

SpiralTOF™

Measurement of a Dendritic MS Reference Standard

Introduction:

A high-quality mass calibration is required to achieve highly accurate mass measurements by mass spectrometry. A polymer or a mixture of peptides is commonly used to calibrate a MALDI-TOF MS system. However, peptides do not necessarily have long-term stability, and a monodisperse polymer does not have a wide m/z range. Sometimes these standards are not well suited for calibration over a wide m/z range.

We used a new dendritic MS calibrant (SpheriCal®) to resolve these issues. Here we demonstrate measurement and calibration using the new calibrant with the JEOL SpiralTOF MALDI mass spectrometer.

Experimental:

The new SpheriCal® High Range dendritic MS reference standard was obtained from the Polymer Factory

(<http://www.polymerfactory.com/>). The sample was dissolved in tetrahydrofuran at a concentration of 10 mg/mL. A 0.5 μ L sample was deposited and dried on the MALDI target plate. An additional matrix was not required because it is already included in the SpheriCal® reference standard mixture.

Results:

The MALDI mass spectrum is shown in Figure 1, and the comparison of measured and theoretical isotopic distribution for m/z 6000 are shown in Figure 2. The delay time was set to achieve the highest mass resolving power at m/z 6000. Therefore, the resolving power was approximately 85,000 for the $[C_{320}H_{372}O_{110}Na]^+$ peak, well in excess of that needed to separate isotope peaks.

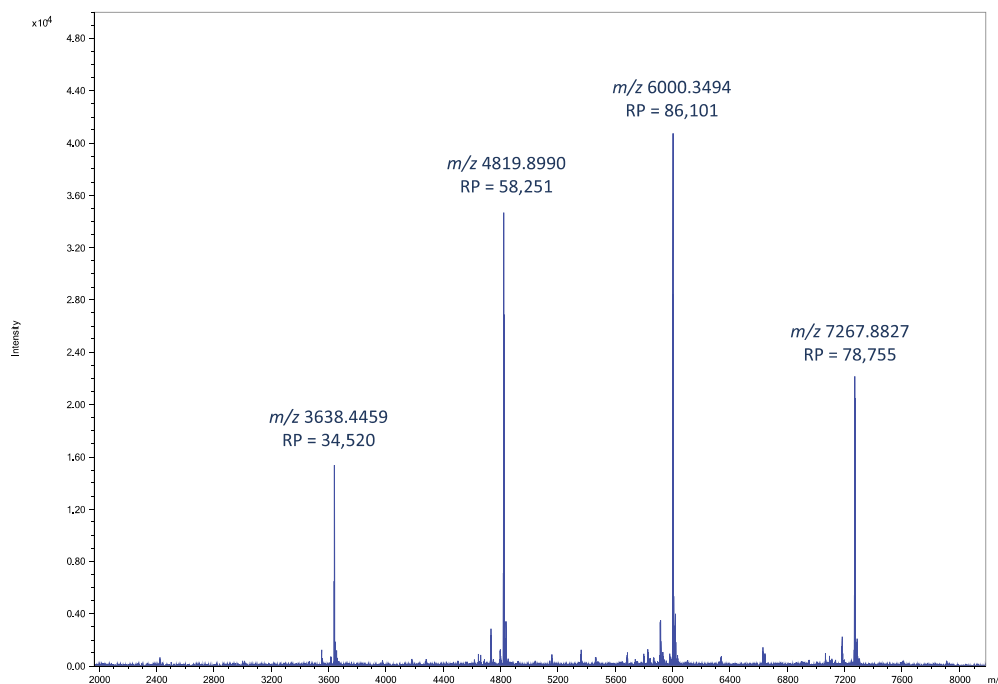
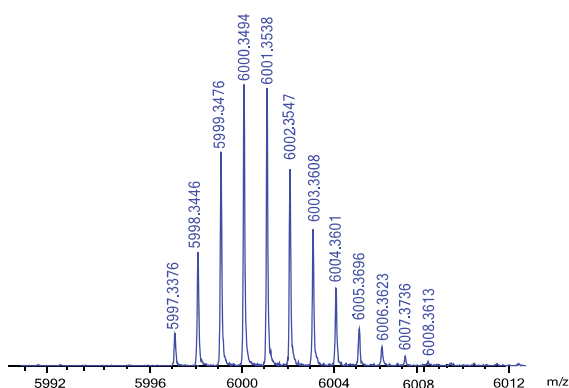


Figure 1. MALDI mass spectrum of SpheriCal® High Range standard.

Measured isotopic distribution



Theoretical isotopic distribution

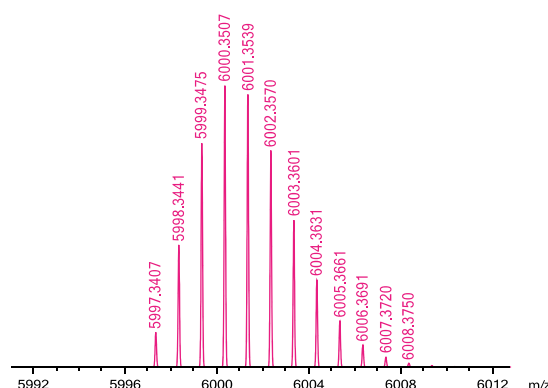
$$C_{320}H_{372}O_{110}Na^+ \text{ (RP = 85,000)}$$


Figure 2. The comparison of measured and theoretical isotopic distribution.

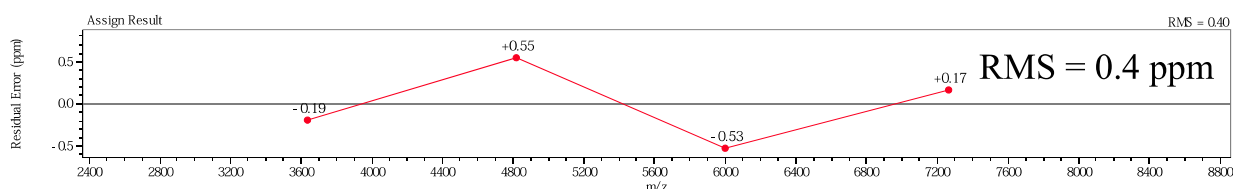


Figure 3. The residual plot for the calibration curve obtained by using the SpheriCal[®] High Range standard.

A residual plot for the calibration curve is shown in Figure 3. We were able to calibrate the system by using the monoisotopic ions for each dendrimer because the SpiralTOF is able to detect these species with enough intensity to achieve a high-quality mass calibration (see Figure 2). The Root Mean Square (RMS) mass error of actual measured m/z value against the calibration curve was just 0.4 ppm with this calibrant.

Conclusion:

In this study we demonstrated measurement and calibration using a new dendritic mass reference standard with the JEOL SpiralTOF MALDI mass spectrometer.

The SpiralTOF provides:

- Ultra high resolving power sufficient to separate isotopic ions and signal-to-noise ratios sufficient to detect monoisotopic ions in the high m/z region.

- Routine high mass accuracy (less than 1ppm)

A high-quality mass calibration curve over a wide m/z range was achieved by using the new dendritic calibrant and the JEOL SpiralTOF.

Reference:

1. Yeija Li, Jessica N. Hoskins, Subramanya G. Sreerama, Michael A. Grayson and Scott M. Grayson. *The identification of synthetic homopolymer end groups and verification of their transformations using MALDI-TOF mass spectroscopy*. *J. Mass Spectroscopy*, 2010, 45, 587-611.
2. http://www.polymerfactory.com/images/articles/Grayson-Universal_MS_calibrants_ASMS%202011.pdf