AIMS

Mass Spectrometry Laboratory

CHEMISTRY

UNIVERSITY OF TORONTO

AIMS Instrumentation & Sample Report Documentation

JEOL AccuTOF GCx plus

AIMS Mass Spectrometry Laboratory
Department of Chemistry, University of Toronto
80 St. George Street, Toronto ON, M5S 3H6

JMS-T200 AccuTOF Gcx-plus

Manufacturer: JEOL USA Inc.
Peabody MA

Features

Ion Sources:	Electron Ionization (EI) Field Desorption (FD) Field Ionization (FI)
Ion Polarity:	Positive and negative
Mass Range:	7-10 000 *Da*
Resolution:	>10 000 mass resolution @ *m/z* 609
Mass Accuracy:	+/- ~1.5 *mDa*
GC System:	Agilent 7890B

AccuTOF 4G DART Results Format

EI-MS Spectrum

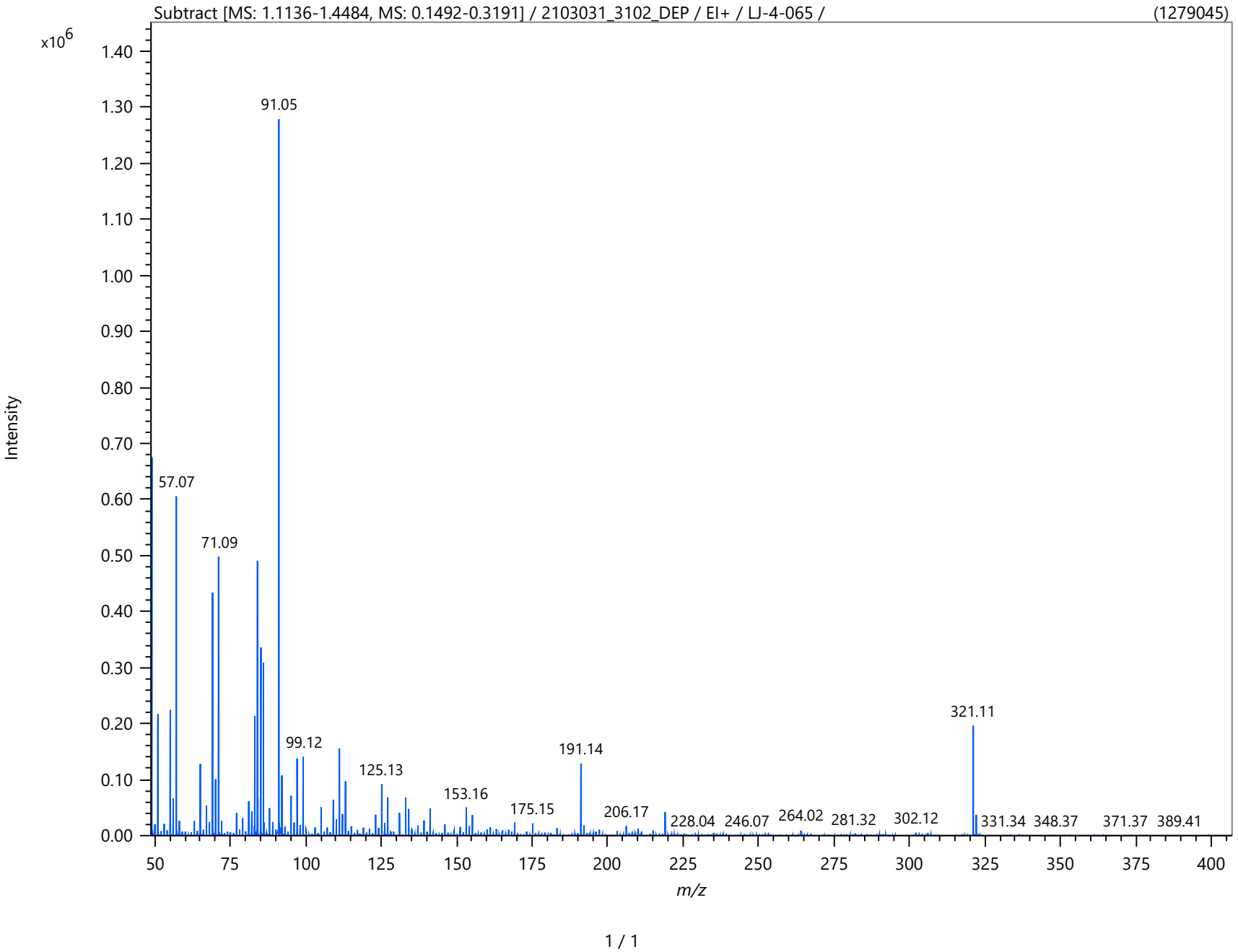
The *msAxel* Spectrum Report consists of a profile mass spectrum showing *m/z* versus intensity. Spectral peaks are labeled with *m/z* values rounded to two decimal places. The standard data acquisition range is *m/z* 50-850 *Da* but printed mass spectra are normally expanded to display an appropriate region of interest. EI mass spectra are normally acquired in positive ion mode and the analyte species of interest appear as radical molecular ions $[M]^{+\cdot}$.

High Resolution Mass Spectrometry (HRMS) Report

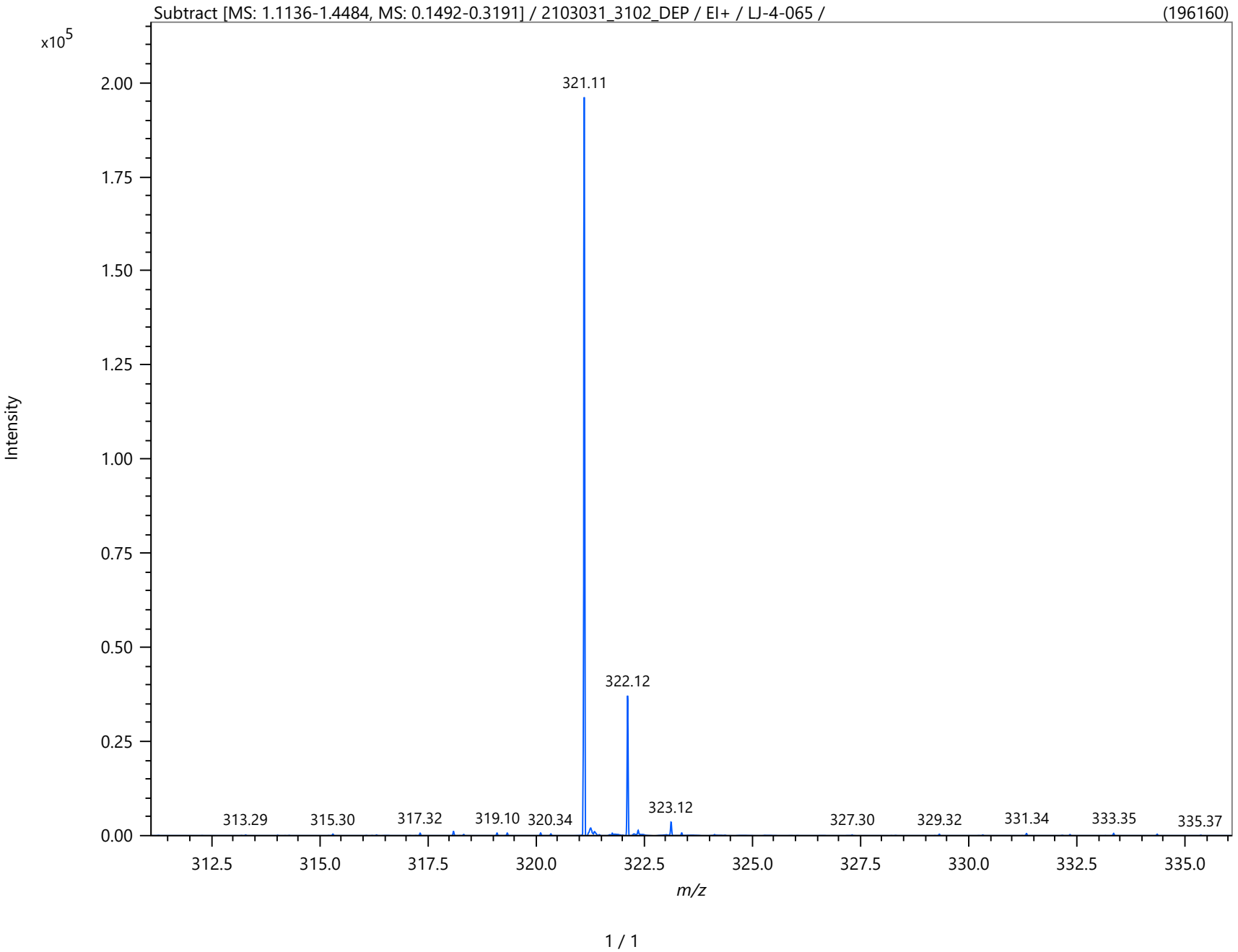
The EI-HRMS report is generated using the *Elemental Composition* feature implemented in the JEOL *msAxel* software package. The report provides the measured *m/z* value and a list of possible molecular formulae and calculated exact *m/z* values. All of the values contained in the report correspond to the *ionic species of interest, despite the table heading*. All ionic formulae are reported as charged species accounting appropriately for the mass of the electron (0.00054 Da).

Suggested reporting format for compound characterization:

"HRMS (EI-TOF+): *m/z* [M]+. calc'd for $C_{18}H_{15}NF_4^+$ *m/z* 321.11351, measured *m/z* 321.1142"

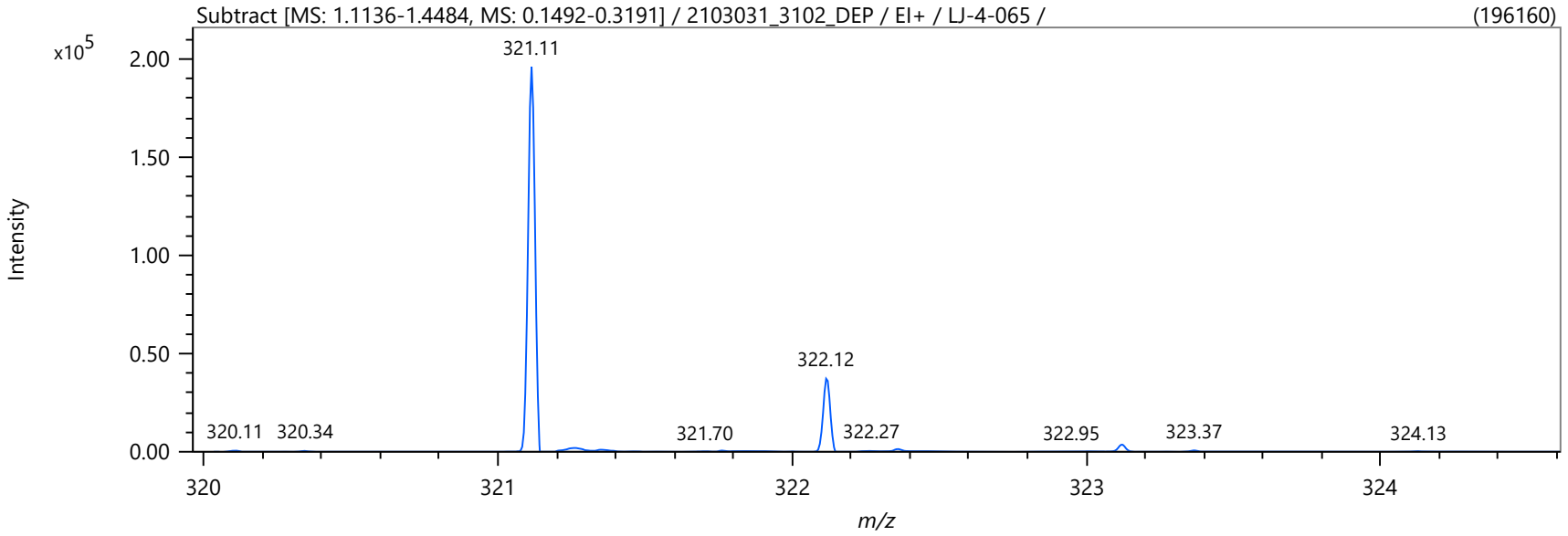

Subtract [MS: 1.1136-1.4484, MS: 0.1492-0.3191] / 2103031_3102_DEP / EI+ / LJ-4-065 / (1279045)
x10^6
Intensity
1.40
1.30
1.20
1.10
1.00
0.90
0.80
0.70
0.60
0.50
0.40
0.30
0.20
0.10
0.00
91.05
57.07
71.09
99.12
125.13
153.16
175.15
191.14
206.17
228.04
246.07
264.02
281.32
302.12
321.11
331.34
348.37
371.37
389.41
50
75
100
125
150
175
200
225
250
275
300
325
350
375
400
m/z

1 / 1


Subtract [MS: 1.1136-1.4484, MS: 0.1492-0.3191] / 2103031_3102_DEP / EI+ / LJ-4-065 / (196160)
x10^5
2.00
1.75
1.50
1.25
1.00
0.75
0.50
0.25
0.00
Intensity
321.11
322.12
323.12
313.29
315.30
317.32
319.10
320.34
327.30
329.32
331.34
333.35
335.37
312.5
315.0
317.5
320.0
322.5
325.0
327.5
330.0
332.5
335.0
m/z

1 / 1

Spectrum



Elemental Composition

Parameters	
Tolerance:	±5.00 mDa
Electron:	Odd/Even
Charge:	+1
DBE:	-1.5 - 40.0

Elements Set 1:

Symbol	C	H	N	O	F
Min	0	0	0	0	4
Max	50	100	10	10	4

Results

Mass	Intensity	Formula	Calculated Mass	Mass Difference [mDa]	Mass Difference [ppm]	DBE
321.11416	196160.25	C18 H15 N F4	321.11351	0.65	2.03	10.0
		C5 H13 N10 O2 F4	321.11536	-1.19	-3.72	2.5
		C7 H15 N7 O3 F4	321.11670	-2.54	-7.90	2.0
		C15 H17 O3 F4	321.11083	3.33	10.37	5.5
		C9 H17 N4 O4 F4	321.11804	-3.88	-12.08	1.5
		C13 H15 N3 O2 F4	321.10949	4.67	14.55	6.0