# Utilization of Monodisperse Fully Porous Particles for Chromatographic Improvement in Mass Spectrometry based Metabolomics for Disease Detection

Introduction

Traditionally, metabolomics is a difficult analysis with conventional chromatographic tools in the lab. MAC-MOD worked in collaboration with Dr. Tim Garrett at the University of Florida to develop an application with the goal of improving quantitative and qualitative analytical capabilities. Here is an untargeted metabolomic screen of a plasma extract via a dried blood spot analysis. We are utilizing monodisperse fully porous particle technology to achieve increased performance and efficiency. The Evosphere® C18/PFP column was chosen for this analysis due to its combination of regioisomer and hydrophobic selectivity as well as polar retention capacity.

Fig 1: Total ion chromatogram from untargeted profiling using LC-HRMS. Several key metabolites are identified and the extracted ion chromatograms are displayed to the right
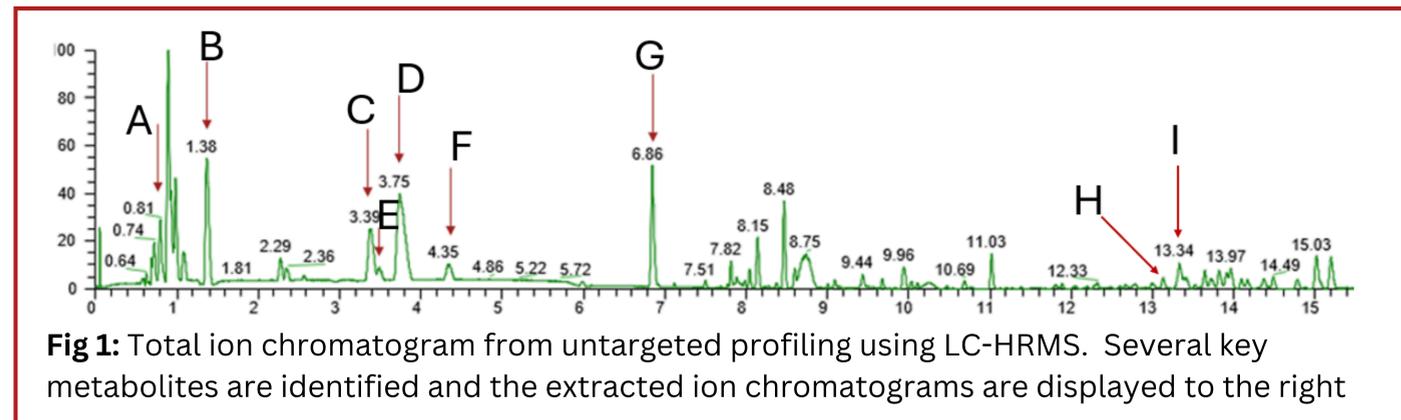
Gradient Table

Time	%B	Flow Rate
3	0	0.35
13	80	0.35
16	80	0.35
16.5	0	0.35
16.8	0	0.60
20	0	0.60
20.5	0	0.60

Experimental Conditions

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PN#:	EVO18FP020503
Column:	Evosphere C18/PFP 100 Å, 3µm, 2.1 x 100mm Monodisperse Particle Column
Instrument:	Thermo Q-Exactive with Dionex Ultimate UHPLC
Sample:	Plasma Extract
Mobile Phase A	0.1% Formic Acid in H_2O
Mobile Phase B	Acetonitrile
Temerature:	25 ºC
Injection Volume	2 µl

Polar Retention
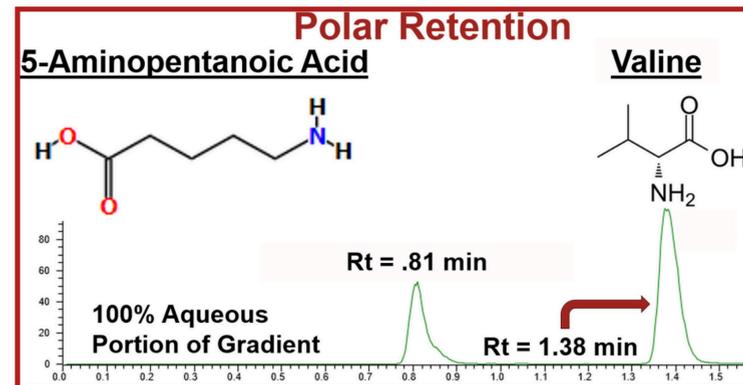
Fig 2: A- 5-Aminopentoic Acid, B- Valine

Optimal Peak Shape

Fig 4: E- Acetyl-Carnitine

Lysophospholipid Isomers sn-1 vs sn-2 with C18/PFP
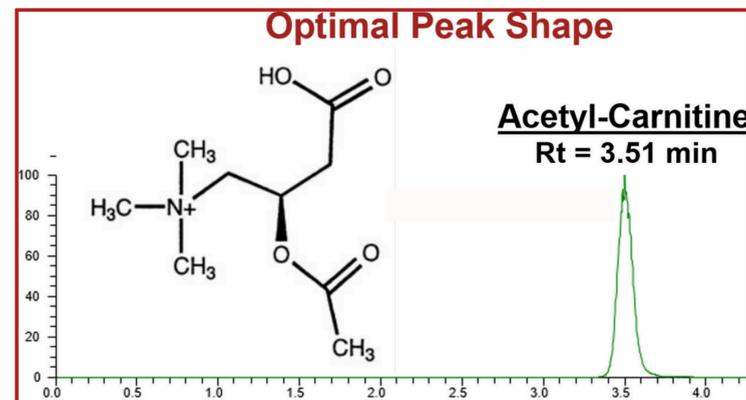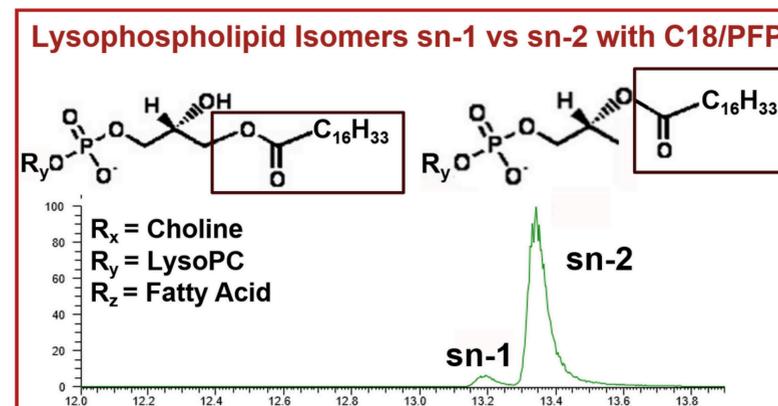
Fig 6: H- Lysophospholipid sn-1, I- Lysophospholipid sn-2

Methyl Position Switch
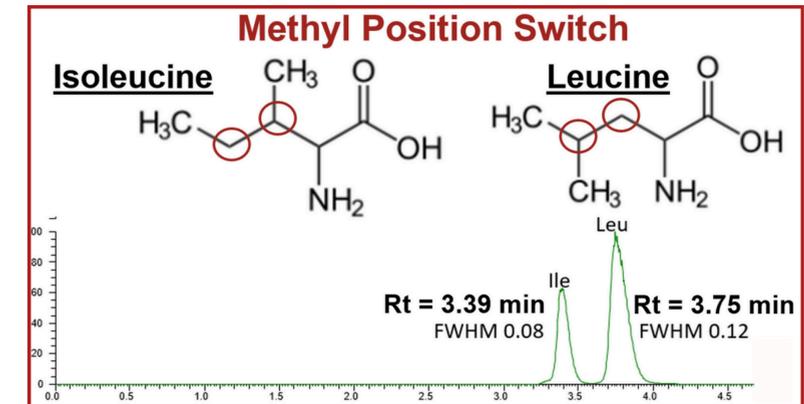
Fig 3: C- Isoleucine, D- Leucine

Strong Isomeric Selectivity
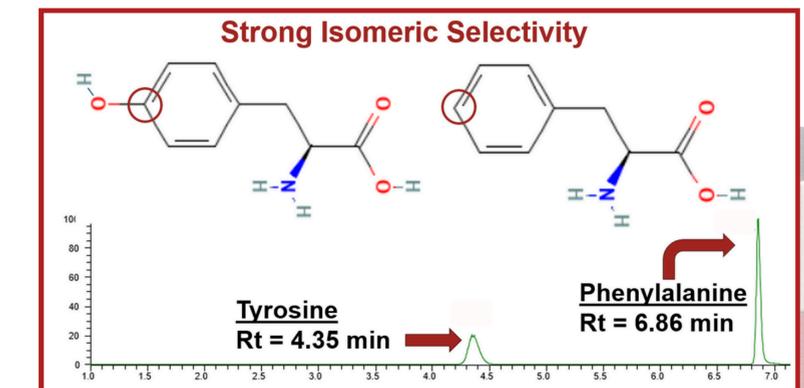
Fig 5: F- Tyrosine, G- Phenylalanine

Conclusion

We tested the use of new monodisperse columns for global metabolomic profiling. Our results indicate excellent separation for polar metabolites. We showed separation of several isomers pairs including valine and 5-aminopentanoic acid, isoleucine and leucine, and lysophophatidylcholine. Peak shape, retention and reproducibility were excellent.

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