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Application Note

The Use of Enhanced Ion Mobility Resolution with MALDI SYNAPT G2 HDMS for Total Solvent-Free Analysis (TSA) of Palimitic Acid

Emmanuelle Claude

Waters Corporation

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

Abstract

Differentiation of fatty acids from isobaric species by efficient ionization, ion mobility separation, and MS/MS fragmentation with positive ion MALDI mass spectrometry.

Benefits

The MALD I SYNA PT G2 HDMS System allows the successful separation and parallel fragmentation of isobaric species, enabling more confident detection and identification of fatty acids.

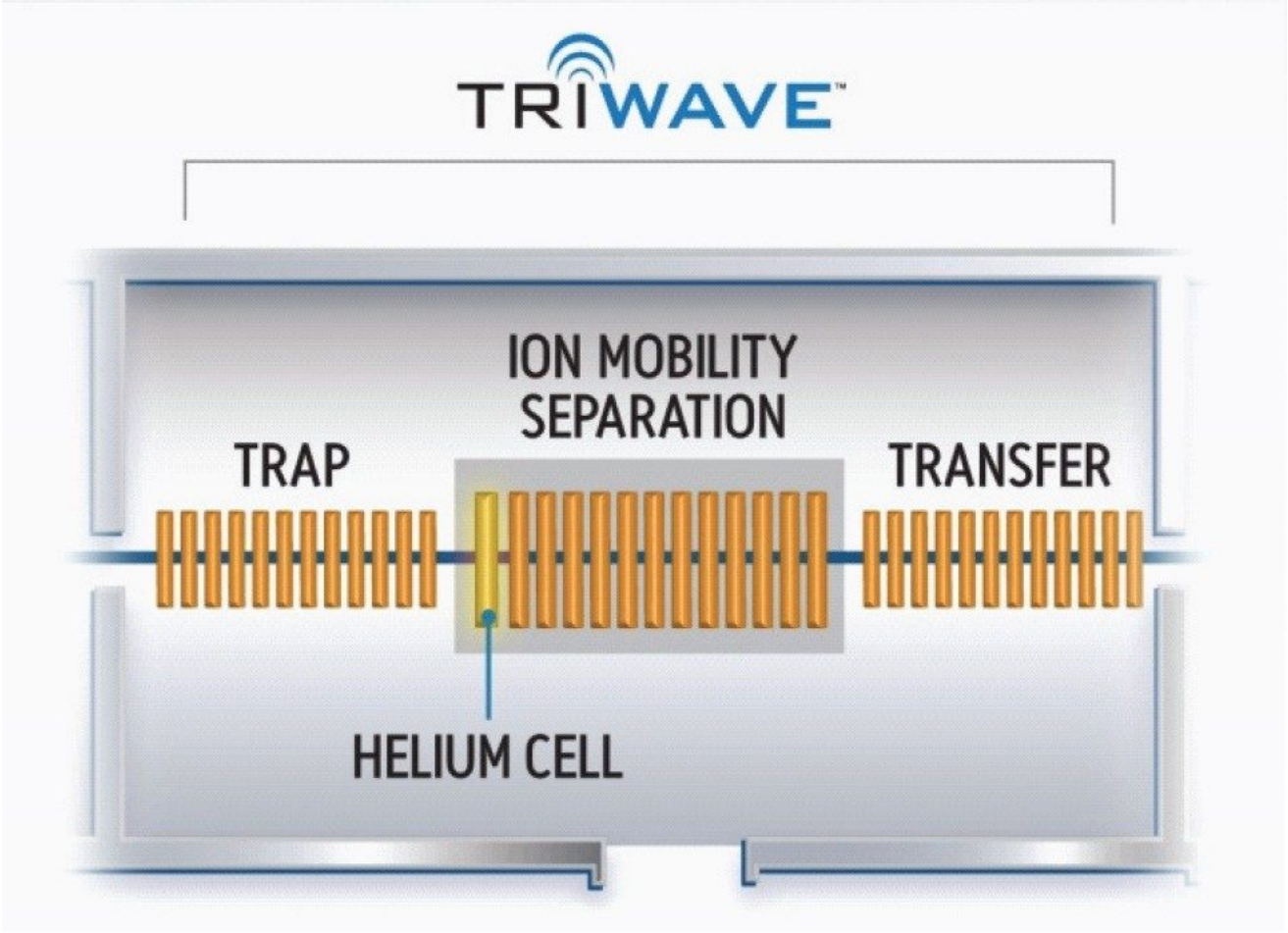
Introduction

Total Solvent-free Analysis (TSA)[1-3] is an alternative way of preparing sample to improve its solubility. It consists of grinding the matrix and analyte together, regardless of solubility. A homogenous layer of matrix/analyte

sample is ionized using laser ablation[4] and is followed by ion mobility separation and mass measurement. This solvent free approach simplifies sample preparation and, as shown here, enables efficient ionization and separation of samples.

This technique is particularly useful for fatty acids, which are a difficult class of compound to ionize as a MH+ species. By using TSA, the fatty acid can be converted into a doubly–lithiated, singly-charged ion with the general formula $[M-H+2Li]^+$.

The MALDI SYNAPT G2 HDMS System provides an ideal platform to conduct this type of analysis on fatty acids, since data is acquired at high resolution, enabling exact mass measurements to be made on both precursor and fragment ions. More importantly it has the incomparable ability to separate isobaric background ions, using the enhanced gas-phase ion mobility separation within the Triwave[5] region of the MALDI SYNAPT G2 HDMS System, as shown in Figure 1.



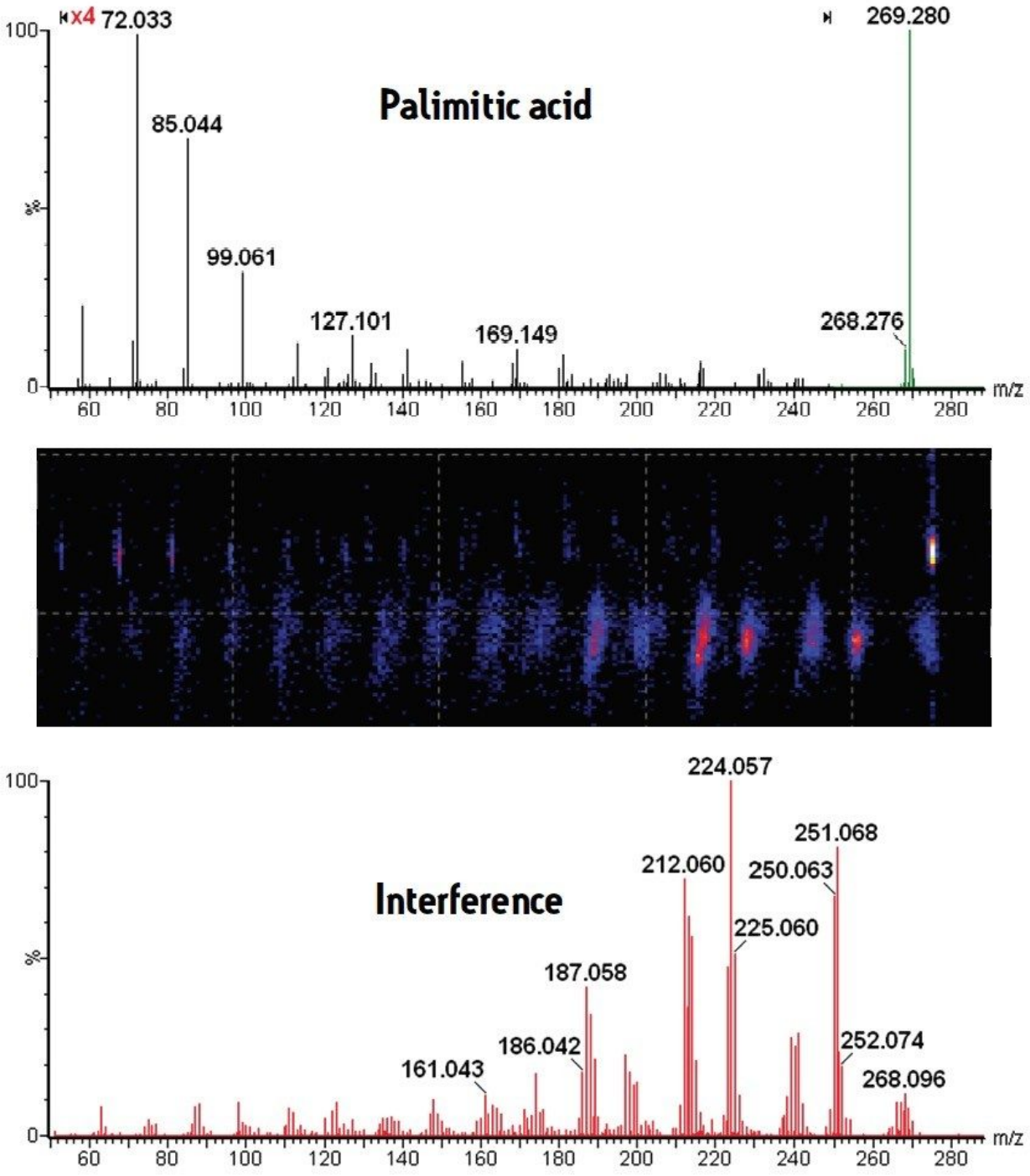
Figures 1. Schematic of the second-generation Triwave Technology in the MALDI SYNAPT G2 HDMS System.

Results and Discussion

Palimitic acid was prepared following TSA sample preparation4 and analyzed on both the MALDI SYNAPT G1 HDMS and MALDI SYNAPT G2 HDMS systems.

In MS mode, the doubly-lithiated, singly-charged ion showed a very strong signal on both instruments at mass-to-charge (*m/z*) 269.278. This m/z was then selected, with the quadrupole set to a 2 Da window, and fragmented in the TRANSFER T-Wave device.

On inspection of the IM dimension (drift time), two different species appear to be present at very similar mass. Their drift time distributions along with their individual MS/MS transfer spectra are displayed in Figure 2. The ion precursor *m/z* 269.278 with the lower mobility, thus more open gas phase structure, corresponds to the expected $[M-H+2Li]^+$. It produces fragments to lower molecular weight ions, showing charge remote fragmentation. The isobaric compound has a higher mobility and gives higher molecular weight fragment ions.



Figures 2. CID transfer fragmentation of palimitic acid on the MALDI SYNAPT G2 HDMS System, where two

isobaric species were separated by ion-mobility.

In Figure 3, we have compared the ability of the MALDI SYNAPT G1 HDMS and MALDI SYNAPT G2 HDMS instruments to separate the palimitic acid and its isobaric interference by ion mobility. There are 12 bins difference between the two species (from the apex of the T-Wave ion mobility arrival time peaks) when analyzed on the MALDI SYNAPT G1 HDMS platform, compared to 30 bins difference when analyzed on the MALDI SYNAPT G2 HDMS platform.

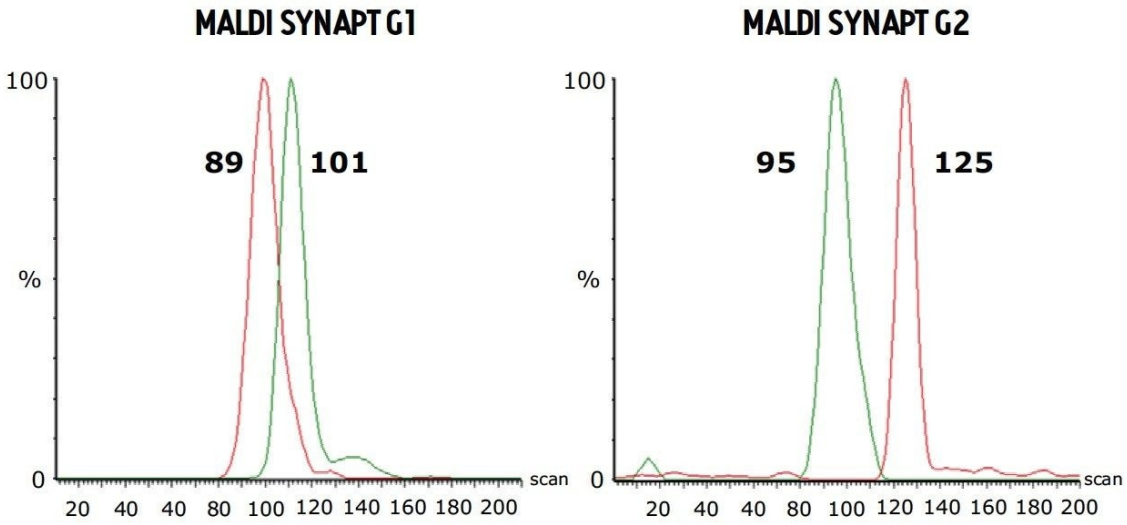


Figure 3. T-Wave ion mobility arrival time (bins) chromatograms of palimitic acid and interference isobaric species when analyzed by transfer fragmentation on the MALDI SYNAPT (G1) HDMS and MALDI SYNAPT G2 HDMS systems.

Conclusion

The MALDI SYNAPT G2 HDMS System allows the successful separation and parallel fragmentation of isobaric species, enabling more confident detection and identification of both components. Here, palimitic acid exhibited a charge remote fragmentation pattern, which is particularly helpful in structural characterization of fatty acids in

general.

The MALDI SYNAPT G2 HDMS System has significantly enhanced ion mobility separation power for the separation of isobaric species.

References

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5. The travelling wave device described here is similar to that described by Kirchner in US Patent 5,206,506 (1993).

Acknowledgments

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