



Analysis Info

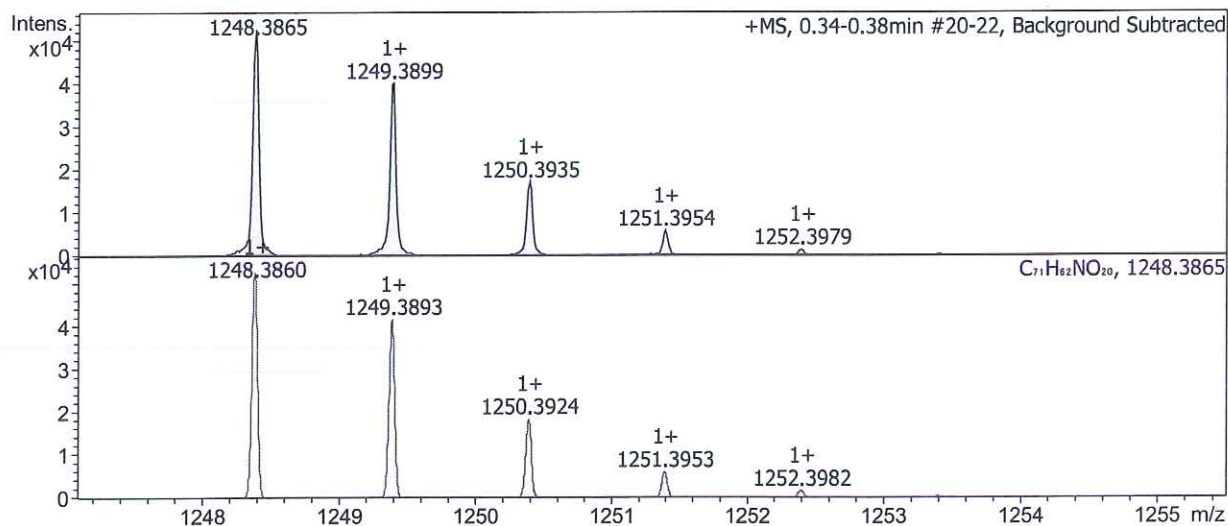
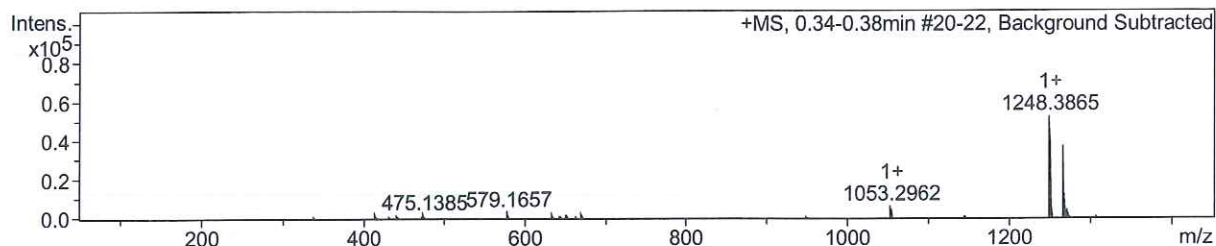
Sample Name **JCJ.13.037**
Analysis Name X005057CYC.d
Method Positif.m

Acquisition Date 12/09/2012 15:59:11

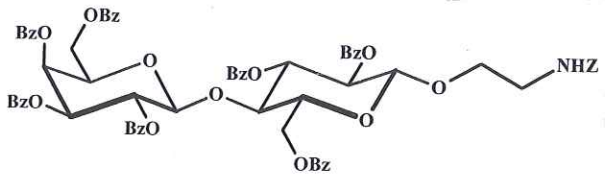
Laboratory
Instrument / Ser# maXis 255552.00
086

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.6 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	1000.0 Vpp	Set Divert Valve	Waste



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
579.165713	1	C34H27O9	579.164959	-1.3	24.2	21.5	even	ok
1053.296162	1	C61H49O17	1053.296427	0.3	8.2	37.5	even	ok
	2	C63H170NO7	1053.297183	1.0	15.2	-20.5	even	ok
	3	C74H41N2O6	1053.295913	-0.2	68.3	55.5	even	ok
1248.386455	1	C71H62NO20	1248.385970	-0.4	14.2	41.5	even	ok
	2	C73H183N2O10	1248.386726	0.2	28.1	-16.5	even	ok
	3	C85H179O3	1248.384876	-1.3	89.8	-3.5	even	ok
1265.412862	1	C71H65N2O20	1265.412519	-0.3	11.1	40.5	even	ok
	1	C73H186N3O10	1265.413276	0.3	24.5	-17.5	even	ok
	1	C85H182NO3	1265.411425	-1.1	86.1	-4.5	even	ok
1270.368237	1	C71H61NNaO20	1270.367914	-0.3	31.8	41.5	even	ok
	1	C73H182N2NaO10	1270.368671	0.3	23.8	-16.5	even	ok
	1	C85H178NaO3	1270.366820	-1.1	50.8	-3.5	even	ok



Handwritten annotations on the left side of the spectrum, including vertical lines and curly braces, likely indicating specific peak regions or integration values.

Integration values for the spectrum peaks:

- 1.99
- 1.05
- 2.03
- 1.88
- 0.96
- 0.98
- 1.00
- 1.96
- 2.95
- 0.91
- 1.94
- 2.92

Integration values for the aromatic region peaks:

- 28.86
- 13.77

Chemical shift scale in ppm (f1):

9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0

ppm (f1)



Analysis Info

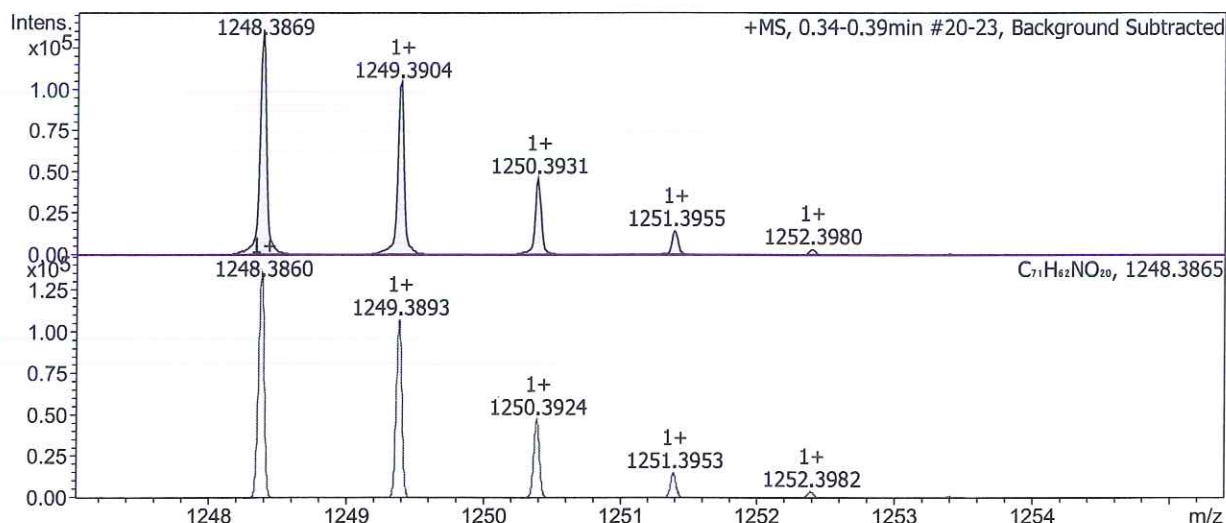
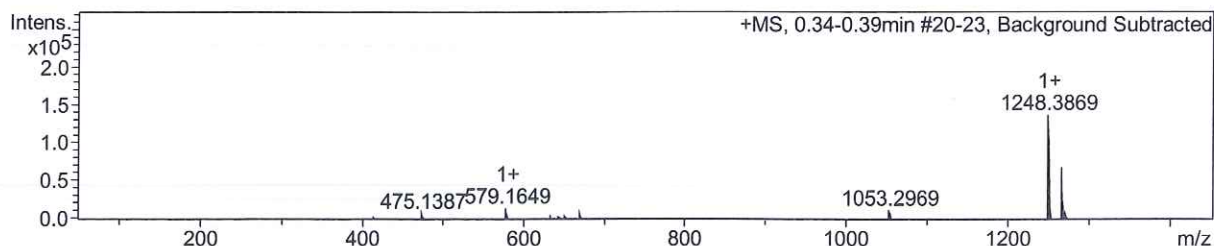
Sample Name **JCJ.13.038**
Analysis Name X005058CYC.d
Method Positif.m

Acquisition Date 12/09/2012 16:01:14

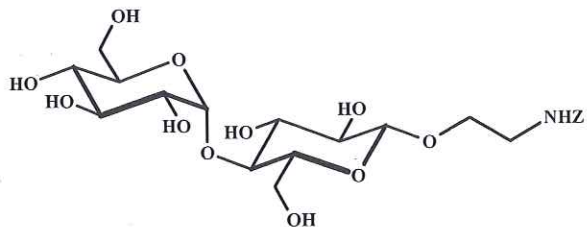
Laboratory
Instrument / Ser# maXis 255552.00
086

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.6 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	1000.0 Vpp	Set Divert Valve	Waste



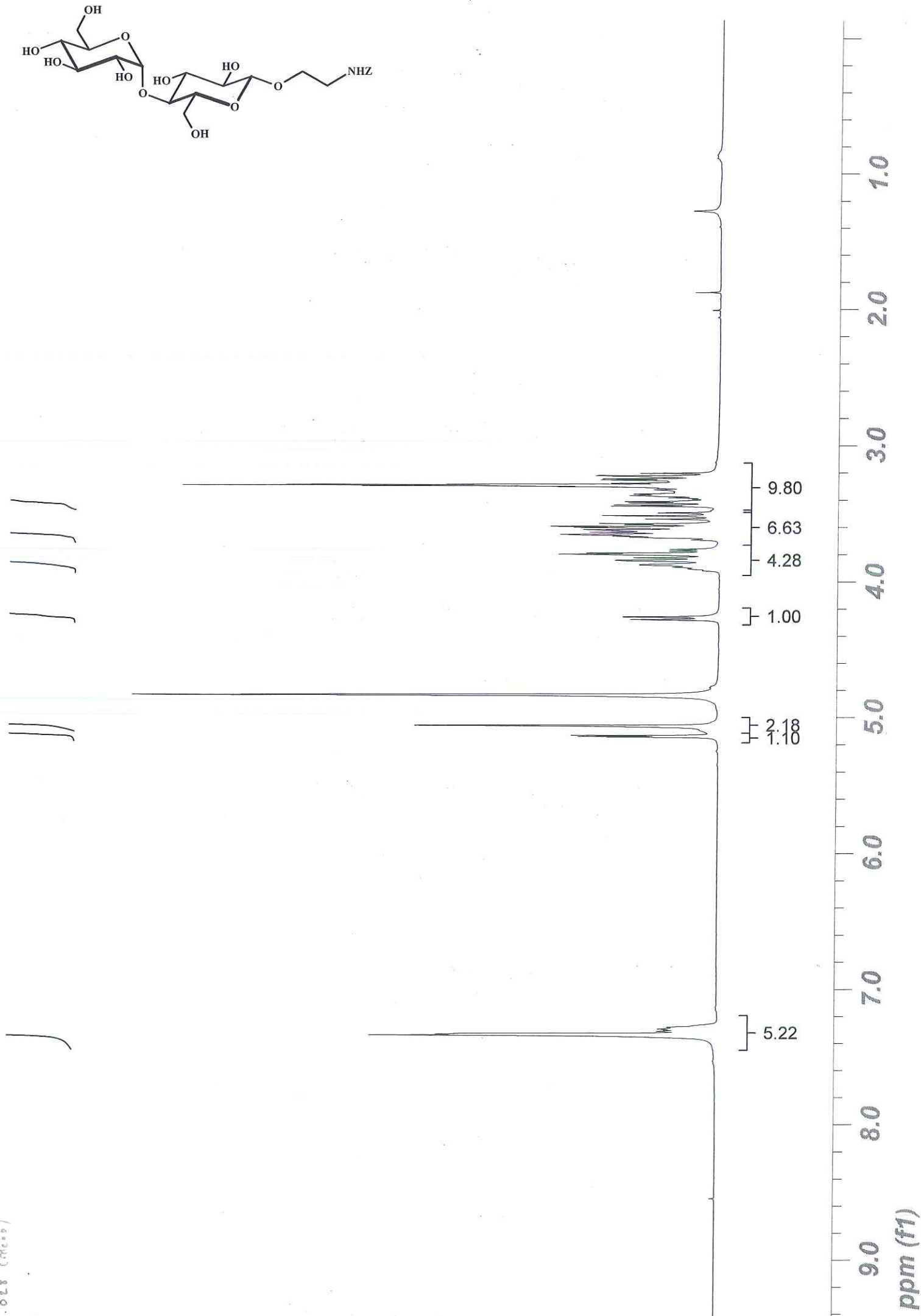
Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
670.227591	1	C37H36NO11	670.228287	1.0	10.1	20.5	even	ok
1248.386907	1	C71H62NO20	1248.385970	-0.8	8.9	41.5	even	ok
	2	C73H183N2O10	1248.386726	-0.1	23.4	-16.5	even	ok
	3	C85H179O3	1248.384876	-1.6	84.5	-3.5	even	ok
1265.413488	1	C71H65N2O20	1265.412519	-0.8	4.7	40.5	even	ok
	1	C73H186N3O10	1265.413276	-0.2	19.0	-17.5	even	ok
	1	C85H182NO3	1265.411425	-1.6	79.5	-4.5	even	ok



12.028 (MeOH)

1

12.028 (MeOH)





Analysis Info

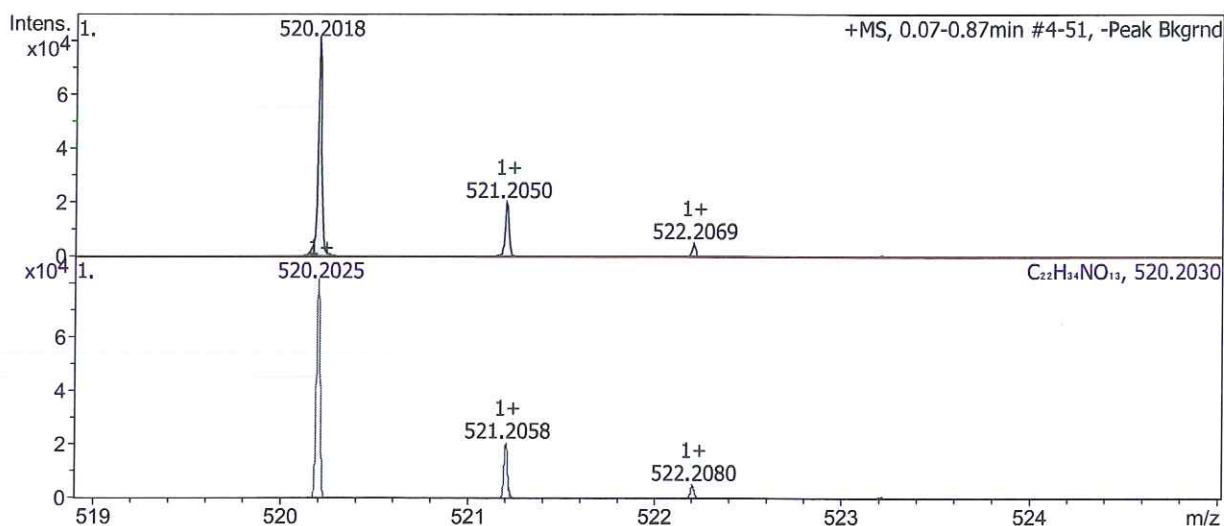
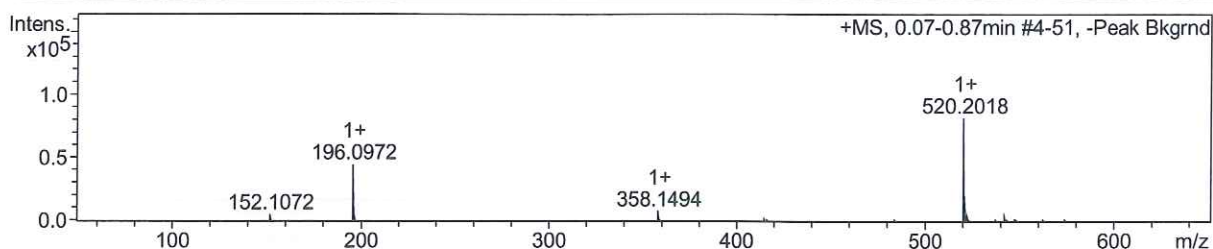
Sample Name **JCJ13.028**
Analysis Name X004321CYC.d
Method Positif.m

Acquisition Date 20/06/2012 13:24:05

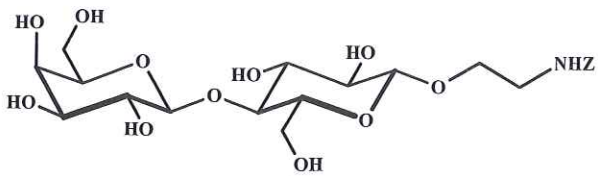
Laboratory
Instrument / Ser# maXis 255552.00
086

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.6 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	1000.0 Vpp	Set Divert Valve	Waste



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	rdB	e ⁻ Conf	N-Rule
196.097168	1	C ₁₀ H ₁₄ NO ₃	196.096820	-1.8	0.5	4.5	even	ok
358.149369	1	C ₁₆ H ₂₄ NO ₈	358.149643	0.8	2.2	5.5	even	ok
520.201820	1	C ₂₂ H ₃₄ NO ₁₃	520.202467	1.2	3.1	6.5	even	ok
542.183153	1	C ₂₂ H ₃₃ NNaO ₁₃	542.184411	2.3	29.0	6.5	even	ok



Handwritten annotations on the left side of the spectrum, including several vertical lines and curly braces, likely indicating specific peak regions or integration values.

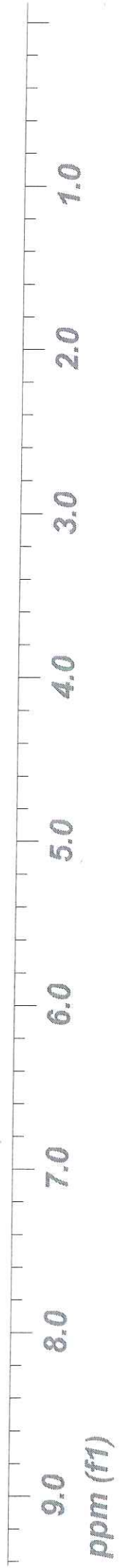
Handwritten annotation on the left side of the spectrum, consisting of a single vertical line.

Handwritten annotation on the left side of the spectrum, consisting of a single vertical line.

13.029 (1000)

4.34
1.99
5.17
2.11
5.09
2.00
2.02

4.76





Analysis Info

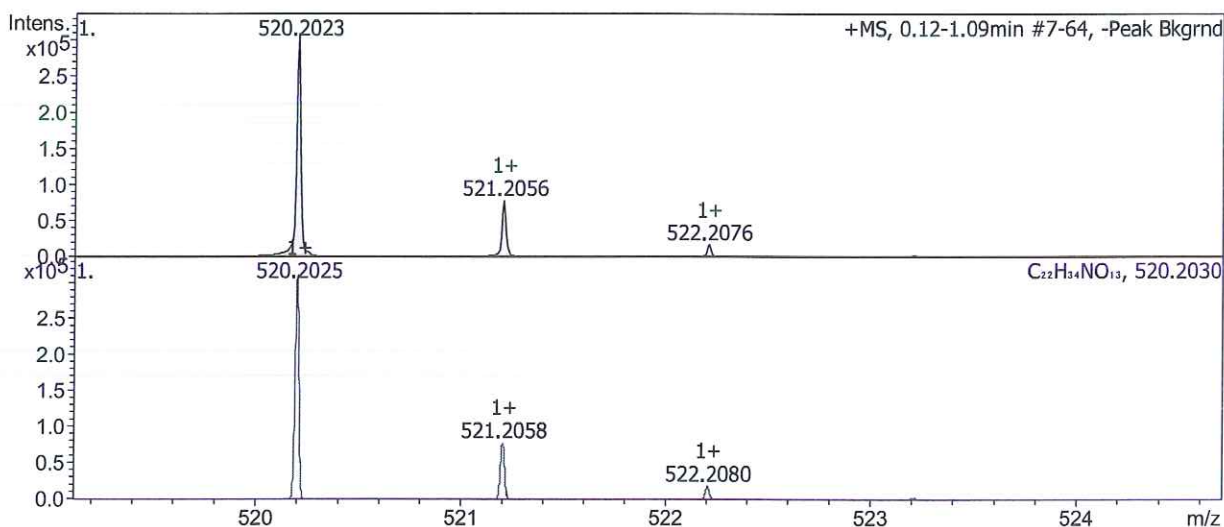
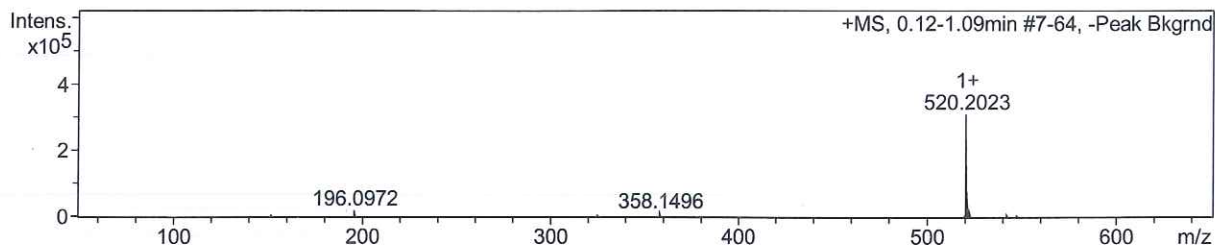
Sample Name **JCJ.13.029**
Analysis Name X004948CYC.d
Method Positif.m

Acquisition Date 29/08/2012 17:50:03

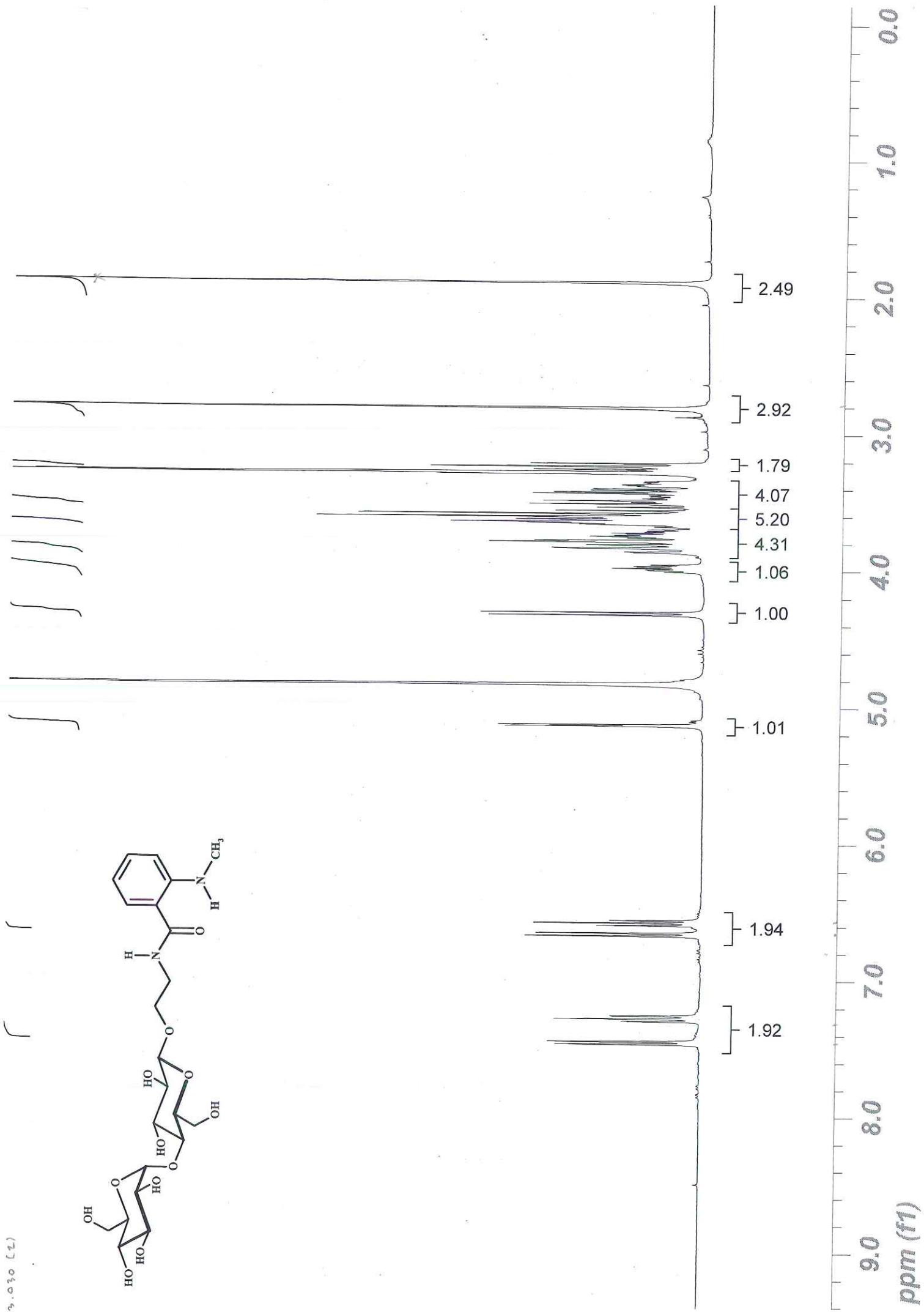
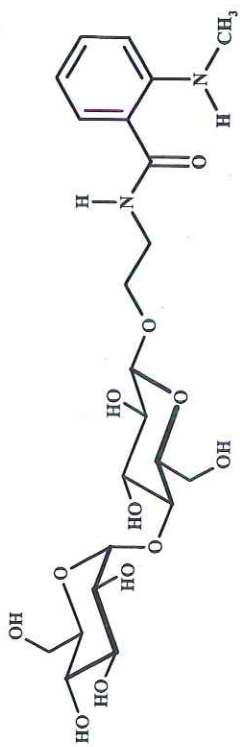
Laboratory
Instrument / Ser# maXis 255552.00
086

Acquisition Parameter

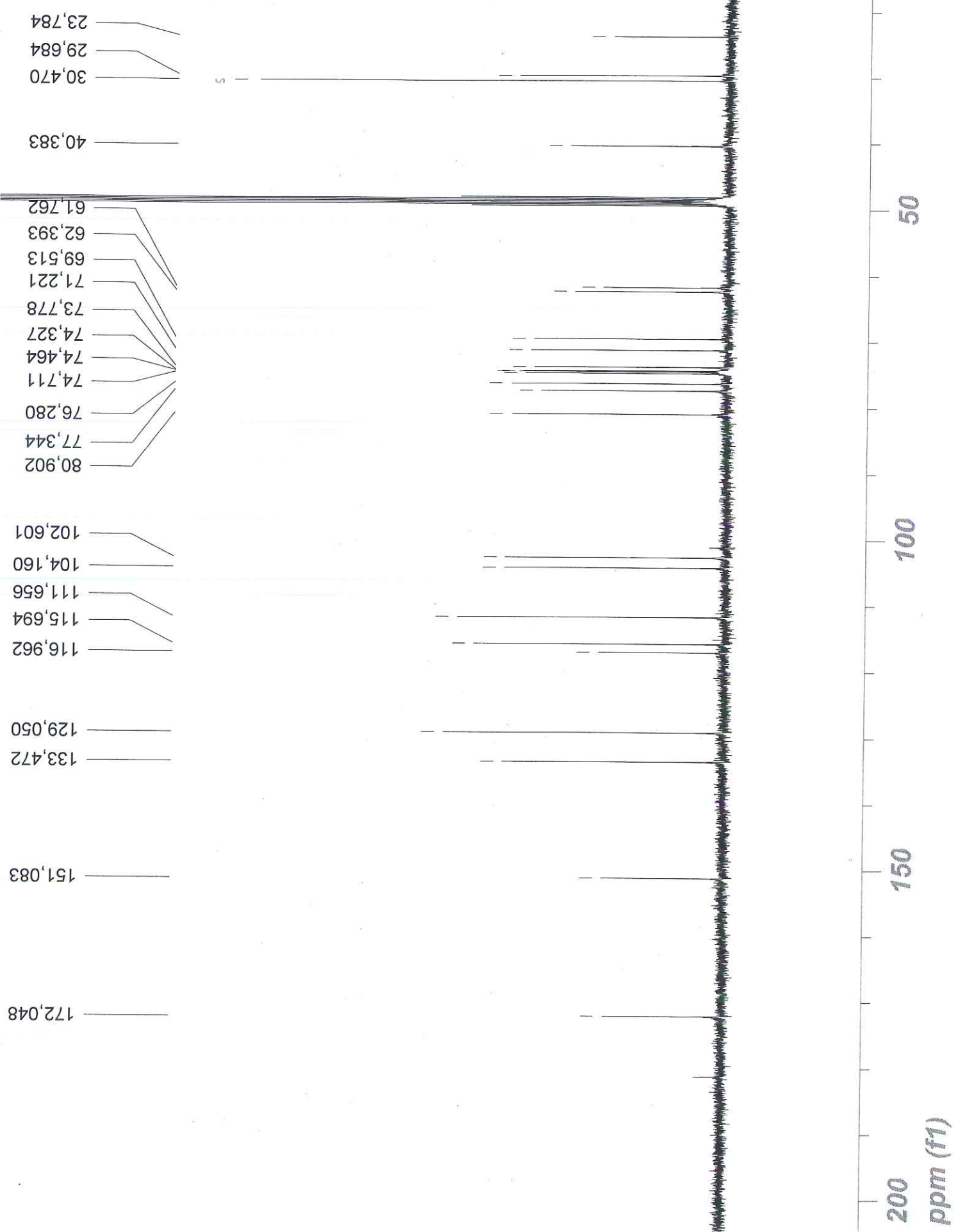
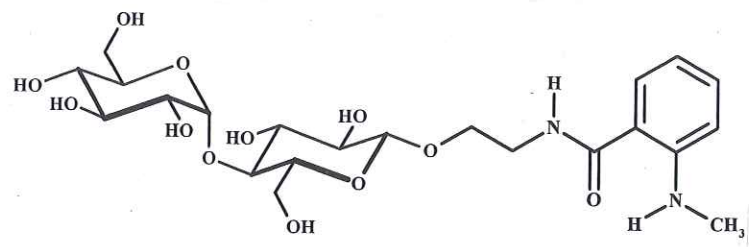
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.6 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	1000.0 Vpp	Set Divert Valve	Waste



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
196.097167	1	C10H14NO3	196.096820	-1.8	7.7	4.5	even	ok
358.149604	1	C16H24NO8	358.149643	0.1	3.3	5.5	even	ok
520.202301	1	C22H34NO13	520.202467	0.3	2.5	6.5	even	ok
542.183739	1	C22H33NNaO13	542.184411	1.2	28.8	6.5	even	ok



13-030-2





Analysis Info

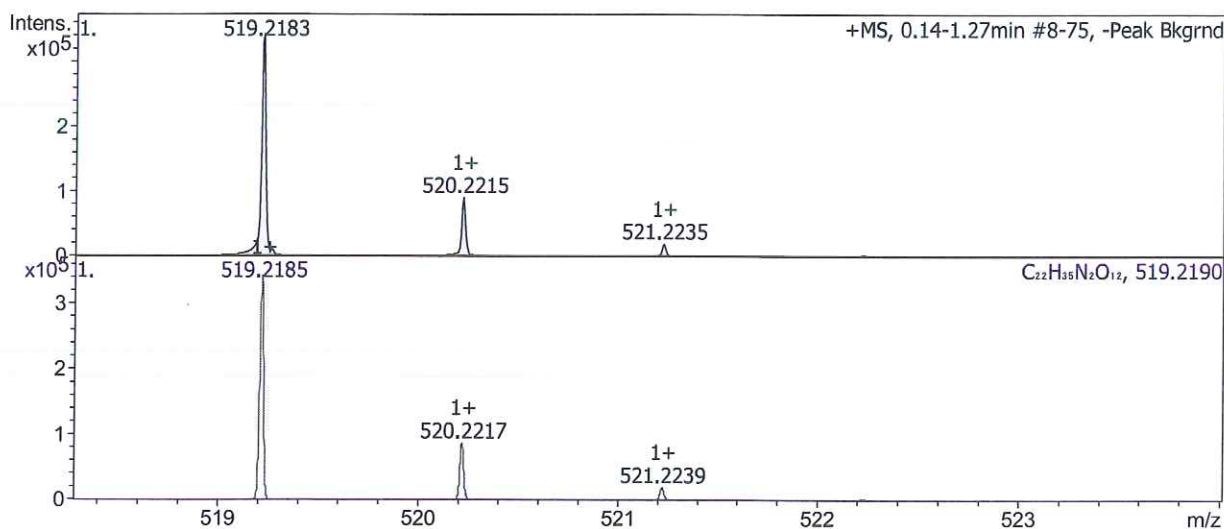
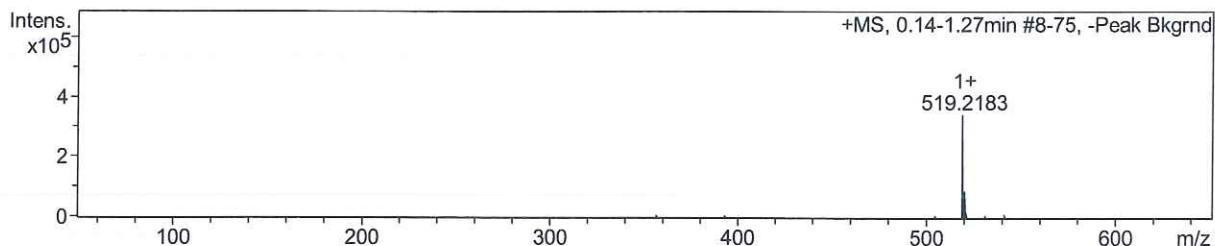
Sample Name **JCJ.13.030**
Analysis Name X004949CYC.d
Method Positif.m

Acquisition Date 29/08/2012 17:52:08

Laboratory
Instrument / Ser# maXis 255552.00
086

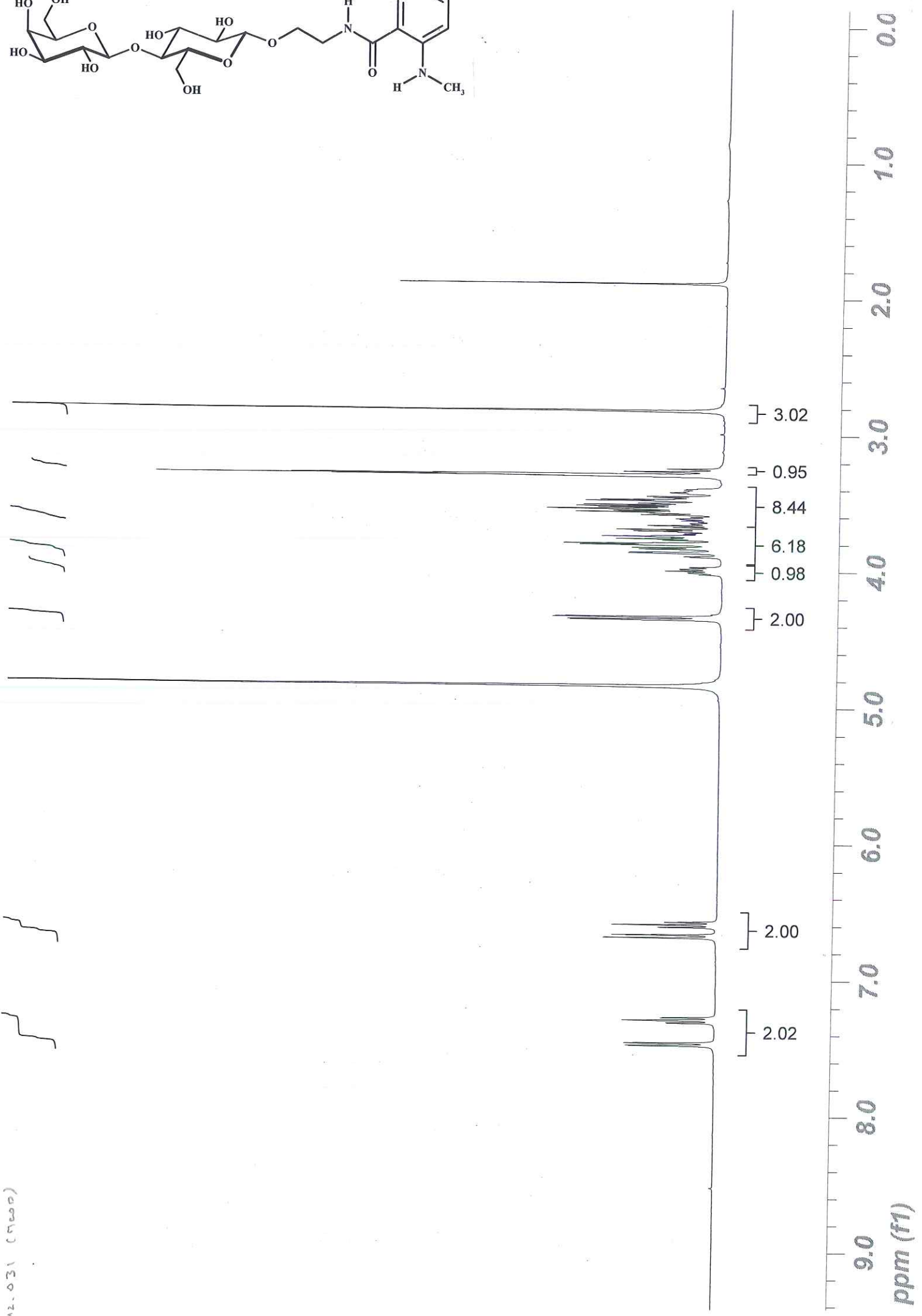
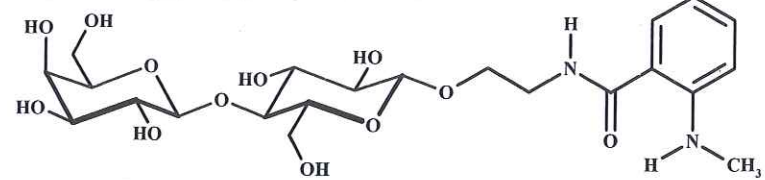
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.6 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	1000.0 Vpp	Set Divert Valve	Waste



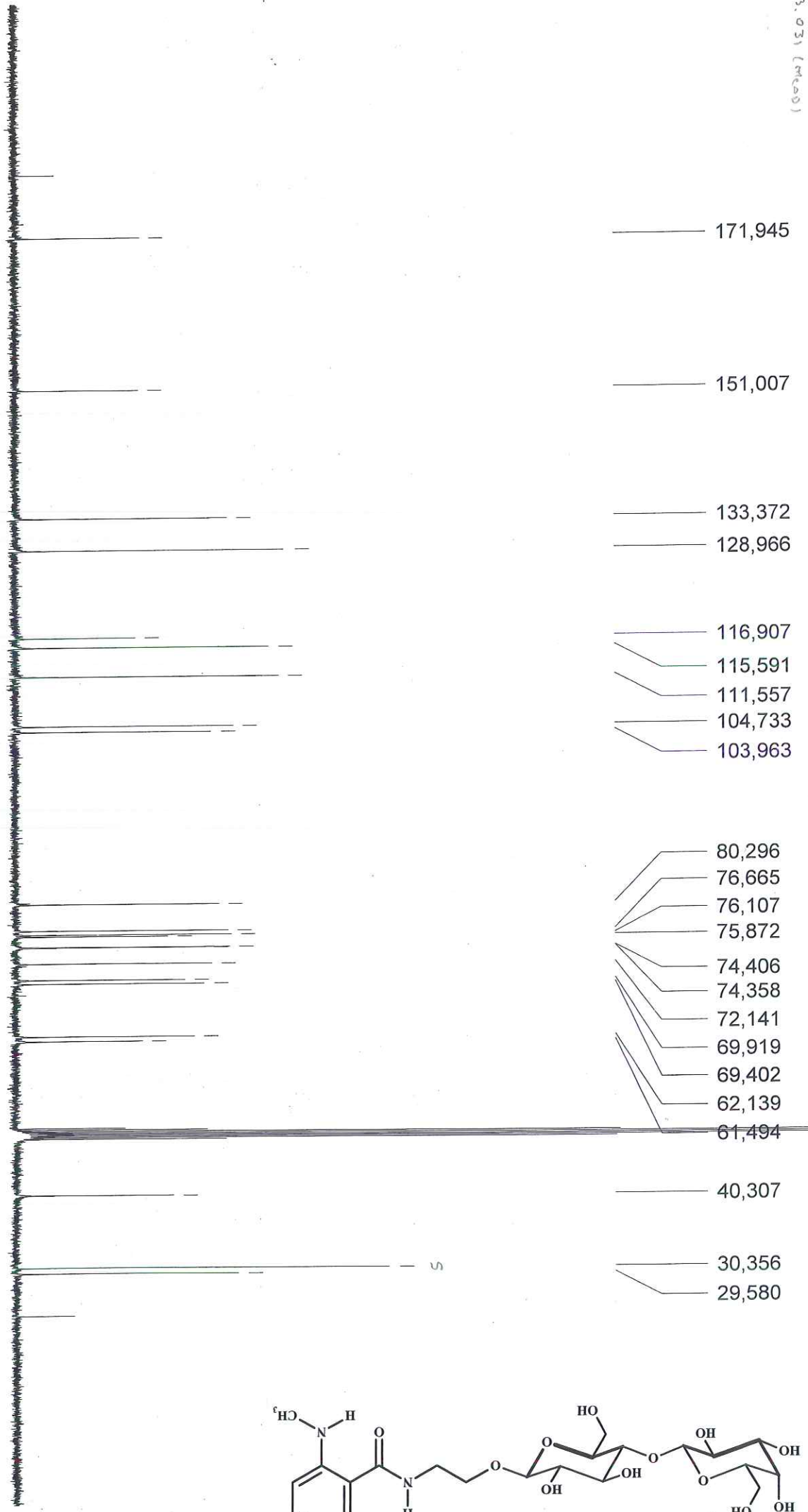
Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	rdB	e ⁻ Conf	N-Rule
519.218254	1	C22H35N2O12	519.218451	0.4	5.7	6.5	even	ok
541.199856	1	C22H34N2NaO12	541.200395	1.0	7.4	6.5	even	ok

12.031 (7600)



ppm (f1)

200
150
100
50
0





Analysis Info

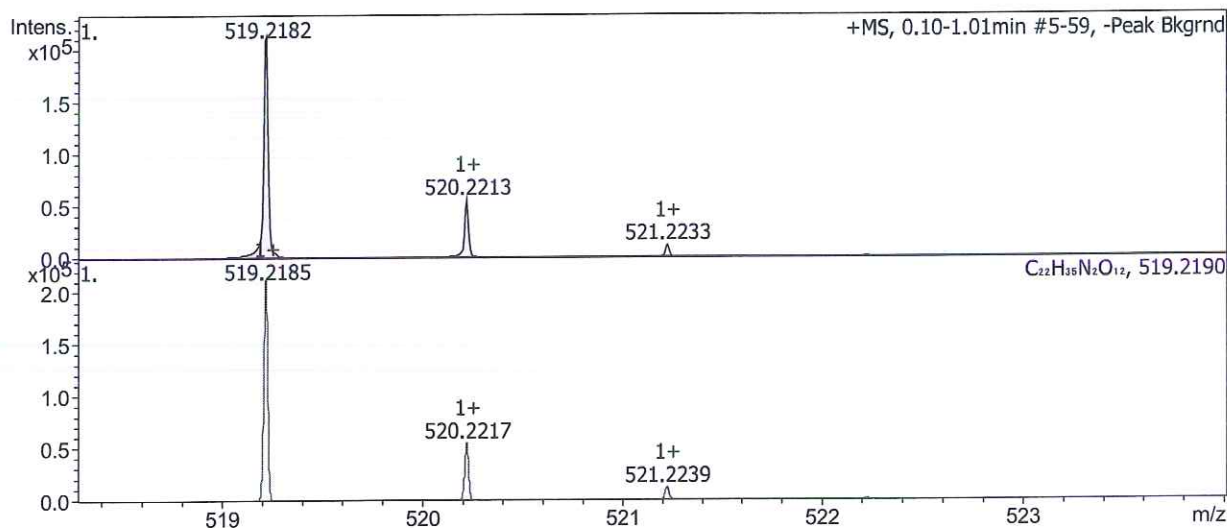
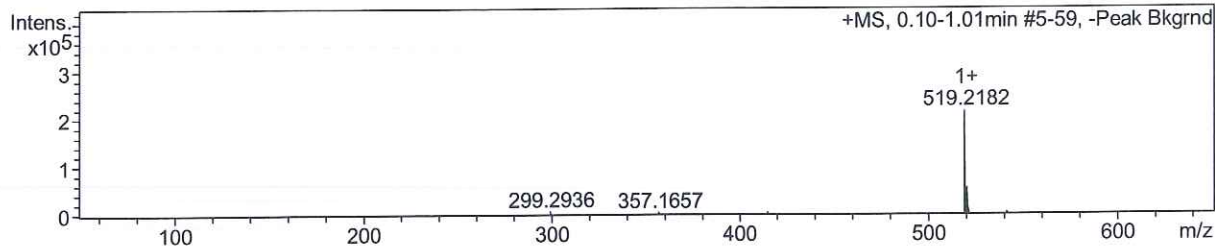
Sample Name **JCJ.13.031**
Analysis Name X004950CYC.d
Method Positif.m

Acquisition Date 29/08/2012 17:54:13

Laboratory
Instrument / Ser# maXis 255552.00
086

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.6 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	1000.0 Vpp	Set Divert Valve	Waste



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
519.218216	1	C22H35N2O12	519.218451	0.5	3.8	6.5	even	ok
541.199739	1	C22H34N2NaO12	541.200395	1.2	29.8	6.5	even	ok