

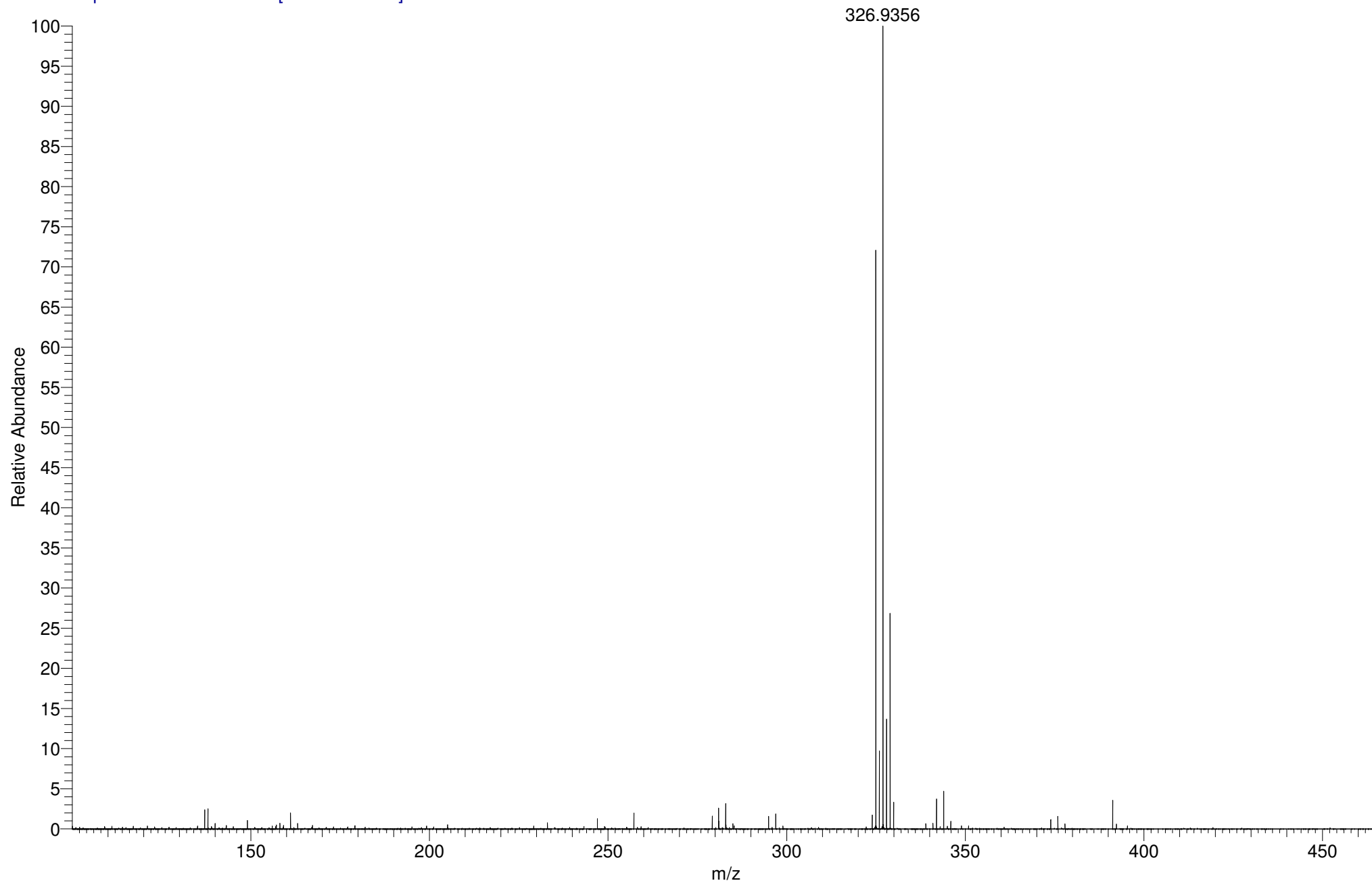
BCCPCA MW=325?
ASAP(SOLID)

EPSRC National Facility Swansea
LTQ Orbitrap XL

Downs
19/09/2013 15:16:33

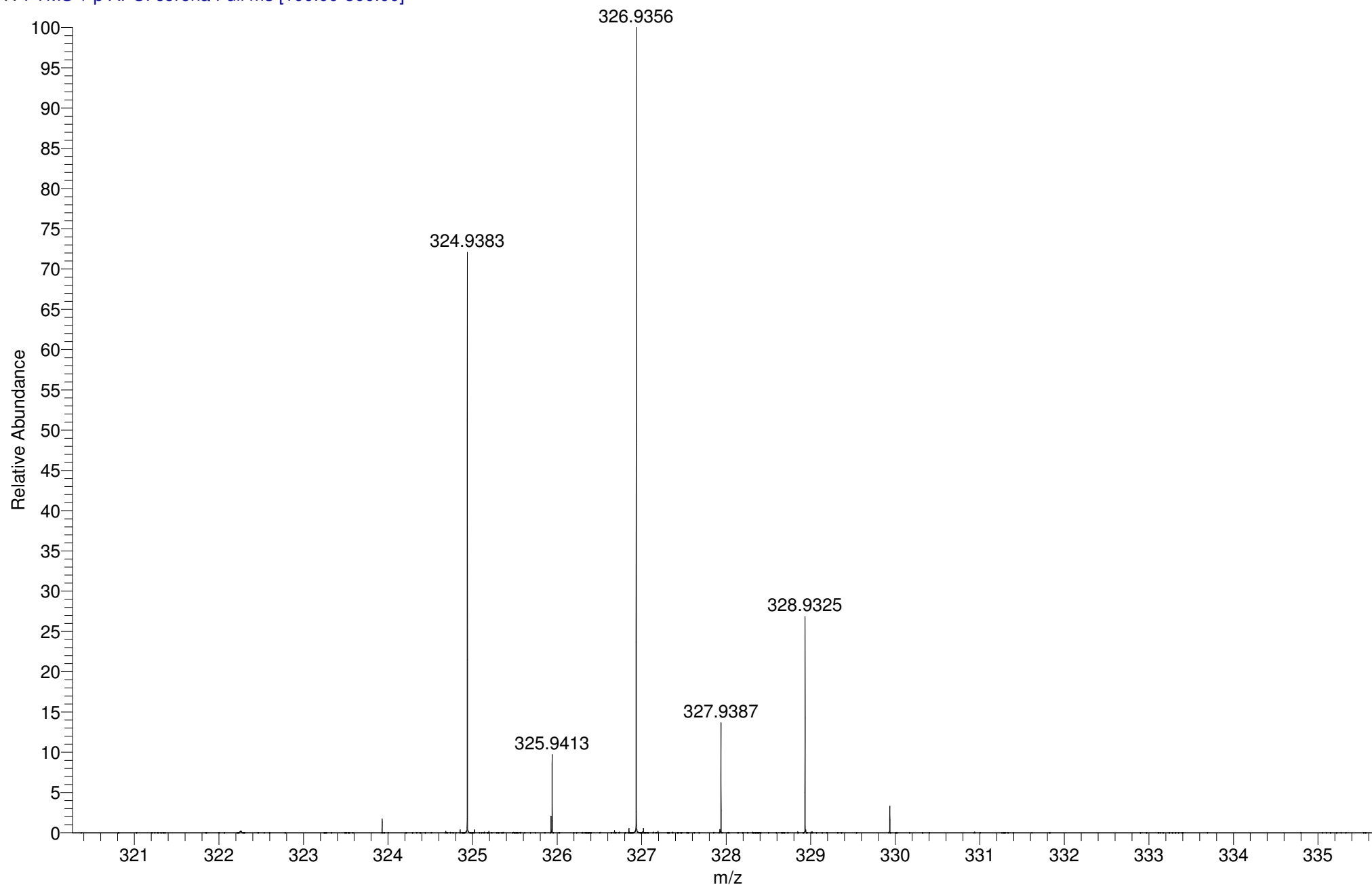
NORPER016-PG-HASP #31-39 RT: 1.77-2.22 AV: 9 SM: 7G NL: 1.23E7

T: FTMS + p APCI corona Full ms [100.00-800.00]

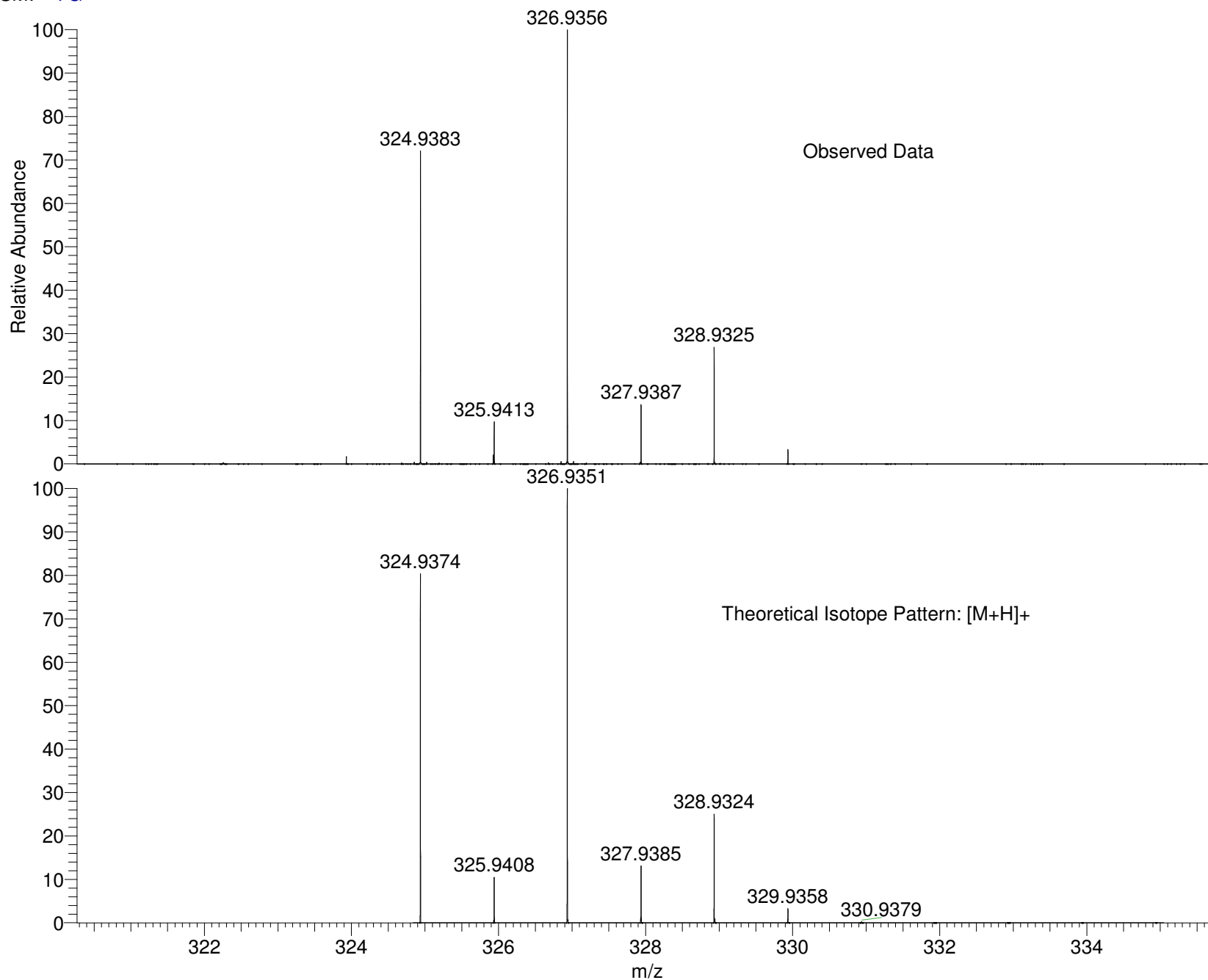


NORPER016-PG-HASP #31-39 RT: 1.77-2.22 AV: 9 SM: 7G NL: 1.23E7

T: FTMS + p APCI corona Full ms [100.00-800.00]



SM: 7G



NL:
1.23E7
NORPER016-PG-HASP#31-39
RT: 1.77-2.22 AV: 9 T: FTMS
+ p APCI corona Full ms
[100.00-800.00]

NL:
9.73E3
C₁₂H₆BrClN₂O₂H:
C₁₂H₇Br₁Cl₁N₂O₂
p (gss, s/p:40) Chrg 1
R: 100000 Res .Pwr . @FWHM

Isotope: Min. .. Max.
 14 N 0....10
 16 O 0....14
 12 C 0....65
 1 H 0....80
 23 Na 0....0
 35 Cl 1....2
 79 Br 1....2
 Tolerance Window: +- 5.00 ppm
 Db/Ring Equiv: -3.. 100
 Fits: 150

N-Rule: Do not use
 Charge: 1

| Mass | Theoretical Mass | Delta [ppm] | RDB | Composition |
|----------|---------------------|----------------|-----|--|
| 324.9383 | 324.9379 | 1.3 | 5.0 | C ₉ H ₁₀ O ₁ N ₃ Br ₁ Cl ₂ |
| | 324.9374 | 2.8 | 9.5 | C ₁₂ H ₇ O ₂ N ₂ Br ₁ Cl ₁ |
| | 324.9392 | -2.8 | 4.5 | C ₁₁ H ₁₂ O ₂ Br ₁ Cl ₂ |