Lipidomics Databases and Online Tools

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University Of California San Diego
LIPID MAPS Bioinformatics Overview

- Lipids
- Genes/proteins
- Standards
- Expt. data

Databases

Core computing infrastructure

Experimental data and metadata

Lipid classification, resources, publications, tutorials

Information display and querying portals

Lipid Structure and Mass Spectrometry Tools
LIPID MAPS Lipidomics gateway
http://www.lipidmaps.org

April, 2013 update

- LIPID MAPS: advancement and innovation in lipidomics

The LIPID MAPS infrastructure is a unique resource for the biomedical community. In addition to providing the largest database of lipid molecular structures, the lipid maps resource contains information on the lipid proteome, quantitative estimates of lipids in the human plasma, the first complete map of the macrophage lipodome, and a host of tools for lipid biology including mass spectrometry tools, structure tools and pathway tools. The LIPID MAPS website is widely regarded as the "one stop shop" for lipid research and a valuable information source for researchers interested in lipid biology and chemistry, and also provides a detailed set of tutorials for the benefit of students and people new to the field. The LIPID MAPS classification and nomenclature system has been adopted worldwide by its guidelines on the organization and structural representation of lipid classes. In addition to numerous citations, LIPID MAPS is cited by the scientific press. For instance LIPID MAPS is referenced by the following popular news articles.

Lipids Take Charge (C&EN News)
LIPID MAPS Classification System (Science News)
Lipidomics in Europe (ASRMS)
Metabolomic databases (Nature Biotechn)

more about the consortium

- LIPID MAPS Highlights

LIPID MAPS Workshop at ED 2013 - Lipidomics Technologies at the End of the First Decade and the Beginning of the Next. Where are we now, and what are the future prospects? Offered in conjunction with the American Society for Nutrition.
8:00 to 10:00 am, April 23, 2013.
Boston Convention Center Room 161 AB - The Education Track Room.

more highlights

- Lipid of the month

Psicosine (Galactosylsphingosine) is a basic glycosphingolipid present in low concentrations in animal cells. It consists of sphingosine having a beta-D-galactosyl residue attached at the C1 position. Psicosine accumulates in tissues in
LIPID MAPS Databases

LIPID MAPS Structure Database (LMSD)
Lipid structures and related references/annotations

LIPID MAPS Proteome Database (LMPD)
Gene and protein information for lipid-related sequences

LIPID MAPS Lipid MS Standards
MS/MS spectra and annotations of synthetic lipid standards
Defining a lipid:
Fundamental biosynthetic units of lipids

Acetyl
Propionyl
Ketoacyl "building blocks"
Isoprene "building block"
## LIPID MAPS Classification System
### Categories and Examples

<table>
<thead>
<tr>
<th>Category</th>
<th>Abbreviation</th>
<th>Example</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fatty acyls</td>
<td>FA</td>
<td>Dodecanoic acid</td>
</tr>
<tr>
<td>Glycerolipids</td>
<td>GL</td>
<td>1-hexadecanoyl-2-(9Z-octadecenoyl)-sn-glycerol</td>
</tr>
<tr>
<td>Glycerophospholipids</td>
<td>GP</td>
<td>1-hexadecanoyl-2-(9Z-octadecenoyl)-sn-glycero-3-phosphocholine</td>
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<tr>
<td>Sphingolipids</td>
<td>SP</td>
<td>N-(tetradecanoyl)-sphing-4-enine</td>
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<tr>
<td>Sterol lipids</td>
<td>ST</td>
<td>Cholest-5-en-3β-ol</td>
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<tr>
<td>Prenol lipids</td>
<td>PR</td>
<td>2E,6E-farnesol</td>
</tr>
<tr>
<td>Saccharolipids</td>
<td>SL</td>
<td>UDP-3-O-(3R-hydroxy-tetradecanoyl)-αD-N-acetylglucosamine</td>
</tr>
<tr>
<td>Polyketides</td>
<td>PK</td>
<td>Aflatoxin B₁</td>
</tr>
</tbody>
</table>

**International Lipid Classification and Nomenclature Committee (ILCNC)**  
*Journal of Lipid Research, Vol. 46, 839-862, 2005*  
*Journal of Lipid Research, Vol. 50, S9-S14, 2009*
LIPID MAPS: Compound ID

- **LIPID MAPS compound ID**
  - LMGP01010005

- **Database identifier**
  - Digits 1-2: Database: LM (LIPID MAPS)
  - Digits 3-4: Category: GP (Glycerophospholipids)
  - Digits 5-6: Class: 01 (Glycerophosphocholines)
  - Digits 7-8: Subclass: 01 (Diacylglycerophosphocholines)
  - Digits 9-?: Optional additional class levels (typically not required)
  - Last 4 digits: Unique identifier within subclass: 0005

1-hexadecanoyl-2-(9Z-octadecenoyl)-sn-glycero-3-phosphocholine
Consistent structure representation across classes

Fatty Acyls (FA)

Glycerolipids (GL)

Glycerophospholipids (GP)

Sphingolipids (SP)

Sterol Lipids (ST)

Prenol Lipids (PR)
Structural comparison of SM and PC

Sphingomyelin (SM)
(Example: N-palmitoyl-sphingomyelin)

Phosphatidylcholine (PC)
(Example: 1-myristoyl-2-palmitoyl-sn-glycero-phosphocholine)
LIPID MAPS Structure Database (LMSD)

Lipids per category in LMSD

Total: 37,500

- FA
- GL
- GP
- SP
- ST
- PR
- SL
- PK

Lipids per category.
LIPID MAPS Structure Database (LMSD)

#Lipids in LMSD by year

- 2004
- 2005
- 2006
- 2007
- 2008
- 2009
- 2010
- 2011
- 2012
Populating the LIPID MAPS Structure Database

Structures from core labs and partners

New structures identified by LIPID MAPS experiments

Computationally generated structures

Public databases

Websites, Publications

LIPID MAPS structure database

37,500 structures as of Apr 2013
Search LMSD by browsing classification hierarchy
Search LMSD by text, mass, formula, classification.
Search LMSD with ontology terms

e.g. find all lipids with 20 carbons, 3 double bonds, at least 3 hydroxyl groups and 1 epoxy group
Search LMSD by substructure
### LMSD Detail view for a lipid structure

#### Structure

![Lipid Structure](image)

<table>
<thead>
<tr>
<th>LM_ID</th>
<th>LMFA03010002</th>
</tr>
</thead>
<tbody>
<tr>
<td>Common Name</td>
<td>PGF2α (W)</td>
</tr>
<tr>
<td>Systematic Name</td>
<td>9,11,15,18-tetrahydroxy-5Z,13E-prostaglandin acid</td>
</tr>
<tr>
<td>Synonyms</td>
<td>Prostaglandin F2α; Prostaglandin F2α; Enzaprost; Dinoprost; Amoglandin; Cycladin</td>
</tr>
<tr>
<td>Exact Mass</td>
<td>354.2405 (neutral)</td>
</tr>
<tr>
<td>Formula</td>
<td>C_{22}H_{34}O_{5}</td>
</tr>
<tr>
<td>Category</td>
<td>Fatty Acids [FA]</td>
</tr>
<tr>
<td>Main Class</td>
<td>Fatty acids [FA03]</td>
</tr>
<tr>
<td>Sub Class</td>
<td>Prostaglandins [FA0301]</td>
</tr>
<tr>
<td>LIPIDBANK ID</td>
<td>A4R1501</td>
</tr>
<tr>
<td>PubChem Substance ID (SID)</td>
<td>4285063</td>
</tr>
<tr>
<td>METACOMMENTS ID</td>
<td>-</td>
</tr>
<tr>
<td>KEGG ID</td>
<td>C00639</td>
</tr>
<tr>
<td>HMDB ID</td>
<td>HMDB01139</td>
</tr>
<tr>
<td>CHEBI ID</td>
<td>15553</td>
</tr>
<tr>
<td>InChIKey</td>
<td>PXQPLTODNUVGFL-YNNPMVKQSA-N</td>
</tr>
<tr>
<td>InChI</td>
<td>5n</td>
</tr>
<tr>
<td>Status</td>
<td>Active</td>
</tr>
<tr>
<td>MS Standard</td>
<td>View lipid standard</td>
</tr>
</tbody>
</table>

#### LM_ID

<table>
<thead>
<tr>
<th>Calculated physicochemical properties (22)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Heavy Atoms</td>
</tr>
<tr>
<td>van der Waals Molecular Volume</td>
</tr>
<tr>
<td>Molecular Volume</td>
</tr>
<tr>
<td>LogP</td>
</tr>
<tr>
<td>Topological Polar Surface Area</td>
</tr>
<tr>
<td>Hydrogen Bond Donors</td>
</tr>
<tr>
<td>Rotatable Bonds</td>
</tr>
<tr>
<td>Hydrogen Bond Acceptors</td>
</tr>
<tr>
<td>Molar Refractivity</td>
</tr>
</tbody>
</table>

#### Names, synonyms

- Prostaglandin F2α
- Prostaglandin F2α
- Enzaprost
- Dinoprost
- Amoglandin
- Cycladin

#### m/z calculation tool

- Calculate m/z: [Select m/z](select)

#### Lipid classification

- Fatty Acids [FA]
- Fatty acids [FA03]
- Prostaglandins [FA0301]

#### Database cross-references

- PubChem Substance ID (SID): 4285063
- METACOMMENTS ID: -
- KEGG ID: C00639
- HMDB ID: HMDB01139
- CHEBI ID: 15553
- InChIKey: PXQPLTODNUVGFL-YNNPMVKQSA-N
- InChI: 5n|7,12,13,15-19,21-23H,2-3,5-8,9-11-14H2,1H3,(H,2,4),7-07,-13,-12,-15,16-,17-18-19-Imol01
- Status: Active
- MS Standard: View lipid standard

### Other structure formats

- Static Image
- MarvinView Applet
- JmolApplet
- ChemDraw

### Structure viewing options

- Download file
- MOLMLC
Use InChIKey to find structures differing only in stereochemistry, double-bond geometry or isotopic labeling

Show lipids differing only in stereochemistry/bond geometry
Use InChIKey (full or partial) to perform a Google structure search
Example: PGE2
Lipidomics Data Display: MS Standards library
http://www.lipidmaps.org/data/standards/index.html
Lipid Proteome Database (LMPD)
Search protein database by pathway (KEGG pathway)
Querying Lipidomics Gateway website as well as LIPID MAPS databases via “Quick search”

- **Multi-purpose**
- **Small “footprint”**
- **High visibility (on home page)**

Search the Lipidomics Gateway html pages by keyword, or the databases by lipid class, common name, systematic name or synonym, mass, formula, InChIKey, LIPID MAPS ID, gene or protein term.
<table>
<thead>
<tr>
<th>Quick search query types</th>
<th>Example</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>LIPID MAPS LM_ID</strong></td>
<td>LMFA03010003</td>
</tr>
<tr>
<td>Lipid classification term</td>
<td>“Choline”, “prostaglandin”, “diterpene”</td>
</tr>
<tr>
<td>Lipid common/systematic name or synonym</td>
<td>“Linoleic”, “HETE”, ””, “PAF”, “PGE”, “5Z,8Z,14Z-eicosatrienoic”, “PC(16:0/18:1(9Z))” “MGDG “docosa”, “phytosphingosine”</td>
</tr>
<tr>
<td>Lipid molecular formula</td>
<td>C$<em>{12}$H$</em>{24}$O$_2$</td>
</tr>
<tr>
<td>InChI Key</td>
<td>XEYBRNLFEZDVAW-ARSRFYASSA-N</td>
</tr>
<tr>
<td>Lipid standard (name or LMID)</td>
<td>sterol</td>
</tr>
<tr>
<td>Gene/protein name/synonym</td>
<td>FABP</td>
</tr>
<tr>
<td>Keywords on Lipidomics Gateway website pages (personnel, publications, news, updates, etc.)</td>
<td>“Atherosclerosis”, “Dennis”, “homeostasis”</td>
</tr>
</tbody>
</table>
LIPID MAPS experimental data section

Experimental data

Lipidomics studies on human plasma

- NIDDK / NIST human plasma sample analysis

Lipidomics studies on macrophages

- RAW 264.7 cells
  - Kdo2-Lipid A time course experiments
  - CompaatrueKdo2-Lipid A time course experiments

- Primary macrophages
  - Thiglycollate-elicited peritoneal macrophages (TGEM)
    - CompaatrueKdo2-Lipid A time course experiments
  - Kern cell study with wildtype and LDLR(-/-) mice
  - Bone marrow-derived macrophages (BMMDD)
    - Kdo2-Lipid A time course experiments
    - ATPKdo2-Lipid A time course experiments
    - 2-hydroxyprostacholat time course experiments
  - Compare results from TGEM and BMMDD treated with Kdo2-Lipid A (3 time points: 0, 6, 24 hrs)

- Compare results from RAW, TGEM, and BMMDD for steroids treated with Kdo2-Lipid A (full time course: 9 time points)

Microarray analysis of macrophages

- RAW 264.7 cells
  - Kdo2-Lipid A time course experiments
  - CompaatrueKdo2-Lipid A time course experiments (2 time points: 12, 24hrs)
  - CompaatrueKdo2-Lipid A time course experiments (full time course: 7 time points)

- Primary macrophages
  - Thiglycollate-elicited macrophages
    - Kern cell study with LDLR(-/-) and wildtype mice
Overview of Quantitative Lipid Analysis by Mass Spectrometry as performed by LIPID MAPS consortium on bone marrow derived macrophages (BMDM)

Extract bone marrow cells
Transfer to plates
Perform timecourse experiment on plated cells
Aliquot samples for shipping to core research labs

Repeat 3x (replicates)

- Fatty acids
  - Methanolic HCl/isooctane extraction
    - GC/MS analysis (normal phase)
      - Deuterated standards
    - LC/MS analysis (reverse phase)
      - ESI-QTRAP viaMRM methods
      - Deuterated standards
  - Methanol/HCl/CICl3 extraction
    - LC/MS analysis (normal phase)
      - ESI-QTRAP viaMRM methods
      - Odd-chain standards

- Eicosanoids
  - Methanol/HCl/CICl3 extraction
  - Methanol/CHCl3 extraction
  - EtOAc/isooctane extraction
  - DFPI derivatization of DAGs
  - ESI-QTRAP [M+NH4]+ detection mode
  - Deuterated standards

- Glycerophospholipids
  - Methanol/HCl/CICl3 extraction
  - Methanol/CHCl3 extraction
  - EtOAc/isooctane extraction
  - SPE extraction
  - ESI-QTRAP viaMRM methods
  - Odd-chain standards

- Cardiolipins
  - Methanol/HCl/CICl3 extraction
  - Methanol/CHCl3 extraction
  - EtOAc/isooctane extraction
  - SPE extraction
  - ESI-QTRAP [M+NH4]+/neutral loss detection mode
  - Deuterated standards

- Glycerolipids
  - Methanol/HCl/CICl3 extraction
  - Methanol/CHCl3 extraction
  - EtOAc/isooctane extraction
  - SPE extraction
  - ESI-QTRAP [M+NH4]+/neutral loss detection mode
  - Deuterated standards

- Cholesteryl esters
  - Methanol/HCl/CICl3 extraction
  - Methanol/CHCl3 extraction
  - Combination of GC/MS, LC/MS (reverse phase)
    - Deuterated standards
    - Triple Quad detection with MRM methods
    - C12 analog standards

- Sterols
  - Methanol/CHCl3 extraction
  - Methanol/HCl/CHCl3 extraction
  - Combination of GC/MS, LC/MS (reverse phase)
  - Deuterated standards
  - Deuterated standards

- Sphingolipids
  - Methanol/HCl/isooctane extraction
  - Methanol/CHCl3 extraction
  - LC/MS analysis (normal phase)
  - ESI-QSTAR-XL via MRM methods
  - Nor-dolichol/CoQ6 standards

- Prenols
  - Methanol/HCl/isooctane extraction
  - Methanol/CHCl3 extraction
  - Methanol/HCl/Isooctane extraction
  - Combination of LC-C18, LC-Si and LC-NH2 separation
  - ESI-QTRAP and API-3000 Triple Quad detection with MRM methods

BIOINFORMATICS
Data consolidation, normalization, statistical analysis and databasing
Presentation in tabular and graphical formats

For details of extraction, purification and quantitation by MS, see:
MACROPHAGE LIPID METABOLISM

- Sphingolipids
- Glycerophospholipids
- Glycerolipids

- Eicosanoids
- Fatty Acids
- Sterol esters
- Sterols
- Prenols

- Carbohydrates
- Acetyl CoA
- Proteins

- Fatty acid synthesis
- β-oxidation

- TCA cycle
- Oxidative phosphorylation

Dennis et al (2010)
J. Biol. Chem, 51, 39976-85
Data presentation formats

**Tabular:**

**Graphical:**

**Heatmap:**

**Integrated pathway/heatmap:**

**Lipids**

**Genes**
Integrated lipids, genes, and pathways data across timecourse experiments for RAW 264.7 cells treated with Kdo₂-lipid A
Cholesterol Biosynthesis Pathway
(Yellow:Lipids Green:Enzymes)
TLR4 signaling pathway
Online lipid structure-drawing tools

http://www.lipidmaps.org/tools/index.html

Online drawing tools for various lipid categories (FA, GL, GP, SP, ST)

Structures viewable in Javascript, Java (Marvin, Jmol) and Chemdraw format. May be saved as Molfiles
Online generation of glycan structures in full chair conformation

http://www.lipidmaps.org/tools/index.html

Sugars
Glc
Gal
GlcNAc
GalNac
Xyl
Fuc
Man
NeuAc
NeuGc
KDN

Anomeric Carbon
α or β linkages may be specified
Template-based combinatorial enumeration of virtual compound libraries for lipids

Command-line Perl scripts

Template-based combinatorial enumeration of virtual compound libraries for lipids.
Workflow for the template-based combinatorial enumeration of virtual compound libraries

MG(*::*0:0/0:0)

PC(*::*/*::*)

Cer(*::*0:0)

CL(1'->[***/0:0],
   3'->[***/0:0])
Mass spectrometry tools
m/z calculation, m/z prediction

- Using virtual databases of structures based on commonly occurring core structures and chains
- Using known lipids in the LIPID MAPS structure database (LMSD)

Online Tools

- **Mass Spectrometry**: Perform searches with precursor ion or product ion peaklists on a variety of lipid classes, where structures are generated by computational methods or are present in the LIPID MAPS structure database. Display various structural properties (exact mass, formula, abbreviation, etc.) for matched ions with links to molecular structures and isotopic distribution profiles where appropriate. Generate *in-silico* product ion peaklists for glycosphingolipids.
  - Calculate the exact mass (m/z) for a lipid. Display structure and isotopic distribution profile
  - Search the LUSD for lipids with a given mass (m/z) value. Display structure and isotopic distribution profile
  - Glycerophospholipid MS analysis
  - Glycerolipid (Mono Dio/Triacylglycerol) MS analysis
  - Sphingolipid MS analysis
  - Glycosphingolipid MS precursor ion analysis (Search computationally generated glycosphingolipid structures)
  - Glycosphingolipid MS/MS product ion search tool (Match your tandem MS data with computationally generated glycosphingolipid structures)
  - Create *in-silico* Glycosphingolipid MS/MS peaklist with permethylation options
  - Compare/contrast 2 different *in-silico* Glycosphingolipid MS/MS peaklists
  - Cardiolipin MS analysis
  - Fatty acid MS analysis (based on structures in the LIPID MAPS database)
  - Fatty acid MS analysis (based on computationally generated structures)
  - Cholesteryl ester MS analysis (based on fatty acid structures in the LIPID MAPS database)
  - Cholesteryl ester MS analysis (based on computationally generated structures)
  - Search a database of MS/MS spectra of Eicosanoids for precursor and production ions (negative ion mode)
  - Species-specific lipidomes
    - *Mycobacterium tuberculosis* lipid MS analysis (based on a database of computationally generated ions)
LMSD detail page: m/z calculator

Structure database (LMSD)

- **LM ID**: LMFA03010003
- **Common Name**: PGE2 (W)
- **Systematic Name**: 9-oxo-11R,15S-dihydroxy-5Z,13E-prostaglandin acid; Prostine E2
- **Synonyms**: Prostaglandin E2; Dinoprostone
- **Exact Mass**: 352.2250 (neutral)  
  Calculate m/z: [M-H]- 351.2177 (C20H31O5)
- **Formula**: C20H32O5
- **Category**: Fatty Acyls [FA]
- **Main Class**: Eicosanoids [FA03]
- **Sub Class**: Prostaglandins [FA0301]

Isotopic distribution profile

m/z for selected ion type/adduct
Calculate m/z value for selected lipid categories
Use pull-down menus to select chains/headgroups

<table>
<thead>
<tr>
<th>Fatty acids</th>
<th>Wax esters</th>
<th>Acyl carnitines</th>
<th>CoA esters</th>
<th>Glycerolipids</th>
<th>Phospholipids</th>
<th>Sphingolipids</th>
<th>Cardiolipins</th>
<th>Cholesteryl esters</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ion [M+H]+</td>
<td>Alcohol</td>
<td>Acid 16.0</td>
<td>Acid 16.0</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
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<td></td>
</tr>
</tbody>
</table>

Note: Chains containing double bonds and/or functional groups with defined regiochemistry, geometry and stereochemistry are meant to serve as examples for structure-drawing purposes. In many cases there may be alternative isobaric structures.
Calculate m/z value for selected lipid categories:

### Glycerophospholipid Mass calculation

**Note:** Chains containing double bonds and/or functional groups with defined regiochemistry, geometry and stereochemistry are meant to serve as examples for structure-drawing purposes. In many cases there may be alternative isobaric structures.

<table>
<thead>
<tr>
<th>m/z</th>
<th>Abbreviation</th>
<th>Formula</th>
<th>Ion</th>
</tr>
</thead>
<tbody>
<tr>
<td>762.6007</td>
<td>PC(16:0/18:0)</td>
<td>C_{42}H_{84}N_{2}O_{10}P</td>
<td>[M+H]^+</td>
</tr>
<tr>
<td>784.5827</td>
<td>Return to main form</td>
<td>C_{42}H_{84}N_{2}O_{10}Na</td>
<td>[M+Na]^+</td>
</tr>
</tbody>
</table>

Select alternative ion-type/adduct

Copy, paste or download structure

**Abbreviation**
PC(16:0/18:0)

**Systematic Name**
1-hexadecanoyl-2-octadecanoyl-sn-glycero-3-phosphocholine

View Structure using
- GGAKetcher
- MarvinView Applet
- JmolApplet
- ChemDraw

Download MDL_MOL file containing only structure data or SDF file with structure and other associated data.
Prediction: Search LMSD (37,000+ lipids) with an m/z value
Search LMSD with an m/z value: Output page
Links to LMSD record details, isotopic distribution profiles

### Possible Lipid Structures

**Note:** Chains containing double bonds and/or functional groups with defined regiochemistry, geometry and stereochemistry are meant to serve as examples for structure-drawing purposes. In many cases there may be alternative isobaric structures.

<table>
<thead>
<tr>
<th>LM_ID</th>
<th>Name</th>
<th>Systematic Name</th>
<th>Input m/z</th>
<th>Exact m/z</th>
<th>Formula</th>
<th>Ion</th>
</tr>
</thead>
<tbody>
<tr>
<td>LMGP01011520</td>
<td>PC(17:0/22:4(7Z,10Z,13Z,16Z))</td>
<td>1-heptadecanoyl-2-(7Z,10Z,13Z,16Z-docosatetraenoyl)-glycerol-3-phosphocholine</td>
<td>824.7</td>
<td>824.6163</td>
<td>C_{47}H_{57}NO_{9}P</td>
<td>M+H</td>
</tr>
<tr>
<td>LMGP01011578</td>
<td>PC(17:2(9Z,12Z)/22:2(13Z,16Z))</td>
<td>1-(9Z,12Z-heptadecadienoyl)-2-(13Z,16Z-docosadienoyl)-glycerol-3-phosphocholine</td>
<td>824.7</td>
<td>824.6163</td>
<td>C_{47}H_{57}NO_{9}P</td>
<td>M+H</td>
</tr>
<tr>
<td>LMGP01011726</td>
<td>PC(18:4(5Z,9Z,12Z,15Z)/21:0)</td>
<td>1-(5Z,9Z,12Z,15Z-octadecatetraenoyl)-2-heneicosanoyl-glycerol-3-phosphocholine</td>
<td>824.7</td>
<td>824.6163</td>
<td>C_{47}H_{57}NO_{9}P</td>
<td>M+H</td>
</tr>
<tr>
<td>LMGP01011748</td>
<td>PC(19:0/20:4(5Z,8Z,11Z,14Z))</td>
<td>1-nonadecanoyl-2-(5Z,8Z,11Z,14Z-eicosatetraenoyl)-glycerol-3-phosphocholine</td>
<td>824.7</td>
<td>824.6163</td>
<td>C_{47}H_{57}NO_{9}P</td>
<td>M+H</td>
</tr>
<tr>
<td>LMGP01011778</td>
<td>PC(19:1(9Z)/20:3(8Z,11Z,14Z))</td>
<td>1-(9Z-nonadecenoyl)-2-(8Z,11Z,14Z-eicosatrienoyl)-glycerol-3-phosphocholine</td>
<td>824.7</td>
<td>824.6163</td>
<td>C_{47}H_{57}NO_{9}P</td>
<td>M+H</td>
</tr>
<tr>
<td>LMGP01011884</td>
<td>PC(20:3(8Z,11Z,14Z)/19:1(9Z))</td>
<td>1-(8Z,11Z,14Z-eicosatrienoyl)-2-(9Z-nonadecenoyl)-glycerol-3-phosphocholine</td>
<td>824.7</td>
<td>824.6163</td>
<td>C_{47}H_{57}NO_{9}P</td>
<td>M+H</td>
</tr>
<tr>
<td>LMGP01011913</td>
<td>PC(20:4(5Z,8Z,11Z,14Z)/19:0)</td>
<td>1-(5Z,8Z,11Z,14Z-eicosatetraenoyl)-2-nonadecanoyl-glycerol-3-phosphocholine</td>
<td>824.7</td>
<td>824.6163</td>
<td>C_{47}H_{57}NO_{9}P</td>
<td>M+H</td>
</tr>
<tr>
<td>LMGP01011967</td>
<td>PC(21:0/18:4(6Z,9Z,12Z,15Z))</td>
<td>1-heneicosanoyl-2-(6Z,9Z,12Z,15Z-octadecatetraenoyl)-glycerol-3-phosphocholine</td>
<td>824.7</td>
<td>824.6163</td>
<td>C_{47}H_{57}NO_{9}P</td>
<td>M+H</td>
</tr>
<tr>
<td>LMGP01012045</td>
<td>PC(22:2(13Z,16Z)/17:2(9Z,12Z))</td>
<td>1-(13Z,16Z-docosadienoyl)-2-(9Z,12Z-heptadecadienoyl)-glycerol-3-phosphocholine</td>
<td>824.7</td>
<td>824.6163</td>
<td>C_{47}H_{57}NO_{9}P</td>
<td>M+H</td>
</tr>
<tr>
<td>LMGP01012074</td>
<td>PC(22:4(7Z,10Z,13Z,16Z)/17:0)</td>
<td>1-(7Z,10Z,13Z,16Z-docosatetraenoyl)-2-heptadecanoyl-glycerol-3-phosphocholine</td>
<td>824.7</td>
<td>824.6163</td>
<td>C_{47}H_{57}NO_{9}P</td>
<td>M+H</td>
</tr>
<tr>
<td>LMGP01020215</td>
<td>PC(O-18:0/22:4(7Z,10Z,13Z,16Z))</td>
<td>1-octadecyl-2-(7Z,10Z,13Z,16Z-docosatetraenoyl)-glycerol-3-phosphocholine</td>
<td>824.7</td>
<td>824.6527</td>
<td>C_{48}H_{51}NO_{7}P</td>
<td>M+H</td>
</tr>
<tr>
<td>LMGP01020238</td>
<td>PC(O-20:0/20:4(5Z,8Z,11Z,14Z))</td>
<td>1-eicosyl-2-(5Z,8Z,11Z,14Z-eicosatetraenoyl)-glycerol-3-phosphocholine</td>
<td>824.7</td>
<td>824.6527</td>
<td>C_{48}H_{51}NO_{7}P</td>
<td>M+H</td>
</tr>
</tbody>
</table>

**Possible Lipid Structures**

**Note:** Chains containing double bonds and/or functional groups with defined regiochemistry, geometry and stereochemistry are meant to serve as examples for structure-drawing purposes. In many cases there may be alternative isobaric structures.
MS precursor ion prediction tools example:
Glycerophospholipids (http://www.lipidmaps.org/data/index.html)
MS precursor ion prediction in “bulk” mode:
Individual chains are not specified

<table>
<thead>
<tr>
<th>Input Mass</th>
<th>Matched Mass</th>
<th>Delta</th>
<th>Abbreviation</th>
<th>Formula</th>
<th>Ion</th>
</tr>
</thead>
<tbody>
<tr>
<td>496.4773</td>
<td>496.3762</td>
<td>.1011</td>
<td>LPE(O-20:0)</td>
<td>$C_{26}H_{54}NO_3P$</td>
<td>[M+H]^+</td>
</tr>
<tr>
<td>496.4773</td>
<td>496.3398</td>
<td>.1375</td>
<td>LPC(16:0)</td>
<td>$C_{24}H_{57}NO_3P$</td>
<td>[M+H]^+</td>
</tr>
<tr>
<td>496.4773</td>
<td>496.3398</td>
<td>.1375</td>
<td>LPE(19:0)</td>
<td>$C_{24}H_{57}NO_3P$</td>
<td>[M+H]^+</td>
</tr>
<tr>
<td>524.4802</td>
<td>524.3711</td>
<td>.1091</td>
<td>LPE(21:0)</td>
<td>$C_{26}H_{54}NO_3P$</td>
<td>[M+H]^+</td>
</tr>
<tr>
<td>524.4802</td>
<td>524.3711</td>
<td>.1091</td>
<td>LPC(18:0)</td>
<td>$C_{24}H_{57}NO_3P$</td>
<td>[M+H]^+</td>
</tr>
<tr>
<td>524.4802</td>
<td>524.3347</td>
<td>.1455</td>
<td>PE(20:0)</td>
<td>$C_{24}H_{57}NO_3P$</td>
<td>[M+H]^+</td>
</tr>
<tr>
<td>524.4802</td>
<td>524.2983</td>
<td>.1819</td>
<td>LPS(18:1)</td>
<td>$C_{24}H_{57}NO_3P$</td>
<td>[M+H]^+</td>
</tr>
<tr>
<td>675.6826</td>
<td>675.5323</td>
<td>.1503</td>
<td>PA(P-35:0)</td>
<td>$C_{38}H_{79}O_5P$</td>
<td>[M+H]^+</td>
</tr>
<tr>
<td>675.6826</td>
<td>675.5323</td>
<td>.1503</td>
<td>PA(O-35:1)</td>
<td>$C_{38}H_{79}O_5P$</td>
<td>[M+H]^+</td>
</tr>
<tr>
<td>675.6826</td>
<td>675.4960</td>
<td>.1866</td>
<td>PA(34:1)</td>
<td>$C_{38}H_{79}O_5P$</td>
<td>[M+H]^+</td>
</tr>
</tbody>
</table>
**MS precursor/product ion prediction tools example:**

**Glycerophospholipids** (http://www.lipidmaps.org/data/index.html)

### Glycerophospholipid MS/MS Prediction

Match MS/MS peaklist to a database of precursor/product ions

(Compromised on background information for glycerophospholipids)

Enter peaklist

Space-delimiter

Possible Glycerophospholipid Structures matching input data

(m/z values in green denote matches within selected tolerance limits)

Number of precursor ions: 1

1 of 1 Precursor mass: 871.6 Charge: 1

<table>
<thead>
<tr>
<th>Abbreviation</th>
<th># of matches</th>
<th>m/z (delta)</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>PI(O-18:0/20:4(6Z,8Z,11Z,14Z))</td>
<td>11</td>
<td>871.5706</td>
<td>Precursor ion [M-H]-</td>
</tr>
<tr>
<td></td>
<td></td>
<td>709.5178 (0.0622)</td>
<td>Loss of inositol from [M-H]-</td>
</tr>
<tr>
<td></td>
<td></td>
<td>585.3409 (0.0591)</td>
<td>Loss of sn2 acyl chain as (RCH=C=O) from [M-H]-</td>
</tr>
<tr>
<td></td>
<td></td>
<td>567.3304 (0.1606)</td>
<td>Neutral loss of sn2 RCOOH group from [M-H]-</td>
</tr>
<tr>
<td></td>
<td></td>
<td>423.2881</td>
<td>Loss of sn2 acyl chain as (RCH=C=O) and inositol from [M-H]-</td>
</tr>
<tr>
<td></td>
<td></td>
<td>405.2775 (0.0775)</td>
<td>Neutral loss of sn2 RCOOH group and inositol from [M-H]-</td>
</tr>
<tr>
<td></td>
<td></td>
<td>315.0487 (0.1513)</td>
<td>Glycerophosphoinositol - H2O</td>
</tr>
<tr>
<td></td>
<td></td>
<td>303.2330 (0.0330)</td>
<td>sn2 RCOO- ion</td>
</tr>
<tr>
<td></td>
<td></td>
<td>297.0381 (0.1619)</td>
<td>Glycerophosphoinositol - 2H2O</td>
</tr>
<tr>
<td></td>
<td></td>
<td>259.2431 (0.0431)</td>
<td>Loss of CO2 from sn2 RCOO- ion (PUFA)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>241.0119 (0.0119)</td>
<td>Inositol phosphate ion</td>
</tr>
<tr>
<td></td>
<td></td>
<td>223.0013 (0.0013)</td>
<td>Inositol phosphate ion - H2O</td>
</tr>
<tr>
<td></td>
<td></td>
<td>204.9908</td>
<td>Inositol phosphate ion - 2 H2O</td>
</tr>
<tr>
<td></td>
<td></td>
<td>152.9958 (0.1042)</td>
<td>Glycerol-3-phosphate ion with loss of H2O</td>
</tr>
<tr>
<td></td>
<td></td>
<td>96.9696</td>
<td>H2PO4- ion</td>
</tr>
<tr>
<td></td>
<td></td>
<td>78.9591</td>
<td>PO3- ion</td>
</tr>
<tr>
<td>PI(20:4(6Z,8Z,11Z,14Z)/17:0)</td>
<td>10</td>
<td>871.5342</td>
<td>Precursor ion [M-H]-</td>
</tr>
<tr>
<td></td>
<td></td>
<td>709.4814 (0.1186)</td>
<td>Loss of inositol from [M-H]-</td>
</tr>
</tbody>
</table>
MS precursor/product ion prediction tools:
Information sources and criteria for commonly occurring product ions

Information sources:
Glycerophospholipid tandem mass spectra displayed in [LIPID MAPS Standards Library](http://www.lipidmaps.org).  
Glycerophospholipid Identification and Quantitation by Electrospray Ionization Mass Spectrometry  
Pavlina T. Ivanova, Stephen B. Milne, Mark O. Byrne, Yun Xiang, and H. Alex Brown.  

Electrospray mass spectrometry of phospholipids  
Melissa Pulfer and Robert C. Murphy  

Characterization of phosphatidylinositol, phosphatidylinositol- 4-phosphate, and phosphatidylinositol-4, 5-bisphosphate by electrospray ionization tandem mass spectrometry: A mechanistic study.  
Fong-Fu Hsu and John Turk  

Algorithm for Processing Raw Mass Spectrometric Data to Identify and Quantitate Complex Lipid Molecular Species in Mixtures by Data-Dependent Scanning and Fragment Ion Database Searching  
Haowei Song, Fong-Fu Hsu, Jack Ladenson, and John Turk  
*J Am Soc Mass Spectrom. 18(10) 1848-1858 (2007).*
Educating the public about lipids
Educating the public about lipids: LIPID MAPS tutorials

http://www.lipidmaps.org

Tutorials and instructions

- Tutorials and lectures on lipids
- Lipidomics methods
- LIPID MAPS databases
- Bioinformatics tools
- Author recommendations and tools

LIPID MAPS databases

- LIPID MAPS Structure Database (LMSD)
  The LIPID MAPS Structure Database (LMSD) is comprised of structures and annotations of biologically relevant lipids, and includes representative examples from each category of the LIPID MAPS Lipid Classification system.
  - Command line access of the LIPID MAPS Structure Database (LMSD) - Instructions for command line data retrieval as CSV, TSV, and SDIF files. Command line parameter options are explained and a number of examples are provided.
  - How to search LMSD by structure or sub-structure - Instructions and screen shots demonstrating how to use the Marvin Sketch API to search for lipids by drawing a complete or partial structure, and optionally specifying a partial lipid name.
  - How to search LMSD by text or ontology - Instructions and screen shots demonstrating how to use the text ontology search form to search for lipids by various combinations of lipid annotations, including name, classification, and ontology parameters.
  - How to search LMSD by text and ontology, (2.22) - Screencast demo

- LIPID MAPS Proteome Database (LMP)
  The LIPID MAPS Proteome Database (LMPD) is an object-relational database of lipid-associated human and mouse protein sequences and annotations.
  - Introduction to the LIPID MAPS Proteome Database (LMPD) - Screencast demo (2.58)

  Lipidomics Gateway "Quick search"
  The Quick search can be used to search the entire Lipidomics Gateway, including all text and database entries.
  - Quick Search Tutorial - Instructions and examples demonstrating how to search by lipid class, name, synonym, abbreviation or lipid-related gene/protein name, lipid abbreviation, SwissProt ID, gene symbol or annotation, chemical formula, lipid mass, LIPID MAPS ID, or LINCID.

Tutorial Series on Lipid Chemistry and Lipid Metabolomics

Presented as a set of PowerPoint files

A: Lipid Chemistry
- Lipid chemistry and classification

B: Lipid Metabolomics
1. Fatty Acid Biosynthesis
2. Fatty Acid Oxidation
3. Ketone Bodies and Essential Fatty Acids
4. Prostaglandins and Other Eicosanoids
5. Glycosphingolipids, Glycoconjugates and Glycolipids
6. Phospholipids
7. Cholesterol and Other Sterols
8. Lipoproteins
9. Fat Soluble Vitamins

Author recommendations and tools

- Lipid classification, nomenclature and structure drawing - detailed instructions for describing and drawing your lipid according to LIPID MAPS guidelines
- Web forms for submitting structures to the LIPID MAPS Structure Database (LMSD) - Web based forms allow you to draw a lipid structure, classify, and enter annotations
- How to cite the Lipidomics Gateway - how to cite LIPID MAPS resources, Lipidomics Update articles, and the Lipidomics Gateway as a general resource

Bioinformatics tools

- LIPID MAPS MS Prediction Tool
  The LIPID MAPS MS Prediction Tool is a standalone Windows application for predicting possible molecular species for a given MS ion.
  - MS Prediction Tutorial - examples of how to use the tool to predict possible glycosylphosphatidylinositol structure. A help interface is also included in the application.

- LIPID MAPS tools package
  The LIPID MAPS tools package is a set of command line Perl scripts to generate SD files containing structure and ontological data for various lipid categories.
  - LIPID MAPS tools package documentation - Both downloadable and online documentation are available along with the LIPID MAPS Tools Package on our Tools page under "Stand-alone tools."

- LIPID MAPS Pathway Editor
  The LIPID MAPS Pathway Editor is a program for managing, visualizing, and editing signaling and metabolic pathways.
  - Pathways Editor tutorial - an overview of Pathway Editor features, including how to start the Pathway Editor, access LIPID MAPS pathways and display LIPID MAPS and user-provided experimental data, create pathways from scratch, and edit and save pathway files and images. Instructions for working with SBML and BioPAX formats are also provided.
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