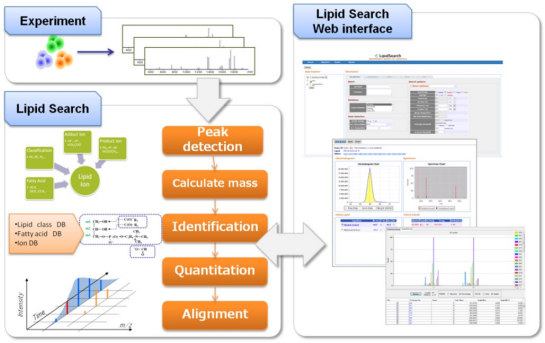
LipidSearch



LipidSearch 4.2: Automated Identification Engine For Lipidomics

We utilize LipidSearch® as our main lipid identification/data processing software. The LipidSearch® software package searches a proprietary MS/MS database for lipid identification. The workflow is described below:

1. Identify features in the LC-MS data (peak picking)
2. Identify lipid ions by their MS/MS spectra (search against library, 1.5 million lipid ions)
3. Integrate peaks that correspond to identified lipid ions
4. Normalize peak areas to class-specific internal standards

Data visualization can be customized and tailored to the client's preference.

Our laboratory has a BSL-2 laboratory to aid in sample preparation and/or extraction from complex biological matrices. If you have questions about the lipid content or lipid species in your samples, please reach out to our Core to discover how we can help you.

Lipidomics at UNC

	Lipid Profiling*	Quantitation*	FAMES**
UNC/ NCSU	50.85	50.85	50.00
External	79.00	79.00	78.00
External Non-Academic	100.00	100.00	150.00

Additional charges may apply for BSL 2 sample extraction and/or sample preparation.

*Pricing is PER SAMPLE.

**Pricing is PER HOUR of instrument time utilized

This method development work was funded and supported by UNC's Core Facility Advocacy Committee (CFAC) under the Method Development Award program (Spring 2019).

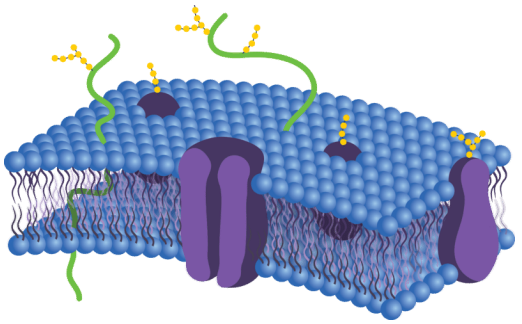
Image on Front Panel is copied from: https://www.ck12.org/biology/phospholipid-bilayer/lesson/Phospholipid-Bilayers-BIO/

UNC CHEMISTRY
MASS SPECTROMETRY LAB

Brandie M. Ehrmann
Caudill 052
125 South Road
Chapel Hill, NC 27599

Phone: 919-962-6813
Email: behrmann@email.unc.edu

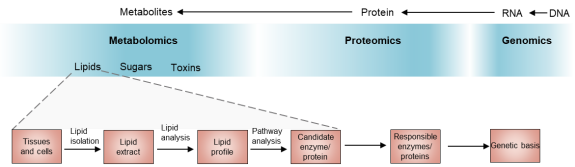
Lipidomics via Mass Spectrometry at the University of North Carolina Chapel Hill



Department of Chemistry
Mass Spectrometry Core Laboratory

Dr. Brandie M Ehrmann, Director
Tel: 919-962-6813
behrmann@email.unc.edu

Why Lipidomics?

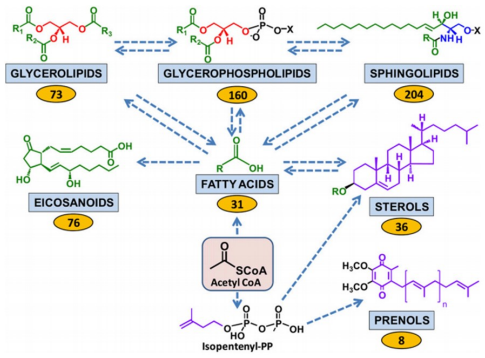


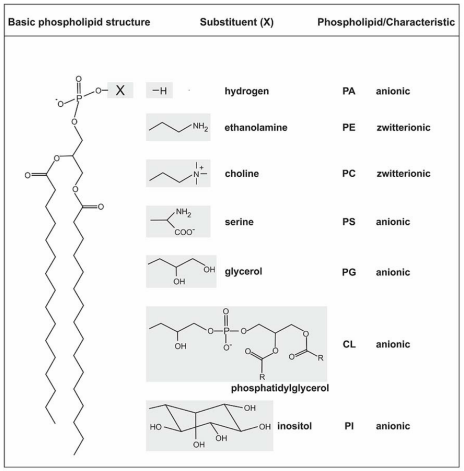
Wenk, M. R. *Nat. Rev. Drug Discov.* **2005**, *4* (7), 594–610.

System-level analysis of lipids as a biochemical snapshot of phenotype

Structural Diversity of Lipids

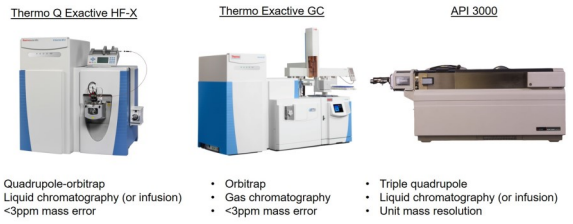
Our methodology targets a diverse array of lipid compounds and aims to characterize the most comprehensive profile of lipid compounds the mass spectrometry methods will allow.





Quehenberger, O., et al. *J. Lipid Res.* **2010**, *51*, 3299–3305.
Aktas, M., et al. *Front. Plant. Sci.* **2014**, *5*, 1-14.

Our Instruments



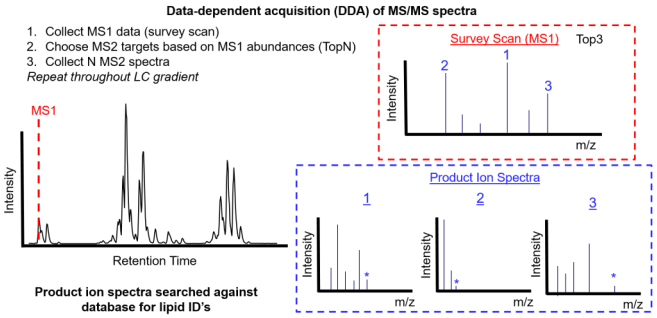
Quadrupole-orbitrap
Liquid chromatography (or infusion)
<3ppm mass error

- Orbitrap
- Gas chromatography
- <3ppm mass error

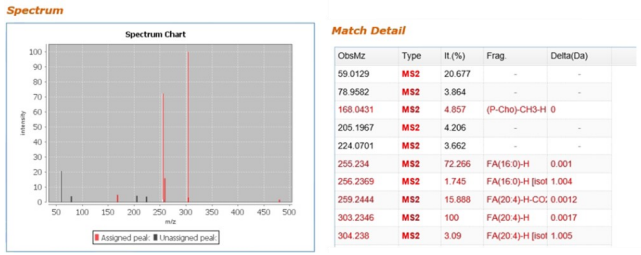
- Triple quadrupole
- Liquid chromatography (or infusion)
- Unit mass resolution

Our instrumentation suite allows for comprehensive profiling of lipids in complex matrices by both LC and GC methods. We also have quantitative profiling capabilities should a researcher need that level of detail.

Untargeted Lipidomics on HF-X Platform



MS2 Spectral Matching

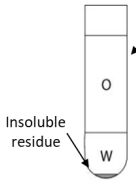


Match: PC (20:4_16:0)

Our data-dependent acquisition methods allow for comprehensive lipid identification through spectral matching in our ThermoFisher® LipidSearch® software.

Workflow

MTBE Extraction



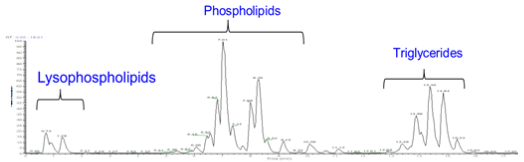
Contains deuterated internal standards

Lipid	Chemical Formula	Exact Mass
15:0-18:1(d7) PC	$C_{41}H_{73}D_7NO_8P$	752.6061
18:1(d7) Lyso PC	$C_{26}H_{45}D_7NO_7P$	528.3921
15:0-18:1(d7) PE	$C_{38}H_{67}D_7NO_8P$	710.5591
18:1(d7) Lyso PE	$C_{23}H_{39}D_7NO_7P$	486.3451
15:0-18:1(d7) PG (Na Salt)	$C_{39}H_{68}D_7O_{10}P$	741.5537
15:0-18:1(d7) PI (NH_4 Salt)	$C_{42}H_{72}D_7O_{13}P$	829.5698
15:0-18:1(d7) PS (Na Salt)	$C_{39}H_{67}D_7NO_{10}P$	754.5490
15:0-18:1(d7)-15:0 TAG	$C_{61}H_{88}D_7O_6$	811.7646
15:0-18:1(d7) DAG	$C_{36}H_{61}D_7O_5$	587.5506
18:1(d7) MAG	$C_{21}H_{33}D_7O_4$	363.3366
18:1(d7) Chol Ester	$C_{45}H_{71}D_7O_2$	657.6441
d18:1-18:1(d9) SM	$C_{41}H_{72}D_9N_2O_6P$	737.6397
C15 Ceramide-d7	$C_{33}H_{58}D_7NO_3$	530.5404

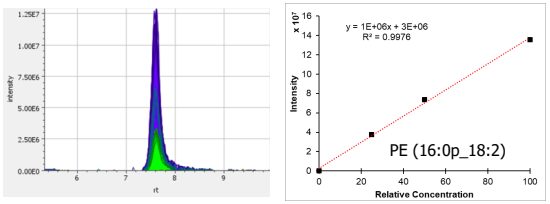
- 10-100 µL plasma
- 10^6 - 10^7 cells
- 10 - 100 mg tissue

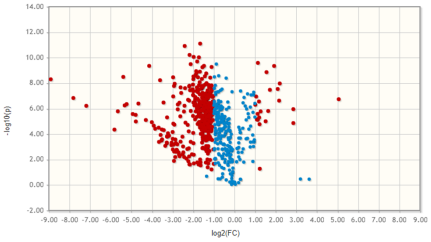
Our extraction procedure utilizes methyl tert-butyl ether to extract lipids from sample matrix and we spike in Avanti® Lipid class standards for normalization/internal standards.

LC-MS



Profiling and Relative Quantification





Our data reports can be tailored to provide a broad overview of the lipids in the sample and/or specific lipid [class] information.

We offer both targeted and untargeted lipid analysis for phenotype differentiation.