

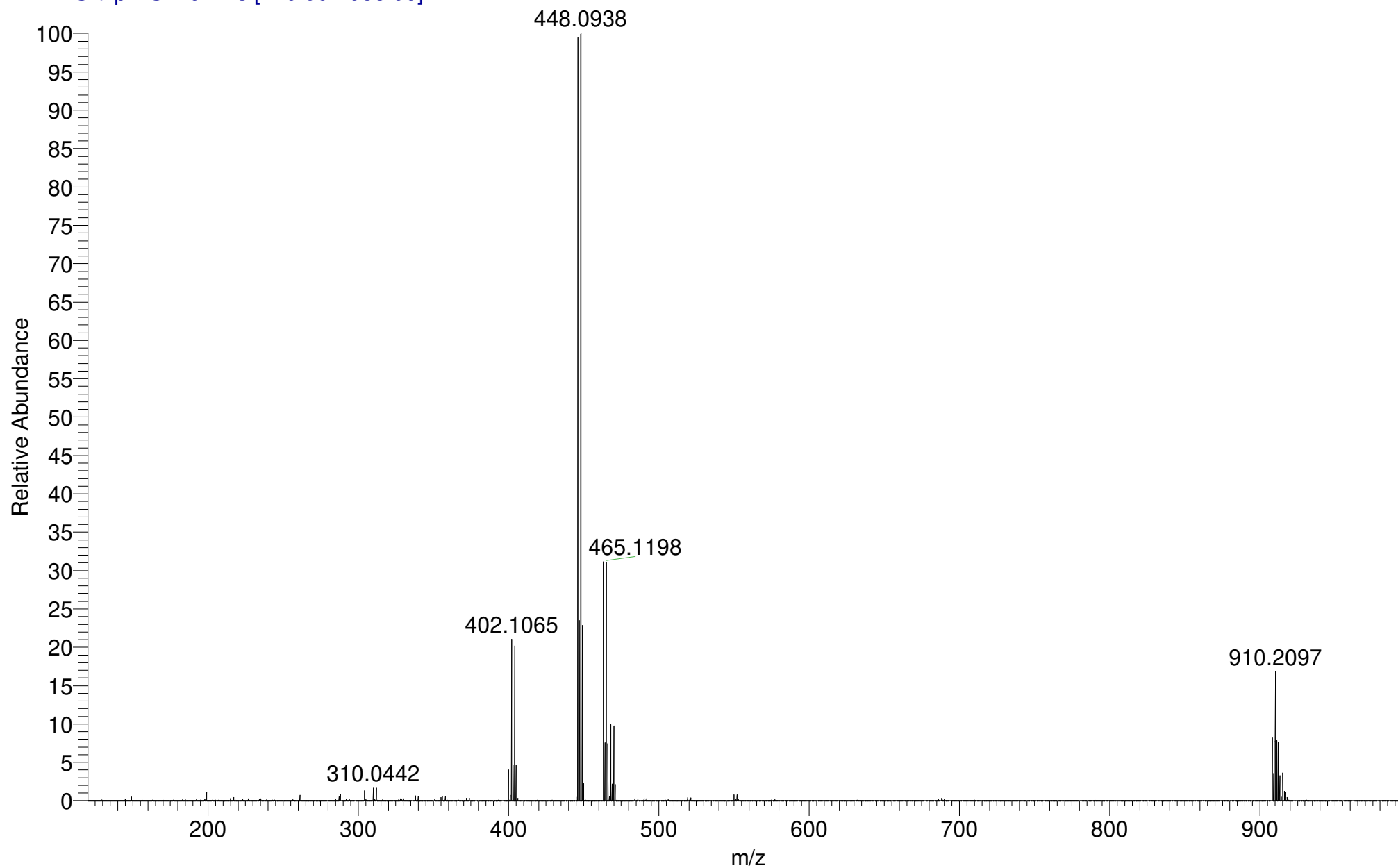
AB5-489
(DCM)/MeOH + NH₄OAc
C₂₂H₂₄BrNO₄

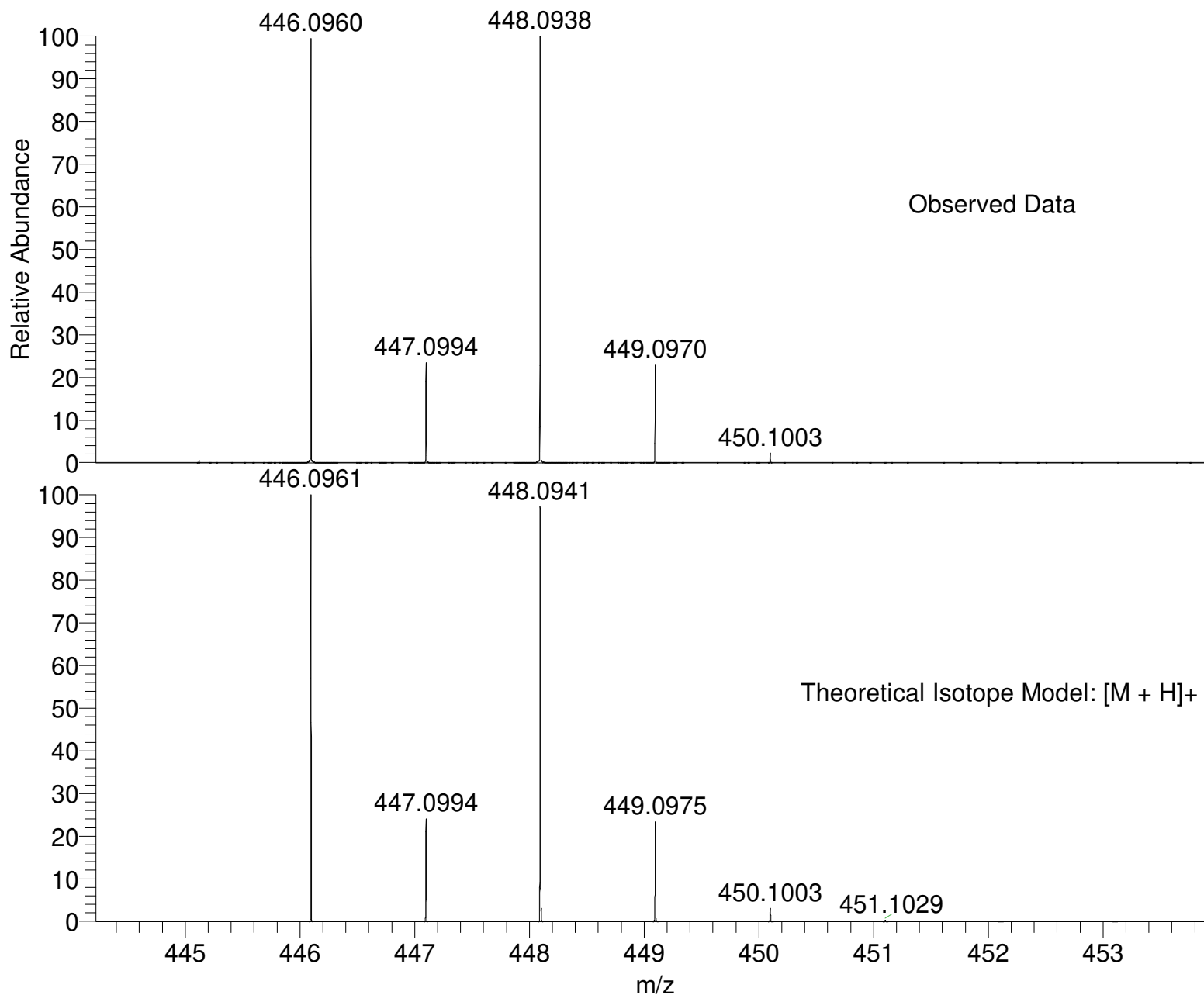
EPSRC National Facility Swansea
LTQ Orbitrap XL

IMPBUL-AJB
24/07/2018 13:00:49

IMPBUL_TVJYU_47153 #42-55 RT: 0.74-1.04 AV: 12 SM: 7G NL: 2.15E7

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





NL:
2.15E7
IMPBUL_TVJYU_47153#42-55
RT: 0.74-1.04 AV: 12 T:
FTMS + p NSI Full ms
[120.00-1935.00]

NL:
9.24E3
C₂₂H₂₄BrNO₄H:
C₂₂H₂₅Br₁N₁O₄
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
446.0960	446.0959	0.3	-9.5	C ₉ H ₃₈ O ₈ N ₁ Br ₂
	446.0959	0.3	-4.0	C ₈ H ₃₂ O ₃ N ₆ Br ₂
	446.0961	-0.3	10.5	C ₂₂ H ₂₅ O ₄ N ₁ Br ₁
	446.0956	0.9	13.0	C ₂₀ H ₁₈ O ₁₀ N ₂
	446.0956	0.9	18.5	C ₁₉ H ₁₂ O ₅ N ₉
	446.0964	-1.0	30.5	C ₃₅ H ₁₂ N ₁
	446.0967	-1.5	-2.0	C ₈ H ₂₇ O ₁₀ N ₆ Br ₁
	446.0953	1.5	-1.5	C ₆ H ₂₅ O ₉ N ₉ Br ₁
	446.0969	-2.1	18.0	C ₂₁ H ₁₄ O ₆ N ₆
	446.0948	2.7	11.0	C ₂₀ H ₂₃ O ₃ N ₄ Br ₁
	446.0972	-2.7	-4.5	C ₁₀ H ₃₄ O ₄ N ₅ Br ₂
	446.0945	3.3	-9.0	C ₇ H ₃₆ O ₇ N ₄ Br ₂
	446.0975	-3.3	15.5	C ₂₃ H ₂₁ N ₅ Br ₁
	446.0943	3.9	13.5	C ₁₈ H ₁₆ O ₉ N ₅
	446.0980	-4.5	3.0	C ₉ H ₂₃ O ₆ N ₁₀ Br ₁
	446.0980	-4.5	-2.5	C ₁₀ H ₂₉ O ₁₁ N ₃ Br ₁
	446.0940	4.5	-6.5	C ₅ H ₂₉ O ₁₃ N ₅ Br ₁