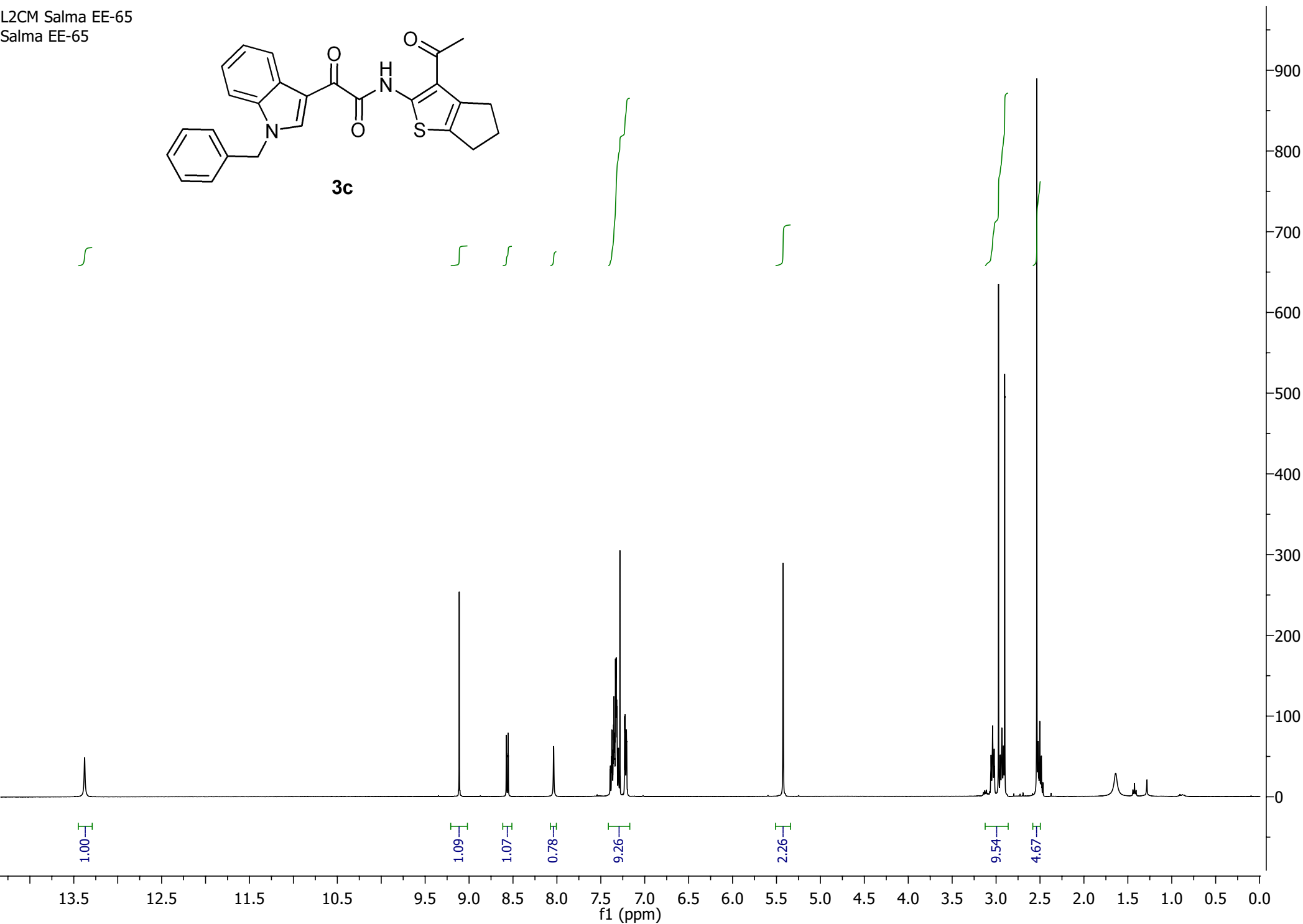
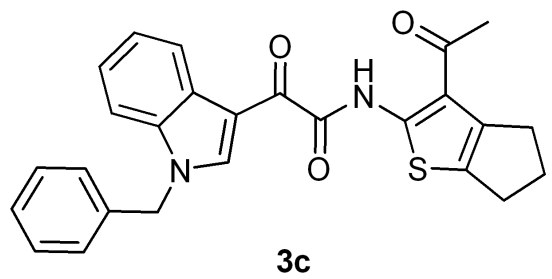
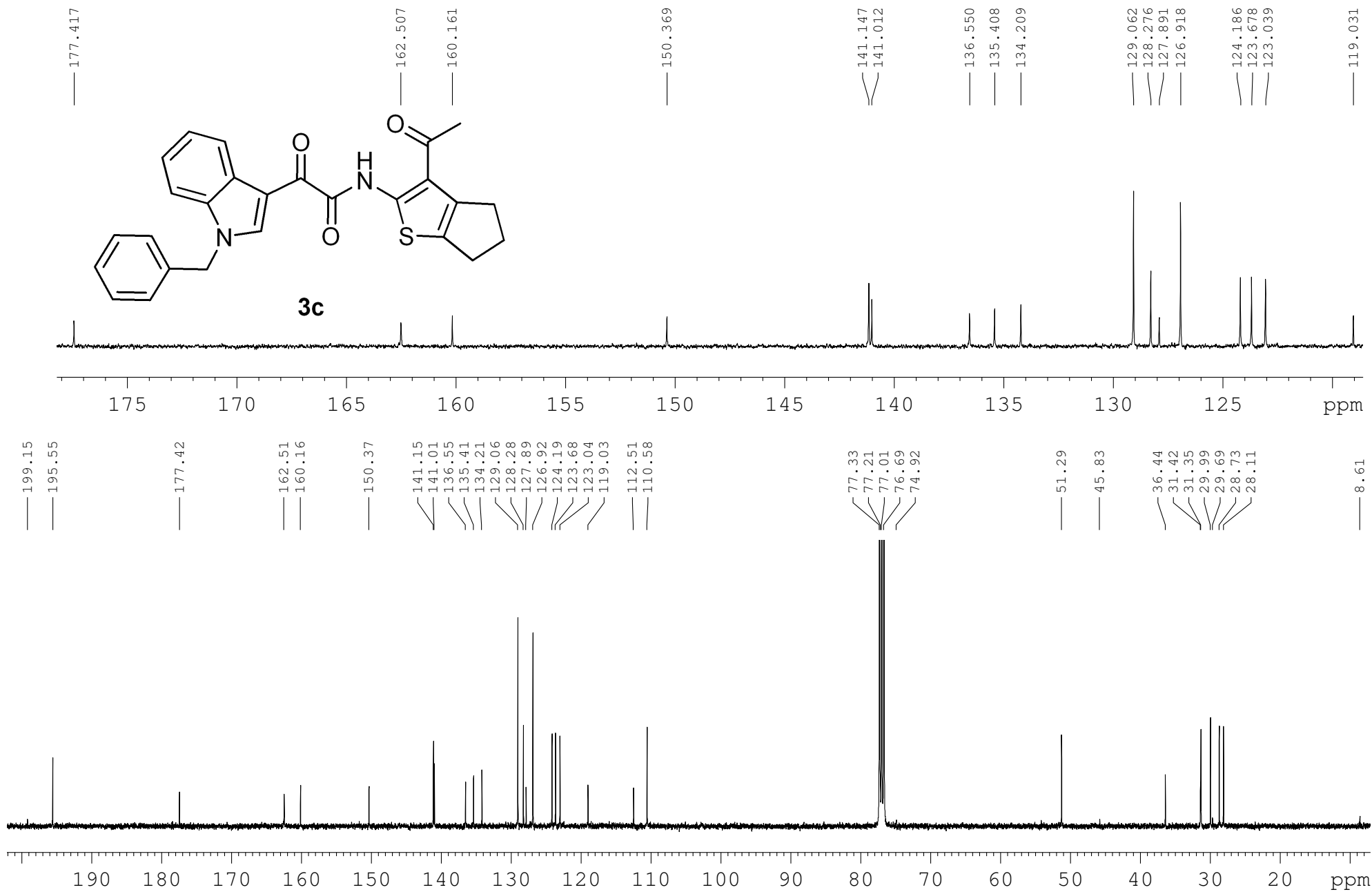


L2CM Salma EE-65
Salma EE-65



L2CM Salma EE-65 13C CPD



Mass Spectrum SmartFormula Report

Analysis Info

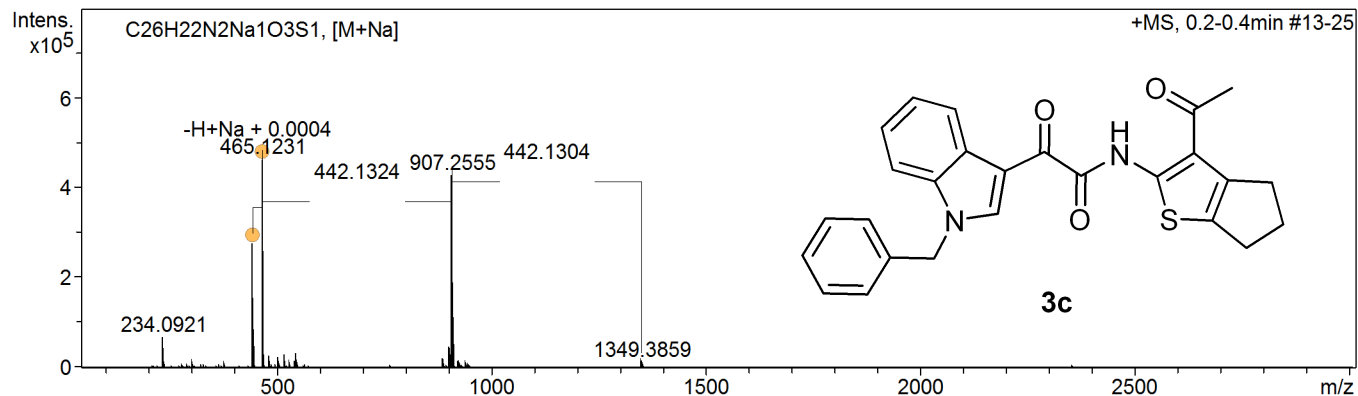
Analysis Name D:\Data\2018\180920000002.d
Method Tuneposlow.m
Sample Name 180913799///EE65
Comment CH2Cl2/MeOH

Acquisition Date 9/20/2018 3:05:08 PM

Operator fabien
Instrument micrOTOF-Q 228888.00098

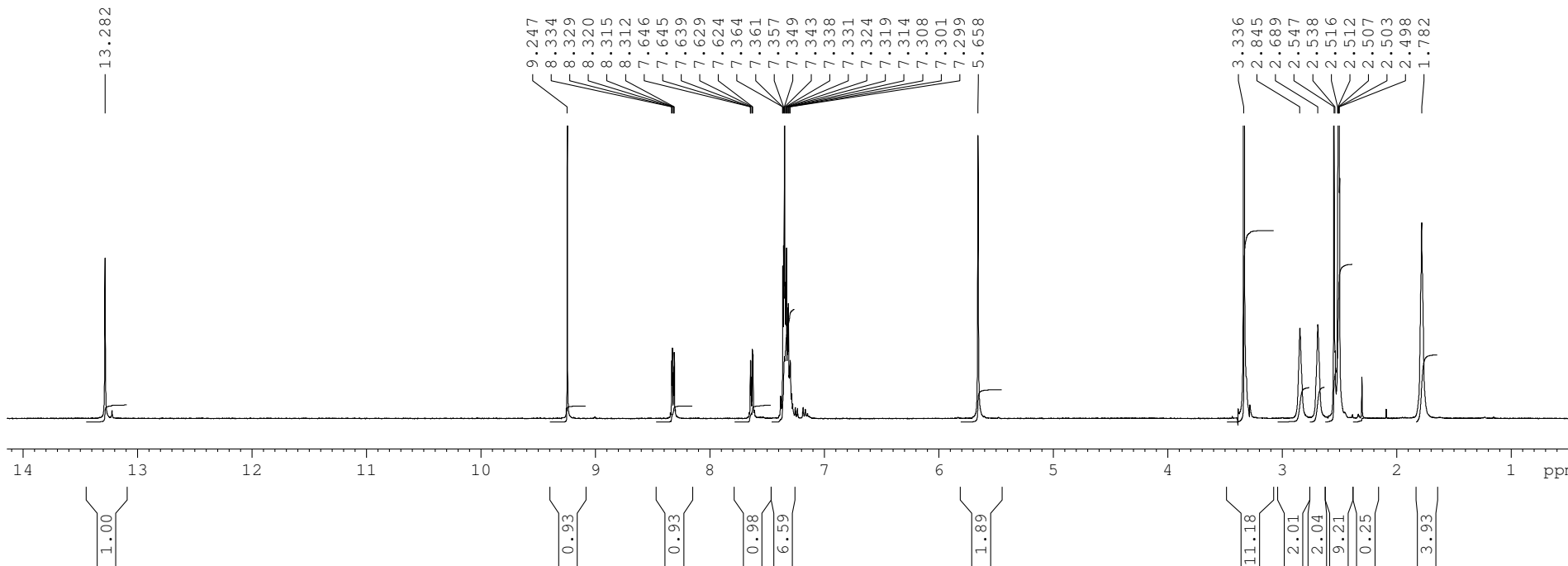
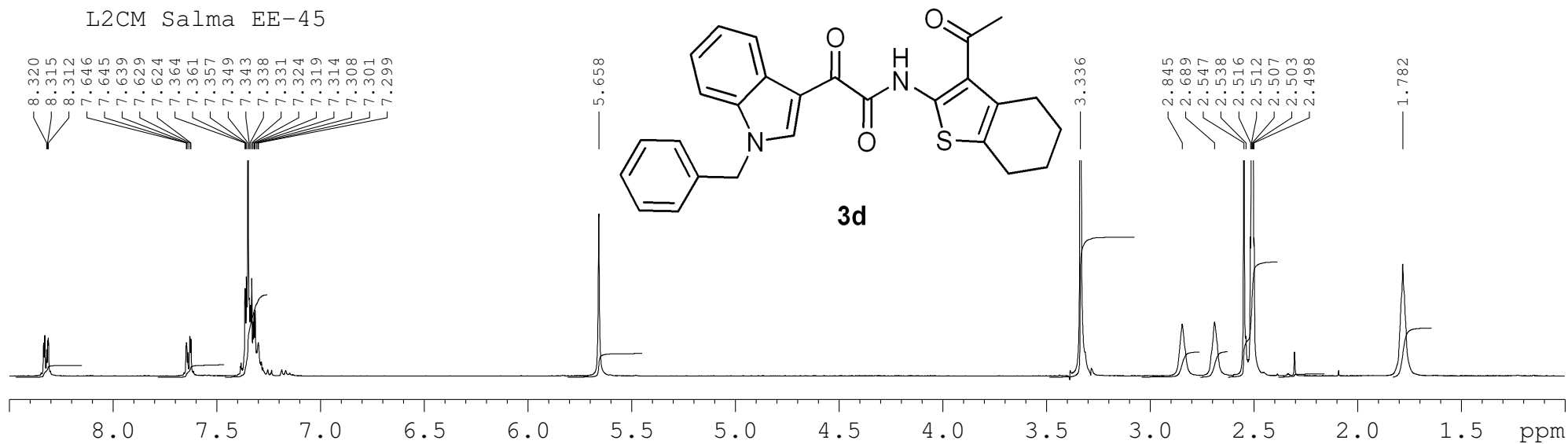
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	190 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Source

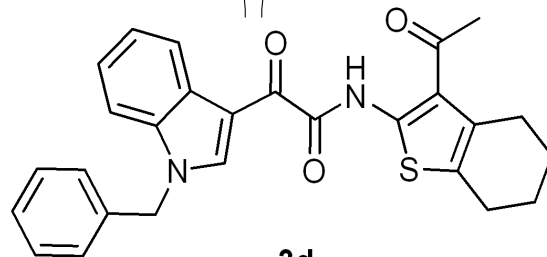


Meas. m/z	#	Ion Formula	m/z	err [mDa]	err [ppm]	mSigma	# mSigma	Score	rdB	e ⁻	Conf	N-Rule
443.1407	1	C26H23N2O3S	443.1424	1.7	3.7	3.5	1	100.00	16.5	even		ok
465.1231	1	C26H22N2NaO3S	465.1243	1.3	2.7	1.7	1	100.00	16.5	even		ok

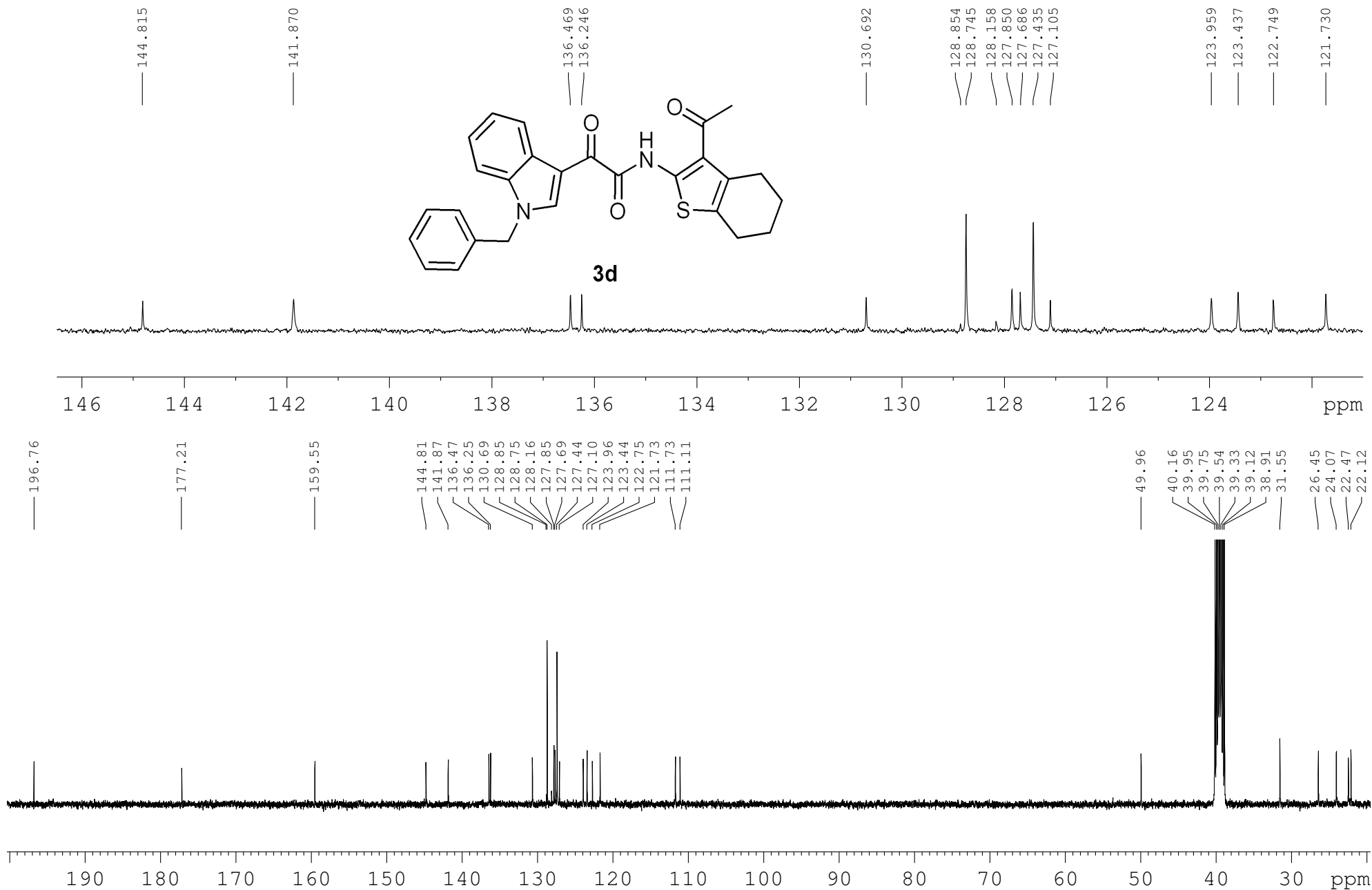
L2CM Salma EE-45



L2CM Salma EE-45 13cpd



3d



Mass Spectrum SmartFormula Report

Analysis Info

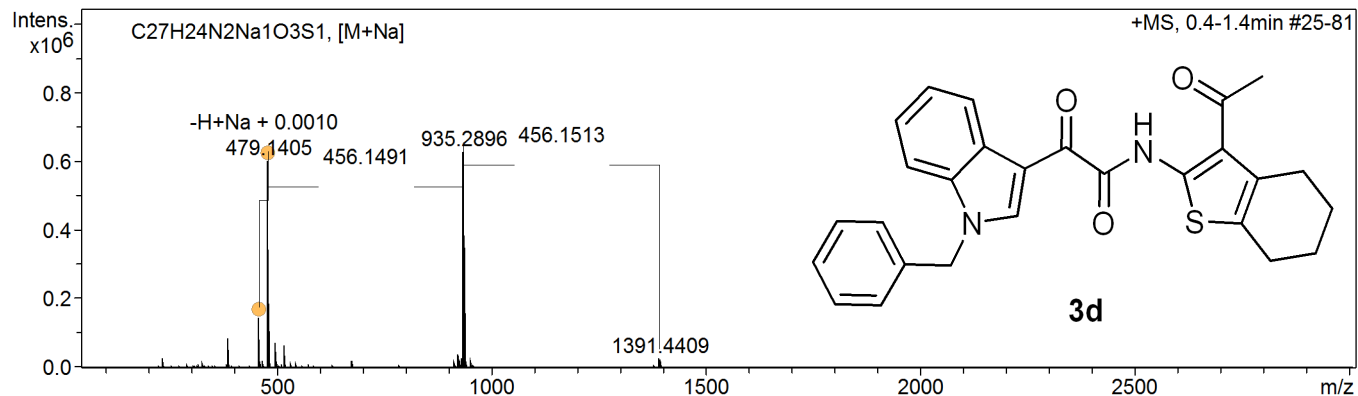
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Method Tuneposlow.m
Sample Name 180913800///EE45
Comment CH2Cl2/MeOH

Acquisition Date 9/20/2018 3:21:17 PM

Operator fabien
Instrument micrOTOF-Q 228888.00098

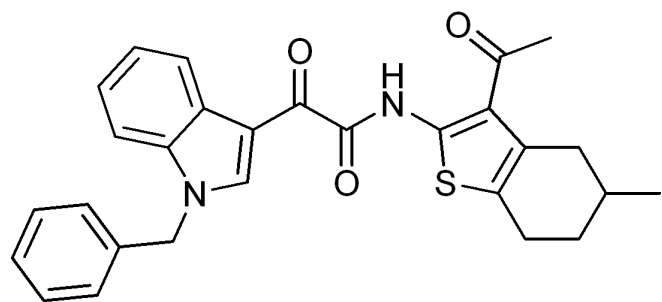
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	190 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Source

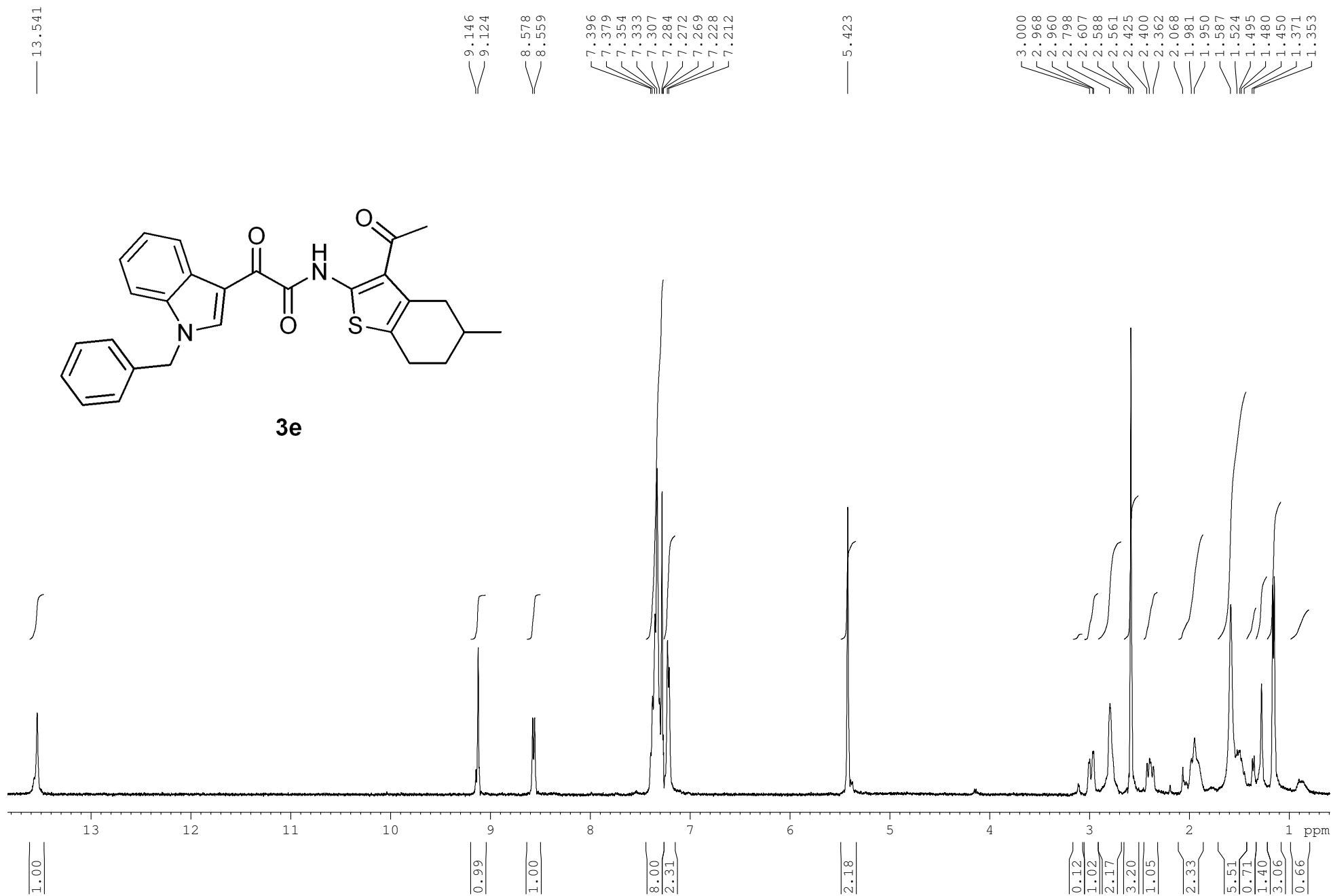


Meas. m/z	#	Ion Formula	m/z	err [mDa]	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻	Conf	N-Rule
457.1576	1	C ₂₇ H ₂₅ N ₂ O ₃ S	457.1580	0.4	0.9	4.3	1	100.00	16.5	even		ok
479.1405	1	C ₂₇ H ₂₄ N ₂ NaO ₃ S	479.1400	0.6	-1.2	1.5	1	100.00	16.5	even		ok

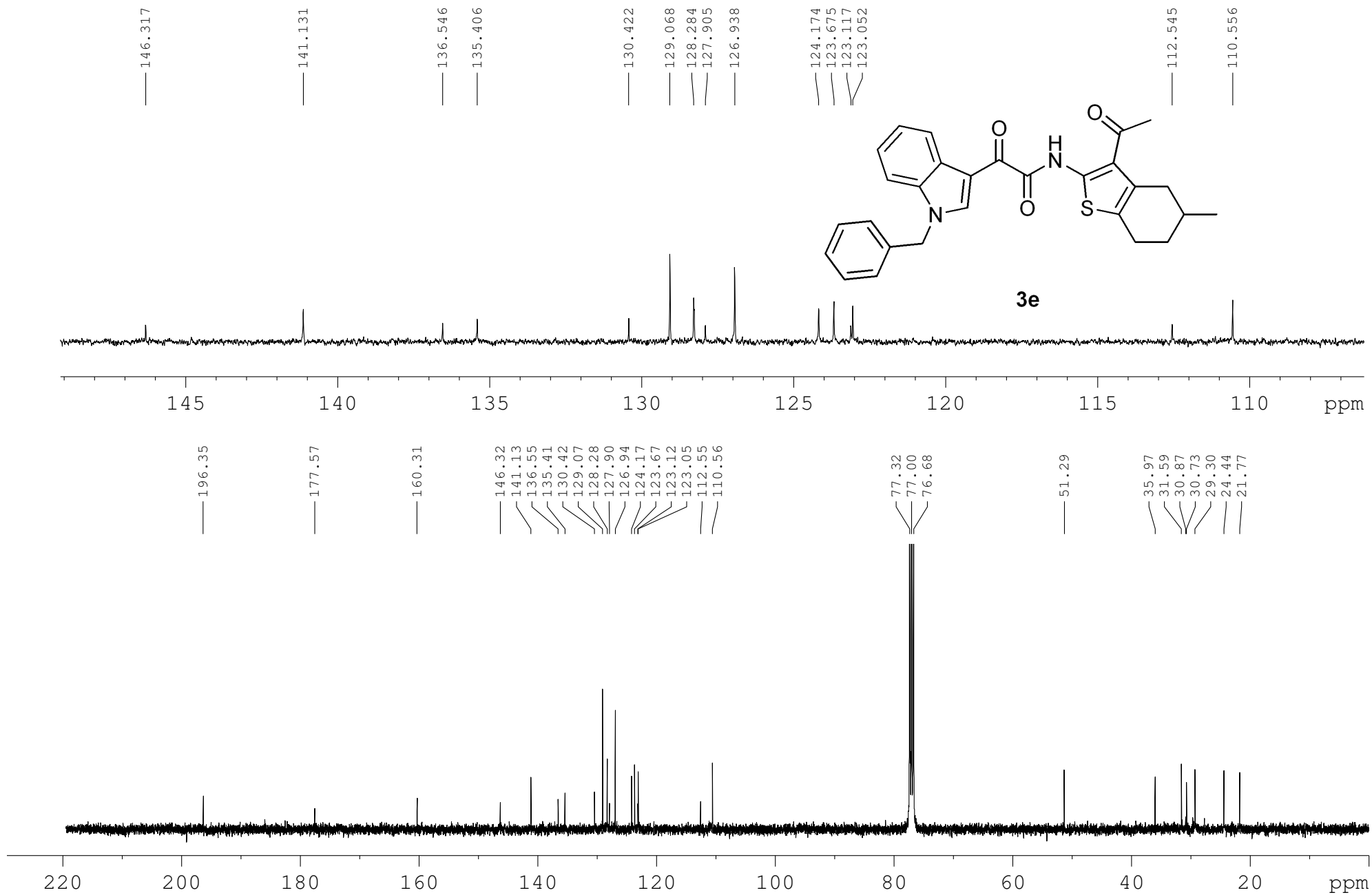
L2CM Salma AE-47



3e



L2CM Salma EE-47 ¹³C



Mass Spectrum SmartFormula Report

Analysis Info

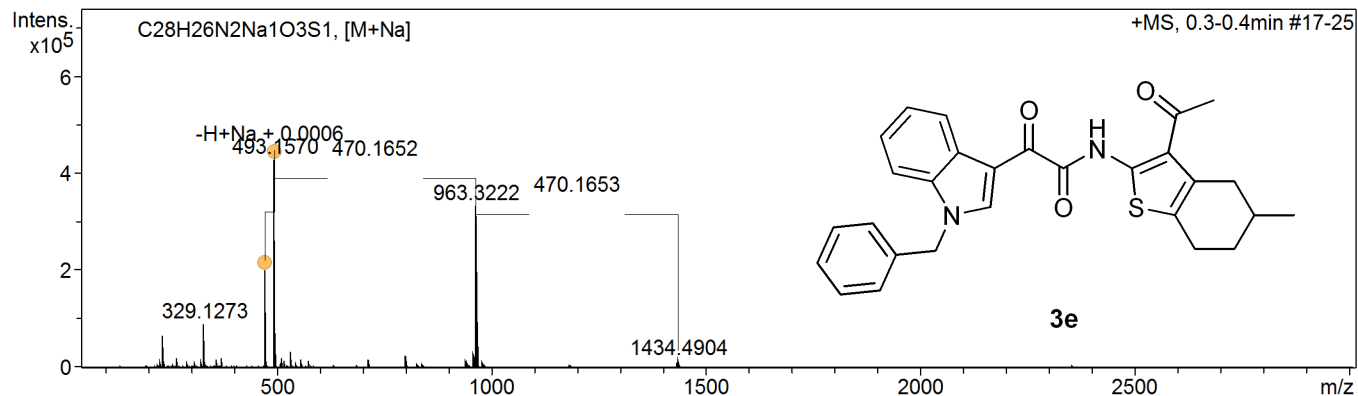
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 Method Tuneposlow.m
 Sample Name 180913801///EE47
 Comment CH2Cl2/MeOH

Acquisition Date 9/20/2018 3:36:36 PM

Operator fabien
 Instrument micrOTOF-Q 228888.00098

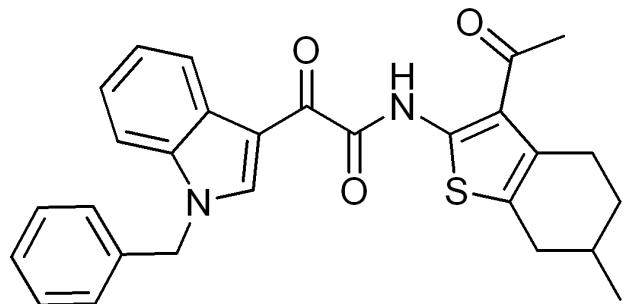
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	190 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Source

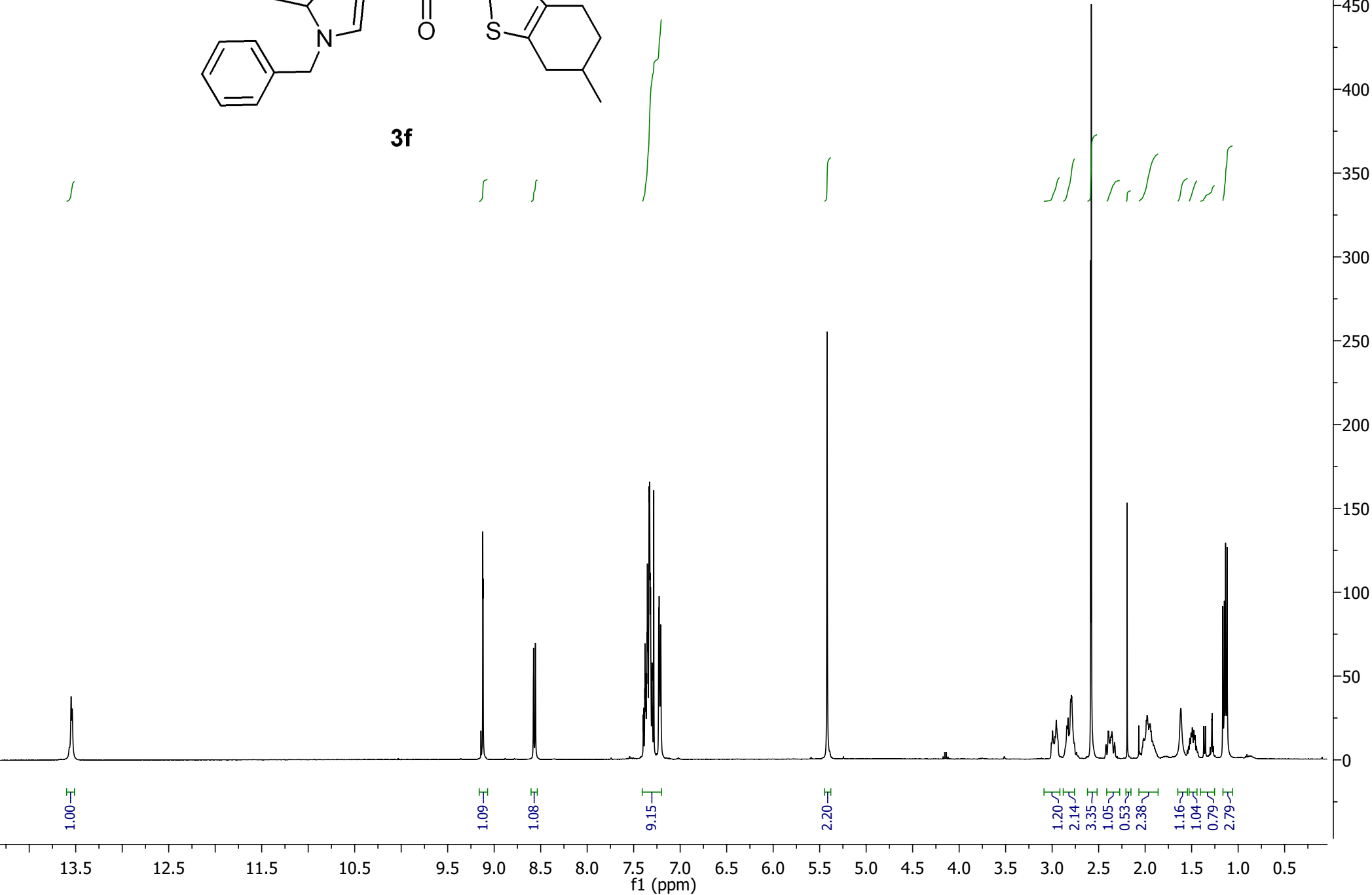


Meas. m/z	#	Ion Formula	m/z	err	[mDa]	err [ppm]	mSigma	# mSigma	Score	rdB	e ⁻	Conf	N-Rule
471.1744	1	C28H27N2O3S	471.1737	0.7	0.7	-1.5	5.5	1	100.00	16.5	even	ok	ok
493.1570	1	C28H26N2NaO3S	493.1556	1.4	1.4	-2.8	5.7	1	100.00	16.5	even	ok	ok

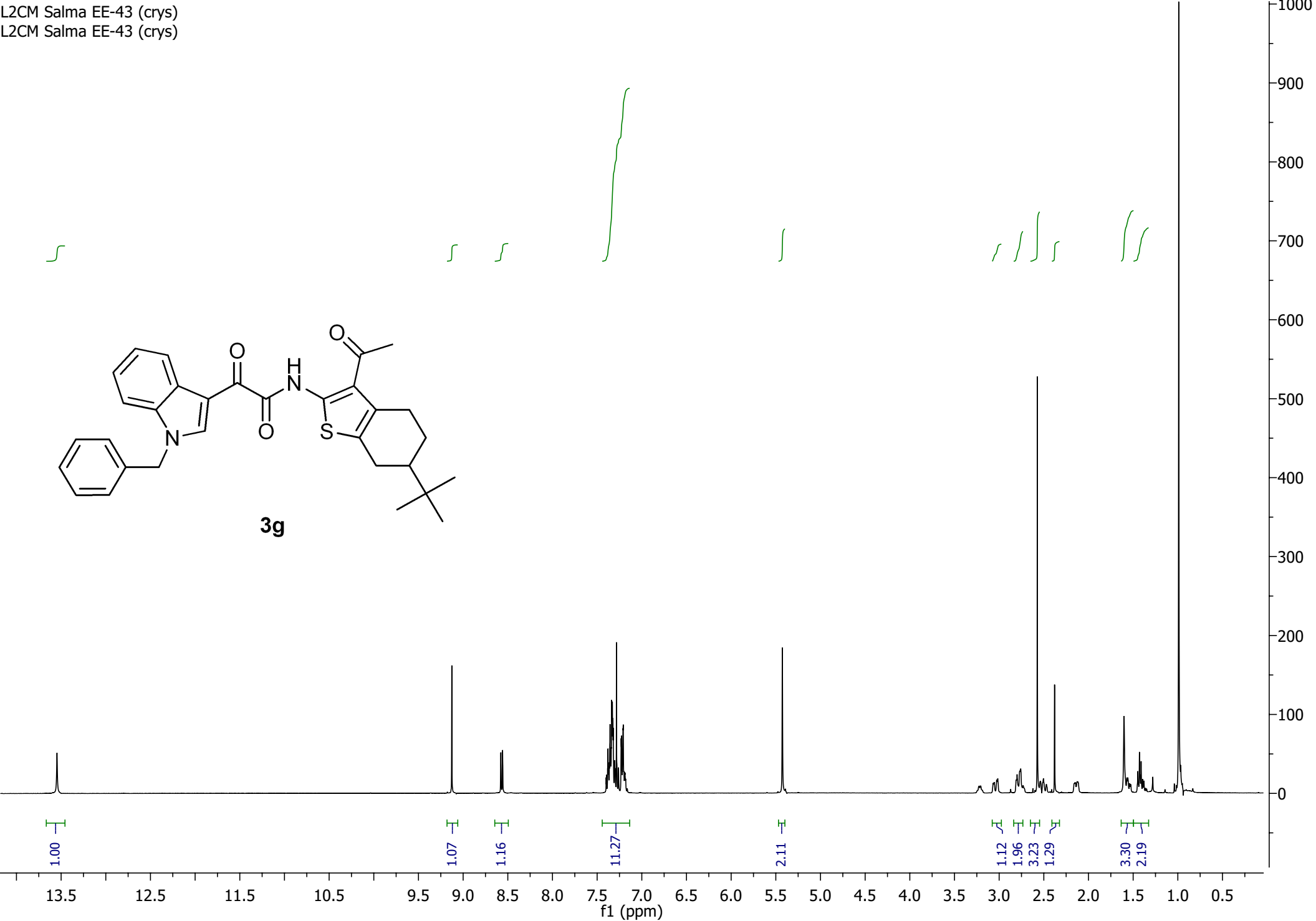
L2CM Salma EE-46
L2CM Salma EE-46



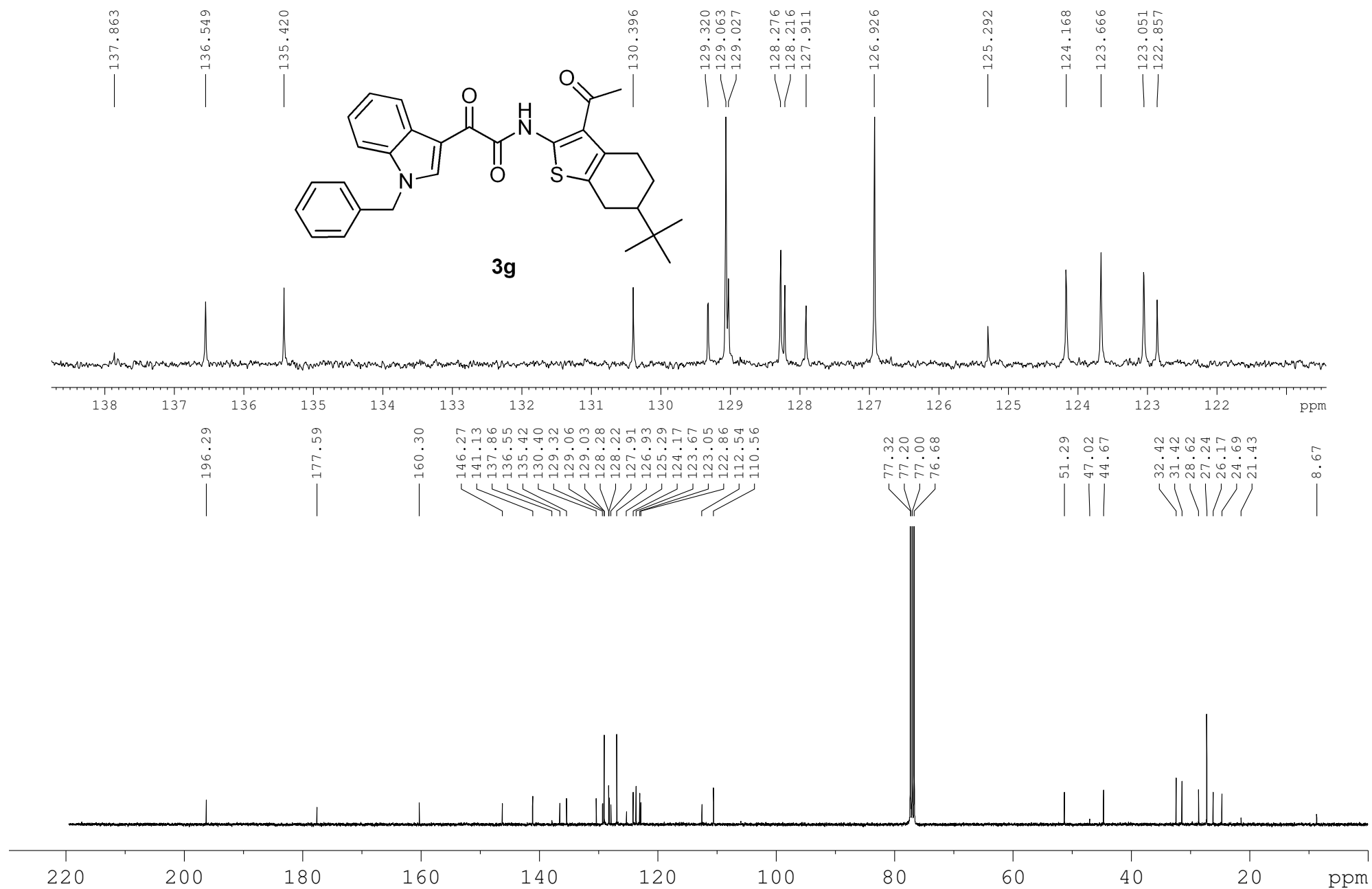
3f



L2CM Salma EE-43 (crys)
L2CM Salma EE-43 (crys)



L2CM Salma EE-43 (crys) ¹³C



Display Report

Analysis Info

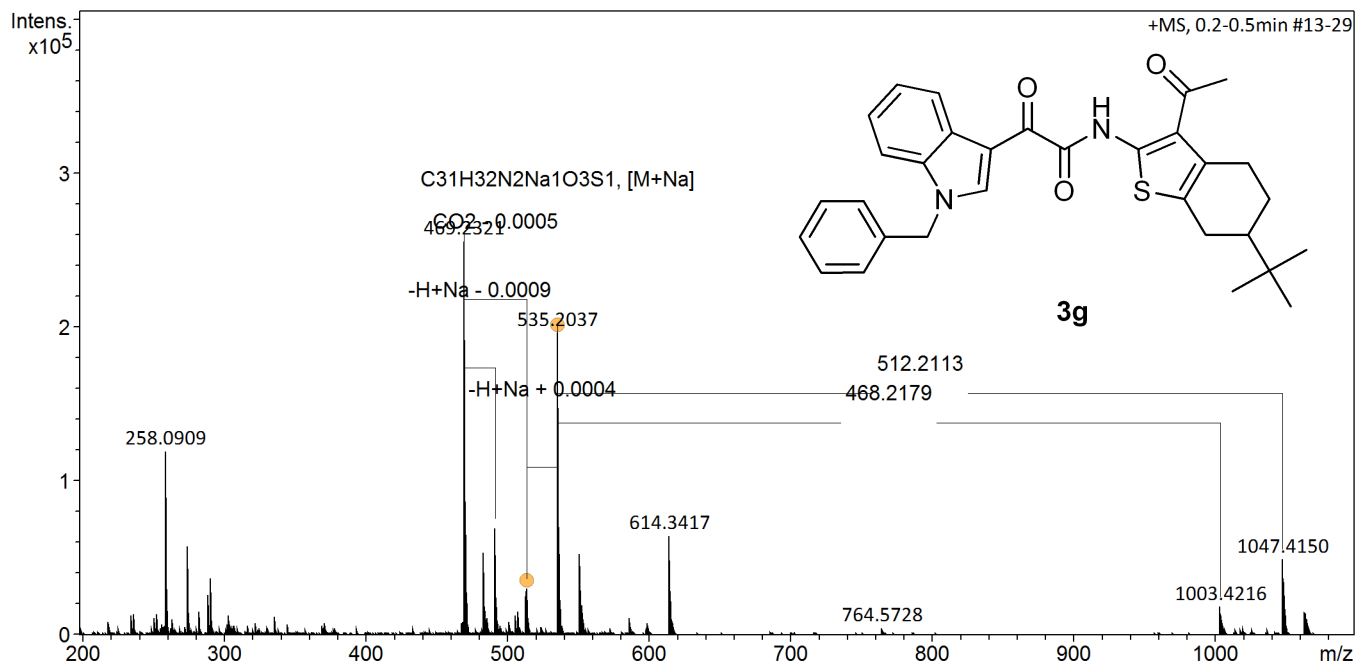
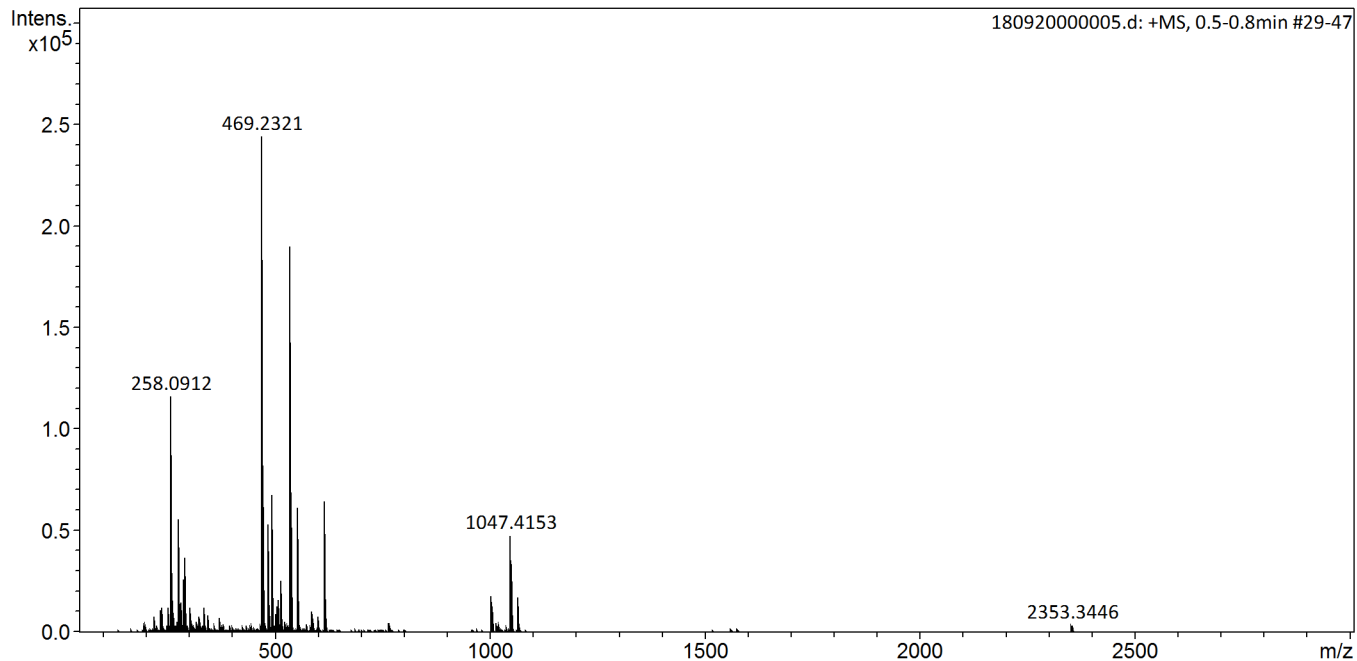
Analysis Name D:\Data\2018\180920000005.d
Method Tuneposlow.m
Sample Name 180913802///EE43
Comment CH2Cl2/MeOH

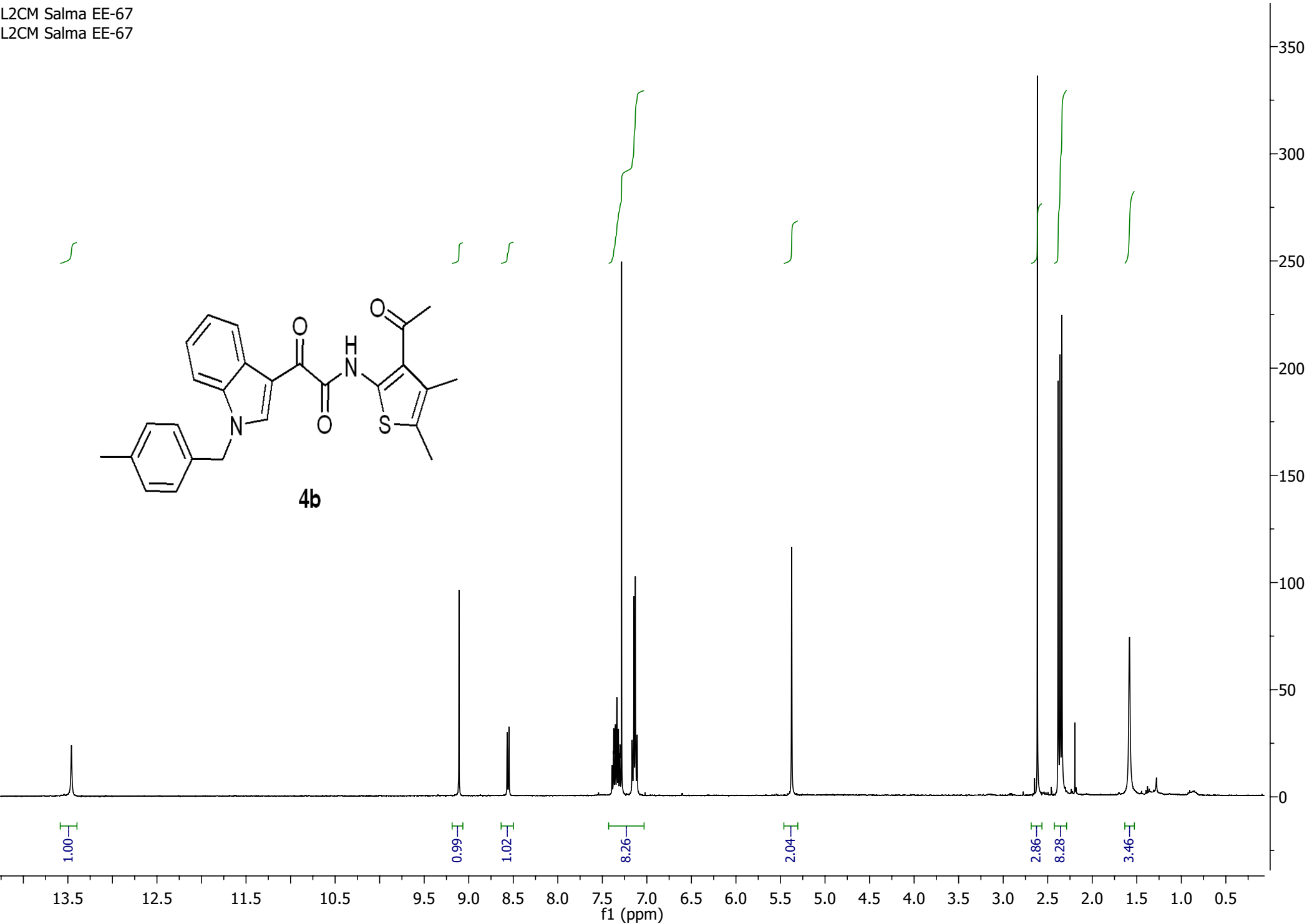
Acquisition Date 9/20/2018 3:56:39 PM

Operator fabien
Instrument micrOTOF-Q 228888.00098

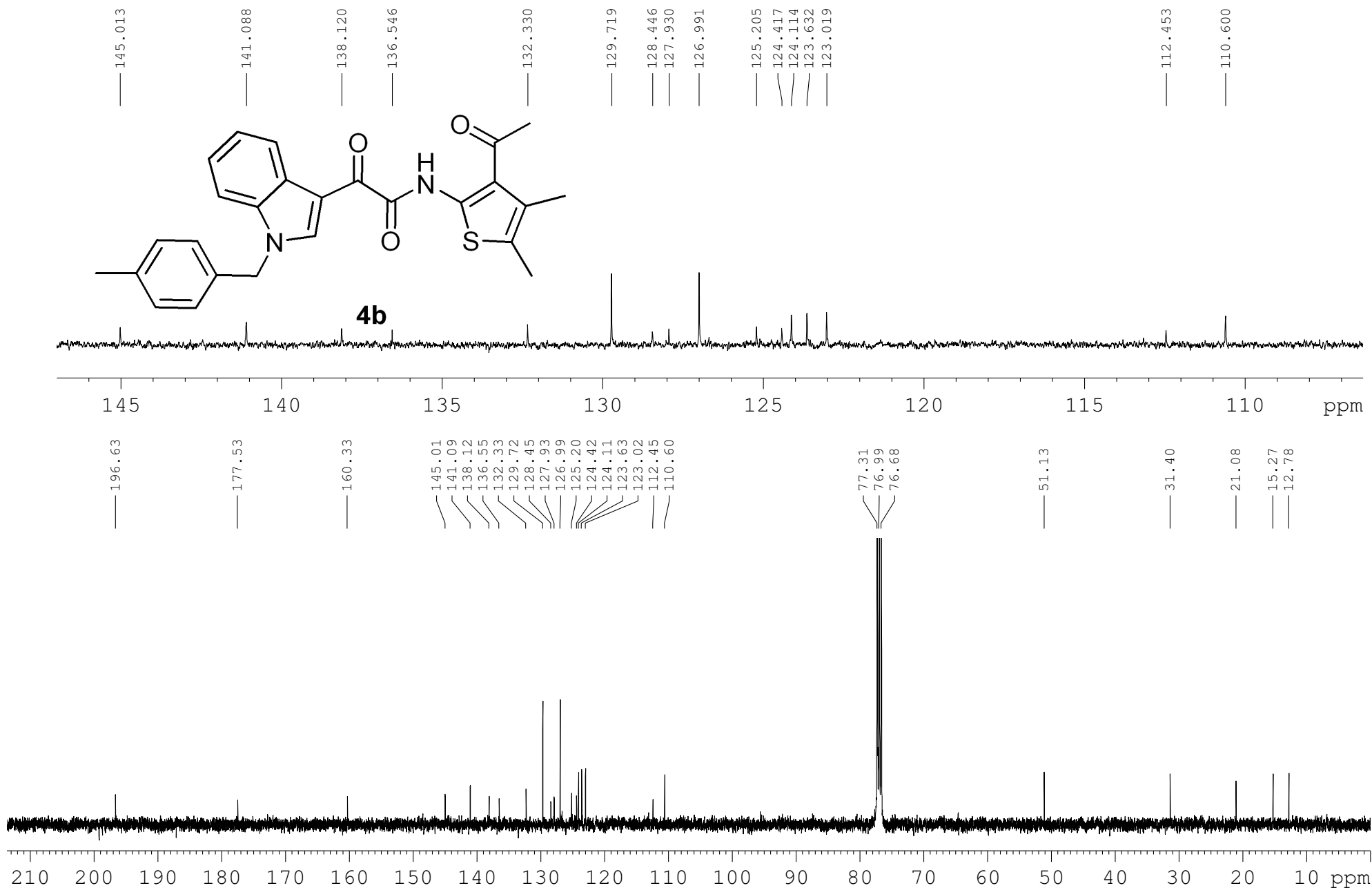
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	190 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Source





L2CM Salma EE-67 13cpd



Mass Spectrum SmartFormula Report

Analysis Info

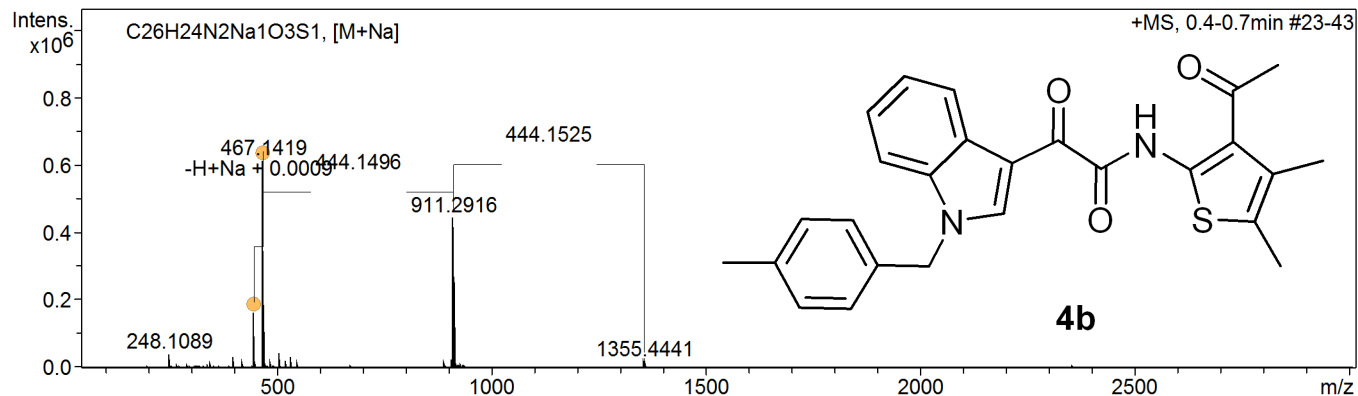
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Method Tuneposlow.m
Sample Name 180913804///EE67
Comment CH2Cl2/MeOH

Acquisition Date 9/20/2018 4:41:19 PM

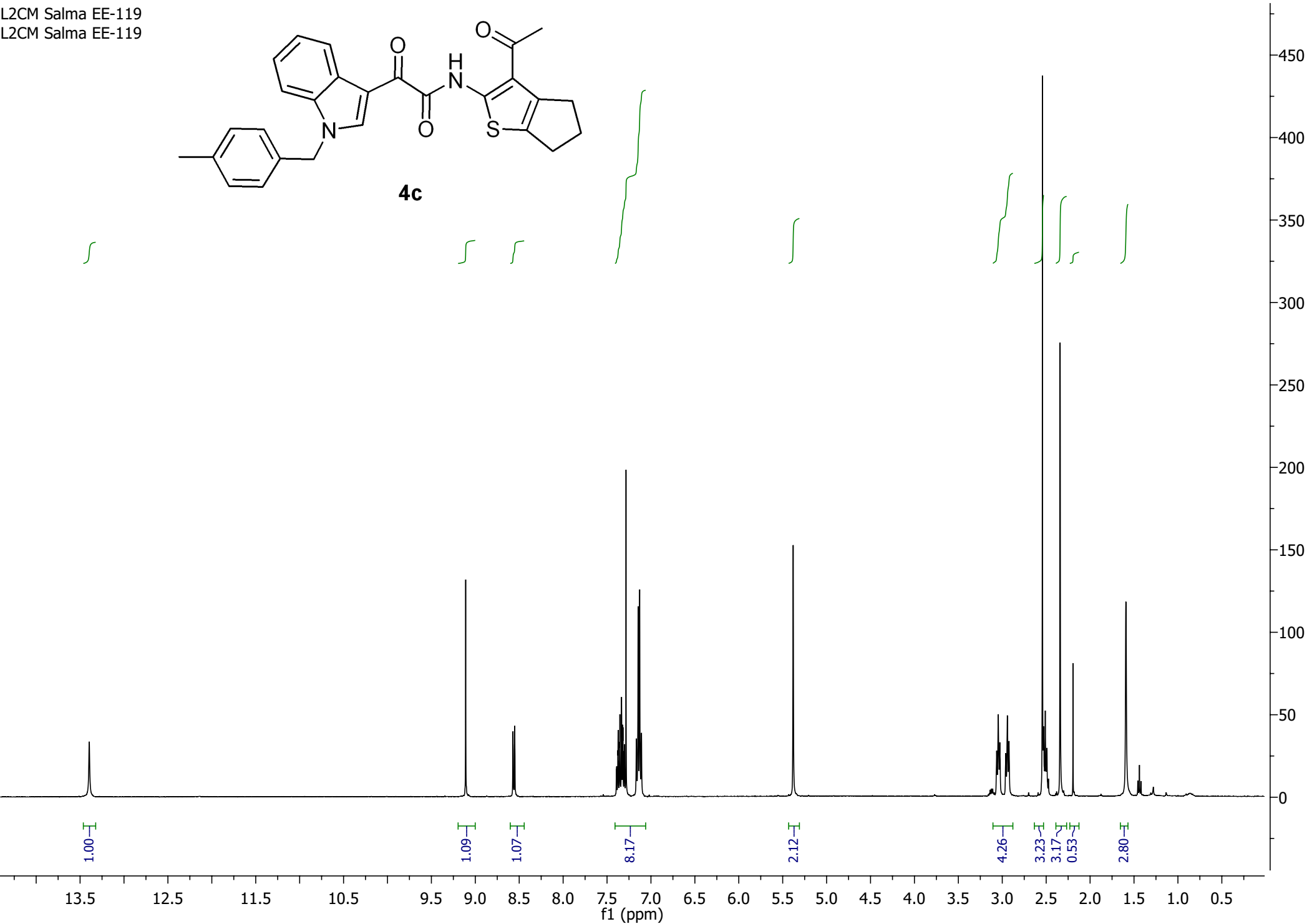
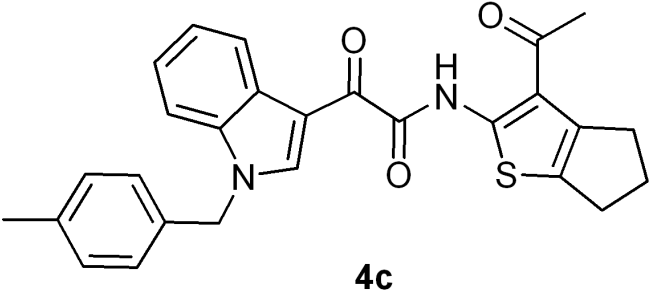
Operator fabien
Instrument micrOTOF-Q 228888.00098

Acquisition Parameter

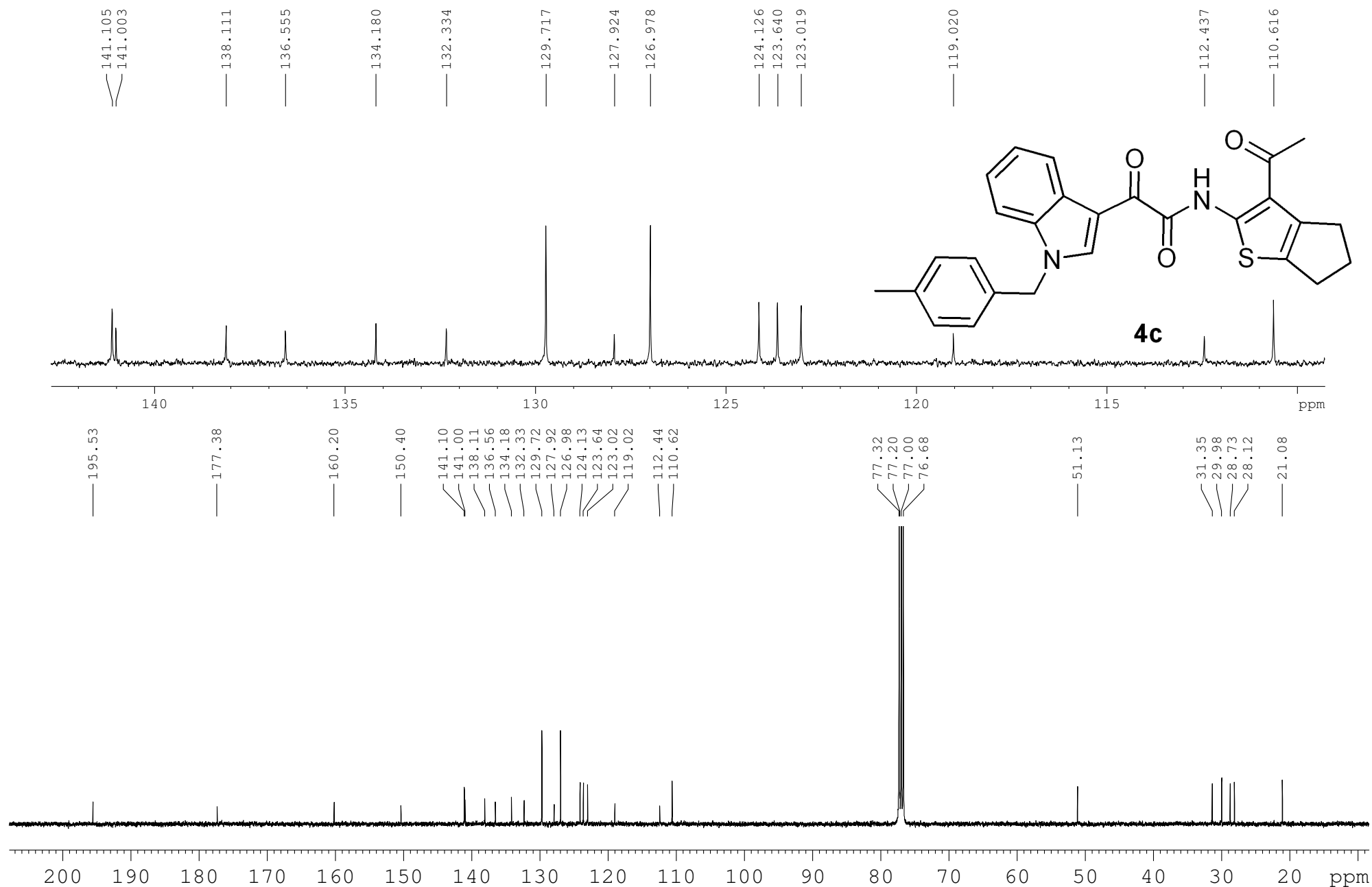
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	190 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Source



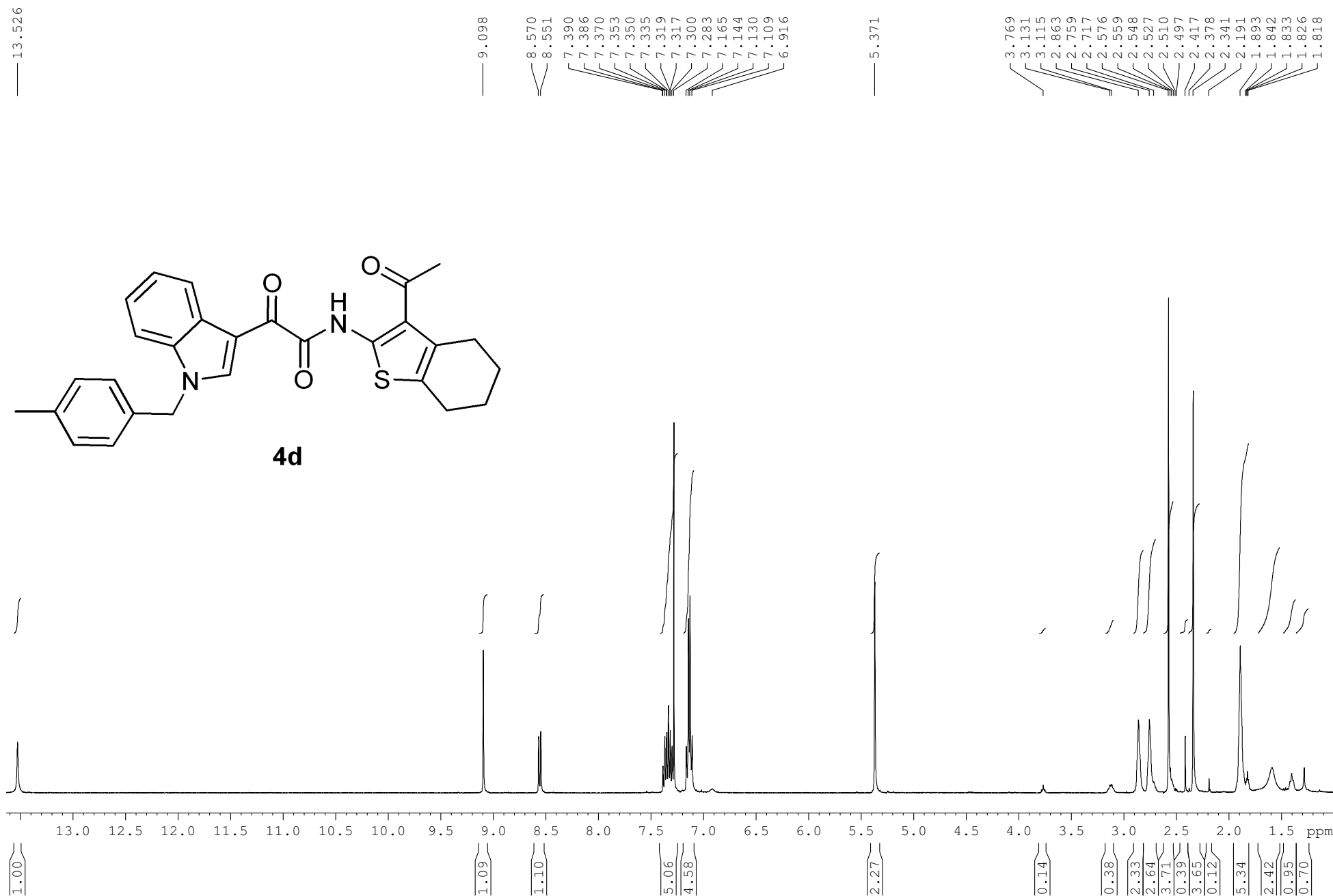
Meas. m/z	#	Ion Formula	m/z	err [mDa]	err [ppm]	mSigma	# mSigma	Score	rdB	e ⁻	Conf	N-Rule
445.1590	1	C26H25N2O3S	445.1580	1.0	-2.2	2.2	1	100.00	15.5	even		ok
467.1419	1	C26H24N2NaO3S	467.1400	1.9	-4.1	2.4	1	100.00	15.5	even		ok



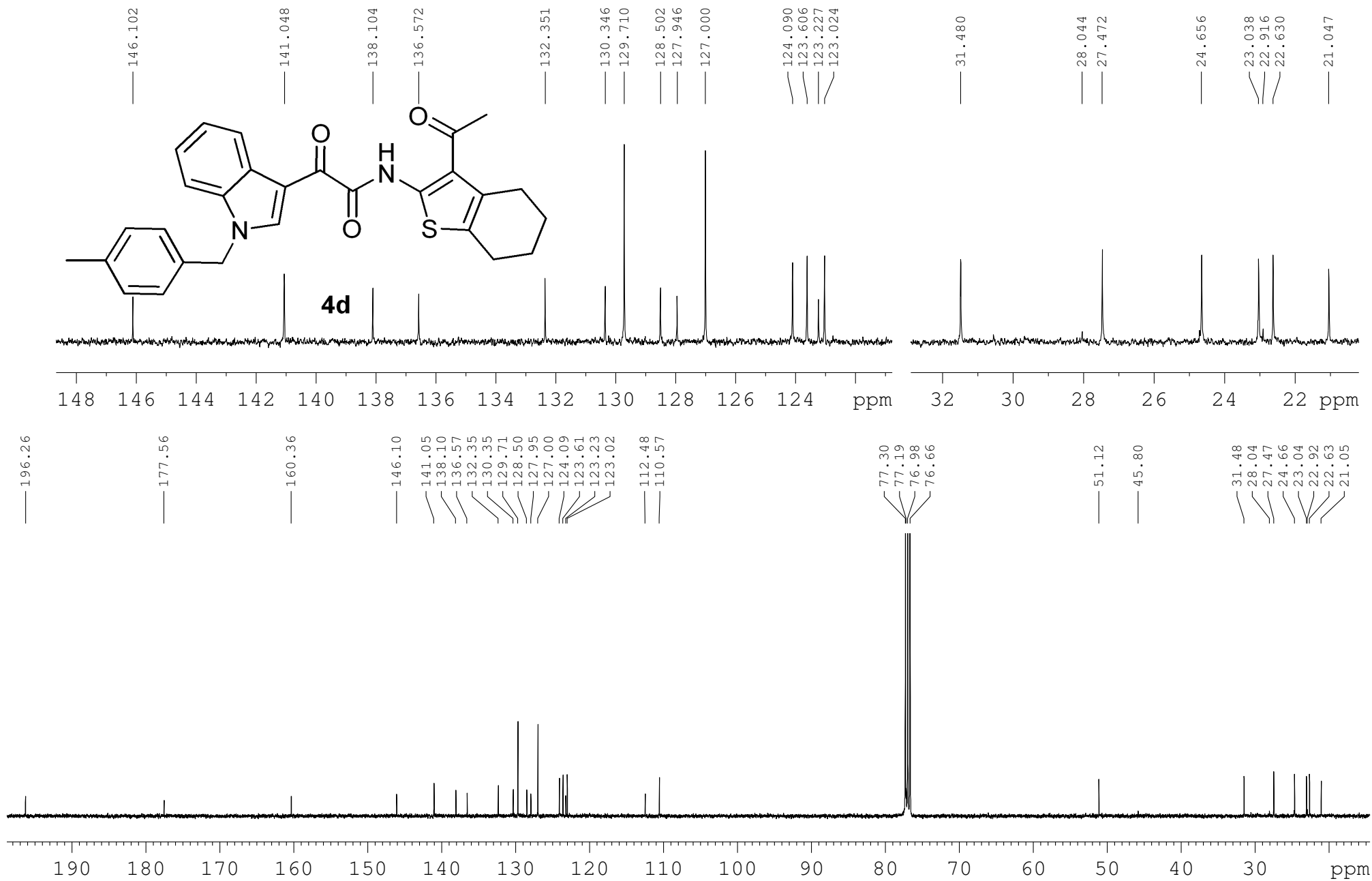
L2CM Salma EE-119 13cpd



L2CM Salma EE-69



L2CM Salma EE-69 13C



Mass Spectrum SmartFormula Report

Analysis Info

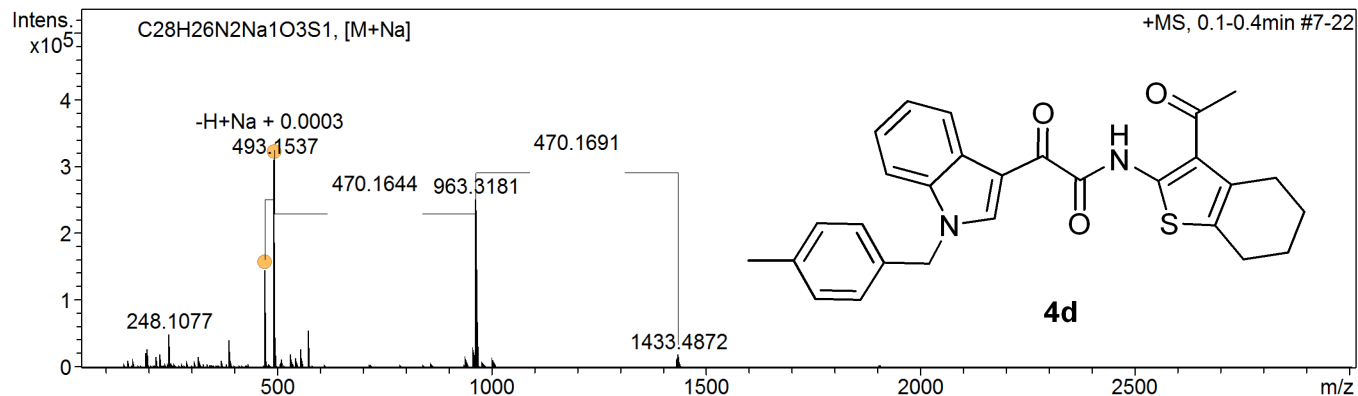
Analysis Name D:\Data\2018\180924000001.d
Method Tuneposlow.m
Sample Name 180913805///EE-69
Comment MeOH/CH₂Cl₂

Acquisition Date 9/24/2018 11:53:25 AM

Operator fabien
Instrument micrOTOF-Q 228888.00098

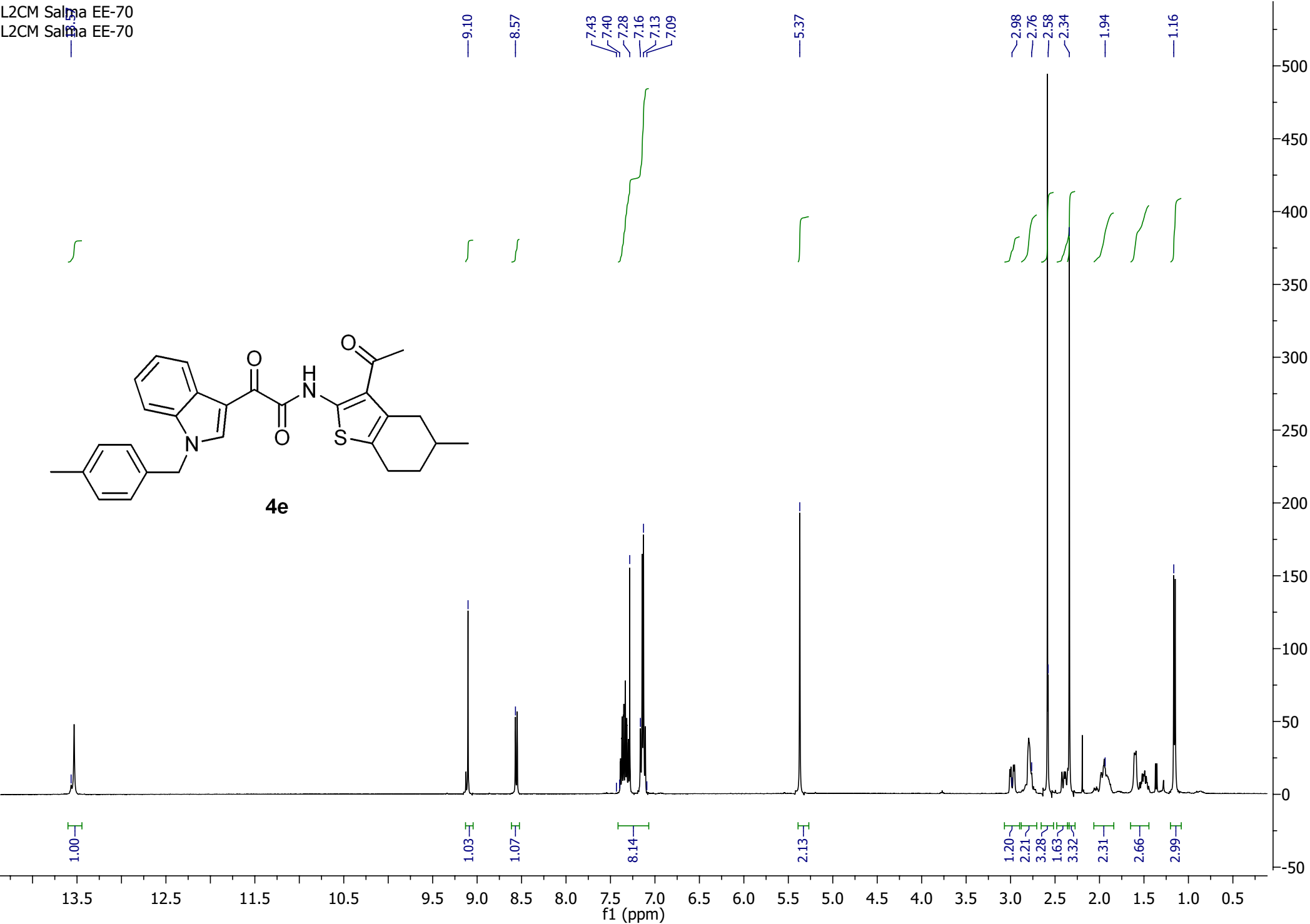
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	190 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Source

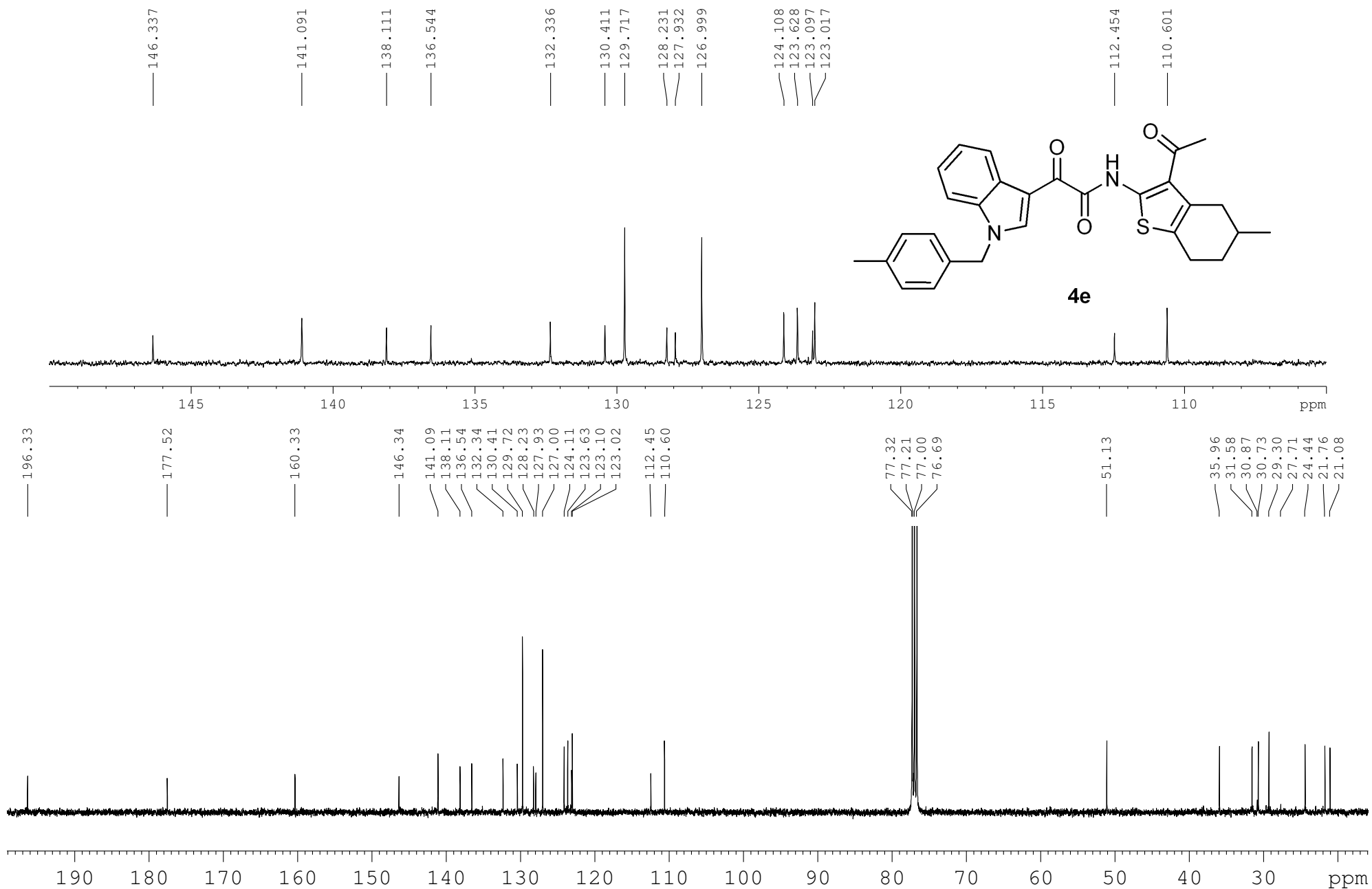


Meas. m/z	#	Ion Formula	m/z	err	[mDa]	err [ppm]	mSigma	# mSigma	Score	rdB	e ⁻	Conf	N-Rule
471.1715	1	C28H27N2O3S	471.1737	2.2		4.7	3.7	1	100.00	16.5	even		ok
493.1537	1	C28H26N2NaO3S	493.1556	1.9		3.8	1.5	1	100.00	16.5	even		ok

L2CM Salma EE-70
L2CM Salma EE-70



L2CM Salma EE-70 13C



Mass Spectrum SmartFormula Report

Analysis Info

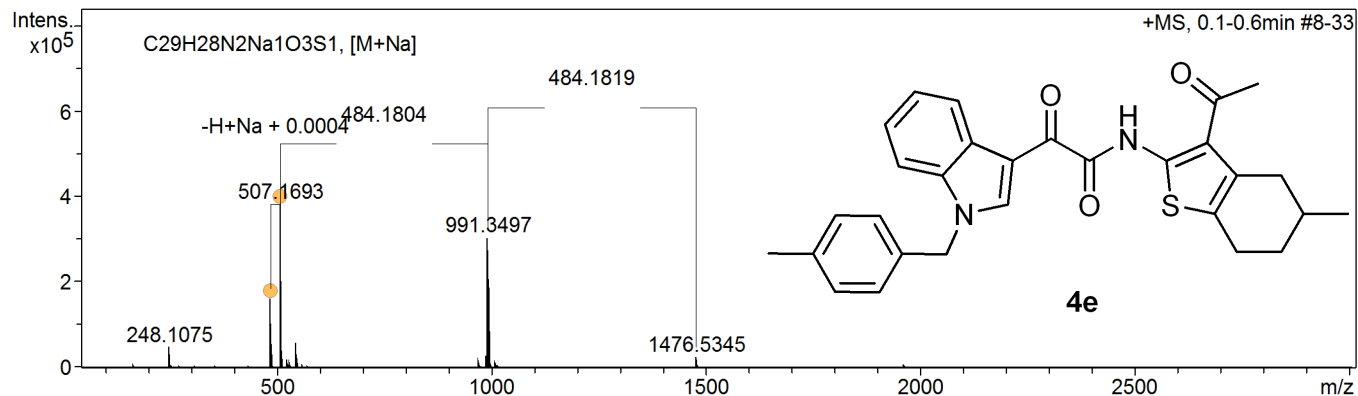
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 Method Tuneposlow.m
 Sample Name 180913806///EE-70
 Comment MeOH/CH₂Cl₂

Acquisition Date 9/24/2018 12:02:18 PM

Operator fabien
 Instrument micrOTOF-Q 228888.00098

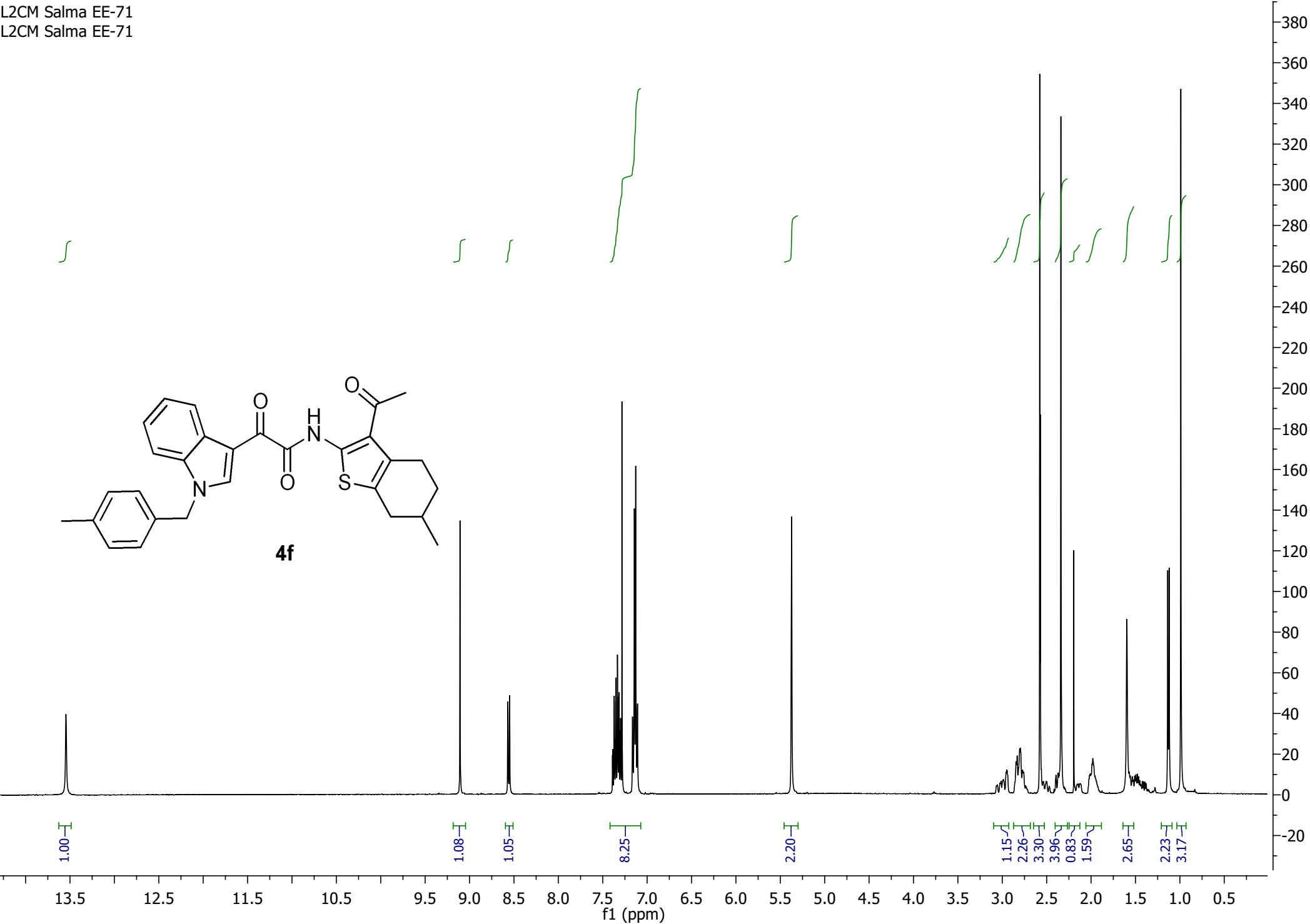
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	190 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Source

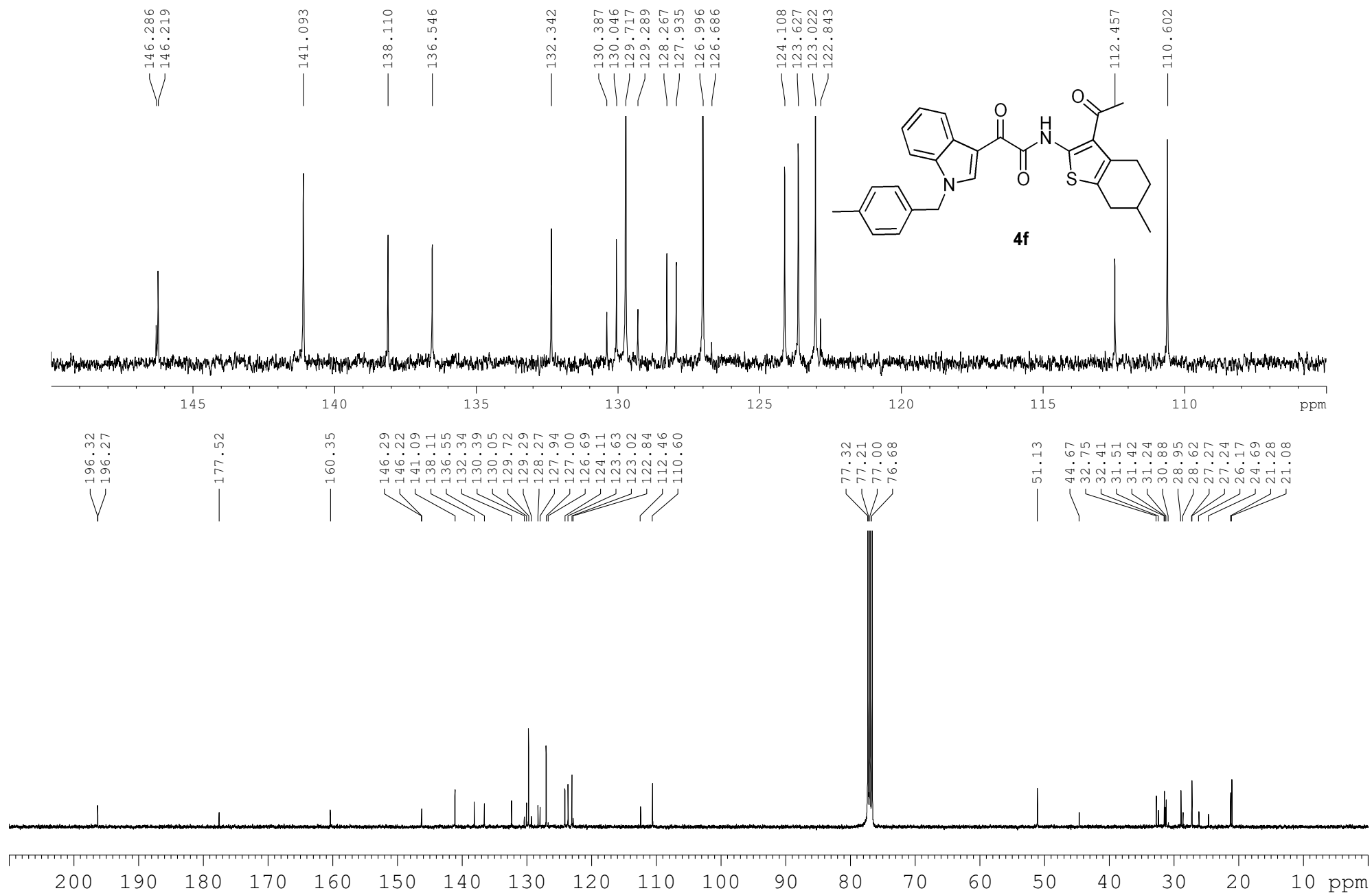


Meas. m/z	#	Ion Formula	m/z	err [mDa]	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻	Conf	N-Rule
485.1869	1	C ₂₉ H ₂₉ N ₂ O ₃ S	485.1893	2.4	5.0	2.7	1	100.00	16.5	even		ok
507.1693	1	C ₂₉ H ₂₈ N ₂ NaO ₃ S	507.1713	2.0	4.0	2.6	1	100.00	16.5	even		ok

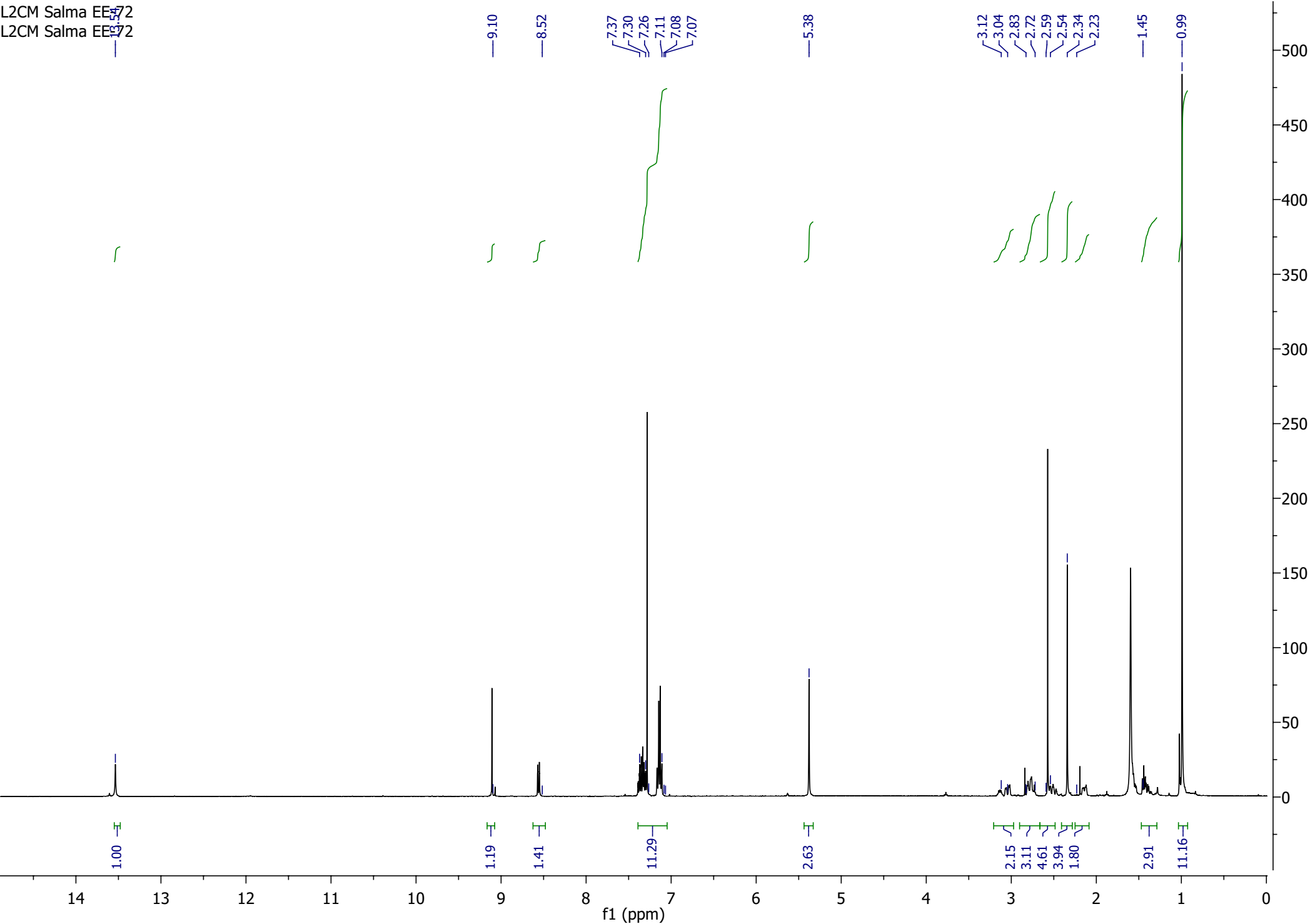
L2CM Salma EE-71
L2CM Salma EE-71



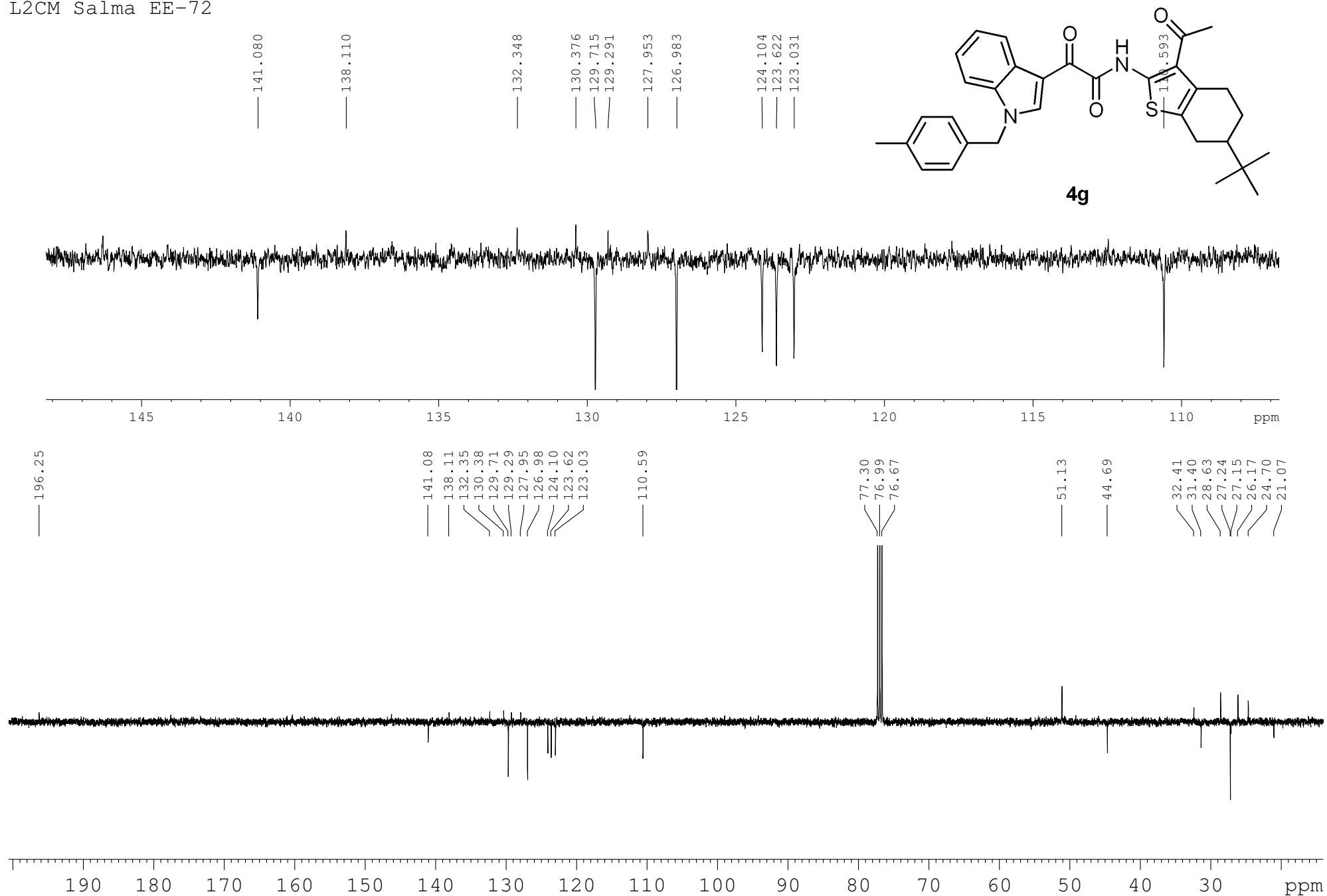
L2CM Salma EE-71



L2CM Salma EE-72
L2CM Salma EE-72



L2CM Salma EE-72



L2CM Salma EE-73
L2CM Salma EE-73

10.83
10.41

8.89

8.21

7.67

7.65

7.36

7.34

7.22

7.20

7.17

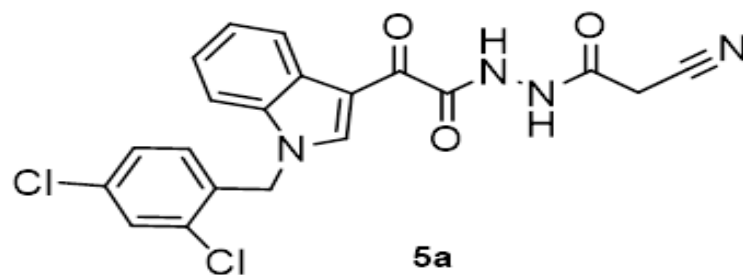
7.15

5.56

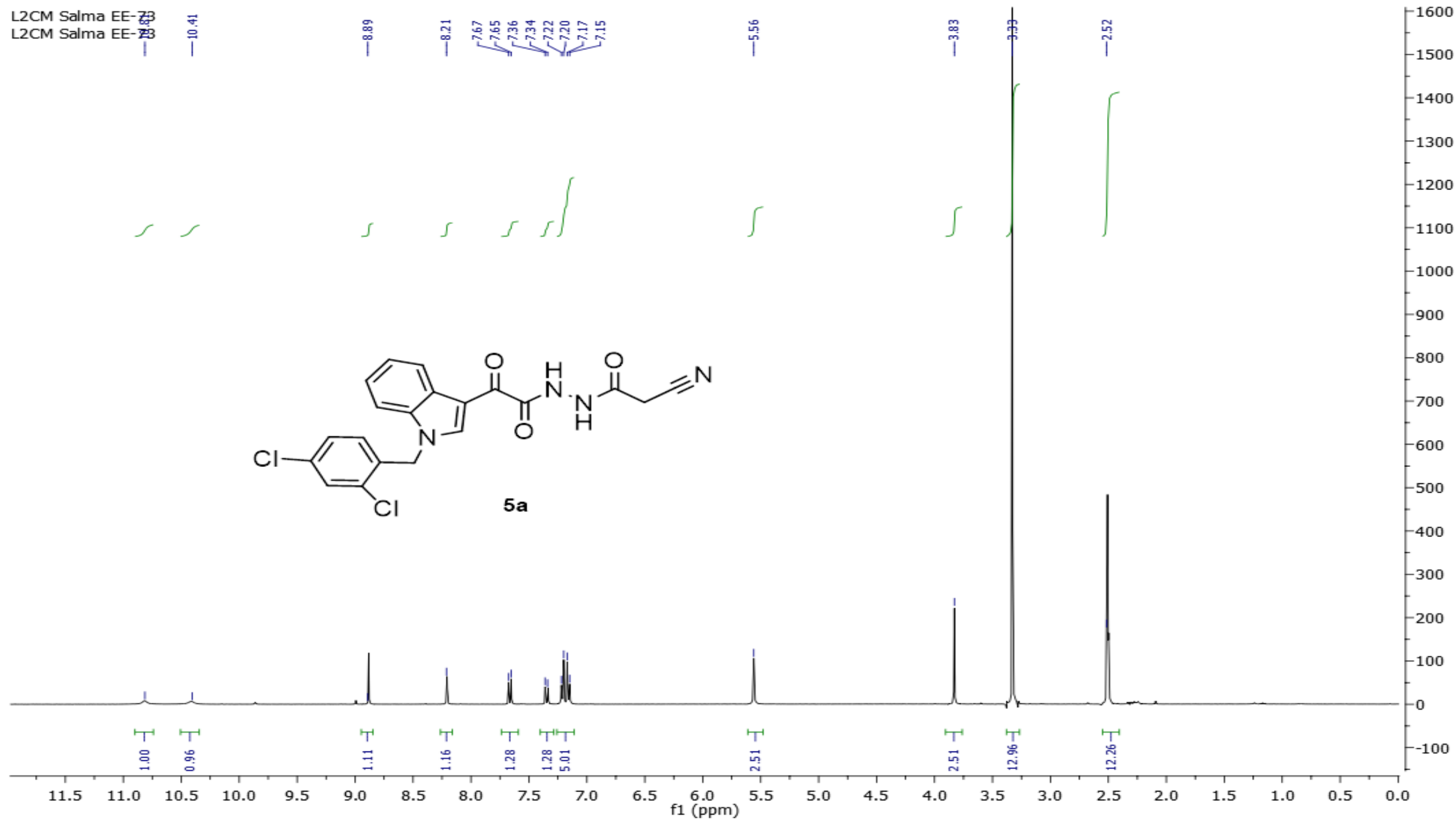
3.83

3.33

2.52



5a



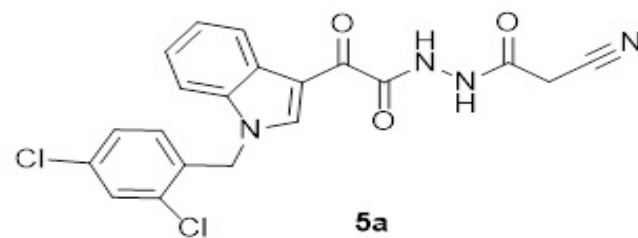
L2cm Salms -73
L2cm Salms -73

162.03
161.47

141.95
137.40
135.07
133.25
129.46
129.37
129.31
128.14
127.86
127.56
127.47
123.90
120.66
115.55
113.56
111.24

69.79

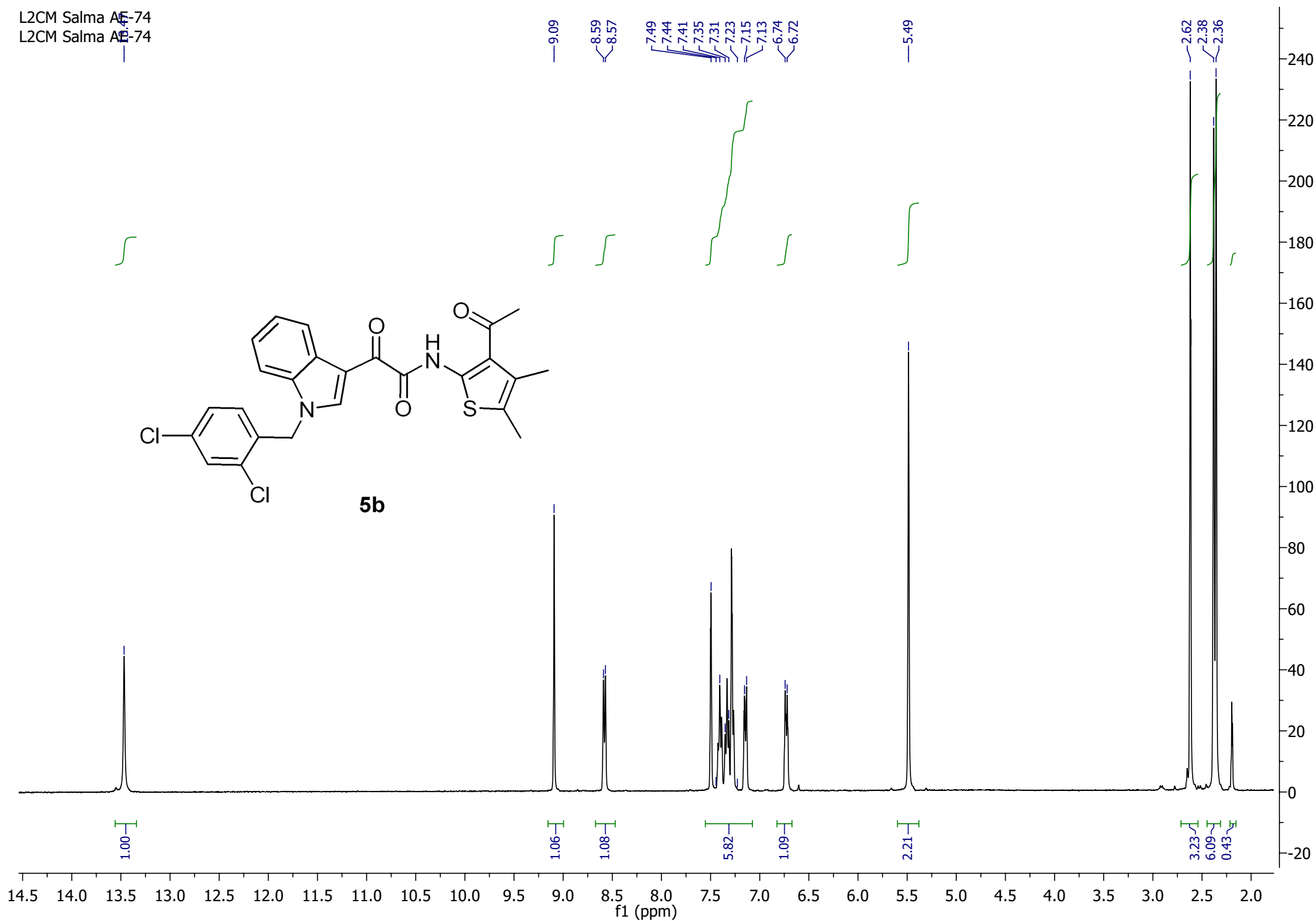
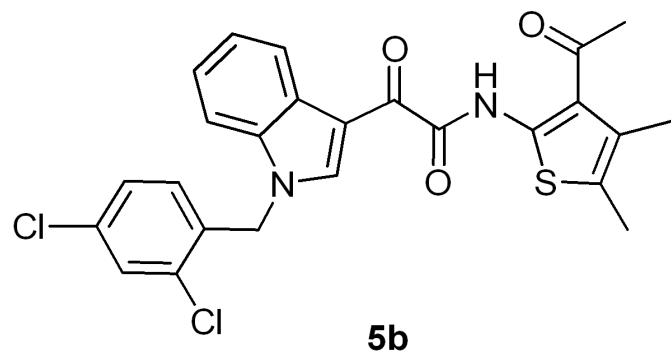
50.04
45.84
40.31
40.10
39.90
39.69
39.48
39.27
39.06



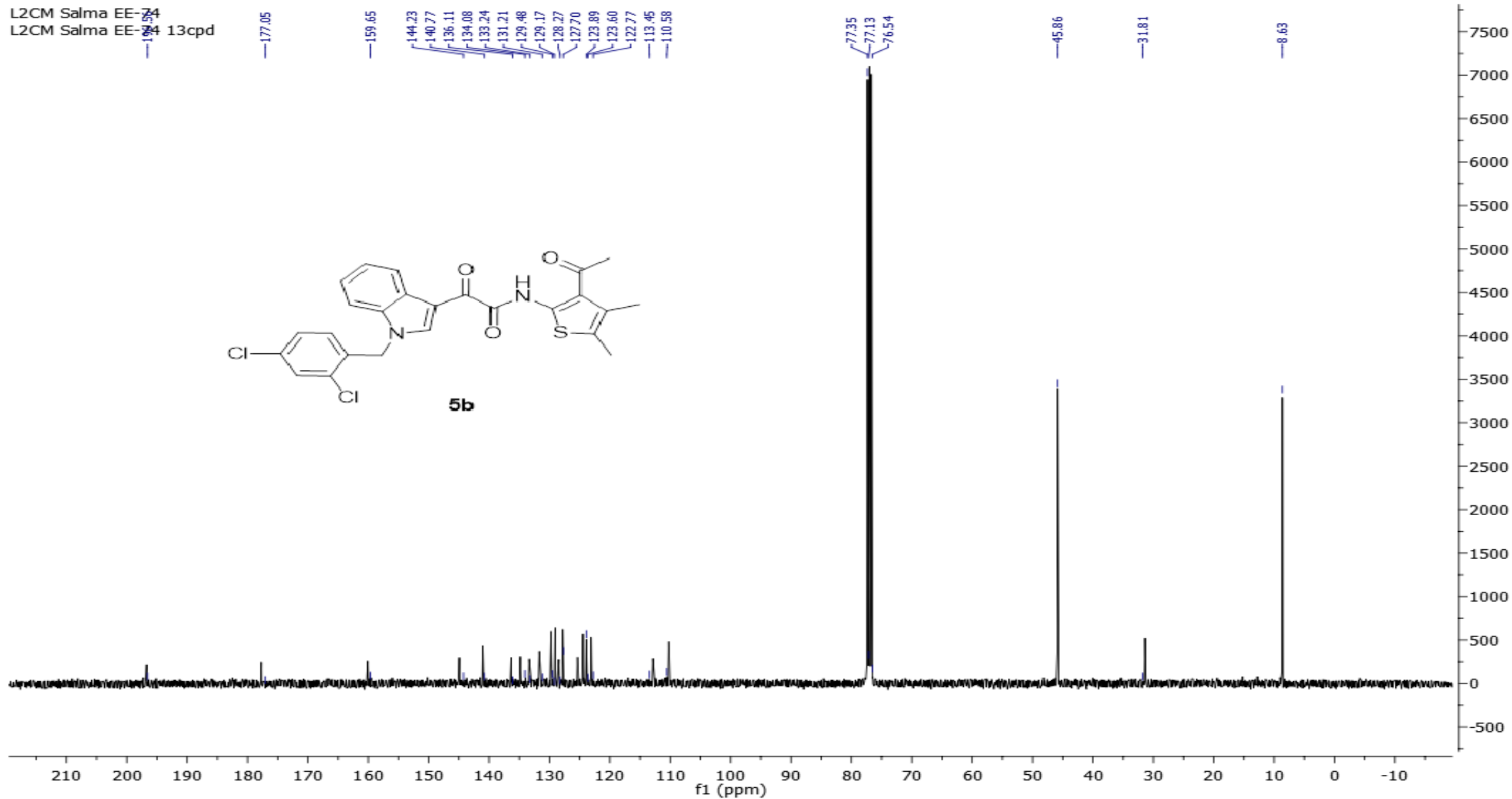
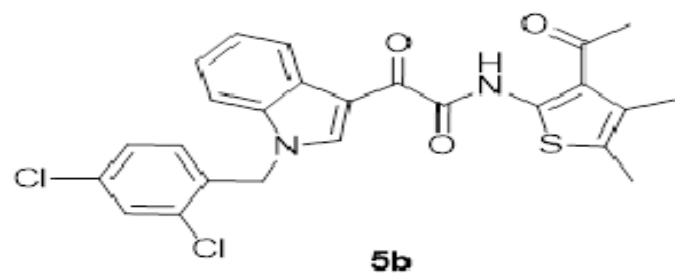
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

1E+05
1E+05
1E+05
1E+05
1E+05
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
-10000

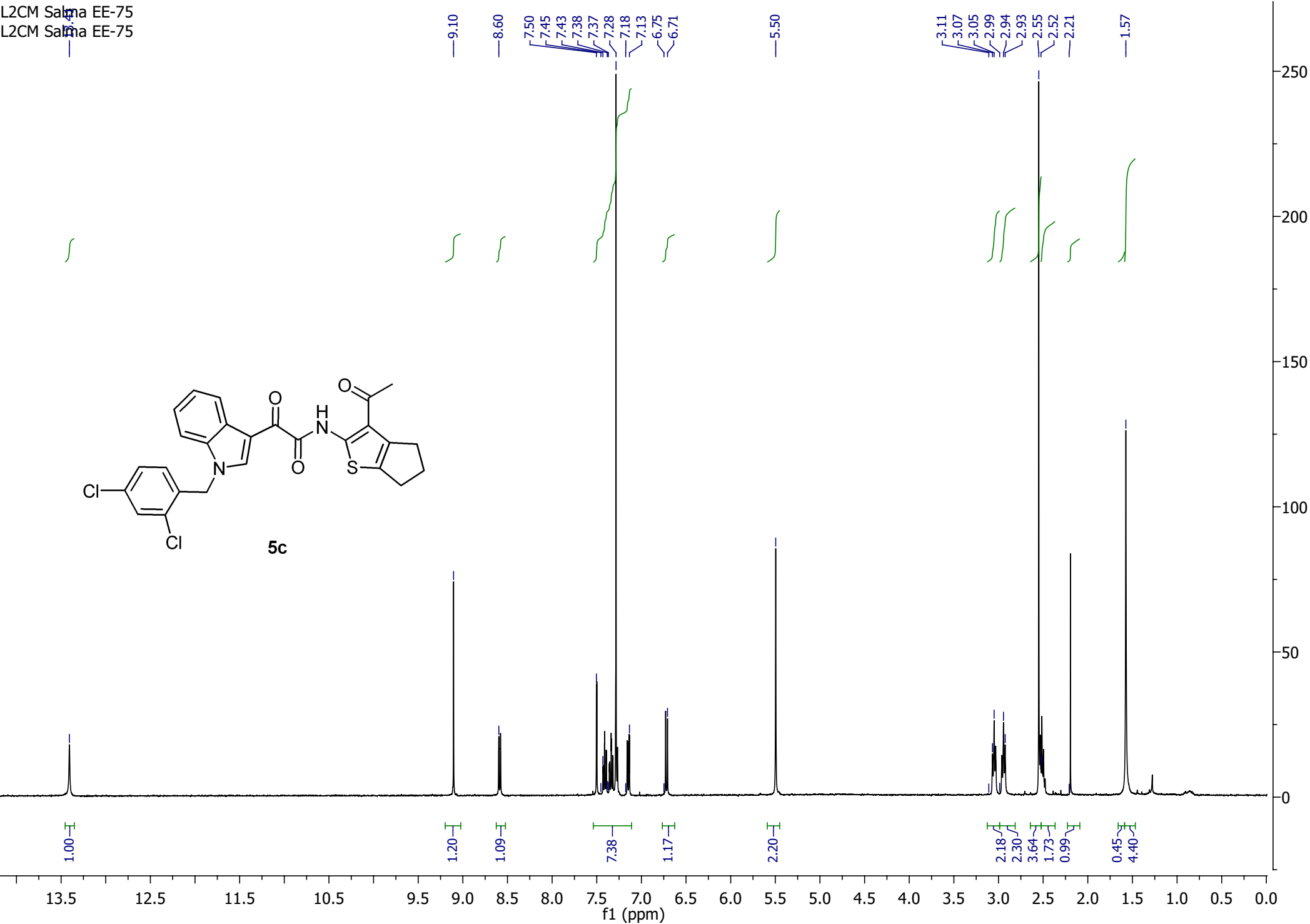
L2CM Salma A-74
L2CM Salma A-74



L2CM Salma EE-74
L2CM Salma EE-74 13cpd



L2CM Salma EE-75
L2CM Salma EE-75



Mass Spectrum SmartFormula Report

Analysis Info

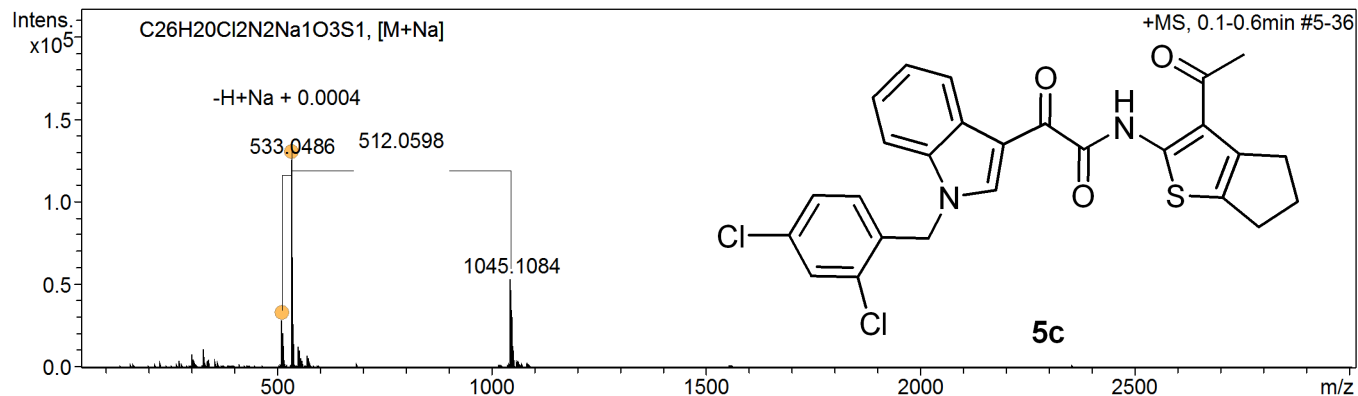
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Method Tuneposlow.m
Sample Name 180913809///EE-75
Comment MeOH/CH₂Cl₂

Acquisition Date 9/24/2018 1:42:55 PM

Operator fabien
Instrument micrOTOF-Q 228888.00098

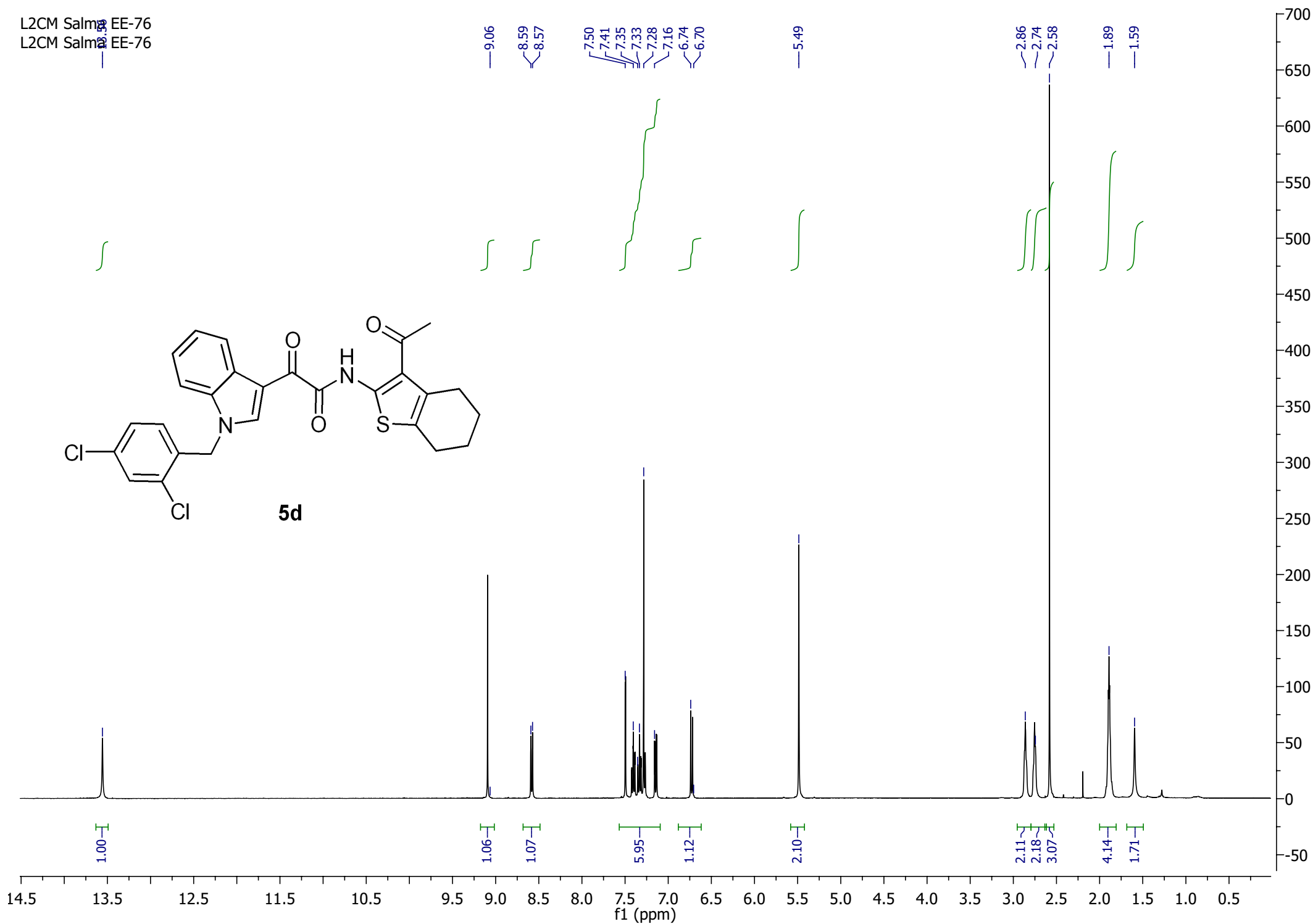
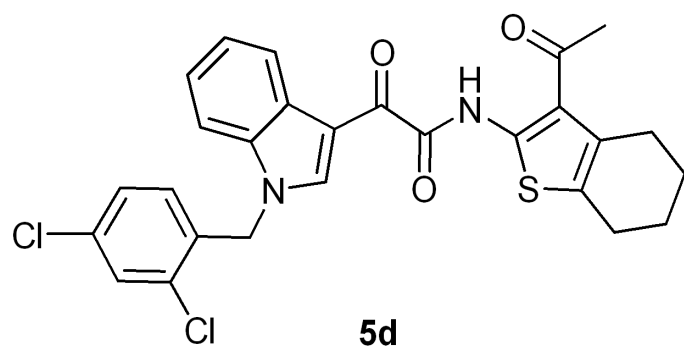
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	190 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Source

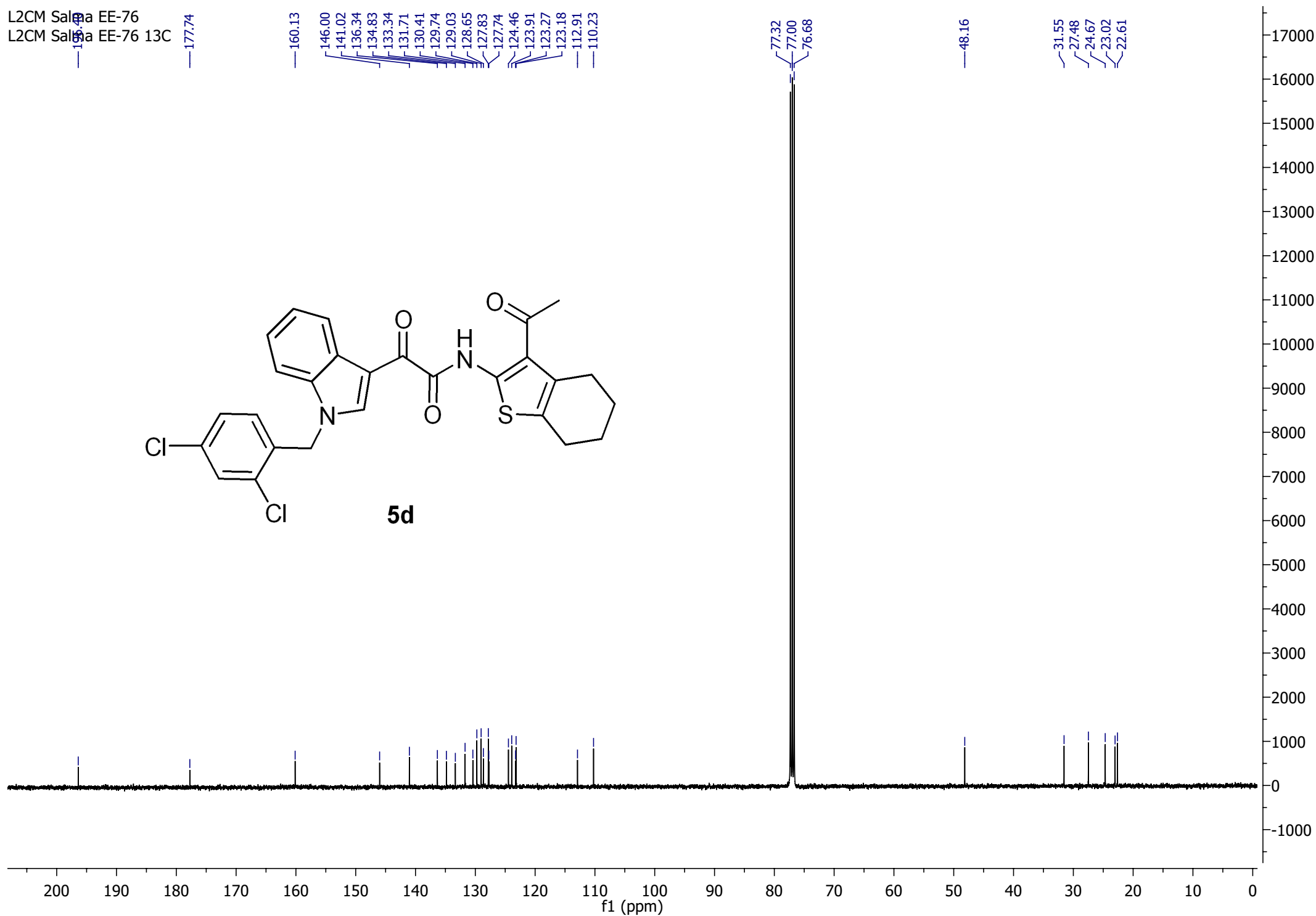
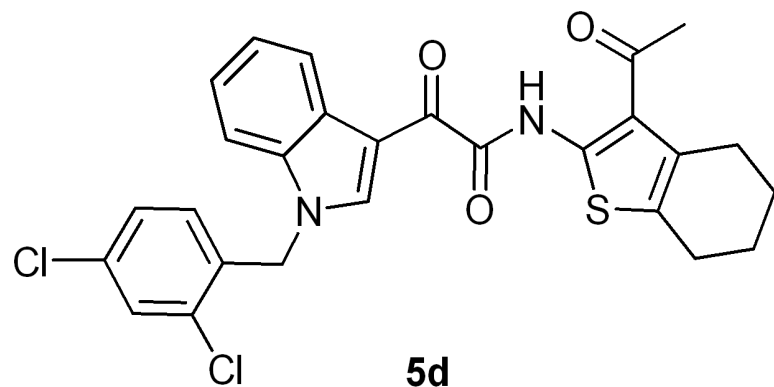


Meas. m/z	#	Ion Formula	m/z	[err] [mDa]	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻	Conf	N-Rule
511.0662	1	C ₂₆ H ₂₁ Cl ₂ N ₂ O ₃ S	511.0644	1.8	-3.4	3.2	1	100.00	16.5	even		ok
533.0486	1	C ₂₆ H ₂₀ Cl ₂ N ₂ NaO ₃ S	533.0464	2.2	-4.1	0.7	1	100.00	16.5	even		ok

L2CM Salma EE-76
L2CM Salma EE-76



L2CM Sala EE-76
L2CM Sala EE-76 13C



Mass Spectrum SmartFormula Report

Analysis Info

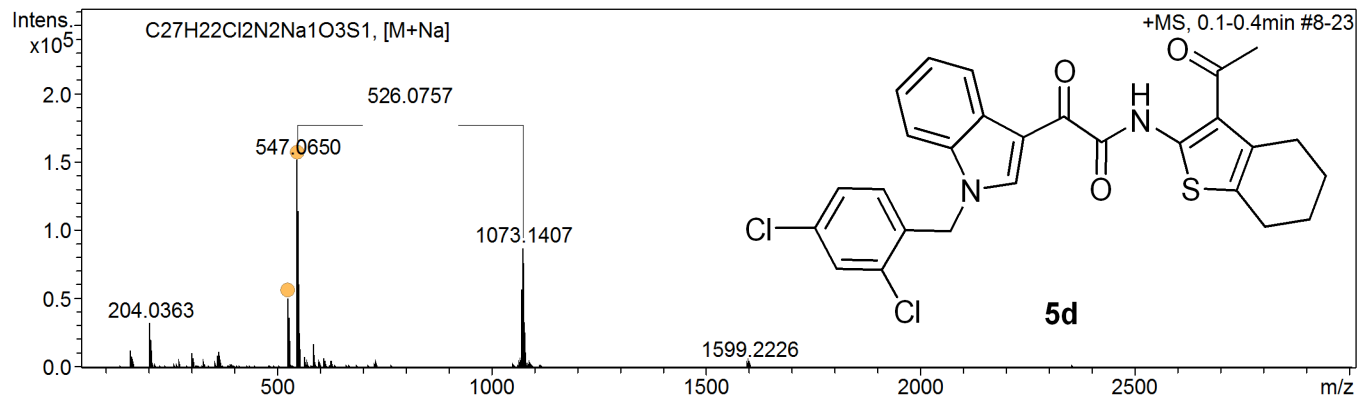
Analysis Name D:\Data\2018\180924000006.d
 Method Tuneposlow.m
 Sample Name 180913810///EE-76
 Comment MeOH/CH₂Cl₂

Acquisition Date 9/24/2018 1:48:49 PM

Operator fabien
 Instrument micrOTOF-Q 228888.00098

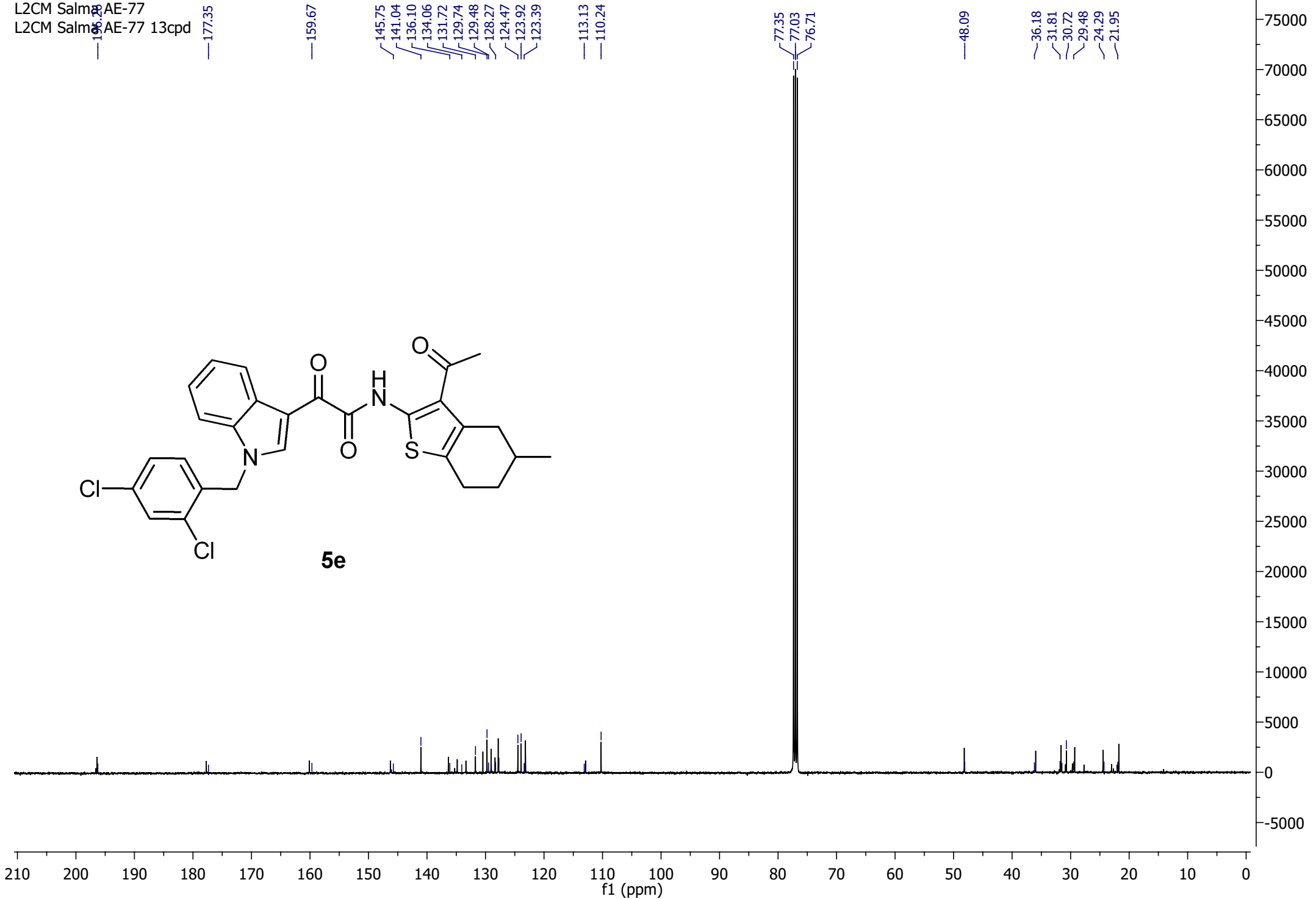
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	190 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Source

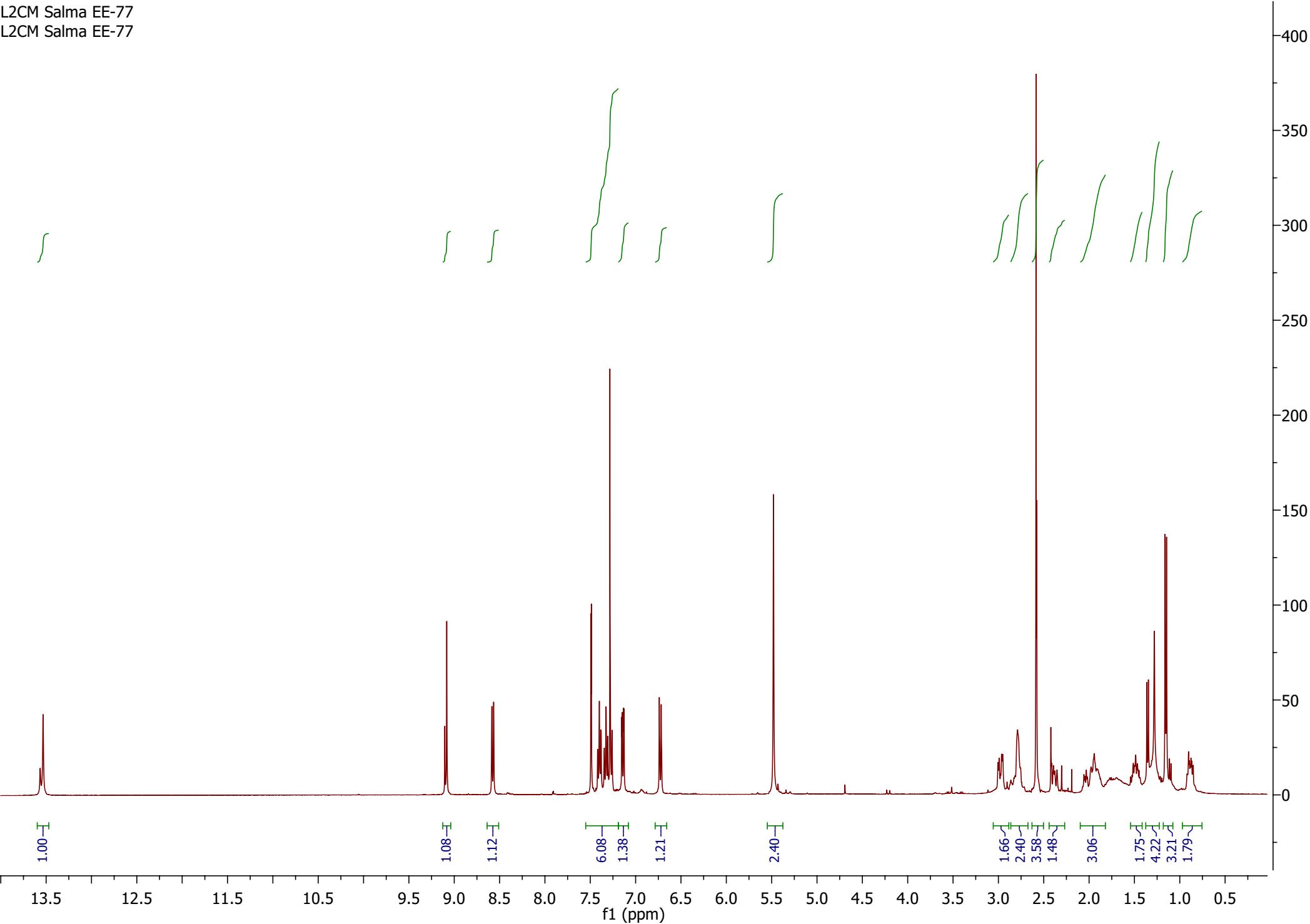


Meas. m/z	#	Ion Formula	m/z	err [mDa]	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻	Conf	N-Rule
525.0828	1	C ₂₇ H ₂₃ Cl ₂ N ₂ O ₃ S	525.0801	2.7	-5.2	6.8	1	100.00	16.5	even		ok
547.0650	1	C ₂₇ H ₂₂ Cl ₂ N ₂ NaO ₃ S	547.0620	3.0	-5.5	7.5	1	100.00	16.5	even		ok

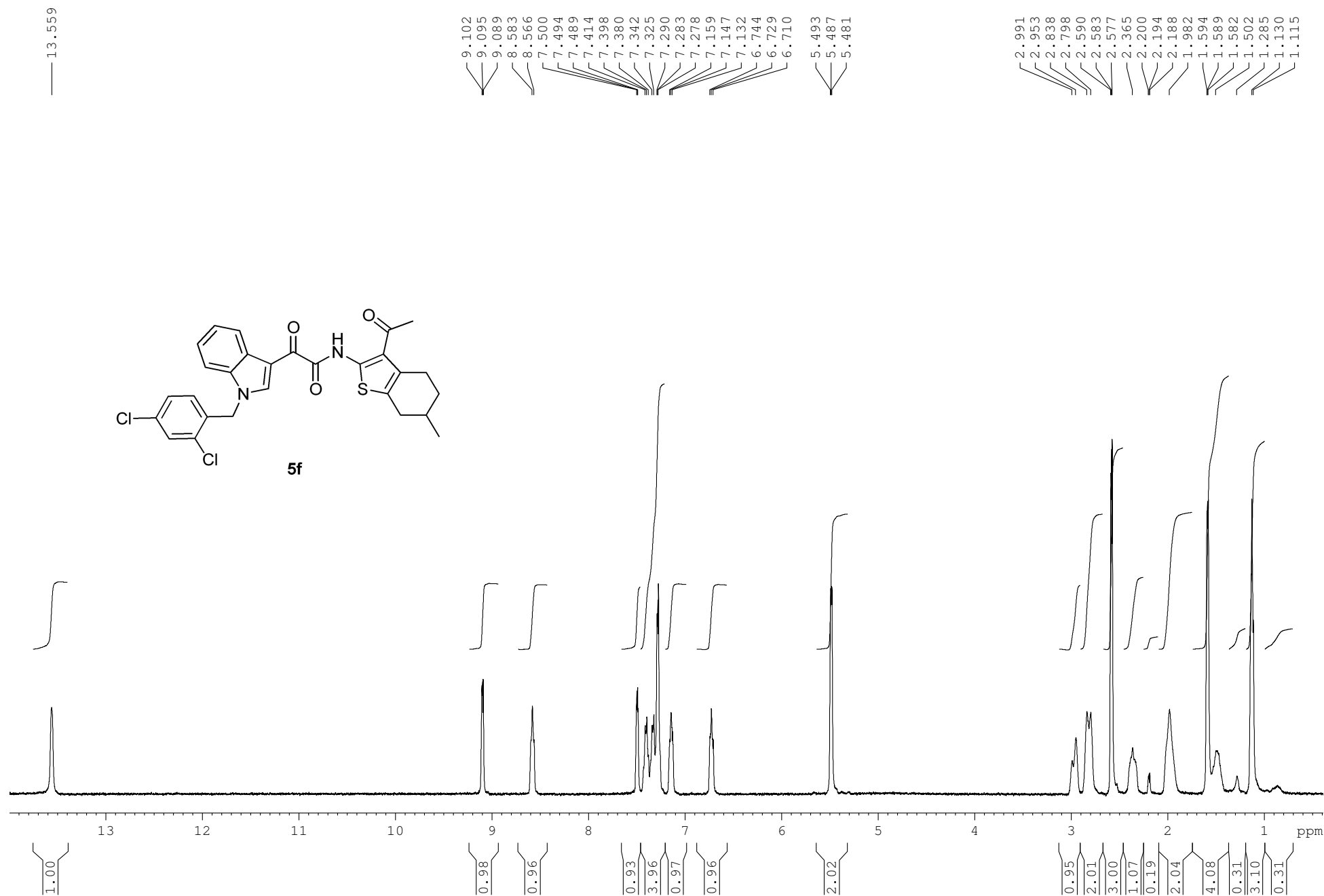
L2CM Salma AE-77
L2CM Salma AE-77 13cpd



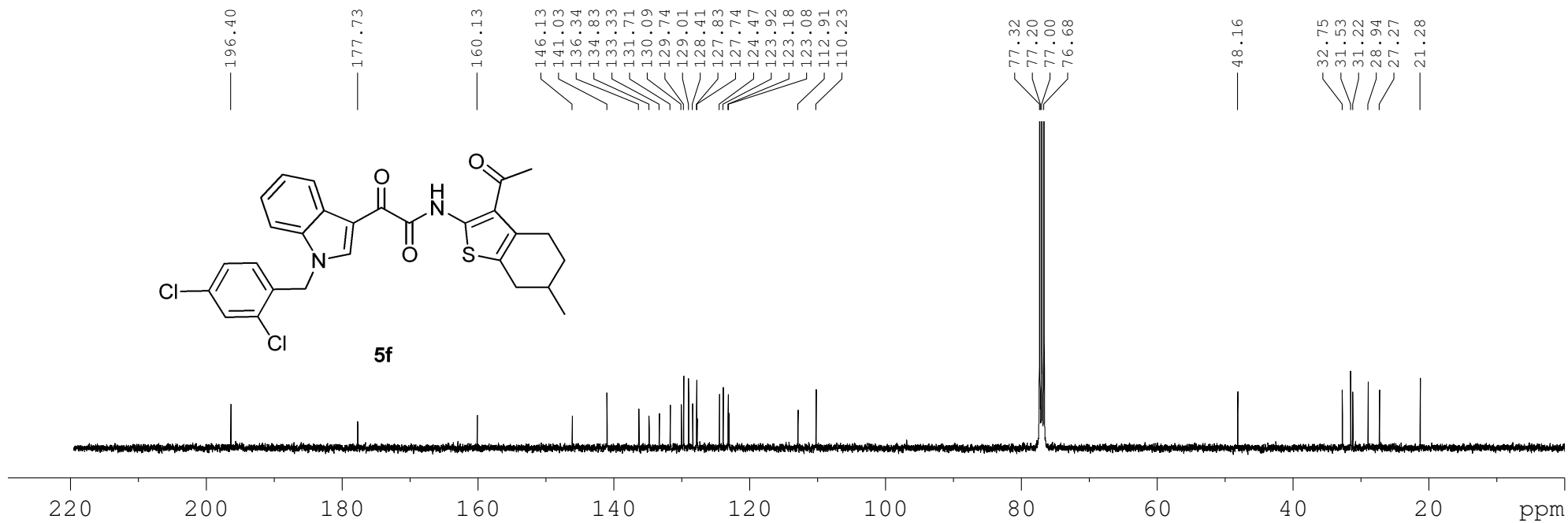
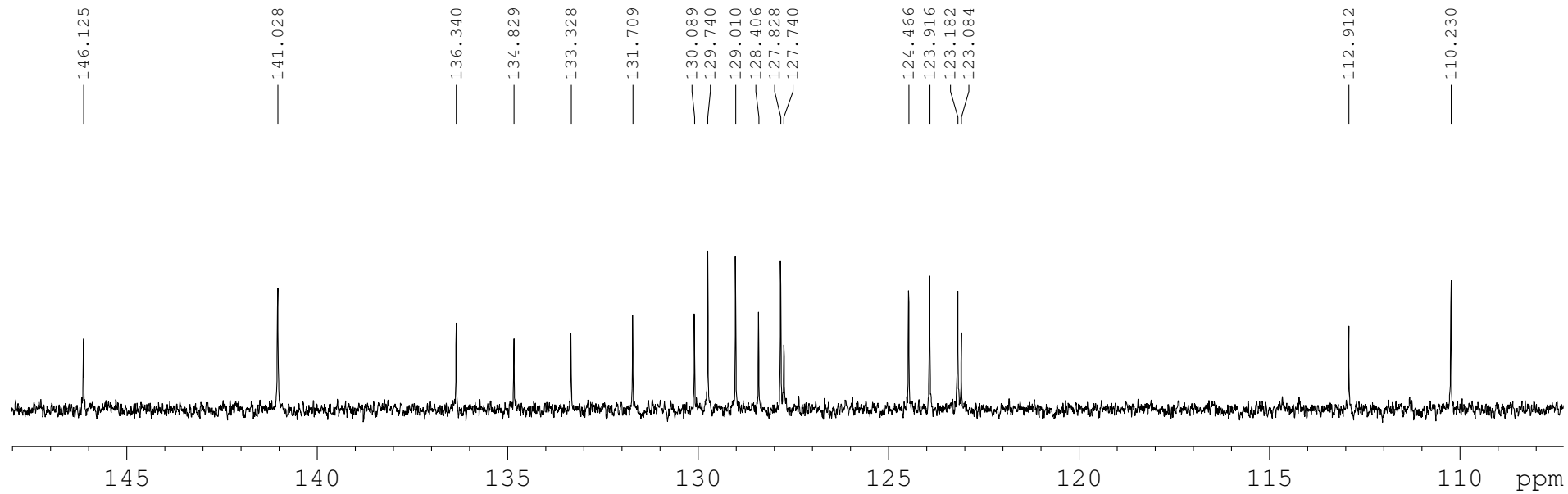
L2CM Salma EE-77
L2CM Salma EE-77



L2CM Salma AE-78



L2CM Salma EE-78 ¹³C



Mass Spectrum SmartFormula Report

Analysis Info

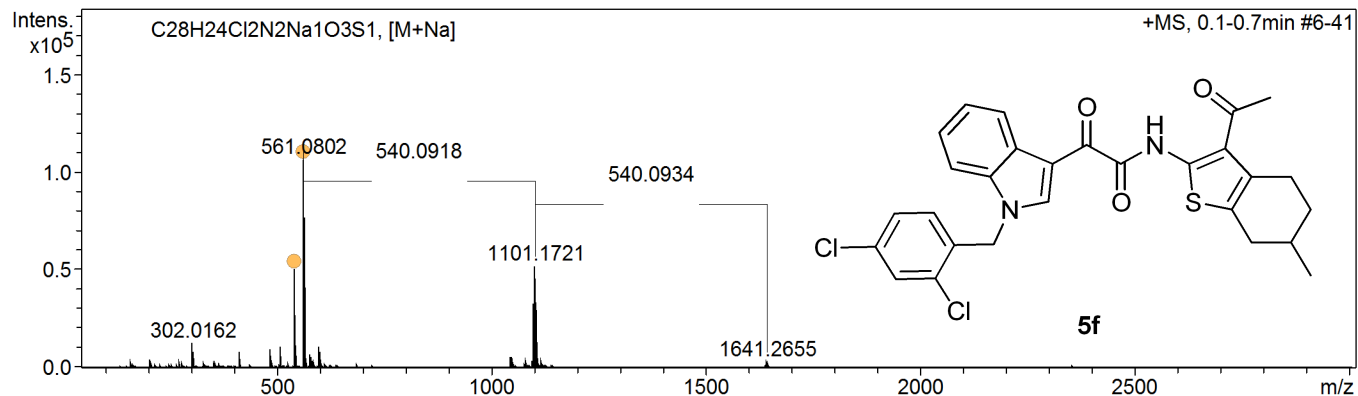
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 Method Tuneposlow.m
 Sample Name 180913811///EE-78
 Comment MeOH/CH₂Cl₂

Acquisition Date 9/24/2018 1:55:36 PM

Operator fabien
 Instrument micrOTOF-Q 228888.00098

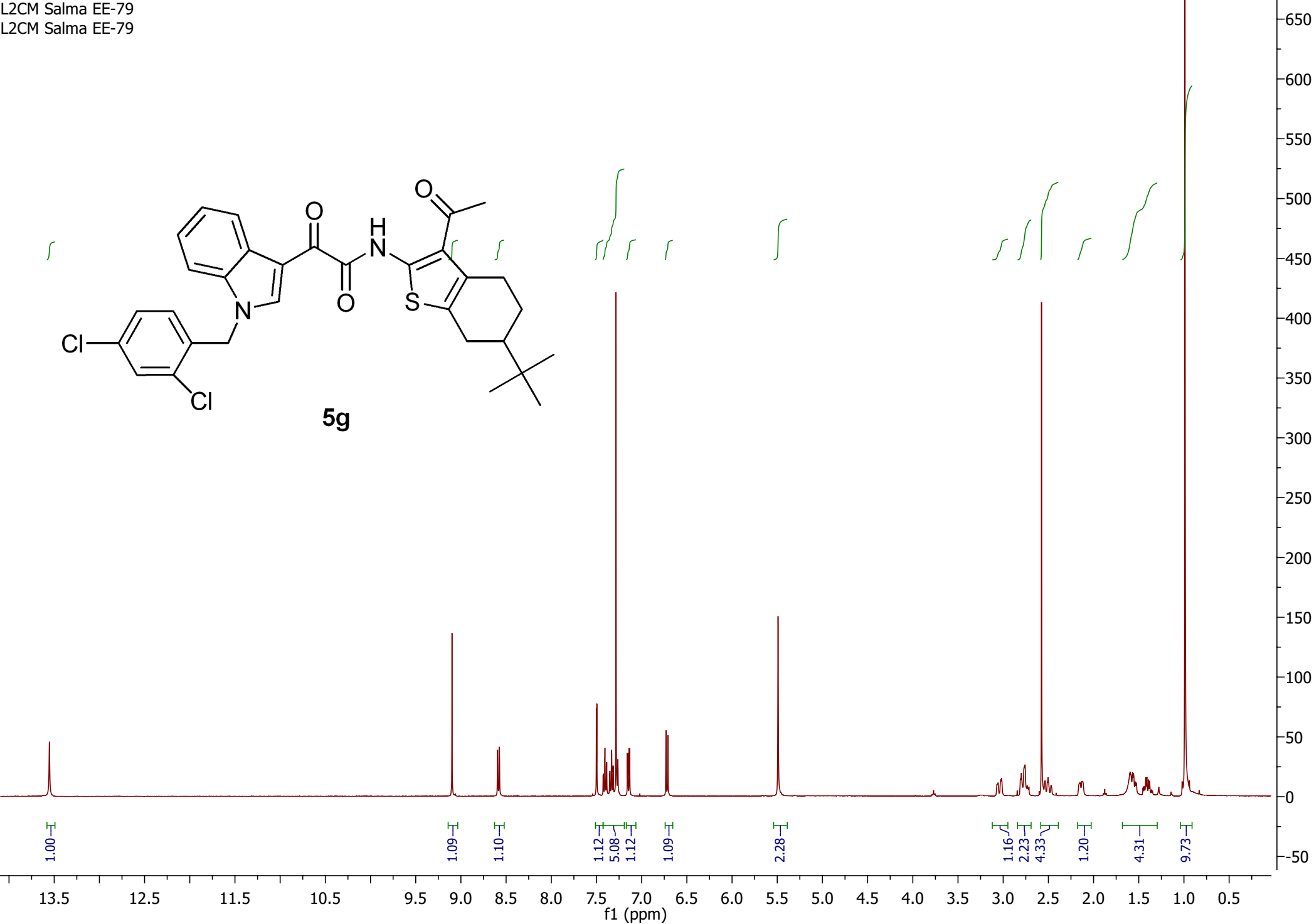
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	190 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Source

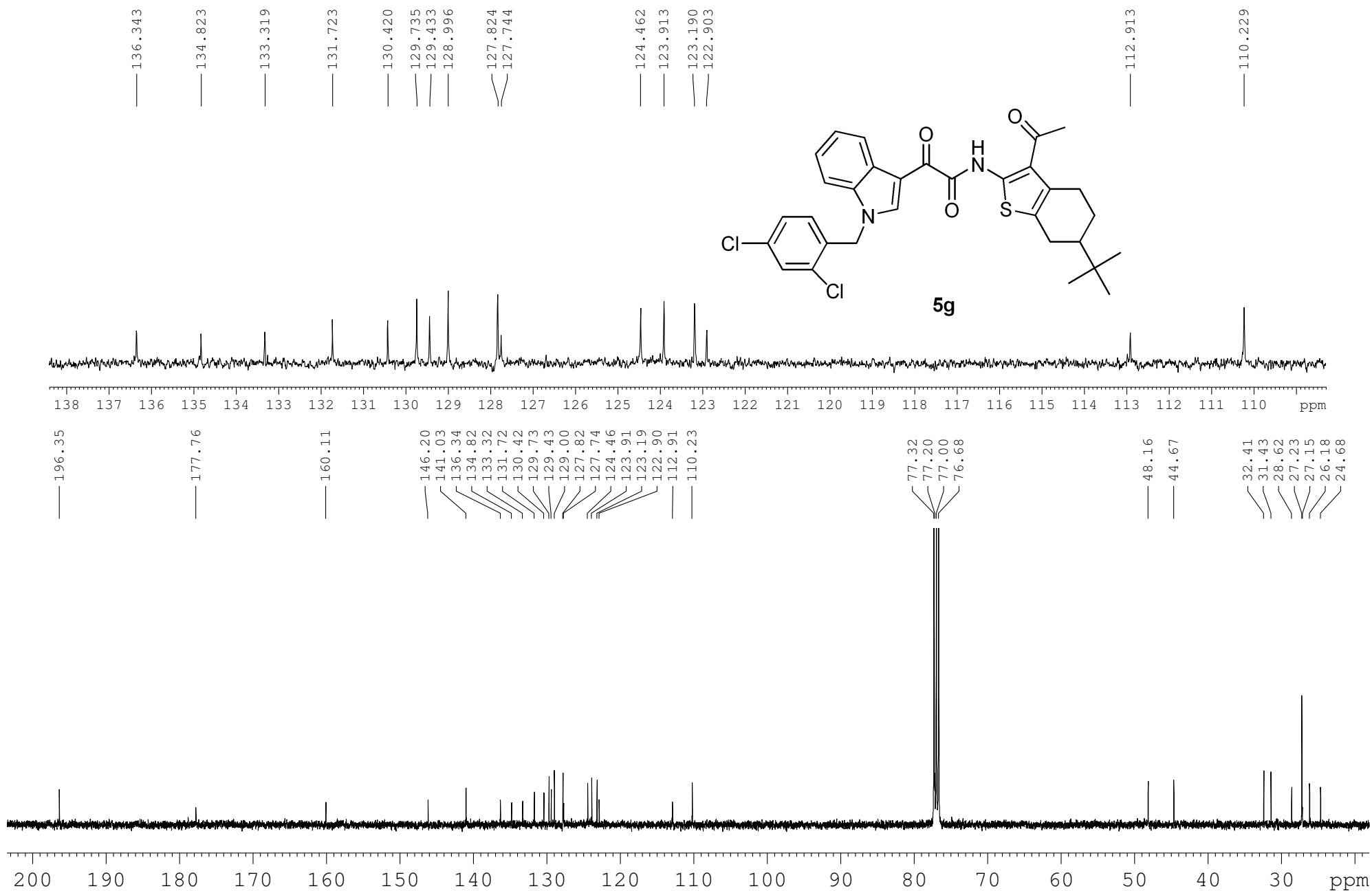


Meas. m/z	#	Ion Formula	m/z	err [mDa]	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻	Conf	N-Rule
539.0979	1	C ₂₈ H ₂₅ Cl ₂ N ₂ O ₃ S	539.0957	2.2	-4.1	13.3	1	100.00	16.5	even	ok	ok
561.0802	1	C ₂₈ H ₂₄ Cl ₂ N ₂ NaO ₃ S	561.0777	2.5	-4.5	8.7	1	100.00	16.5	even	ok	ok

L2CM Salma EE-79
L2CM Salma EE-79



L2cm salma EE-79



Mass Spectrum SmartFormula Report

Analysis Info

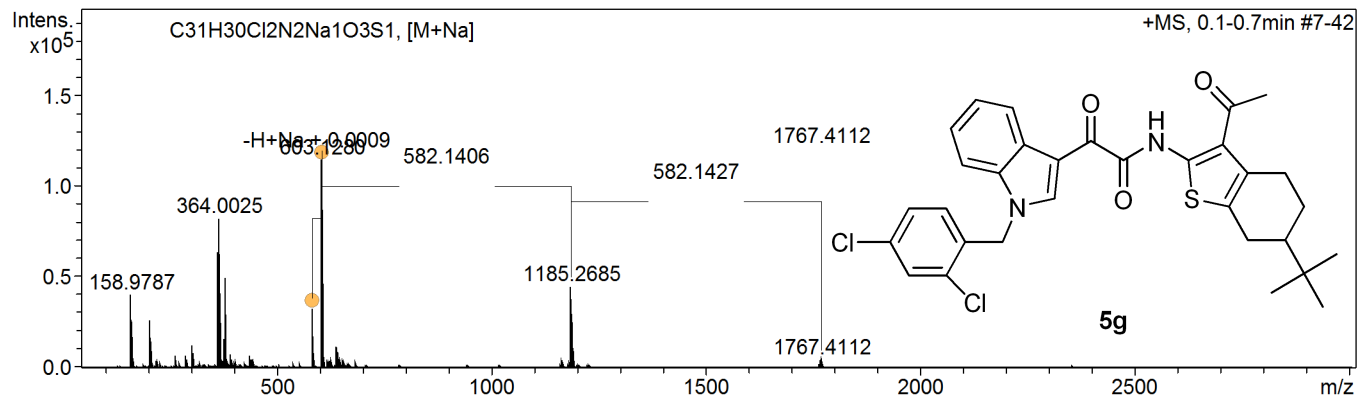
Analysis Name D:\Data\2018\180924000008.d
 Method Tuneposlow.m
 Sample Name 180913812///EE-79
 Comment MeOH/CH₂Cl₂

Acquisition Date 9/24/2018 2:20:41 PM

Operator fabien
 Instrument micrOTOF-Q 228888.00098

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	190 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	[err] [mDa]	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻	Conf	N-Rule
581.1451	1	C ₃₁ H ₃₁ Cl ₂ N ₂ O ₃ S	581.1427	2.4	-4.2	10.9	1	100.00	16.5	even	ok	ok
603.1280	1	C ₃₁ H ₃₀ Cl ₂ N ₂ NaO ₃ S	603.1246	3.3	-5.5	3.2	1	100.00	16.5	even	ok	ok