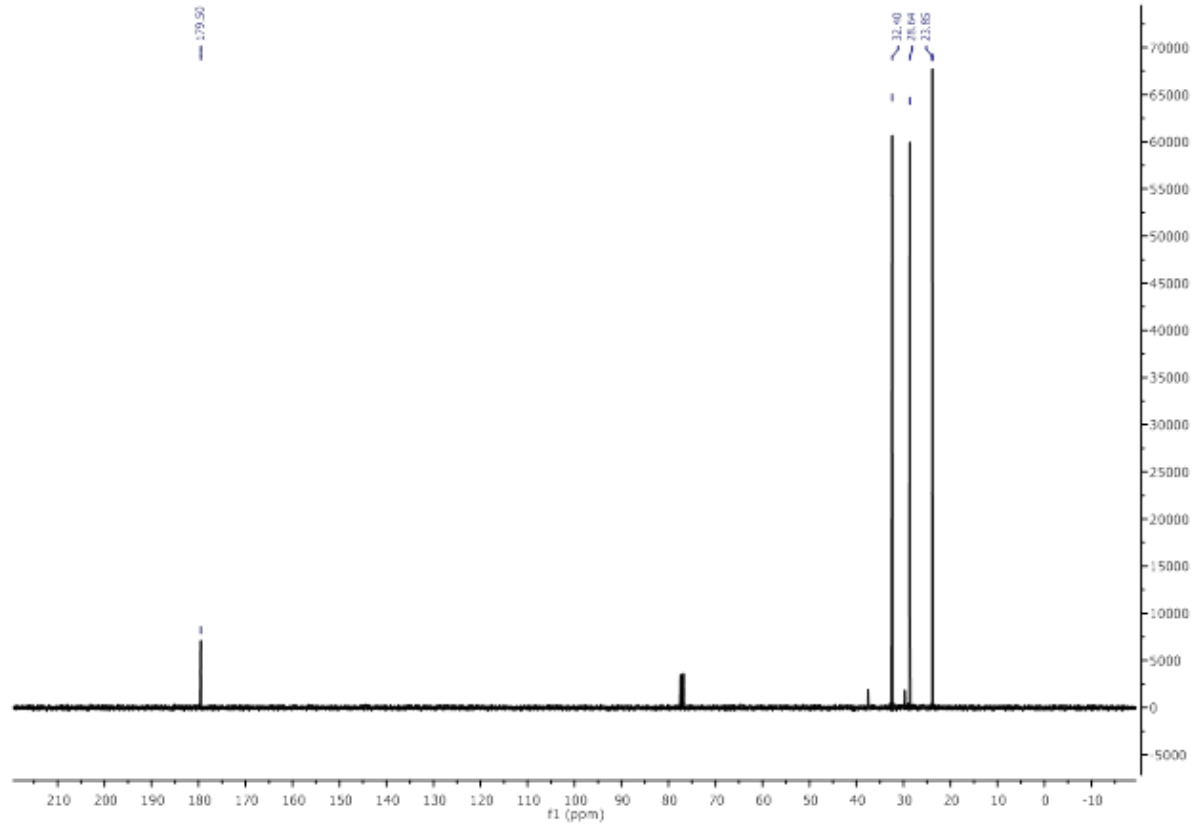


Compound 216

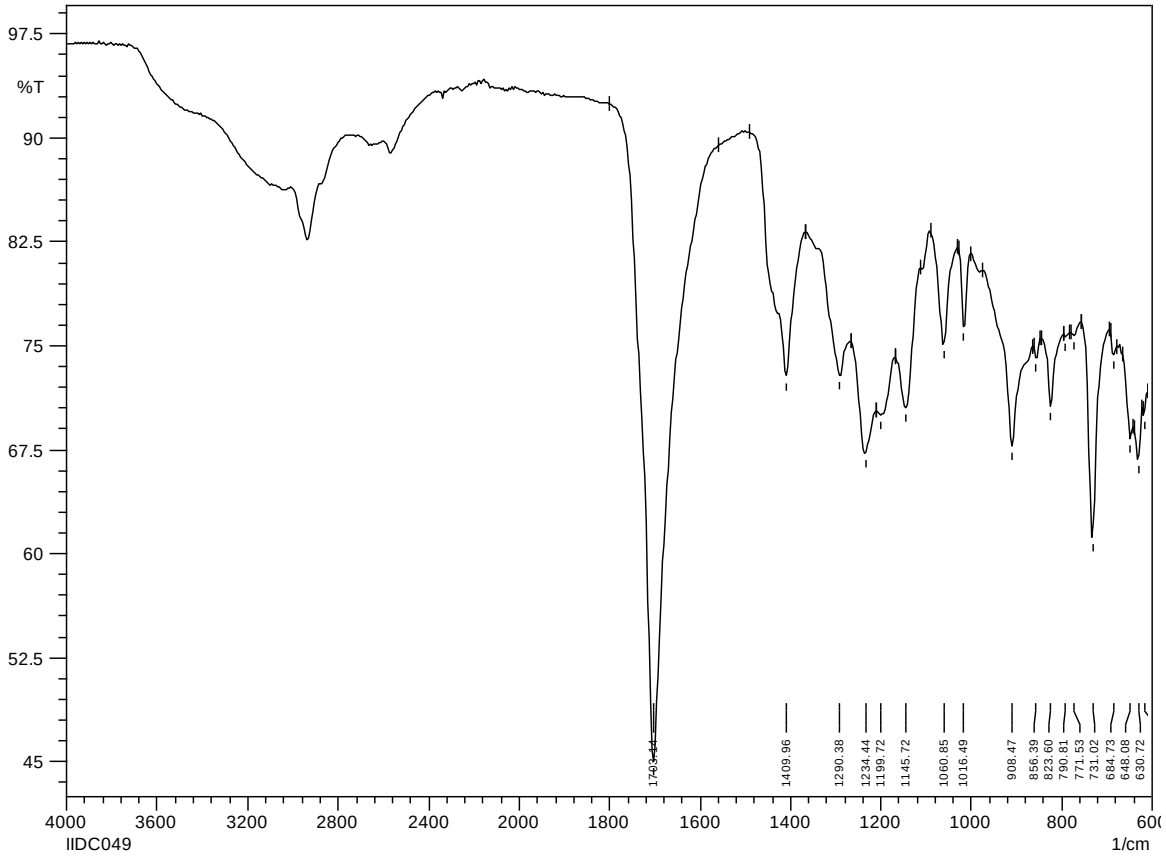
^{1}H NMR



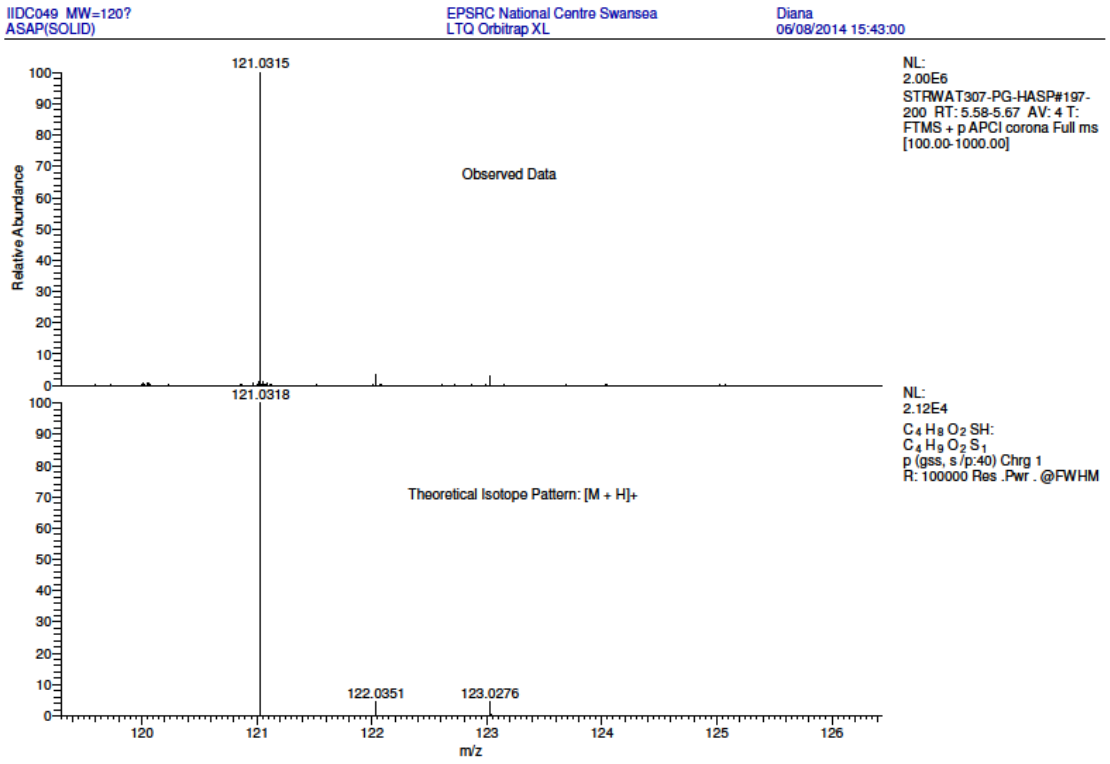
^{13}C NMR of 216



IR of 216

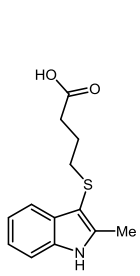


HRMS of 216



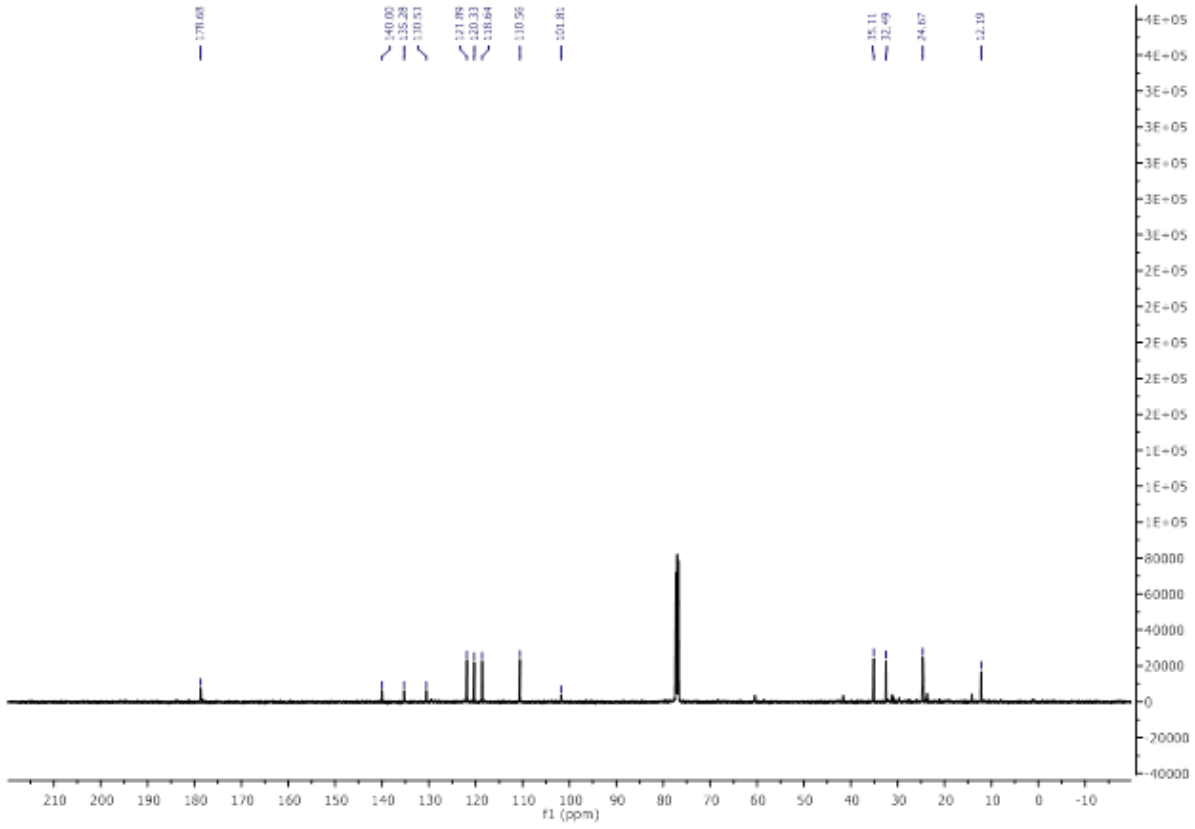
Compound 218

^{1}H NMR

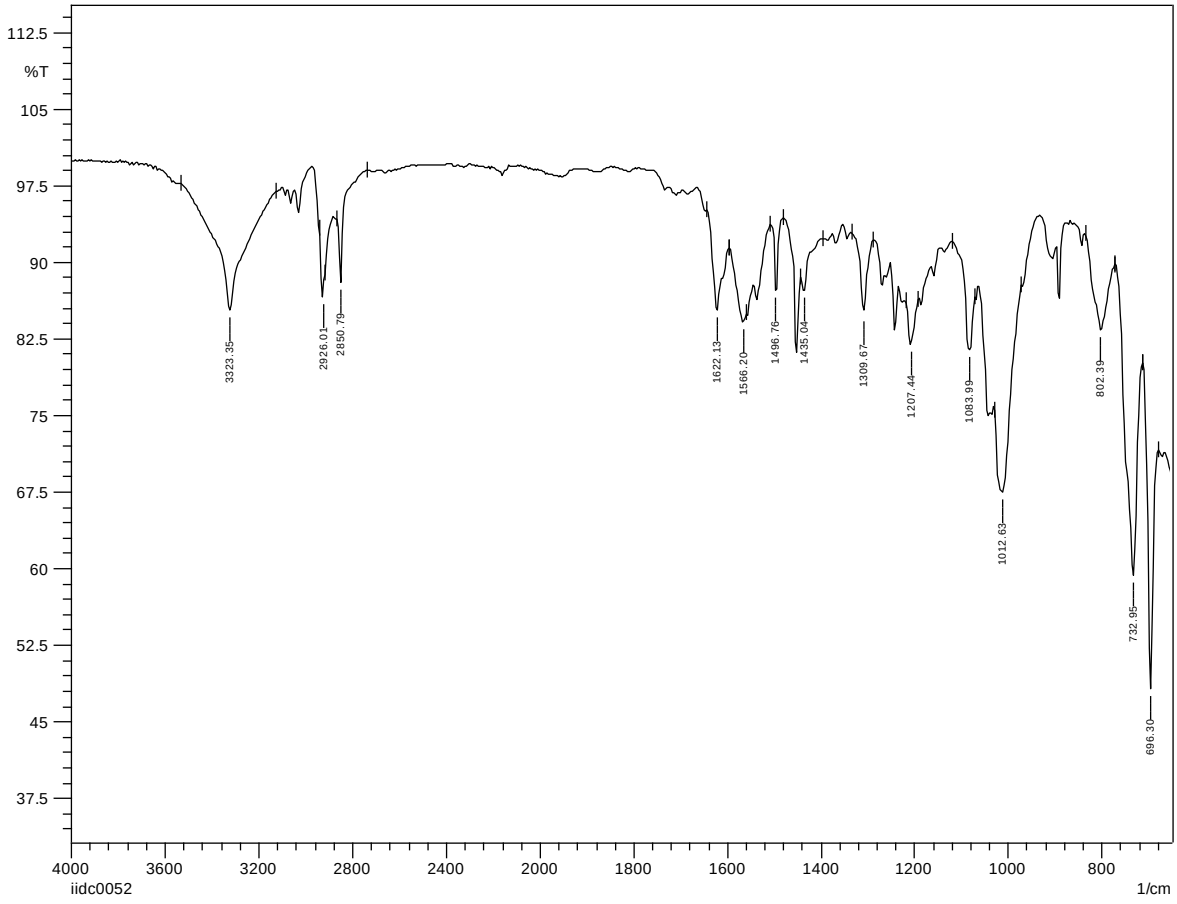


218

^{13}C NMR of 218



IR of 218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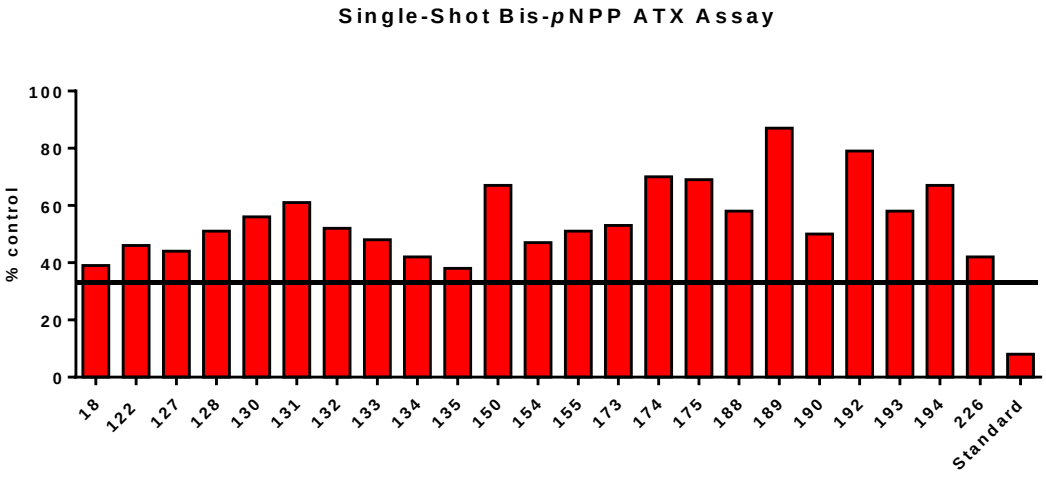
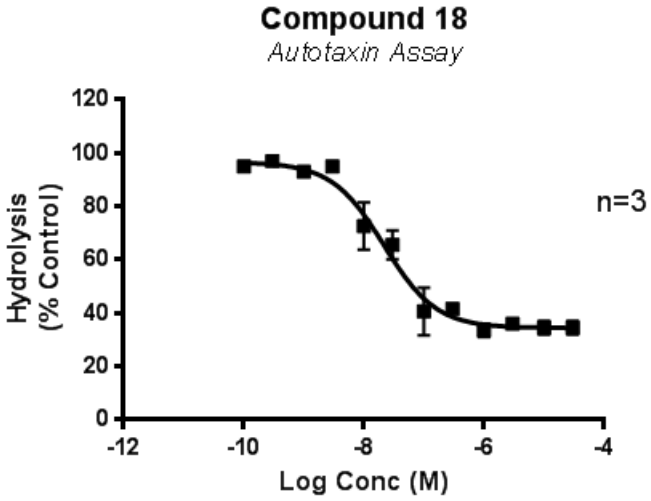
%T
105
97.5
90
82.5
75
67.5
60
52.5
45
37.5
3323.35
2926.01
2850.79
1622.13
1566.20
1496.76
1435.04
1309.67
1207.44
1083.99
1012.63
802.39
732.95
696.30
4000
3600
3200
2800
2400
2000
1800
1600
1400
1200
1000
800
iidc0052
1/cm

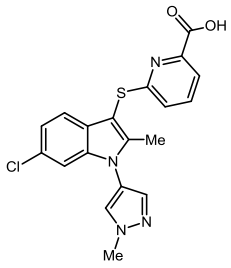
2. Bis-*p*NPP Assay Data

2.1 Bis-*p*NPP Single Shot Data



2.2 Full Curve Assay Results





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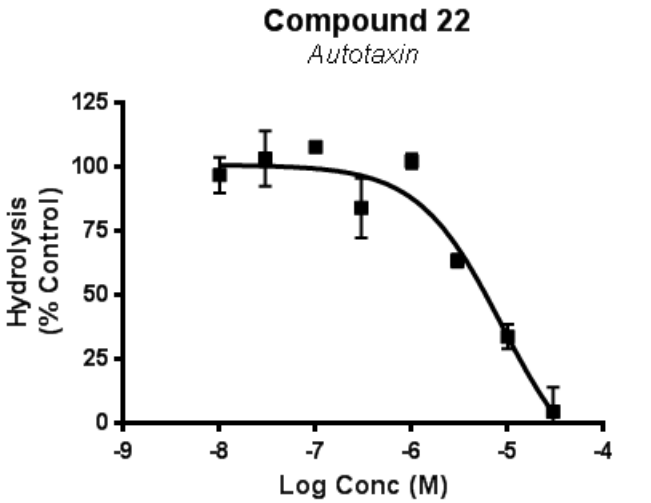

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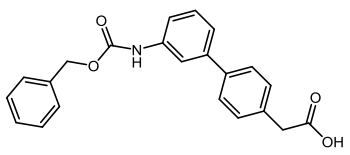

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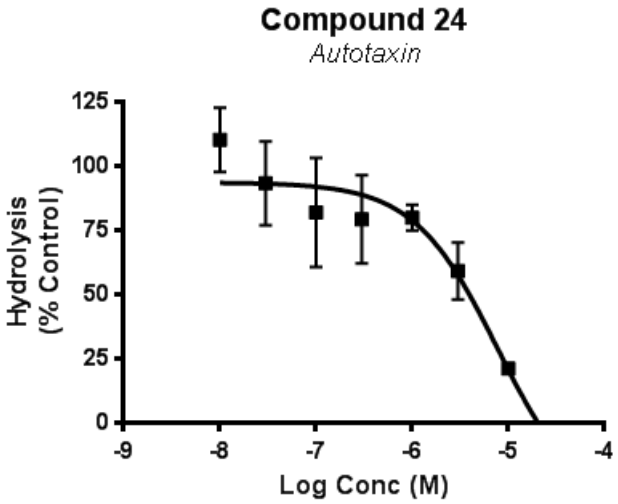

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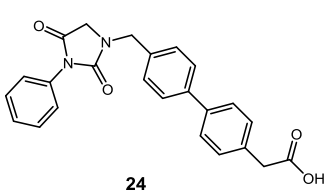

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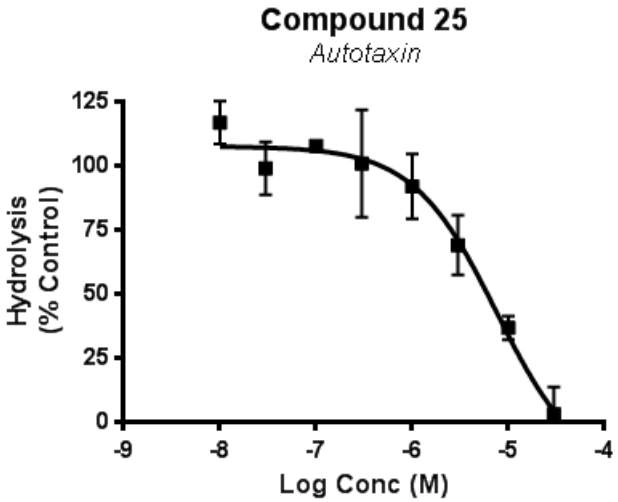

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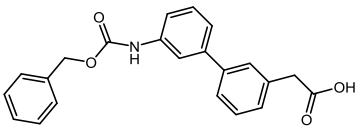

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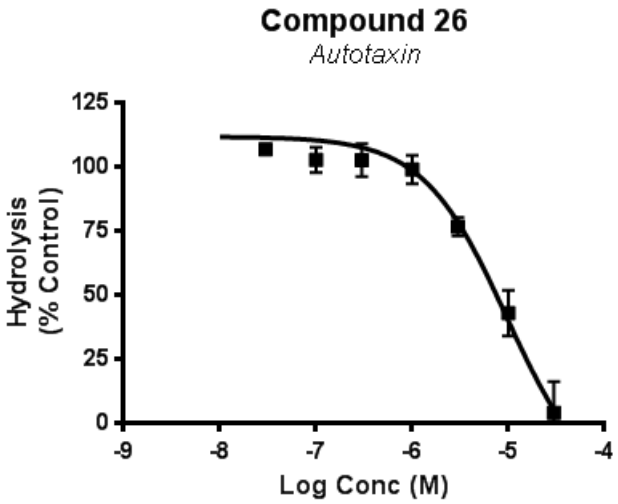

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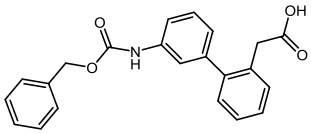
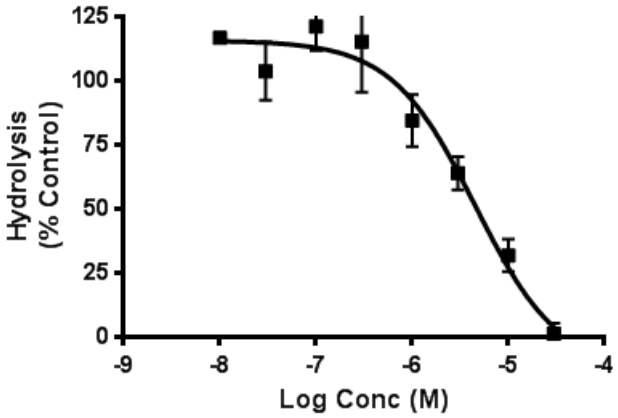


26

Compound 29

Autotaxin



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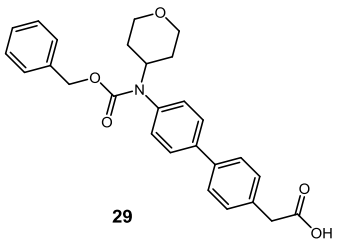
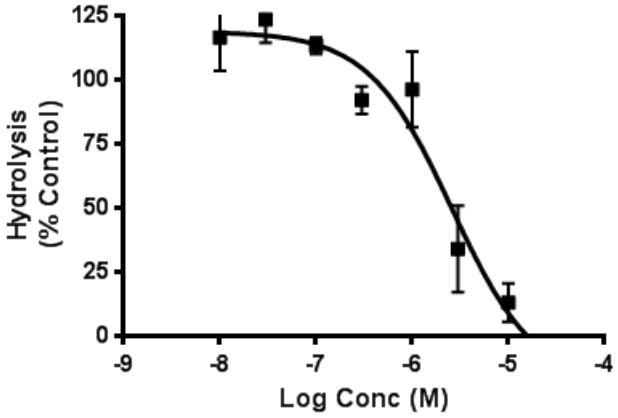


29

Compound 32

Autotaxin



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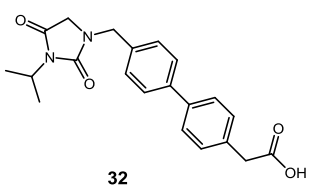
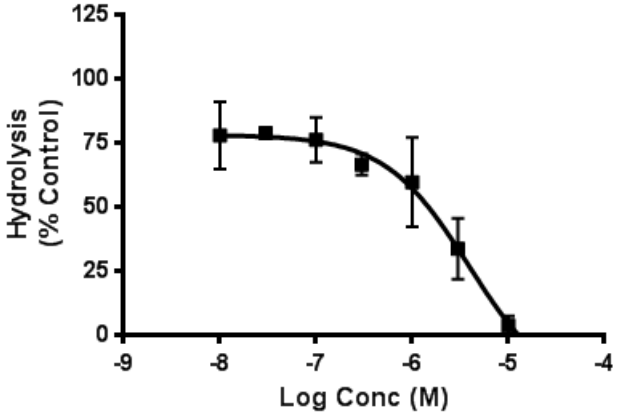


32

Compound 33

Autotaxin



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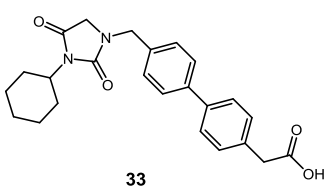

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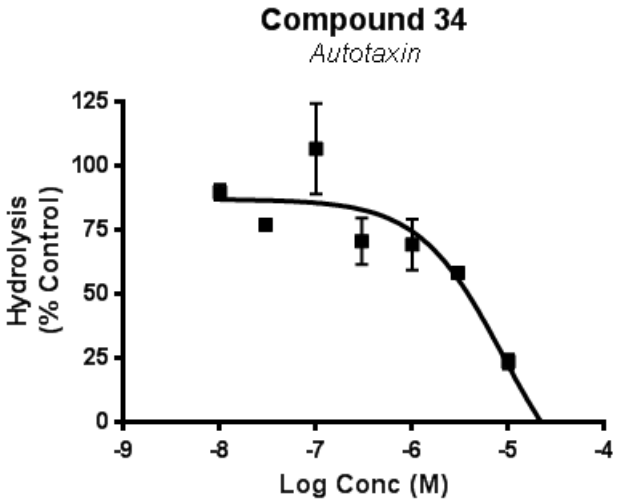

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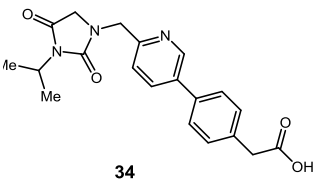
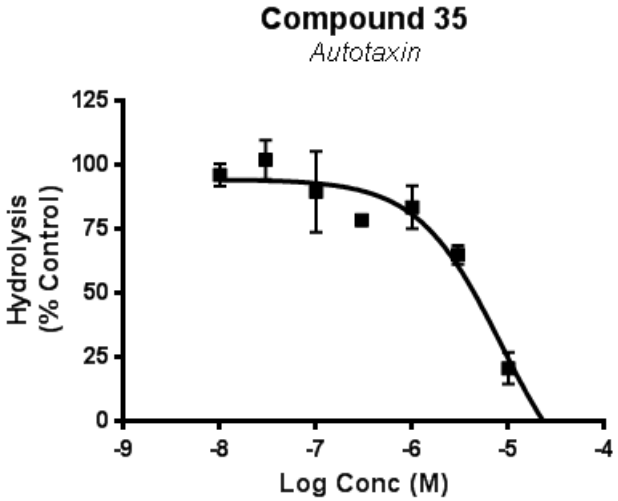


34



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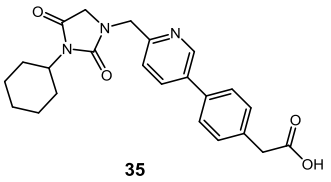

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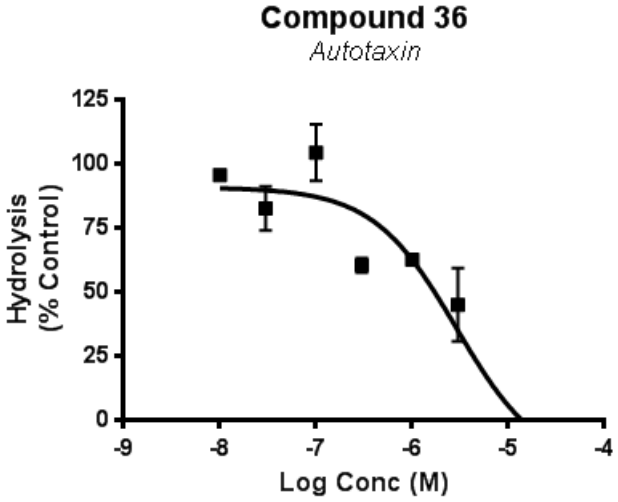

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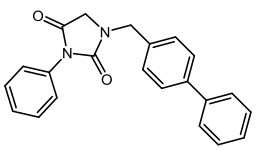
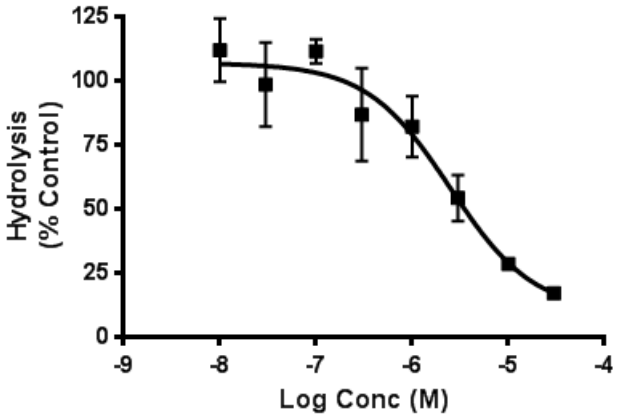


36

Compound 75

Autotaxin



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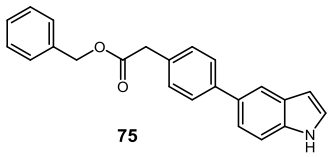
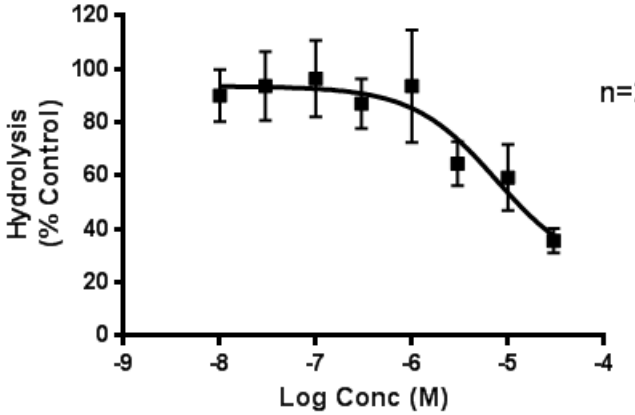


75

Compound 104

Autotaxin Assay



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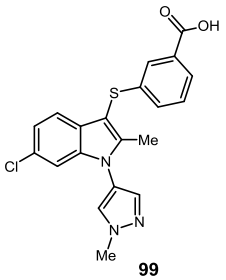
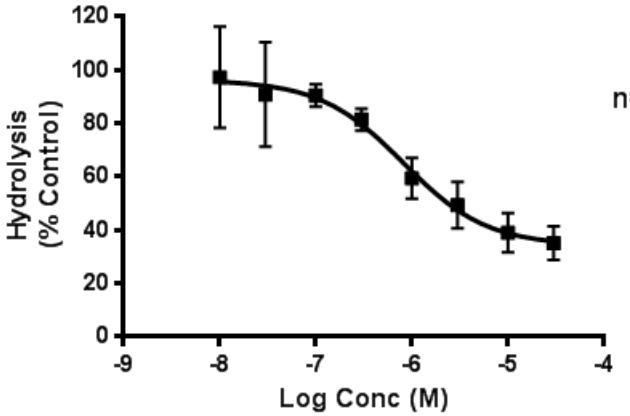


99

Compound 134

Autotaxin Assay



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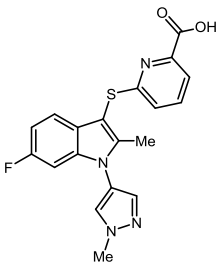
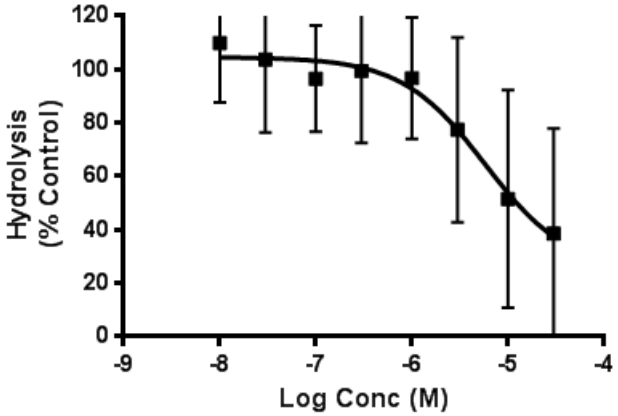
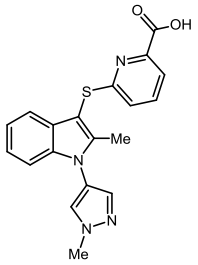


130

Compound 136

Autotaxin Assay

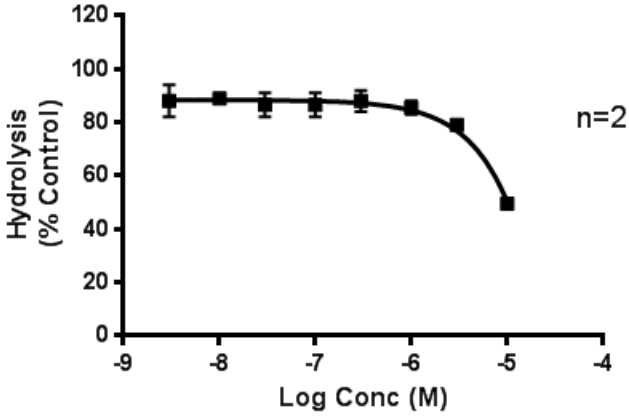




131

Compound 137

Autotaxin Assay



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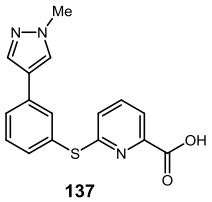
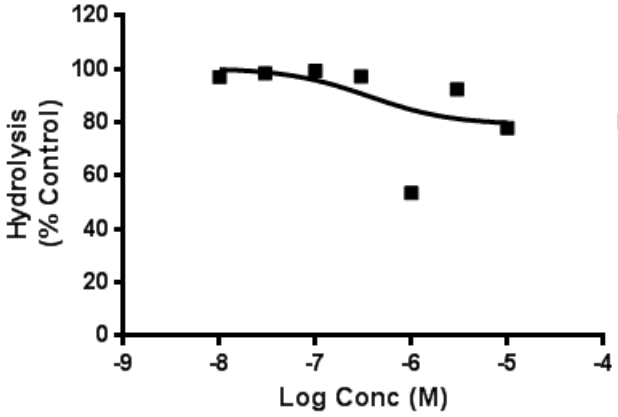


137

Compound 138

Autotaxin Assay



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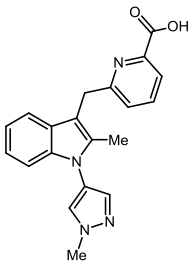
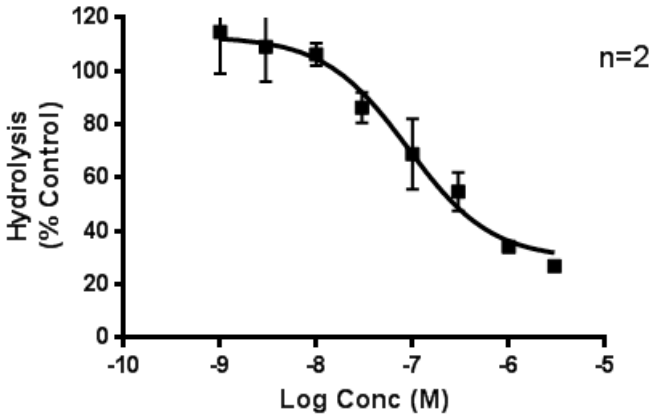


132

Compound 140

Autotaxin Assay



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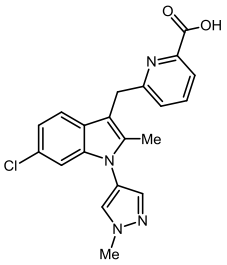
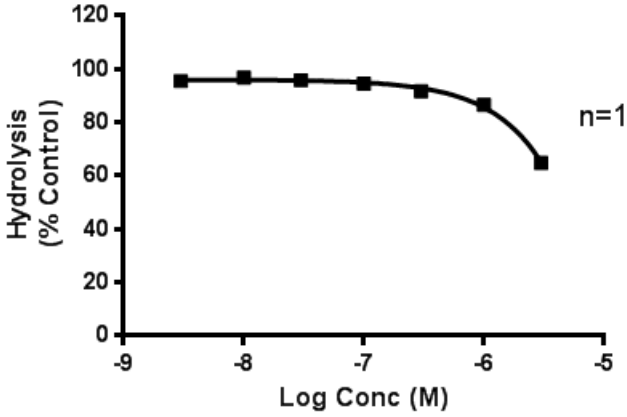


140

Compound 142

Autotaxin Assay



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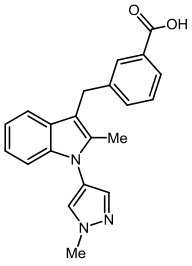
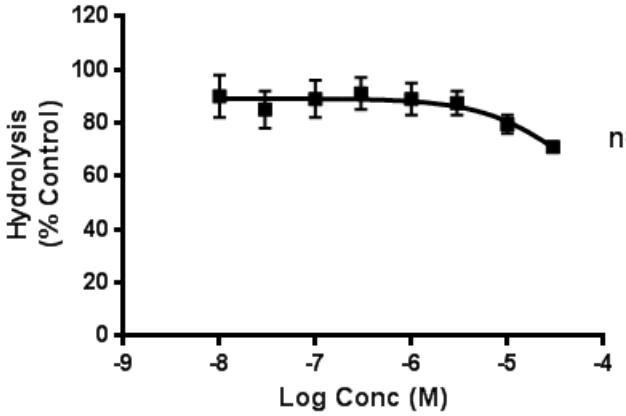


142

Compound 143

Autotaxin Assay



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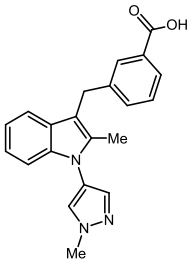
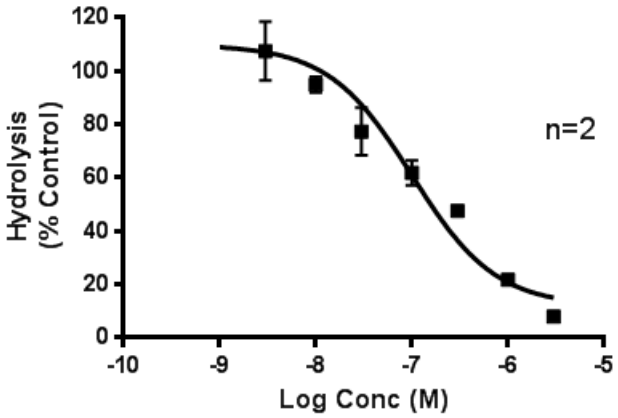
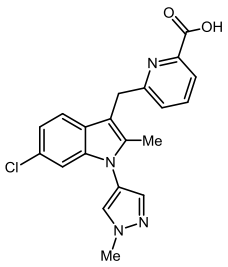


143

Compound 144

Autotaxin Assay

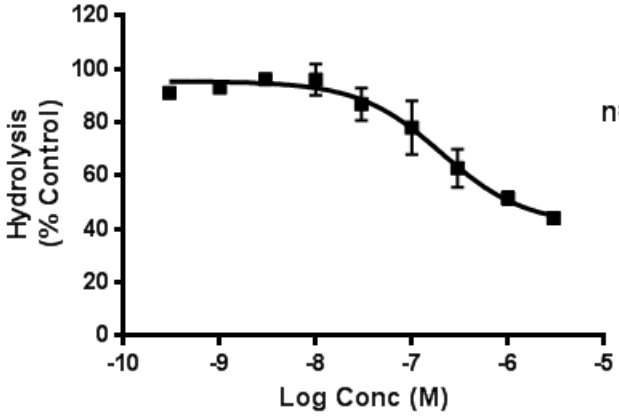


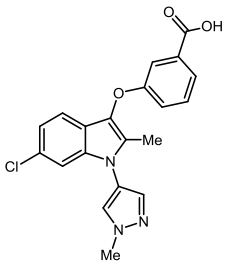


144

Compound 145

Autotaxin Assay

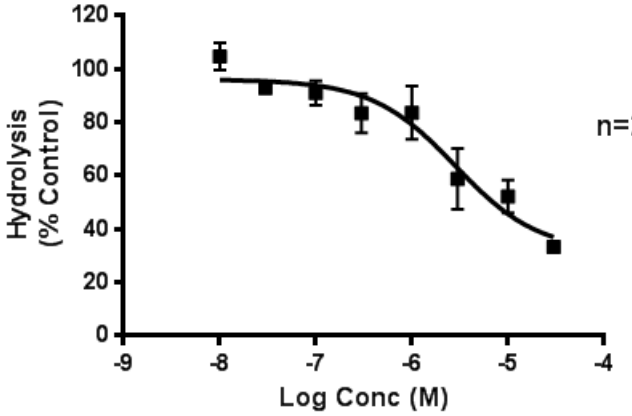


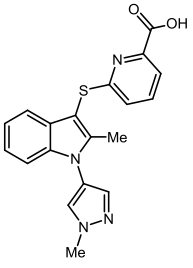


145

Compound 146

Autotaxin Assay

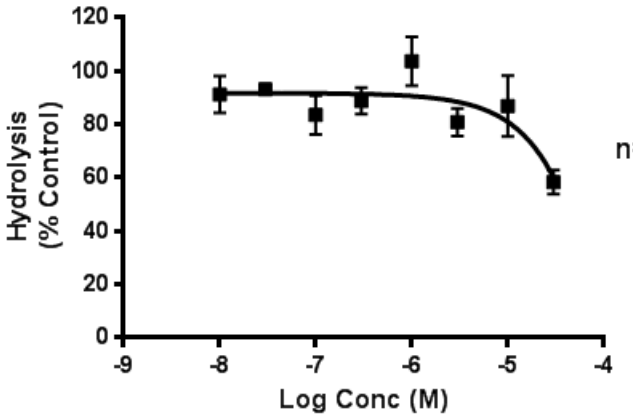




146

Compound 149

Autotaxin Assay



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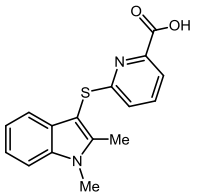
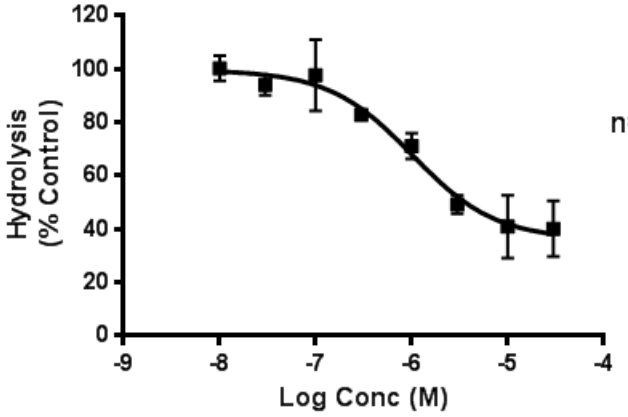


149

Compound 151

Autotaxin Assay



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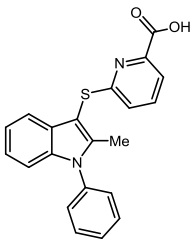
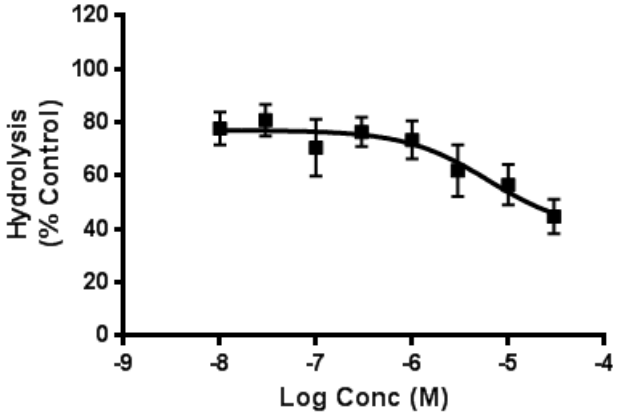


151

Compound 152

Autotaxin Assay



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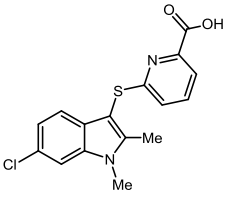
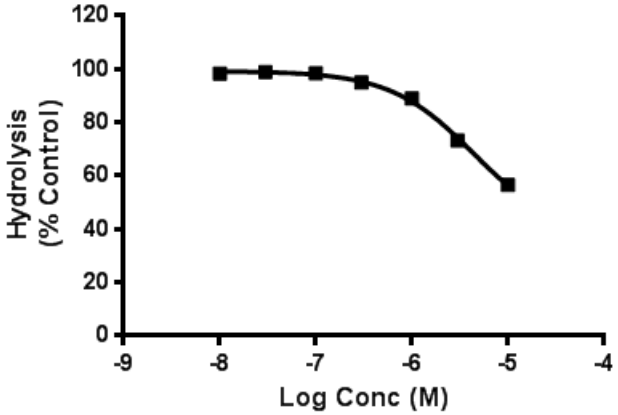
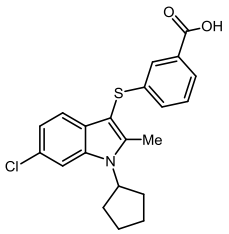


152

Compound 153

Autotaxin Assay

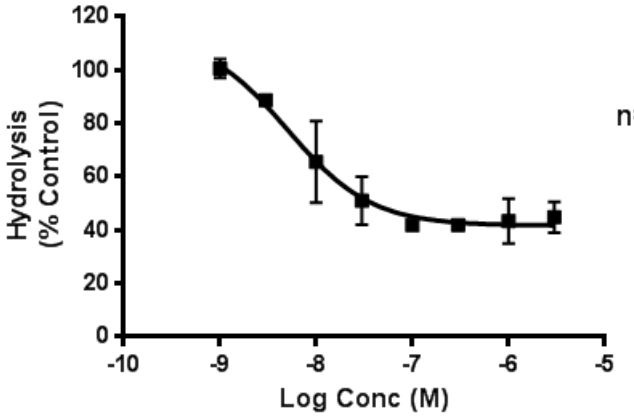




153

Compound 154

Autotaxin Assay



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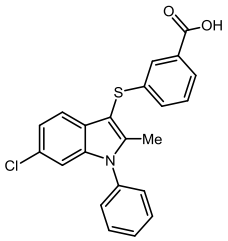
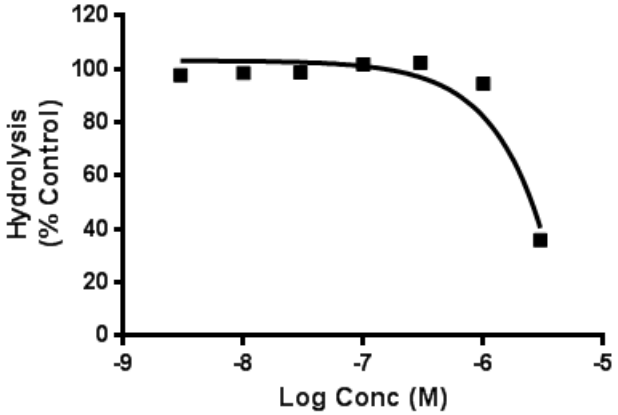
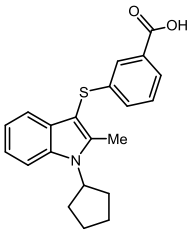


154

Compound 156

Autotaxin Assay

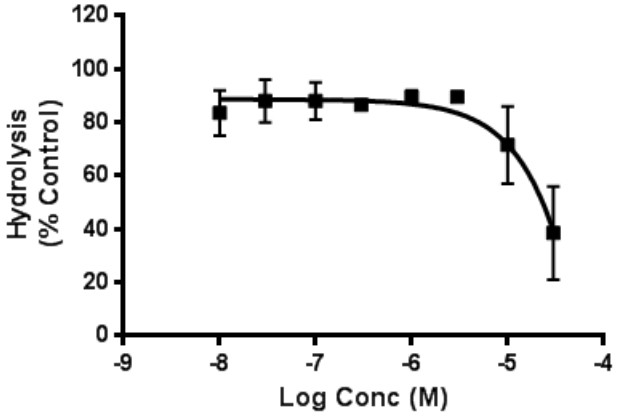




156

Compound 157

Autotaxin Assay



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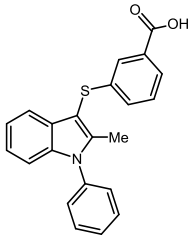
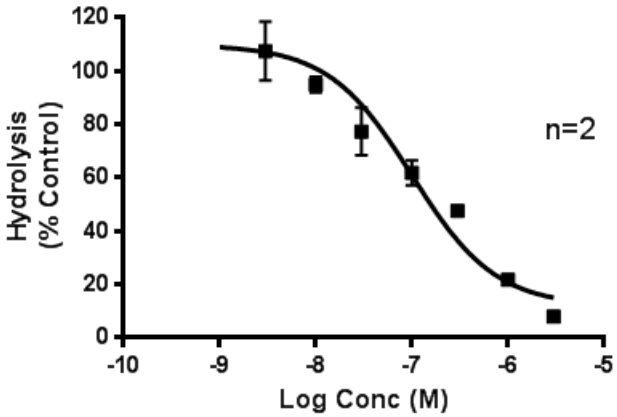


157

Compound 158

Autotaxin Assay



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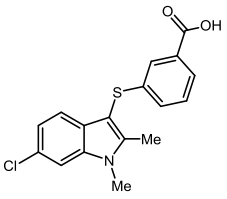
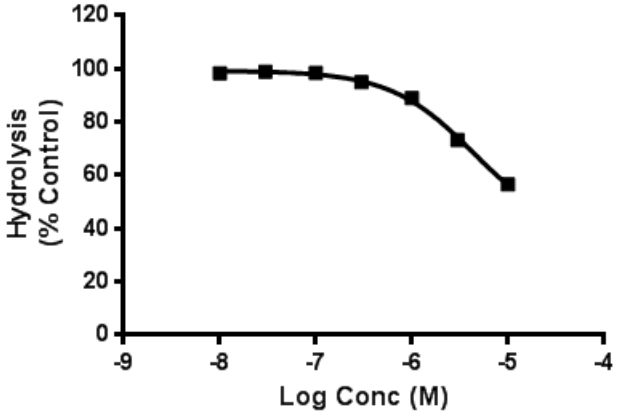
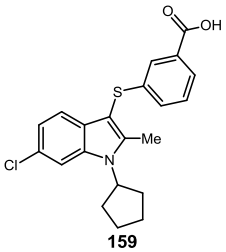


158

Compound 159

Autotaxin Assay

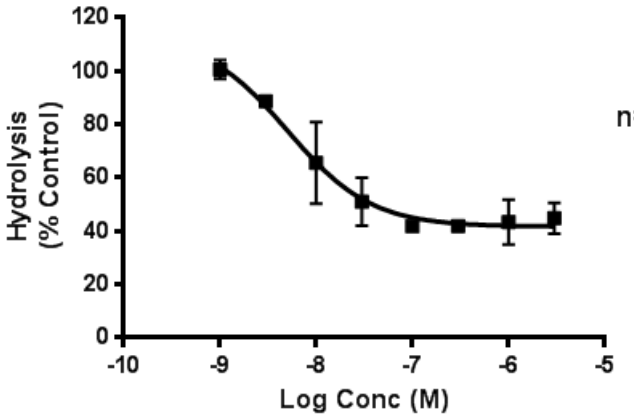




159

Compound 160

Autotaxin Assay



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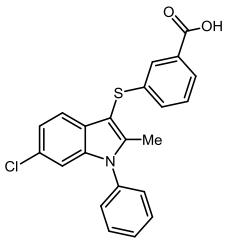
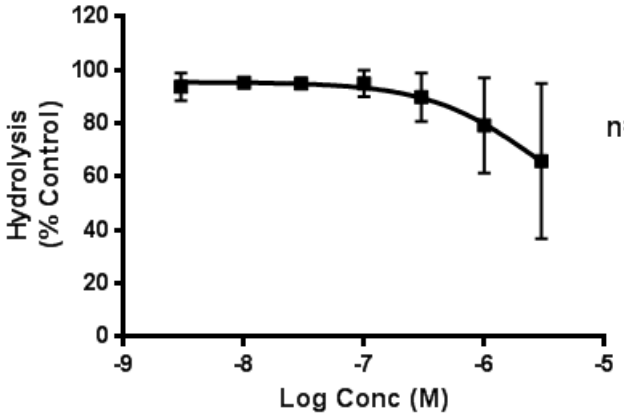


160

Compound 227

Autotaxin Assay



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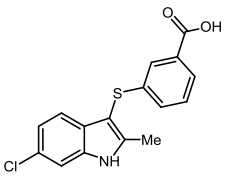

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3. LPC Assay Full Curve Data