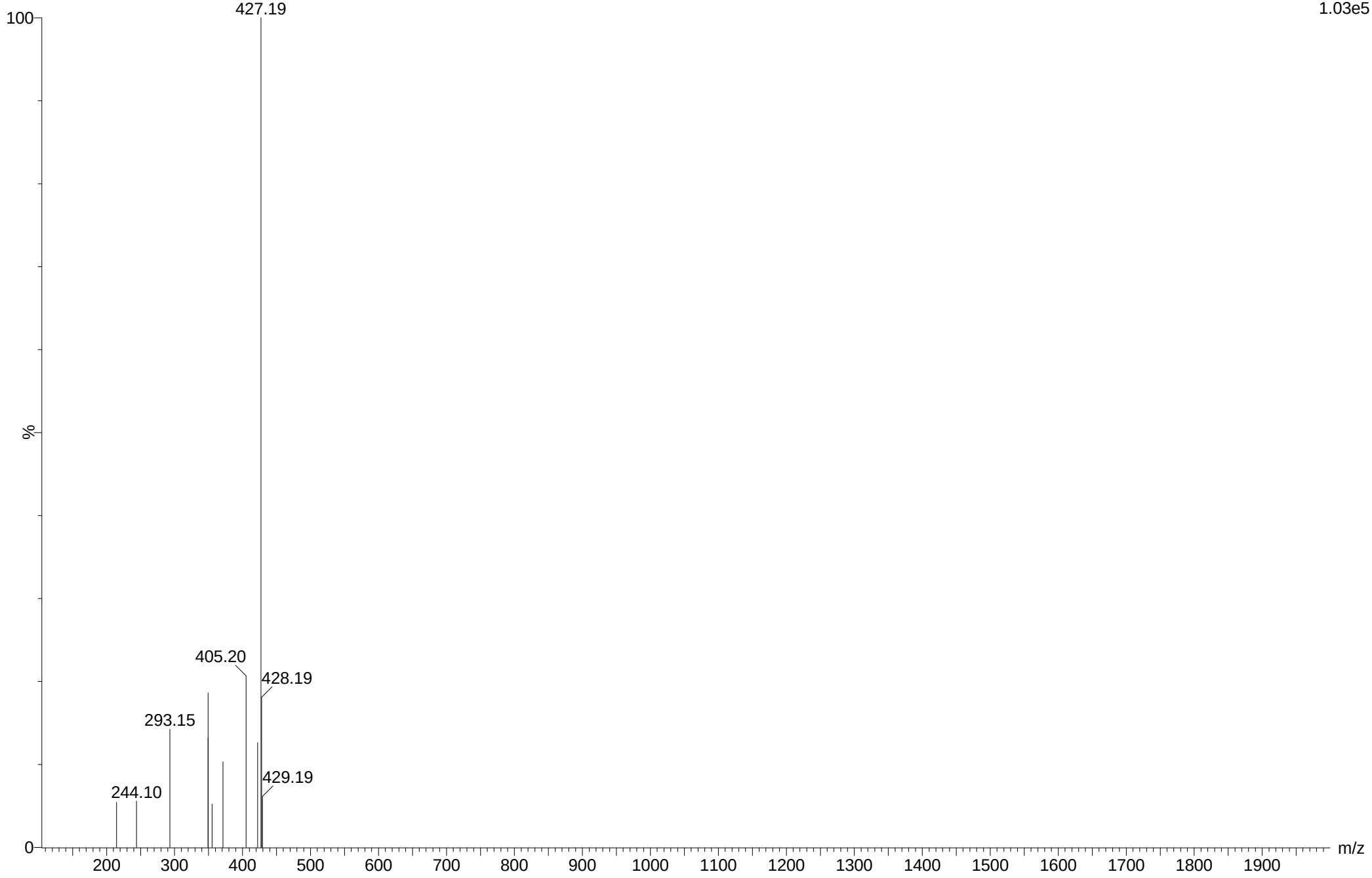
LNB0367-100-P C18H32N2O6S MW=404
Methanol

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

Daniel Kovari
11-Dec-2020 21:06:01

LRC-DXK-3U9VK-ESI-Pos-2 10 (0.707) AM2 (Ar,30000.0,0.00,0.00); ABS

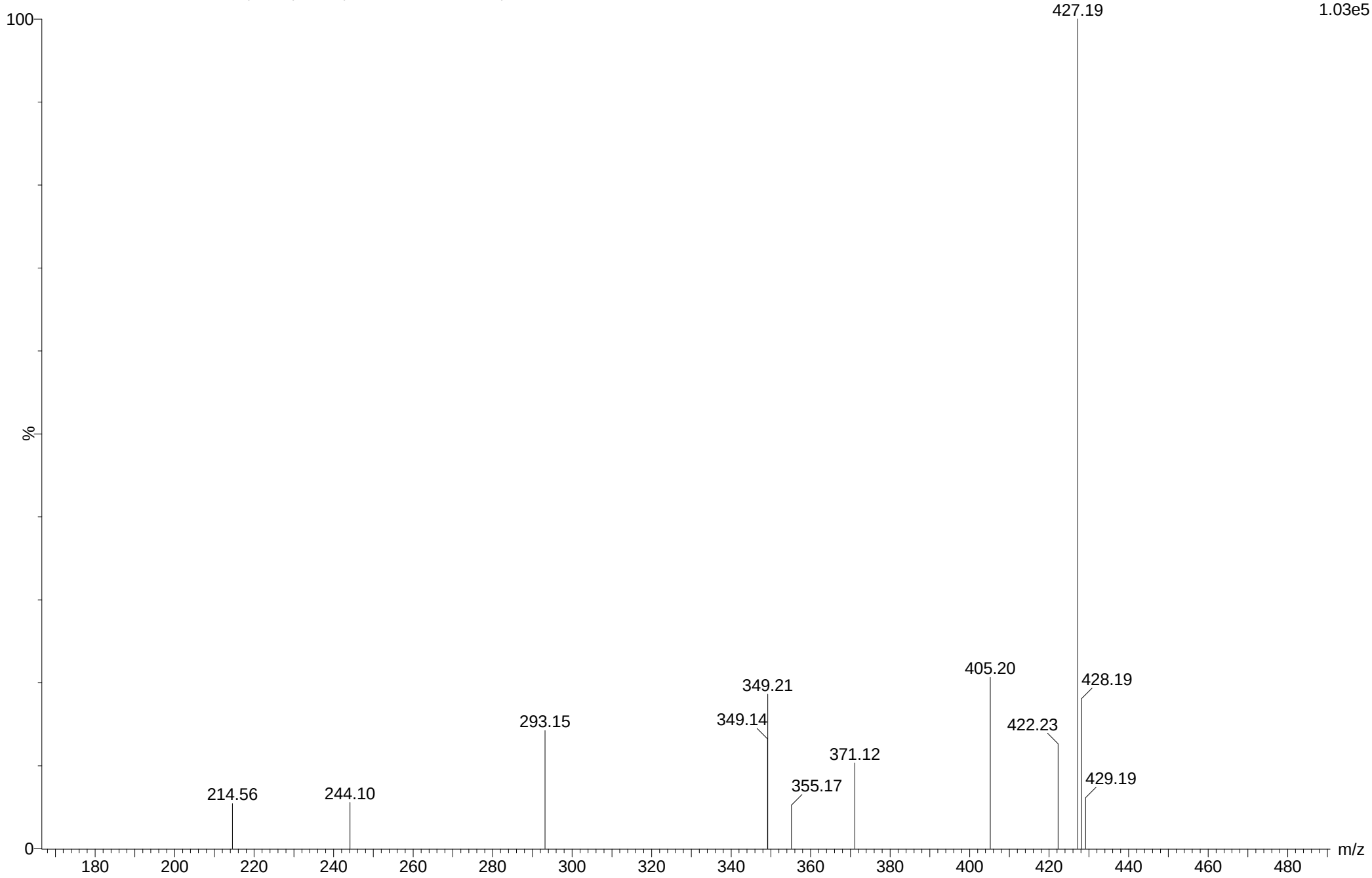
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1.03e5



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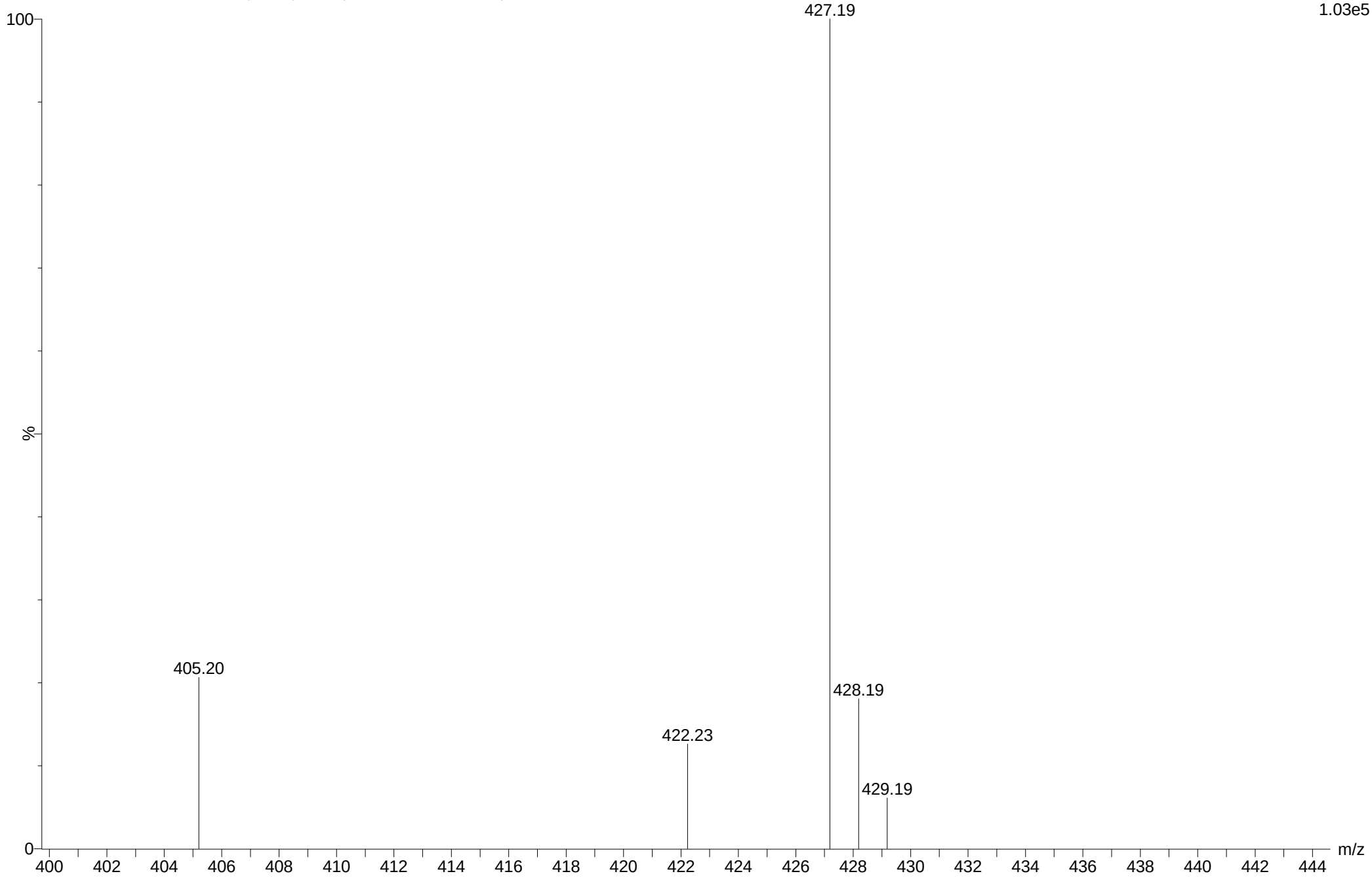
Daniel Kovari
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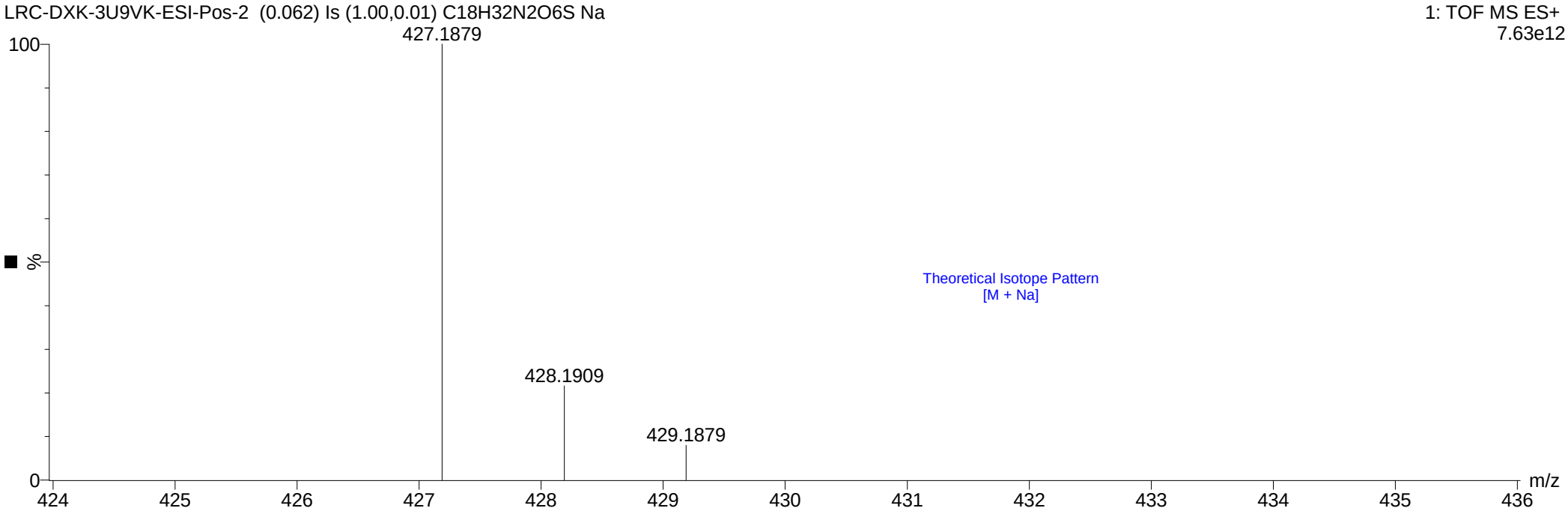
Daniel Kovari
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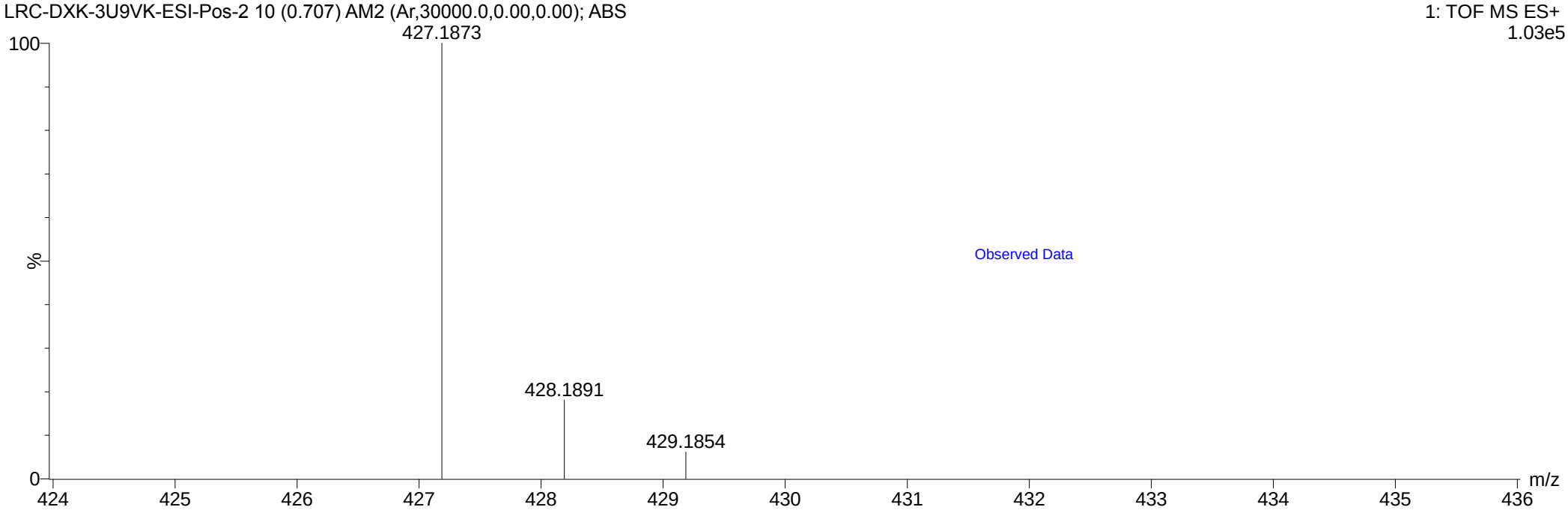


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Single Mass Analysis

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
1199 formula(e) evaluated with 5 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 Na: 0-1

Minimum:				-10.0				
Maximum:		5.0	5.0	100.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
427.1873	427.1876	-0.3	-0.7	7.5	38.0	1.000	36.80	C16 H27 N8 O4 S
	427.1879	-0.6	-1.4	3.5	40.0	2.938	5.30	C18 H32 N2 O6 S Na
	427.1863	1.0	2.3	2.5	38.6	1.606	20.06	C15 H31 N4 O8 S
	427.1892	-1.9	-4.4	8.5	40.4	3.369	3.44	C19 H28 N6 O2 S Na
	427.1852	2.1	4.9	4.5	38.1	1.067	34.40	C14 H28 N8 O4 S Na