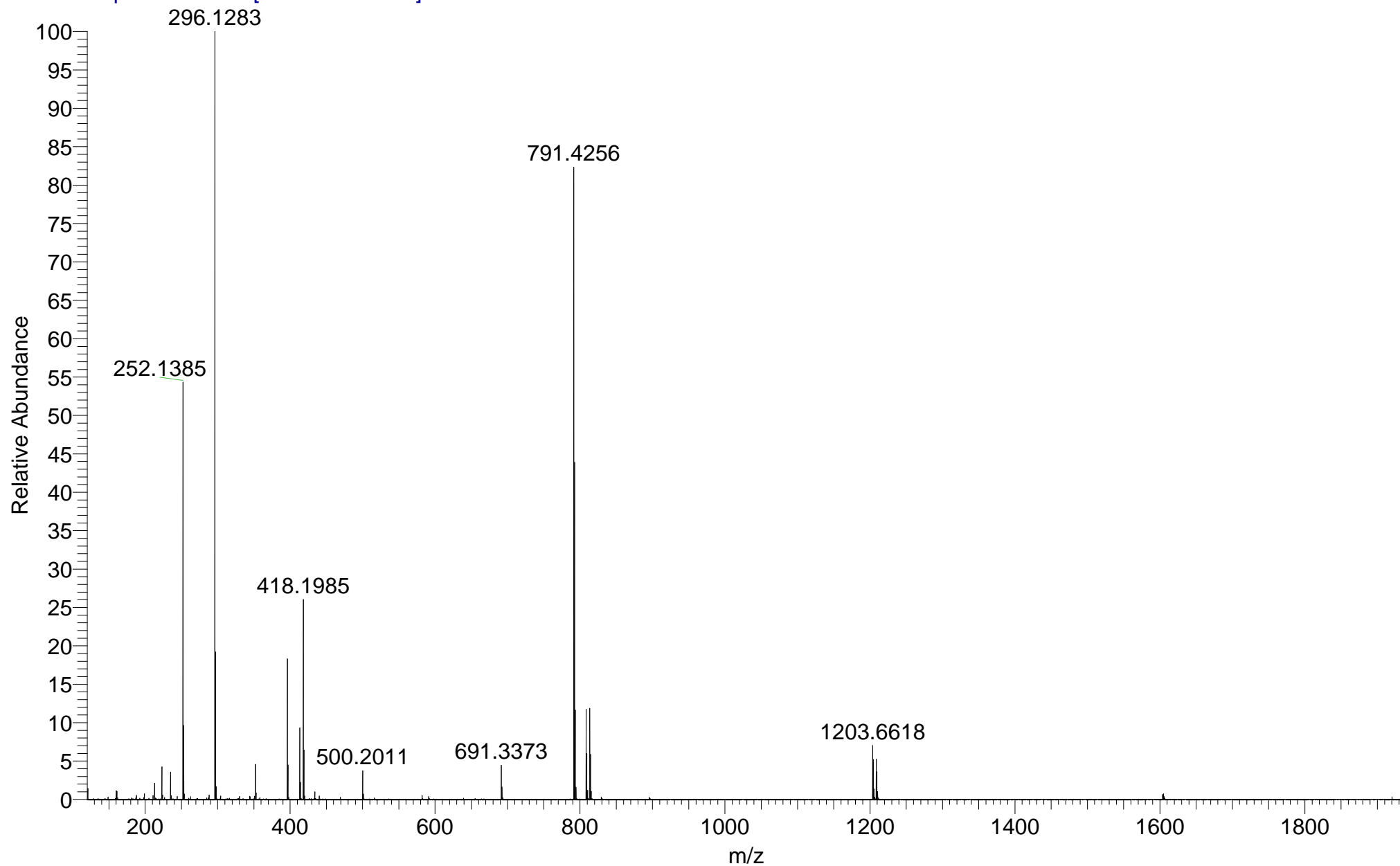


IMPBUL_CN4VU_47916 #38-55 RT: 0.66-1.04 AV: 16 SM: 7G NL: 3.12E7

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

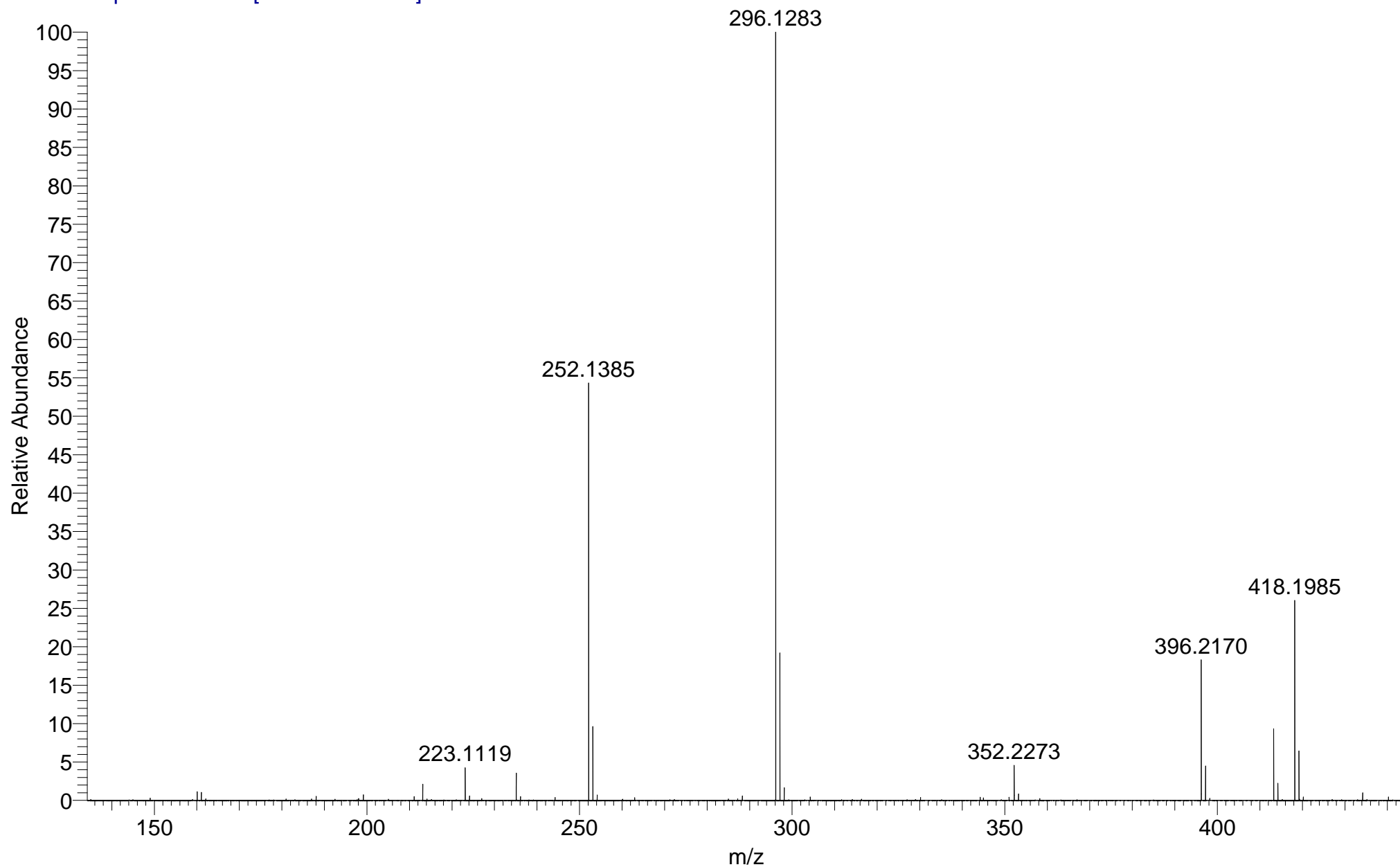


O:\IMPBUL_CN4VU_47916
(DCM)/MeOH + NH4OAc
JR1-171

EPSRC UK National MS Facility
LTQ Orbitrap XL

C24H29NO4
13/08/2018 16:01:38

IMPBUL_CN4VU_47916 #38-55 RT: 0.66-1.04 AV: 16 SM: 7G NL: 3.12E7
T: FTMS + p NSI Full ms [120.00-1935.00]

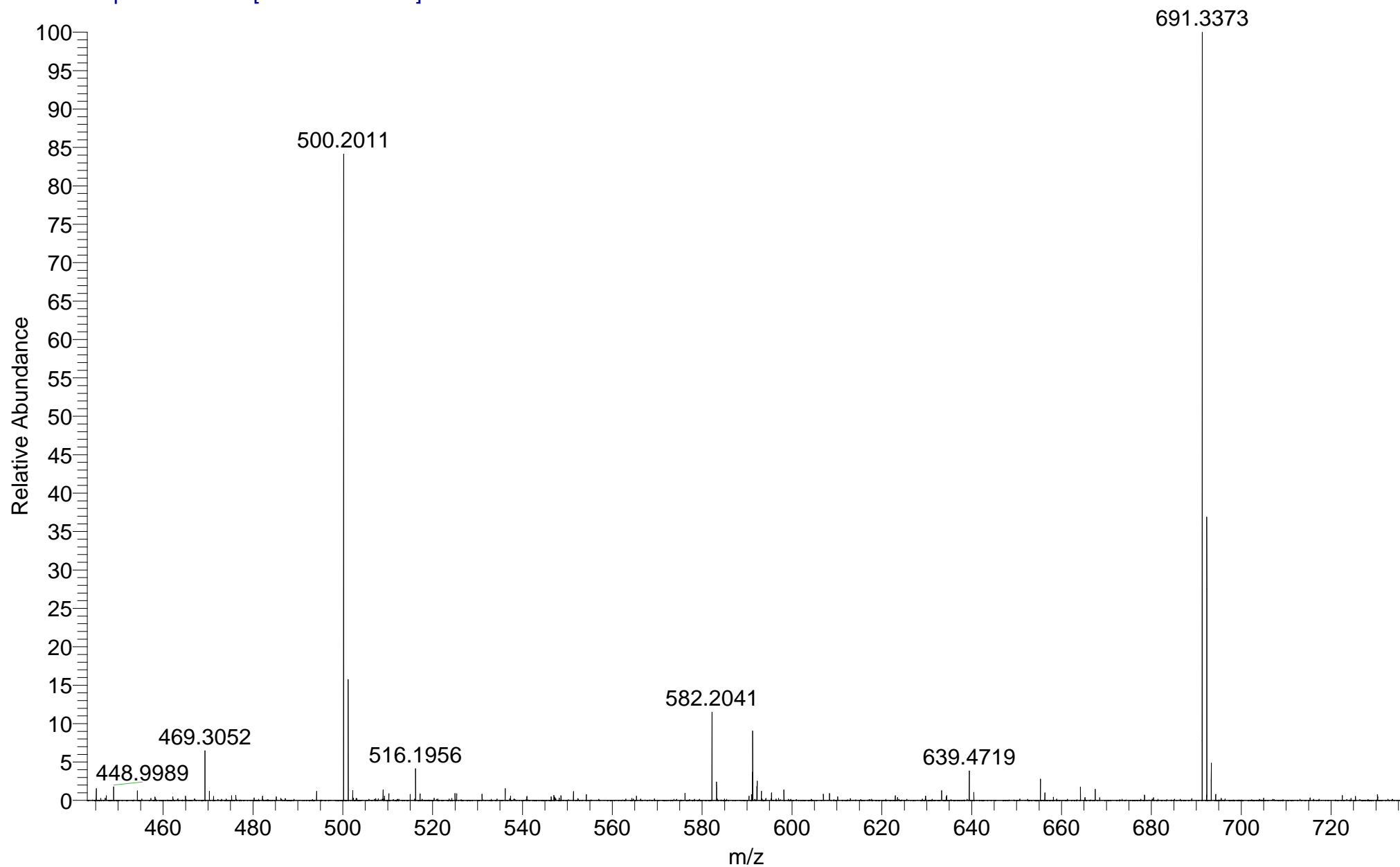


O:\IMPBUL_CN4VU_47916
(DCM)/MeOH + NH4OAc
JR1-171

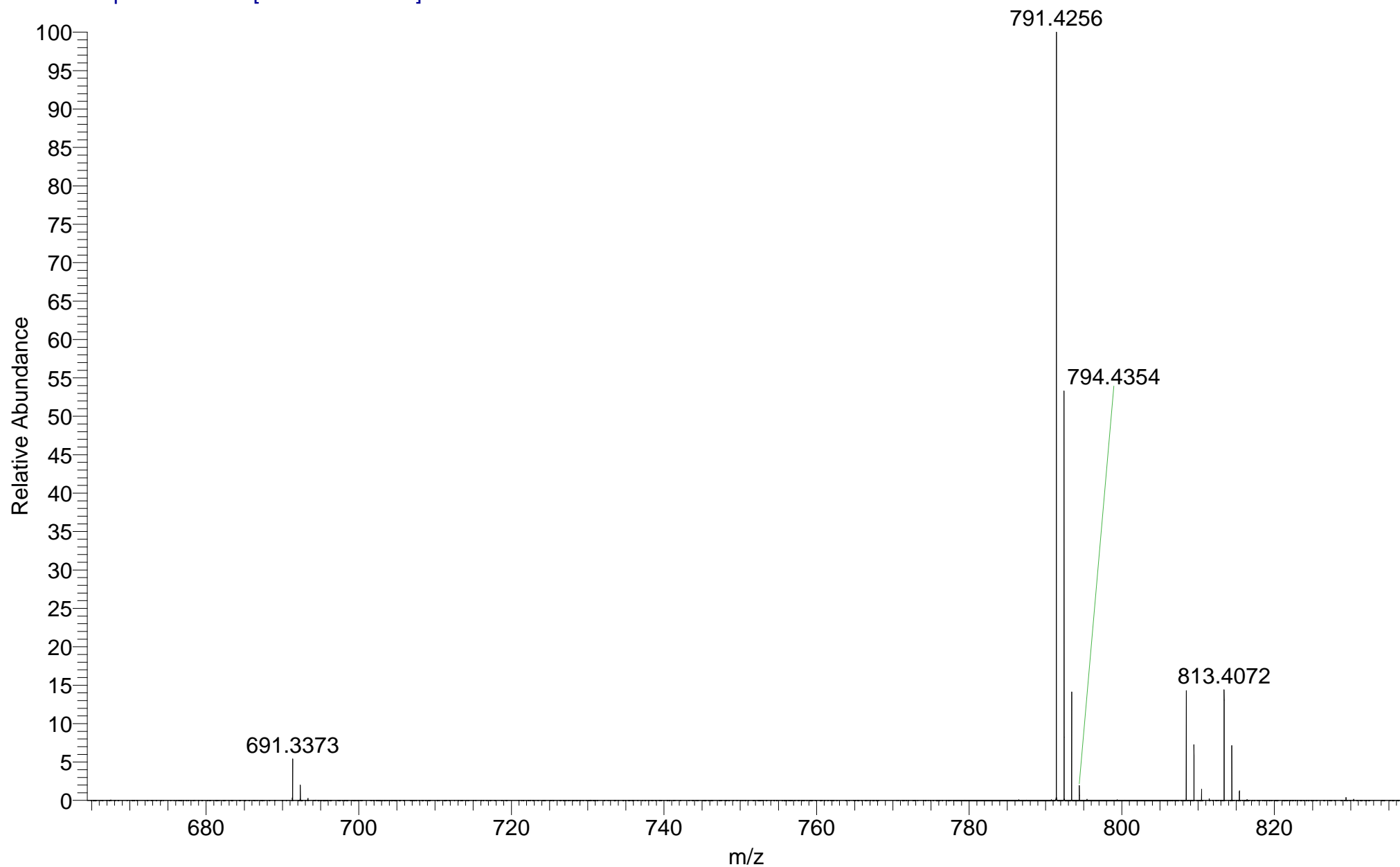
EPSRC UK National MS Facility
LTQ Orbitrap XL

C24H29NO4
13/08/2018 16:01:38

IMPBUL_CN4VU_47916 #38-55 RT: 0.66-1.04 AV: 16 SM: 7G NL: 1.39E6
T: FTMS + p NSI Full ms [120.00-1935.00]



IMPBUL_CN4VU_47916 #38-55 RT: 0.66-1.04 AV: 16 SM: 7G NL: 2.57E7
T: FTMS + p NSI Full ms [120.00-1935.00]

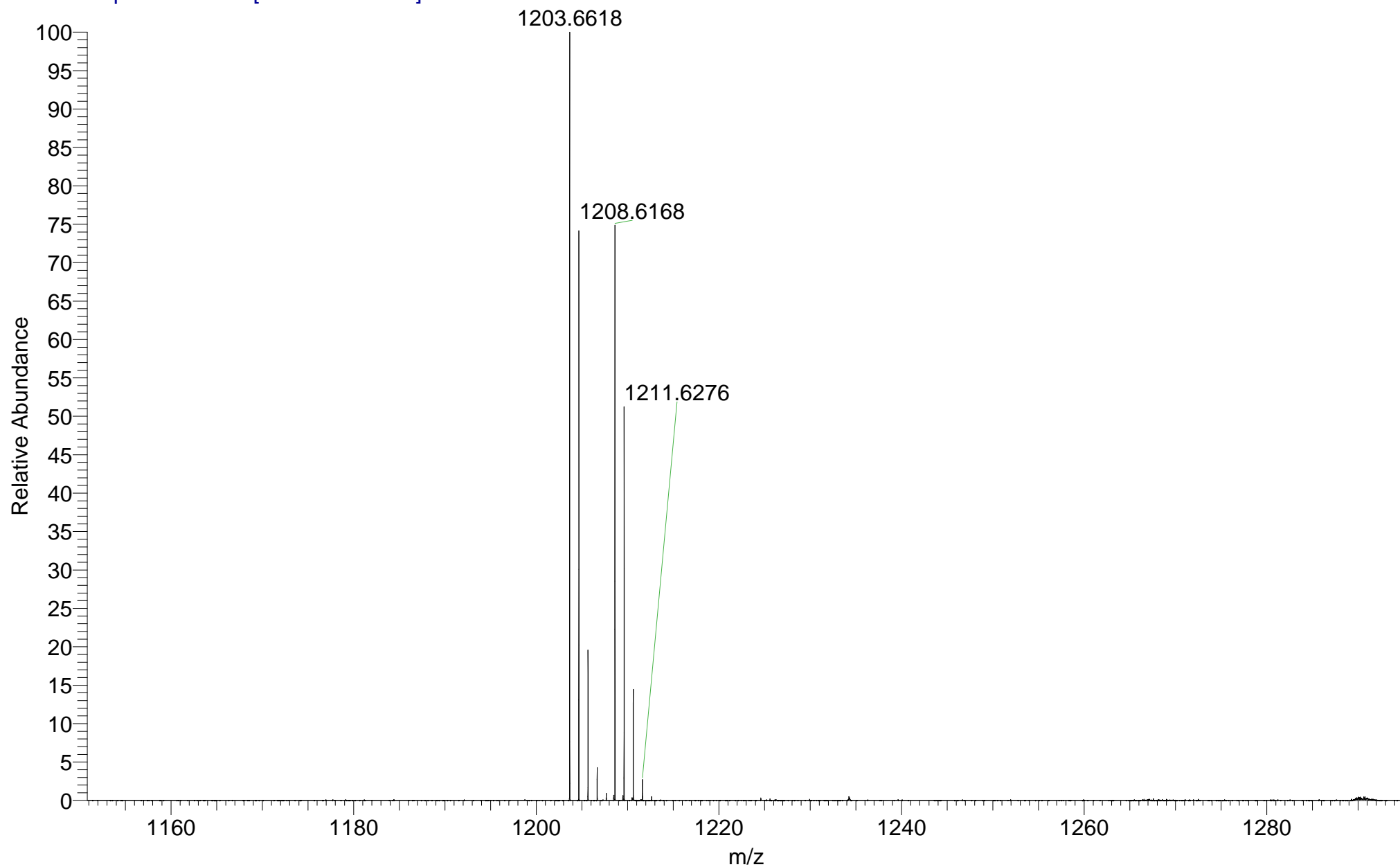


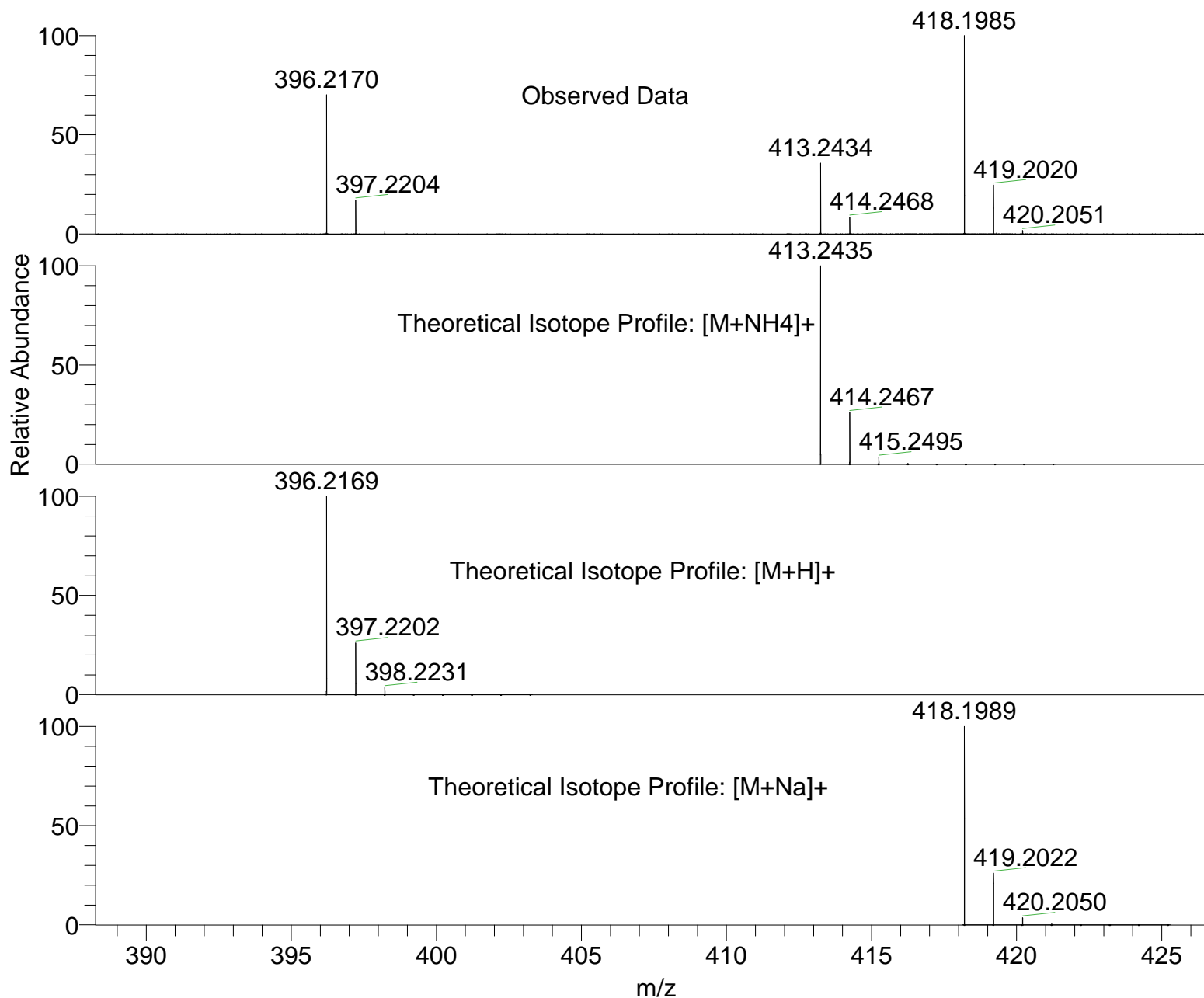
O:\IMPBUL_CN4VU_47916
(DCM)/MeOH + NH4OAc
JR1-171

EPSRC UK National MS Facility
LTQ Orbitrap XL

C24H29NO4
13/08/2018 16:01:38

IMPBUL_CN4VU_47916 #38-55 RT: 0.66-1.04 AV: 16 SM: 7G NL: 2.19E6
T: FTMS + p NSI Full ms [120.00-1935.00]





NL:
8.14E6
IMPBUL_CN4VU_47916#38-
55 RT: 0.66-1.04 AV: 16 T:
FTMS + p NSI Full ms
[120.00-1935.00]

NL:
1.78E4
C₂₄H₂₉NO₄NH₄:
C₂₄H₃₃N₂O₄
p (gss, s /p:40) Chrg 1
R: 100000 Res .Pwr . @FWHM

NL:
1.78E4
C₂₄H₂₉NO₄H:
C₂₄H₃₀N₁O₄
p (gss, s /p:40) Chrg 1
R: 100000 Res .Pwr . @FWHM

NL:
1.78E4
C₂₄H₂₉NO₄Na:
C₂₄H₂₉N₁O₄Na₁
p (gss, s /p:40) Chrg 1
R: 100000 Res .Pwr . @FWHM

Isotope: Min. .. Max.
 14 N 0....20
 16 O 0....20
 12 C 0....120
 1 H 0....150
 23 Na 0....1
 Tolerance Window: +- 5.00 ppm
 Db/Ring Equiv: -3...100
 Fits: 300

N-Rule: Do not use
 Charge: 1

Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
396.2169	396.2169	-0.1	10.5	C ₂₄ H ₃₀ O ₄ N ₁
	396.2174	-1.3	9.0	C ₈ H ₂₀ N ₂₀
	396.2174	-1.4	3.5	C ₉ H ₂₆ O ₅ N ₁₃
	396.2174	-1.4	-2.0	C ₁₀ H ₃₂ O ₁₀ N ₆
	396.2161	2.0	-1.5	C ₈ H ₃₀ O ₉ N ₉
	396.2161	2.0	4.0	C ₇ H ₂₄ O ₄ N ₁₆
	396.2156	3.3	11.0	C ₂₂ H ₂₈ O ₃ N ₄
	396.2183	-3.5	15.5	C ₂₅ H ₂₆ N ₅
	396.2188	-4.7	8.5	C ₁₀ H ₂₂ O ₁ N ₁₇
	396.2188	-4.7	3.0	C ₁₁ H ₂₈ O ₆ N ₁₀
	396.2188	-4.8	-2.5	C ₁₂ H ₃₄ O ₁₁ N ₃
413.2434	413.2435	-0.2	9.5	C ₂₄ H ₃₃ O ₄ N ₂
	413.2440	-1.4	2.5	C ₉ H ₂₉ O ₅ N ₁₄
	413.2440	-1.4	-3.0	C ₁₀ H ₃₅ O ₁₀ N ₇
	413.2426	1.8	-2.5	C ₈ H ₃₃ O ₉ N ₁₀
	413.2426	1.8	3.0	C ₇ H ₂₇ O ₄ N ₁₇
	413.2421	3.0	10.0	C ₂₂ H ₃₁ O ₃ N ₅
	413.2448	-3.4	14.5	C ₂₅ H ₂₉ N ₆
	413.2453	-4.7	7.5	C ₁₀ H ₂₅ O ₁ N ₁₈
	413.2453	-4.7	2.0	C ₁₁ H ₃₁ O ₆ N ₁₁
418.1985	418.1986	-0.2	14.5	C ₂₂ H ₂₄ O ₂ N ₇
	418.1986	-0.3	9.0	C ₂₃ H ₃₀ O ₇
	418.1989	-0.9	10.5	C ₂₄ H ₂₉ O ₄ N ₁ Na ₁
	418.1980	1.1	-1.5	C ₈ H ₂₉ O ₉ N ₉ Na ₁
	418.1980	1.1	4.0	C ₇ H ₂₃ O ₄ N ₁₆ Na ₁
	418.1991	-1.4	7.5	C ₇ H ₂₀ O ₃ N ₁₉
	418.1991	-1.5	2.0	C ₈ H ₂₆ O ₈ N ₁₂
	418.1978	1.7	-3.0	C ₇ H ₃₀ O ₁₂ N ₈
	418.1978	1.8	2.5	C ₆ H ₂₄ O ₇ N ₁₅
	418.1994	-2.1	9.0	C ₈ H ₁₉ N ₂₀ Na ₁
	418.1994	-2.1	3.5	C ₉ H ₂₅ O ₅ N ₁₃ Na ₁
	418.1994	-2.1	-2.0	C ₁₀ H ₃₁ O ₁₀ N ₆ Na ₁

Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
	418.1975	2.3	11.0	C ₂₂ H ₂₇ O ₃ N ₄ Na ₁
	418.1973	3.0	9.5	C ₂₁ H ₂₈ O ₆ N ₃
	418.1973	3.0	15.0	C ₂₀ H ₂₂ O ₁ N ₁₀
	418.1999	-3.4	14.0	C ₂₄ H ₂₆ O ₃ N ₄
	418.2002	-4.1	15.5	C ₂₅ H ₂₅ N ₅ Na ₁
	418.1967	4.3	-1.0	C ₆ H ₂₇ O ₈ N ₁₂ Na ₁
	418.1967	4.3	4.5	C ₅ H ₂₁ O ₃ N ₁₉ Na ₁
	418.2004	-4.7	7.0	C ₉ H ₂₂ O ₄ N ₁₆
	418.2004	-4.7	1.5	C ₁₀ H ₂₈ O ₉ N ₉
	418.1964	5.0	-2.5	C ₅ H ₂₈ O ₁₁ N ₁₁
	418.1964	5.0	3.0	C ₄ H ₂₂ O ₆ N ₁₈