

PSB 119

Scan Speed vs Cycle Time on an Ion Trap Mass Spectrometer

Page 1 of 3

One of the key advantages of ion trap mass spectrometry is the ability to perform multiple MS/MS (or MSⁿ) fragmentation steps on a single precursor ion and its product ions to create a cascade of product-precursor ion relationships that yield extensive amounts of structural information. To achieve maximum benefit in an LC/MSⁿ experiment, the series of events starting from the process of filling the ion trap through detecting the ions must be optimized for a chromatographic timescale. The time taken to complete this series of events is referred to as the analytical cycle time.

The analytical cycle time in a high-performance ion trap device consists of the following major components which are also depicted in Figure 1.

- 1–AGC (Automatic Gain Control) pre-scan*,
- 2–Ion injection (usually the rate-determining step),
- 3–Isolation and activation of the parent ion within the trap,
- 4–Scanning the ions out of the trap (mass analysis).

* The AGC pre-scan is patented technology and only available on Thermo Scientific ion trap instruments. It ensures the trap is always filled to the optimum number of charges for mass accuracy and sensitivity.

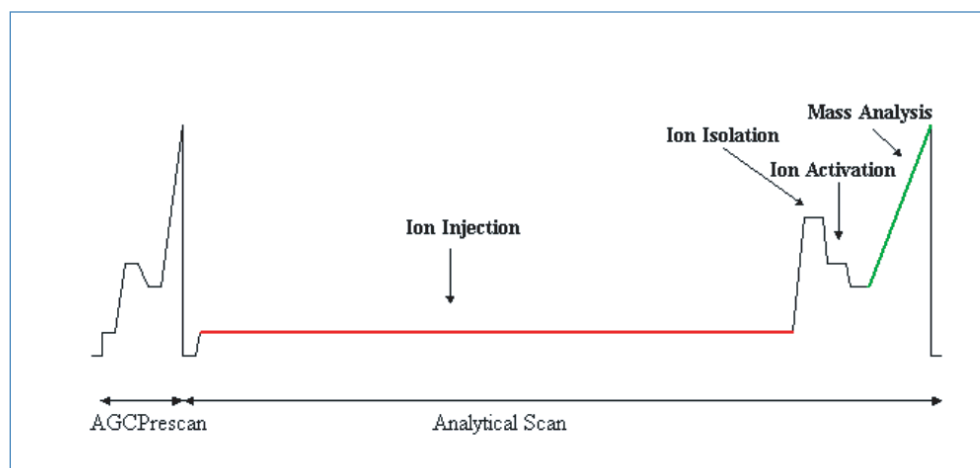


Figure 1: Major components of an ion trap analytical cycle

The ability to perform multiple experiments on a chromatographic peak and to increase the precision of quantitative experiments relies on the number of scans across the LC peak. Scan speed refers only to the time required to scan ions out of the trap during mass analysis, which represents a small fraction of the overall analytical cycle time. Scan speed is not the major time constraint in the overall analytical cycle time. As illustrated in Figure 1, only the ion injection and mass analysis times vary; whereas the other times are fixed. The ion injection time is determined by the rate of ions entering the trap.

Scan Speed vs Cycle Time on an Ion Trap Mass Spectrometer

Page 2 of 3

The mass analysis time is a function of the selected mass range and the scan speed. At low concentrations, where cycle time is particularly important, an optimal ion injection time is likely to be in the order of 500 ms. Table 1 shows typical times for different stages of an ion trap scan. As is shown, increasing the scan speed by 25 times (5000 amu/s to 125,000 amu/s) results in only an 11% time saving in cycle time (603 ms down from 675 ms). The net result is an increase of between 1 and 2 MS/MS scans across a 10-second wide chromatographic peak. The only way to significantly increase the sampling rate across the peak is to reduce the injection time, which can be achieved in two ways:

1. Set a lower maximum injection time, which reduces the number of ions in the trap, and hence sensitivity.
2. Increase the efficiency of the API source and lens stack to improve the transmission of ions, filling the trap to the same level in a shorter period of time. (This has been achieved on the Thermo Scientific ion traps by the addition of the Ion Max™ source, which increases signal and reduces chemical noise.)

	5000 amu/s	16,700 amu/s	125,000 amu/sec
AGC Scan	50 ms	50 ms	50 ms
Ion Injection	500 ms	500 ms	500 ms
Isolation and Activation	50 ms	50 ms	50 ms
Mass Analysis	75 ms	23 ms	3 ms
Total Cycle Time	675 ms	623 ms	603 ms

Table 1: Time components of a typical ion trap analytical scan.

Scan Speed vs Cycle Time on an Ion Trap Mass Spectrometer

Page 3 of 3

For good quantitative reproducibility, it is necessary to acquire enough data points to precisely determine the chromatographic peak shape particularly at the take-off point. Increasing the scan speed in the ion trap does not significantly increase the number of data points taken across a peak. Figure 2 shows the same chromatographic peak scanned at three different scan speeds. In Figure 2a, the ions are scanned out of the ion trap at 125,000 amu/s, which produces 19 scans across the LC peak. At 16,700 amu/s (Figure 2b), 18 points across the peak are acquired, and in the final case with the ions ejected at 5,000 amu/s 17 points were recorded. The times given above are valid if a single scan is used with no averaging. If spectral averaging is required (often required by 3D traps to compensate for lower ion capacities), then the above calculation must be multiplied by the number of scans averaged.

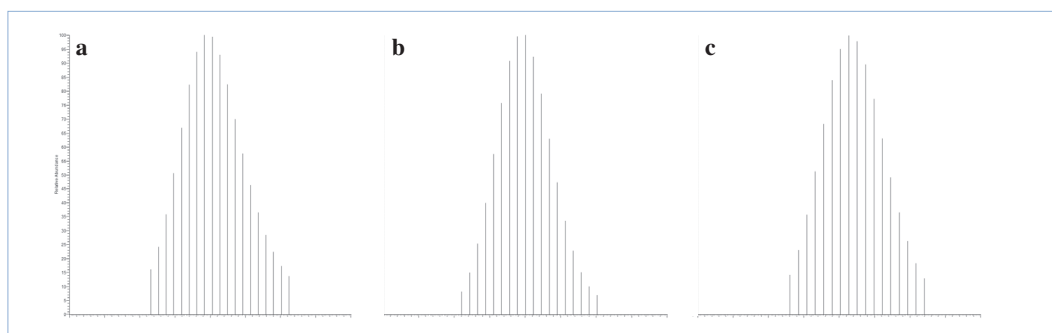


Figure 2: Number of MS/MS scans across a chromatographic peak at **a)** 125,000 amu/s, **b)** 16,700 amu/s, and **c)** 5,000 amu/s. Example is for MS/MS scans from m/z 135–510 and a maximum injection time of 500 ms.

Conclusion

When analyzing samples at low levels in complex matrices, maximum information is achieved with fast analytical cycle times and high spectral quality. While part of the cycle time is determined by how fast the ions are scanned out from the trap (scan speed), filling the trap (injection time) accounts for the largest proportion of the cycle time by far, particularly for low level components. The use of AGC allows a maximum injection time to be set for low abundance ions while regulating the ion injection time for species of higher concentration. This ensures optimum sensitivity and mass accuracy for the widest range of sample concentrations.

It is also useful to remember that, with all other things being equal, an increase in the scan speed will reduce the mass resolution of the spectrum. This means that simply increasing the scan speed will not significantly increase the number of analytical scans acquired across a chromatographic peak and it can adversely affect the quality of the data, making interpretation more difficult.