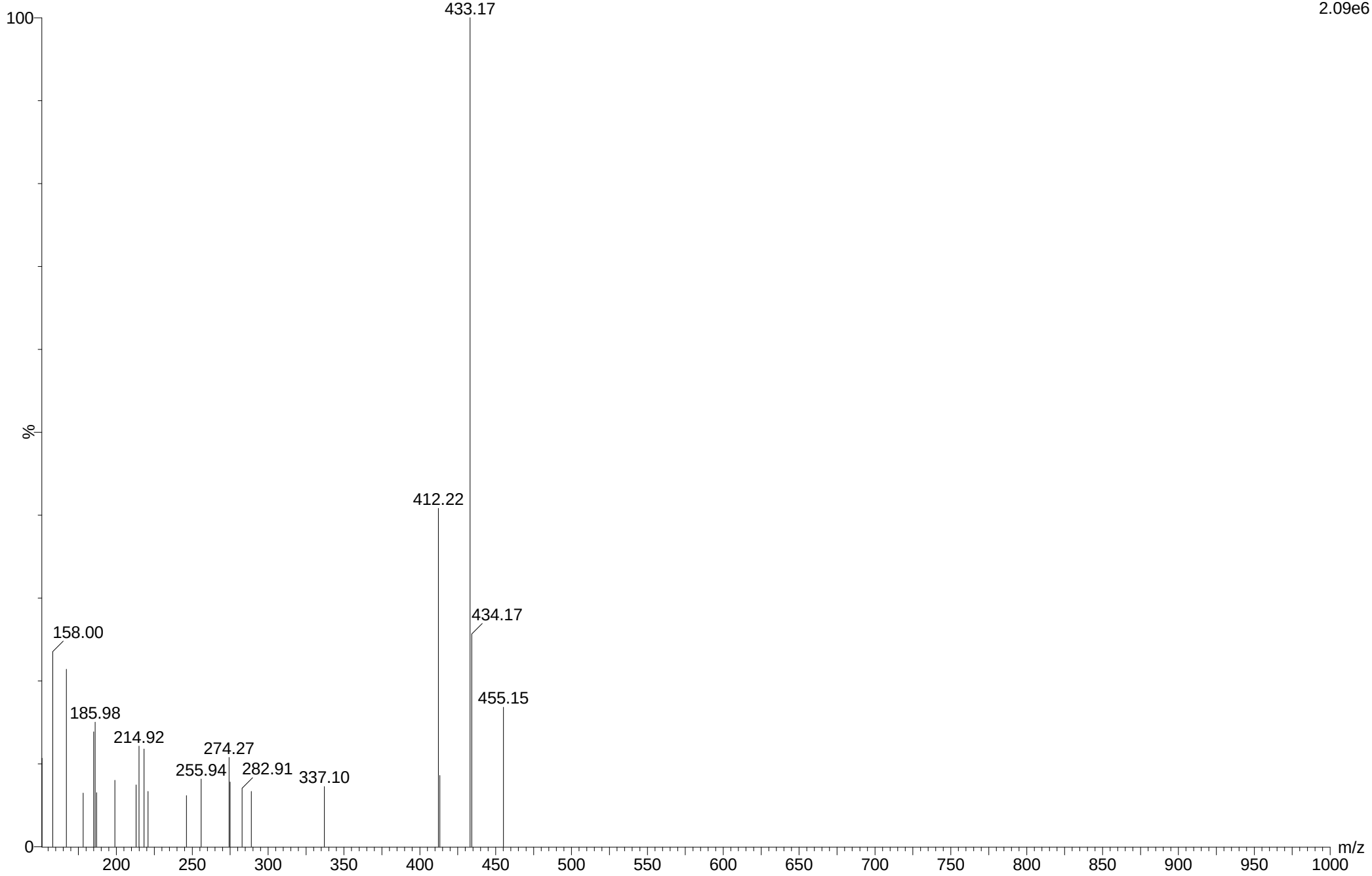
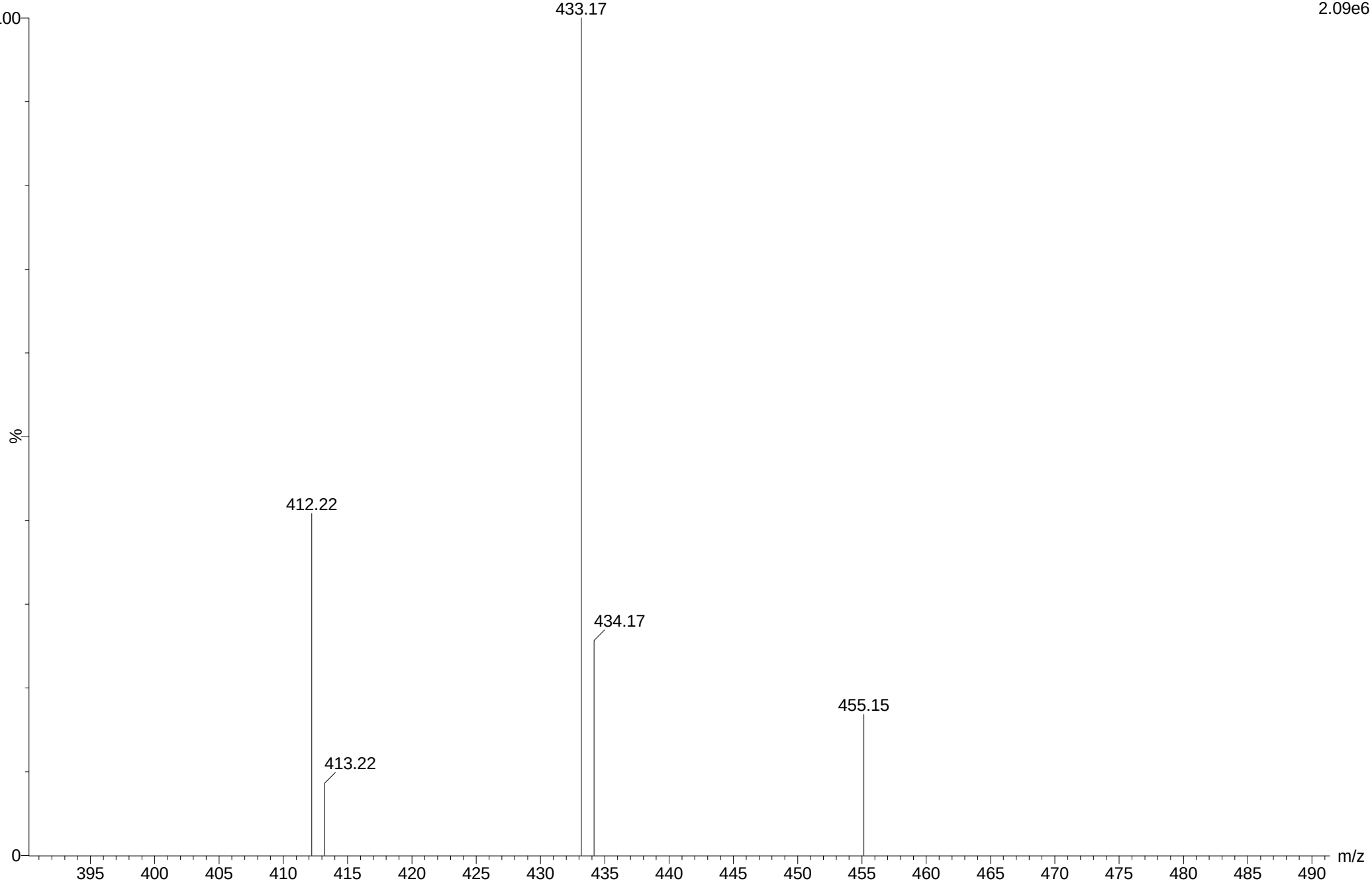
NAT384-652694 C21H22F2N4O4 MW=432
Methanol:Water
LRC-HVA-4U7HL-ESI-Pos-1 13 (0.774) AM2 (Ar,27500.0,0.00,0.00); ABS; Cm (9:19-(4+55))

University of Birmingham, School of Chemistry
Waters Xevo G2-XS

Holly Adcock
16-Apr-2021 18:16:24
2: TOF MS ES+
2.09e6



NAT384-652694 C21H22F2N4O4 MW=432 University of Birmingham, School of Chemistry Holly Adcock
Methanol:Water Waters Xevo G2-XS 16-Apr-2021 18:16:24
LRC-HVA-4U7HL-ESI-Pos-1 13 (0.774) AM2 (Ar,27500.0,0.00,0.00); ABS; Cm (9:19-(4+55)) 2: TOF MS ES+
2.09e6



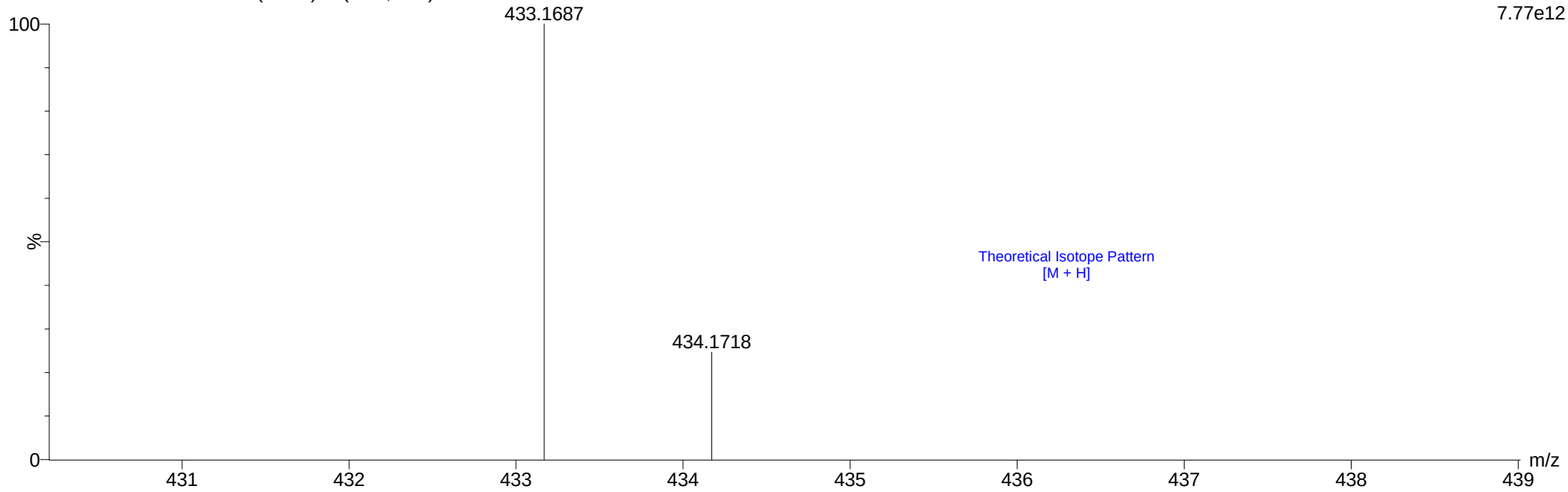
NAT384-652694 C21H22F2N4O4 MW=432
Methanol:Water

University of Birmingham, School of Chemistry
Waters Xevo G2-XS

Holly Adcock
16-Apr-2021 18:16:24

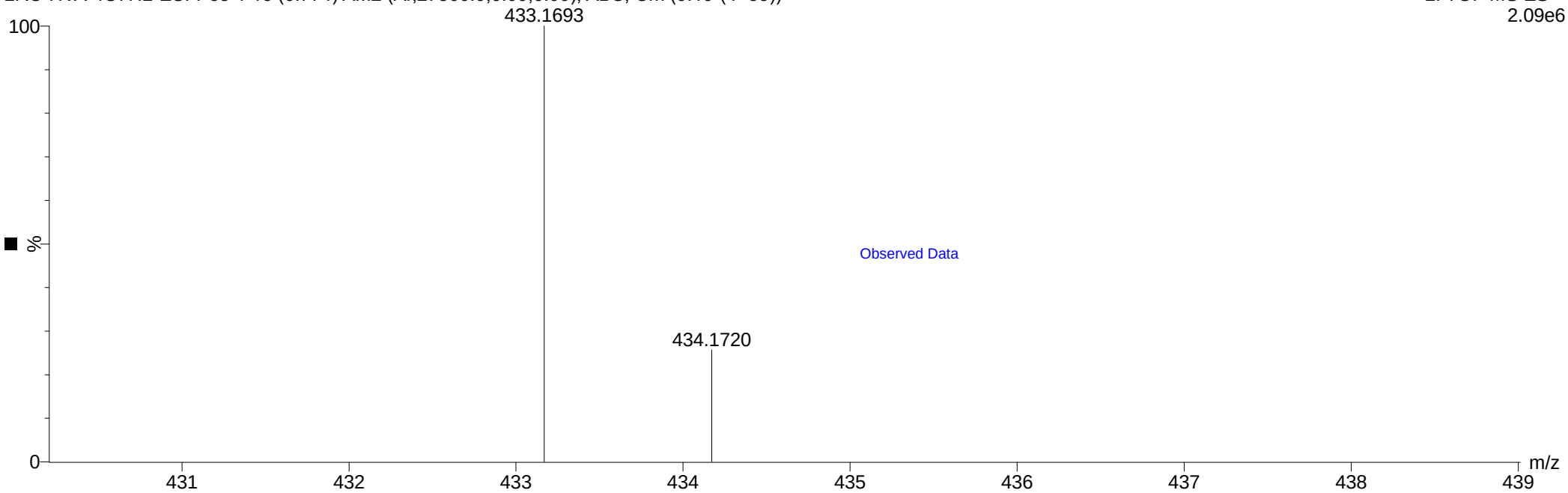
LRC-HVA-4U7HL-ESI-Pos-1 (0.290) Is (1.00,0.01) C21H22F2N4O4 H

2: TOF MS ES+
7.77e12



LRC-HVA-4U7HL-ESI-Pos-1 13 (0.774) AM2 (Ar,27500.0,0.00,0.00); ABS; Cm (9:19-(4+55))

2: TOF MS ES+
2.09e6



Single Mass Analysis

Tolerance = 3.0 PPM / DBE: min = -4.0, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
1521 formula(e) evaluated with 6 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 1-40 H: 0-60 N: 0-10 O: 0-10 F: 2-4

Minimum:				-4.0				
Maximum:		3.0	3.0	100.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
433.1693	433.1697	-0.4	-0.9	-1.5	43.6	2.356	9.48	C14 H29 O10 F4
	433.1699	-0.6	-1.4	7.5	42.9	1.608	20.02	C18 H24 N4 O5 F3
	433.1687	0.6	1.4	11.5	42.4	1.202	30.06	C21 H23 N4 O4 F2
	433.1685	0.8	1.8	2.5	43.1	1.835	15.97	C17 H28 O9 F3
	433.1701	-0.8	-1.8	16.5	42.9	1.648	19.25	C22 H19 N8 F2
	433.1683	1.0	2.3	4.5	44.2	2.952	5.22	C11 H21 N10 O4 F4