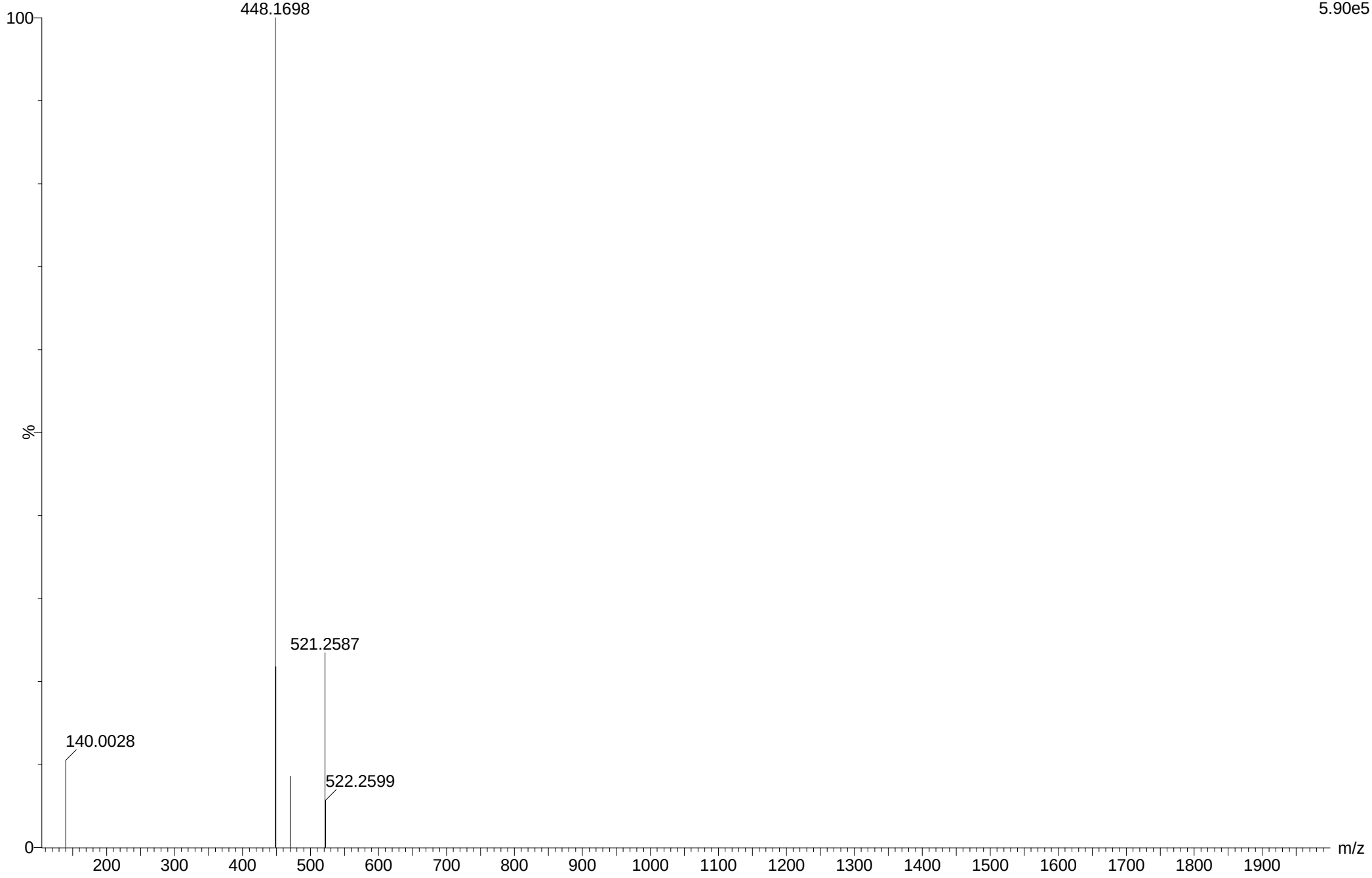
LNB0367-059-P C22H23F2N3O5 MW=447 University of Birmingham, School of Chemistry Daniel Kovari
Methanol Waters Xevo G2-XS 11-Dec-2020 19:22:14
LRC-DXK-3TXCJ-ESI-Pos-1 14 (1.018) AM2 (Ar,30000.0,0.00,0.00); ABS; Cm (14) 1: TOF MS ES+
5.90e5

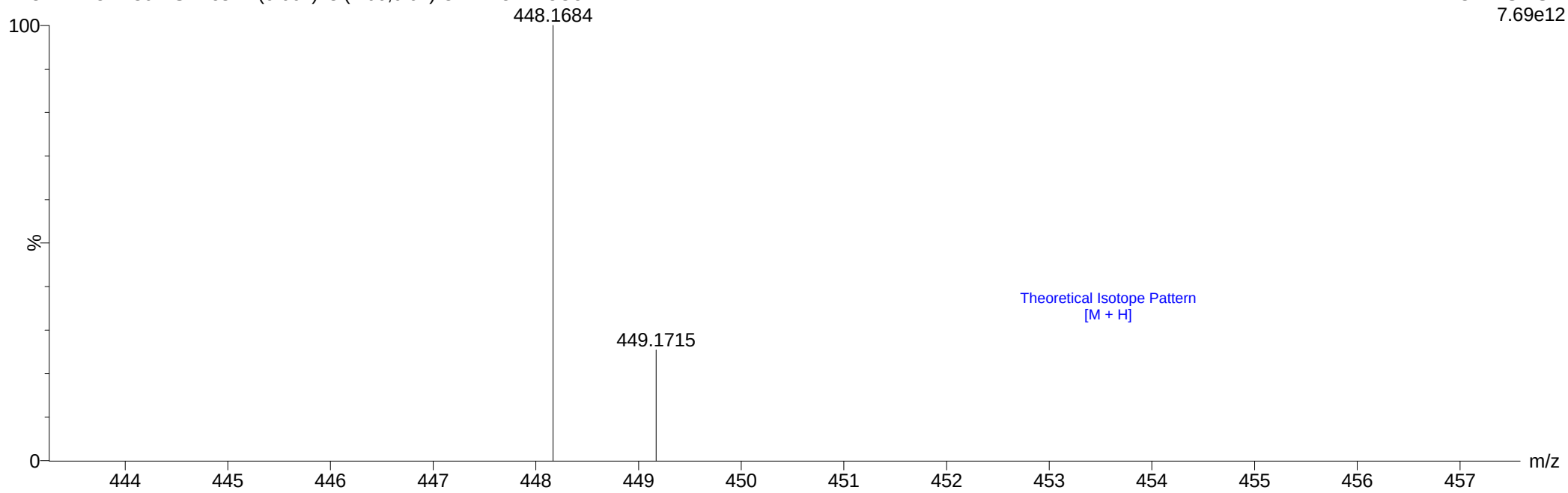


LNB0367-059-P C22H23F2N3O5 MW=447 University of Birmingham, School of Chemistry Daniel Kovari
Methanol Waters Xevo G2-XS 11-Dec-2020 19:22:14
LRC-DXK-3TXCJ-ESI-Pos-1 14 (1.018) AM2 (Ar,30000.0,0.00,0.00); ABS; Cm (14) 1: TOF MS ES+
5.90e5

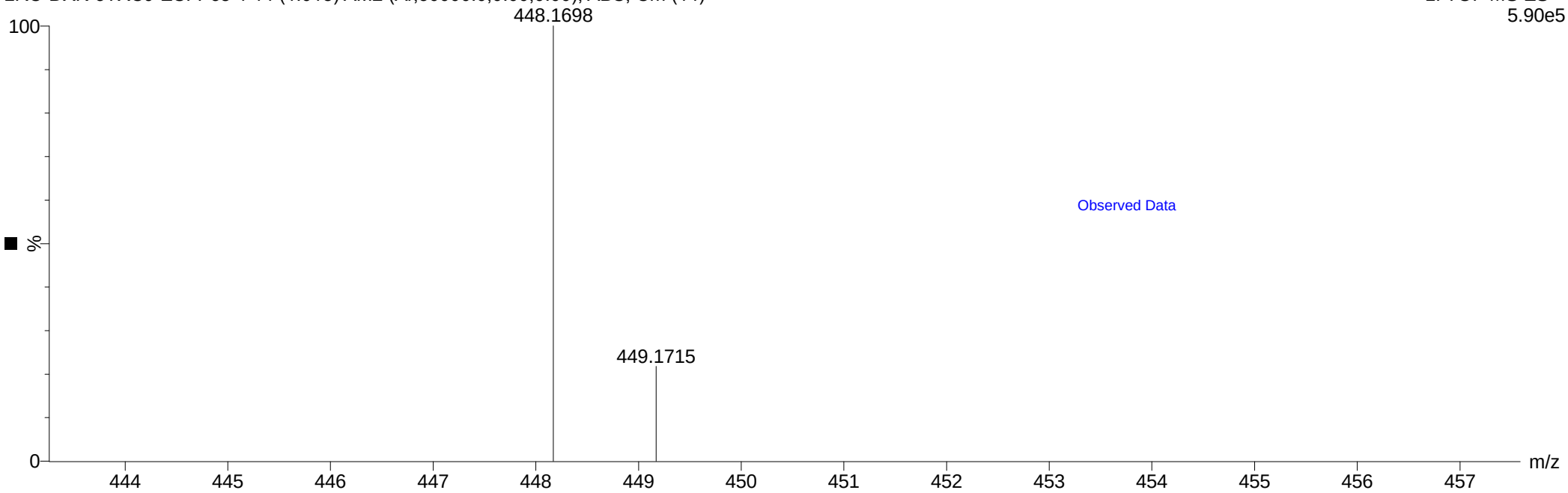


LNB0367-059-P C22H23F2N3O5 MW=447 University of Birmingham, School of Chemistry Daniel Kovari
Methanol Waters Xevo G2-XS 11-Dec-2020 19:22:14

LRC-DXK-3TXCJ-ESI-Pos-1 (0.062) Is (1.00,0.01) C22H23F2N3O5 H
1: TOF MS ES+
7.69e12



LRC-DXK-3TXCJ-ESI-Pos-1 14 (1.018) AM2 (Ar,30000.0,0.00,0.00); ABS; Cm (14)
1: TOF MS ES+
5.90e5



Single Mass Analysis

Tolerance = 4.0 PPM / DBE: min = -10.0, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 4

Monoisotopic Mass, Even Electron Ions
1856 formula(e) evaluated with 8 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-50 H: 0-60 N: 0-10 O: 0-10 F: 0-2

Minimum:				-10.0				
Maximum:		5.0	4.0	100.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
448.1698	448.1697	0.1	0.2	16.5	46.9	1.988	13.69	C23 H20 N7 O F2
	448.1701	-0.3	-0.7	23.5	48.7	3.804	2.23	C33 H22 N O
	448.1693	0.5	1.1	11.5	45.9	0.974	37.76	C17 H22 N9 O6
	448.1704	-0.6	-1.3	7.5	46.3	1.450	23.46	C14 H23 N9 O7 F
	448.1686	1.2	2.7	20.5	47.2	2.297	10.06	C26 H19 N7 F
	448.1684	1.4	3.1	11.5	47.7	2.807	6.04	C22 H24 N3 O5 F2
	448.1713	-1.5	-3.3	19.5	49.4	4.528	1.08	C30 H23 N O2 F
	448.1716	-1.8	-4.0	3.5	47.8	2.868	5.68	C11 H24 N9 O8 F2