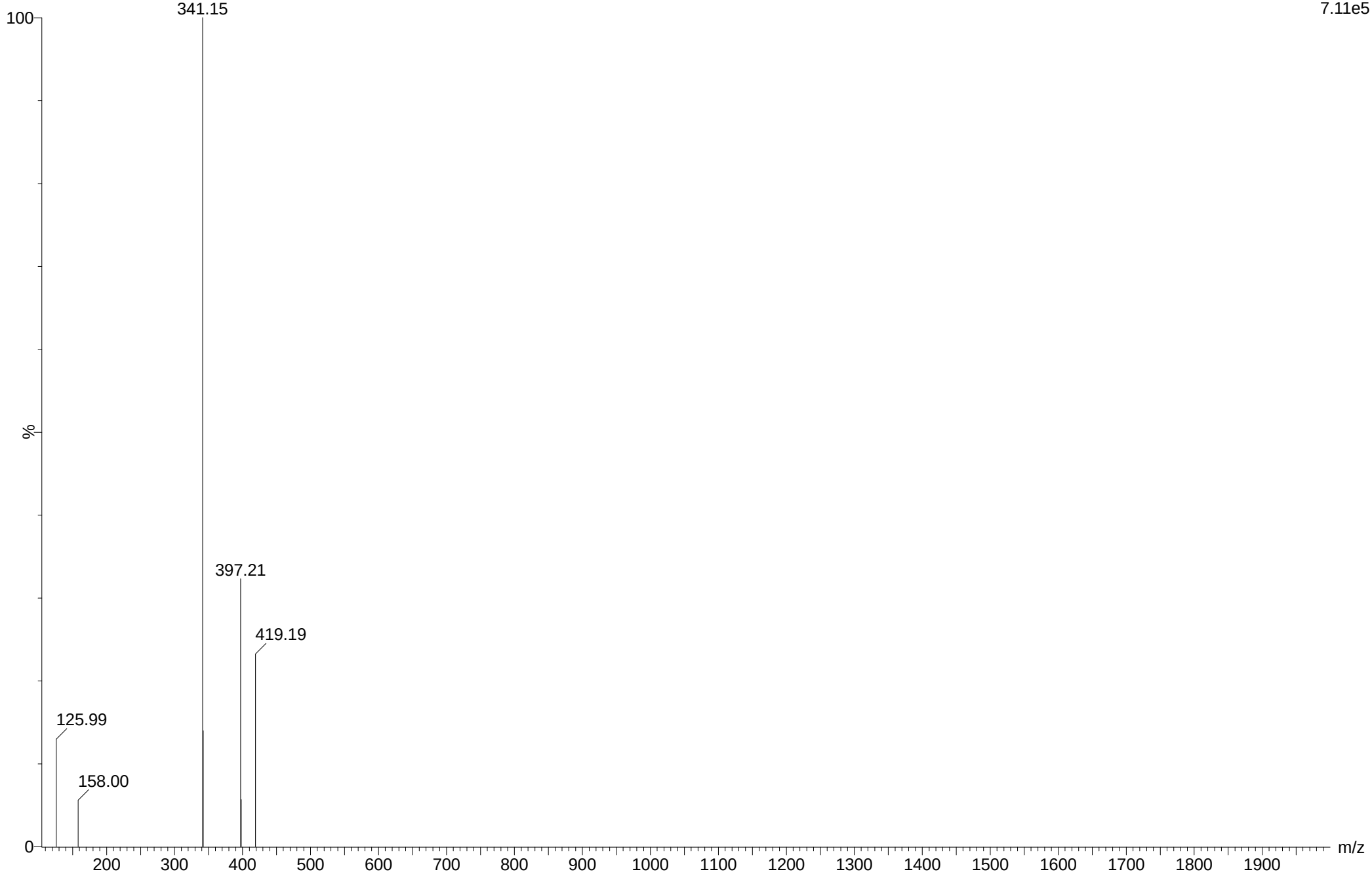
LNB0367-147-P C18H28N4O6 MW=396
Methanol

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

Daniel Kovari
11-Dec-2020 22:43:20

LRC-DXK-3UUWY-ESI-Pos-1 6 (0.615) AM2 (Ar,30000.0,0.00,0.00); ABS

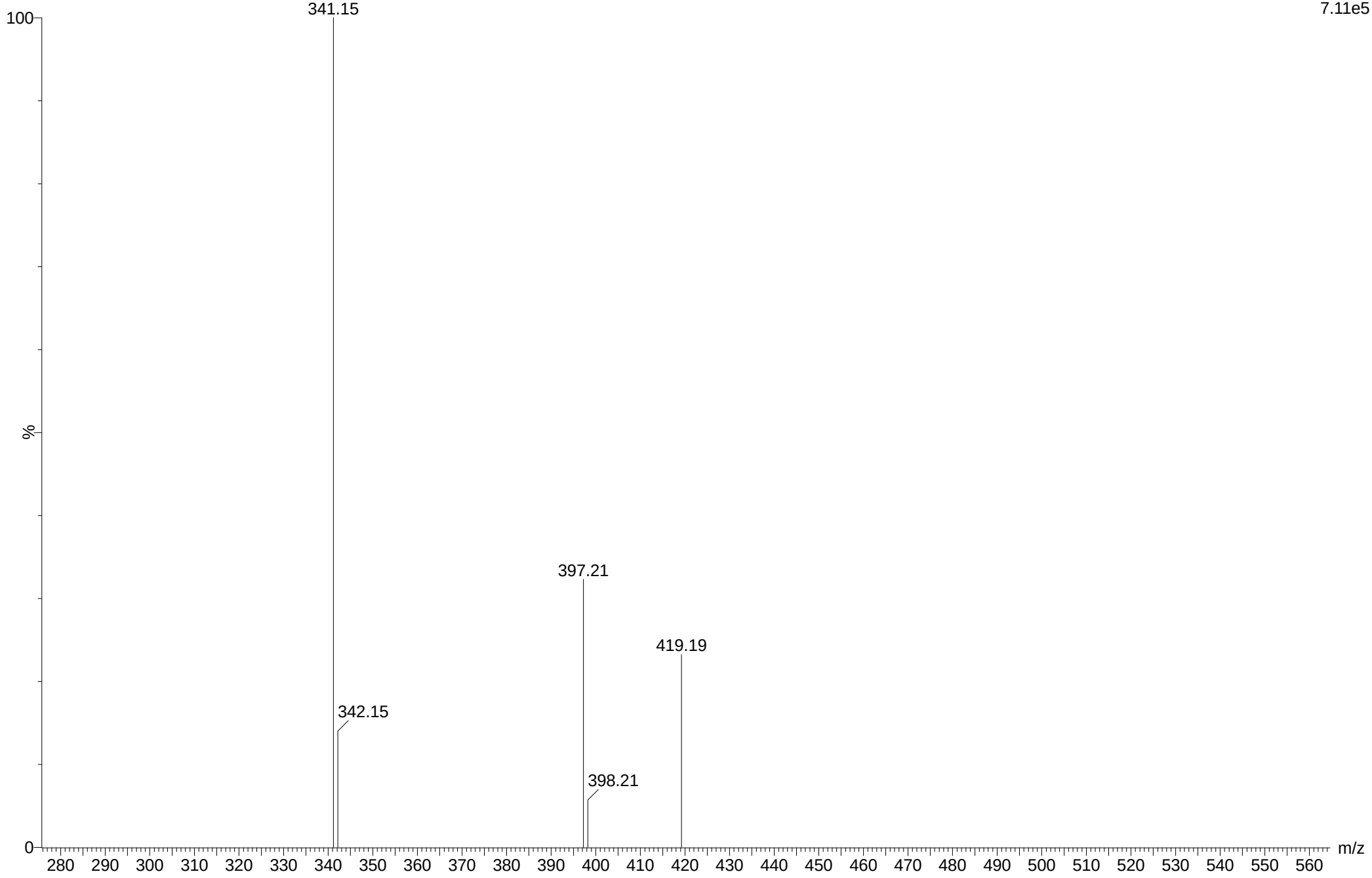
1: TOF MS ES+
7.11e5



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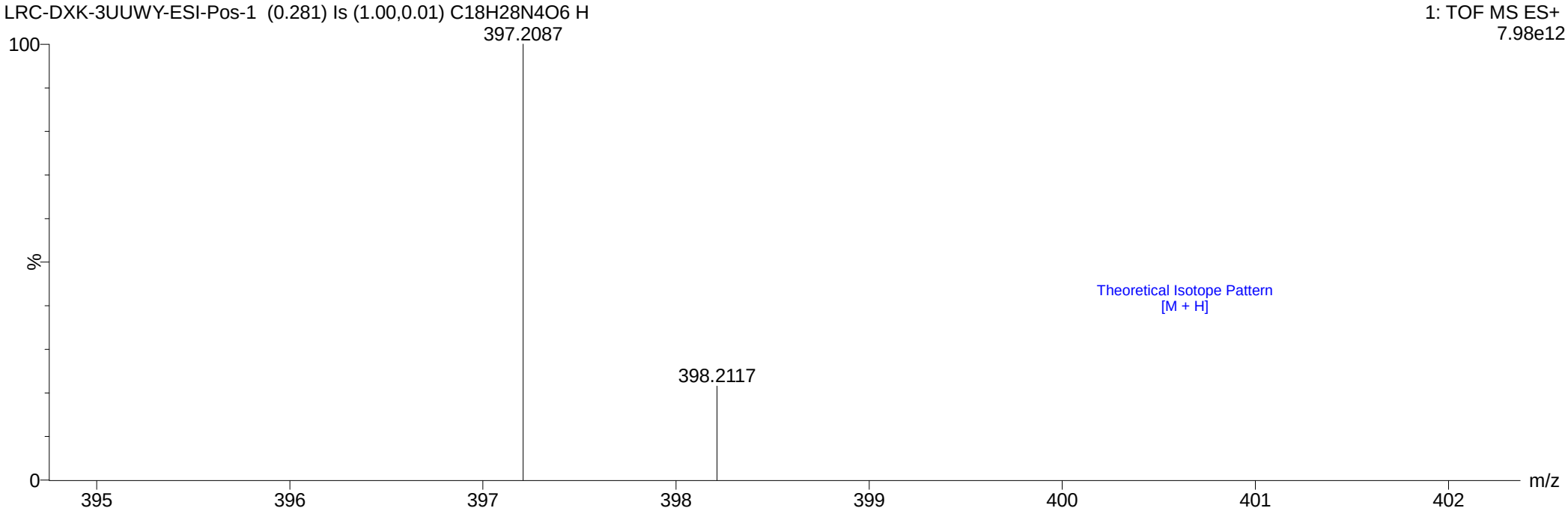
Daniel Kovari
11-Dec-2020 22:43:20
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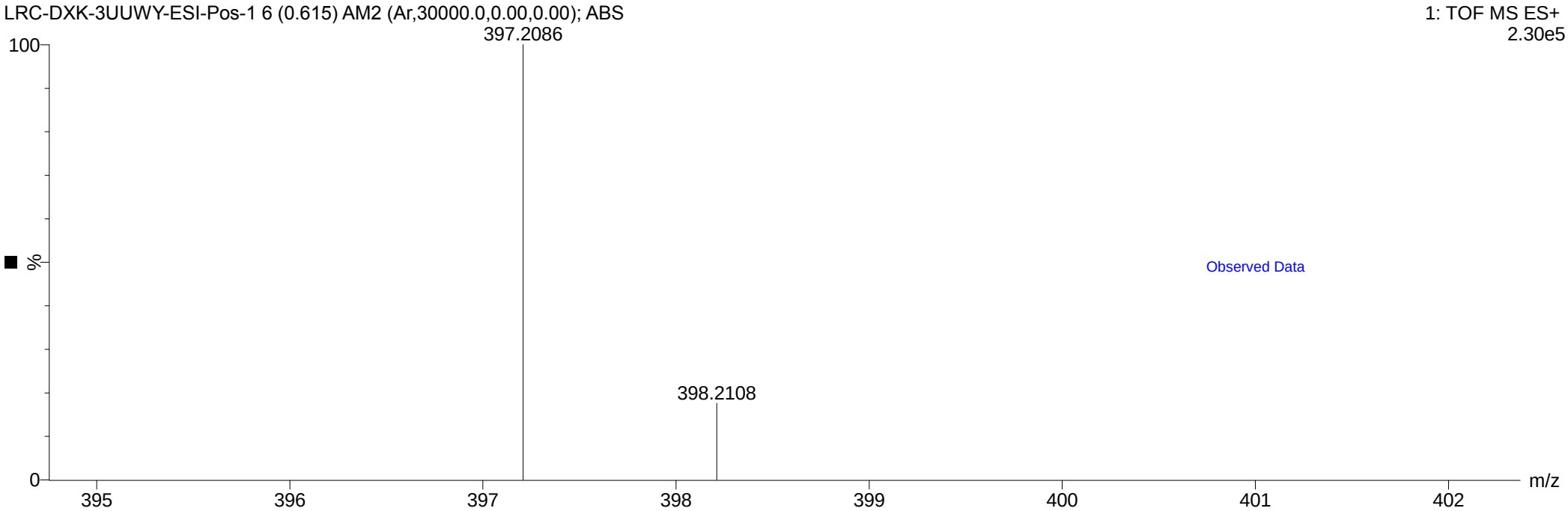


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Methanol

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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
611 formula(e) evaluated with 3 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

Minimum:				-10.0				
Maximum:		5.0	5.0	100.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
397.2086	397.2087	-0.1	-0.3	6.5	42.6	0.551	57.63	C18 H29 N4 O6
	397.2074	1.2	3.0	1.5	43.8	1.784	16.80	C17 H33 O10
	397.2100	-1.4	-3.5	11.5	43.4	1.364	25.57	C19 H25 N8 O2