

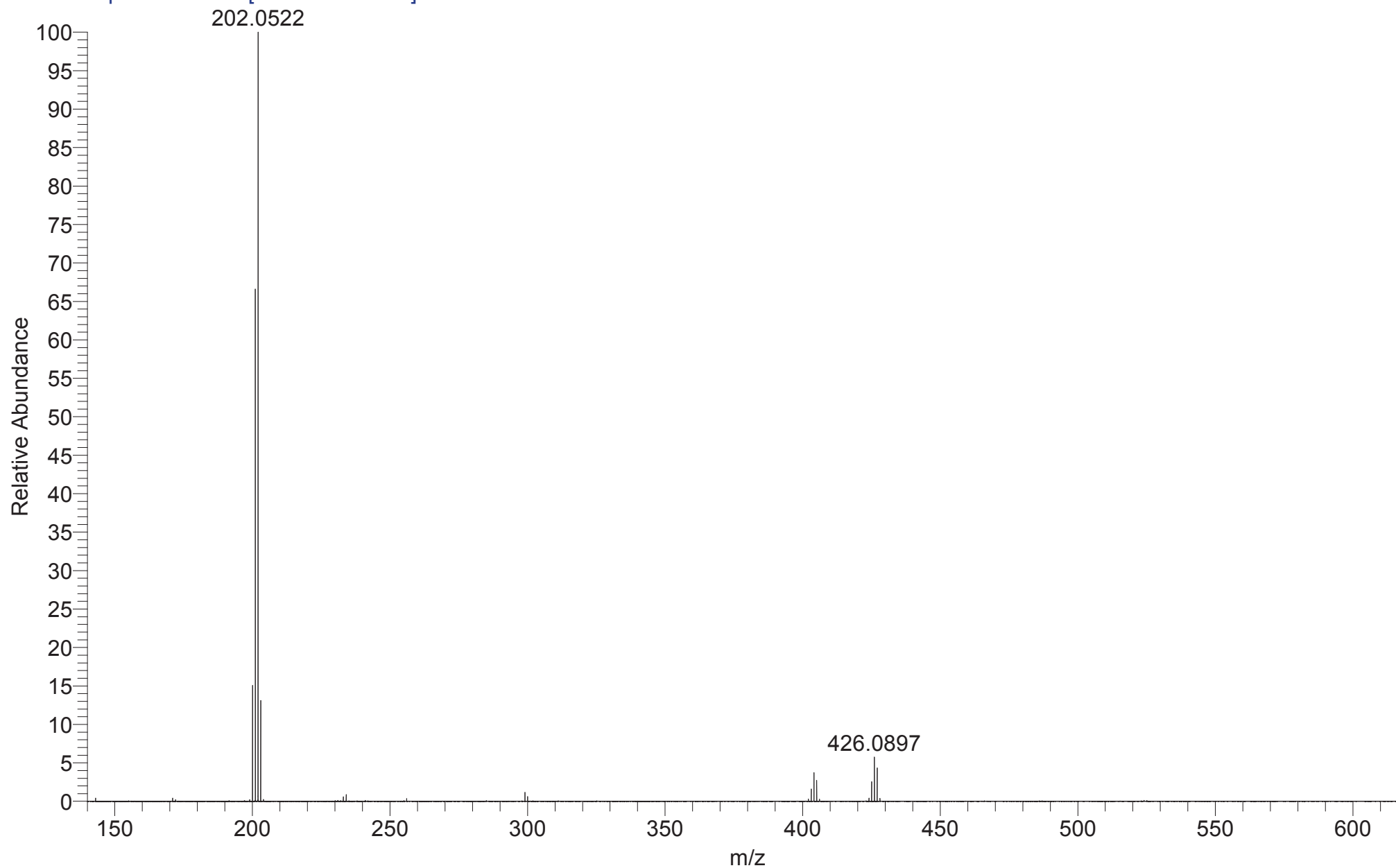
O:\NTTWAL_8C12M_38_2
NAP173
NTTWAL

EPSRC UK National MS Facility
LTQ Orbitrap XL

(MeOH)/MeOH+DEA
07/11/2016 10:02:32
C12H8O3

NTTWAL_8C12M_38_2 #6-17 RT: 0.14-0.42 AV: 11 NL: 8.62E7

T: FTMS - p NSI Full ms [140.00-1935.00]



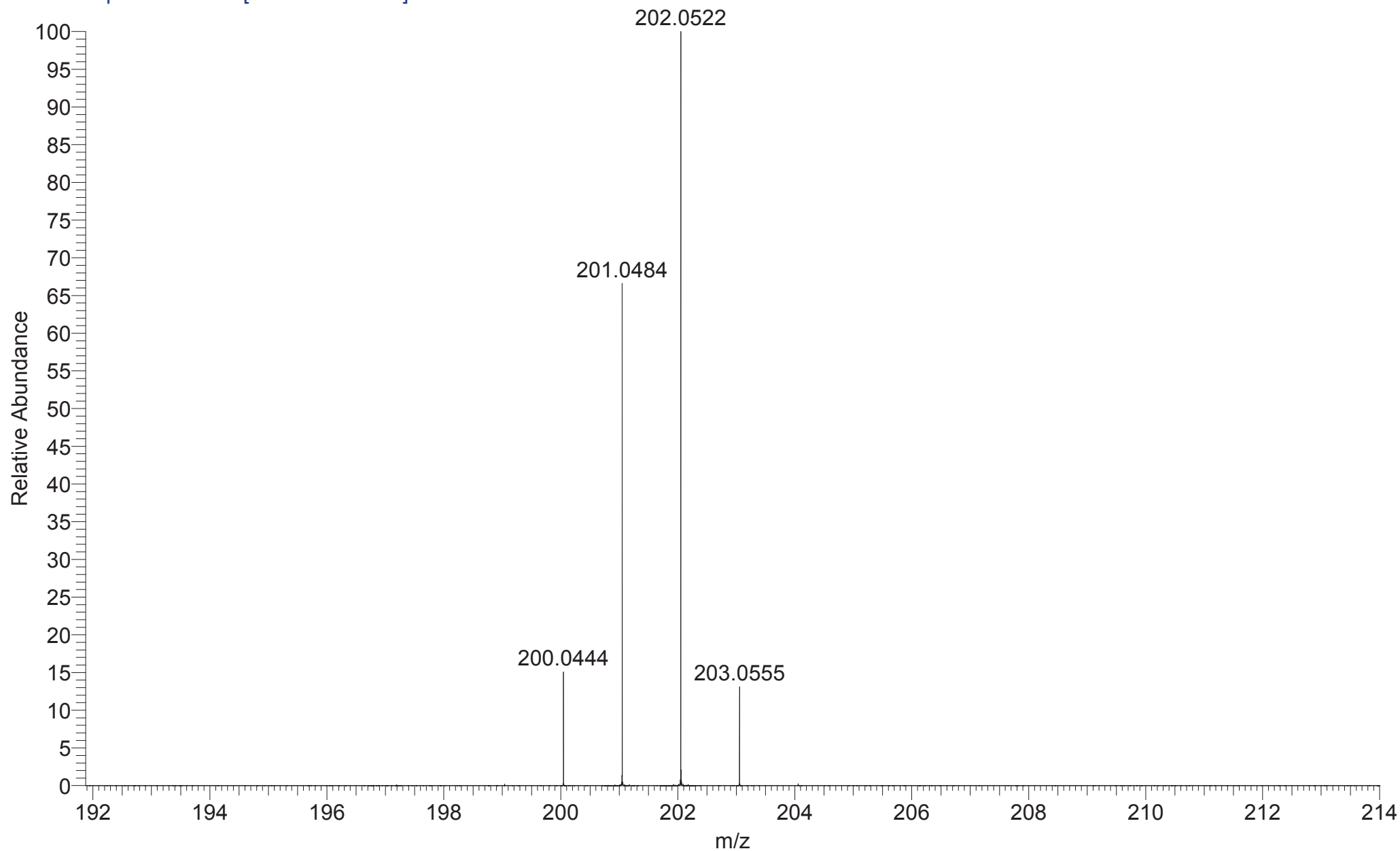
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NTTWAL_8C12M_38_2 #6-17 RT: 0.14-0.42 AV: 11 NL: 8.62E7

T: FTMS - p NSI Full ms [140.00-1935.00]



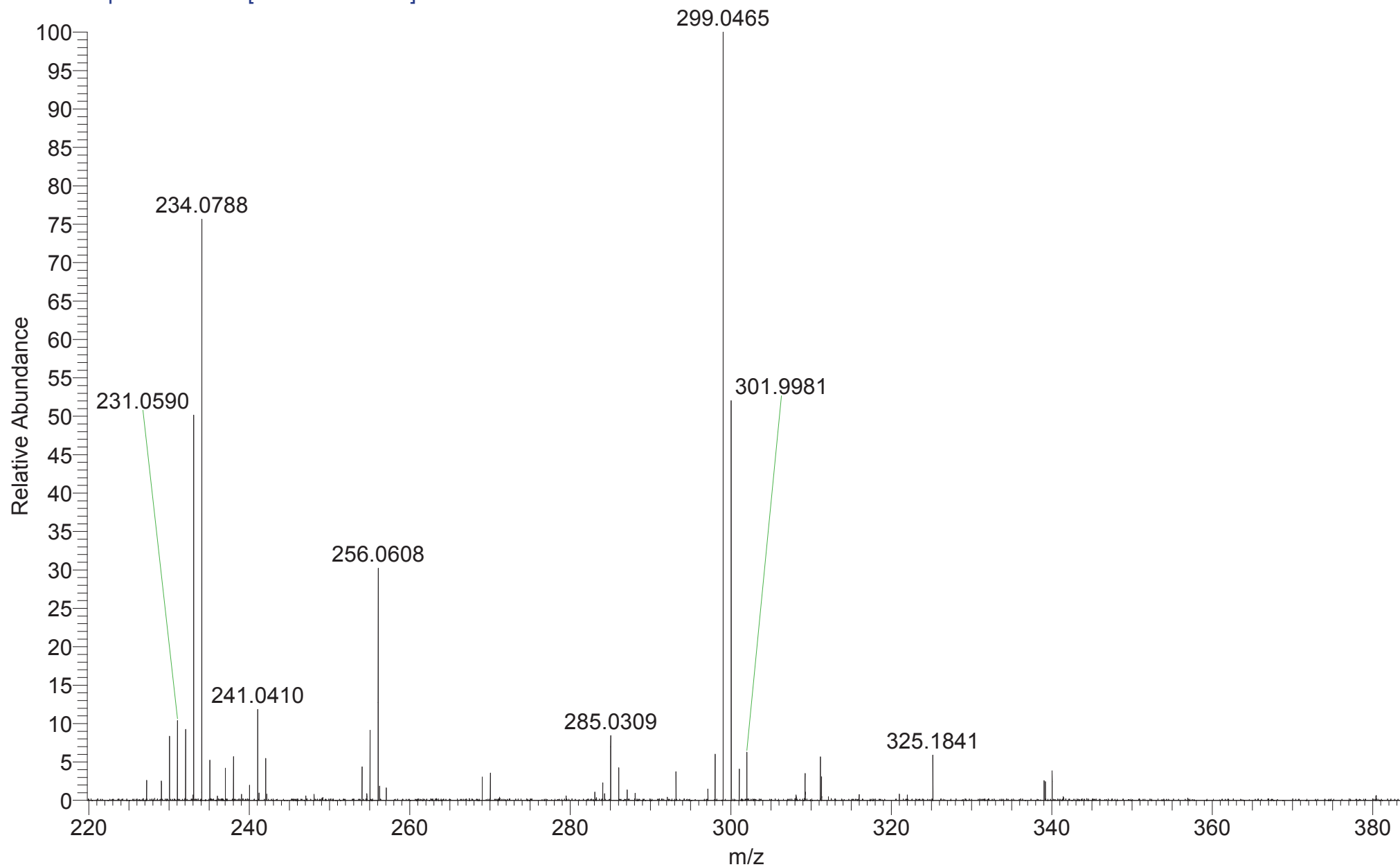
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NAP173
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(MeOH)/MeOH+DEA
07/11/2016 10:02:32
C12H8O3

NTTWAL_8C12M_38_2 #6-17 RT: 0.14-0.42 AV: 11 NL: 1.02E6

T: FTMS - p NSI Full ms [140.00-1935.00]

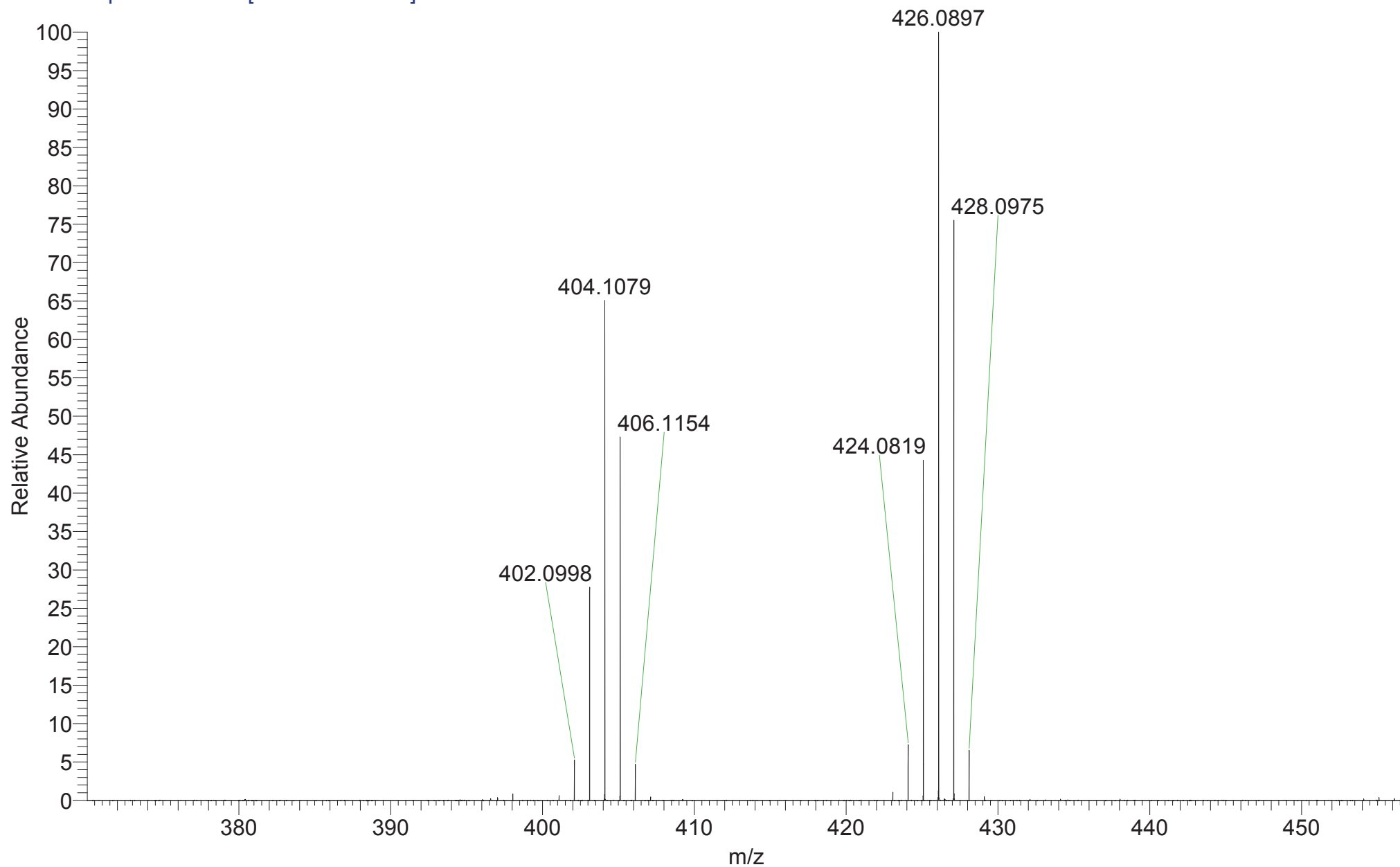


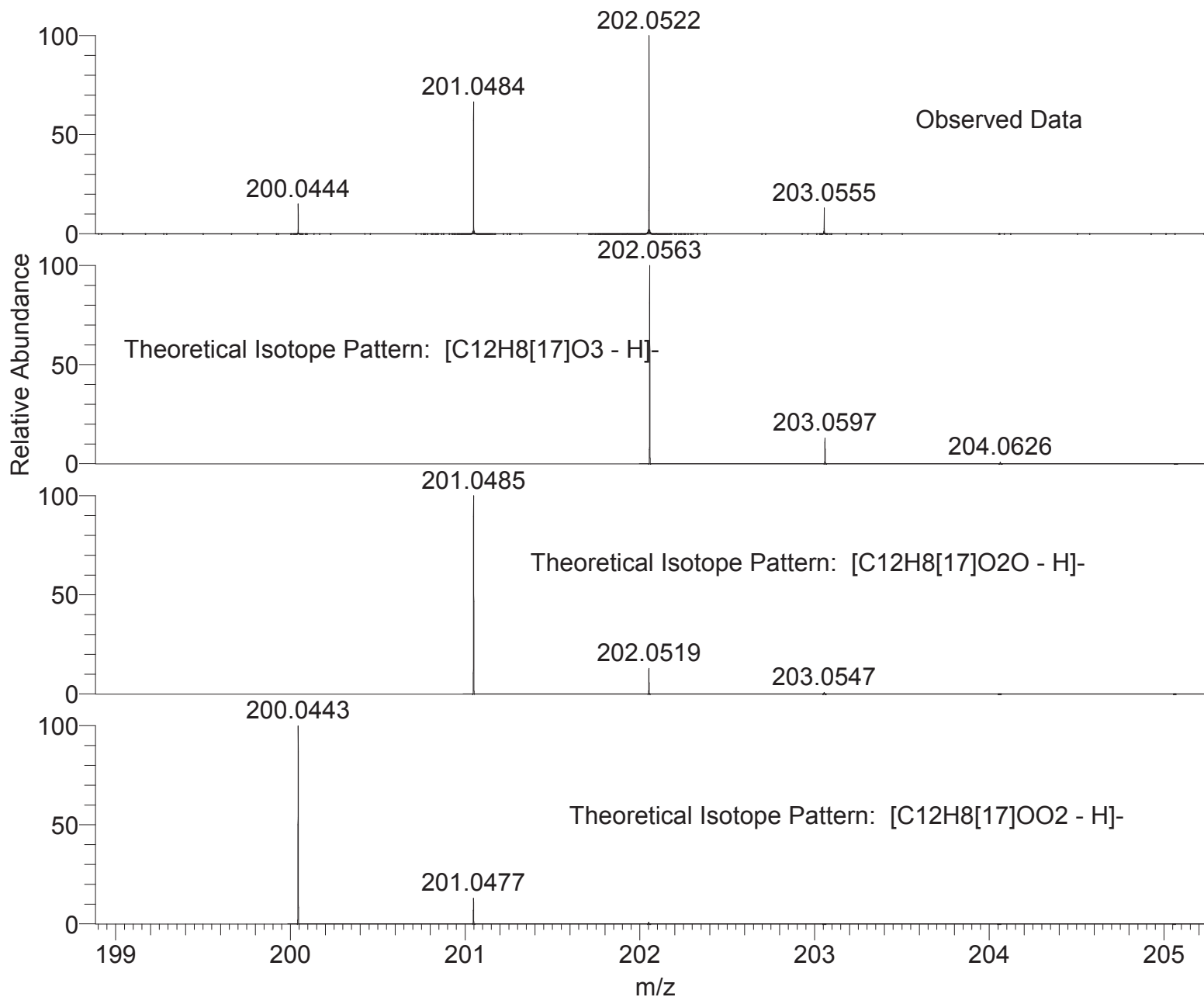
O:\NTTWAL_8C12M_38_2
NAP173
NTTWAL

EPSRC UK National MS Facility
LTQ Orbitrap XL

(MeOH)/MeOH+DEA
07/11/2016 10:02:32
C12H8O3

NTTWAL_8C12M_38_2 #6-17 RT: 0.14-0.42 AV: 11 NL: 4.97E6
T: FTMS - p NSI Full ms [140.00-1935.00]





NL:
8.62E7
NTTWAL_8C12M_38_2#6-17
RT: 0.14-0.42 AV: 11 T: FTMS
- p NSI Full ms
[140.00-1935.00]

NL:
2.06E4
 $^{17}O_2 C_{12} H_8 O:$
 $^{17}O_2 C_{12} H_8 O_1$
p (gss, s /p:40) Chrg -1
R: 100000 Res .Pwr . @FWHM

NL:
2.06E4
 $^{17}O_2 C_{12} H_7 O:$
 $^{17}O_2 C_{12} H_7 O_1$
p (gss, s /p:40) Chrg -1
R: 100000 Res .Pwr . @FWHM

NL:
2.05E4
 $^{17}OC_{12} H_7 O_2:$
 $^{17}O_1 C_{12} H_7 O_2$
p (gss, s /p:40) Chrg -1
R: 100000 Res .Pwr . @FWHM

Isotope: Min. .. Max.
 14 N 0....8
 16 O 0....8
 12 C 0....30
 1 H 0....50
 23 Na 0....0
 17 O 0....3
 Tolerance Window: +- 5.00 ppm
 Db/Ring Equiv: -3.. 100
 Fits: 200

N-Rule: Do not use
 Charge: -1

Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
200.0444	200.0443	0.6	9.5	C ₁₂ H ₇ O ₂ ¹⁷ O ₁
	200.0443	0.6	6.5	C ₆ H ₅ O ₁ ¹⁷ O ₃ N ₄
	200.0439	2.7	5.0	C ₇ H ₈ O ₅ N ₂
	200.0439	2.7	2.0	C ₁ H ₆ O ₄ ¹⁷ O ₂ N ₆
	200.0452	-4.0	1.5	C ₃ H ₈ O ₅ ¹⁷ O ₂ N ₃
	200.0452	-4.0	10.0	C ₈ H ₄ O ₁ N ₆
201.0484	201.0485	-0.5	9.5	C ₁₂ H ₇ O ₁ ¹⁷ O ₂
	201.0481	1.6	5.0	C ₇ H ₈ O ₄ ¹⁷ O ₁ N ₂
	201.0481	1.6	2.0	C ₁ H ₆ O ₃ ¹⁷ O ₃ N ₆
	201.0490	-3.0	5.5	C ₃ H ₅ O ₃ N ₈
	201.0490	-3.1	0.0	C ₄ H ₁₁ O ₈ N ₁
	201.0477	3.6	0.5	C ₂ H ₉ O ₇ N ₄
202.0522	202.0523	-0.5	5.0	C ₇ H ₈ O ₃ ¹⁷ O ₂ N ₂
	202.0519	1.5	0.5	C ₂ H ₉ O ₆ ¹⁷ O ₁ N ₄
	202.0527	-2.6	9.5	C ₁₂ H ₇ ¹⁷ O ₃

SPECTRUM - MS

NTTWAL_8C12M_38_2.raw

FTMS - p NSI Full ms [140.00-1935.00]

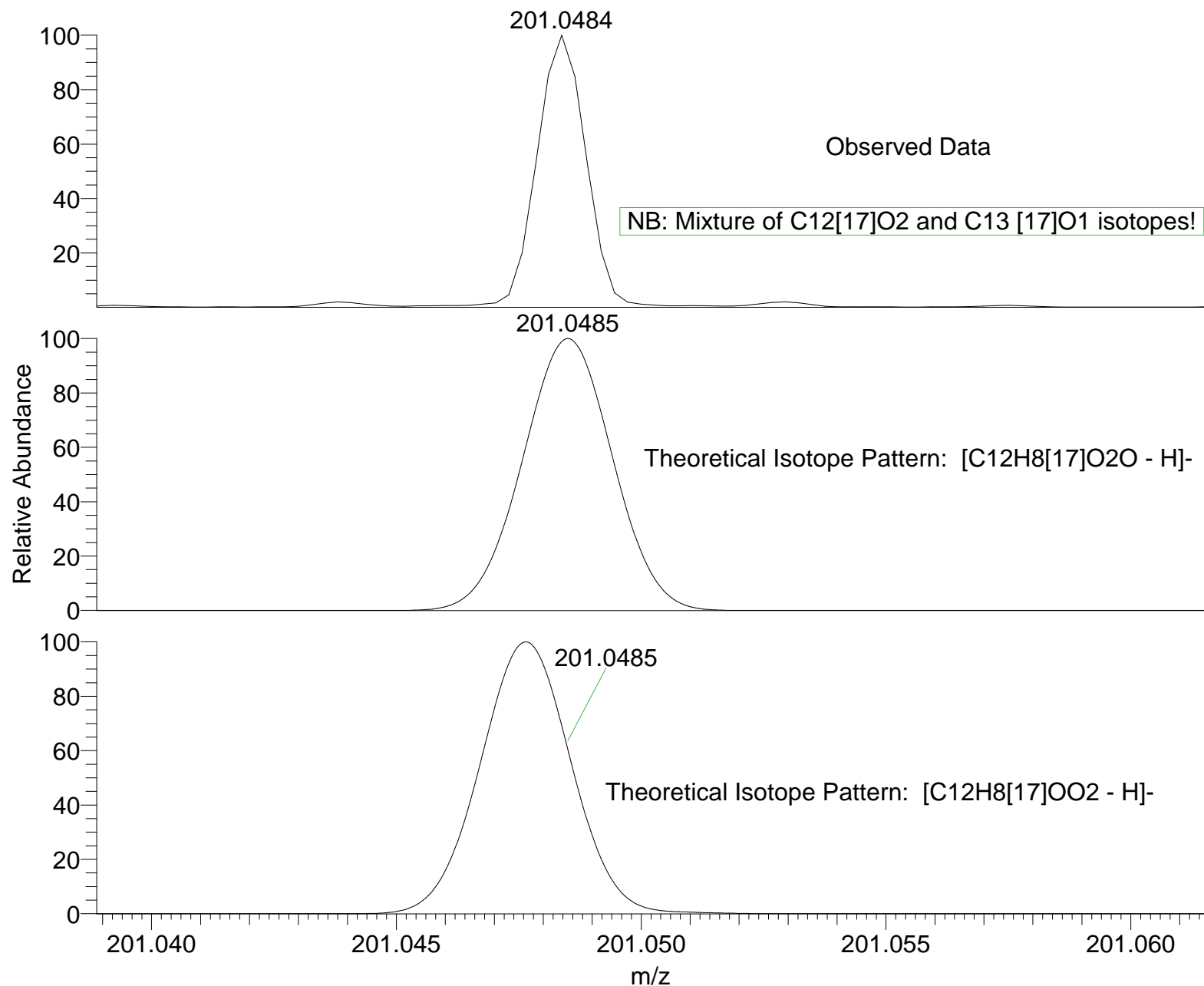
Scan #: 6-16

RT: 0.14-0.42

AV: 11

m/z Intensity Relative

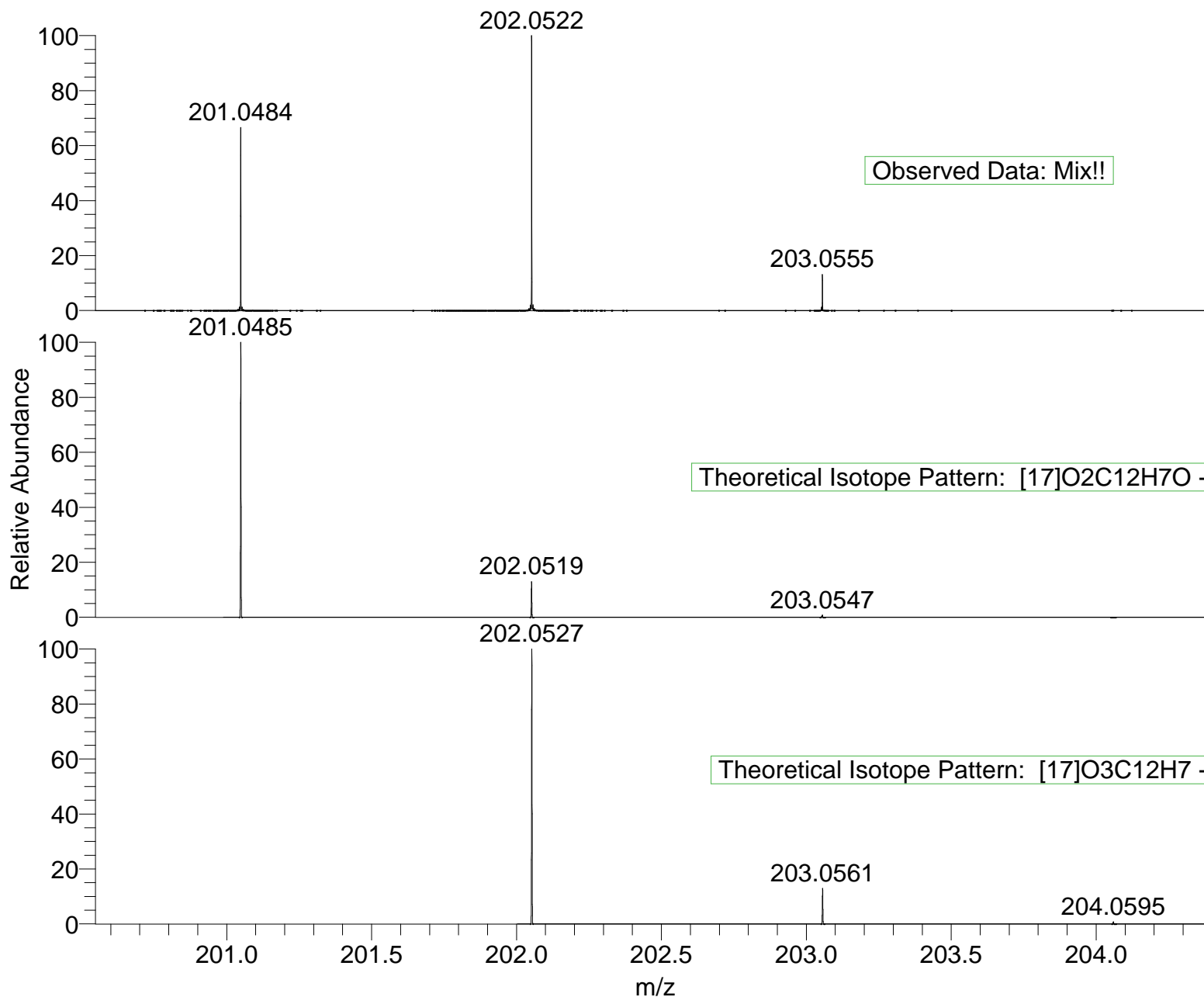
200.0399	260373.3	0.29
200.0444	13129591.0	14.86
200.0489	266248.3	0.30
201.0393	428876.8	0.49
201.0438	1154149.5	1.31
201.0484	57437968.0	65.00
201.0510	365408.8	0.41
201.0529	1169655.4	1.32
201.0575	420407.0	0.48
202.0385	293517.2	0.33
202.0431	656640.4	0.74
202.0477	1773048.4	2.01
202.0522	88364848.0	100.00
202.0549	547984.9	0.62
202.0568	1819005.4	2.06
202.0587	226809.5	0.26
202.0614	655714.3	0.74
202.0661	307628.2	0.35
203.0525	1101475.0	1.25
203.0555	11299534.0	12.79



NL:
5.74E7
NTTWAL_8C12M_38_2#6-17
RT: 0.14-0.42 AV: 11 T: FTMS
- p NSI Full ms
[140.00-1935.00]

NL:
2.06E4
 $^{17}\text{O}_2 \text{C}_{12} \text{H}_7 \text{O}$:
 $^{17}\text{O}_2 \text{C}_{12} \text{H}_7 \text{O}_1$
p (gss, s /p:40) Chrg -1
R: 100000 Res .Pwr . @FWHM

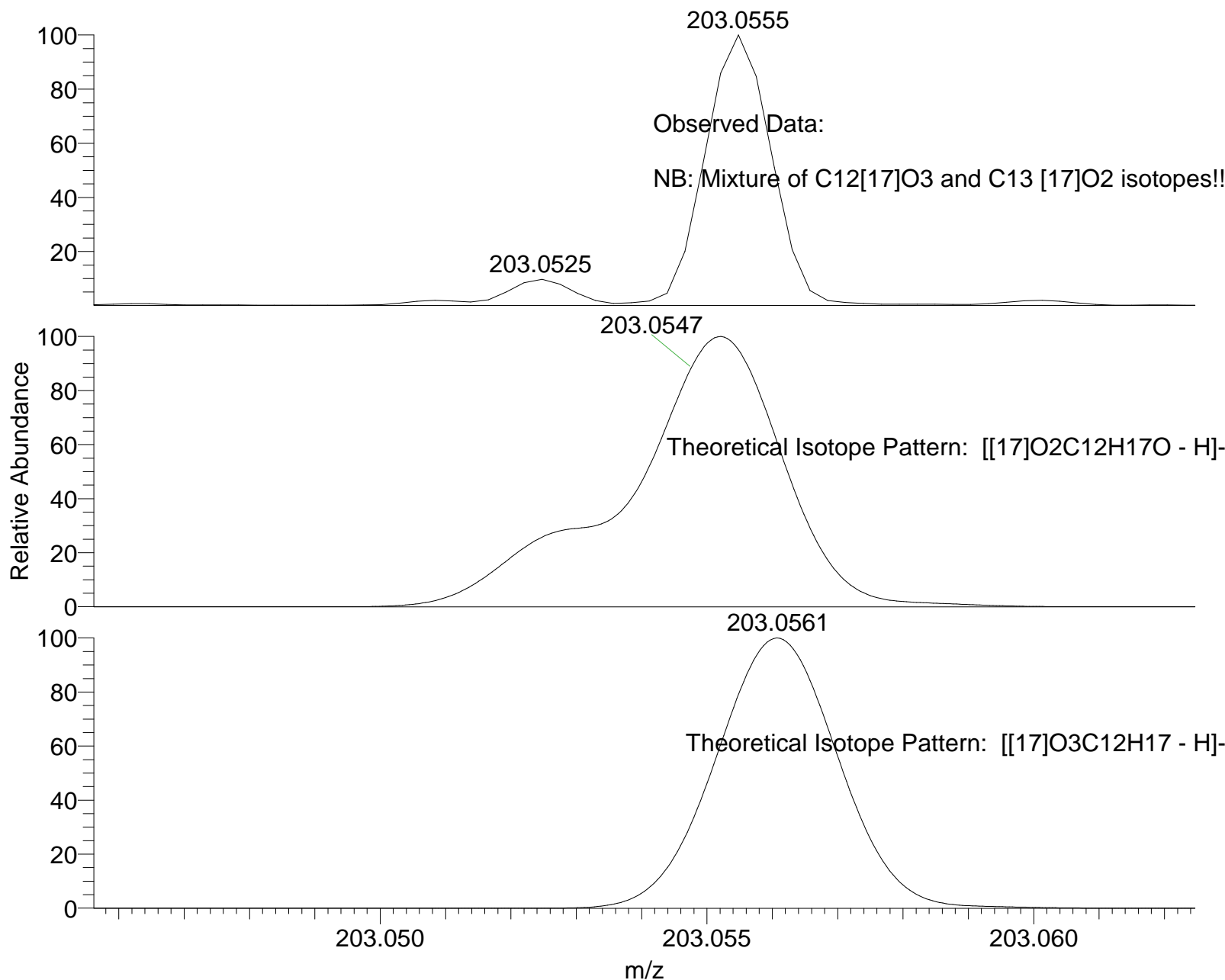
NL:
2.67E3
 $^{17}\text{O} \text{C}_{12} \text{H}_7 \text{O}_2$:
 $^{17}\text{O}_1 \text{C}_{12} \text{H}_7 \text{O}_2$
p (gss, s /p:40) Chrg -1
R: 100000 Res .Pwr . @FWHM



NL:
8.62E7
NTTWAL_8C12M_38_2#6-17
RT: 0.14-0.42 AV: 11 T: FTMS
- p NSI Full ms
[140.00-1935.00]

NL:
2.06E4
 $^{17}\text{O}_2\text{C}_{12}\text{H}_7\text{O}$:
 $^{17}\text{O}_2\text{C}_{12}\text{H}_7\text{O}_1$
p (gss, s /p:40) Chrg -1
R: 100000 Res .Pwr . @FWHM

NL:
2.06E4
 $^{17}\text{O}_3\text{C}_{12}\text{H}_7$:
 $^{17}\text{O}_3\text{C}_{12}\text{H}_7$
p (gss, s /p:40) Chrg -1
R: 100000 Res .Pwr . @FWHM



NL:
1.13E7
NTTWAL_8C12M_38_2#6-17
RT: 0.14-0.42 AV: 11 T: FTMS
- p NSI Full ms
[140.00-1935.00]

NL:
1.60E2
 $^{17}\text{O}_2 \text{C}_{12} \text{H}_7 \text{O}$:
 $^{17}\text{O}_2 \text{C}_{12} \text{H}_7 \text{O}_1$
p (gss, s /p:40) Chrg -1
R: 100000 Res .Pwr . @FWHM

NL:
2.67E3
 $^{17}\text{O}_3 \text{C}_{12} \text{H}_7$:
 $^{17}\text{O}_3 \text{C}_{12} \text{H}_7$
p (gss, s /p:40) Chrg -1
R: 100000 Res .Pwr . @FWHM