

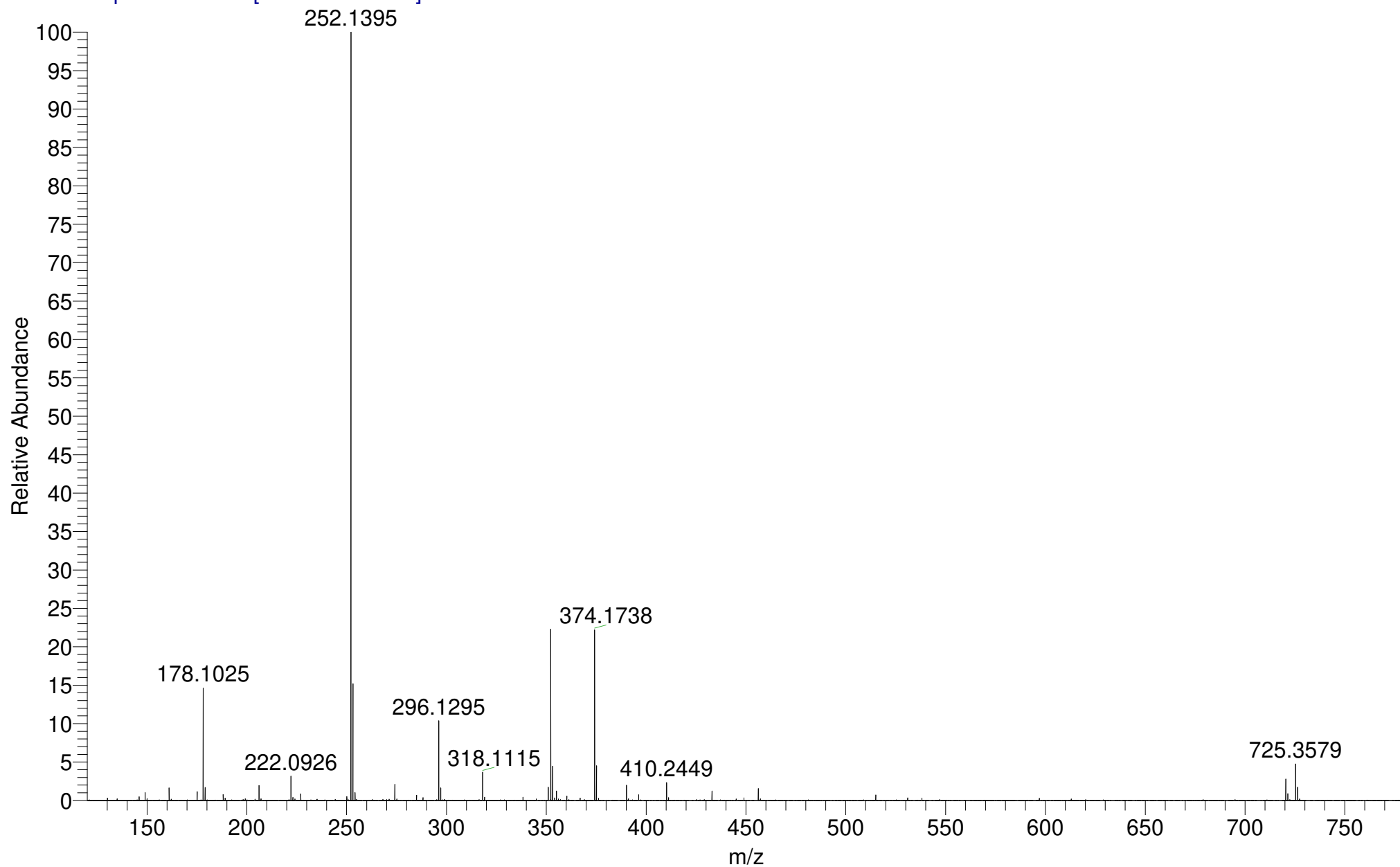
AB3-318
(DCM)/MeOH + NH₄OAc
C₁₉H₂₆FNO₄

EPSRC National Facility Swansea
LTQ Orbitrap XL

IMPBUL-AJB
22/02/2018 16:58:20

IMPBUL_CLWJP_42210 #32-39 RT: 0.74-1.02 AV: 6 SM: 7G NL: 1.79E7

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

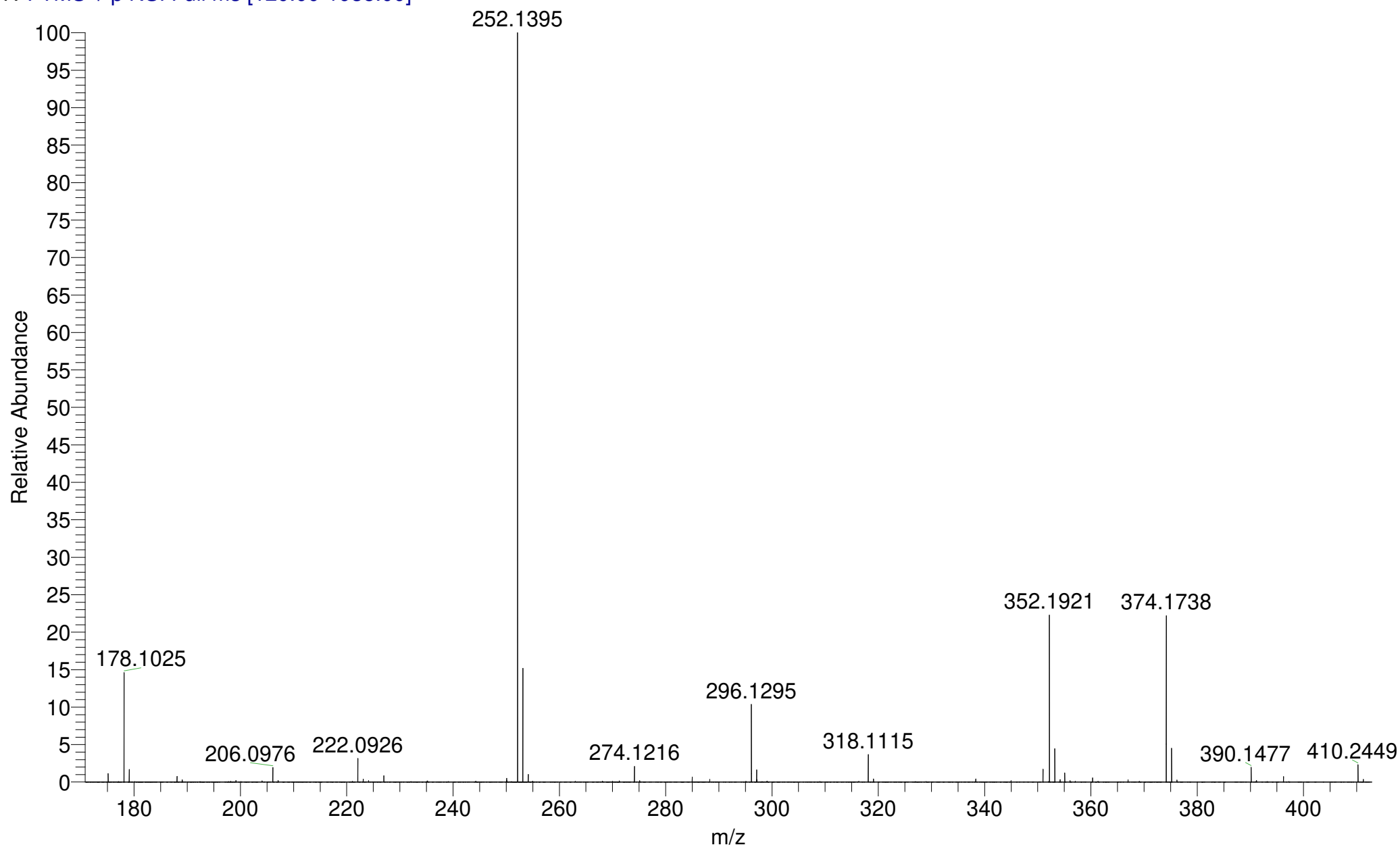


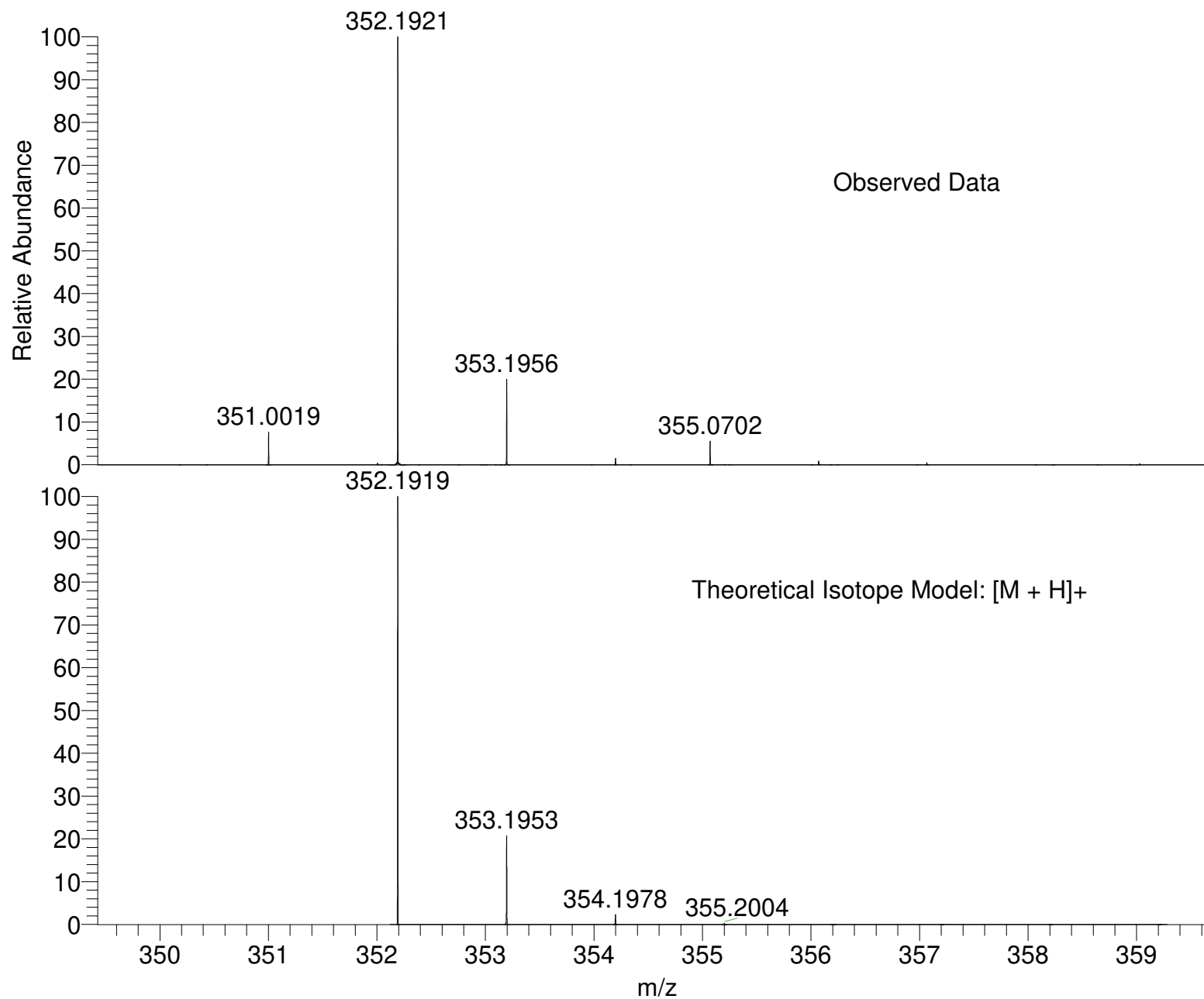
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(DCM)/MeOH + NH₄OAc
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IMPBUL_CLWJP_42210 #32-39 RT: 0.74-1.02 AV: 6 SM: 7G NL: 1.79E7
T: FTMS + p NSI Full ms [120.00-1935.00]





NL:
3.98E6
IMPBUL_CLWJP_42210#32-
39 RT: 0.74-1.02 AV: 6 T:
FTMS + p NSI Full ms
[120.00-1935.00]

NL:
1.88E4
C₁₉H₂₆FNO₄H:
C₁₉H₂₇F₁N₁O₄
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
 19 F 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
352.1921	352.1919	0.7	6.5	C ₁₉ H ₂₇ O ₄ N ₁ F ₁
	352.1924	-0.8	-0.5	C ₄ H ₂₃ O ₅ N ₁₃ F ₁
	352.1917	1.2	3.0	C ₁₄ H ₂₆ O ₄ N ₄ F ₂
	352.1926	-1.3	3.0	C ₉ H ₂₄ O ₅ N ₁₀
	352.1926	-1.3	-2.5	C ₁₀ H ₃₀ O ₁₀ N ₃
	352.1926	-1.4	1.0	C ₅ H ₂₀ N ₁₄ F ₄
	352.1915	1.8	-0.5	C ₉ H ₂₅ O ₄ N ₇ F ₃
	352.1928	-2.0	4.5	C ₁₀ H ₂₁ N ₁₁ F ₃
	352.1928	-2.0	-1.0	C ₁₁ H ₂₇ O ₅ N ₄ F ₃
	352.1912	2.5	-2.0	C ₈ H ₂₈ O ₉ N ₆
	352.1912	2.5	3.5	C ₇ H ₂₂ O ₄ N ₁₃
	352.1930	-2.6	8.0	C ₁₅ H ₂₂ N ₈ F ₂
	352.1930	-2.6	2.5	C ₁₆ H ₂₈ O ₅ N ₁ F ₂
	352.1932	-3.1	11.5	C ₂₀ H ₂₃ N ₅ F ₁
	352.1932	-3.2	4.0	C ₁₇ H ₂₅ N ₂ F ₅
	352.1934	-3.7	15.0	C ₂₅ H ₂₄ N ₂
	352.1907	3.9	10.5	C ₂₂ H ₂₆ O ₃ N ₁
	352.1906	4.4	-0.5	C ₁₄ H ₂₇ O ₃ N ₁ F ₅
	352.1905	4.5	7.0	C ₁₇ H ₂₅ O ₃ N ₄ F ₁
	352.1937	-4.6	-1.0	C ₆ H ₂₅ O ₆ N ₁₀ F ₁
	352.1937	-4.7	-3.0	C ₂ H ₂₁ O ₁ N ₁₄ F ₅