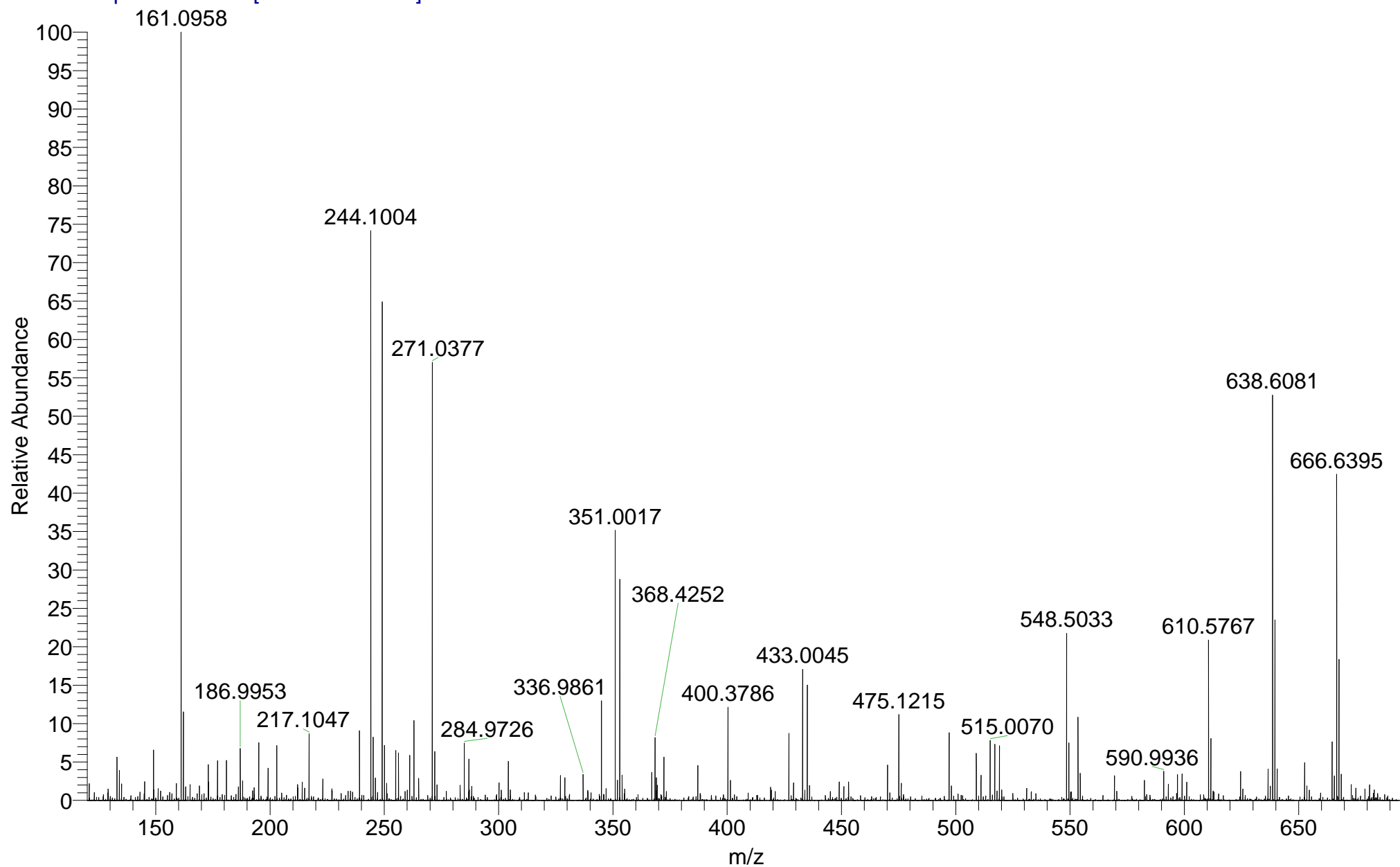


rc5-643
(H₂O)/MeOH + NH₄OAc
C₁₁H₁₃NaO₃S

EPSRC National Facility Swansea EPSRC National IMPBUL-RACea
LTQ Orbitrap XL
03/04/2017 16:41:23

IMPBUL_AYVN7_A #32-38 RT: 0.74-1.02 AV: 6 SM: 7G NL: 3.29E6

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

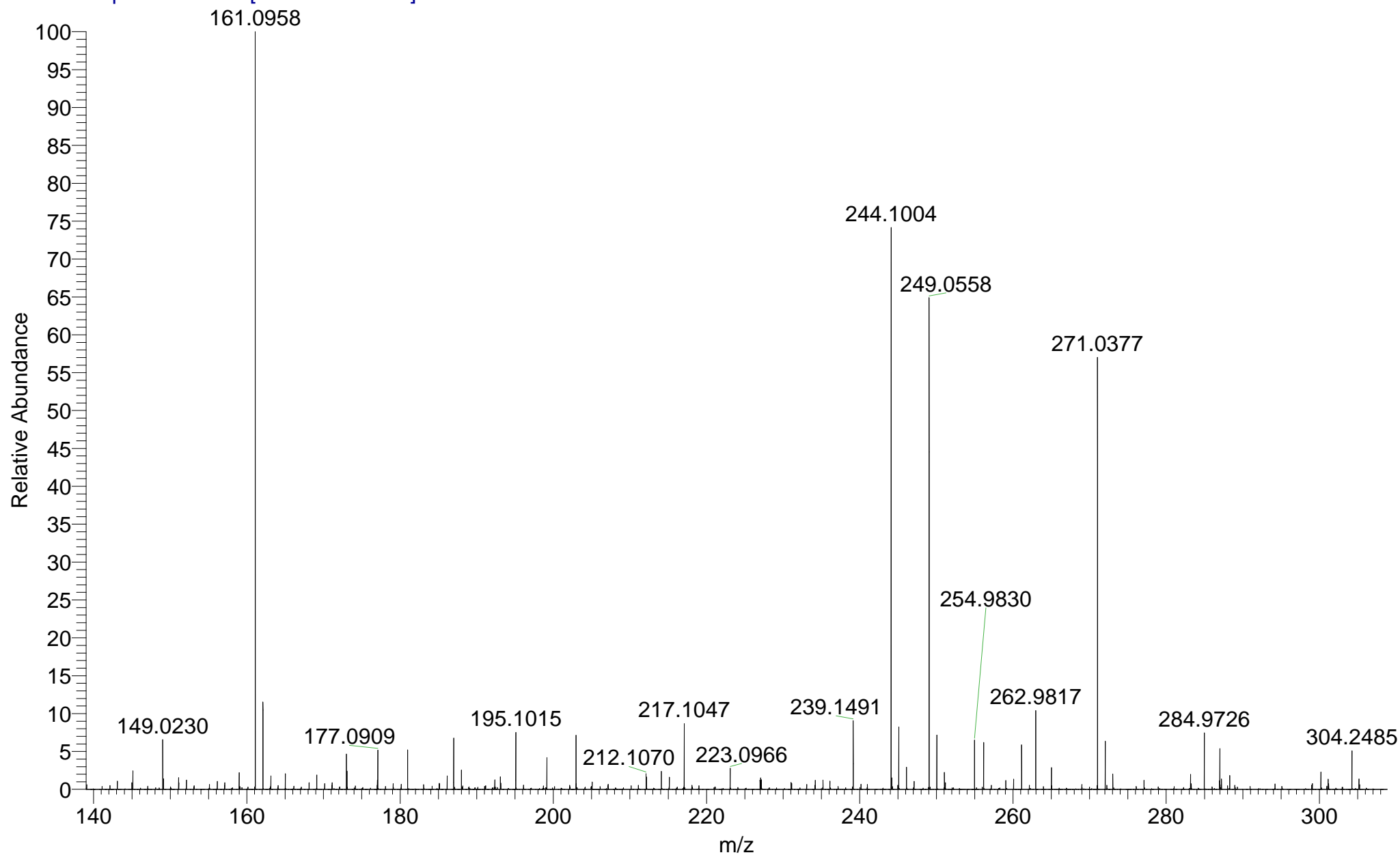


rc5-643
(H₂O)/MeOH + NH₄OAc
C₁₁H₁₃NaO₃S

EPSRC National Facility Swansea EPSRC National IMPBUL-RACea
LTQ Orbitrap XL 03/04/2017 16:41:23

IMPBUL_AYVN7_A #32-38 RT: 0.74-1.02 AV: 6 SM: 7G NL: 3.29E6

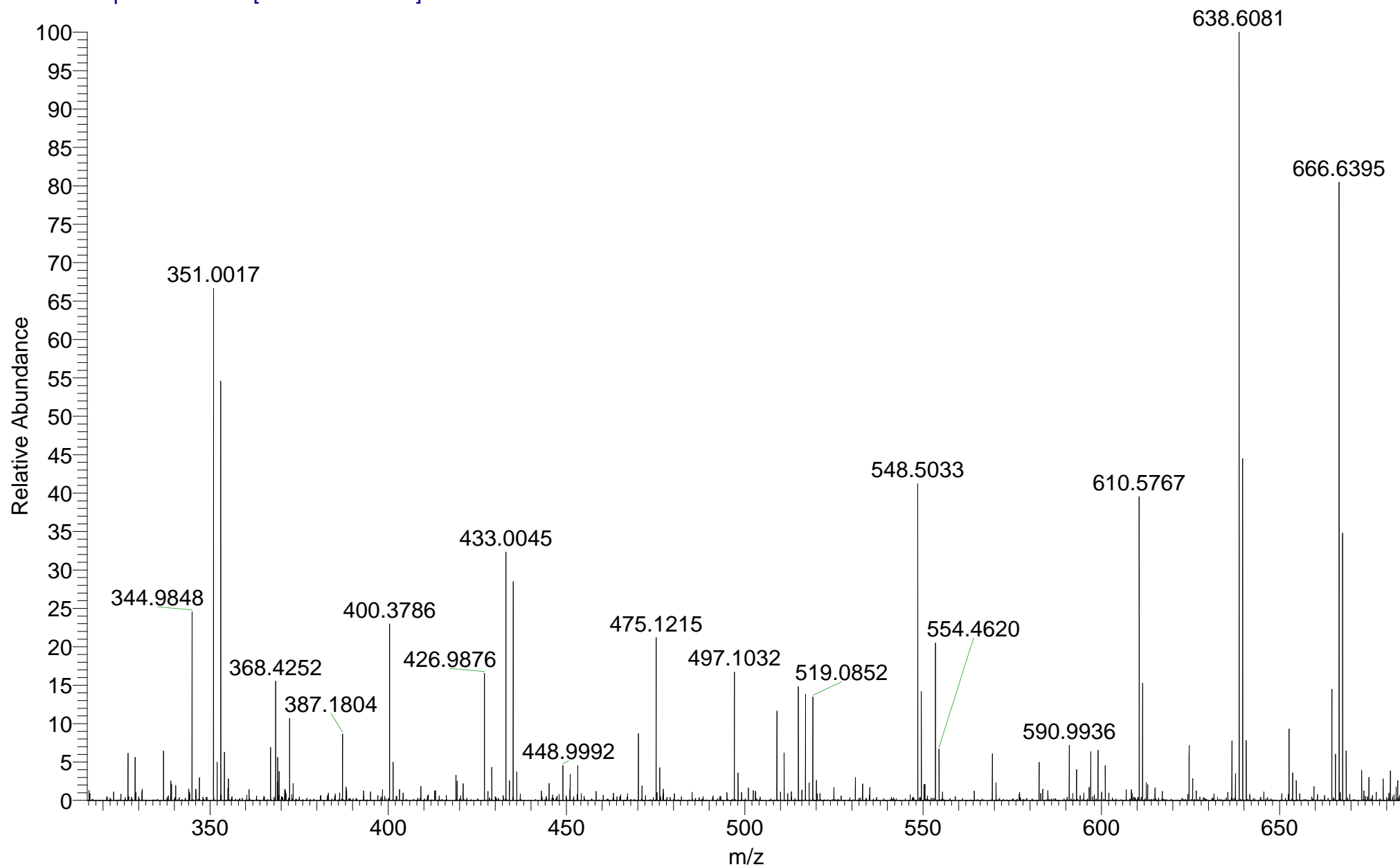
T: FTMS + p NSI Full ms [120.00-1935.00]

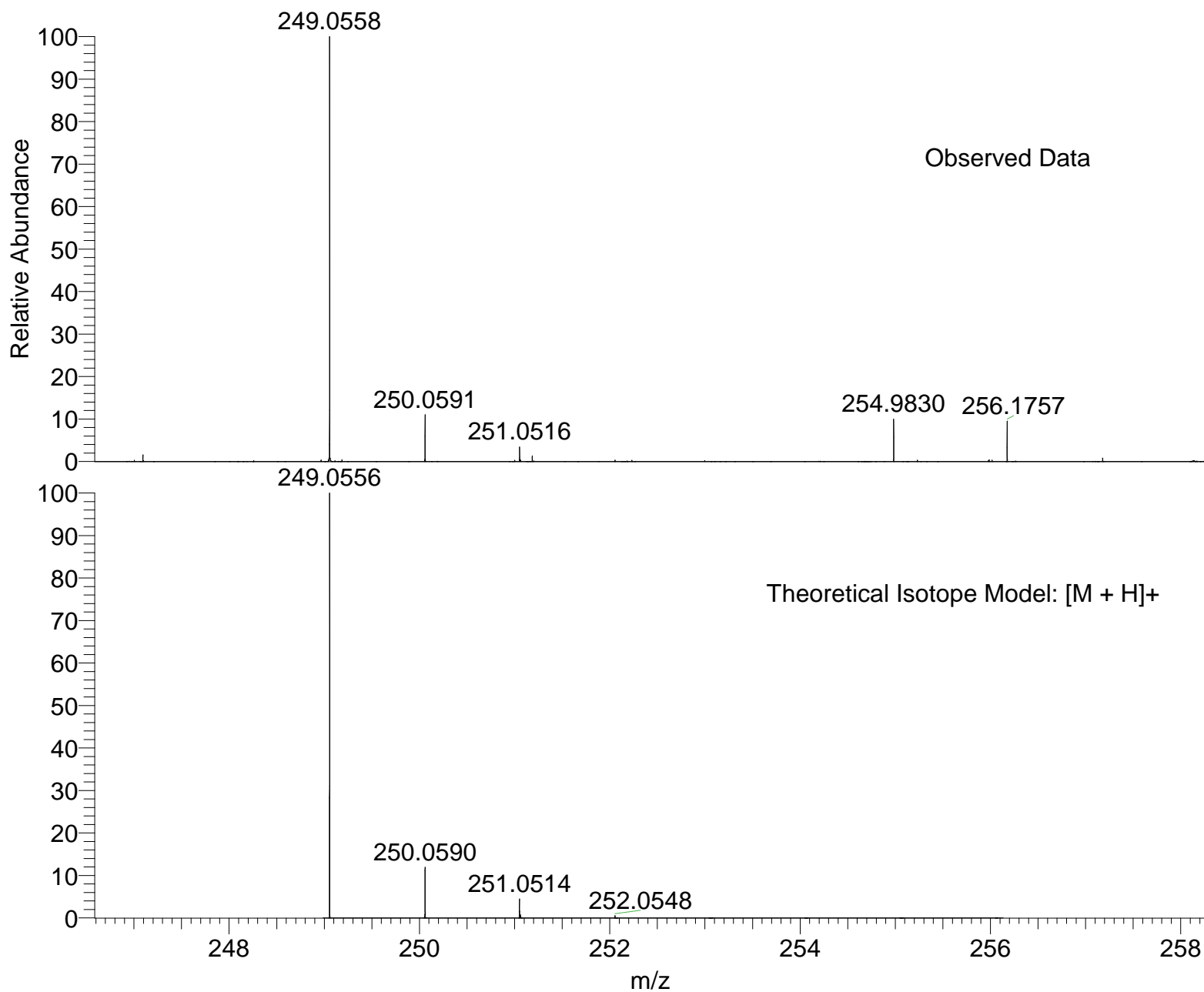


rc5-643
(H₂O)/MeOH + NH₄OAc
C₁₁H₁₃NaO₃S

EPSRC National Facility Swansea EPSRC National IMPBUL-RACe
LTQ Orbitrap XL 03/04/2017 16:41:23

IMPBUL_AYVN7_A #32-38 RT: 0.74-1.02 AV: 6 SM: 7G NL: 1.74E6
T: FTMS + p NSI Full ms [120.00-1935.00]





NL:
2.14E6
IMPBUL_AYVN7_A#32-38 RT:
0.74-1.02 AV: 6 T: FTMS + p
NSI Full ms [120.00-1935.00]

NL:
1.96E4
C₁₁H₁₃NaO₃SH:
C₁₁H₁₄Na₁O₃S₁
p (gss, s /p:40) Chrg 1
R: 100000 Res .Pwr . @FWHM

Isotope: Min. .. Max.
 14 N 0....15
 16 O 0....15
 12 C 0....60
 1 H 0....70
 23 Na 0....5
 32 S 0....5
 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
249.0558	249.0559	-0.2	6.0	C ₁₂ H ₁₃ N ₁ Na ₂ S ₁
	249.0557	0.5	-2.5	C ₅ H ₁₅ O ₈ Na ₂
	249.0557	0.5	3.0	C ₄ H ₉ O ₃ N ₇ Na ₂
	249.0560	-0.6	4.5	C ₅ H ₈ N ₈ Na ₃
	249.0560	-0.6	-1.0	C ₆ H ₁₄ O ₅ N ₁ Na ₃
	249.0560	-0.8	-1.0	C ₃ H ₁₅ O ₄ N ₅ S ₂
	249.0556	0.9	4.5	C ₁₁ H ₁₄ O ₃ Na ₁ S ₁
	249.0554	1.6	1.5	C ₃ H ₁₀ O ₆ N ₆ Na ₁
	249.0554	1.6	7.0	C ₂ H ₄ O ₁ N ₁₃ Na ₁
	249.0562	-1.7	0.5	C ₇ H ₁₃ O ₂ N ₂ Na ₄
	249.0563	-1.9	0.5	C ₄ H ₁₄ O ₁ N ₆ Na ₁ S ₂
	249.0553	2.0	8.5	C ₉ H ₉ O ₁ N ₆ S ₁
	249.0552	2.4	-3.0	C ₄ H ₁₇ O ₂ N ₃ Na ₂ S ₂
	249.0565	-2.7	5.0	C ₃ H ₇ O ₅ N ₉
	249.0565	-2.7	-0.5	C ₄ H ₁₃ O ₁₀ N ₂
	249.0551	2.7	0.0	C ₂ H ₁₁ O ₉ N ₅
	249.0551	2.7	5.5	C ₁ H ₅ O ₄ N ₁₂
	249.0566	-3.4	8.0	C ₁₁ H ₁₁ O ₂ N ₃ S ₁
	249.0549	3.5	1.0	C ₂ H ₁₂ N ₉ Na ₁ S ₂
	249.0549	3.6	14.0	C ₁₇ H ₈ N ₁ Na ₁
	249.0549	3.7	1.0	C ₅ H ₁₁ O ₁ N ₅ Na ₄
	249.0567	-3.8	6.5	C ₄ H ₆ O ₂ N ₁₀ Na ₁
	249.0567	-3.8	1.0	C ₅ H ₁₂ O ₇ N ₃ Na ₁
	249.0548	3.9	2.5	C ₉ H ₁₇ N ₂ S ₃
	249.0568	-4.1	-2.0	C ₇ H ₁₈ N ₁ Na ₃ S ₂
	249.0547	4.6	-0.5	C ₁ H ₁₃ O ₃ N ₈ S ₂
	249.0546	4.7	12.5	C ₁₆ H ₉ O ₃
	249.0546	4.8	-0.5	C ₄ H ₁₂ O ₄ N ₄ Na ₃
	249.0570	-4.9	2.5	C ₆ H ₁₁ O ₄ N ₄ Na ₂