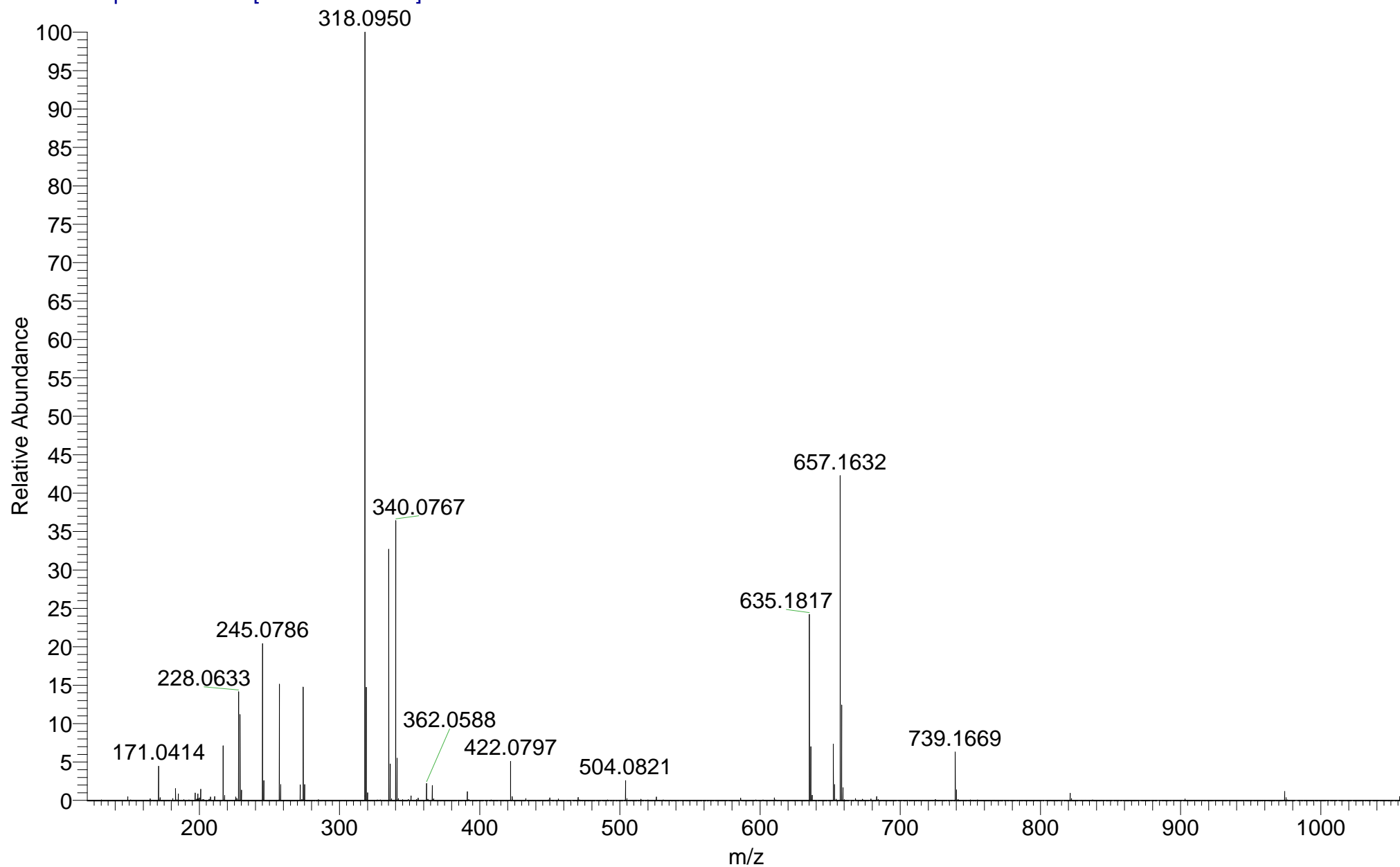


IMPBUL_TW7JN_50398 #37-53 RT: 0.66-1.04 AV: 16 SM: 7G NL: 2.56E7

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

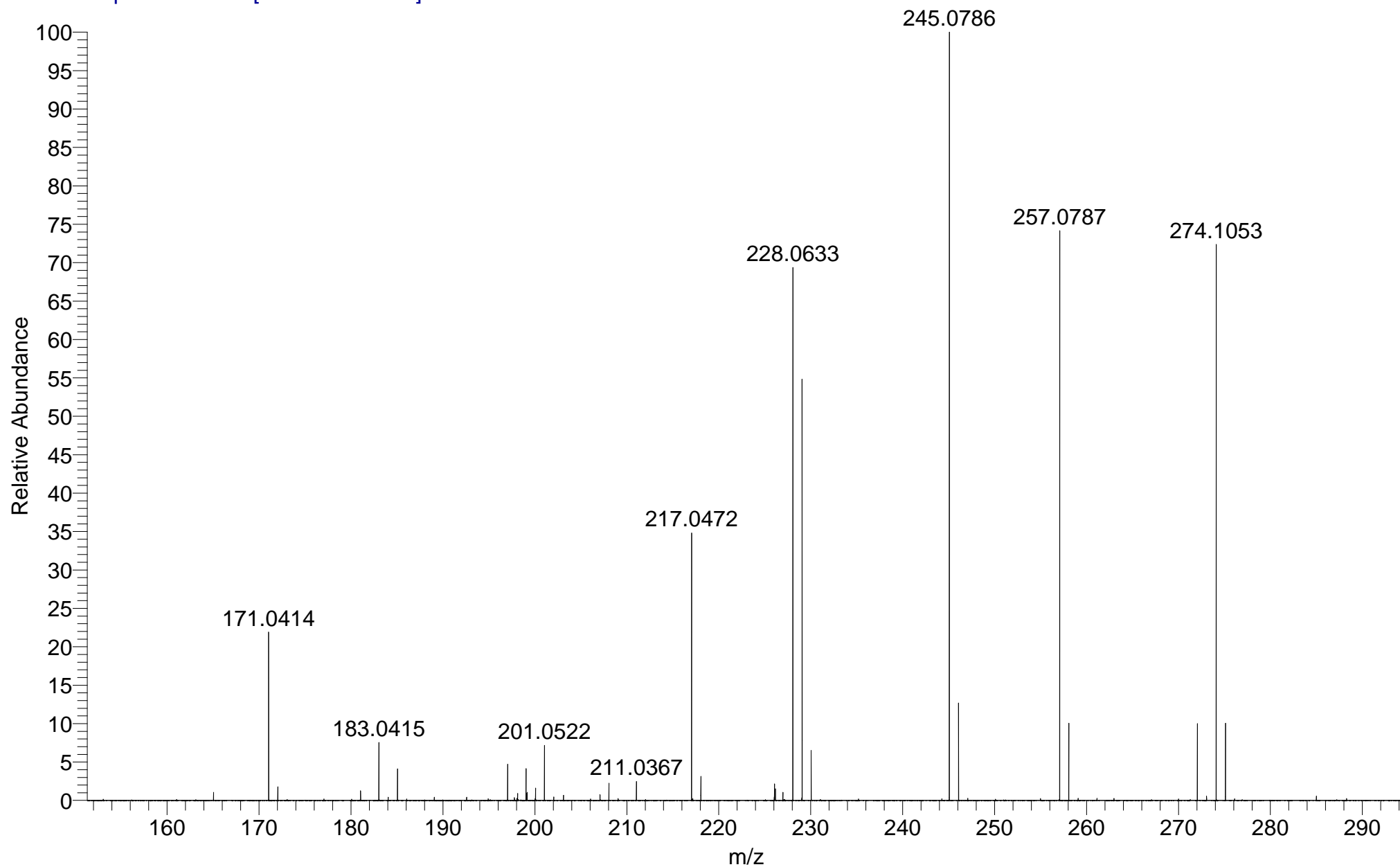


O:\IMPBUL_TW7JN_50398
(MeOH)/MeOH + NH4OAc
AB5-546

EPSRC UK National MS Facility
LTQ Orbitrap XL

C14H14F3NO4
26/11/2018 08:22:19

IMPBUL_TW7JN_50398 #37-53 RT: 0.66-1.04 AV: 16 SM: 7G NL: 5.22E6
T: FTMS + p NSI Full ms [120.00-1935.00]



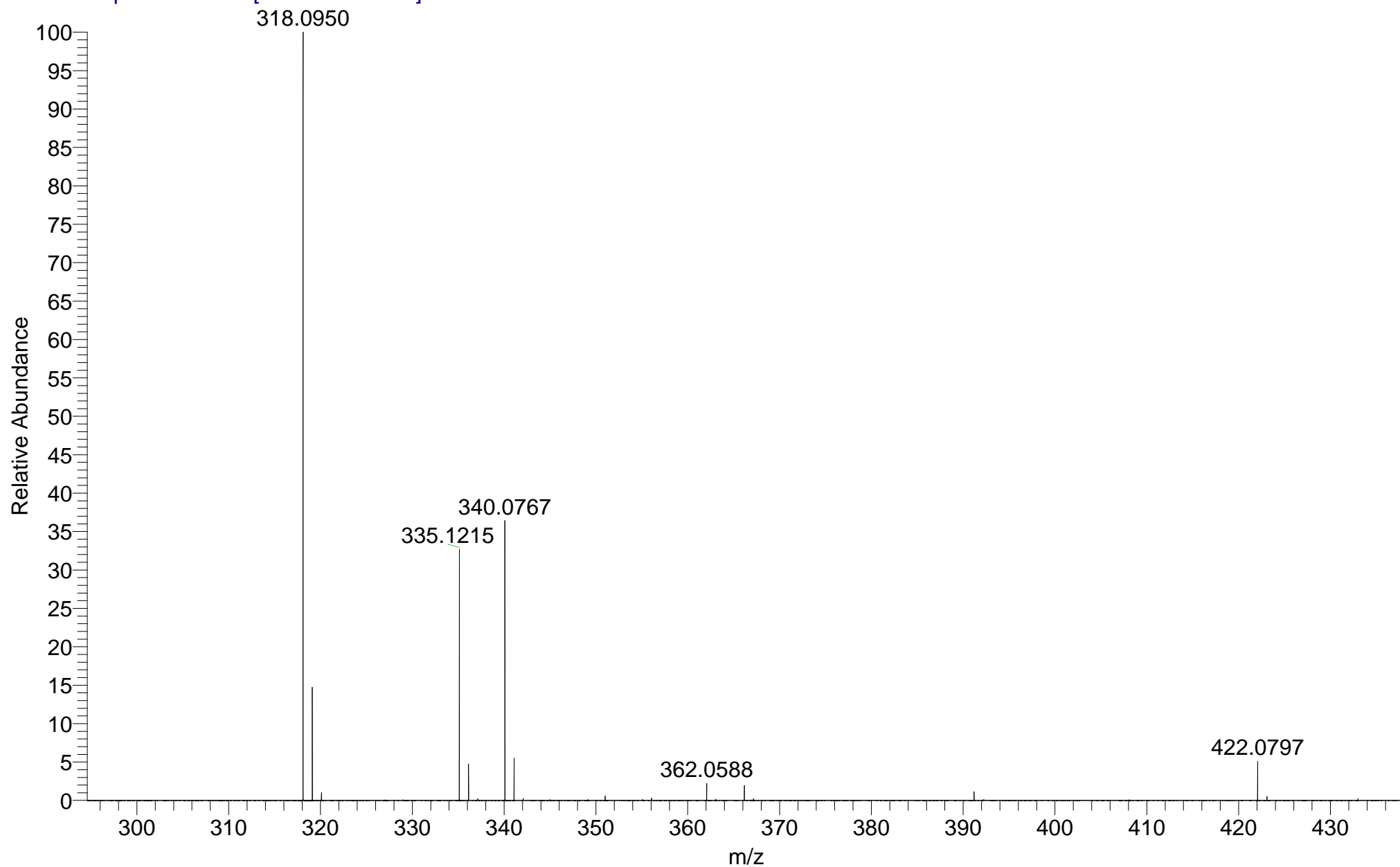
O:\IMPBUL_TW7JN_50398
(MeOH)/MeOH + NH4OAc
AB5-546

EPSRC UK National MS Facility
LTQ Orbitrap XL

C14H14F3NO4
26/11/2018 08:22:19

IMPBUL_TW7JN_50398 #37-53 RT: 0.66-1.04 AV: 16 SM: 7G NL: 2.56E7

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

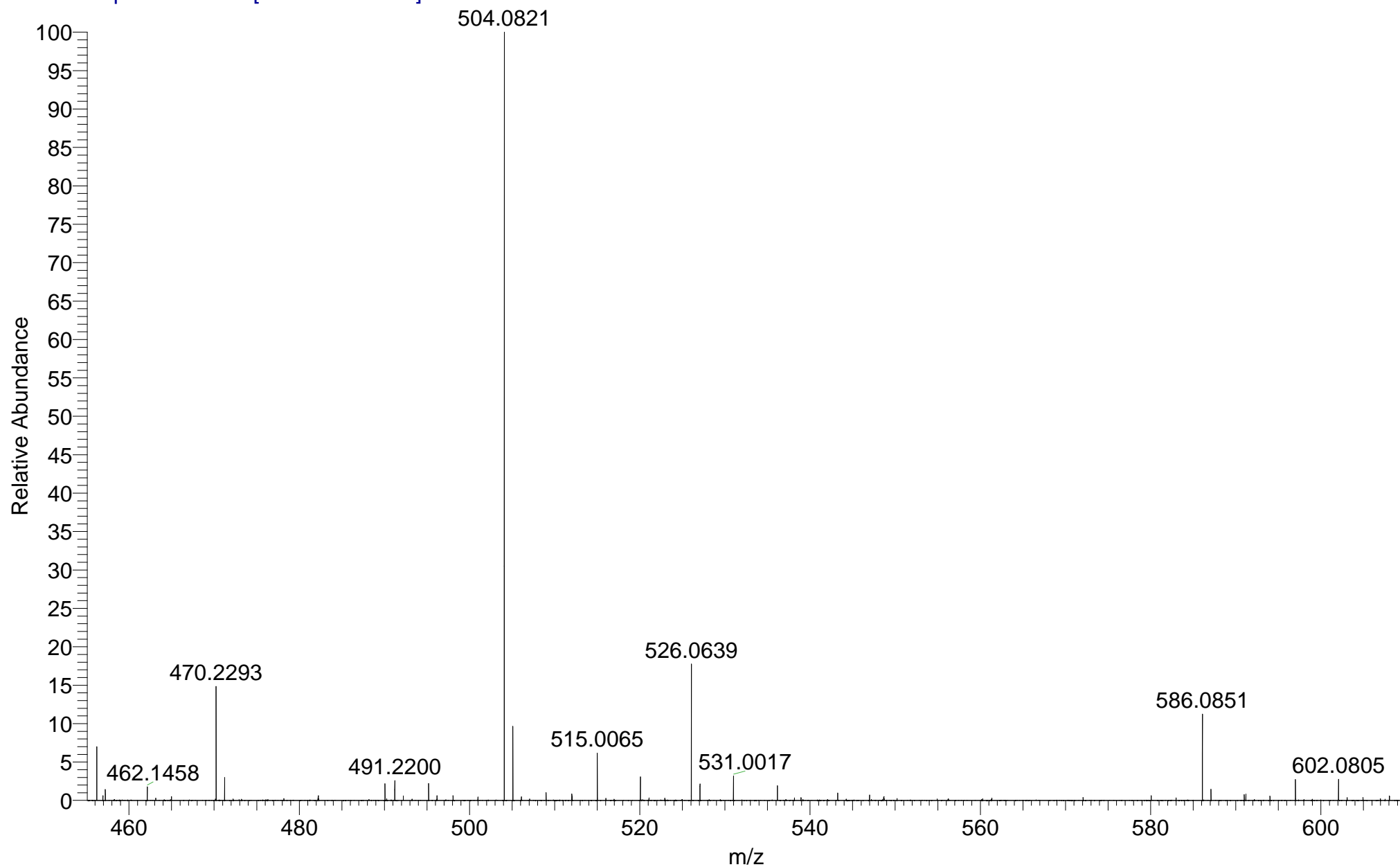


O:\IMPBUL_TW7JN_50398
(MeOH)/MeOH + NH₄OAc
AB5-546

EPSRC UK National MS Facility
LTQ Orbitrap XL

C₁₄H₁₄F₃NO₄
26/11/2018 08:22:19

IMPBUL_TW7JN_50398 #37-53 RT: 0.66-1.04 AV: 16 SM: 7G NL: 6.64E5
T: FTMS + p NSI Full ms [120.00-1935.00]

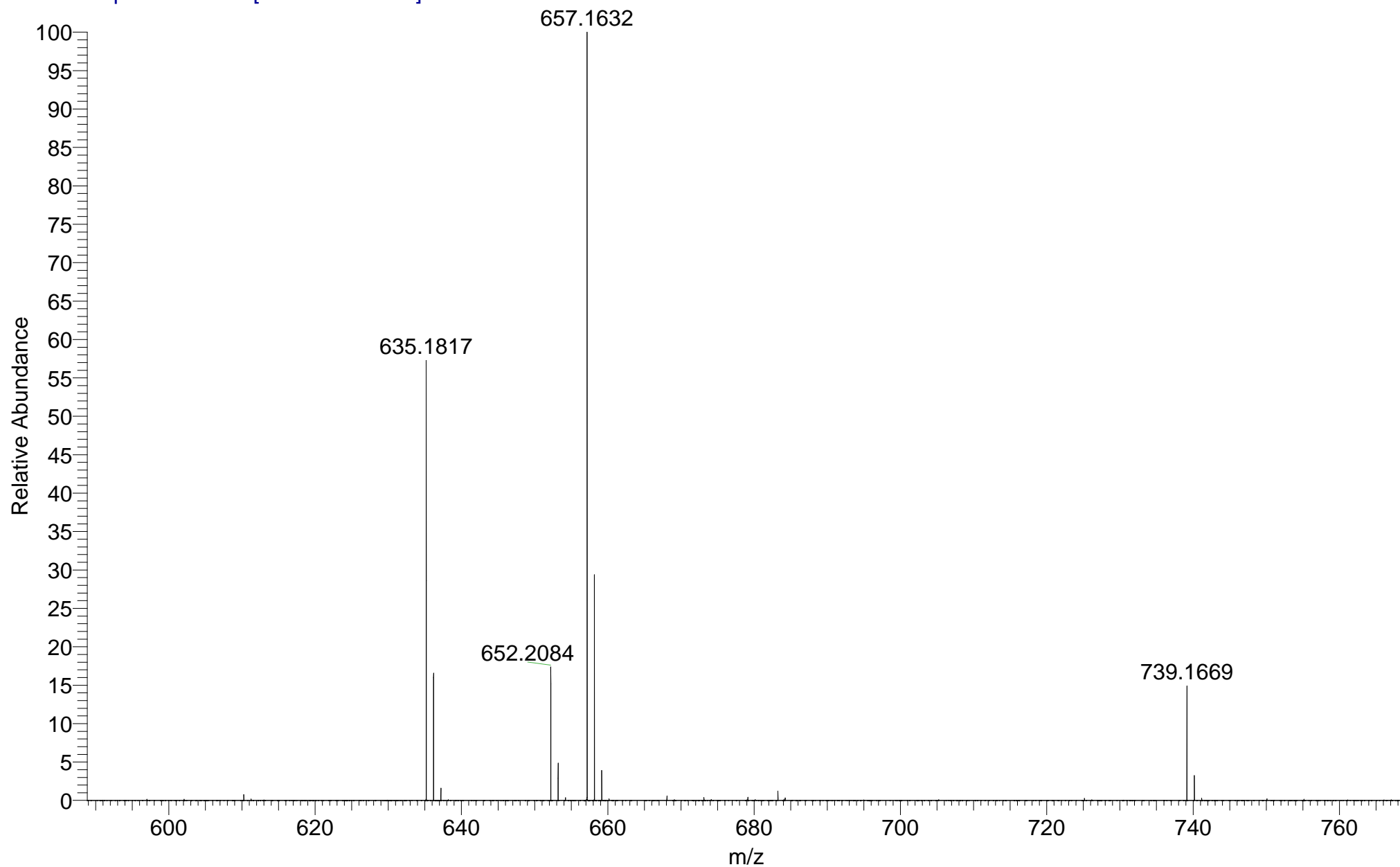


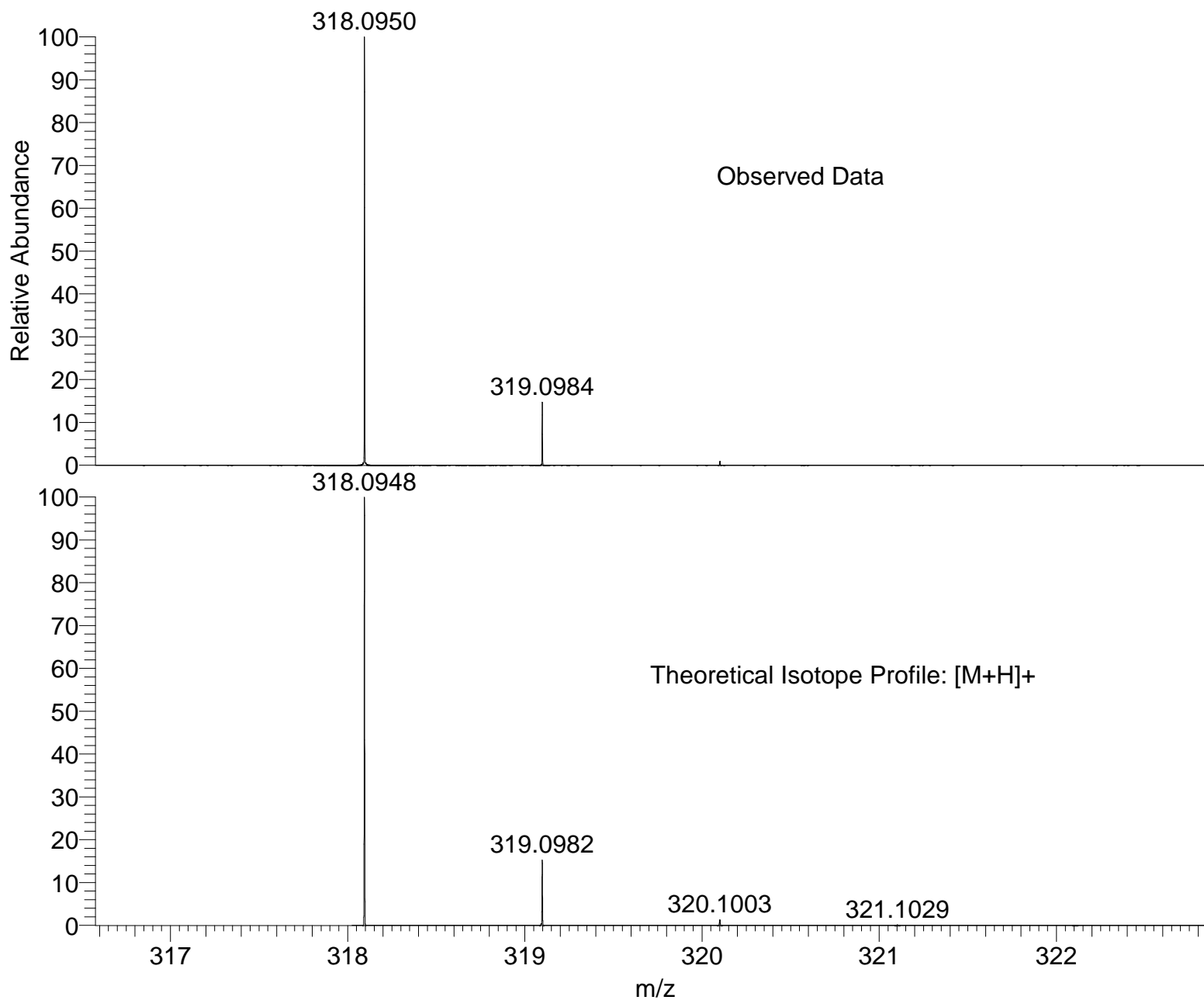
O:\IMPBUL_TW7JN_50398
(MeOH)/MeOH + NH4OAc
AB5-546

EPSRC UK National MS Facility
LTQ Orbitrap XL

C₁₄H₁₄F₃NO₄
26/11/2018 08:22:19

IMPBUL_TW7JN_50398 #37-53 RT: 0.66-1.04 AV: 16 SM: 7G NL: 1.08E7
T: FTMS + p NSI Full ms [120.00-1935.00]





NL:
2.56E7
IMPBUL_TW7JN_50398#37-
53 RT: 0.66-1.04 AV: 16 T:
FTMS + p NSI Full ms
[120.00-1935.00]

NL:
1.99E4
C₁₄H₁₄F₃NO₄H:
C₁₄H₁₅F₃N₁O₄
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
 19 F 0....7
 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
318.0950	318.0948	0.7	6.5	C ₁₄ H ₁₅ O ₄ N ₁ F ₃
	318.0953	-0.9	-6.0	H ₁₇ O ₁₀ N ₆ F ₃
	318.0946	1.4	3.0	C ₉ H ₁₄ O ₄ N ₄ F ₄
	318.0945	1.5	5.0	C ₁₃ H ₁₈ O ₉
	318.0955	-1.5	3.0	C ₄ H ₁₂ O ₅ N ₁₀ F ₂
	318.0945	1.5	10.5	C ₁₂ H ₁₂ O ₄ N ₇
	318.0955	-1.5	-2.5	C ₅ H ₁₈ O ₁₀ N ₃ F ₂
	318.0955	-1.6	1.0	H ₈ N ₁₄ F ₆
	318.0955	-1.6	-4.5	C ₁ H ₁₄ O ₅ N ₇ F ₆
	318.0955	-1.6	-10.0	C ₂ H ₂₀ O ₁₀ F ₆
	318.0944	2.0	-6.0	C ₅ H ₁₉ O ₉ F ₅
	318.0944	2.0	-0.5	C ₄ H ₁₃ O ₄ N ₇ F ₅
	318.0957	-2.1	12.0	C ₈ H ₇ N ₁₄ F ₁
	318.0943	2.1	1.5	C ₈ H ₁₇ O ₉ N ₃ F ₁
	318.0957	-2.1	6.5	C ₉ H ₁₃ O ₅ N ₇ F ₁
	318.0943	2.1	7.0	C ₇ H ₁₁ O ₄ N ₁₀ F ₁
	318.0957	-2.1	1.0	C ₁₀ H ₁₉ O ₁₀ F ₁
	318.0957	-2.2	4.5	C ₅ H ₉ N ₁₁ F ₅
	318.0957	-2.2	-1.0	C ₆ H ₁₅ O ₅ N ₄ F ₅
	318.0942	2.6	-9.5	H ₁₈ O ₉ N ₃ F ₆
	318.0959	-2.7	15.5	C ₁₃ H ₈ N ₁₁
	318.0941	2.7	-2.0	C ₃ H ₁₆ O ₉ N ₆ F ₂
	318.0959	-2.7	10.0	C ₁₄ H ₁₄ O ₅ N ₄
	318.0941	2.7	3.5	C ₂ H ₁₀ O ₄ N ₁₃ F ₂
	318.0959	-2.9	8.0	C ₁₀ H ₁₀ N ₈ F ₄
	318.0959	-2.9	2.5	C ₁₁ H ₁₆ O ₅ N ₁ F ₄
	318.0961	-3.5	11.5	C ₁₅ H ₁₁ N ₅ F ₃
	318.0961	-3.6	4.0	C ₁₂ H ₁₃ N ₂ F ₇
	318.0963	-4.1	15.0	C ₂₀ H ₁₂ N ₂ F ₂
	318.0936	4.3	10.5	C ₁₇ H ₁₄ O ₃ N ₁ F ₂
	318.0964	-4.3	-2.5	H ₁₆ O ₁₁ N ₉