

The Convergence of Differential Ion Mobility Spectrometry and Mass Spectrometry: *Next Generation Global and Targeted Lipid Analysis*

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The Lipidome

Comprised of multiple, structurally distinct lipid classes and sub-classes



Fundamental Challenge in Lipidomic Analysis: Isobaric Overlap

There are as many as 180,000 different lipid molecular species possible in a narrow mass range of ~700 amu

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LipidView[™] Software calculator exercise:

Select mass of 762.4 with a tolerance of 0.1 amu \rightarrow 41 lipids identified, many of which are isoelemental

Problem: Identification and quantification of lipids based on high resolution MS alone is not possible.



Challenges in Lipidomic Analysis: Isobaric Overlap

There are as many as 180,000 different lipid molecular species that are found in a narrow mass range of ~700 amu; most LC applications require 2D separation or multiple injections

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LipidViewTM Software calculator exercise:

Select mass of 762.4 with a tolerance of 1.2 amu \rightarrow 290 Lipids identified

Due to the wide Q1 isolation window, isobaric overlap makes unambiguous identification and quantification nearly impossible



Isobaric Overlap of Phospholipids

Experiment: EMS scan of Bovine Heart Extract (BHE)





Current Strategies in Lipidomics

Separation approaches:

- SPE extraction
- Fractionation
- Chemical derivatization
- Chromatography

Mass spectrometry approaches:

- Dedicated precursor and neutral loss scans (Qtrap[®] Systems)
- IDA-based methodologies (Triple TOF Instruments[®] Systems and Qtrap[®] Systems)
- MS/MS^{ALL} (Triple TOF[®] Systems Instruments)

New approach: Differential Ion Mobility Spectrometry



SelexION[™] Technology for Lipid Analysis

SelexION™ Hardware Configuration

Compatible with QTRAP® and TTOF technology

- Differential Mobility Spectrometry (DMS)
- Installation / removal of DMS in < 2mins no tools required







SelexION™ Hardware Configuration

- Compatible with QTRAP® and TTOF technology
- Installation / removal of DMS in < 2mins no tools required
- Resolves analytes prior to MS analysis







Differential Mobility Spectrometry- DMS

SelexION[™] Technology



DMS Dimensions

• Planar geometry

- Gas flow towards MS draws ions (transport gas)
- Asymmetric waveform applied which alternates between high field, K(E) and low field, K(0) – separation voltage (SV)
 - Moves charged ion back and forth between plates
 - Ion will have net drift base on its high and low field mobility
- Compensation voltage (COV) is small DC offset between the plates – filtering voltage



Relationship Between Dipole Moment and CoV



Theoretical dipole moments were calculated using isopropanol as a modifying solvent Head Group Dipole Moment (D) 6 PC **O** PE 5 O P/ 4 p-value < 0.0142 PG O PS -6 -2 0 CV, V

Molecules that have different dipole moments can be separated by DMS



SelexION[™] Technology Separates Phospholipid Sub-Classes



Experiment: MRM scan of 6 phospholipid standards with COV ramp

Proof of concept: DMS separates different lipid classes **Implications**: High degree of lipid class specificity without LC



Isobaric Interference Among Different Lipid Molecular Species

Isobaric interference makes 'unassisted' MRM analysis by infusion non-specific. SelexION[™] Technology makes it possible



Experiment: mrm analysis of CSF (PE 40:5; 792.6/283.2)

SelexION[™] Device Off

Multiple different lipids have the same MRM transition:

Isobaric Interference

Resolution of Glucosylceramides (Cerebrosides)

- Galactosylceramide (Galβ1-1'Cer) is the principal glycosphingolipid in brain tissue and is an essential structural component of myelin
- Glucosylceramide (Glcβ1-1'Cer) is found in animal tissues, and is a major component of skin lipids and neuronal tissue.



Due to identical product ion spectra, mrm transitions and similar physical properties, LC separation and individual characterization/quantitation of these two lipid classes is challenging.

For Research Use Only. Not for use in diagnostic procedures.



DMS Resolves Glycosylceramide Isomers without Chromatography



For Research Use Only. Not for use in diagnostic procedures



Resolution of Retinoic Acid Isomers by SelexION[™] Technology



Complete resolution of RA isomers is possible, but the sensitivity is affected such that it is not a biologically relevant assay.

 \rightarrow Combine LC and DMS to balance need for selectivity and sensitivity

For Research Use Only. Not for use in diagnostic procedures



SelexION Separation of PI(3)P and PI(4)P

Baseline separation without chromatography



Experimental Conditions

SelexION Conditions	
Separation Voltage (SV):	4100V
DMS Resolution Enhancement (DR):	42
Modifier:	None
DMS Temperature (DT):	Low=150 °C

6500 QTRAP Conditions

IonSpray Voltage (IS):	4500
Temperature (TEM):	100
Gas 1 (GS1):	30
Gas 2 (GS2):	40
Curtain Gas (CUR):	15
Declustering Potential (DP):	100
Entrance Potential (EP):	10

MRM: 953.5 → 613.4 (CE=30)



PI(3)P



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Resolution of PI(3,5)P₂ and PI(4,5)P₂ by DMS

Traditional methods to separate the PIP₂ molecular species rely on chromatography and derivatization





Applying SelexION[™] Technology to MS/MS^{ALL} with the TripleTOF[®] 5600+

MSMS^{ALL} Introduction

Product ion spectrum generated for every precursor ion



Ståhlman, M et al. High-throughput shotgun lipidomics by quadrupole time-of-flight mass spectrometry, J Chrom B 2009 Ekroos, K., Methods in Pharmacology and Toxicology: Biomarker Methods in Drug Discovery and Development, Humana Press 2008



MS/MS^{ALL} Information-Independent Data Collection



Direct infusion, flow injection, and lipidclass targeted LC techniques

Fast Q1 precursor selection step-wise through mass range

CID Fragmentation

Precursor mass range 200-1250; total analysis time 3-5 min



MS/MS^{ALL}



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6600 TripleTOF with FIA Configuration



6600 TripleTOF[®] Mass Spectrometer With SelexION[®] Technology



Eluting Profile and Data Acquisition Window





Excellent Reproducibility in Elution Profile and MS Intensity





Quantitative Level Carryover





MS/MS^{ALL –} Fragment and Neutral Loss Filter



MS/MS^{ALL} with SelexION[™]

Use the SelexION[™] technology to isolate individual lipid classes for analysis

- Identify CoV values for each lipid class of interest
- Focus mass list to analyze only masses that are germane to lipid class of interest (e.g., PC: 675-925)
- Run MS/MS^{All} sequence for all lipid classes

Primary Benefits

- Clean MS/MS data without isobaric contamination
- Reduced background
- Improved ID confidence







MS/MS^{ALL} with SelexION[™]

Use the SelexIONTM technology to isolate individual lipid classes for analysis







MS/MS^{ALL} with SelexION[™]

Use the SelexION[™] technology deconvolves complex spectra



The Power of DMS to Deconvolute Product Ion Spectra

MS/MS of 814.5 (PC 36:5 + Cl and PC 34:3 + AcO)



31 Experiment: Krill oil analyzed by MS/MS^{ALL} (negative ion mode) with and without DMS

TOFMS data show 2 peaks at 814.5



Resolution = \sim 33,0000

Resolution of these adducts is not possible during precursor ion isolation on ANY instrument unless DMS is used. Extensive chromatography or careful selection of quantitative fragments is required otherwise



The Power of DMS to Deconvolve Product Ion Spectra

MS/MS of 840.6 (PC 38:6 + Cl and PC 36:4 + AcO)



32 Experiment: Krill oil analyzed by MS/MS^{ALL} (negative ion mode) with and without DMS



Acknowledgements

SCIEX

- Paul Baker
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- Eva Duchoslav
- Larry Campbell
- Leo Wang
- Pauline Vollmerhaus
- Fadi Abdi
- Aaron Hudson
- Cyrus Papan

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