Waters™

Applikationsbericht

LCT Premier – Enhanced Spectral Resolution for Improved Analytical Specificity

Waters Corporation

Abstract

The Waters Micromass LCT Premier is the next generation of oa-TOF mass spectrometer that provides the user with high resolution mass spectrometry in a bench-top LC-MS instrument. LCT Premier incorporates a new time-of-flight mass analyzer that allow the user to switch between patented 'V' and 'W' TOF analyzer optics, with W-Optics providing an additional 2x spectral resolution for a single analytical experiment. This results in improved specificity.

Benefits

LCT Premier provides an oa-TOF instrument with unsurpassed resolution, specificity, and exact mass measurement, even at low *m/z* masses, for wide ranging analytical applications.

Introduction

Enhanced MS resolution is vital for identifying components in complex analytical mixtures and is essential for enabling automated exact mass measurement. High resolution MS minimizes potential interferences to the peak shape of your analyte of interest. By removing interferences due to contaminants/matrix effects, a more accurate measurement of mass-to-charge ratio (*m/z*) can be made. The inherent high resolution capability of oa- TOF (orthogonal acceleration time-of-flight) mass spectrometry allows exact mass measurement and the unambiguous determination of elemental composition, enabling compounds to be easily identified.

The Waters Micromass LCT Premier is the next generation of oa-TOF mass spectrometer that provides the user with high resolution mass spectrometry in a bench-top LC-MS instrument. LCT Premier incorporates a new time-of-flight mass analyzer that allow the user to switch between patented 'V' and 'W' TOF analyzer optics, with W-Optics providing an additional 2x spectral resolution for a single analytical experiment. This results in improved specificity.

V-Optics and W-Optics

W-Optics is a novel method of enhancing spectral resolution without increasing the instrument footprint. By activating an additional ion mirror in the TOF analyzer, at the single click of a button, the unique flight path of the ions is effectively doubled, producing a 2x improvement in resolution. Although the ions have a second pass through the analyzer for W-Optics, the unique flight path ensures the wide mass range of the analyzer is not compromised.

With LCT Premier, V-mode provides >5,000 FWHM resolution (full width half maximum, Figure 1) while W-

mode provides >10,000 FWHM resolution (Figure 2). Figure 3 shows the typical spectral resolution obtained on an LCT Premier with both V-Optics (5000 FWHM) and W-Optics (10,000 FWHM) and compares this to the spectral resolution that is typically obtainable from a scanning quadrupole or ion trap style instrument. The benefit of having high resolution from a TOF instrument is improved specificity of data resulting in the ability to determine an exact mass measurement with high precision during a real time LC-MS experiment.

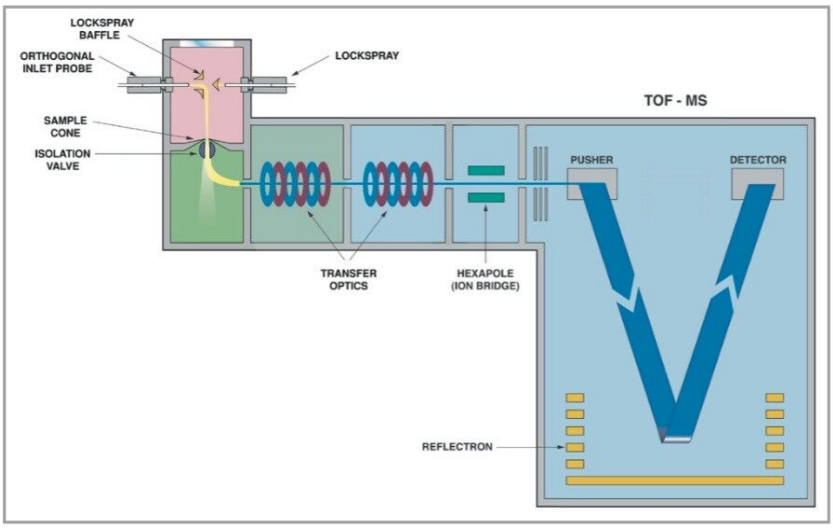

Figure 1. V-Optics.

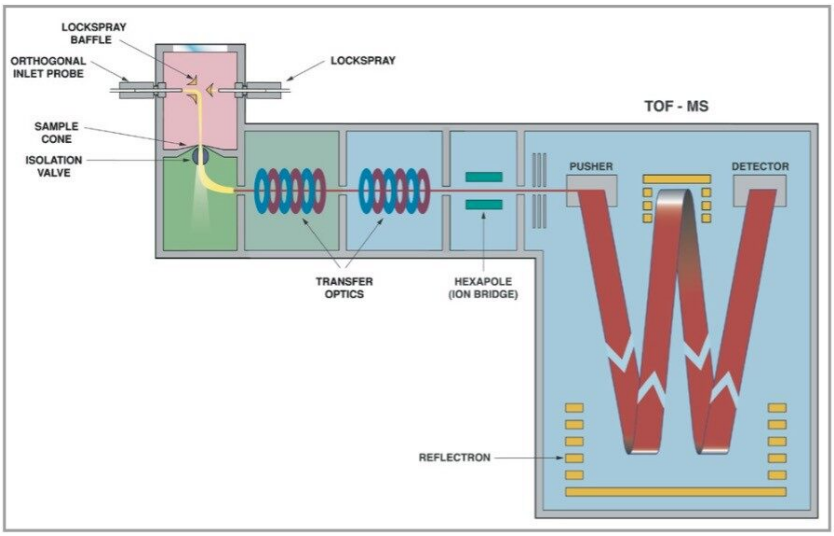

Figure 2. W-Optics.

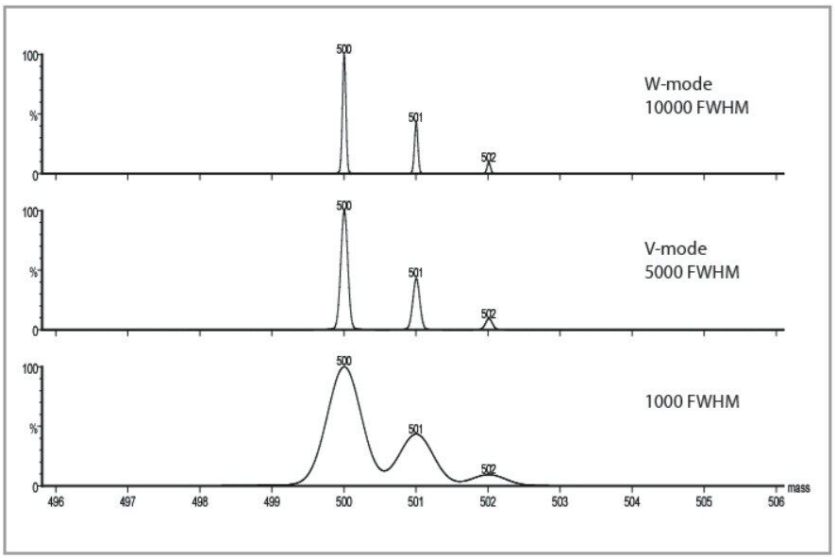

Figure 3. Comparison of V and W-mode resolution on LCT Premier with typical scanning quadrupole/ion trap resolution.

To take full advantage of the enhanced resolution provided by the LCT Premier's improved TOF analyzer, ions are detected and recorded using a 4 GHz time-to-digital converter (TDC). Assuming an ultimate instrument spectral resolution of 11,000 FWHM (ignoring any detector effects), Figure 4 compares the typical displayed resolution obtainable against *m/z* with a TDC based system to that of an ADC (analog-to-digital converter) based system. This graph is based on a edge detecting TDC with a 0.5 nsec jitter (as used on LCT Premier) and an ADC with a 2 nsec peak width.

The outcome is enhanced resolution with superior peak definition even for low mass ions with LCT Premier - resulting in unsurpassed specificity and exact mass measurement.

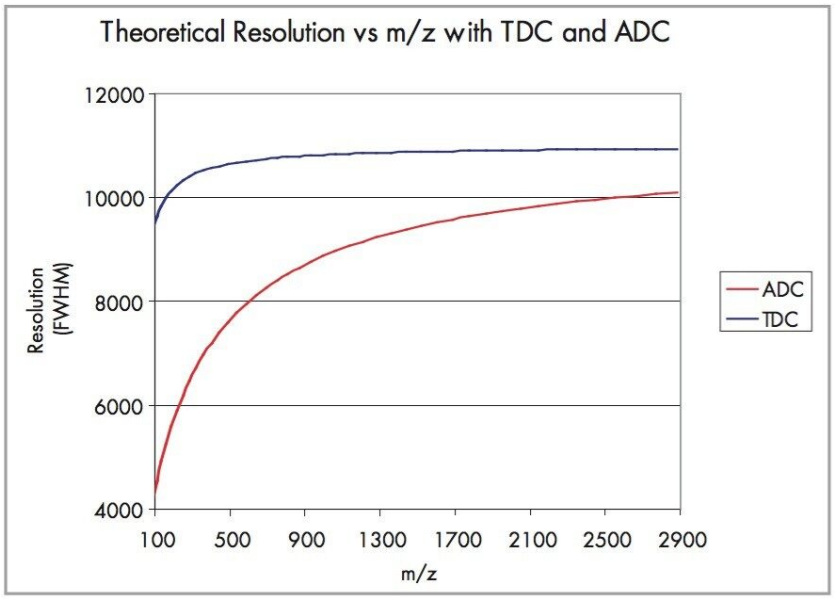

Figure 4. Theoretical spectral resolution of TDC to ADC.

Results and Discussion

Examples of Spectral Resolution on the LCT Premier

Figure 5 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. In terms of sensitivity, acquiring data in W-mode optics reduces the signal intensity by a factor of 4 due to a second pass through the reflectron.

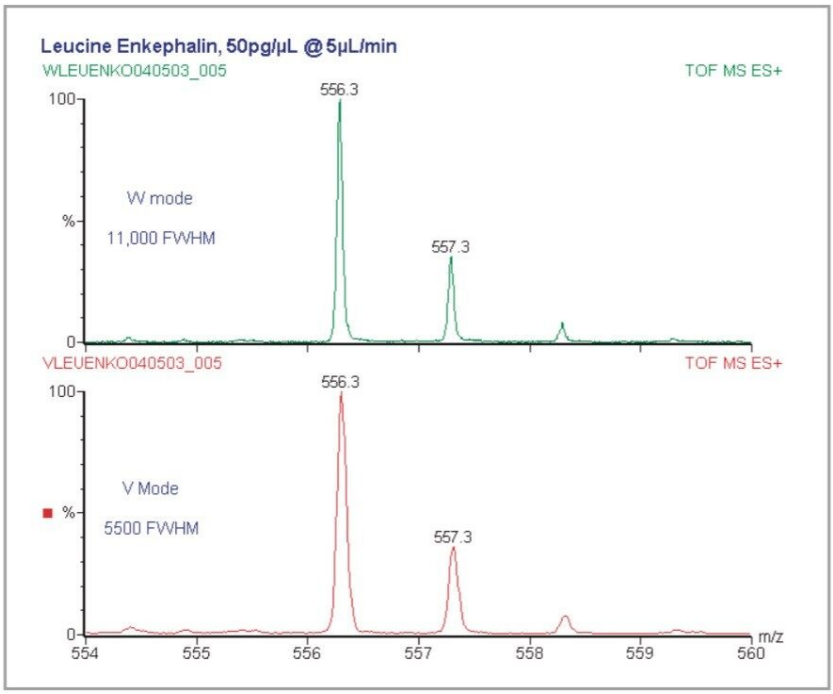

Figure 5. V and W-mode mass spectra of leucine enkephalin.

Figures 6 and 7 show the applicability of the enhanced resolution available with LCT Premier to the measurement of multiply charged species. 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.

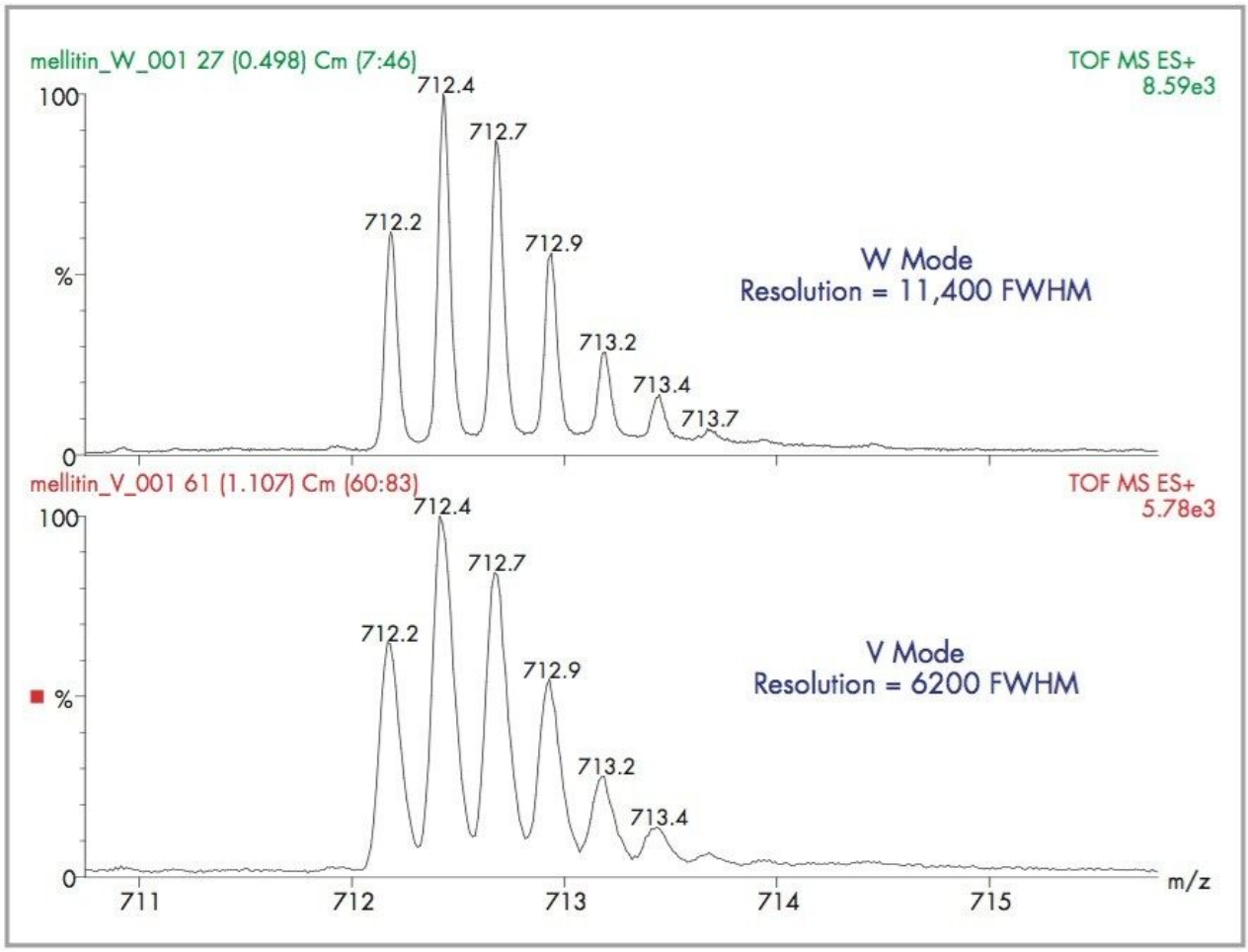

Figure 6. V and W-mode mass spectra of $[M+4H]^{4+}$ isotope pattern of mellitin.

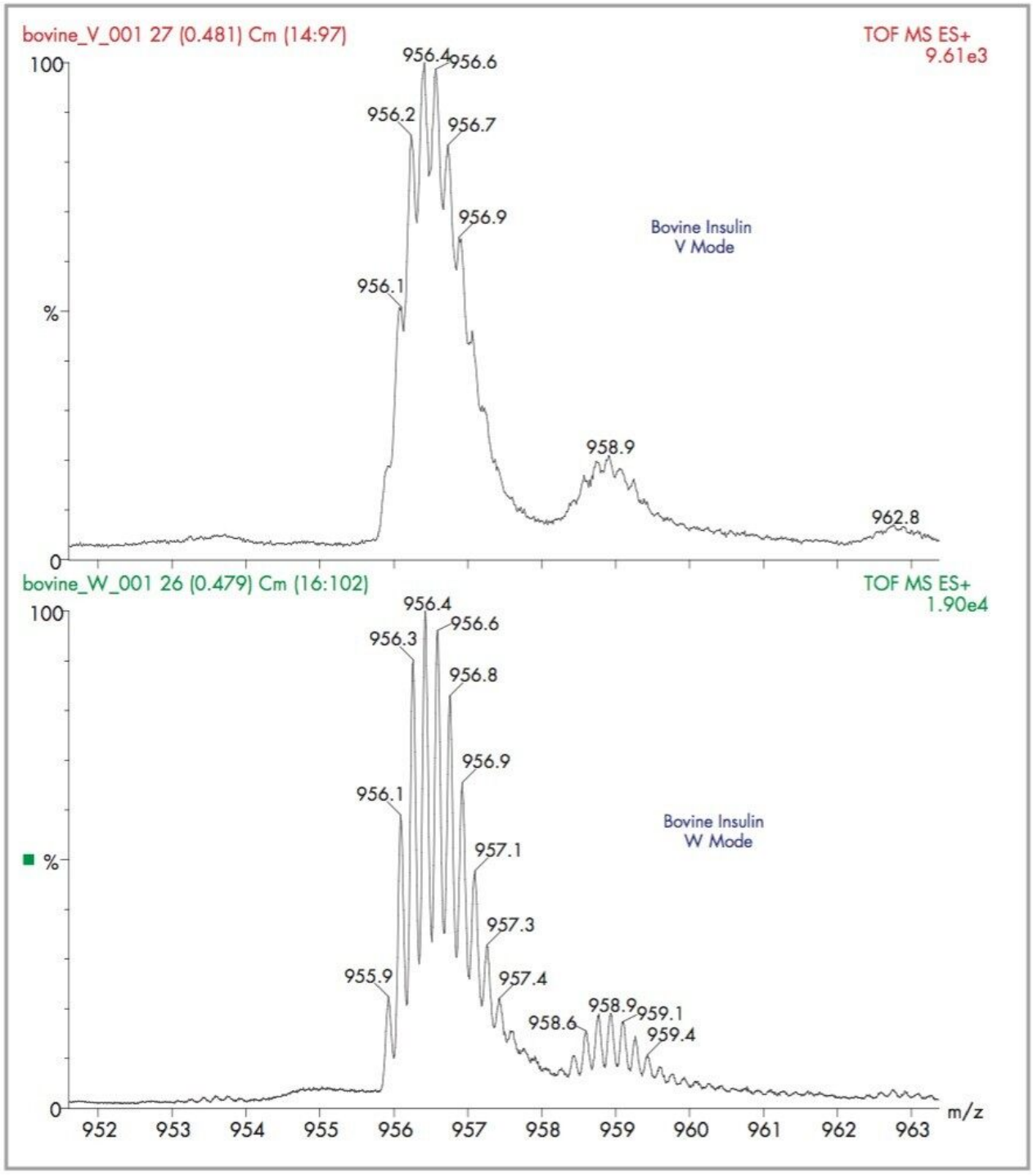

Figure 7. V and W-mode mass spectra of $[M+6H]^{6+}$ isotope pattern of bovine insulin.

Figure 7 shows the mass spectra of the $[M+6H]^{6+}$ isotope pattern at m/z 956 of bovine insulin acquired in both V and W-Optics. Clearly the figure shows the benefit of having the additional resolution available with W-Optics. Additional to this, the data acquired in W-mode was processed through the MaxEnt1 package available

within MassLynx to produce the theoretically protonated mass. The resolution provided by W-Optics allowed an exact mass measurement of the singly charged ion to be calculated at *m/z* 5733.5815, 0.9ppm from the theoretical (*m/z* = 5733.5765) (Figure 8). Such high resolution obtained using W-Optics on LCT Premier affords excellent mass measurement accuracy, even for high molecular weight proteins, ultimately providing the analyst with enhanced specificity and an increased confidence in the analytical answer.

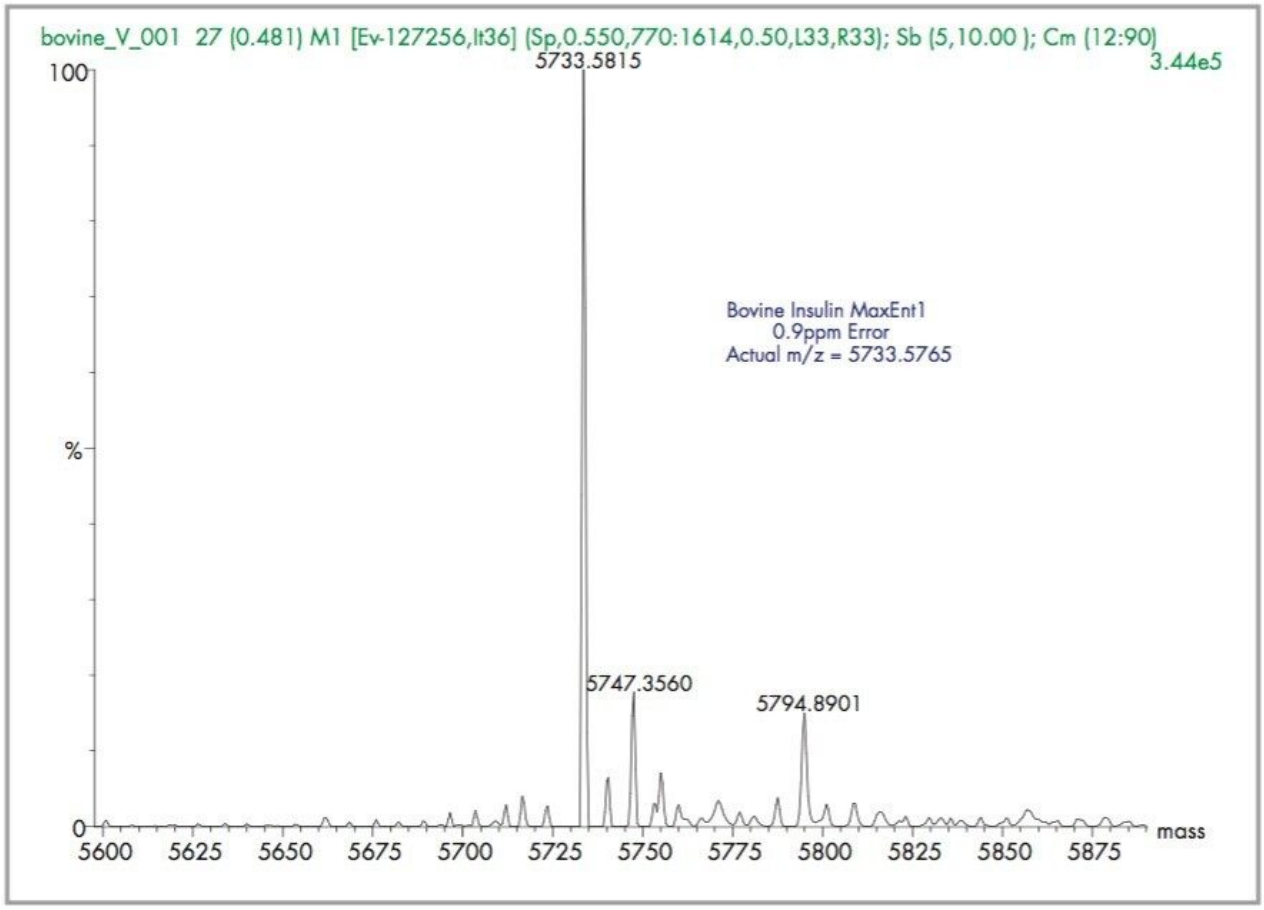

Figure 8. MaxEnt1 processed spectrum of the singly charged ion of bovine insulin.

Conclusion

LCT Premier is the next generation of oa-TOF mass spectrometer that provides the user high resolution mass spectrometry in a bench-top LC-MS instrument. Incorporating a new TOF mass analyzer with an additional ion mirror, V or W-Optics can be easily selected for either 5,000 or 10,000 FWHM spectral resolution. Coupled

with the 4 GHz TDC for superior peak definition, LCT Premier provides an oa TOF instrument with unsurpassed resolution, specificity, and exact mass measurement, even at low *m/z* masses, for wide ranging analytical applications.

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