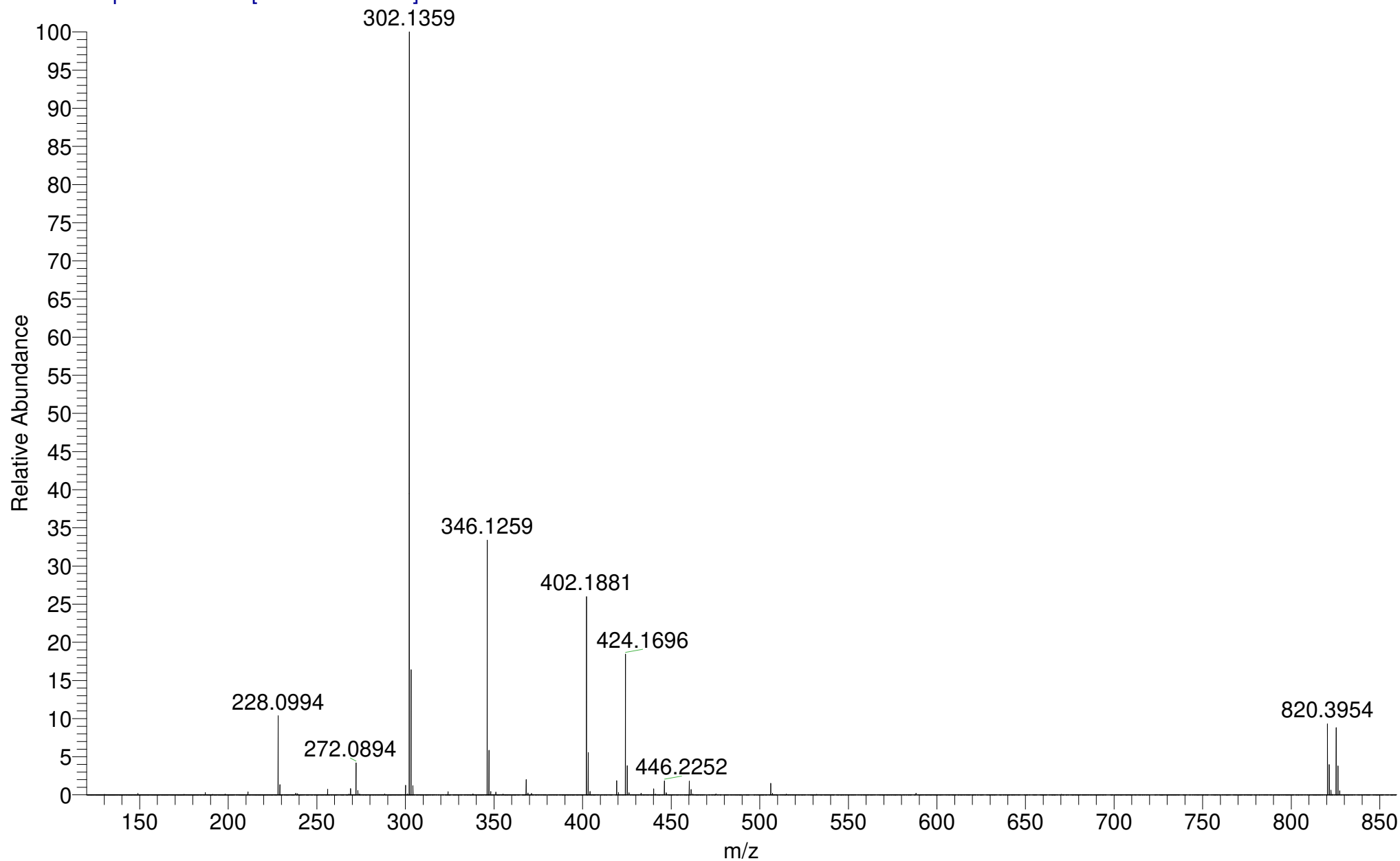


IMPBUL_CNURC_42211 #13-19 RT: 0.15-0.50 AV: 7 SM: 7G NL: 5.87E7

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



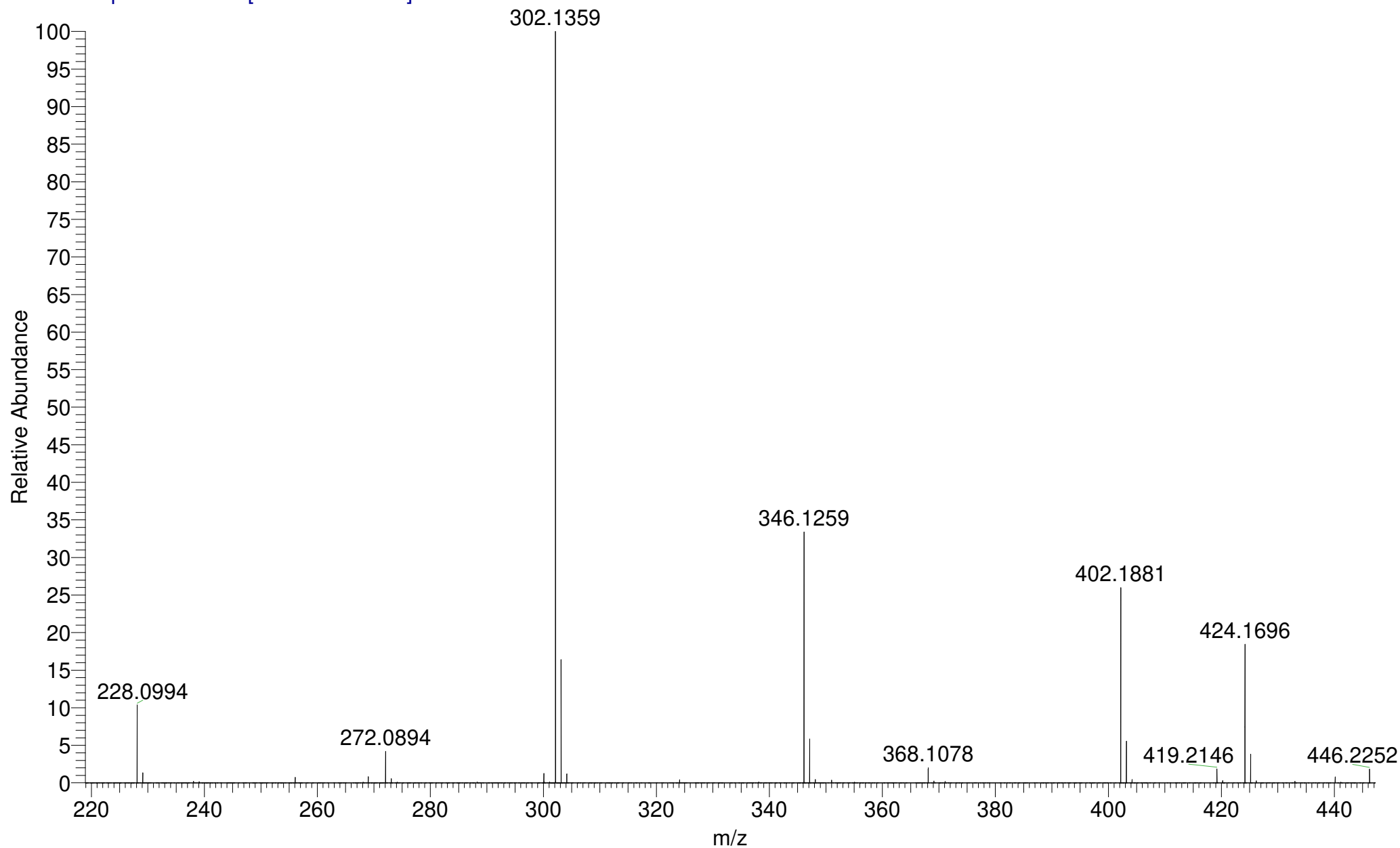
AB3-324
(DCM)/MeOH + NH₄OAc
C₂₀H₂₆F₃NO₄

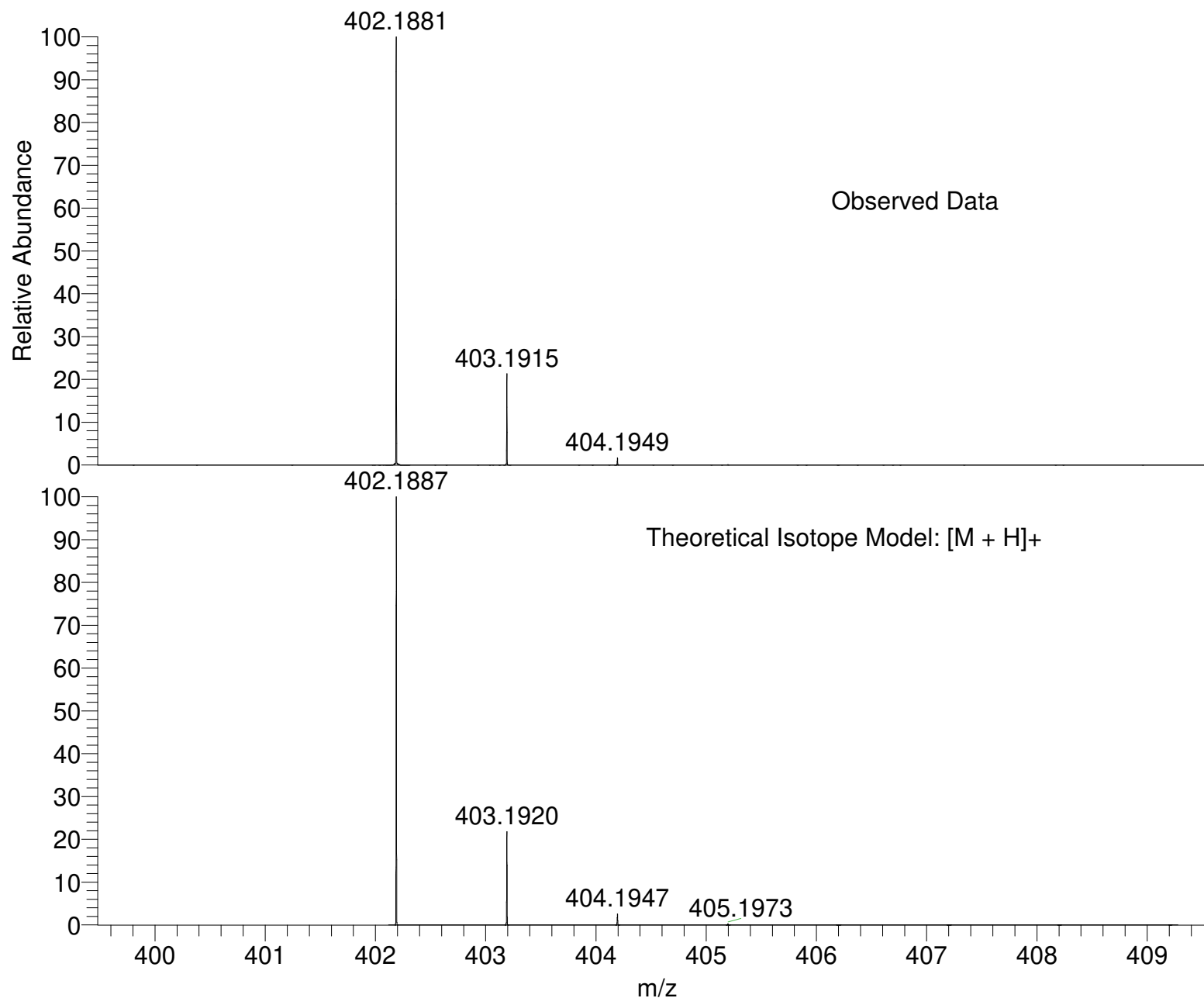
EPSRC National Facility Swansea
LTQ Orbitrap XL

IMPBUL-AJB
22/02/2018 17:21:39

IMPBUL_CNURC_42211 #13-19 RT: 0.15-0.50 AV: 7 SM: 7G NL: 5.87E7

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





NL:
1.53E7
IMPBUL_CNURC_42211#13-
19 RT: 0.15-0.50 AV: 7 T:
FTMS + p NSI Full ms
[120.00-1935.00]

NL:
1.86E4
C₂₀H₂₆F₃NO₄H:
C₂₀H₂₇F₃N₁O₄
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....10
 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
402.1881	402.1880	0.2	-2.0	C ₉ H ₂₈ O ₉ N ₆ F ₂
	402.1880	0.2	3.5	C ₈ H ₂₂ O ₄ N ₁₃ F ₂
	402.1882	-0.3	7.0	C ₁₃ H ₂₃ O ₄ N ₁₀ F ₁
	402.1882	-0.3	1.5	C ₁₄ H ₂₉ O ₉ N ₃ F ₁
	402.1883	-0.4	-0.5	C ₁₀ H ₂₅ O ₄ N ₇ F ₅
	402.1884	-0.8	10.5	C ₁₈ H ₂₄ O ₄ N ₇
	402.1884	-0.8	5.0	C ₁₉ H ₃₀ O ₉
	402.1885	-0.9	3.0	C ₁₅ H ₂₆ O ₄ N ₄ F ₄
	402.1876	1.3	-1.5	C ₂ H ₂₄ O ₉ N ₁₅
	402.1887	-1.4	6.5	C ₂₀ H ₂₇ O ₄ N ₁ F ₃
	402.1875	1.4	10.5	C ₂₃ H ₂₆ O ₃ N ₁ F ₂
	402.1874	1.8	-0.5	C ₁₅ H ₂₇ O ₃ N ₁ F ₇
	402.1873	1.9	7.0	C ₁₈ H ₂₅ O ₃ N ₄ F ₃
	402.1889	-2.1	-2.0	C ₄ H ₂₆ O ₁₀ N ₁₂
	402.1871	2.4	-2.0	C ₁₄ H ₃₀ O ₈ F ₄
	402.1871	2.4	3.5	C ₁₃ H ₂₄ O ₃ N ₇ F ₄
	402.1871	2.5	5.5	C ₁₇ H ₂₈ O ₈ N ₃
	402.1871	2.5	11.0	C ₁₆ H ₂₂ O ₃ N ₁₀
	402.1892	-2.7	-0.5	C ₅ H ₂₃ O ₅ N ₁₃ F ₃
	402.1869	2.9	0.0	C ₈ H ₂₃ O ₃ N ₁₀ F ₅
	402.1869	3.0	2.0	C ₁₂ H ₂₇ O ₈ N ₆ F ₁
	402.1869	3.0	7.5	C ₁₁ H ₂₁ O ₃ N ₁₃ F ₁
	402.1894	-3.2	3.0	C ₁₀ H ₂₄ O ₅ N ₁₀ F ₂
	402.1894	-3.2	-2.5	C ₁₁ H ₃₀ O ₁₀ N ₃ F ₂
	402.1894	-3.3	1.0	C ₆ H ₂₀ N ₁₄ F ₆
	402.1867	3.5	-1.5	C ₇ H ₂₆ O ₈ N ₉ F ₂
	402.1896	-3.6	12.0	C ₁₄ H ₁₉ N ₁₄ F ₁
	402.1896	-3.7	6.5	C ₁₅ H ₂₅ O ₅ N ₇ F ₁
	402.1896	-3.7	1.0	C ₁₆ H ₃₁ O ₁₀ F ₁
	402.1896	-3.7	4.5	C ₁₁ H ₂₁ N ₁₁ F ₅
	402.1896	-3.8	-1.0	C ₁₂ H ₂₇ O ₅ N ₄ F ₅

Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
	402.1896	-3.8	-3.0	C ₈ H ₂₃ N ₈ F ₉
	402.1898	-4.1	15.5	C ₁₉ H ₂₀ N ₁₁
	402.1898	-4.2	10.0	C ₂₀ H ₂₆ O ₅ N ₄
	402.1898	-4.2	8.0	C ₁₆ H ₂₂ N ₈ F ₄
	402.1898	-4.3	2.5	C ₁₇ H ₂₈ O ₅ N ₁ F ₄
	402.1864	4.3	14.5	C ₂₆ H ₂₅ O ₂ N ₁ F ₁
	402.1898	-4.3	0.5	C ₁₃ H ₂₄ N ₅ F ₈
	402.1862	4.7	3.5	C ₁₈ H ₂₆ O ₂ N ₁ F ₆
	402.1900	-4.7	11.5	C ₂₁ H ₂₃ N ₅ F ₃
	402.1862	4.8	11.0	C ₂₁ H ₂₄ O ₂ N ₄ F ₂
	402.1900	-4.8	4.0	C ₁₈ H ₂₅ N ₂ F ₇