



Società Chimica Italiana

Divisione di Spettrometria  
di Massa



# XXII International Mass Spectrometry Conference

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# ABSTRACT BOOK

application in several biological situations.

### References

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### ThP-125 / MICRO-UPLC-MS HIGH-THROUGHPUT SCREENING ASSAY FOR SPHINGOLIPIDS PATHWAY ANALYSIS

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**Keywords:** microflow liquid chromatography, high-throughput screening, lipidomics

### Introduction

In the presentation we will describe the Micro-UPLC-MS system based on Vanquish Focused+ LC (Thermo) and TSQ Altis Triple Quadrupole Mass spectrometer (Thermo) for lipid analysis.

### Methods

Replacing conventional tubing of the system with micro ID tubing, adding a second pump and optimizing the injection strategy allows us to convert conventional system to micro with parallel chromatography capabilities. Run time using a 5 cm length column was less than one min per injection.

### Results

This system was successfully used for affinity screening of biomarkers from lipid pathways. This strategy is valuable when highly sensitive biomarker quantification in large sample set (library screening) is required.

### Conclusions

In the poster we will demonstrate performance of the micro-LC-MS system using endogenous sphingolipid biomarkers from cell extracts at sub ng/ml (limit of quantitation is 0.05 ng/ml) concentration. We have evaluated Acclaim C8 0.3 mm i.d. and BEH C18 1 mm i.d. columns using gradient and isocratic chromatography. C8 was found to be more rugged but C18 enabled us to discriminate isobaric lipids.

### Novel Aspect

We have developed LC-MS based screens using microflow chromatography.

### ThP-126 / CERAMIDOME PLASTICITY THROUGH ISO-ENERGETIC PRECURSOR AND NEUTRAL LOSS DISCOVERY SCANS

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**Keywords:** Ceramide, epidermoside, collision-induced dissociation, screening, triple quadrupole,

### Introduction

Mass spectrometric methods of identification and measurement are pivotal to investigate the multi-faceted biological role of ceramides and the dose-effect relationship of pharmaceuticals that modulate ceramide flux. Triple-quadrupole tandem MS embodies the highest flexibility to discover, identify and measure expected and unexpected molecular species, and an unprecedented scan mode is presented [1].

### Methods

An API3000 LTQ LC-MS system is operated under manufacturer's instructions to perform extensive tandem MS fragmentation studies on standard ceramides with C<sub>6</sub>-C<sub>24</sub> fatty acids, lipid extracts of animal tissues and of nutraceutical seeds and nuts. LC separation and MS operation is optimized for the separation, detection, identification and quantification of expected and unexpected ceramides.

### Results

The equation linking instrumental to center-of-mass collision energy (CoM-CE) in collision-induced dissociation is rearranged to calculate laboratory-frame inter-quadrupole potential drop (LF-CE) corresponding to distinctive positions, such as that of the CoM-CE maximum fragment yield, in the breakdown curves for protonated ceramides with molecular masses up to 1,000 Th. The value of the CoM-CE for distinctive fragments is calculated for representative ceramide FA homologs from accurate recordings of the spectra in the 0 to 90 DV interval of LF-CE. A scan function of the q2 collision cell is synchronized with the Q1 scan in the precursor ion mode and with the Q1 and Q3 scans in the Neutral Loss mode. Several lipid extracts containing ceramides are examined by infusion and by LC, and unexpected components, such as Z-ceramides in nut extracts are tentatively identified.

### Conclusions

Precursor and Neutral Loss scans with iso-energetic CID in the triple quadrupole MS allow to characterize ceramide mixtures that contain unexpected components with a common substructure to known ones. Individual response factors for (semi)-quantification of unexpected components can be calculated from the fractional intensity of the reporter fragment in the spectra of known components.

### Novel Aspect

A novel scan function of a triple quadrupole instrument allows to measure tandem mass spectra at a constant center-of-mass collision energy.

### References

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## ThP-127 / SERUM LIPIDOMIC CHANGES IN ZIKA AND DENGUE VIRUS INFECTION REVEALS POTENTIAL TARGETS FOR ASSERTIVE CLINICAL DIAGNOSIS

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**Keywords:** Zika virus, Dengue virus, lipidomic, serum

### Introduction

The Zika (ZKV) and Dengue (DENV) Virus have been a major public health challenge in the world due to