# Agilent 500 Ion Trap LC/MS with Enhanced Charge Capacity (ECC)

## Technical Overview

### Introduction

Historically, ion traps were limited by the amount of charge that could be stored in them. If too much charge was in the trap, the electric field from the trapped charge would influence the ion ejection process and shift the apparent mass position. In addition, the mass resolution would be degraded. Software techniques were developed to ensure that the trap would always have a relatively constant amount of charge by controlling the ionization time. Although this automatic charge regulation was able to limit the charge in the trap to values that did not cause unacceptable mass shifts and resolution losses, it required limiting the total number of sample and matrix ions.

Modifying the electrical multipole content of the trapping field can have dramatic effects on the performance of the ion trap [1,2]. The Agilent 500 Ion Trap LC/MS employs a trapping field that has additional mechanically formed octapole and electrically generated hexapole components to the trapping field, resulting in significant increases in the number of ions that can be trapped and therefore, an EEC. A relative comparison was made between an Agilent 500 Ion Trap and a competitive ion trap.

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## Experimental Conditions

The test sample was the mass calibration compound Ultramark, a perfluorinated amine having ions with mass-to-charge ratios (*m/z*) up to 2200. The ion cluster at mass-to-charge 1122 was selected as the test ion. The fixed ionization time duration was increased and the mass shift and mass resolution full width at half maximum (FWHM) was measured. The ion times were adjusted to give approximately the same signal-to-noise on both instruments (Figure 1).

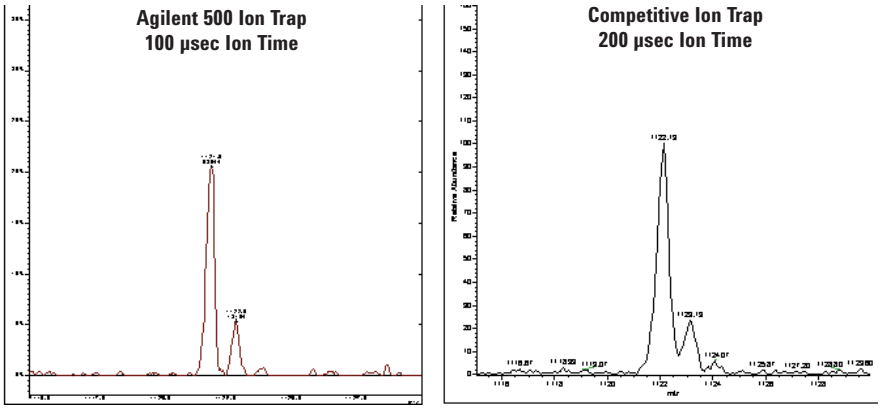


*Figure 1. Similar S/N ratios with only half the ionization time for the Agilent 500 Ion Trap. Note that this latter system is baseline resolved while the competitive ion trap has a 10% valley.*

The ion times were then adjusted to values that produced similar mass resolution (Figure 2). It was observed that the Agilent 500 Ion Trap could tolerate a 100-fold increase in the ion time, equivalent to increasing the charge in the trap by a factor of 100, with little noticeable decrease in the mass resolution. The competitive ion trap on the other hand could only tolerate an increase in ion time of 10 before the mass resolution was noticeably degraded. Therefore, the Agilent 500 Ion Trap could store 10 times the number of ions without affecting its performance.

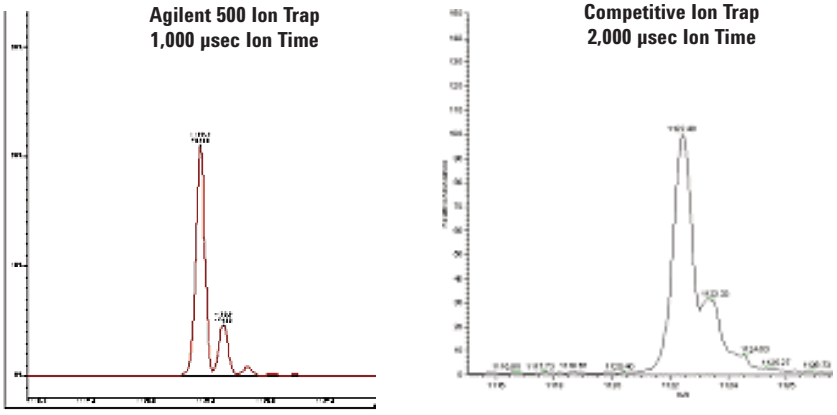


*Figure 2. Excellent mass resolution and extended charge capacity for the Agilent 500 Ion Trap versus degraded mass resolution and limited charge capacity for the competitive ion trap.*

## Discussion and Results

Figure 3 shows a plot of peakwidth at half height as a function of ion time for both the Agilent 500 Ion Trap and the competitive ion trap. The figure illustrates how the 500 Ion Trap (blue trace) maintains 0.5 peakwidth at half height while the competitive ion trap starts to increase peakwidth significantly after only a 10-fold ion concentration increase.

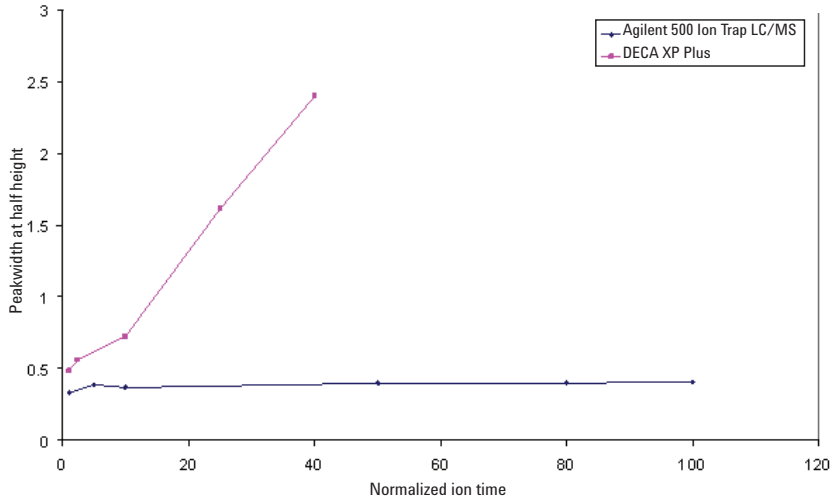


*Figure 3. Peakwidth versus normalized ion time for the Agilent 500 Ion Trap and a competitive ion trap.*

Figure 4 shows mass shift versus normalized ion time for the 500 Ion Trap and competitive ion trap. Reliable detection of trace amounts in the presence of high concentration of coeluting analytes and heavy matrix requires the ion trap to have a large charge capacity. Alprazolam, with a parent ion at *m/z* 309 at 500 fg level and alprazolam-d5 with parent ion at *m/z* 314 at 50 pg level, extracted from bovine serum albumin (BSA) was injected into the 500 Ion Trap LC/MS. The two analytes coeluted under the conditions we used. Despite the 100-fold concentration difference between the d5 analog and native compound, the signal-to-noise ratio obtained for alprazolam is excellent. The 500 Ion Trap signal was not suppressed due to the large amount of matrix, the coeluting d5 analog (Figure 5).

The 500 fg alprazolam, extracted from BSA is present only at 1/100 of the concentration of the coeluting labeled compound, alprazolam-d5 at 50 pg. This coelution is a manufactured matrix contribution, present at 100-fold concentration and only five masses away from the target analyte mass, which produced good detection on the Agilent 500 Ion Trap LC/MS.

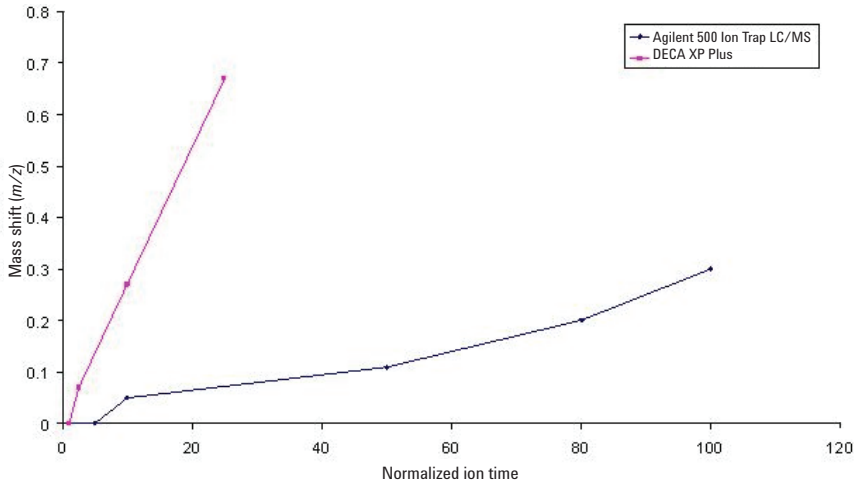


*Figure 4. Mass shift versus normalized ion time for the Agilent 500 Ion Trap and a competitive ion trap.*

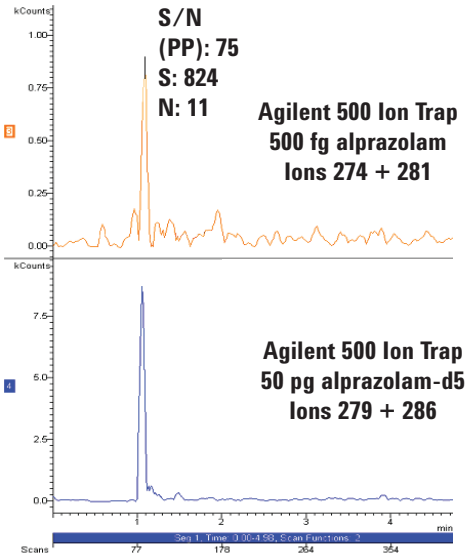


*Figure 5. No signal suppression observed with the Agilent 500 Ion Trap for alprazolam with the presence of large amount of coeluting compound.*

## Benefits

Enhanced charge capacity (EEC) provides the ion trap with the capability to reliably detect trace amounts in a high concentration of coeluting analytes in heavy matrices.

## References


1. "A new ion ejection method employing an asymmetric trapping field to improve mass scanning performance of an electrodynamic ion trap," International Journal of Mass Spectrometry Vol. 190/191; (1999) 129-143.
2. "Mass scanning in an asymmetric trapping field," Proc. 44th Ann. ASMS Conf. on Mass Spectrometry and Allied Topics, Portland, OR, May 12-16, 1996, p.126.

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