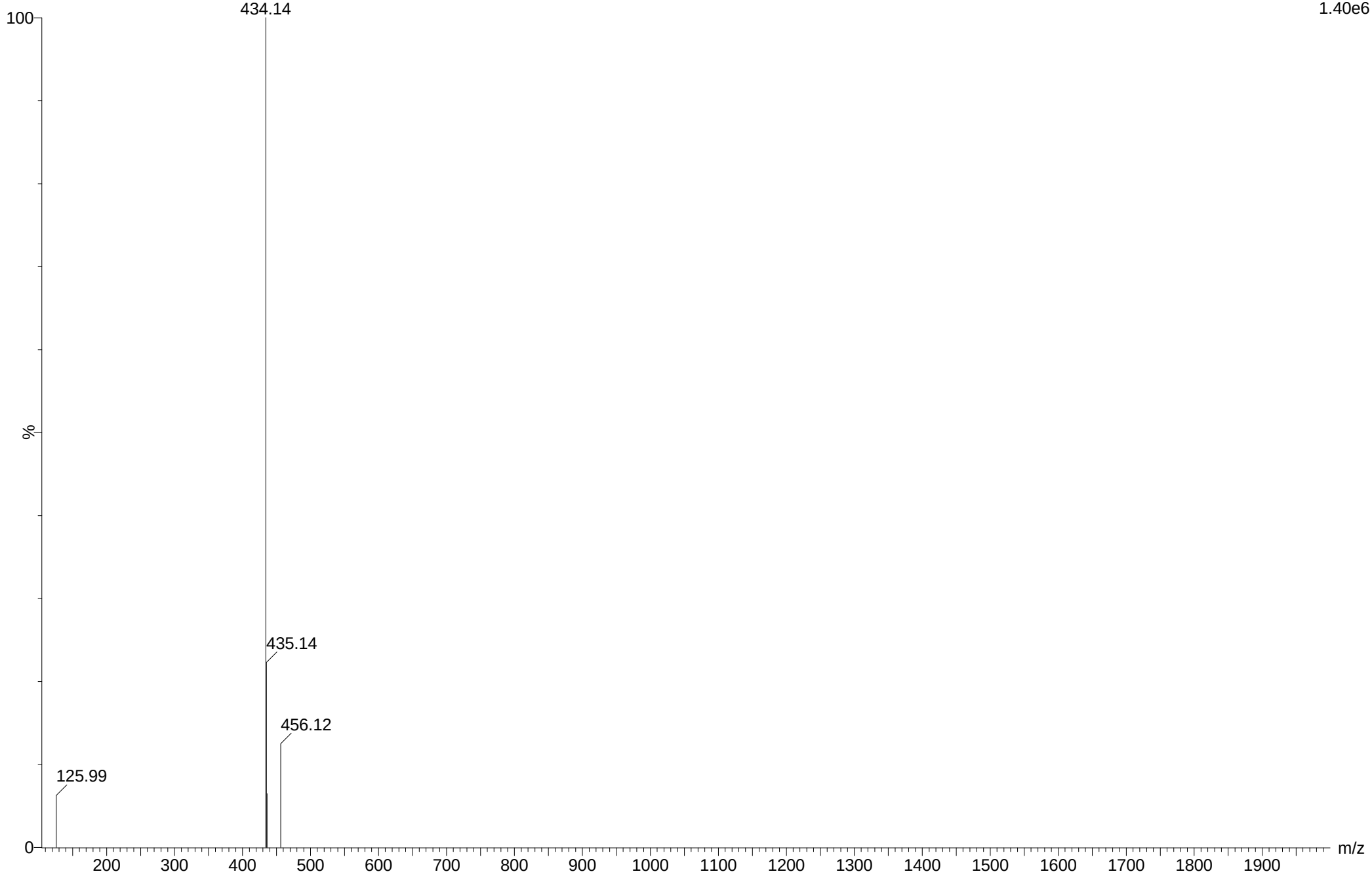
LNB0367-027-P C20H23N3O6S MW=433
Methanol

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

Daniel Kovari
11-Dec-2020 21:38:19

LRC-DXK-3UNLR-ESI-Pos-1 7 (0.492) AM2 (Ar,30000.0,0.00,0.00); ABS

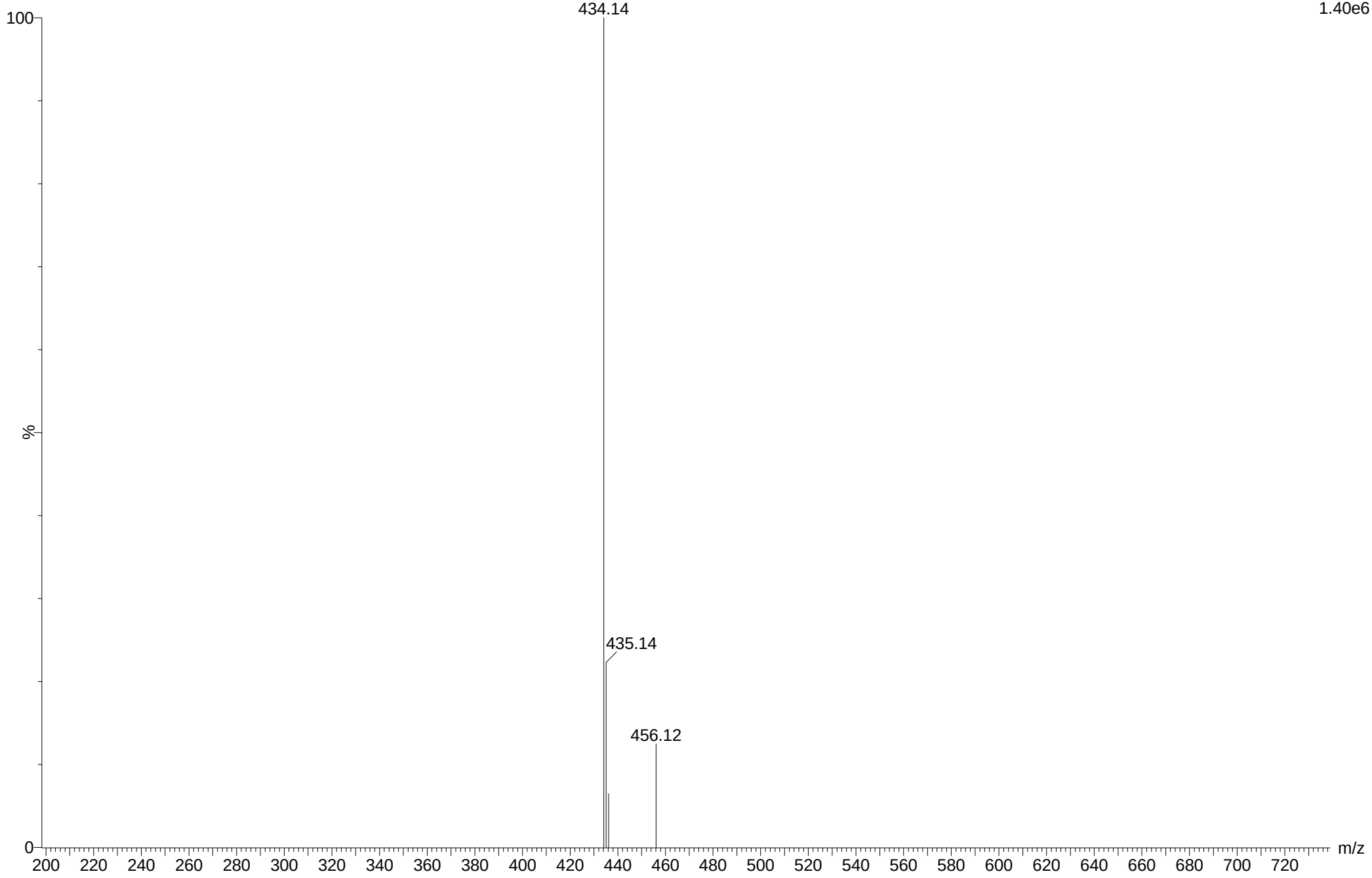
1: TOF MS ES+
1.40e6



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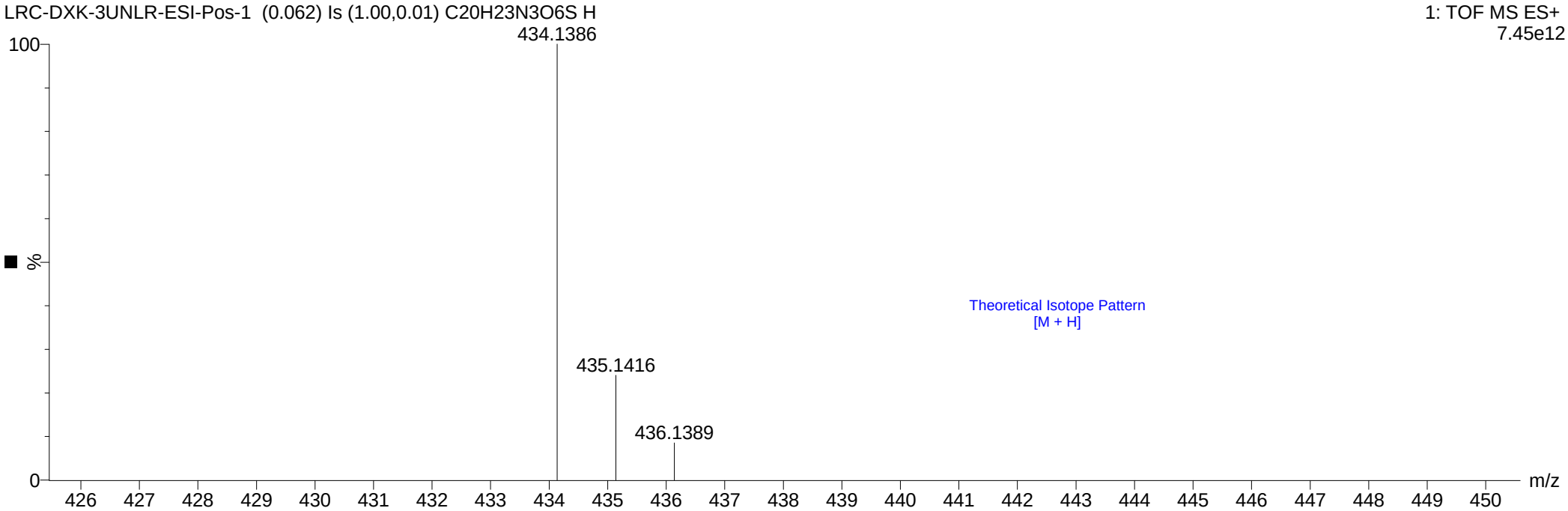
Daniel Kovari
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1: TOF MS ES+
1.40e6

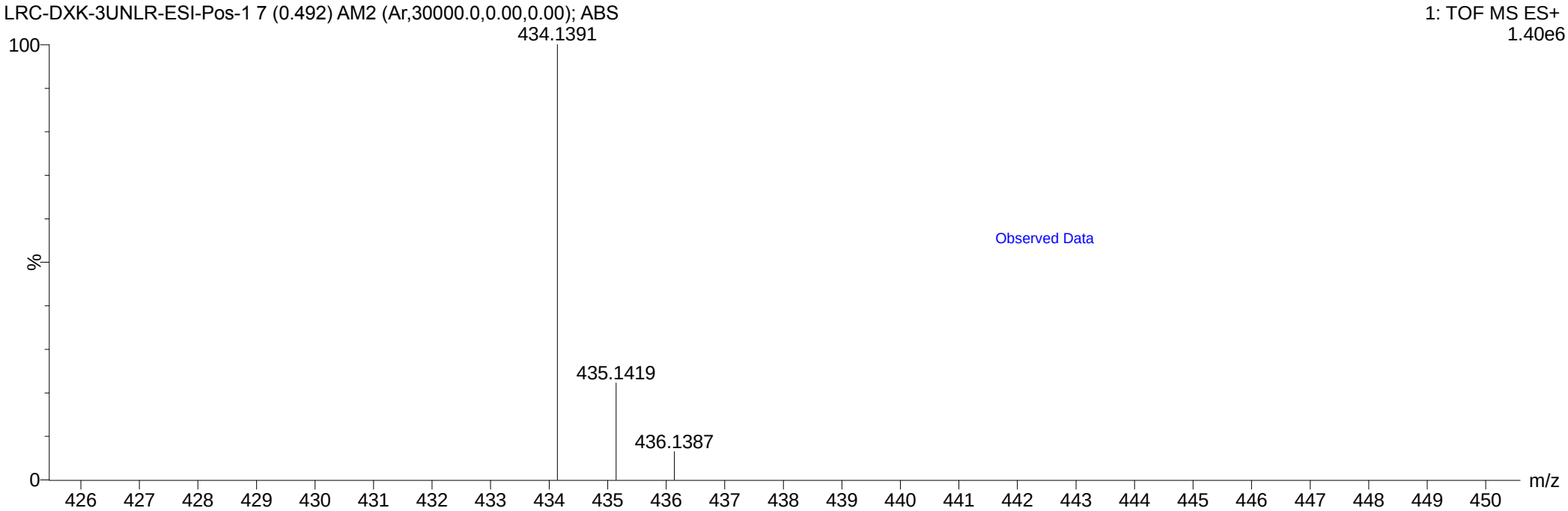


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Single Mass Analysis

Tolerance = 5.0 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
608 formula(e) evaluated with 2 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 S: 1-1

Minimum:				-10.0				
Maximum:		5.0	5.0	100.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
434.1391	434.1386	0.5	1.2	10.5	47.2	0.539	58.35	C20 H24 N3 O6 S
	434.1399	-0.8	-1.8	15.5	47.6	0.876	41.65	C21 H20 N7 O2 S