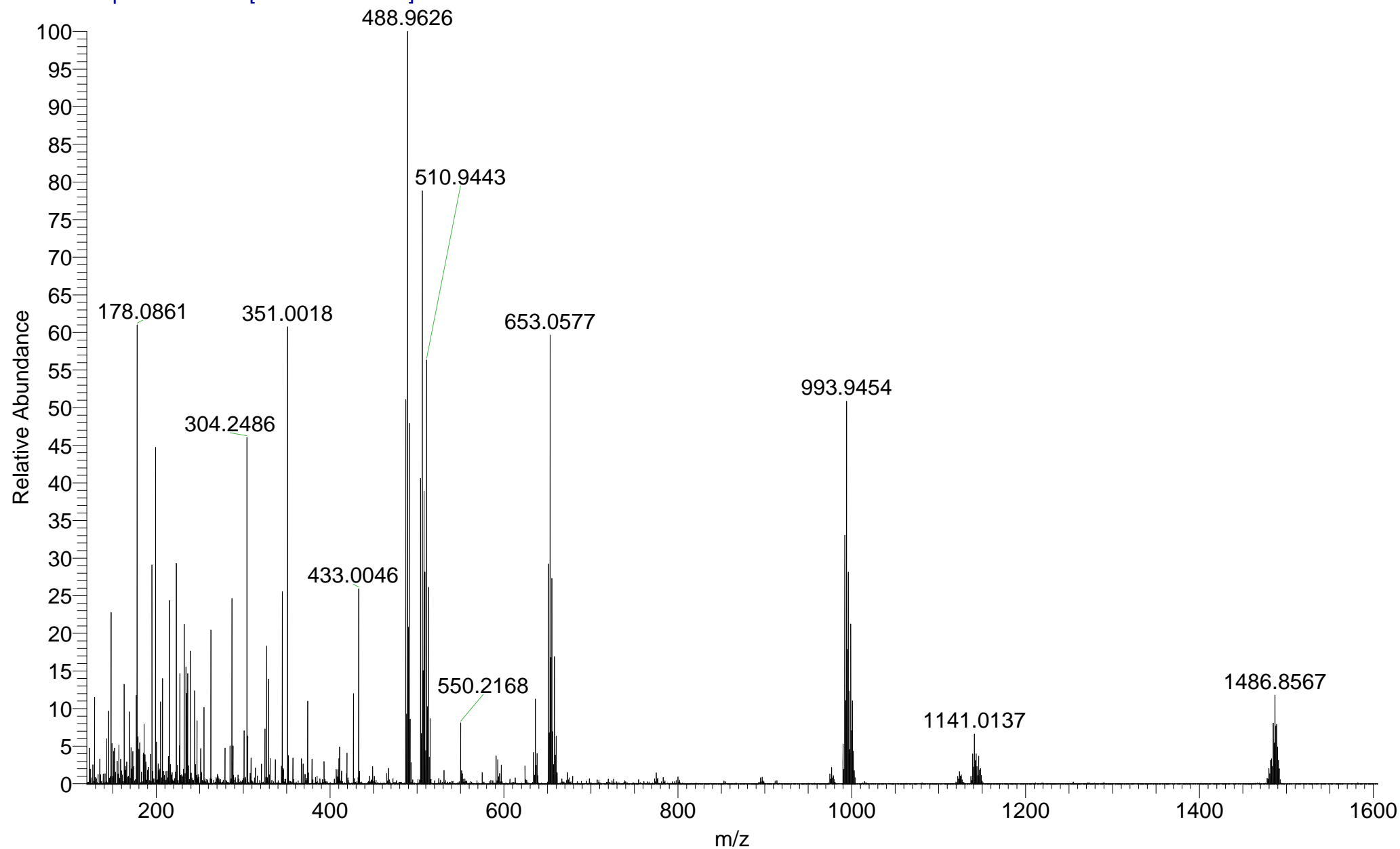


BATJAM_LTKUL_32800 #45-60 RT: 0.72-1.02 AV: 12 SM: 7G NL: 6.85E5
T: FTMS + p NSI Full ms [120.00-1935.00]



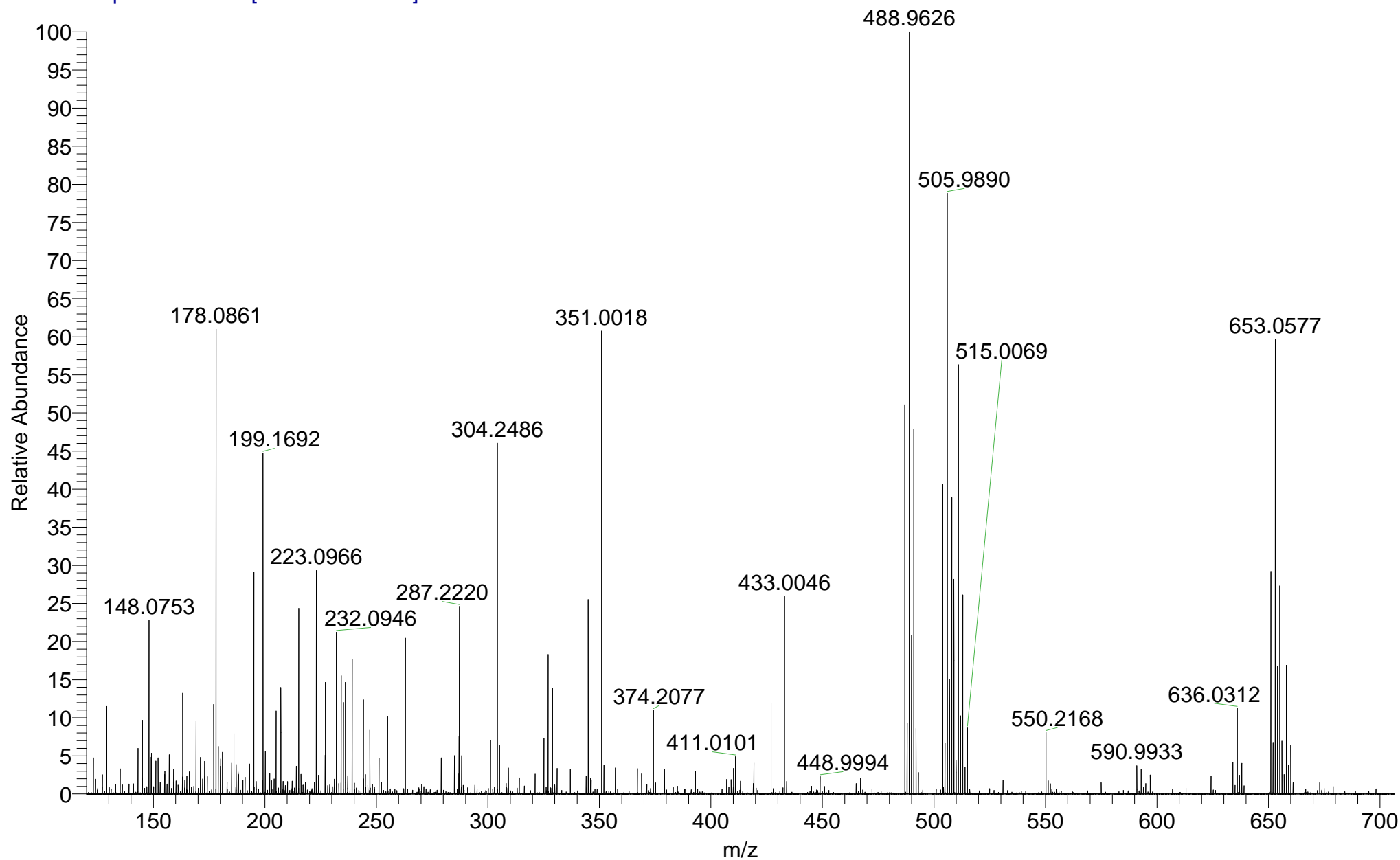
MLO111
(MeOH)/MeOH+NH4OAc
C21H16Br2N2O2

EPSRC National Facility Swansea
LTQ Orbitrap XL

BATJAM-MO
16/06/2017 12:44:37

BATJAM_LTKUL_32800 #45-60 RT: 0.72-1.02 AV: 12 SM: 7G NL: 6.85E5

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

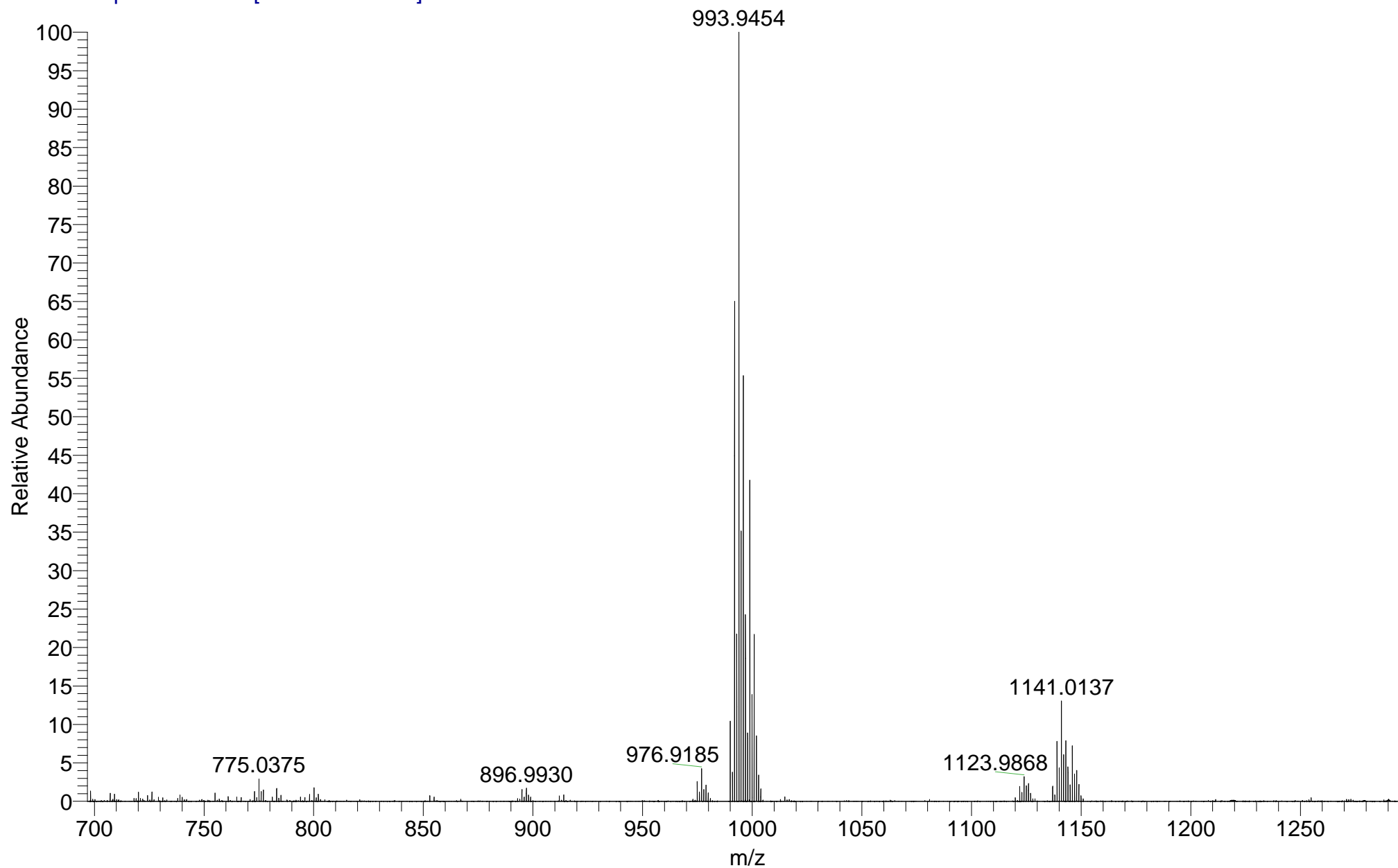


MLO111
(MeOH)/MeOH+NH4OAc
C21H16Br2N2O2

EPSRC National Facility Swansea
LTQ Orbitrap XL

BATJAM-MO
16/06/2017 12:44:37

BATJAM_LTKUL_32800 #45-60 RT: 0.72-1.02 AV: 12 SM: 7G NL: 3.48E5
T: FTMS + p NSI Full ms [120.00-1935.00]

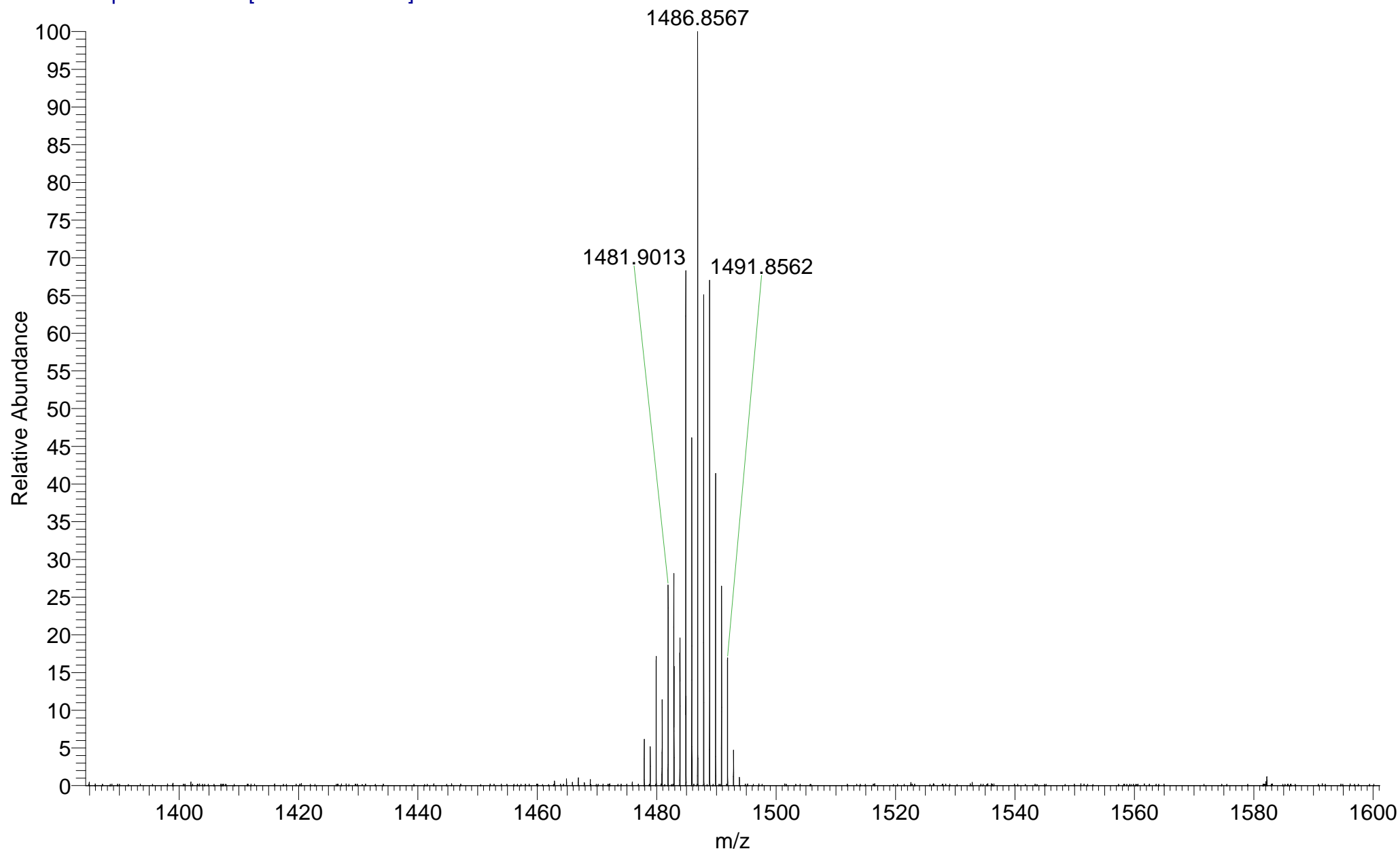


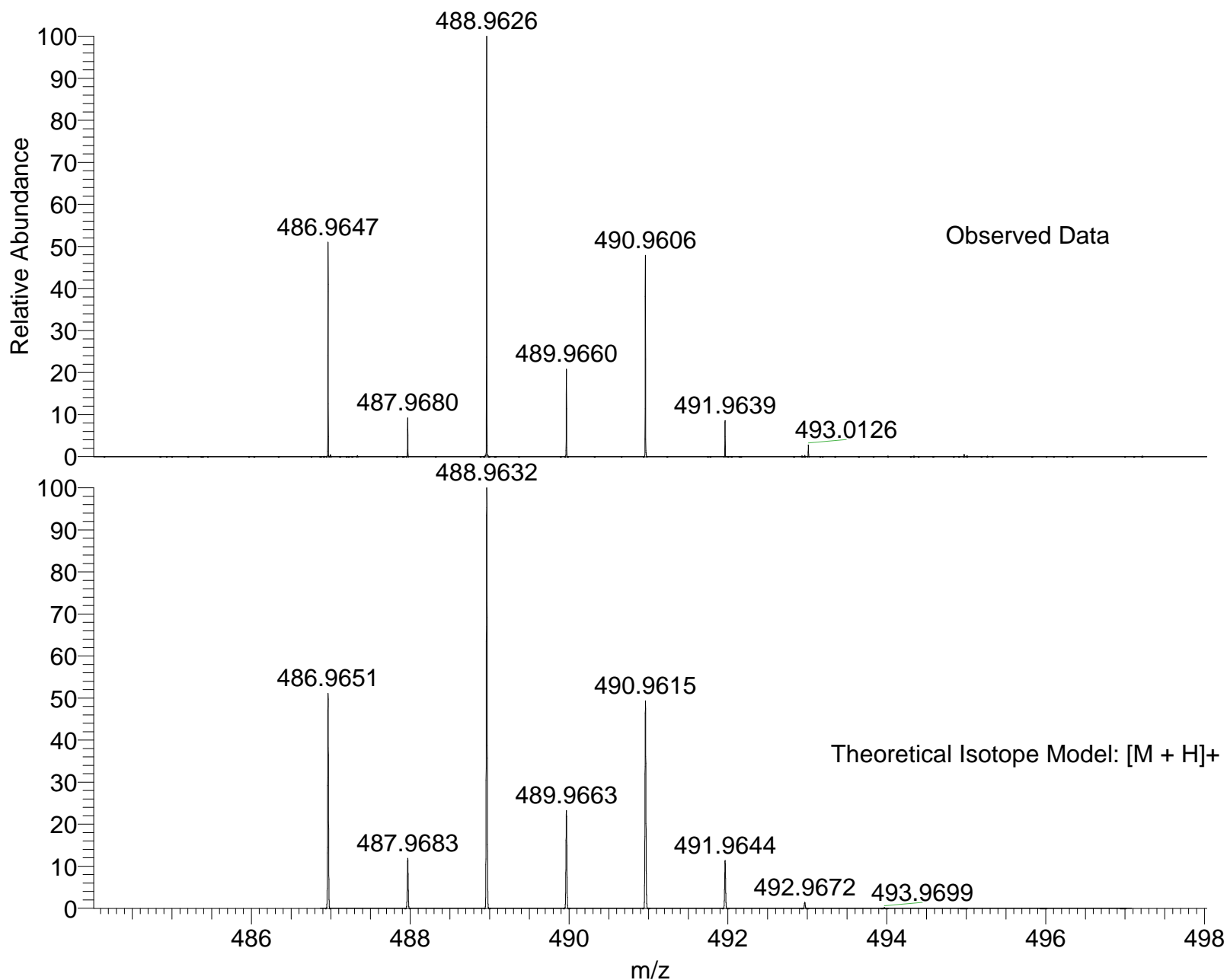
MLO111
(MeOH)/MeOH+NH₄OAc
C₂₁H₁₆Br₂N₂O₂

EPSRC National Facility Swansea
LTQ Orbitrap XL

BATJAM-MO
16/06/2017 12:44:37

BATJAM_LTKUL_32800 #45-60 RT: 0.72-1.02 AV: 12 SM: 7G NL: 8.08E4
T: FTMS + p NSI Full ms [120.00-1935.00]





NL:
6.85E5
BATJAM_LTKUL_32800#45-
60 RT: 0.72-1.02 AV: 12 T:
FTMS + p NSI Full ms
[120.00-1935.00]

NL:
9.27E3
C₂₁H₁₆Br₂N₂O₂H:
C₂₁H₁₇Br₂N₂O₂
p (gss, s /p:40) Chrg 1
R: 40000 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 1....2
 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 |
|----------|---------------------|----------------|------|--|
| 486.9647 | 486.9646 | 0.2 | 16.0 | C ₁₉ H ₁₀ O ₈ N ₃ Br ₁ |
| | 486.9646 | 0.3 | 21.5 | C ₁₈ H ₄ O ₃ N ₁₀ Br ₁ |
| | 486.9651 | -0.8 | 9.0 | C ₄ H ₆ O ₉ N ₁₅ Br ₁ |
| | 486.9651 | -0.8 | 3.5 | C ₅ H ₁₂ O ₁₄ N ₈ Br ₁ |
| | 486.9643 | 0.8 | 1.5 | C ₅ H ₁₇ O ₇ N ₁₀ Br ₂ |
| | 486.9651 | -0.9 | 13.5 | C ₂₁ H ₁₇ O ₂ N ₂ Br ₂ |
| | 486.9638 | 1.9 | 14.0 | C ₁₉ H ₁₅ O ₁ N ₅ Br ₂ |
| | 486.9656 | -1.9 | 6.5 | C ₆ H ₁₃ O ₃ N ₁₄ Br ₂ |
| | 486.9656 | -1.9 | 1.0 | C ₇ H ₁₉ O ₈ N ₇ Br ₂ |
| | 486.9637 | 2.0 | 4.0 | C ₃ H ₁₀ O ₁₃ N ₁₁ Br ₁ |
| | 486.9659 | -2.5 | 21.0 | C ₂₀ H ₆ O ₄ N ₇ Br ₁ |
| | 486.9659 | -2.5 | 15.5 | C ₂₁ H ₁₂ O ₉ Br ₁ |
| | 486.9632 | 3.0 | 16.5 | C ₁₇ H ₈ O ₇ N ₆ Br ₁ |
| | 486.9632 | 3.0 | 22.0 | C ₁₆ H ₂ O ₂ N ₁₃ Br ₁ |
| | 486.9664 | -3.5 | 8.5 | C ₆ H ₈ O ₁₀ N ₁₂ Br ₁ |
| | 486.9664 | -3.5 | 3.0 | C ₇ H ₁₄ O ₁₅ N ₅ Br ₁ |
| | 486.9630 | 3.6 | 2.0 | C ₃ H ₁₅ O ₆ N ₁₃ Br ₂ |
| | 486.9624 | 4.6 | 9.0 | C ₁₈ H ₁₉ O ₅ N ₁ Br ₂ |
| | 486.9624 | 4.6 | 14.5 | C ₁₇ H ₁₃ N ₈ Br ₂ |
| | 486.9670 | -4.7 | 6.0 | C ₈ H ₁₅ O ₄ N ₁₁ Br ₂ |
| | 486.9670 | -4.7 | 0.5 | C ₉ H ₂₁ O ₉ N ₄ Br ₂ |
| | 486.9624 | 4.7 | 4.5 | C ₁ H ₈ O ₁₂ N ₁₄ Br ₁ |