

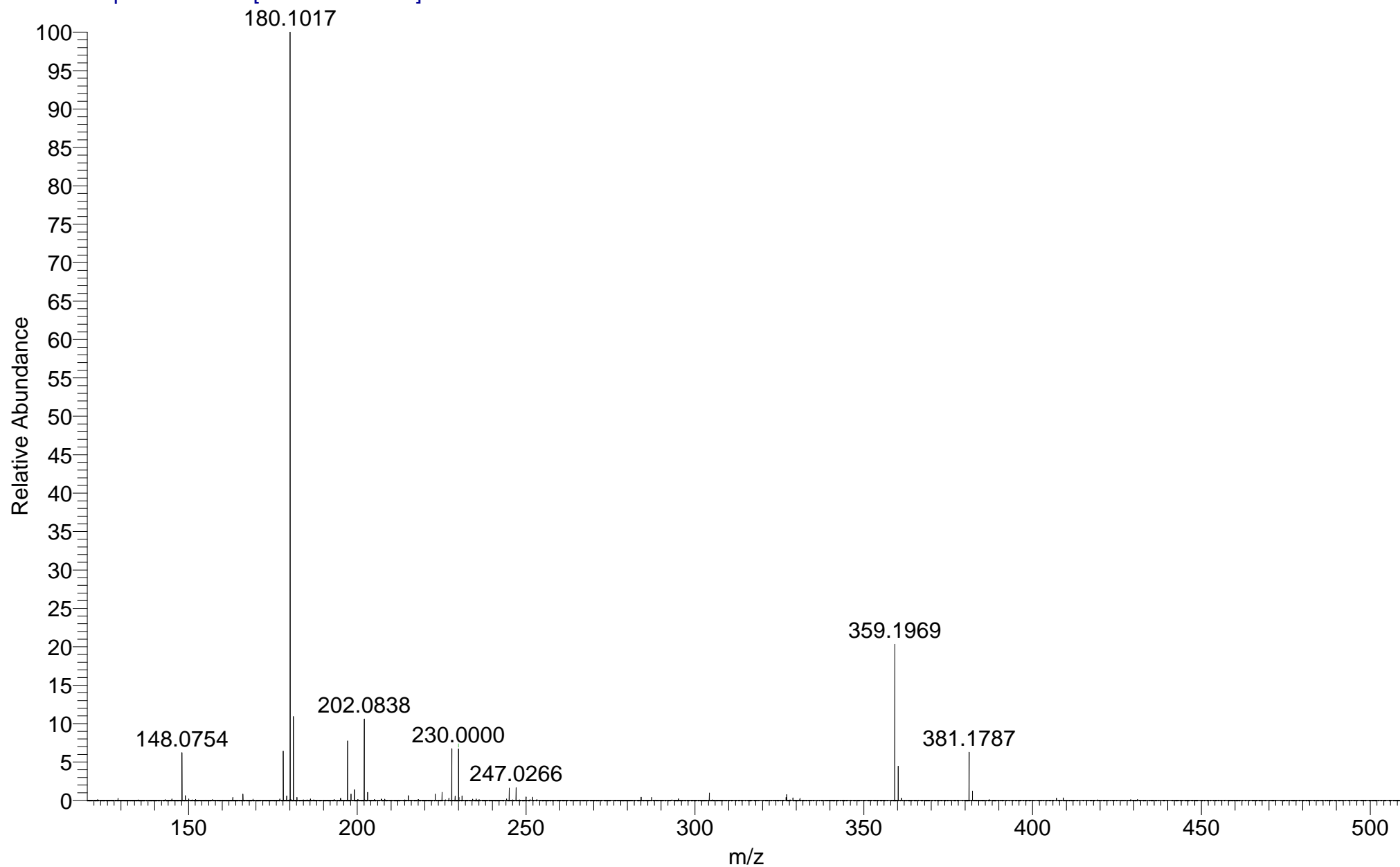
MLO114
(MeOH)/MeOH+NH₄OAc
C₉H₁₀BrNO

EPSRC National Facility Swansea
LTQ Orbitrap XL

BATJAM-MO
16/06/2017 12:53:22

BATJAM_LTU34_33048 #46-58 RT: 0.74-1.05 AV: 12 SM: 7G NL: 1.64E7

T: FTMS + p NSI Full ms [120.00-1935.00]



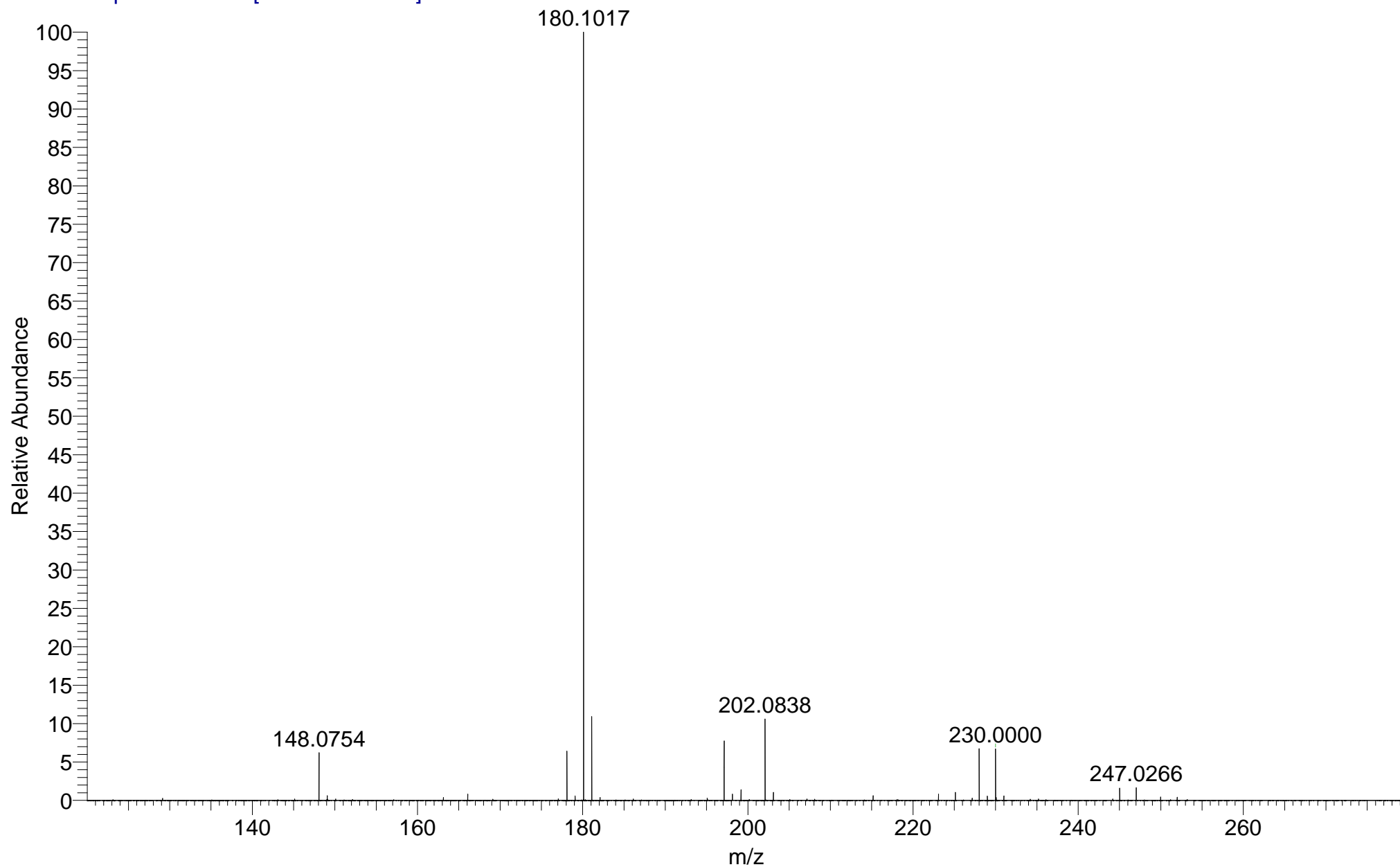
MLO114
(MeOH)/MeOH+NH₄OAc
C₉H₁₀BrNO

EPSRC National Facility Swansea
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16/06/2017 12:53:22

BATJAM_LTU34_33048 #46-58 RT: 0.74-1.05 AV: 12 SM: 7G NL: 1.64E7

T: FTMS + p NSI Full ms [120.00-1935.00]



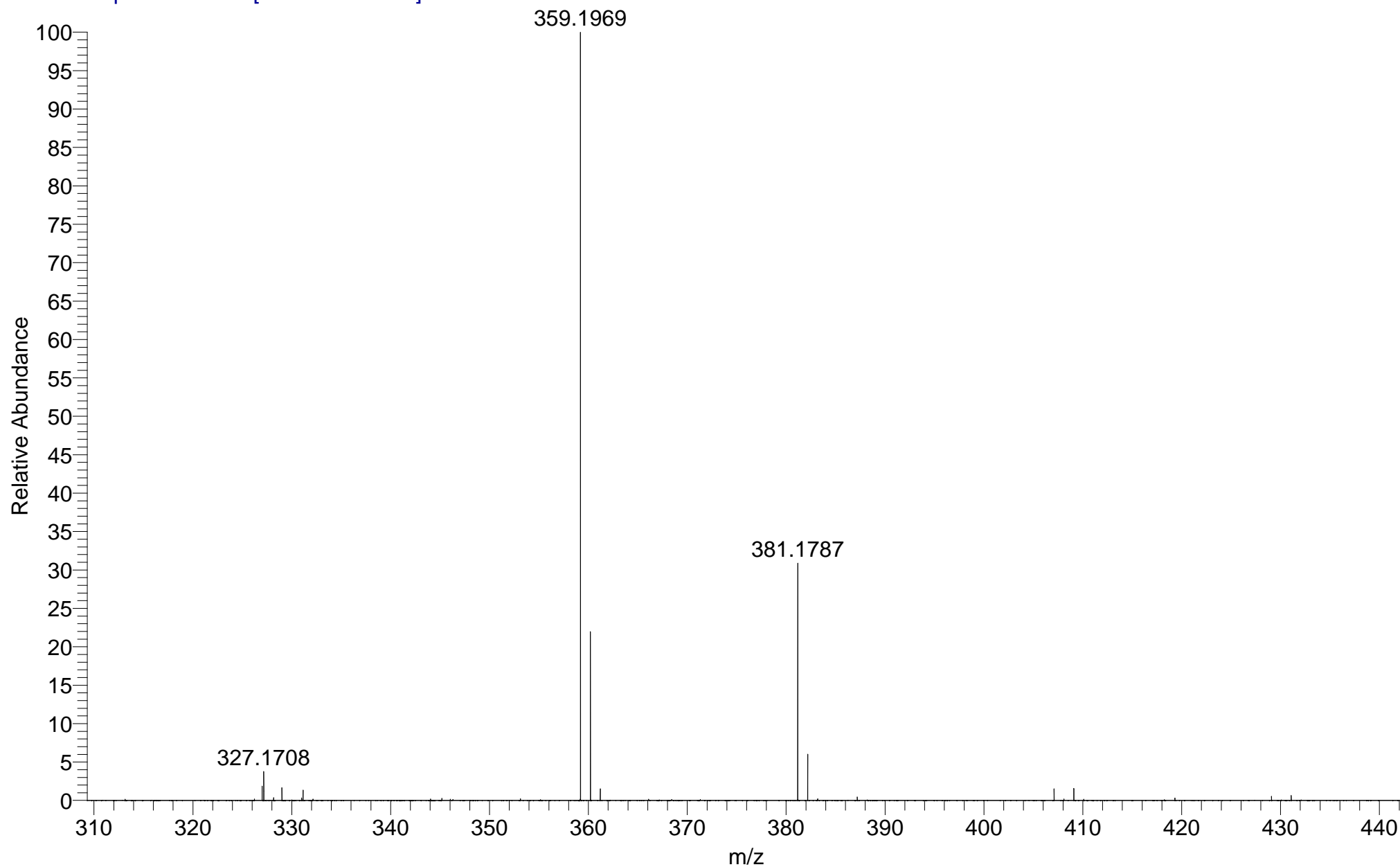
MLO114
(MeOH)/MeOH+NH₄OAc
C₉H₁₀BrNO

EPSRC National Facility Swansea
LTQ Orbitrap XL

BATJAM-MO
16/06/2017 12:53:22

BATJAM_LTU34_33048 #46-58 RT: 0.74-1.05 AV: 12 SM: 7G NL: 3.33E6

T: FTMS + p NSI Full ms [120.00-1935.00]

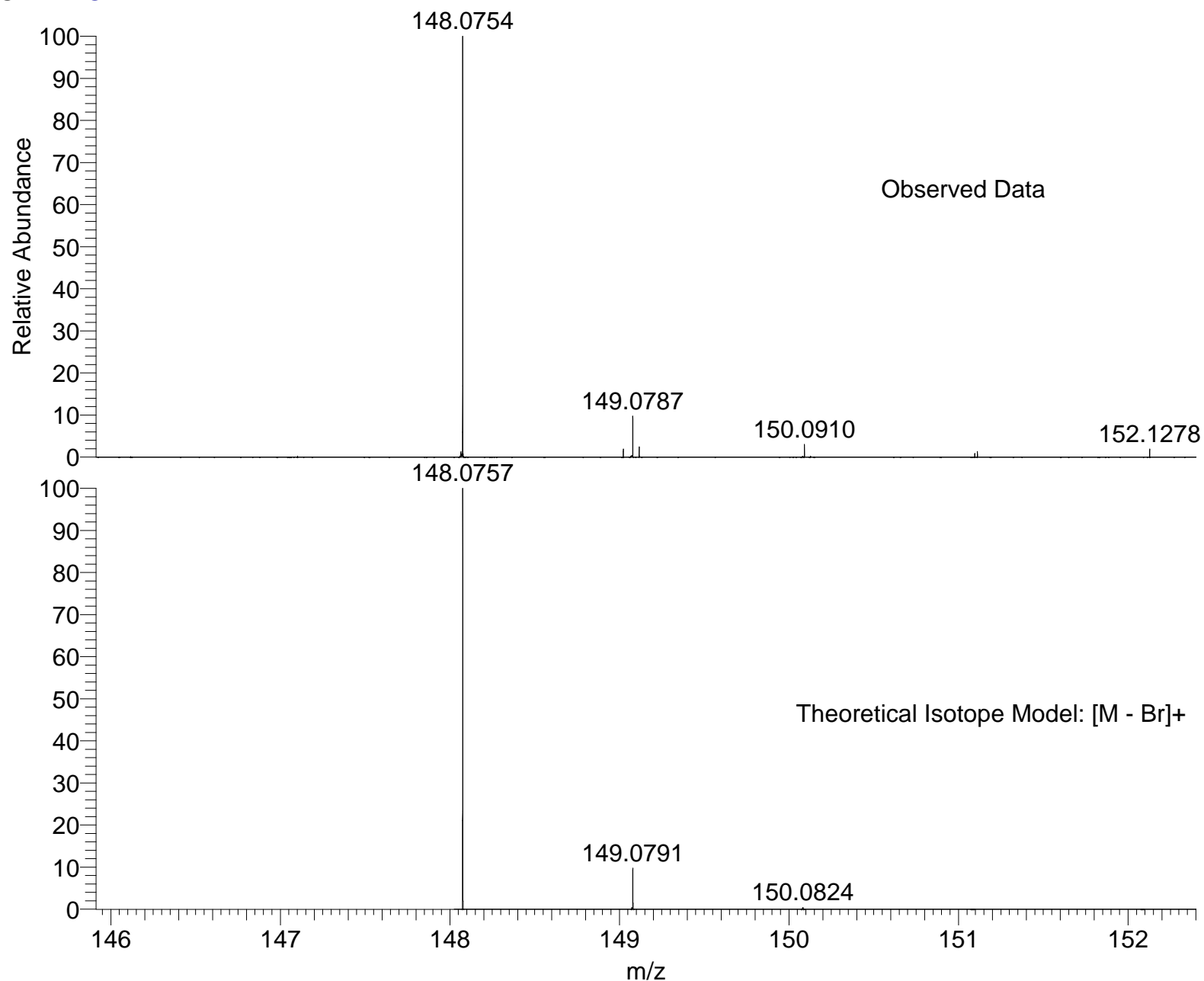


MLO114
(MeOH)/MeOH+NH4OAc
C9H10BrNO

EPSRC National Facility Swansea
LTQ Orbitrap XL

BATJAM-MO
16/06/2017 12:53:22

SM: 7G



NL:
1.02E6
BATJAM_LTU34_33048#46-58
RT: 0.74-1.05 AV: 12 T:
FTMS + p NSI Full ms
[120.00-1935.00]

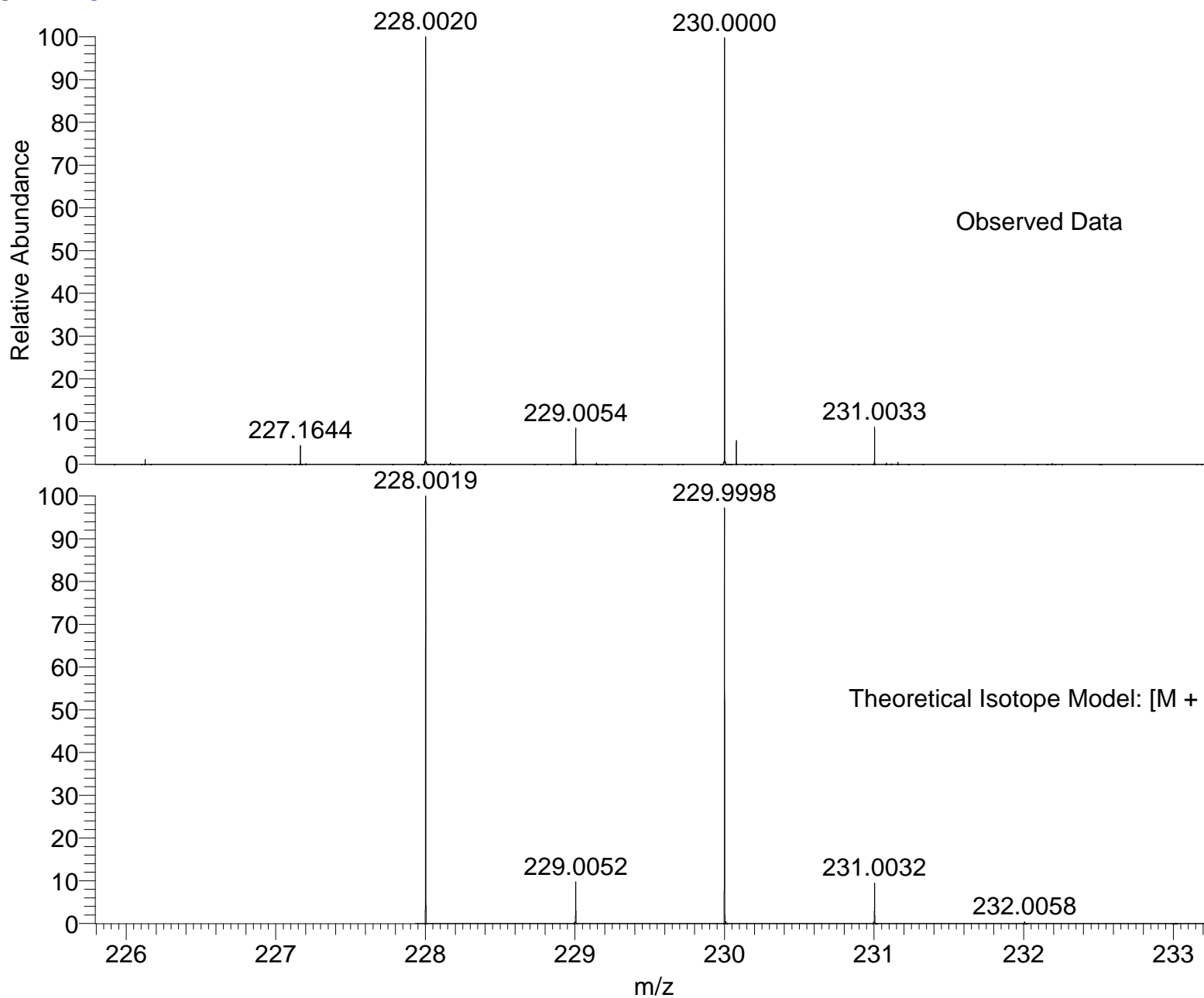
NL:
2.11E4
C₉H₁₀NO:
C₉H₁₀N₁O₁
p (gss, s /p:40) Chrg 1
R: 100000 Res .Pwr . @FWHM

MLO114
(MeOH)/MeOH+NH₄OAc
C₉H₁₀BrNO

EPSRC National Facility Swansea
LTQ Orbitrap XL

BATJAM-MO
16/06/2017 12:53:22

SM: 7G



NL:
1.10E6
BATJAM_LTU34_33048#46-58
RT: 0.74-1.05 AV: 12 T:
FTMS + p NSI Full ms
[120.00-1935.00]

NL:
1.07E4
C₉H₁₀NOBrH:
C₉H₁₁N₁O₁Br₁
p (gss, s /p:40) Chrg 1
R: 100000 Res .Pwr . @FWHM

Isotope: Min. .. Max.
 14 N 0....15
 16 O 0....15
 12 C 0....30
 1 H 0....50
 23 Na 0....0
 79 Br 0....1
 Tolerance Window: +- 5.00 ppm
 Db/Ring Equiv: -3.. 300
 Fits: 300

N-Rule: Do not use
 Charge: 1

Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
148.0754	148.0757	-2.0	5.5	C ₉ H ₁₀ O ₁ N ₁
228.0020	228.0019	0.6	4.5	C ₉ H ₁₁ O ₁ N ₁ Br ₁
	228.0026	-2.8	12.0	C ₈ O ₃ N ₆
	228.0013	3.1	7.0	C ₇ H ₄ O ₇ N ₂