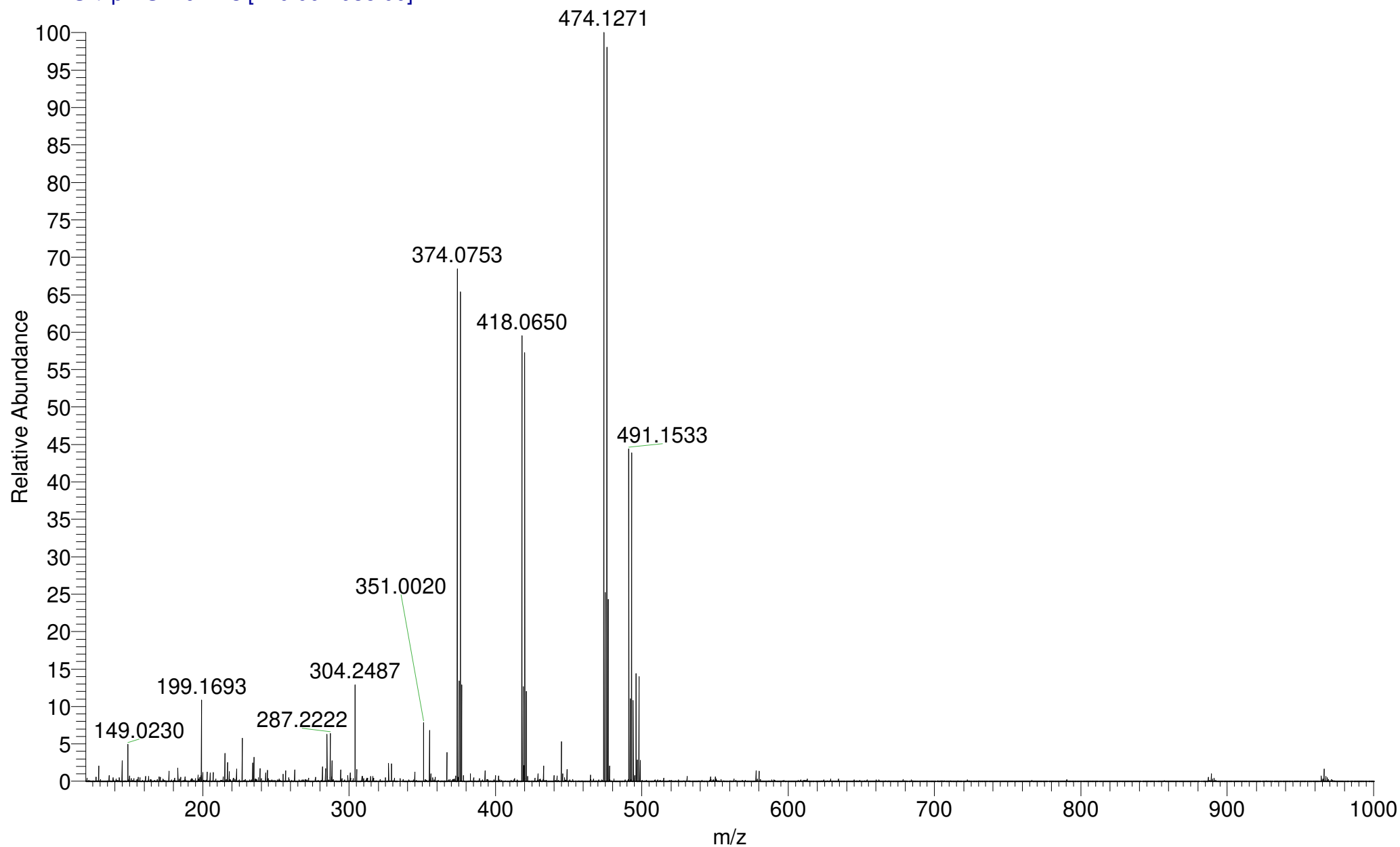


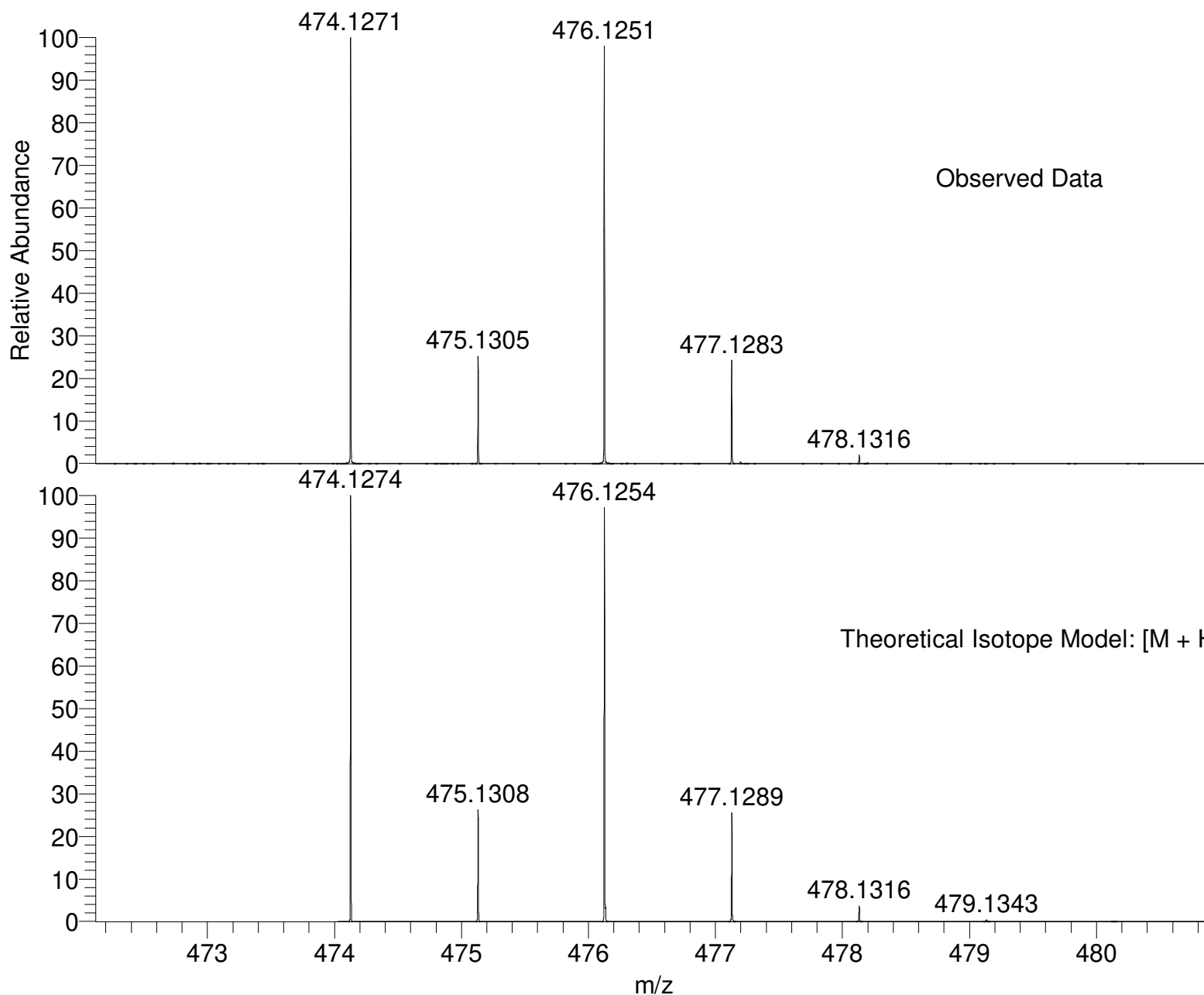
AB5-490
(DCM)/MeOH + NH₄OAc
C₂₄H₂₈BrNO₄

EPSRC National Facility Swansea
LTQ Orbitrap XL

IMPBUL-AJB
24/07/2018 13:03:44

IMPBUL_TVTMV_47154 #41-56 RT: 0.72-1.02 AV: 12 SM: 7G NL: 2.52E6
T: FTMS + p NSI Full ms [120.00-1935.00]





NL:
2.52E6
IMPBUL_TVTMV_47154#41-
56 RT: 0.72-1.02 AV: 12 T:
FTMS + p NSI Full ms
[120.00-1935.00]

NL:
9.04E3
C₂₄H₂₈BrNO₄H:
C₂₄H₂₉Br₁N₁O₄
p (gss, s /p:40) Chrg 1
R: 100000 Res .Pwr . @FWHM

Isotope: Min. .. Max.
 14 N 0....10
 16 O 0....13
 12 C 0....60
 1 H 0....80
 79 Br 0....2
 Tolerance Window: +- 5.00 ppm
 Db/Ring Equiv: -30.. 100
 Fits: 300

N-Rule: Do not use
 Charge: 1

Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
474.1271	474.1272	-0.1	-4.0	C ₁₀ H ₃₆ O ₃ N ₈ Br ₂
	474.1272	-0.1	-9.5	C ₁₁ H ₄₂ O ₈ N ₁ Br ₂
	474.1269	0.4	13.0	C ₂₂ H ₂₂ O ₁₀ N ₂
	474.1269	0.4	18.5	C ₂₁ H ₁₆ O ₅ N ₉
	474.1274	-0.7	10.5	C ₂₄ H ₂₉ O ₄ N ₁ Br ₁
	474.1266	1.0	-1.5	C ₈ H ₂₉ O ₉ N ₉ Br ₁
	474.1277	-1.3	30.5	C ₃₇ H ₁₆ N ₁
	474.1280	-1.8	-2.0	C ₁₀ H ₃₁ O ₁₀ N ₆ Br ₁
	474.1261	2.1	11.0	C ₂₂ H ₂₇ O ₃ N ₄ Br ₁
	474.1282	-2.4	18.0	C ₂₃ H ₁₈ O ₆ N ₆
	474.1258	2.7	-9.0	C ₉ H ₄₀ O ₇ N ₄ Br ₂
	474.1285	-3.0	-4.5	C ₁₂ H ₃₈ O ₄ N ₅ Br ₂
	474.1256	3.3	13.5	C ₂₀ H ₂₀ O ₉ N ₅
	474.1288	-3.6	15.5	C ₂₅ H ₂₅ N ₅ Br ₁
	474.1253	3.8	-6.5	C ₇ H ₃₃ O ₁₃ N ₅ Br ₁
	474.1250	4.3	26.0	C ₃₄ H ₁₈ O ₃
	474.1293	-4.6	3.0	C ₁₁ H ₂₇ O ₆ N ₁₀ Br ₁
	474.1293	-4.6	-2.5	C ₁₂ H ₃₃ O ₁₁ N ₃ Br ₁
	474.1248	4.9	6.0	C ₂₁ H ₃₁ O ₇ Br ₁
	474.1248	4.9	11.5	C ₂₀ H ₂₅ O ₂ N ₇ Br ₁