REAL TIME LIPIDOMIC PROFILING USING DESORPTION IONIZATION WITH ION MOBILITY SEPARATION

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OVERVIEW

A rapid screening and fingerprinting approach for phenotypic identification and comparative lipidomics using DART ion source and ion mobility separation coupled with TOF detection.

INTRODUCTION

The analysis of lipid composition often requires very laborious and time consuming procedures. Furthermore, the detailed spatial distribution of lipid species on a surface is often missed using traditional sample preparation and lipid extraction protocols for lipidomic analysis.

The use of desorption ionization (DI) techniques in lipidomics could provide a new level of description beyond the pure measure of lipid concentration. DI-MS techniques are useful for real-time, rapid, in-situ screening of various materials including food, plant and biological samples [1].

The in situ generation of a particular profile of lipid ions has been proposed for the real-time molecular fingerprinting and diagnosis. Here, we present a rapid (few seconds), real time method to analyze lipidomic profiles in food and biological samples.

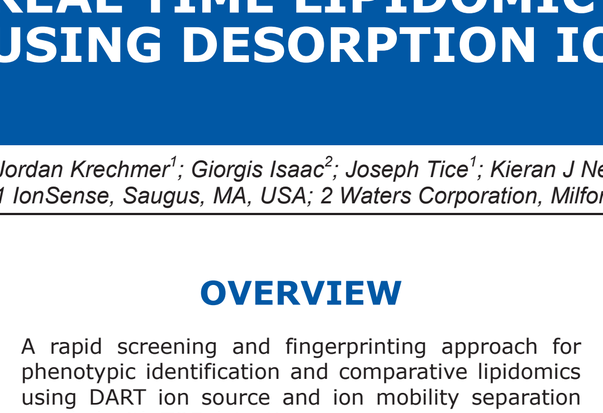
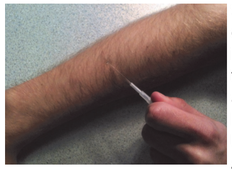


Figure 1. Representative lipid structures analyzed in the study.

Figure 2. Sebum from human skin and edible oils have been used as representative samples for the analyses.

METHODS

Sample preparation. No sample preparation required. Samples were swiped on glass capillaries, which were held in the in metastable gas beam between the ion source and MS. Data were acquired using a Direct Analysis in Real Time (DART, IonSense, MA, USA) coupled with a Waters SYNAPT™ HDMS instrument.



No chromatographic separation required. Acquisition time: 5-10 seconds.

MS Conditions

MS System	Waters Synapt™ HDMS
Ionization	DART +ve and –ve
Cone voltage	20.0 V
Source temp.	120.0 °C
DART temp.	50 to 450 °C
Cone gas	30 L/hr
Desolvation gas	800 L/hr (Nitrogen)
IMS gas	90.0 mL/min (Nitrogen)

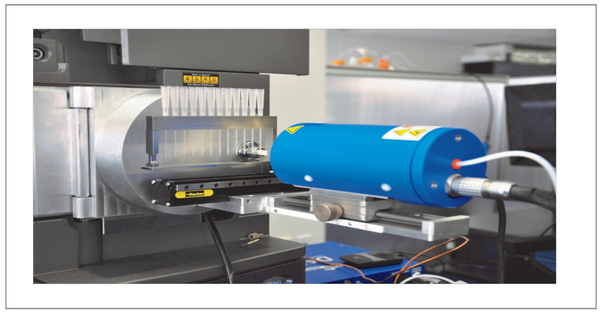


Figure 3. DART can be used as an ion source for the Waters Synapt™ HDMS instrument.

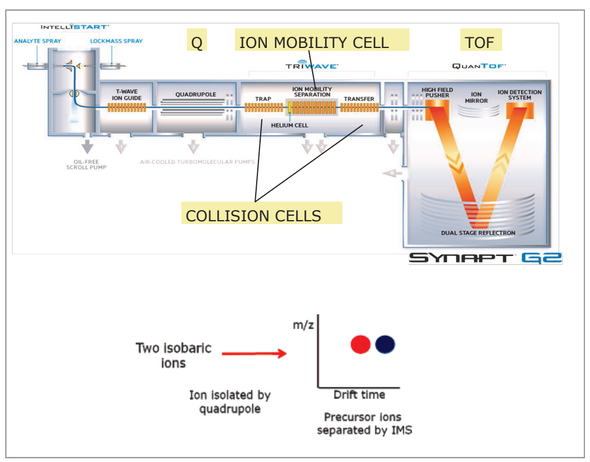


Figure 4. Schematic of the Synapt™ HDMS instrument, which allows ion mobility separation.

RESULTS

For a rapid lipidomic analysis, we combined two emerging technologies - direct analysis in real time (DART) and ion mobility separation [2].

Without the need of chromatographic separation, lipids are ionized by DART and enter in the mass spectrometer, where they pass through the Ion Mobility Separation (IMS) cell. A T-Wave mobility separator uses a repeating train of DC pulses to propel ions through the gas-filled cell in a mobility dependent manner. Lipids migrate with characteristic mobility times (drift times) according to their size and shape before TOF detection.

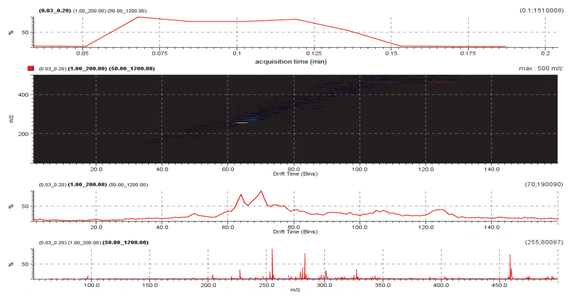


Figure 5. The entire DART-IMS-TOF analysis requires just few seconds (0.1 min). Lipids are separated by ion mobility on the millisecond time-scale.

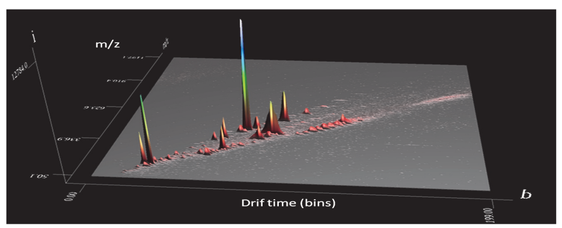


Figure 6. Software processing of the data allows the generation of 3D molecular maps based on drift time, exact mass and intensity of the signal relative to the various analytes present in the oils. Isobaric species are separated by ion mobility.

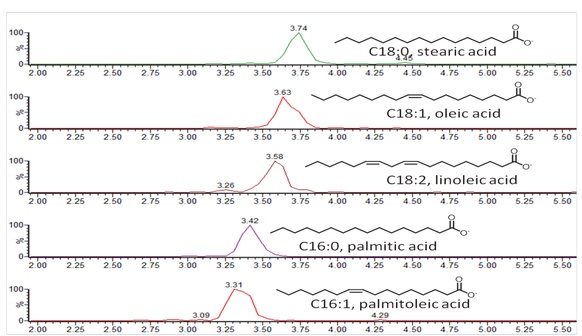


Figure 7. Ion mobility separation of fatty acids from olive oil after rapid DART ionization in negative-ion mode. Differences in the acyl chain length or number of double bonds affect the shape and size of lipid molecules, resulting in characteristic drift times.

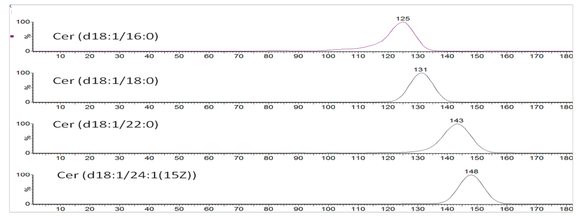


Figure 8. Ion mobility separation of ceramides from human sebum after rapid DART ionization in positive-ion mode.

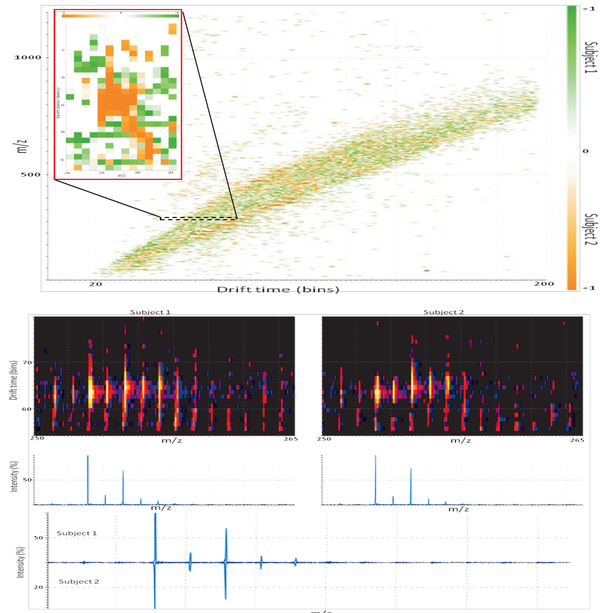


Figure 9. Comparison of human sebum (skin oils) from two subjects (subject 1, green; subject 2, orange) . Overlaying individual molecular maps clearly show areas where the samples are significantly different.

CONCLUSION

- **The combination of DART and ion mobility-TOF offers a convenient solution for lipidomic profiling.**
- **Our approach is suitable for the rapid screening of bioactive lipids, including fatty acids and ceramides.**
- **Potential applications include phenotypic fingerprinting and comparative lipidomics in the areas of personalized medicine, disease diagnostics, food analysis and traditional medicines.**

References

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2. Dear GJ, Munoz-Muriedas J, Beaumont C, Roberts A, Kirk J, Williams JP, Campuzano I. Rapid Commun Mass Spectrom. 2010 Nov 15;24 (21):3157-62.

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