응용 자료

LCT Premier: Enhanced MS Resolution

Waters Corporation

This is an Application Brief and does not contain a detailed Experimental section.

Abstract

The Waters LCT Premier Mass Spectrometer is the highest performance benchtop orthogonal acceleration time-of-flight (oa-TOF) LC-MS system available today.

Benefits

The LCT Premier: for enhanced resolution with superior peak definition that results in unsurpassed specificity and exact mass measurement.

Introduction

The Waters LCT Premier Mass Spectrometer is the highest performance benchtop orthogonal acceleration time-of-flight (oa-TOF) LC-MS system available today. Its innovative design incorporates a TOF analyser that has the capability of switching between two preset modes of resolution operation at the simple click of a button: V transmission providing >5000 Full Width Half Maximum resolution (FWHM) (Figure 1) and W transmission providing >10,000 FWHM resolution (Figure 2). Figure 3 shows how FWHM resolution is calculated.

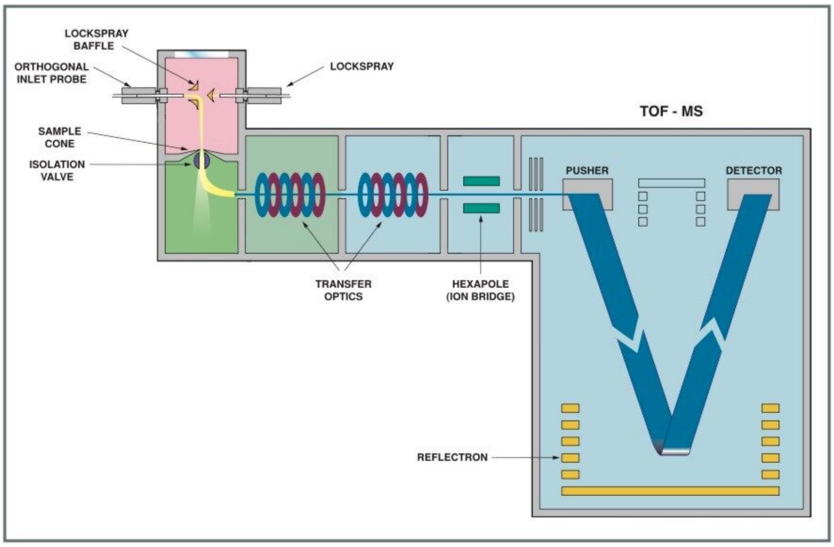

Figure 1. LCT Premier Mass Spectrometer's V transmission.

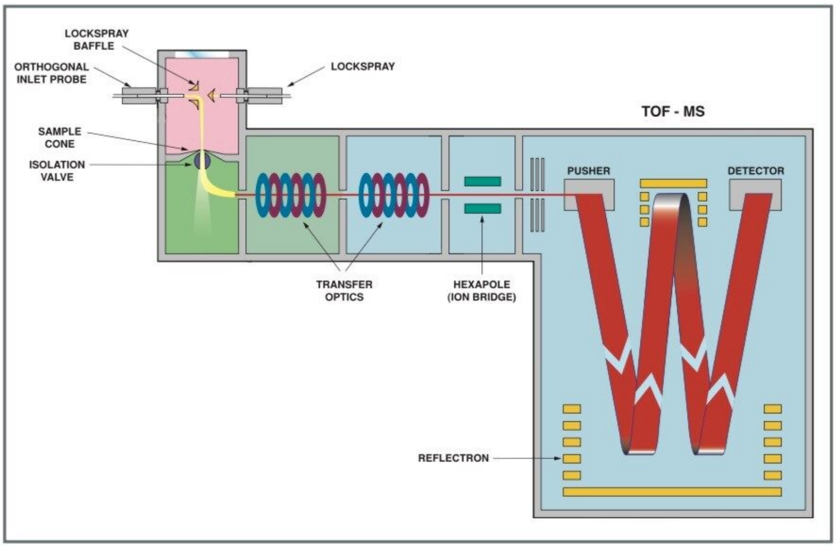

Figure 2. LCT Premier Mass Spectrometer's W transmission.

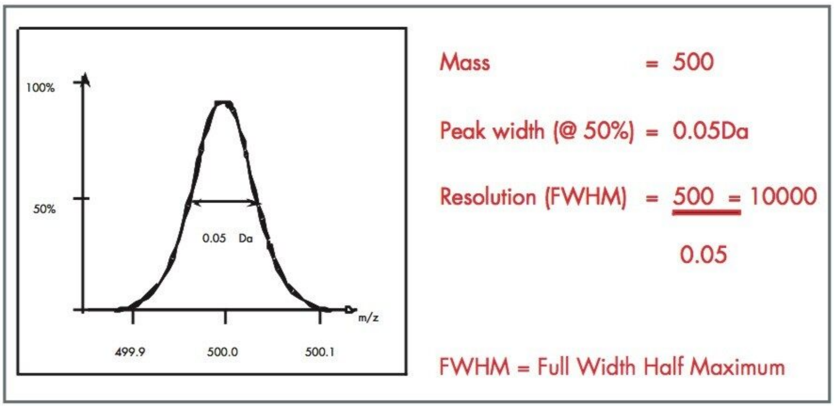

Figure 3. Example of resolution calculation for oa-TOF.

TOF mass spectrometry, with its elevated resolution, provides the user with the ability to perform exact mass measurements to within 3 ppm of the actual mass. This allows enhanced specificity of the analytical answer and therefore a higher confidence that the answer is correct.

Results and Discussion

Figure 4 shows the typical resolution provided by the LCT Premier in both V and W mode transmission and compares the resolution to that of a typical scanning quadrupole or ion trap style instrument. Due to the narrow spectral peaks provided by the LCT Premier, isobaric interferences can be distinguished easily but also provide the ability to accurately determine the peak's center. Because the accuracy of determining the center of the spectral peak is enhanced, an exact mass measurement to within 3 ppm of actual can be determined with a high degree of confidence. All this can be done during an LC-MS experiment, providing the user with a highly specific answer.

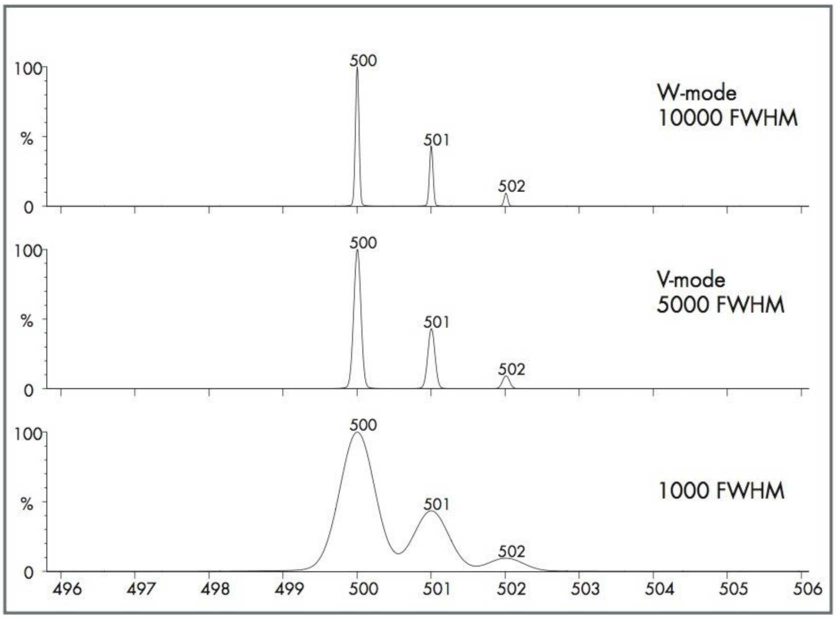

Figure 4. Comparison of V and W mode resolution on the LCT Premier with typical scanning quadrupole/ion trap resolution.

Figure 5 clearly shows the benefit of enhanced resolution provided by the LCT Premier. In this example, a scanning quadrupole instrument and LCT Premier have been used to analyse the same sample. With the quadrupole instrument a single molecular ion is produced at a nominal mass of m/z 215. However, with the LCT Premier with mass resolution of 10,000 FWHM, two distinct ions can be seen - one due to the component of interest and one due to a contaminant ion at the same nominal mass. With the resolving power of LCT Premier, an exact mass measurement for both ions is possible whereas with the quadrupole instrument, the two components would not be detected. Such selectivity obtained with the LCT Premier provides greater confidence in the analytical result.

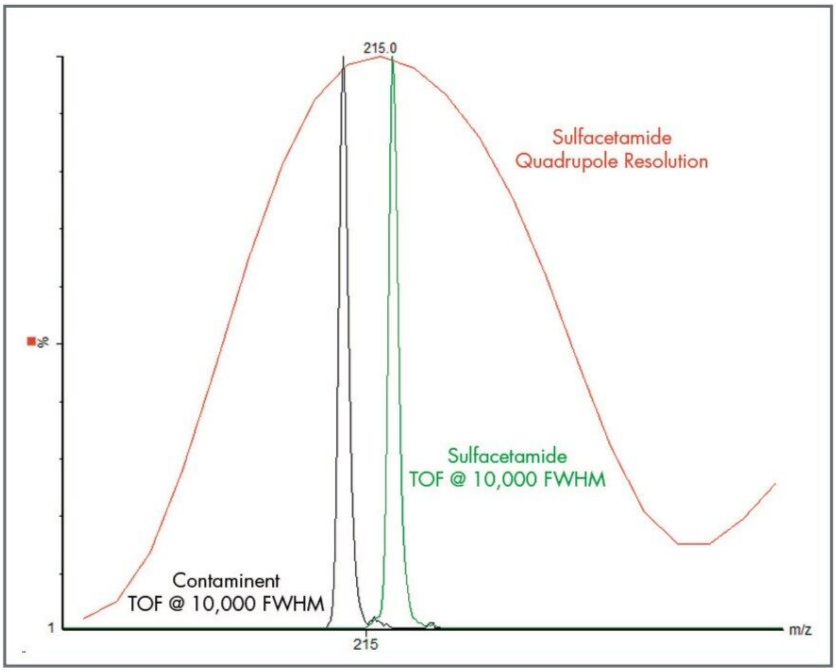

Figure 5. Benefits of oa-TOF against quadrupole resolution.

Figure 6 shows the mass spectrum of the $[M+4H]^{4+}$ isotope pattern of mellitin acquired in both V and W-mode optics. This typical resolution was calculated at 6,200 FWHM in V-mode and 11,400 FWHM in W-mode.

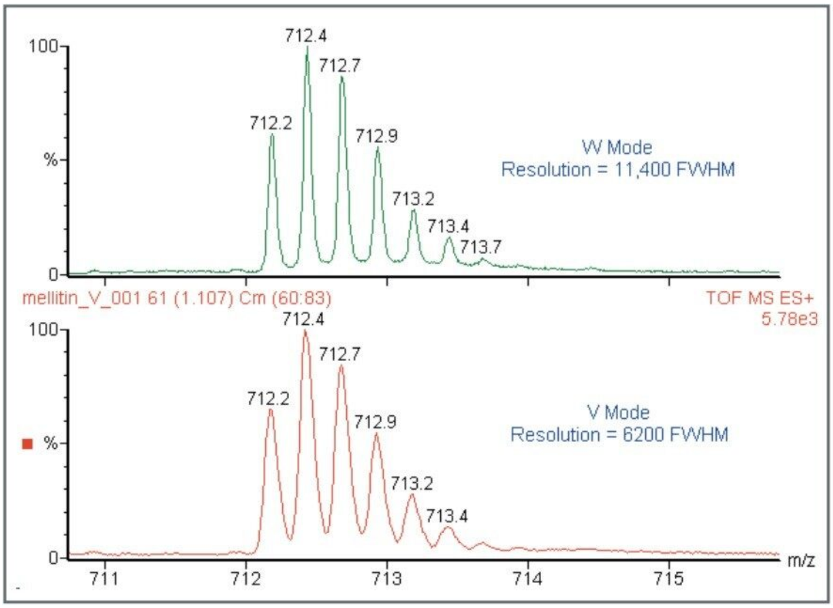

Figure 6. V and W-mode mass spectra of $[M+4H]^{4+}$ isotope pattern of mellitin.

Figure 7 shows the mass spectra of the singly charged molecular ion of leucine enkephalin ($[M+H]^+$ = 556.2771) acquired in both V and W mode optics. By measuring the width at half height, the resolution was calculated at 5,500 FWHM for V-mode and 11,000 FWHM for W-mode.

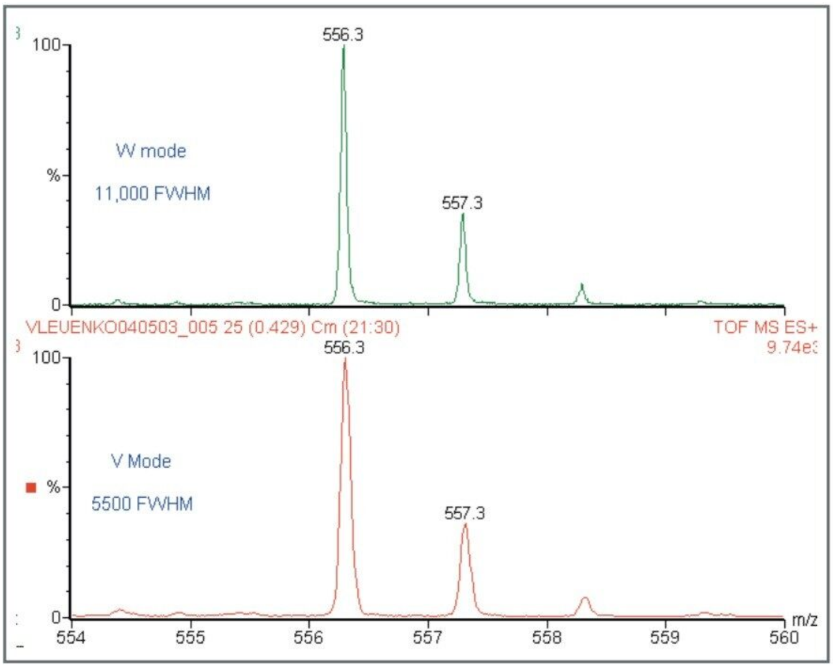

Figure 7. V and W-mode mass spectra of leucine enkephalin.

In addition to the improved TOF analyser in the LCT Premier that provides enhanced resolution, ions are detected and recorded using a 4 GHz time-to-digital converter (TDC). This technology provides unsurpassed peak definition even at low mass (<500 *m/z*), particularly when compared to other TOF detection devices such as an analogue-to-digital converter (ADC). When analysing ions below *m/z* 1,000 with an ADC, there is a significant reduction in peak definition due to the number of points physically acquired across such low mass ions.

With a TDC, there is negligible drop off in resolution definition even down to low *m/z* values. Figures 8a-8e show singly charged $[M+H]^+$ ions of some small pharmaceutical type molecules, from *m/z* 556 to *m/z* 152, where resolution is maintained with the use of a TDC.

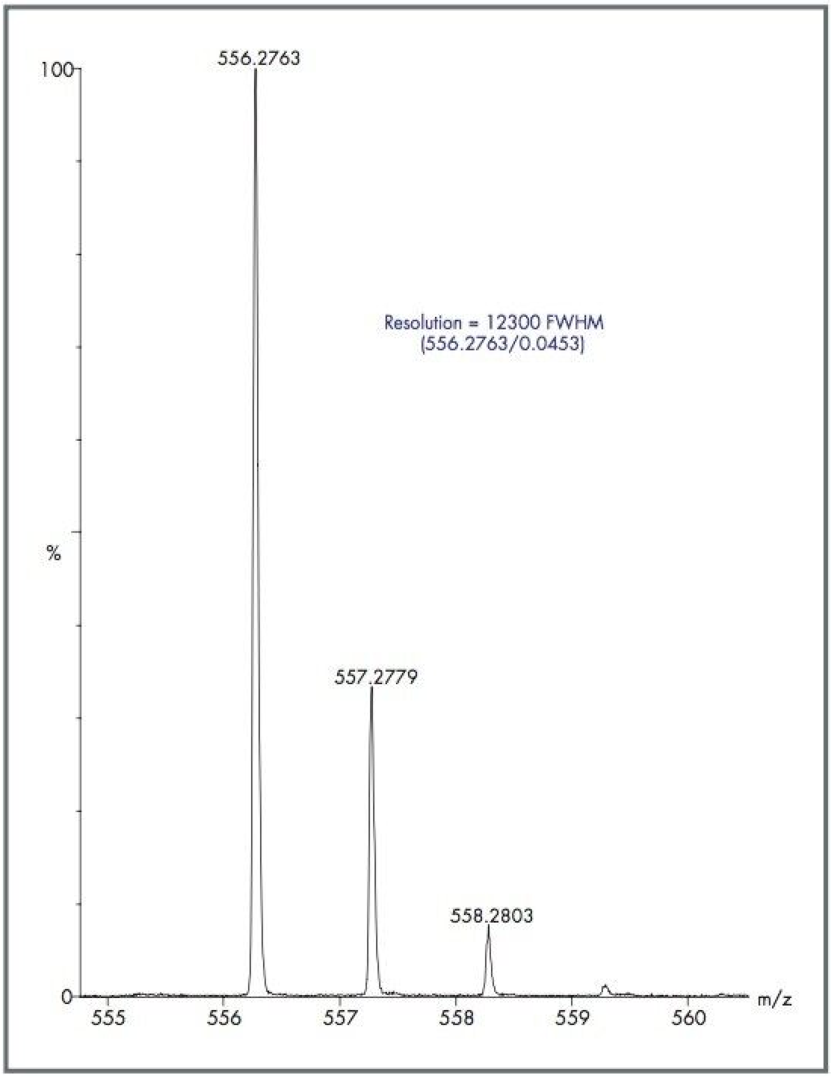

Figure 8a. Resolution measurement at m/z 556.

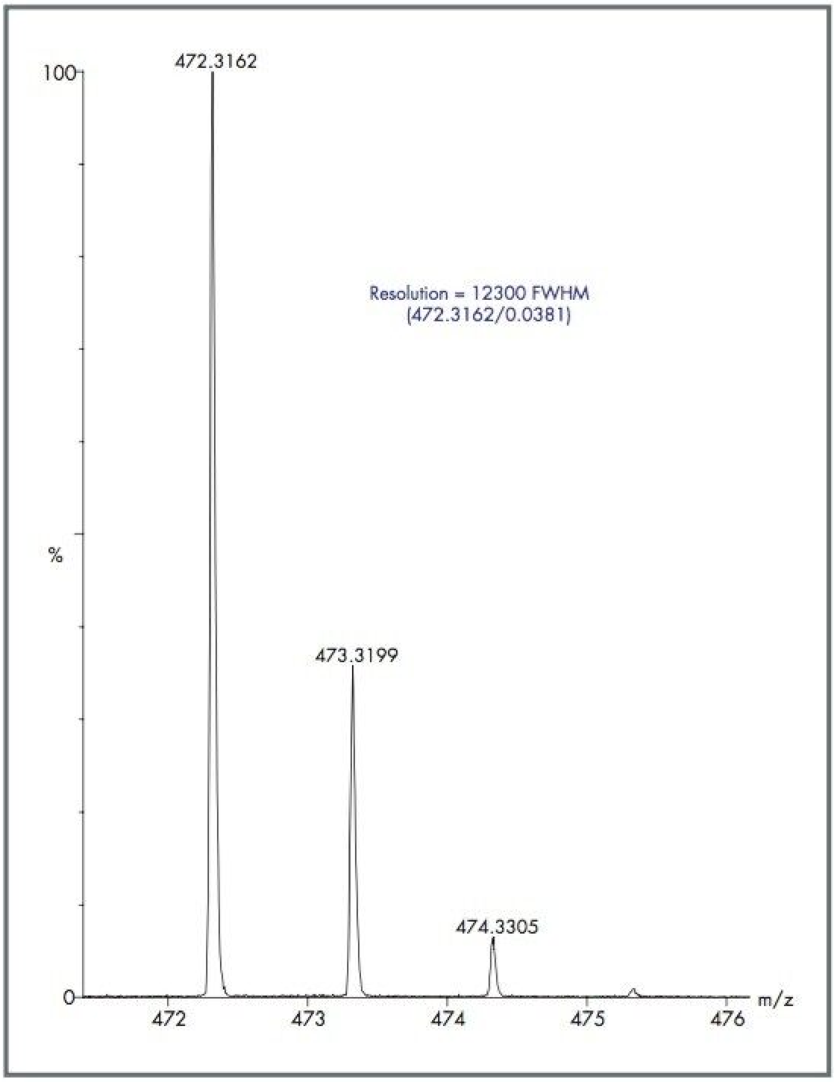

Figure 8b. Resolution measurement at m/z 472.

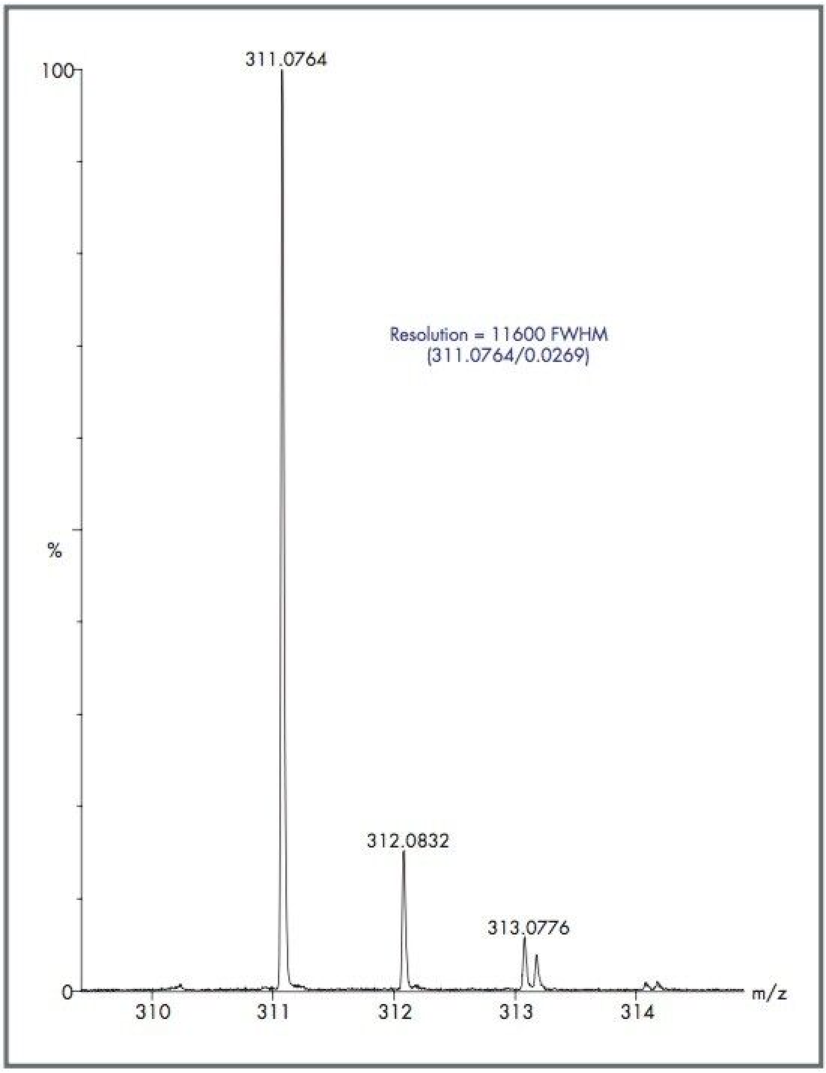

Figure 8c. Resolution measurement at m/z 311.

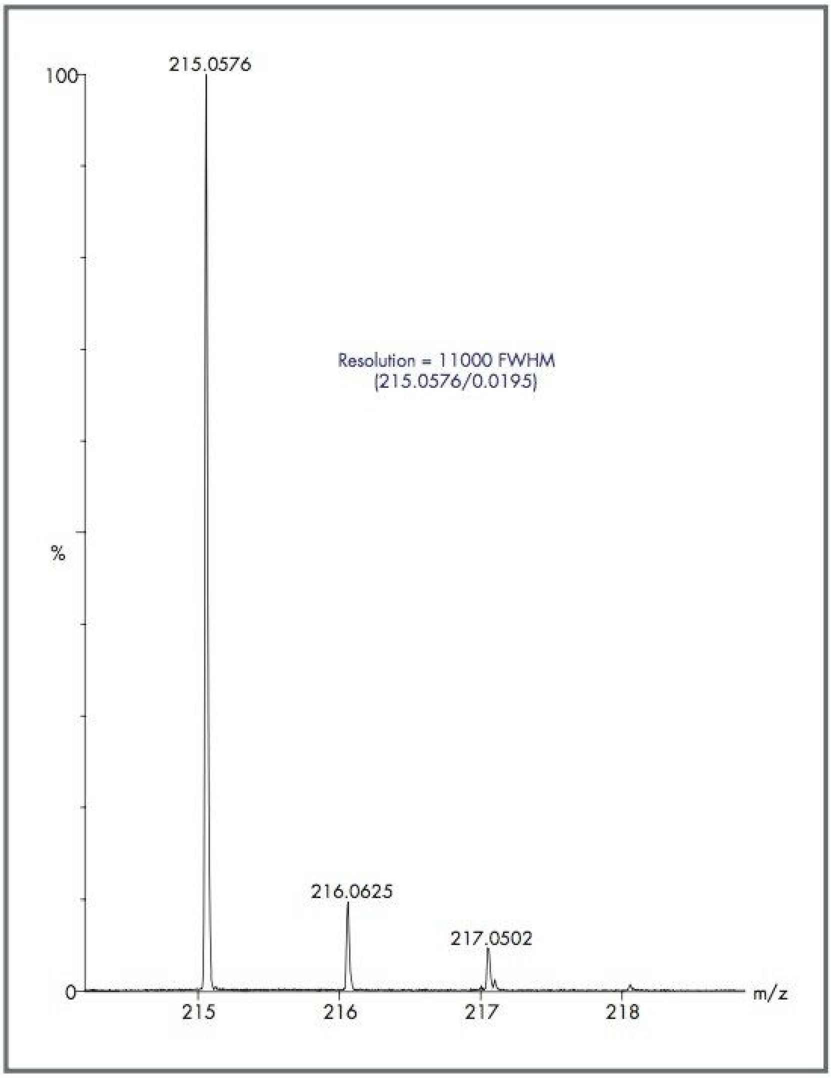

Figure 8d. Resolution measurement at m/z 215.

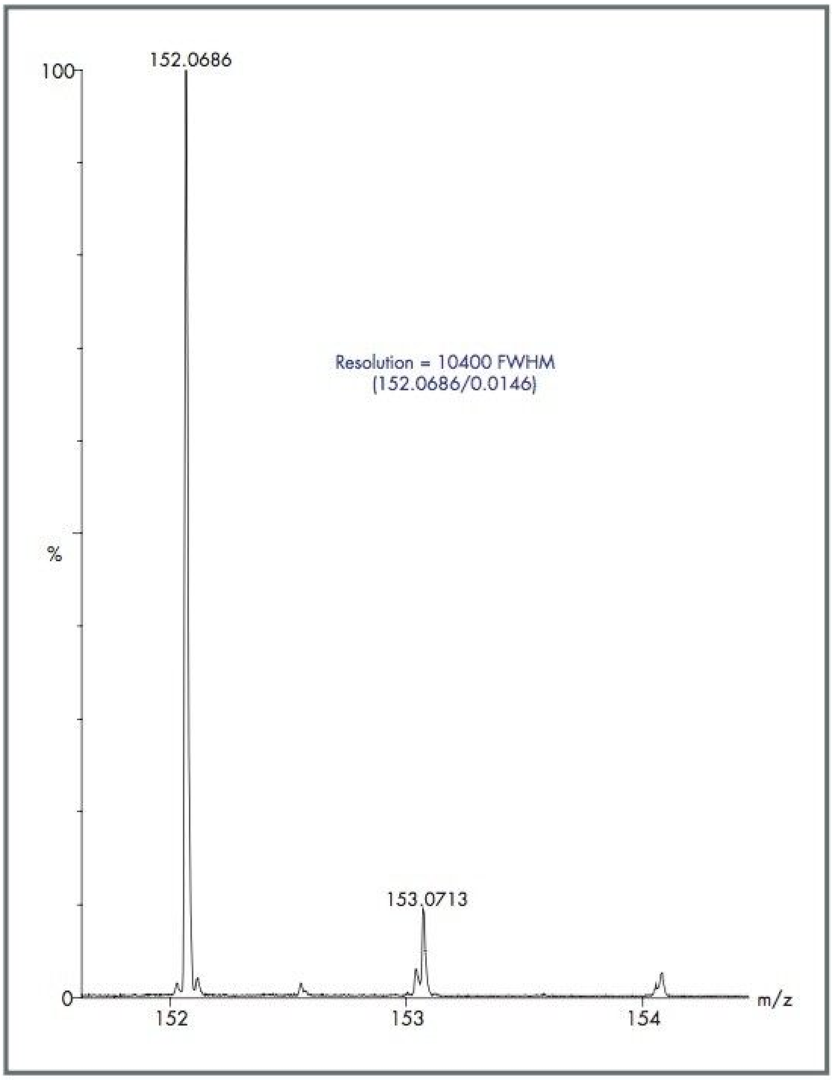

Figure 8e. Resolution measurement at m/z 152.

Conclusion

The LCT Premier: for enhanced resolution with superior peak definition that results in unsurpassed specificity and exact mass measurement.

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