

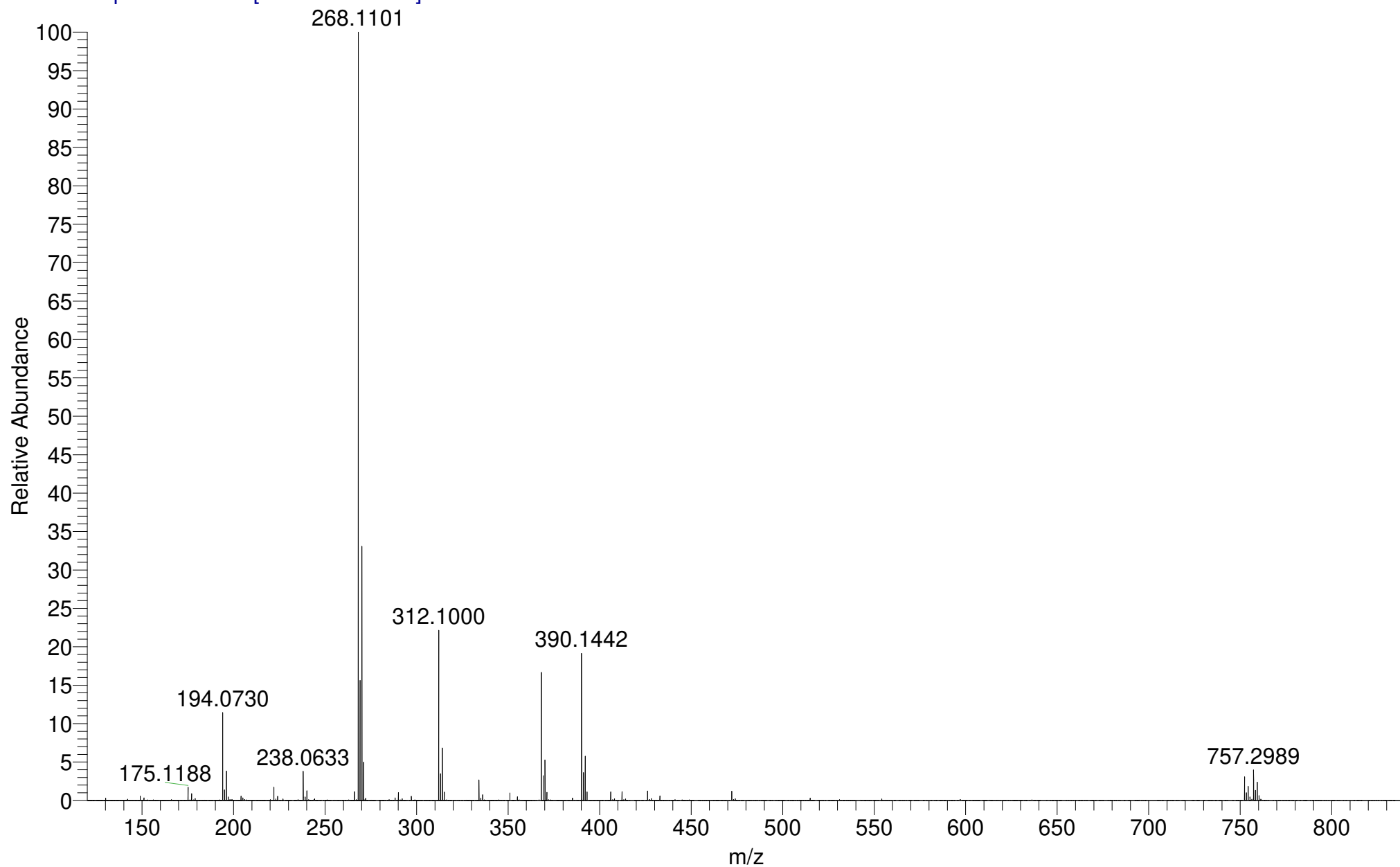
AB3-317
(DCM)/MeOH + NH₄OAc
C₁₉H₂₆ClNO₄

EPSRC National Facility Swansea
LTQ Orbitrap XL

IMPBUL-AJB
22/02/2018 16:52:28

IMPBUL_CLR9P_42200 #33-40 RT: 0.74-1.02 AV: 6 SM: 7G NL: 3.30E7

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

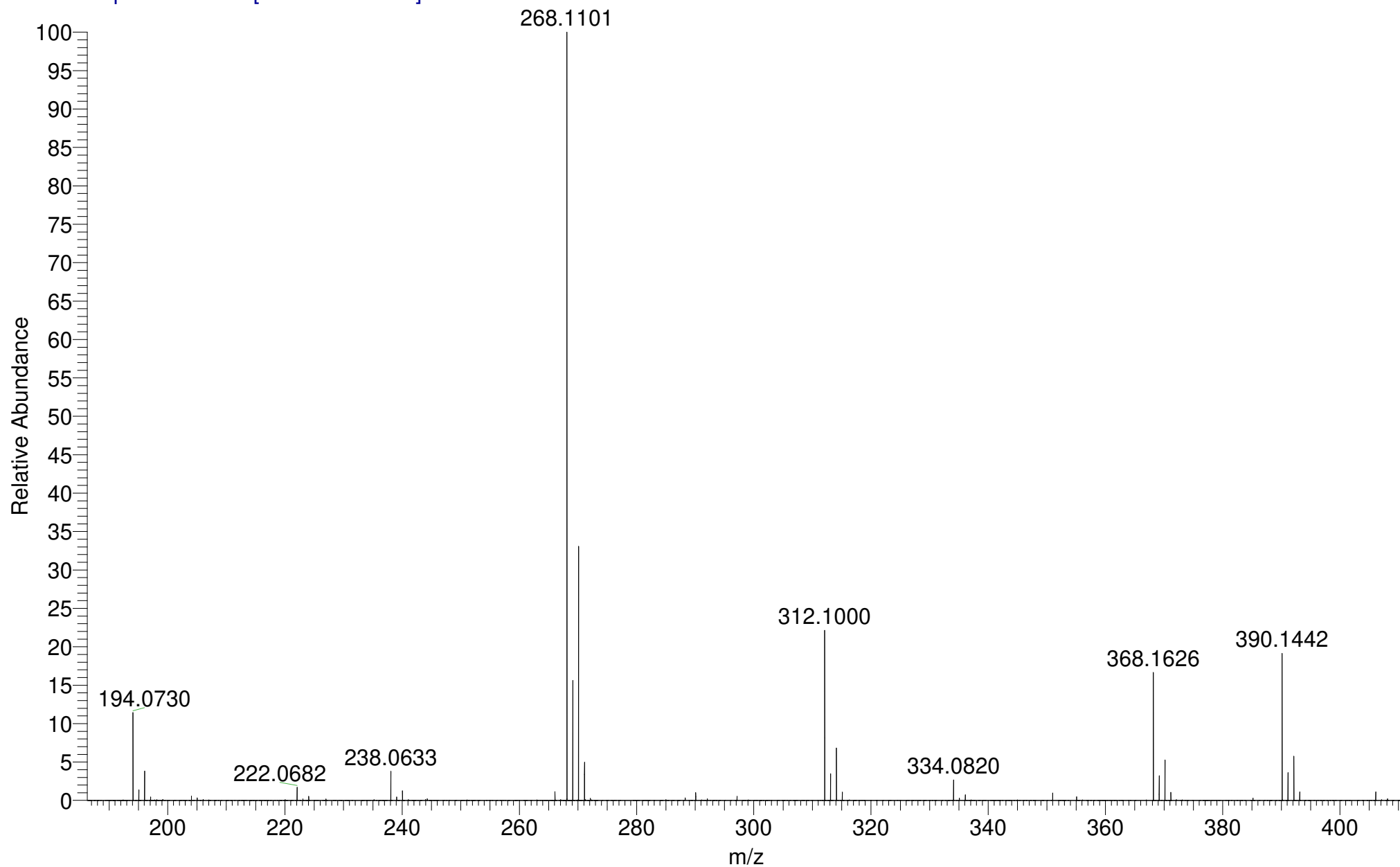


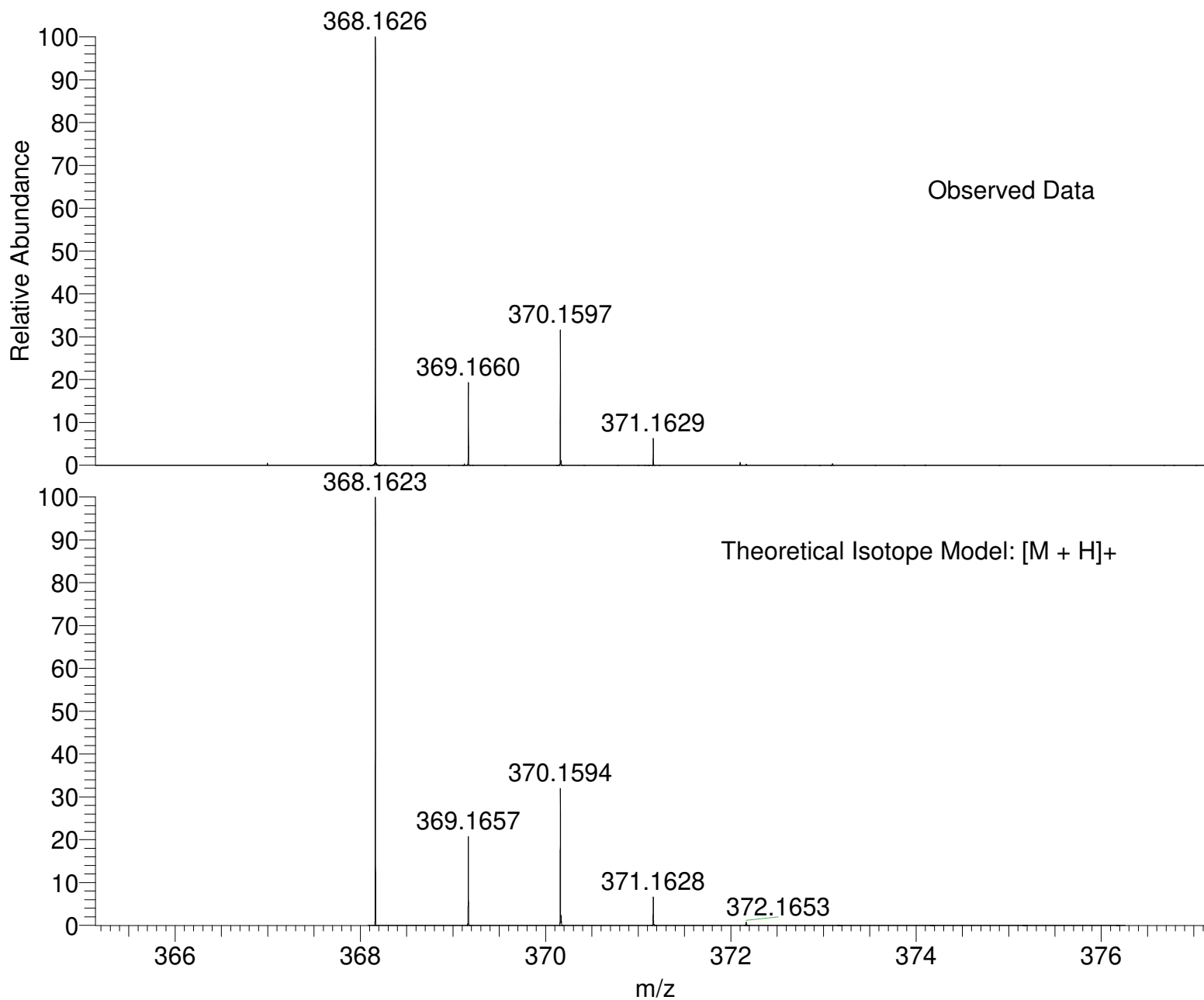
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(DCM)/MeOH + NH₄OAc
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IMPBUL_CLR9P_42200 #33-40 RT: 0.74-1.02 AV: 6 SM: 7G NL: 3.30E7
T: FTMS + p NSI Full ms [120.00-1935.00]





NL:
5.50E6
IMPBUL_CLR9P_42200#33-40
RT: 0.74-1.02 AV: 6 T: FTMS
+ p NSI Full ms
[120.00-1935.00]

NL:
1.43E4
C₁₉H₂₆ClNO₄H:
C₁₉H₂₇Cl₁N₁O₄
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....80
 1 H 0....90
 23 Na 0....0
 35 Cl 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
368.1626	368.1628	-0.5	2.0	C ₁₆ H ₃₀ O ₃ N ₂ Cl ₂
	368.1628	-0.6	-0.5	C ₄ H ₂₃ O ₅ N ₁₃ Cl ₁
	368.1623	0.7	-1.5	C ₈ H ₂₆ O ₁₁ N ₅
	368.1623	0.7	4.0	C ₇ H ₂₀ O ₆ N ₁₂
	368.1623	0.8	6.5	C ₁₉ H ₂₇ O ₄ N ₁ Cl ₁
	368.1632	-1.5	16.0	C ₂₃ H ₂₀ O ₁ N ₄
	368.1619	1.8	-2.0	C ₁₁ H ₃₁ O ₁ N ₆ Cl ₃
	368.1633	-1.9	-2.5	C ₁₃ H ₃₃ O ₂ N ₃ Cl ₃
	368.1618	2.1	11.0	C ₂₂ H ₂₄ O ₅
	368.1618	2.1	16.5	C ₂₁ H ₁₈ N ₇
	368.1636	-2.9	11.5	C ₂₀ H ₂₃ N ₅ Cl ₁
	368.1637	-2.9	3.5	C ₉ H ₂₂ O ₇ N ₉
	368.1637	-2.9	-2.0	C ₁₀ H ₂₈ O ₁₂ N ₂
	368.1615	3.1	2.5	C ₁₄ H ₂₈ O ₂ N ₅ Cl ₂
	368.1642	-4.2	-1.0	C ₆ H ₂₅ O ₆ N ₁₀ Cl ₁
	368.1610	4.4	-1.0	C ₆ H ₂₄ O ₁₀ N ₈
	368.1610	4.4	4.5	C ₅ H ₁₈ O ₅ N ₁₅
	368.1610	4.4	7.0	C ₁₇ H ₂₅ O ₃ N ₄ Cl ₁