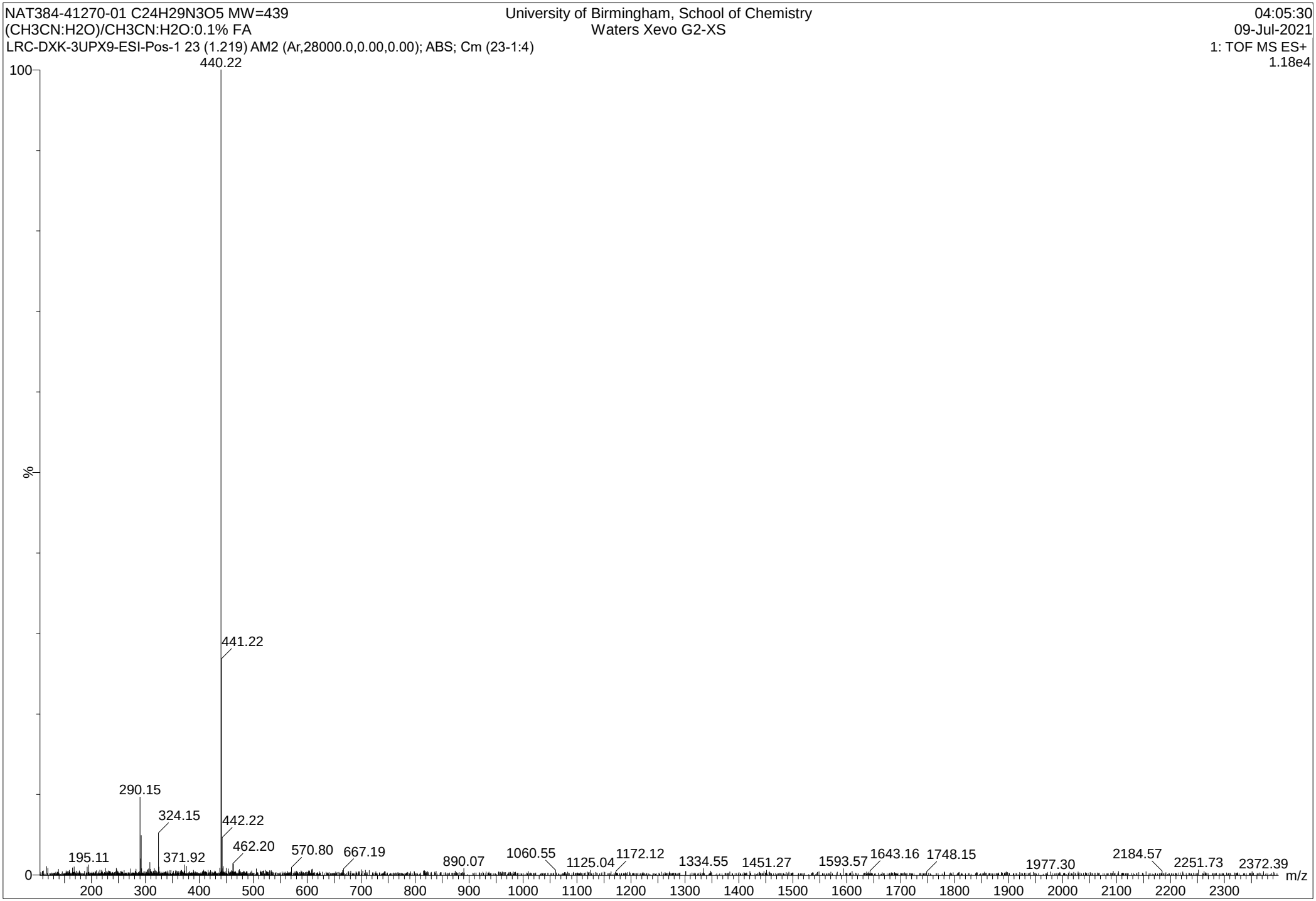
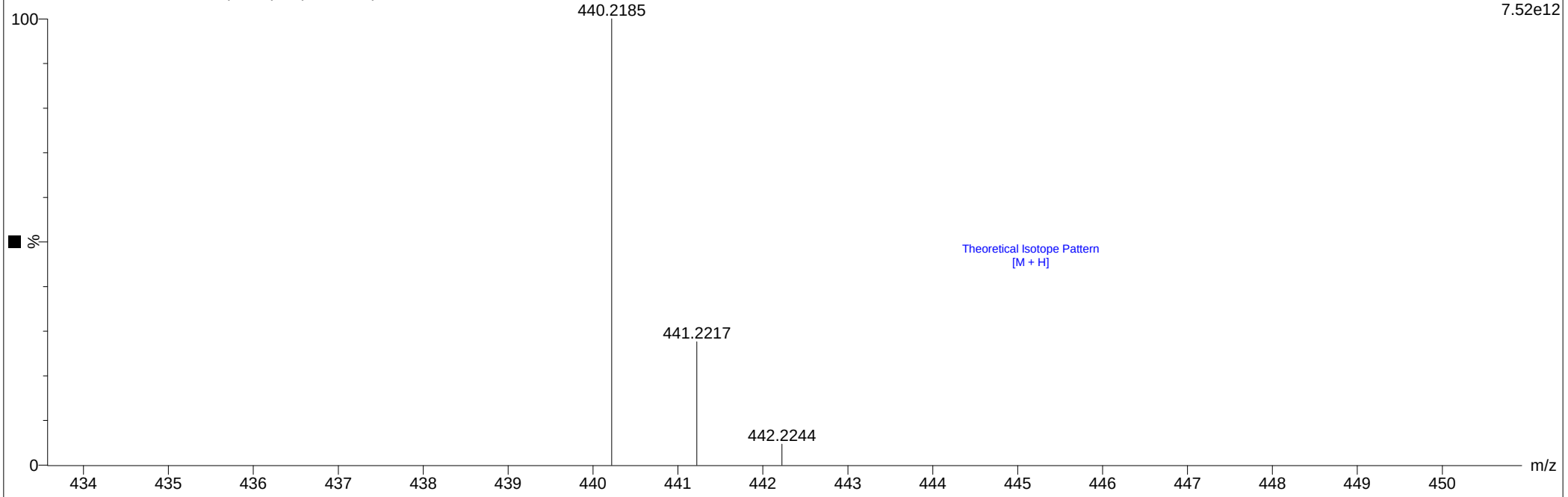

NAT384-41270-01 C24H29N3O5 MW=439
(CH3CN:H2O)/CH3CN:H2O:0.1% FA
LRC-DXK-3UPX9-ESI-Pos-1 23 (1.219) AM2 (Ar,28000.0,0.00,0.00); ABS; Cm (23-1:4)
University of Birmingham, School of Chemistry
Waters Xevo G2-XS
04:05:30
09-Jul-2021
1: TOF MS ES+
1.18e4
100
%
0
440.22
441.22
290.15
324.15
442.22
462.20
195.11
371.92
570.80
667.19
890.07
1060.55
1125.04
1172.12
1334.55
1451.27
1593.57
1643.16
1748.15
1977.30
2184.57
2251.73
2372.39
m/z
200
300
400
500
600
700
800
900
1000
1100
1200
1300
1400
1500
1600
1700
1800
1900
2000
2100
2200
2300

NAT384-41270-01 C24H29N3O5 MW=439
(CH3CN:H2O)/CH3CN:H2O:0.1% FA
LRC-DXK-3UPX9-ESI-Pos-1 (0.062) Is (1.00,1.00) C24H29N3O5 H

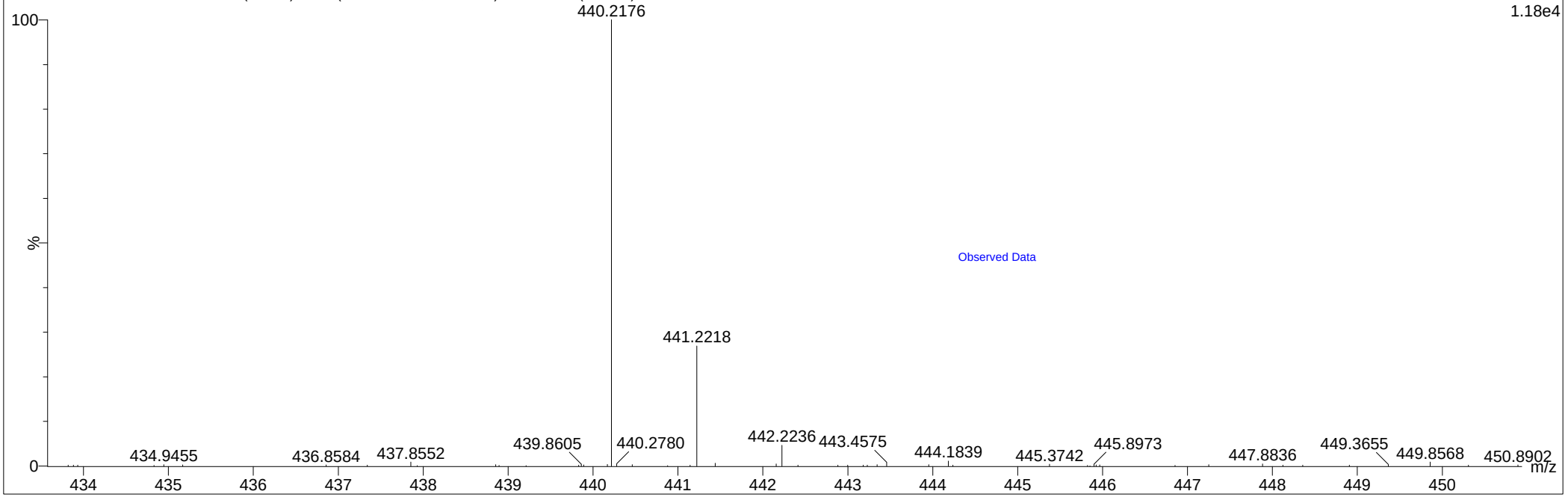
University of Birmingham, School of Chemistry
Waters Xevo G2-XS

04:05:30
09-Jul-2021
1: TOF MS ES+
7.52e12



LRC-DXK-3UPX9-ESI-Pos-1 23 (1.219) AM2 (Ar,28000.0,0.00,0.00); ABS; Cm (23-1:4)

1: TOF MS ES+
1.18e4



Single Mass Analysis

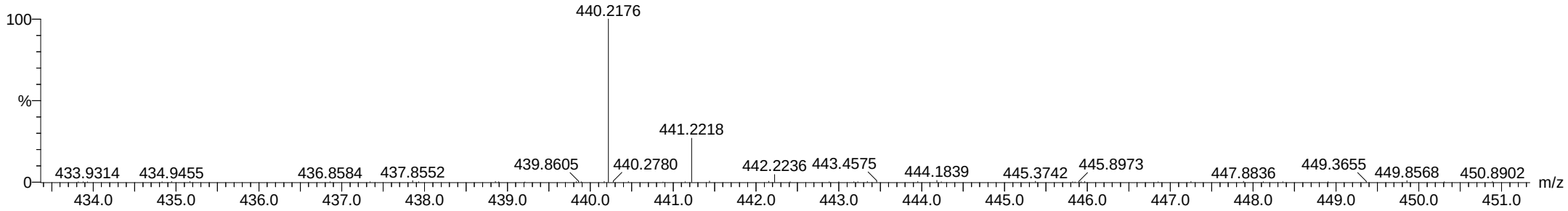
Tolerance = 3.0 PPM / DBE: min = -4.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
1290 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-60 H: 0-100 N: 0-15 O: 0-20

NAT384-41270-01 C24H29N3O5 MW=439
(CH3CN:H2O)/CH3CN:H2O:0.1% FA
LRC-DXK-3UPX9-ESI-Pos-1 23 (1.219) AM2 (Ar,28000.0,0.00,0.00); ABS; Cm (23-1:4)

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

04:05:30
09-Jul-2021
1: TOF MS ES+
1.18e+004



Minimum:				-4.5				
Maximum:		5.0	3.0	100.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
440.2176	440.2177	-0.1	-0.2	-0.5	68.9	14.304	0.00	C8 H30 N11 O10
	440.2185	-0.9	-2.0	11.5	54.6	0.000	100.00	C24 H30 N3 O5