

Development of fast scanning technologies for a triple quadrupole mass spectrometer

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Introduction

We present the development of a triple quadrupole mass spectrometer with a scan speed of 15,000u/sec without loss of sensitivity, resolution and mass stability applied to MS and MS/MS data acquisitions. To achieve a high scan speed in triple quadrupole analysis the design has taken into a number of factors including the dynamics of ion transmission between Q1 and the detector, increased ion energy applied to both Q1-Q3 and the enhanced responsiveness of RF power supplies applied to Q1-Q3. This design was applied to the high scan speed analysis of several sulfa drugs using neutral loss scan, precursor ion scan and product ion scan modes.

Methods

Ion transmission and scan speed on triple quadrupole mass spectrometers is influenced by the loss of ion momentum and energy dispersion between the first quadrupole mass filter and the detector. Momentum loss and energy dispersion is further compounded within the collision cell which contributes to an increased flight time from the end of Q1 to the detector. Longer flight times constrain the effective scan speed and energy dispersion aggravates mass resolution.

UFsweeper Collision Cell

Accelerates ions out of the collision cell by forming a pseudo-potential surface. The result is higher CID efficiency and Ultra Fast ion transport to reduce the sensitivity losses and cross-talk.

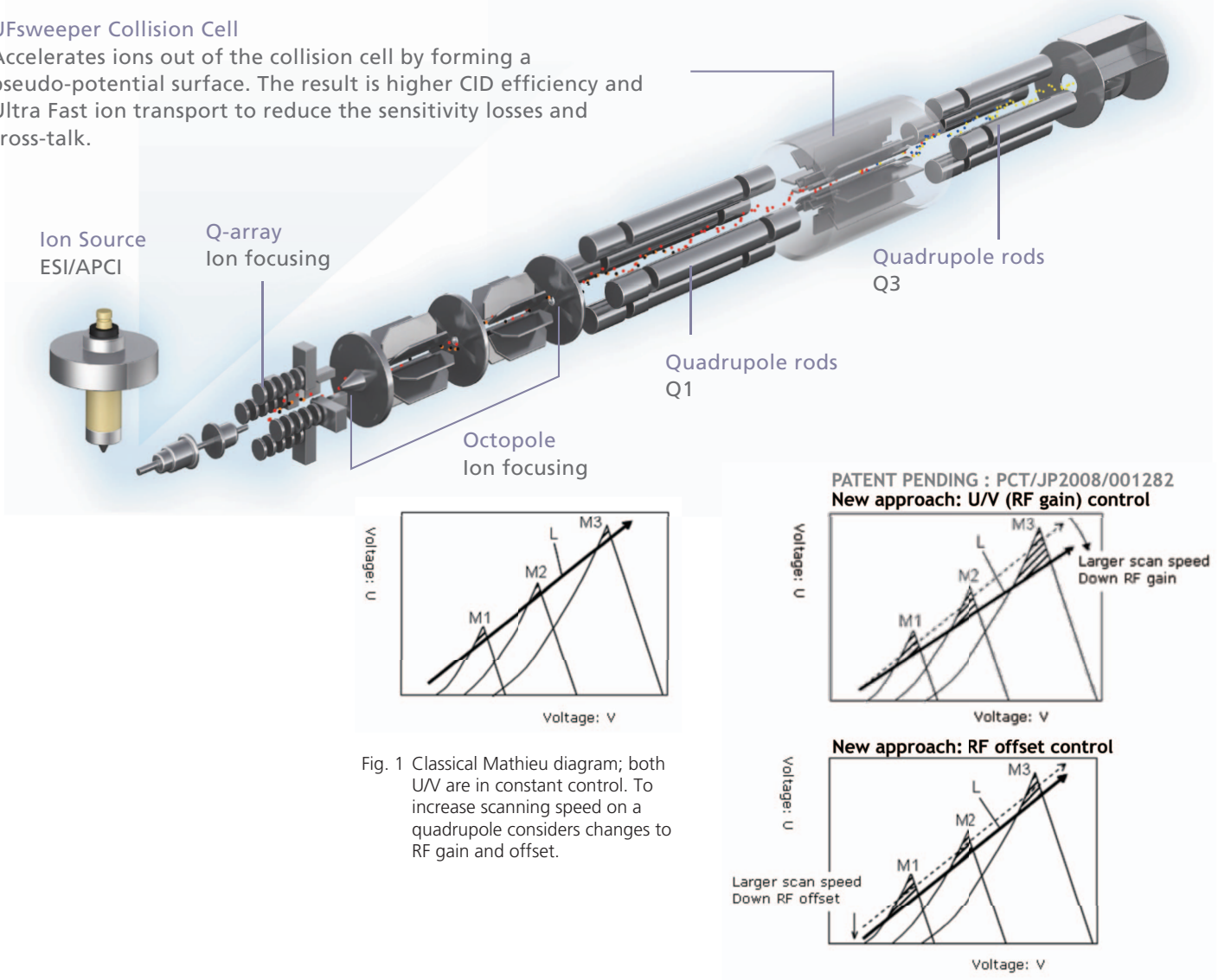


Fig. 1 Classical Mathieu diagram; both U/V are in constant control. To increase scanning speed on a quadrupole considers changes to RF gain and offset.

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Power supply

High scan speed MS and MS/MS data acquisition on a triple quadrupole MS system was achieved by increasing the ion energy on the hyperbolic quadrupole rods (from 1-2eV to 5eV) and by developing an ultra fast RF power supply.

The ultra fast RF power supply delivers a stable RF voltage in 200 μ sec and a stable intensity in 600 μ sec (this

compares with a time frame of 2.5 msec to achieve a stable RF voltage and 3 msec to achieve a stable intensity on previous designs, [Figure2]). High-energy ion transmission between Q1 and the detector improves mass peak shape distortion of Q1 scan under high scan speed and results in improving mass resolution (Figure 3).

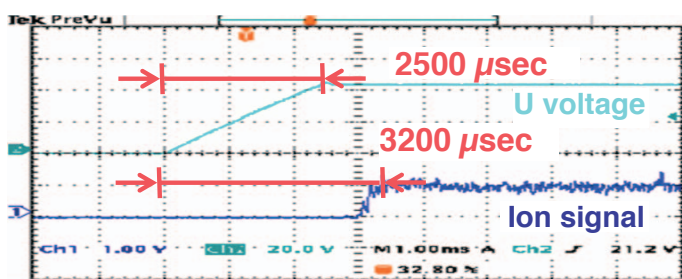


Fig. 2 Conventional RF power supply
Stable RF voltage achieved in 2.5 msec and 3 msec to achieve a stable intensity.

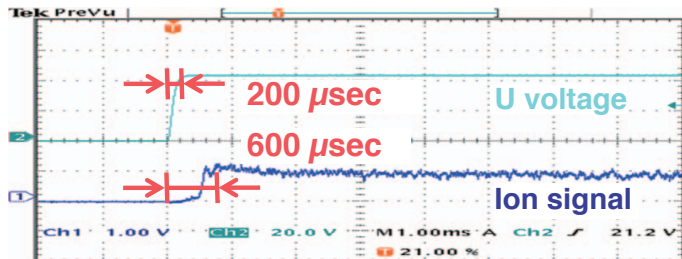


Fig. 3 Enhanced RF power supply
Using an ultra fast RF power supply results in a stable RF voltage in 200 μ sec and a stable intensity in 600 μ sec.

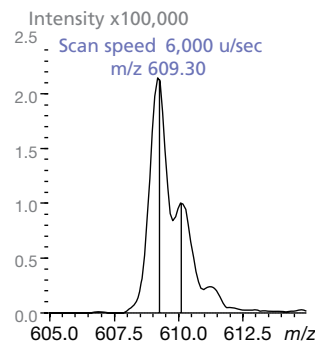
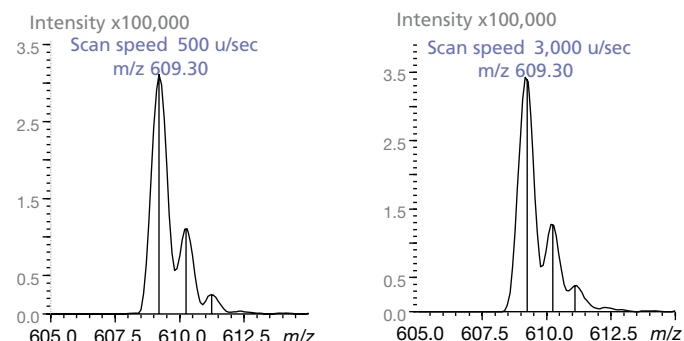


Fig. 4 By applying the high-energy ion transmission algorithm to neutral loss and precursor ion scan, high performance high speed scan analysis was achieved. Precursor ion spectra of reserpine with different speeds up to 6,000u/sec. No mass shift and almost same mass resolution were observed.

Fast scan analysis

As one example, a fast scanning method was developed to screen for a number of sulpha drugs. The method used three precursor ion scans (m/z 65, 92 and 156) and three neutral loss scans (200, 173 and 109) at a scan speed of 6000 μ /sec.

Table 1 Analytical Conditions

LC condition	
Column	: Shim-pack XR-ODSII (2.0 mmI.D. x 150 mmL.)
Mobile phase A	: 0.1% formic acid
Mobile phase B	: Acetonitrile
Gradient program	: 10 %B (0-1min) \rightarrow 95 %B (10-12 min) \rightarrow 5 %B (12.01-17 min)
Flow rate	: 0.25 mL/min

MS condition

Event No.	Scan type	Prec. of m/z	Loss of m/z	Start m/z	END m/z	Speed u/sec
1	Prec.	65	—	200	500	6000
2	Prec.	92	—	200	500	6000
3	Prec.	156	—	200	500	6000
4	NL	—	200	220	500	6000
5	NL	—	173	200	500	6000
6	NL	—	109	200	500	6000

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Table 2 Qualitative data by compounds

Compounds	RT min	m/z	Standard scan for detection					
			Prec of 65	Prec of 92	Prec of 156	NL 200	NL 173	NL 109
Sulfisomidine	3.06	279	○	○	○			
Sulfathiazole	4.78	256	○	○	○			
Sulfamerazine	5.33	265	○	○	○	○	○	○
Sulfamethizole	5.88	271	○	○	○			
Sulfadimidine	5.91	279	○	○	○	○	○	
Sulfamonomethoxine	6.54	281	○	○	○		○	
Sulfamethoxazole	7.20	254	○	○	○			
Sulfaquinoxaline	8.11	301	○	○	○			
Sulfadimethoxine	8.14	311	○	○	○			
Number of Detected Compounds			9	9	9	2	3	1

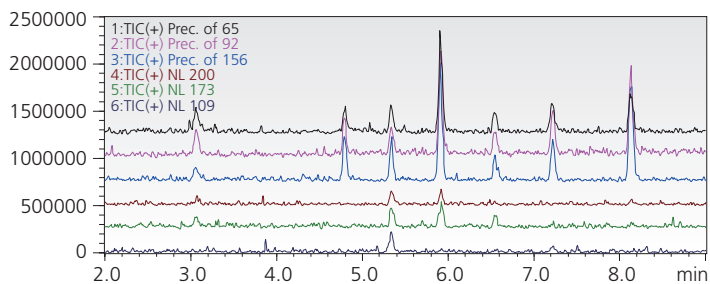


Fig. 5 The advantage of high speed scanning and flexible neutral loss and precursor ion scanning enables multi compound mixtures such as a series of sulpha drugs to be quickly identified in a single MS/MS analysis.

Conclusion

- The results show high speed analysis both precursor ion and neutral loss scanning.
- Supports multiple scan methods in a single analysis, with no mass displacement.
- No precursor ion mass error was identified in this experiment.

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