

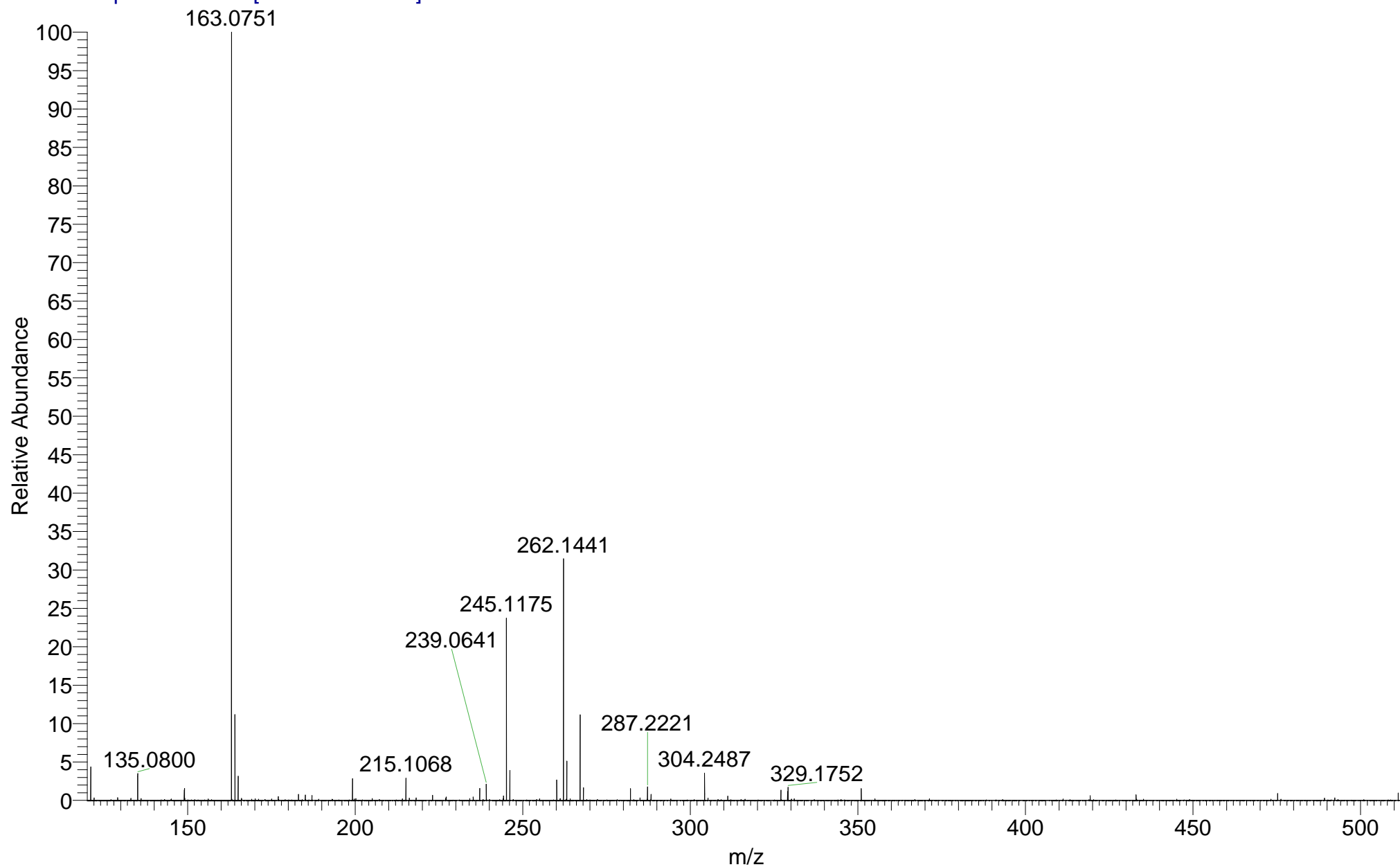
O:\IMPBUL_CLN_XE_45527
(DCM)/MeOH + NH₄OAc
MD-3-024

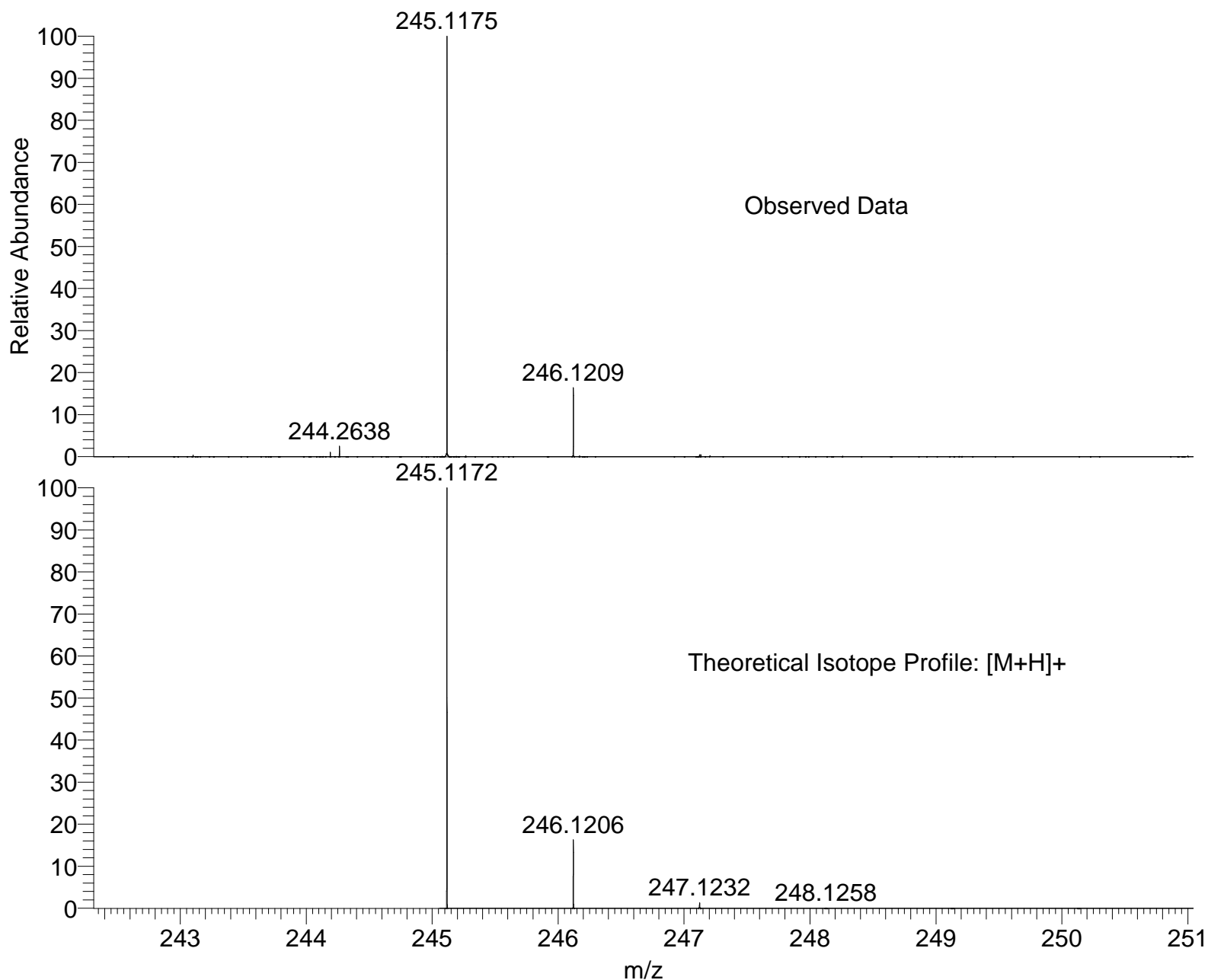
EPSRC UK National MS Facility
LTQ Orbitrap XL

C₁₅H₁₆O₃
30/05/2018 11:04:52

IMPBUL_CLN_XE_45527 #38-53 RT: 0.65-1.05 AV: 16 SM: 7G NL: 1.08E7

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





NL:
2.57E6
IMPBUL_CLN_XE_45527#38-53
RT: 0.65-1.05 AV: 16 T:
FTMS + p NSI Full ms
[120.00-1935.00]

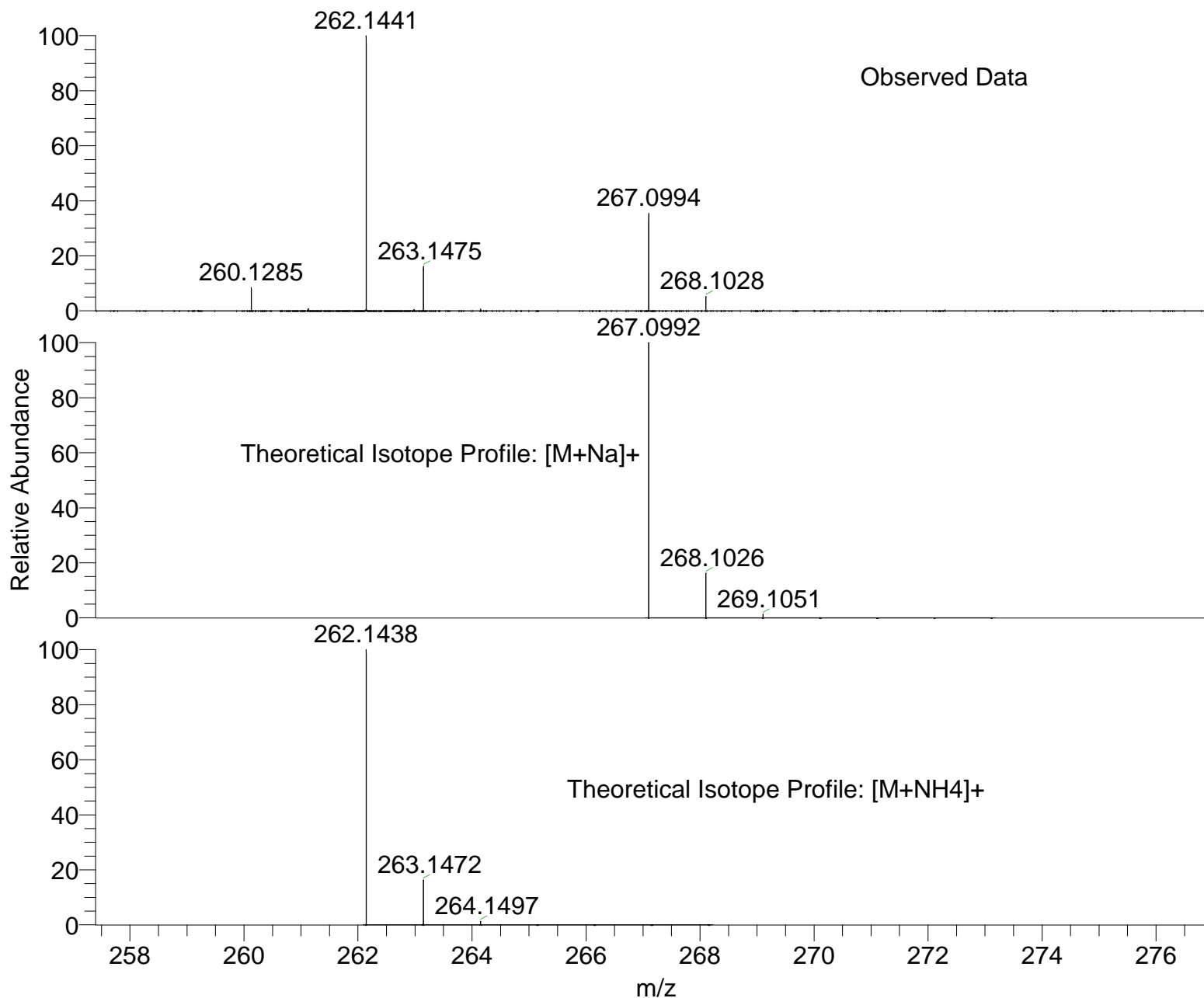
NL:
1.98E4
C₁₅H₁₆O₃H:
C₁₅H₁₇O₃
p (gss, s /p:40) Chrg 1
R: 100000 Res .Pwr . @FWHM

Isotope: Min. .. Max.
 14 N 0....10
 16 O 0....20
 12 C 0....60
 1 H 0....80
 23 Na 0....0
 Tolerance Window: +- 10.00 ppm
 Db/Ring Equiv: -3.. 100
 Fits: 150

N-Rule: Do not use
 Charge: 1

Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
245.1175	245.1172	1.1	7.5	C ₁₅ H ₁₇ O ₃
	245.1191	-6.4	0.0	C ₂ H ₁₅ O ₅ N ₉
	245.1159	6.6	8.0	C ₁₃ H ₁₅ O ₂ N ₃
	245.1199	-9.8	12.0	C ₁₈ H ₁₅ N ₁

SM: 7G



NL:
3.41E6
IMPBUL_CLN_XE_45527#38-53
RT: 0.65-1.05 AV: 16 T:
FTMS + p NSI Full ms
[120.00-1935.00]

NL:
1.98E4
C₁₅H₁₆O₃Na:
C₁₅H₁₆O₃Na₁
p (gss, s /p:40) Chrg 1
R: 100000 Res .Pwr . @FWHM

NL:
1.97E4
C₁₅H₁₆O₃NH₄:
C₁₅H₂₀O₃N₁
p (gss, s /p:40) Chrg 1
R: 100000 Res .Pwr . @FWHM