

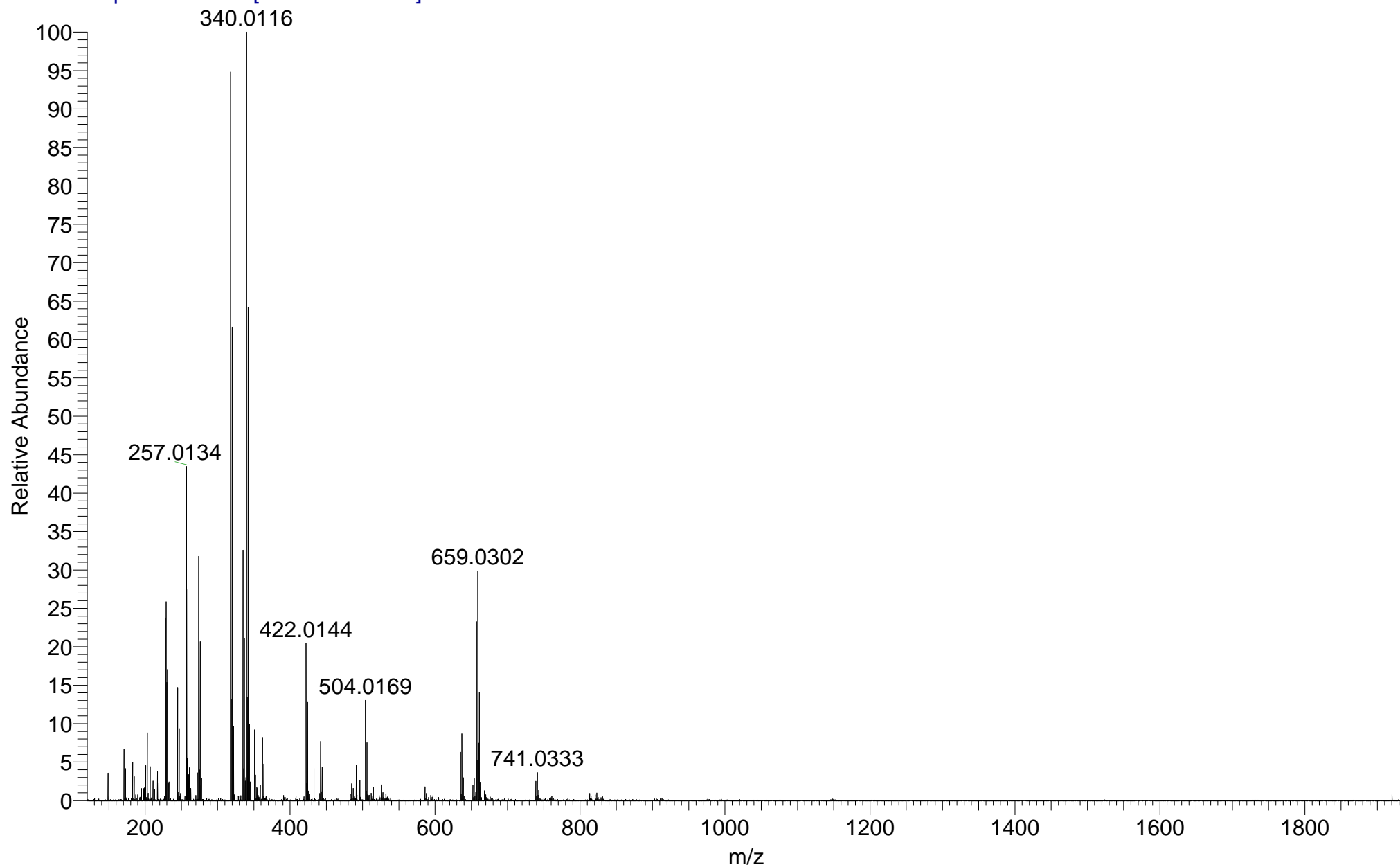
O:\IMPBUL_TW3J3_50397
(MeOH)/MeOH + NH4OAc
AB5-540

EPSRC UK National MS Facility
LTQ Orbitrap XL

C₁₃H₁₃Cl₂NO₄
26/11/2018 08:19:26

IMPBUL_TW3J3_50397 #37-55 RT: 0.66-1.05 AV: 16 SM: 7G NL: 4.00E6

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

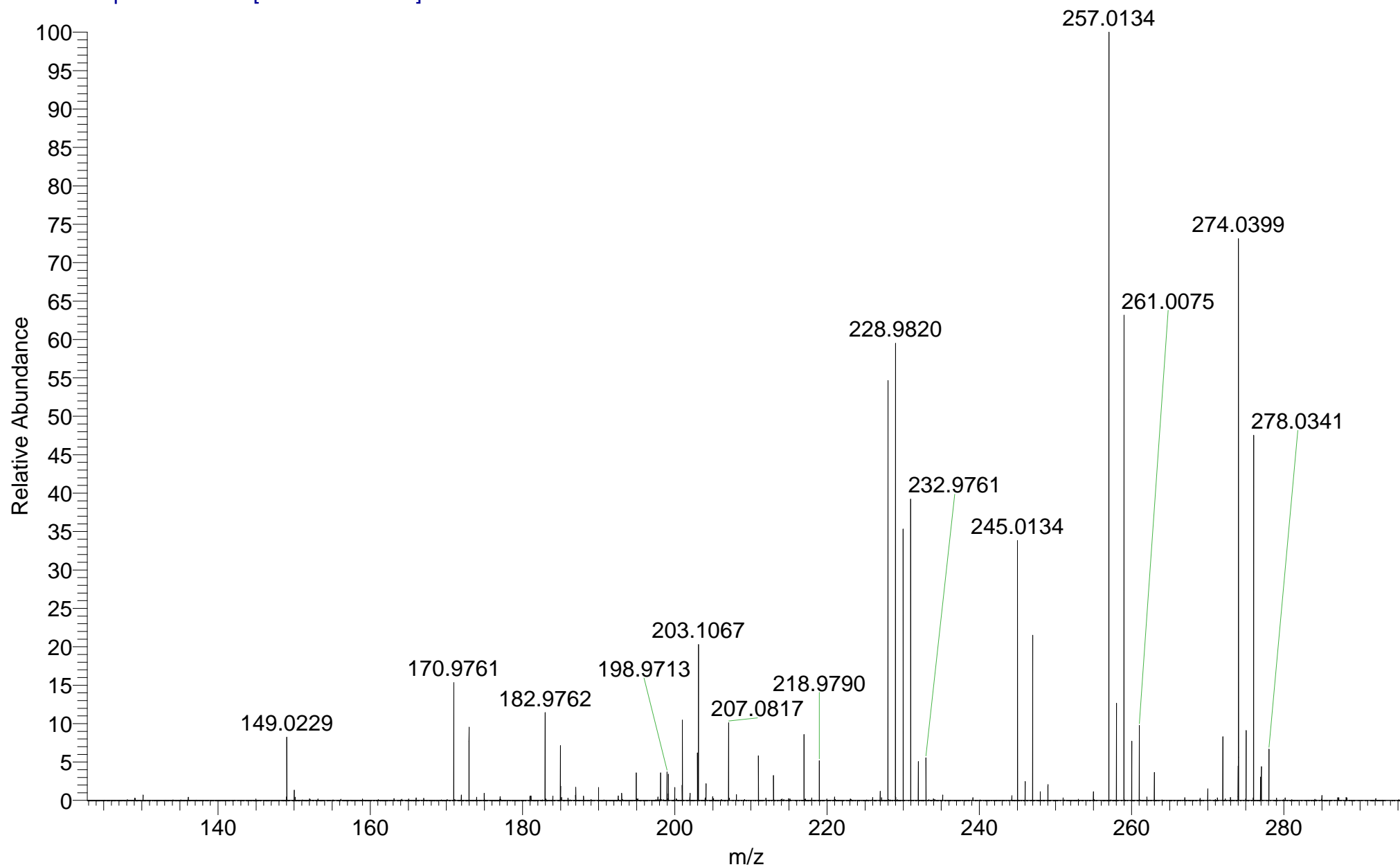


O:\IMPBUL_TW3J3_50397
(MeOH)/MeOH + NH4OAc
AB5-540

EPSRC UK National MS Facility
LTQ Orbitrap XL

C₁₃H₁₃Cl₂NO₄
26/11/2018 08:19:26

IMPBUL_TW3J3_50397 #37-55 RT: 0.66-1.05 AV: 16 SM: 7G NL: 1.74E6
T: FTMS + p NSI Full ms [120.00-1935.00]

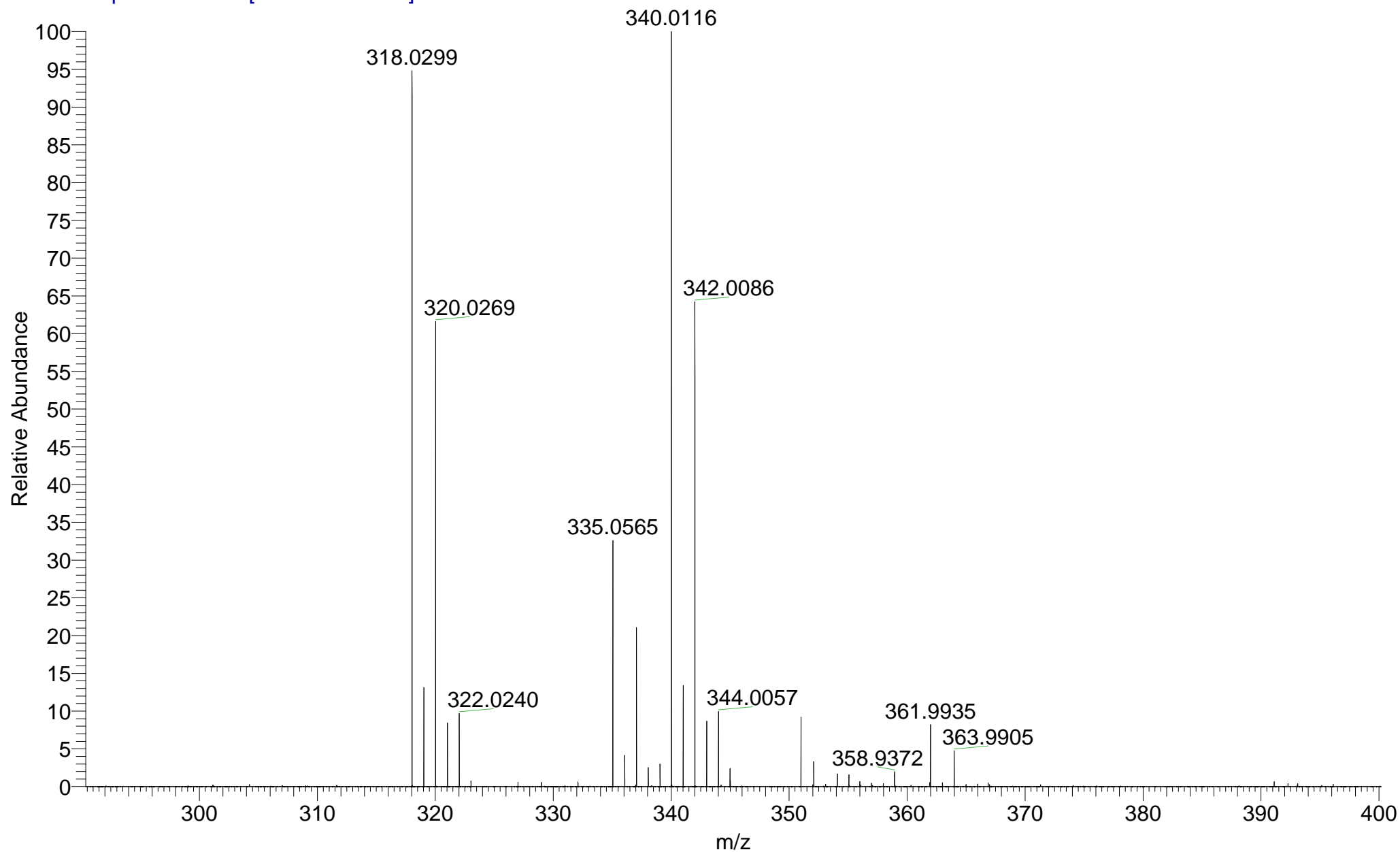


O:\IMPBUL_TW3J3_50397
(MeOH)/MeOH + NH4OAc
AB5-540

EPSRC UK National MS Facility
LTQ Orbitrap XL

C₁₃H₁₃Cl₂NO₄
26/11/2018 08:19:26

IMPBUL_TW3J3_50397 #37-55 RT: 0.66-1.05 AV: 16 SM: 7G NL: 4.00E6
T: FTMS + p NSI Full ms [120.00-1935.00]



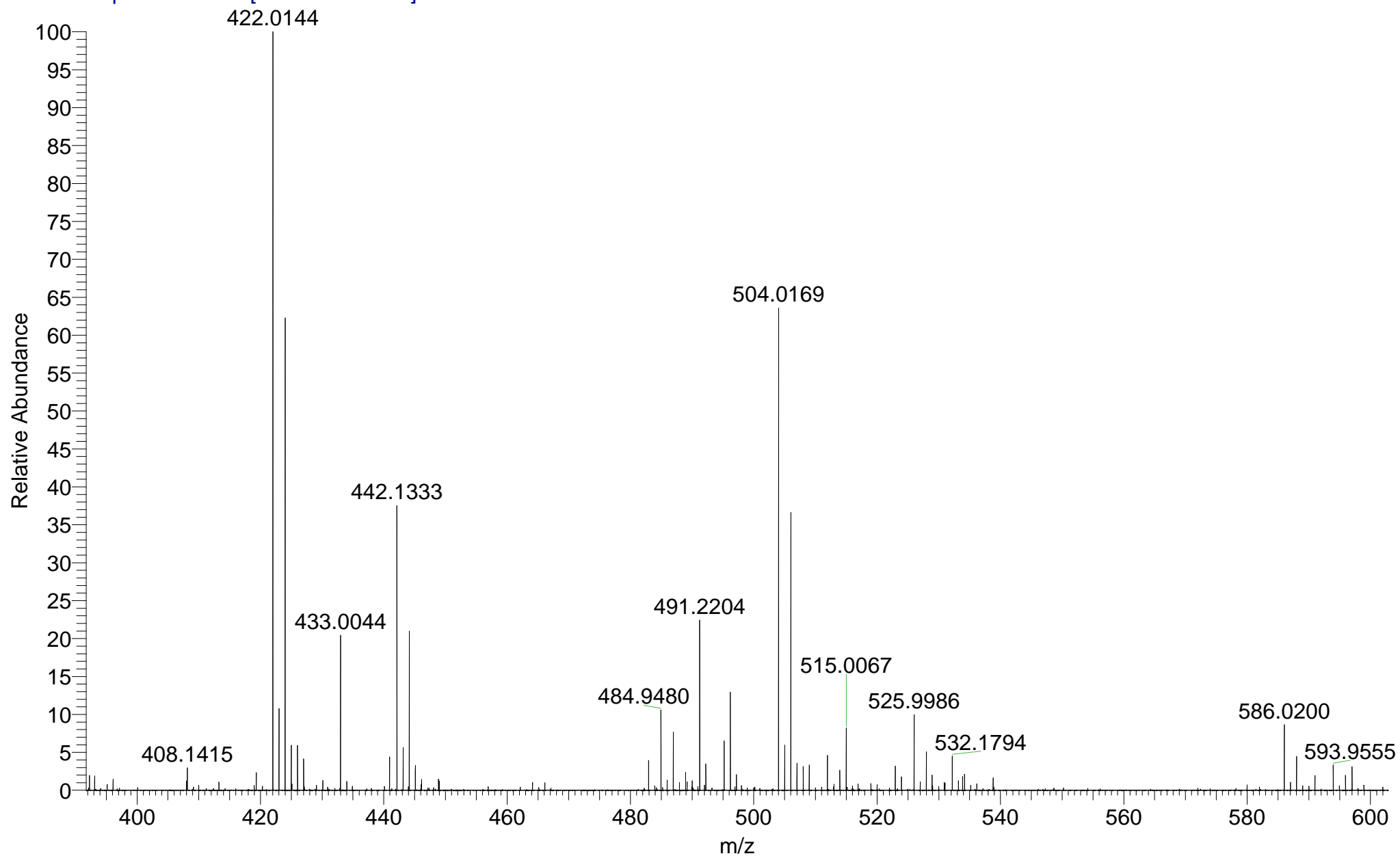
O:\IMPBUL_TW3J3_50397
(MeOH)/MeOH + NH4OAc
AB5-540

EPSRC UK National MS Facility
LTQ Orbitrap XL

C₁₃H₁₃Cl₂NO₄
26/11/2018 08:19:26

IMPBUL_TW3J3_50397 #37-55 RT: 0.66-1.05 AV: 16 SM: 7G NL: 8.19E5

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

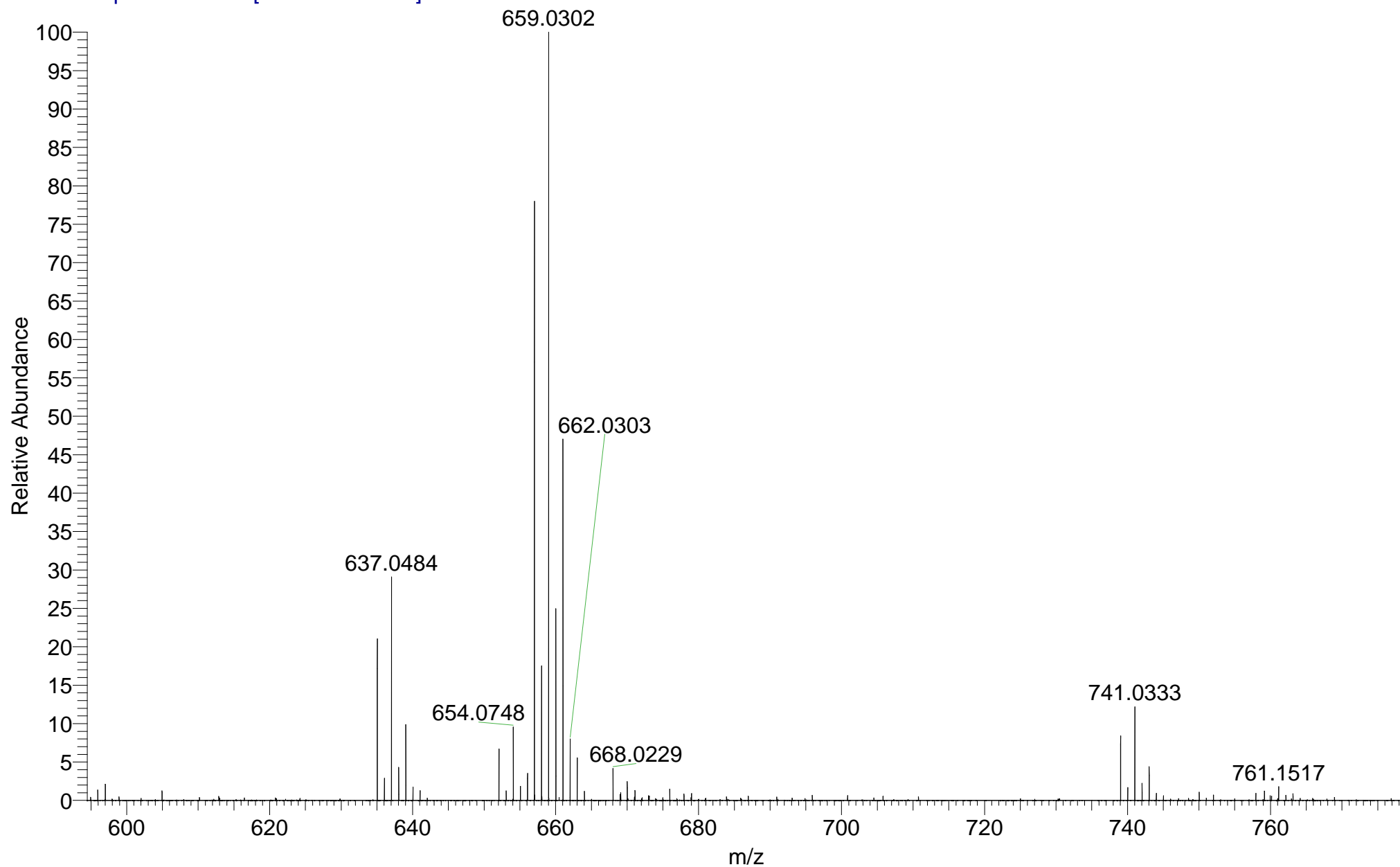


O:\IMPBUL_TW3J3_50397
(MeOH)/MeOH + NH4OAc
AB5-540

EPSRC UK National MS Facility
LTQ Orbitrap XL

C₁₃H₁₃Cl₂NO₄
26/11/2018 08:19:26

IMPBUL_TW3J3_50397 #37-55 RT: 0.66-1.05 AV: 16 SM: 7G NL: 1.19E6
T: FTMS + p NSI Full ms [120.00-1935.00]



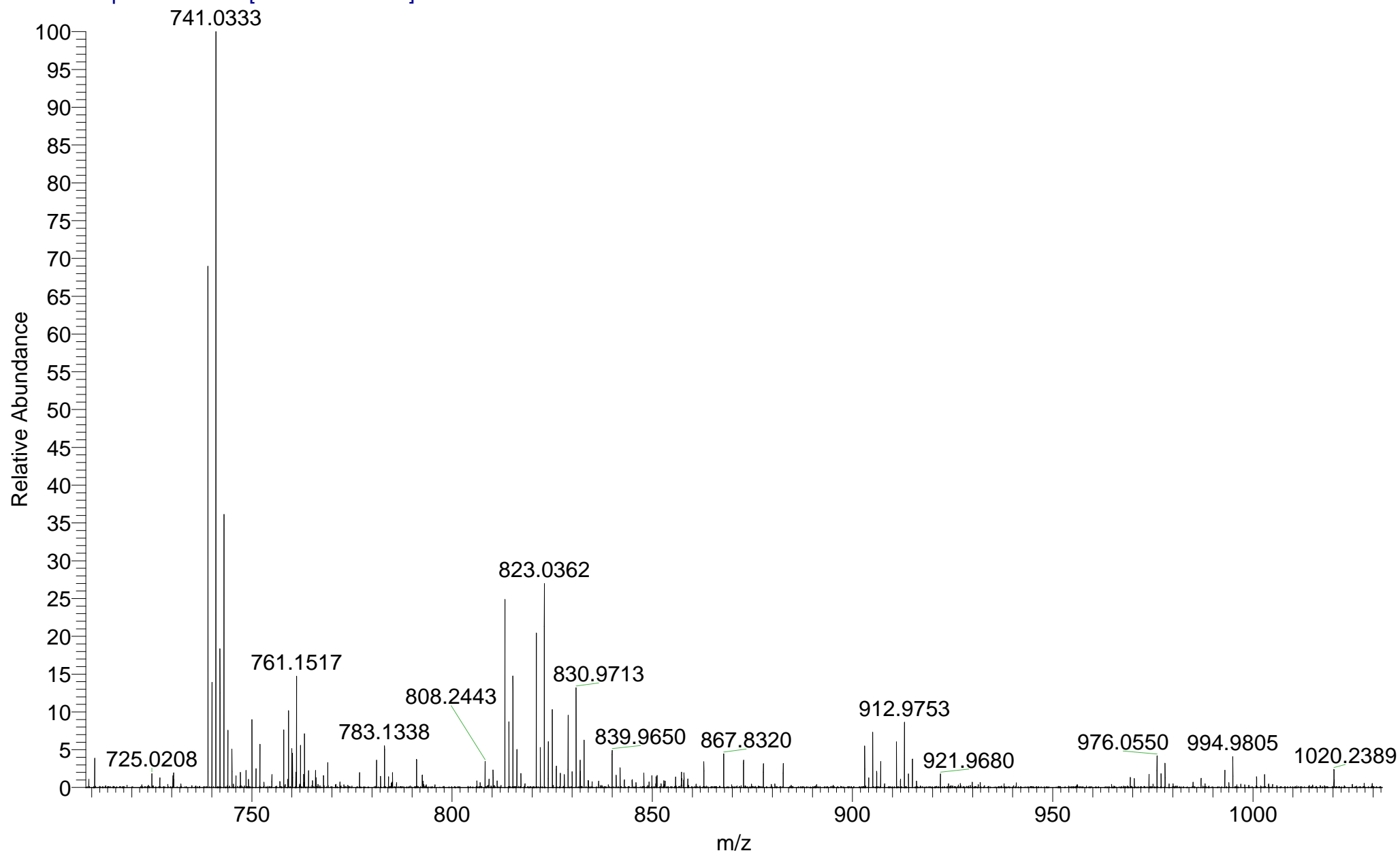
O:\IMPBUL_TW3J3_50397
(MeOH)/MeOH + NH4OAc
AB5-540

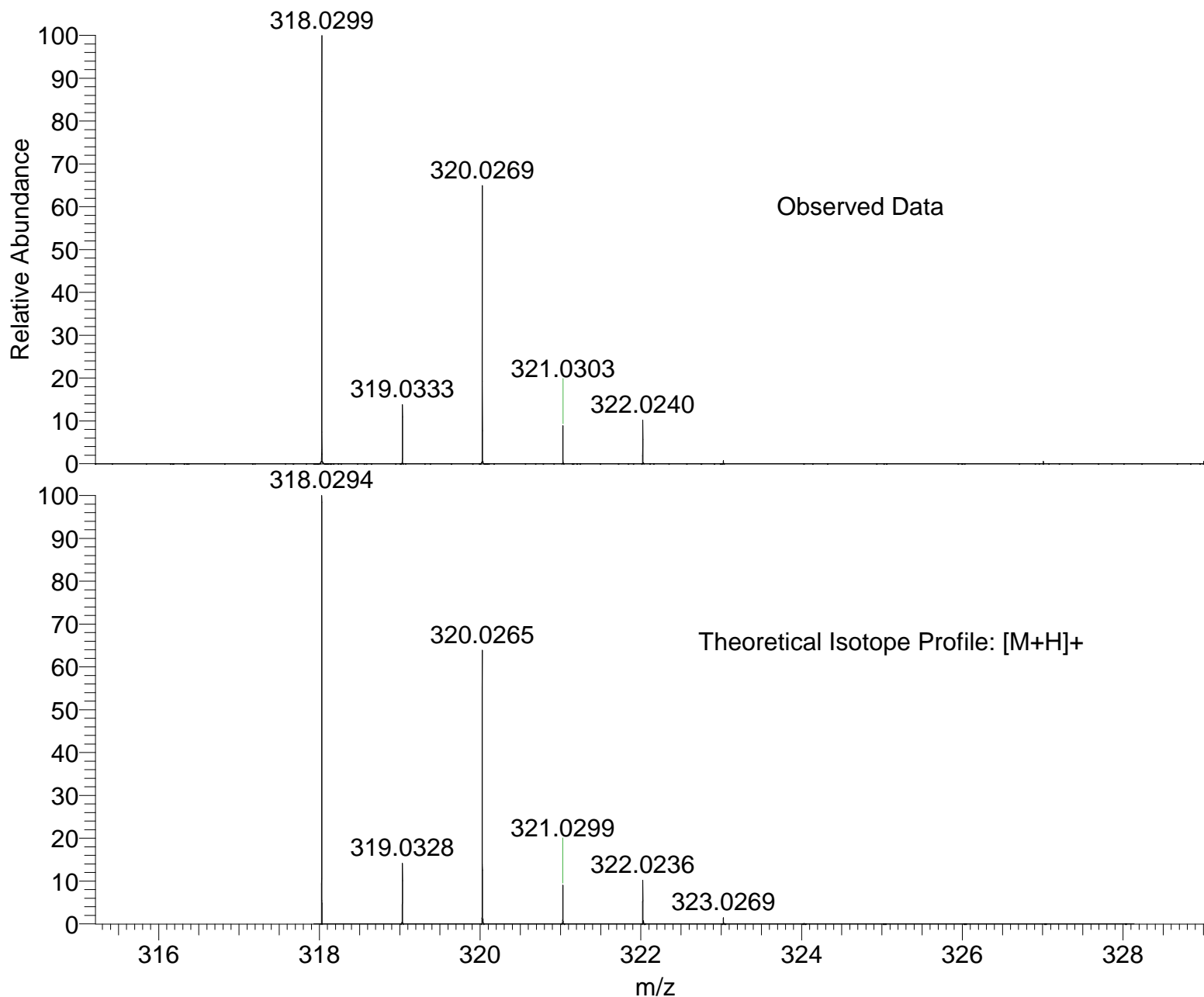
EPSRC UK National MS Facility
LTQ Orbitrap XL

C13H13Cl2NO4
26/11/2018 08:19:26

IMPBUL_TW3J3_50397 #37-55 RT: 0.66-1.05 AV: 16 SM: 7G NL: 1.45E5

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





NL:
3.79E6
IMPBUL_TW3J3_50397#37-55
RT: 0.66-1.05 AV: 16 T:
FTMS + p NSI Full ms
[120.00-1935.00]

NL:
1.15E4
C₁₃H₁₃Cl₂NO₄H:
C₁₃H₁₄Cl₂N₁O₄
p (gss, s /p:40) Chrg 1
R: 100000 Res .Pwr . @FWHM

Isotope: Min. .. Max.
 14 N 0....15
 16 O 0....20
 12 C 0....80
 1 H 0....100
 23 Na 0....0
 35 Cl 0....3
 Tolerance Window: +- 5.00 ppm
 Db/Ring Equiv: -10.. 500
 Fits: 300

N-Rule: Do not use
 Charge: 1

Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
318.0299	318.0299	-0.1	2.0	C ₁₀ H ₁₇ O ₃ N ₂ Cl ₃
	318.0298	0.3	20.5	C ₂₀ H ₄ O ₂ N ₃
	318.0303	-1.2	16.0	C ₁₇ H ₇ O ₁ N ₄ Cl ₁
	318.0303	-1.3	13.5	C ₅ O ₃ N ₁₅
	318.0303	-1.3	8.0	C ₆ H ₆ O ₈ N ₈
	318.0303	-1.3	2.5	C ₇ H ₁₂ O ₁₃ N ₁
	318.0295	1.4	-1.5	C ₂ H ₁₃ O ₁₁ N ₅ Cl ₁
	318.0295	1.4	4.0	C ₁ H ₇ O ₆ N ₁₂ Cl ₁
	318.0294	1.4	6.5	C ₁₃ H ₁₄ O ₄ N ₁ Cl ₂
	318.0308	-2.8	11.5	C ₁₄ H ₁₀ N ₅ Cl ₂
	318.0308	-2.8	3.5	C ₃ H ₉ O ₇ N ₉ Cl ₁
	318.0308	-2.8	-2.0	C ₄ H ₁₅ O ₁₂ N ₂ Cl ₁
	318.0290	2.9	3.0	C ₅ H ₁₀ O ₁₂ N ₄
	318.0290	2.9	8.5	C ₄ H ₄ O ₇ N ₁₁
	318.0290	3.0	11.0	C ₁₆ H ₁₁ O ₅ Cl ₁
	318.0289	3.0	16.5	C ₁₅ H ₅ N ₇ Cl ₁
	318.0311	-3.9	20.0	C ₂₂ H ₆ O ₃
	318.0286	4.1	2.5	C ₈ H ₁₅ O ₂ N ₅ Cl ₃
	318.0313	-4.4	-1.0	H ₁₂ O ₆ N ₁₀ Cl ₂
	318.0313	-4.4	-6.5	C ₁ H ₁₈ O ₁₁ N ₃ Cl ₂
	318.0285	4.5	21.0	C ₁₈ H ₂ O ₁ N ₆