

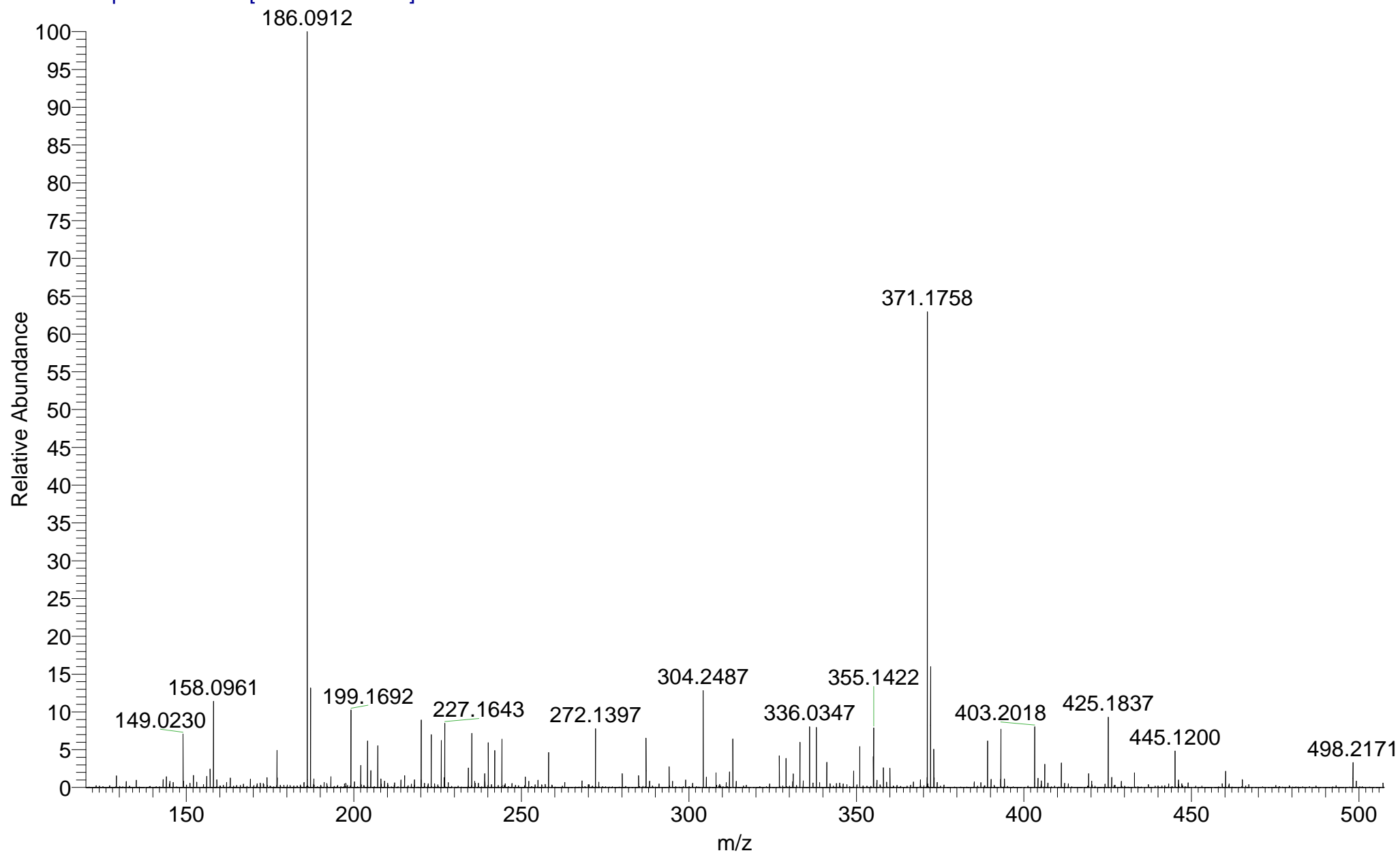
MD-1-052
(DCM)/MeOH + NH₄OAc
C₁₂H₁₃NO₂

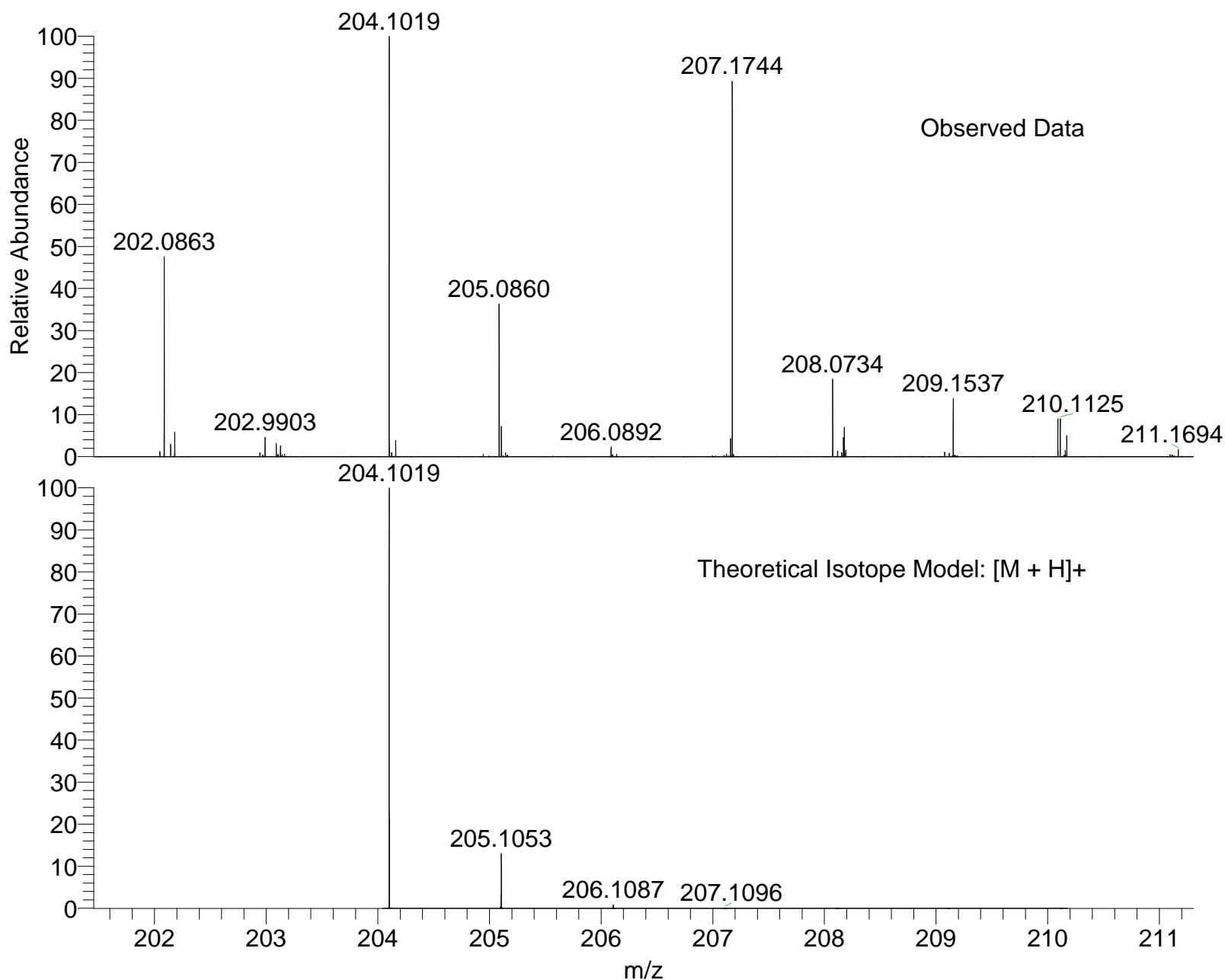
EPSRC National Facility Swansea
LTQ Orbitrap XL

IMPBUL-AJB
02/02/2017 12:02:28

IMPBUL_AXFJV_A #42-56 RT: 0.72-1.03 AV: 12 SM: 7G NL: 1.70E6

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





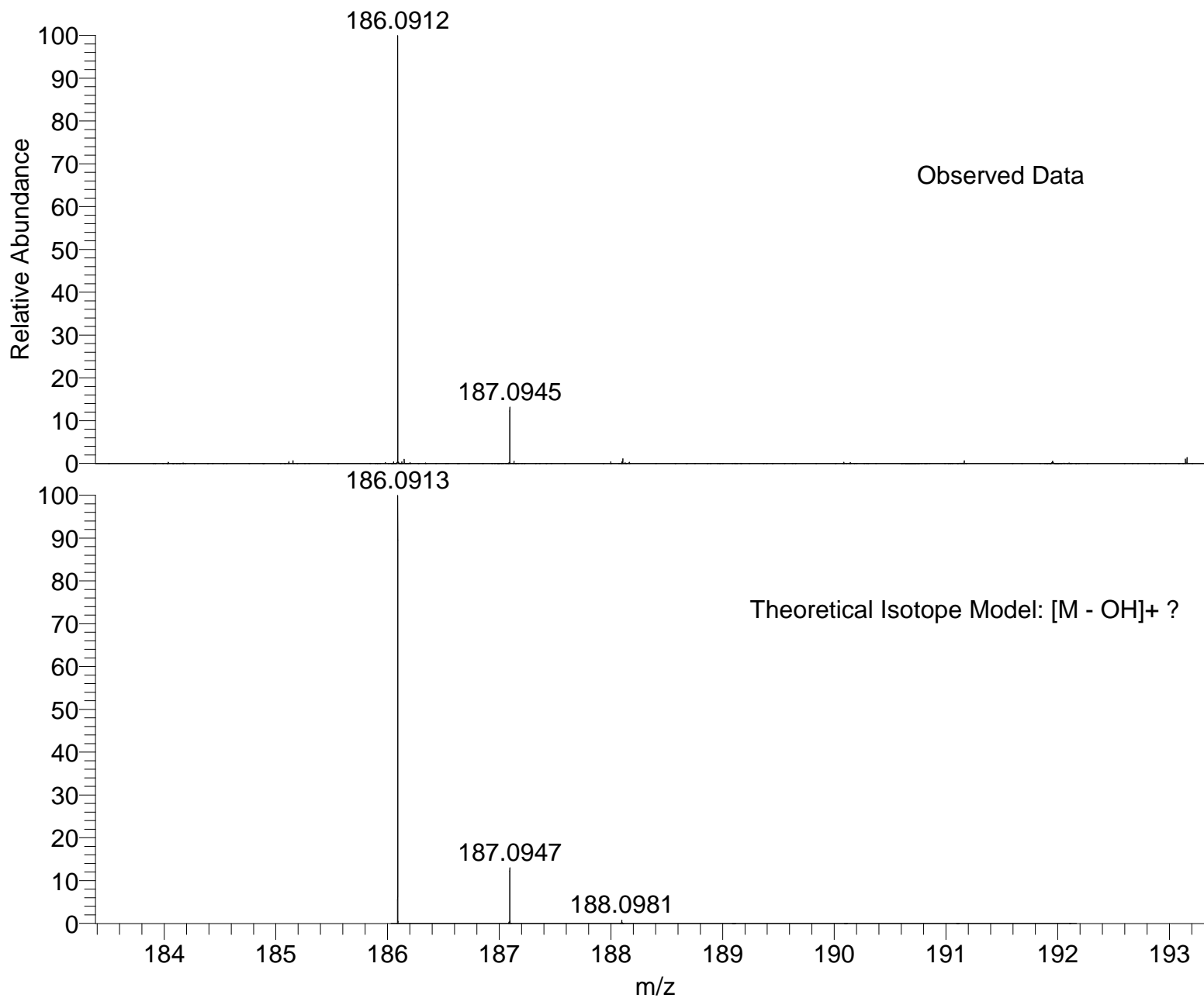
NL:
1.05E5
IMPBUL_AXFJV_A#42-56 RT:
0.72-1.03 AV: 12 T: FTMS + p
NSI Full ms [120.00-1935.00]

NL:
2.04E4
C₁₂H₁₃NO₂H:
C₁₂H₁₄N₁O₂
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....70
1 H	0....80
23 Na	0....0
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
204.1019	204.1019	-0.0	6.5	C ₁₂ H ₁₄ O ₂ N ₁



NL:
1.70E6
IMPBUL_AXFJV_A#42-56 RT:
0.72-1.03 AV: 12 T: FTMS + p
NSI Full ms [120.00-1935.00]

NL:
2.05E4
C₁₂H₁₂NO:
C₁₂H₁₂N₁O₁
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....70
1 H	0....80
23 Na	0....0
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
186.0912	186.0913	-0.8	7.5	C ₁₂ H ₁₂ O ₁ N ₁