Development of High Performance LC-QIT-TOF

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The Need for Highly Precise Mass Spectrometry

- Precision mass spectrometry allows inferring the elemental composition of molecules
- The higher the precision, the more the number of constituent candidates can be reduced

Example: (reserpine) The number of elemental combination candidates listed for a mass of (M+H)⁺=609.2822

Constituent Elements:

Carbon 20 - 40 Nitrogen 3 - 10 Sulfer 0 - 5	Hyd Oxy	30 - 60 5 -15	
Precision	10 ppm	5 ppm	2 ppm
Number of Combinations	29	16	Δ

Objective of LC-QIT-TOF

Ion Trap MS
 Allows MSⁿ
 High precursor resolution

• TOF MS

Highly precise mass values High resolution

QIT-TOF

An instrument that allows high precision MSⁿ spectrometry

Technologies Developed for LC-QIT-TOF

1685 x 685 x 570 mm, 280 kg

Differences Between

MALDI-QIT-TOF and ESI-QIT-TOF

Key newly developed technologies:

- 1. Compressed ion introduction
MALDI: Pulsed ionization(introduction to QIT)
ESI: Continuous ionization
- 2. Improvements to Dual Stage Reflectron (High sensitivity and high resolution for QIT-TOF)
- 3. lonic cooling using argon gas (High resolution)
- 4. Temperature controlled interior of instrument (Stability of mass precision)
- 5. Ballistic Ion Ejection

(Accuracy and stability of mass measurements)

Compressed Ion Introduction





Basic Process of QIT-TOF



Dual Stage Reflectron Improvements

The shape of the electric field was changed for second stage of the dual stage reflectron.

-> Improves the time convergence with respect to ion distribution during acceleration



Cooling with Argon Gas

Bovine Insulin m/z 956 [M+6H]⁶⁺



Controlling the Instrument's Internal Temperature to Stabilize Mass Precision

Temperature Control

- Flight Tube (Representative temperature point)
- High Voltage Switch (Ion Trap EC, Ring)
- High Voltage Power Supply
 (Ion Trap, Flight Tube, Reflectron)
- RF Generator (Ion Trap)

Controls representative temperature point to $40\pm0.3^{\circ}C$

Fundamental Performance Data

Mass Spectrometry of Bovine Insulin 6+(5733m/z)



Mass Spectrometry of Verapamil



MS/MS Measurement of Verapamil

 MS/MS ID
 Expected
 Found
 Error

 C18H27N2O2
 303.2073
 303.2075
 + 0.66ppm



24-Hour Stability of Mass Precision External Standard Method (m/z928)



24-Hour Stability of Mass Precision Internal Standard Method (m/z928)



Precursor Selection Using Ion Trap



MS¹⁰

using NaTFA sample

Inten. (x100,000)									Base Peak: 2,600	. 4826/337, 10	02
MS							m/z 1192.22 Abs.	Inten.	240 Reil.	Inten. 0.0	7
2.5						- I					H
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Inten (x100,000)									Base Peak: 2,606	5165/522,98	90
= 0 (MS) ²	1						m/z 1215.49 Abs.	Inten.	440 Rel.	Inten. 0.0	18
3.0-(MOV						2062.60	2334.5	619	2606.5165		E
0.0 453.9332 64	4.8702 781.7149	974.8244	1382.	7376 165	(4, 6814		h	2470.0360	2742.495	72882.4779	Q
500	750	1000	1250	1500	1750	2000	2250	2500	2750	m/	z
Inten. (x100,000)					:			Inten	Base Peak: 2,334	1.5559/335,91	18
2.5- (MS)*						2062.60	552334.5	559			Ð
475.0331	704.0235 878.1	1737	1246.7718		1790.6563		2198.5847	2470.5421	2706.6420	2909.7973	Q
0.0-4 5do	750	1000	1250	1500	1750	2000	2250	2500	2750	' 'm/	/z
Inten. (x100,000)									Base Peak: 2,062	2.6013/282,16	60
2 5 (MS) ⁴	1					0.000 100	m/z 1243.77 Abs.	Inten.	563 Rel.	Inten. 0.2	0
					1790.6546	2002.00	13			2953. 1939	E
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1.0 (MS) ⁶	750	1000	1250 1246-7517 874	15b0 1518, 7139 165	1750 4.6817 L 1728 7190	2080	m/z_1264.52_Abs.	25b0	2750 Base Peak: 1,518 112 Bel. 2811	m/ 3.7139/ 91,50 Jnten0.1 2999.4887	′z' 06 12 ⊕
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High Speed Pos/Neg Ion Switching (Max 2.5Hz)

Sample: glycosylceramide (C16,18,20,22,23,24:0-d18:1), (C24:1-d18:1) From Riken Imtakt Cadenza 5.0 (x10.00 STIC 4.5 2:TIC 4.0 Column With Pos/Neg Ion TIC **CD-C18** 3.5 Mobile Phase: 5mM 3.0 acetate 2.5 methanol **Neg. Ion TIC** 2.0 solution 1.5 1.0 Flow Rate: 0.2ml/min Pos. Ion TIC 0.5 isocratic 0.0-20 (x10,000,000) (x10,000,000) 2:812.5475 (6,00) 2:840.5843 (6,00) :750, 5841 (6, 00) 778.6174 (6.00) Neg. Ion Mass Spectrum **Pos. Ion Mass Spectrum** 4.0 :832 6649 (6.00) 2:922,6623 (6,00) :806.6493 (6.00) 2:896.6468 (6.00) 820.6635 (6.00) 2:910.6605 (6.00) 2:924,6792 (6,00) :906.2668 (6.00) :980.2865 (6.00) 2.5 2.0 5.0 3.0 4.0 5.0 6.0 7.0 Inten. (x1, 000, 000) Inten. (x1, 000, 000) 1 50 2.00 722. 5527 812. 5475 Expected Expected 1.75 1 25 722.55469 812.54996 1.50 1.00 Error: 2.75PPM Error: 3.02PPM 1.25 0.75 1.00 0.75 0.50 0.50 0.25 0.25 0.00-0.007 1250 250 1000 1500 1750 260 1000 1250 1500 1750 500 500 750

Auto MS/MS



Auto MS/MS



Summary of New Technologies

Compressed Ion Introduction Method (Continuous ionization -> Pulsed ionization)

Ballistic Ion Ejection

(Transfers ions to TOF all at the same time with similar velocities for higher mass accuracy)

Ion Cooling using Argon Gas

(High resolution analysis of multivalent ions)

Dual Stage Reflectron Improvements (Hign sensitivity and high resolution for QIT-TOF)

Temperature controlled interor of instrument housing (Stability of high mass precision)