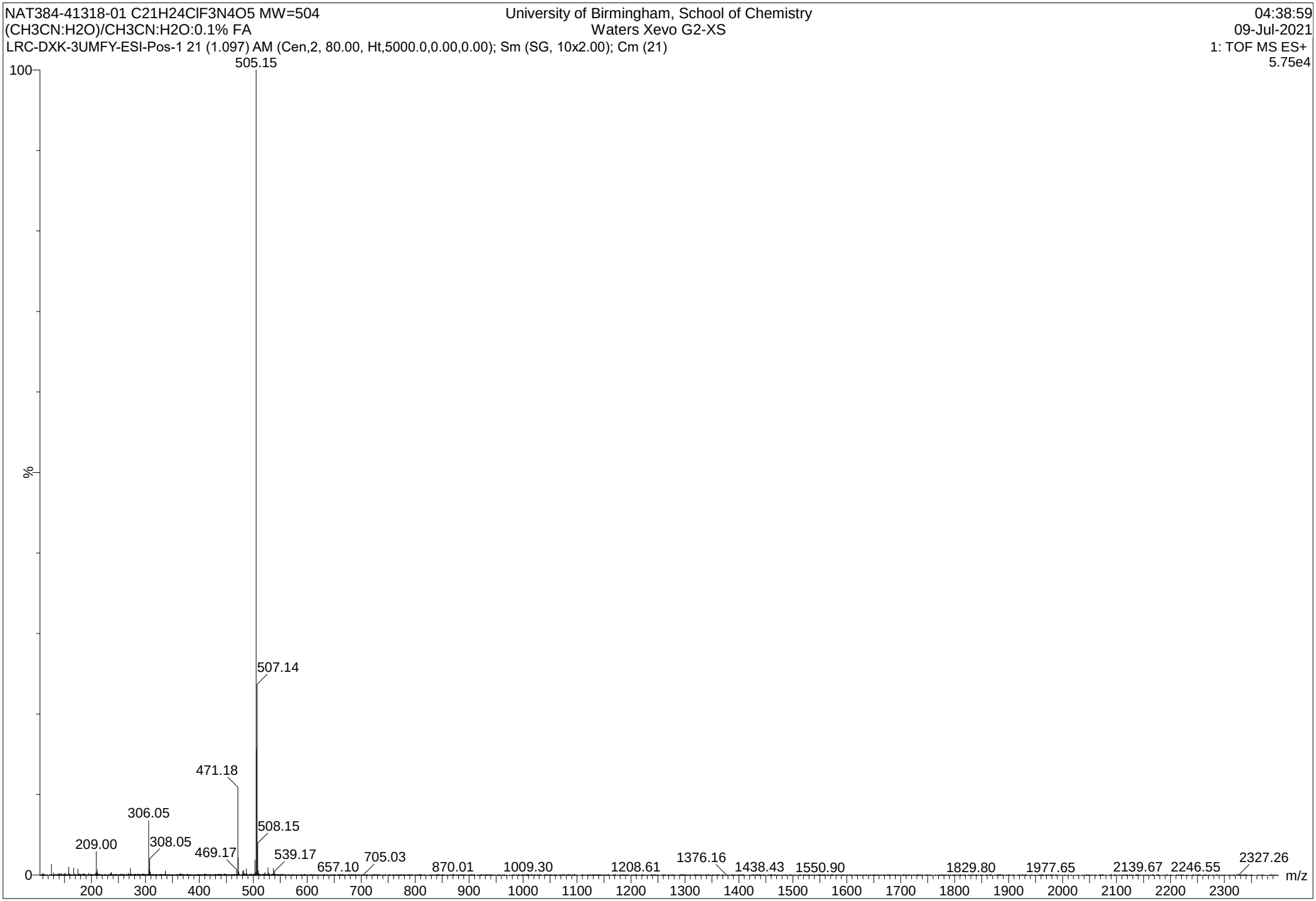
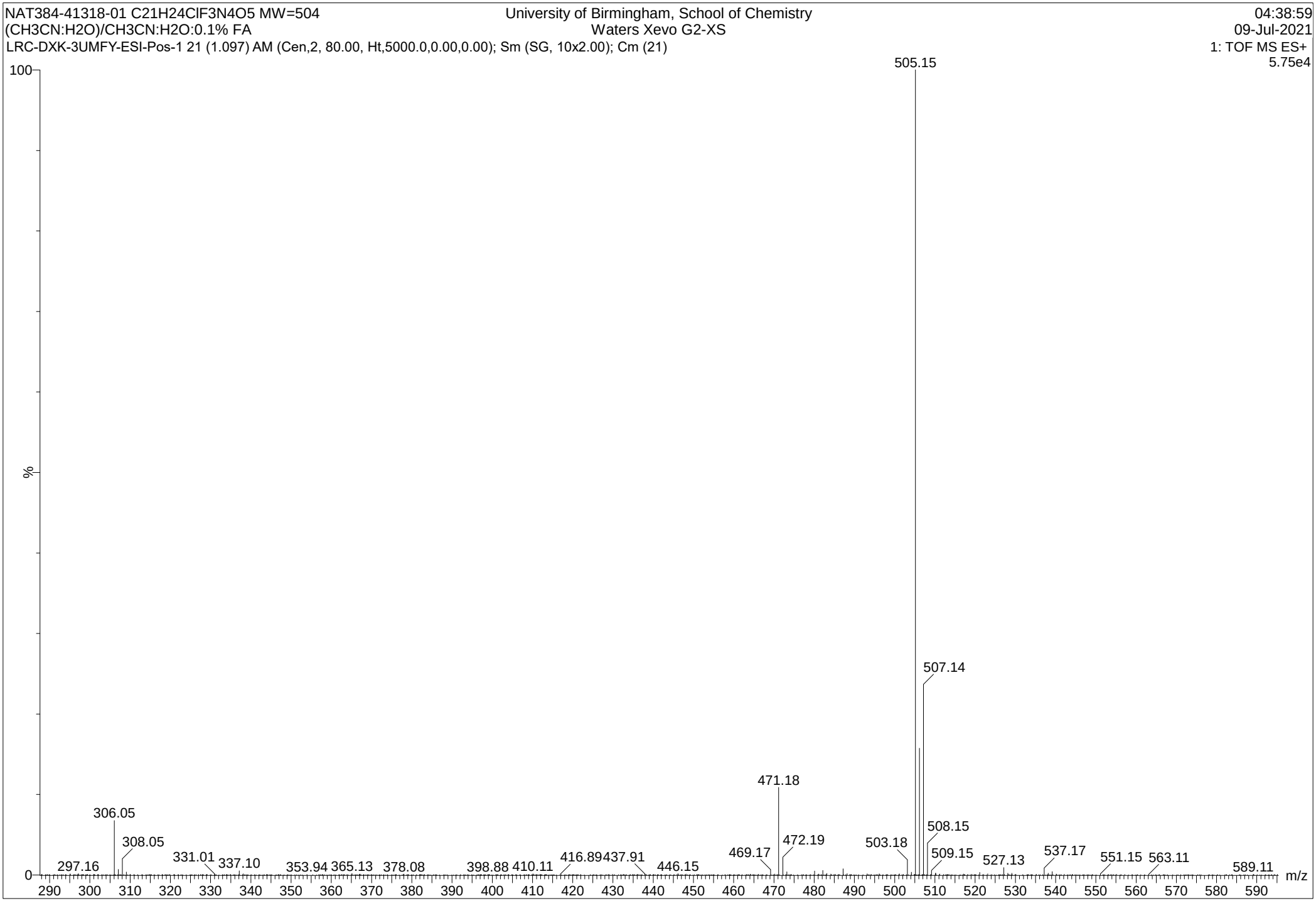
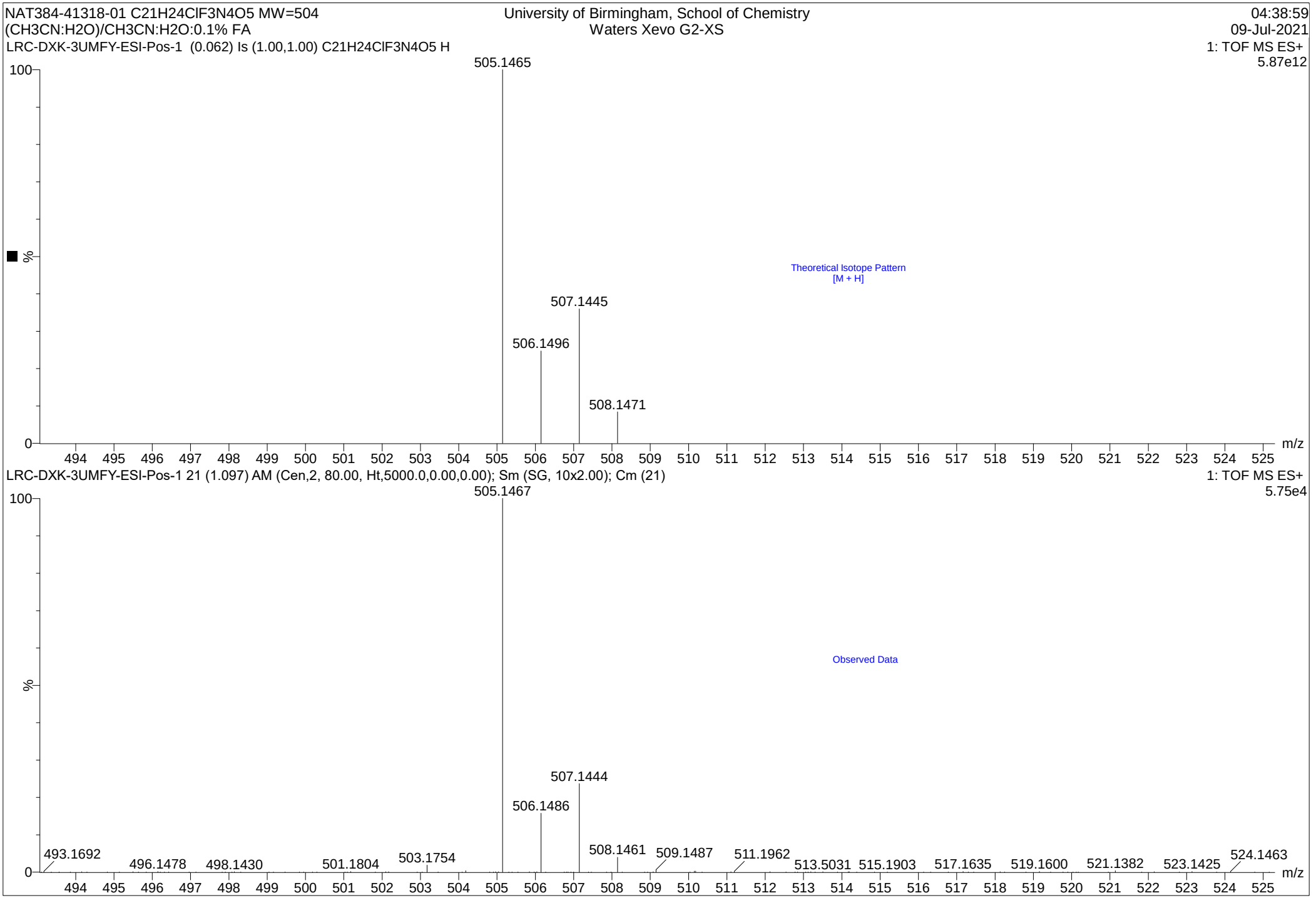

NAT384-41318-01 C21H24ClF3N4O5 MW=504
(CH3CN:H2O)/CH3CN:H2O:0.1% FA
LRC-DXK-3UMFY-ESI-Pos-1 21 (1.097) AM (Cen,2, 80.00, Ht,5000.0,0.00,0.00); Sm (SG, 10x2.00); Cm (21)
University of Birmingham, School of Chemistry
Waters Xevo G2-XS
04:38:59
09-Jul-2021
1: TOF MS ES+
5.75e4
100
%
0
505.15
507.14
471.18
306.05
508.15
308.05
209.00
469.17
539.17
657.10
705.03
870.01
1009.30
1208.61
1376.16
1438.43
1550.90
1829.80
1977.65
2139.67
2246.55
2327.26
m/z
200
300
400
500
600
700
800
900
1000
1100
1200
1300
1400
1500
1600
1700
1800
1900
2000
2100
2200
2300


NAT384-41318-01 C21H24ClF3N4O5 MW=504
(CH3CN:H2O)/CH3CN:H2O:0.1% FA
LRC-DXK-3UMFY-ESI-Pos-1 21 (1.097) AM (Cen,2, 80.00, Ht,5000.0,0.00,0.00); Sm (SG, 10x2.00); Cm (21)
University of Birmingham, School of Chemistry
Waters Xevo G2-XS
04:38:59
09-Jul-2021
1: TOF MS ES+
5.75e4
100
%
0
505.15
507.14
471.18
306.05
308.05
508.15
472.19
469.17
503.18
509.15
331.01
337.10
297.16
353.94
365.13
378.08
398.88
410.11
416.89
437.91
446.15
527.13
537.17
551.15
563.11
589.11
m/z
290
300
310
320
330
340
350
360
370
380
390
400
410
420
430
440
450
460
470
480
490
500
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540
550
560
570
580
590

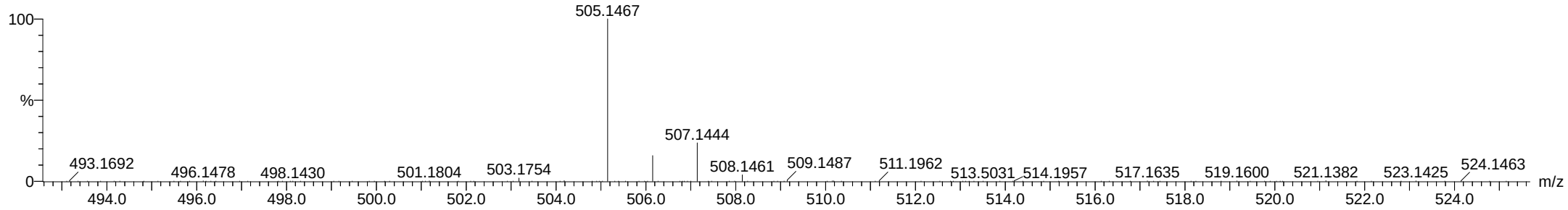

NAT384-41318-01 C21H24ClF3N4O5 MW=504
(CH3CN:H2O)/CH3CN:H2O:0.1% FA
LRC-DXK-3UMFY-ESI-Pos-1 (0.062) Is (1.00,1.00) C21H24ClF3N4O5 H
University of Birmingham, School of Chemistry
Waters Xevo G2-XS
04:38:59
09-Jul-2021
1: TOF MS ES+
5.87e12
505.1465
507.1445
506.1496
508.1471
Theoretical Isotope Pattern
[M + H]
%
m/z
LRC-DXK-3UMFY-ESI-Pos-1 21 (1.097) AM (Cen,2, 80.00, Ht,5000.0,0.00,0.00); Sm (SG, 10x2.00); Cm (21)
1: TOF MS ES+
5.75e4
505.1467
507.1444
506.1486
508.1461
509.1487
511.1962
493.1692
496.1478
498.1430
501.1804
503.1754
513.5031
515.1903
517.1635
519.1600
521.1382
523.1425
524.1463
Observed Data

Single Mass Analysis

Tolerance = 5.0 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
8661 formula(e) evaluated with 42 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 F: 1-4 Na: 0-1 Cl: 1-1

NAT384-41318-01 C21H24ClF3N4O5 MW=504 University of Birmingham, School of Chemistry 04:38:59
(CH3CN:H2O)/CH3CN:H2O:0.1% FA Waters Xevo G2-XS 09-Jul-2021
LRC-DXK-3UMFY-ESI-Pos-1 21 (1.097) AM (Cen,2, 80.00, Ht,5000.0,0.00,0.00); Sm (SG, 10x2.00); Cm (21) 1: TOF MS ES+
5.75e+004



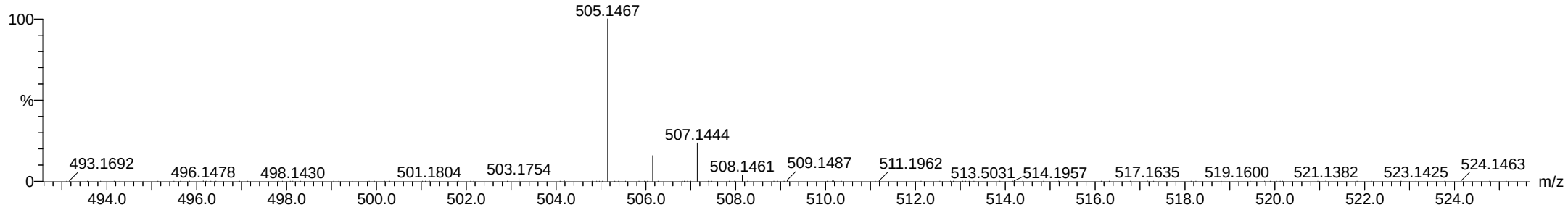
Minimum:				-4.5				
Maximum:		5.0	5.0	100.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
505.1467	505.1466	0.1	0.2	9.5	83.4	4.624	0.98	C21 H25 N4 O5 F3 Cl
	505.1466	0.1	0.2	7.5	81.7	2.909	5.45	C17 H23 N8 O2 F4 Na Cl
	505.1468	-0.1	-0.2	18.5	83.8	4.952	0.71	C25 H20 N8 F2 Cl
	505.1464	0.3	0.6	0.5	83.9	5.144	0.58	C17 H32 O12 F Na Cl
	505.1464	0.3	0.6	11.5	81.0	2.184	11.26	C15 H18 N14 F4 Cl
	505.1464	0.3	0.6	11.5	81.0	2.203	11.04	C15 H20 N14 O2 F Na Cl
	505.1464	0.3	0.6	0.5	83.8	5.013	0.66	C17 H30 O10 F4 Cl
	505.1470	-0.3	-0.6	14.5	85.3	6.452	0.16	C27 H25 N2 O2 F2 Na Cl
	505.1462	0.5	1.0	2.5	80.8	2.011	13.38	C11 H25 N10 O7 F2 Na Cl
	505.1461	0.6	1.2	4.5	81.9	3.099	4.51	C15 H27 N6 O10 F Cl
	505.1473	-0.6	-1.2	0.5	82.0	3.230	3.96	C12 H28 N6 O11 F2 Cl
	505.1473	-0.6	-1.2	-1.5	81.3	2.454	8.60	C8 H26 N10 O8 F3 Na Cl
	505.1475	-0.8	-1.6	7.5	80.8	2.020	13.27	C12 H21 N14 O3 F2 Na Cl
	505.1459	0.8	1.6	18.5	85.4	6.646	0.13	C30 H24 N2 O F Na Cl
	505.1459	0.8	1.6	-4.5	83.5	4.651	0.95	C11 H32 N2 O15 F2 Cl
	505.1475	-0.8	-1.6	9.5	81.9	3.113	4.45	C16 H23 N10 O6 F Cl
	505.1475	-0.8	-1.6	-3.5	84.6	5.778	0.31	C14 H33 O13 F2 Na Cl
	505.1457	1.0	2.0	-2.5	84.2	5.384	0.46	C5 H25 N12 O10 F3 Cl
	505.1477	-1.0	-2.0	5.5	83.9	5.049	0.64	C18 H28 N4 O8 F Na Cl
	505.1477	-1.0	-2.0	5.5	83.7	4.865	0.77	C18 H26 N4 O6 F4 Cl
	505.1455	1.2	2.4	11.5	83.0	4.238	1.44	C20 H22 N8 O F3 Na Cl
	505.1479	-1.2	-2.4	14.5	84.3	5.494	0.41	C22 H21 N8 O F3 Cl
	505.1454	1.3	2.6	13.5	84.3	5.492	0.41	C24 H24 N4 O4 F2 Cl
	505.1453	1.4	2.8	2.5	83.0	4.185	1.52	C16 H27 N4 O6 F4 Na Cl
	505.1482	-1.5	-3.0	10.5	85.8	6.952	0.10	C24 H26 N2 O3 F3 Na Cl

Single Mass Analysis

Tolerance = 5.0 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
8661 formula(e) evaluated with 42 results within limits (all results (up to 1000) for each mass)
Elements Used:
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NAT384-41318-01 C21H24ClF3N4O5 MW=504 University of Birmingham, School of Chemistry 04:38:59
(CH3CN:H2O)/CH3CN:H2O:0.1% FA Waters Xevo G2-XS 09-Jul-2021
LRC-DXK-3UMFY-ESI-Pos-1 21 (1.097) AM (Cen,2, 80.00, Ht,5000.0,0.00,0.00); Sm (SG, 10x2.00); Cm (21) 1: TOF MS ES+
5.75e+004



Minimum:			-4.5	
Maximum:	5.0	5.0	100.0	

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
	505.1452	1.5	3.0	4.5	84.3	5.504	0.41	C20 H29 O9 F3 Cl
	505.1483	-1.6	-3.2	21.5	87.5	8.700	0.02	C32 H23 N2 O F Cl
	505.1451	1.6	3.2	6.5	82.4	3.644	2.62	C14 H24 N10 O6 F Na Cl
	505.1450	1.7	3.4	6.5	82.5	3.656	2.58	C14 H22 N10 O4 F4 Cl
	505.1484	-1.7	-3.4	-3.5	83.7	4.879	0.76	C9 H29 N6 O12 F3 Cl
	505.1449	1.8	3.6	-2.5	83.2	4.392	1.24	C10 H29 N6 O11 F2 Na Cl
	505.1486	-1.9	-3.8	5.5	83.1	4.271	1.40	C13 H24 N10 O7 F2 Cl
	505.1448	1.9	3.8	-0.5	84.0	5.230	0.54	C14 H31 N2 O14 F Cl
	505.1487	-2.0	-4.0	3.5	82.6	3.804	2.23	C9 H22 N14 O4 F3 Na Cl
	505.1488	-2.1	-4.2	14.5	84.0	5.186	0.56	C17 H19 N14 O2 F Cl
	505.1488	-2.1	-4.2	3.5	85.9	7.067	0.09	C19 H31 O12 F Cl
	505.1446	2.1	4.2	1.5	84.0	5.224	0.54	C8 H24 N12 O9 F2 Cl
	505.1489	-2.2	-4.4	1.5	84.7	5.901	0.27	C15 H29 N4 O9 F2 Na Cl
	505.1490	-2.3	-4.6	10.5	85.0	6.245	0.19	C19 H22 N8 O2 F4 Cl
	505.1491	-2.4	-4.8	10.5	85.2	6.421	0.16	C19 H24 N8 O4 F Na Cl
	505.1443	2.4	4.8	17.5	86.1	7.260	0.07	C27 H23 N4 O3 F Cl
	505.1443	2.4	4.8	15.5	85.2	6.379	0.17	C23 H21 N8 F2 Na Cl