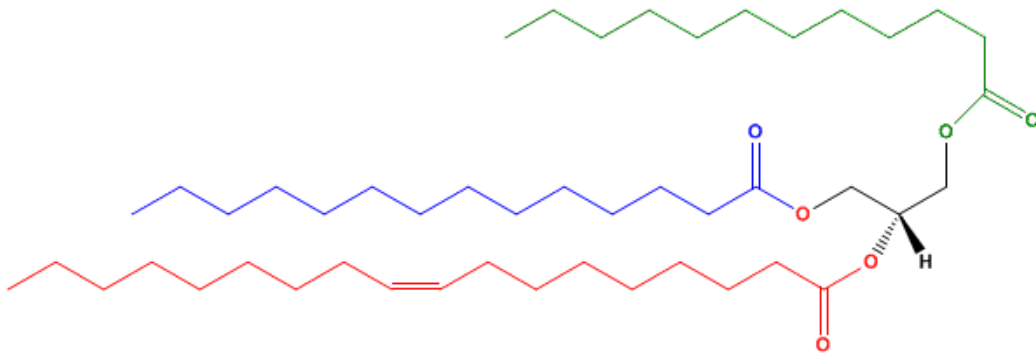
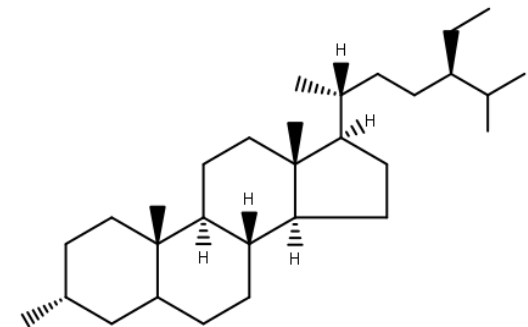


Lipidy a bioinformatika



Aplikovaná bioinformatika, Jaro 2016



LIPIDY

Lipidy jsou heterogenní skupina biomolekul nerozpuštěných ve vodě a rozpustných v organických rozpouštědlech. Jsou to deriváty vyšších monokarboxylových kyselin a alifatických či alicyklických hydroxyderivátů nebo aminoderivátů. Patří do ní následující látky:

1. Tuky a oleje ([acylglyceroly](#))
2. Glycerolipidy ([glycerofosfolipidy](#), [plasmalogeny](#), kardiolipin)
3. [Sfingolipidy](#)
4. [Steroidy](#) ([cholesterol](#), [žlučové kyseliny](#), [steroidní hormony](#))
5. Izoprenoidy ([ubichinon](#), [plastochinon](#), [dolichol](#))
6. [Vitaminy](#) rozpustné v tucích
7. Deriváty mastných kyselin ([leukotrieny](#), [prostaglandiny](#), prostacykliny, [tromboxany](#))

Lipidy hrají v organismu roli jako zásobní látky, strukturální složky membrán, hormony a vitaminy.

***Základní pojmy z biochemie, V. Mikeš, Katedra biochemie PŘF
Masarykovy Univerzity v Brně, 2. doplněné vydání 2001***



LIPIDY

Lipid classification, structures and tools[☆]

Eoin Fahy^{*}, Dawn Cotter, Manish Sud, and Shankar Subramaniam

University of California, San Diego, 9500 Gilman Dr., La Jolla, CA 92093-0411, USA

Abstract

The study of lipids has developed into a research field of increasing importance as their multiple biological roles in cell biology, physiology and pathology are becoming better understood. The Lipid Metabolites and Pathways Strategy (LIPID MAPS) consortium is actively involved in an integrated approach for the detection, quantitation and pathway reconstruction of lipids and related genes and proteins at a systems-biology level. A key component of this approach is a bioinformatics infrastructure involving a clearly defined classification of lipids, a state-of-the-art database system for molecular species and experimental data and a suite of user-friendly tools to assist lipidomics researchers. Herein, we discuss a number of recent developments by the LIPID MAPS bioinformatics core in pursuit of these objectives. This article is part of a Special Issue entitled Lipidomics and Imaging Mass Spectrometry.

**Klasifikační systém zahrnující
8 hlavních tříd, každá je dále
členěná**

LIPID MAPS



LIPID Metabolites and Pathways Strategy (LIPID MAPS)

Lipidomics Gateway

Home | Lipidomics Update | **Resources** | Meetings | Tutorials | Protocols | About

Overview | Publications | **Classification** | Standards | Data | Databases | Pathways | Tools | Services

<http://www.lipidmaps.org/>

Lipid Classification System

The LIPID MAPS Lipid Classification System is comprised of eight lipid categories, each with its own subclassification hierarchy. All lipids in the LIPID MAPS Structure Database (LMSD) have been classified using this system and have been assigned LIPID MAPS ID's (LM_ID) which reflects their position in the classification hierarchy. LMSD can be searched by lipid class, common name, systematic name or synonym, mass, InChIKey or LIPID MAPS ID with the ["Quick Search" tool](#) on the home page, or alternatively, by LIPID MAPS ID, systematic or common name, mass, formula, category, main class, subclass data, or structure or sub-structure with one of the search interfaces in the [LMSD database](#) section. Each LMSD record contains an image of the molecular structure, common and systematic names, links to external databases, Wikipedia pages (where available), other annotations and links to structure viewing tools. In addition to LMSD search interfaces, you can drill down through the classification hierarchy below to the LMSD record for an individual lipid.

LIPID MAPS



LIPID Metabolites and Pathways Strategy (LIPID MAPS)

Lipidomics Gateway

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[Overview](#) | [Publications](#) | [Classification](#) | [Standards](#) | [Data](#) | **[Databases](#)** | [Pathways](#) | [Tools](#) | [Services](#) | [Lir](#)

<http://www.lipidmaps.org/>

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.

- [LIPID MAPS Proteome Database \(LMPD\)](#)

Lipid-associated protein sequences with annotations from UniProt, EntrezGene, ENZYME, GO, KEGG and other public resources. Browse or search by species, lipid class association, and/or keywords.

LIPID MAPS

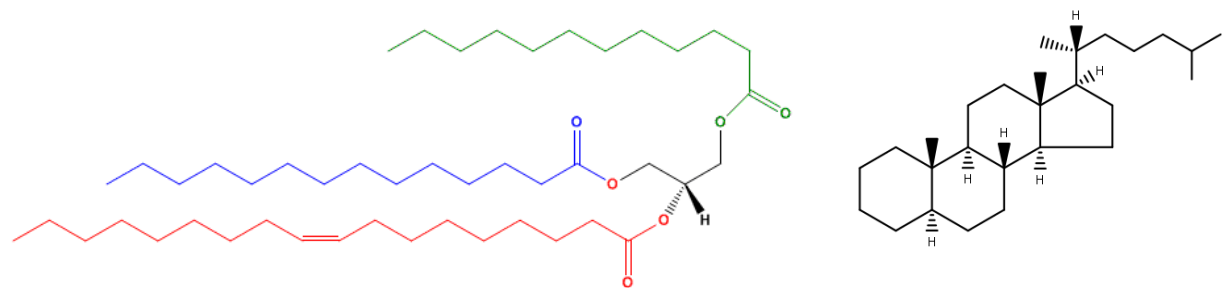


**Nástroje pro MS
analýzu lipidů**

**Algorithms for Automatic Processing of Data from Mass
Spectrometric Analyses of Lipids**

Haowei Song¹, Jack Ladenson², and John Turk^{1,*}

**Nástroje pro grafické
znázornění lipidů**



LipidBank

"LipidBank" is an open, publicly free database of natural lipids including fatty acids, glycerolipids, sphingolipids, steroids, and various vitamins.

The database contains more than 6000 unique molecular structures (ChemDraw cdx format, MDL MOL format), their lipid names (common name, IUPAC), spectral information (mass, UV, IR, NMR and others), and most importantly, literature information.

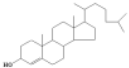
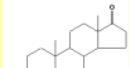
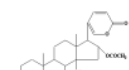
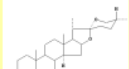
The database lists natural lipids only, and all molecular information is manually curated and approved by experts in lipid research (see Informant in each record).

LipidBank is the official database of the Japanese Conference on the Biochemistry of Lipids (JCBL).

<http://lipidbank.jp/>

479 / 479 matched

1-20 displayed (out of 479 matched) [Next Page](#) [change](#)

1		Allocholesterol / Coprostenol / 4:5-Coprosten-3-ol / Cholest-4-en-3b-ol (No = SST0001)
2		Androsterone / Cis-androsterone / 3a-Hydroxy-17-androstanone / 3(a)-Hydroxyetioallocholan-17-one / 3-Epihydroxyetioallocholan-17 (No = SST0002)
3		Bufotalin / 16-(Acetyloxy)-3,14-dihydroxybufa-20,22-dienolide / 3b,14,16b-Trihydroxy-5b-bufa-20,22-dienolide 16-acetate (No = SST0003)
4		Chlorogenin / 5a-Spirostan-3b,6a-diol (No = SST0004)

Steroid

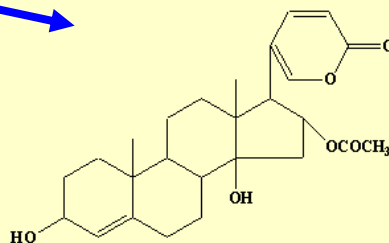
DATA No : SST0003 INFORMANT : Hideaki Nishino

NAME : 16-(Acetyloxy)-3,14-dihydroxybufa-20,22-dienolide / 3b,14,16b-Trihydroxy-5b-bufa-20,22-dienolide 16-acetate

COMMON NAME : Bufotalin

SYMBOL :

FORMULA : C₂₆H₃₆O₆ MOL.WT (average) : 444.560



[Download ChemDraw structure data](#)

LINKS

[Cosmetics oil](#) - [Veeco Finance Export](#) (cashew, h
[Craig Byrdwell Lipid site](#) - Mass analyses of vita
[CREOL](#) - Pilote d'études de graines d'oléagineux
[CTVO-NET](#) (Chemical-Technical Utilization of
definition of the prospects of European oils.
[DHA/EPA Omega-3 Institute](#) - Objective Scienc
[Drug Therapy for Lipid Disorders](#) - Medicine co
[EFA Education](#) - Essential fatty acids
[Eicosanoid Research Division @IGBM](#) - Multid
[Eicosanoids and Vascular Pharmacology](#)
[Essential Nutrient Research Company](#) - Flax inf
[Essential Oil University](#) - R. Pappas web site an
[Essential Oils - Bo Jensen website](#) (A small guid
[European Biofuels Technology Platform](#)
[European Olive oil Medical Information Center](#)
[European Lipidomics Initiative](#) - ELife: The Eur
[Fats for Health](#) - Essential fatty acid informatio
[Fats of life](#) - Information on fatty acids and nutr
[Fats You Need -- Essential Fatty Acids](#)
[Fatty acids](#) : list of composition and trivial name

CYBERLIPID CENTER

RESOURCE SITE FOR LIPID STUDIES

If you are interested in the science of LIPIDS then you're
in the right site.
Add this page to your hotlist now!
Visit these pages regularly to keep up to date with
the latest lipid news.

<http://www.cyberlipid.org/index.htm>

ANALYSIS

CALENDAR

HISTORY

10-12 April 2016 - Authenticity of olive oil and other vegetable oils, Nuremberg, Germany.
For information contact : [website](#)

10-11 May 2016 - Second DGF "Young Investigators in Lipid Science" Meeting, Duesseldorf, Germany.
For information contact : [website](#)

17-18 May 2016 - LIPID MAPS Annual Meeting 2016: Lipidomics Impact on Metabolic, Cancer, Cardiovascular and Inflammatory Diseases. University of California, San Diego, USA.
For information contact : [web site](#)

23-26 May 2016 - 10th International Society of Nutrigenetics/Nutrigenomics (ISNN) Congress, Tel Aviv, Israel.
For information contact : [web site](#)

1- How to preserve and extract lipids?

2- What amount of lipids is present in the sample ?

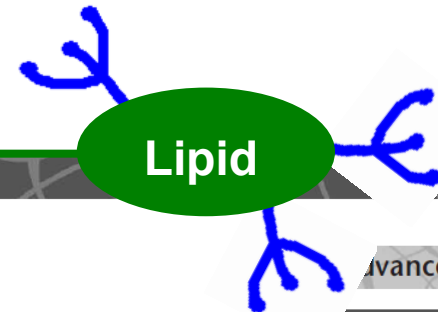
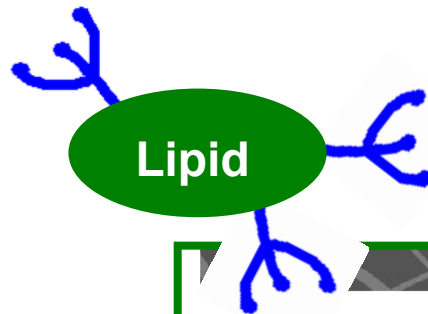
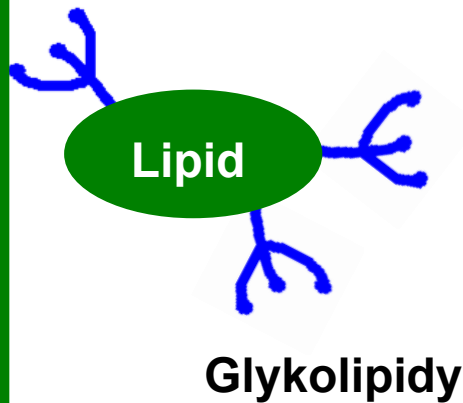
3- How to fractionate a natural lipid extract?

4- What are the components present within each fraction?

5- What amounts of each component are present in the lipid extract?

1783:
Fourcroy AF introduced
alcohol to extract brain
lipids.

LIPIDY + SACHARIDY



- Antigeny
- Receptory
- Adheze

- Lipidová část slouží k ukotvení v membráně

Glycolipids: Animal

Hakomori Sen-itiroh, *Pacific Northwest Research Institute and University of Washington, Seattle, Washington, USA*

Ishizuka Ineo, *Teikyo University School of Medicine, Tokyo, Japan*

Glycolipids are carbohydrates linked to lipid (either ceramide or glyceride). They are found in animal cells and tissues.

Introduction

Glycolipids are ubiquitous components of all animal cell membranes and are particularly abundant at the cell surface membrane. The majority of glycolipids belong to the class 'glycosphingolipids' (GSLs; also called sphingoglycolipids), which have a backbone lipid (termed 'ceramide') consisting of fatty acids and a long-chain aliphatic amino alcohol, discovered and named 'sphingosine' by JLW Thudichum in 1876. Sphingosine has the structure 1,3-dihydroxy-2-amino-octadecene, exhibiting the D-erythro stereoconfiguration with regard to the asymmetric carbon 1 (C1), C2 and C3 (Figure 1a). Fatty acids with various chain lengths are linked to the 2-amino group of sphingosine to form ceramide (Figure 1b). Various sugar residues are linked to the C1 primary hydroxyl group of the sphingosine moiety in ceramide to form galactosylceramide (GalCer) (Figure 1c), glucosylceramide (GlcCer) (Figure 1d), or a variety of more complex oligosaccharides, resulting in a wide variety of GSLs. One example of such a structure, 'GM3',

Advanced article

Article Contents

- Introduction
- Structure
- Synthesis and Degradation
- Function
- Conformational Structure, Distribution and Organization of Glycosphingolipids in Membrane

doi: 10.1002/9780470015902.a0000706.pub2

Another class of glyceroglycolipids is the 'glycosylphosphatidylinositol anchor' (GPI anchor). A large number of functionally important cell-surface proteins are anchored through this class of glycolipids (see below). See also: Glycolipids: distribution and biological function

Structure

The most extensive studies on the structure and function of animal cell glycolipids have been focused on GSLs. GSLs consist of two distinct moieties: ceramide, which is hydrophobic, and carbohydrate, which is hydrophilic. A molecular model of GSL based on X-ray crystallography indicates that the axis of the ceramide is perpendicular to the axis of the carbohydrate chain. GSLs have a strong tendency to aggregate to form micelles in aqueous media, or to form microdomains in the cell membrane bilayer.

LIPIDY + SACHARIDY

- [Generate Fatty Acyl Structures](#)
- [Generate Glycerolipid Structures](#)
- [Generate Glycerophospholipid Structures](#)
- [Generate Cardiolipin Structures](#)
- [Generate Sphingolipid Structures](#)
- [Generate Sterol \(cholestane, ergostane, campestane and stigmasterane\) Structures](#)
- [Generate Glycan structures \(attached to either an R group or ceramide\)](#)
- [Species-specific lipidomes](#)
- [Generate Mycobacterium tuberculosis structures](#)

<http://www.lipidmaps.org/>

ARCHITECTURE AND SHEMATIC STRUCTURE OF AN ENTEROBACTERIAL LIPOPOLYSACCHARIDE



 **GLYCO-SCIENCES.DE**

- **Lipopolysacharidy** jsou součástí vnější membrány gramnegativních bakterií.
- Endotoxin (pyrogen, aktivace imunitního systému, poruchy srážlivosti)

LIPIDY + PROTEINY

LipoP 1.0 Server

Prediction of lipoproteins and signal peptides in Gram negative bacteria

The LipoP 1.0 server produces predictions of lipoproteins and discriminates between lipoprotein signal peptides, other signal peptides and n-terminal membrane helices in Gram-negative bacteria.

Note: Although LipoP 1.0 has been trained on sequences from Gram-negative bacteria only, the following paper reports that it has a good performance on sequences from Gram-positive bacteria also:

[Methods for the bioinformatic identification of bacterial lipoproteins encoded in the genomes of Gram-positive bacteria](#)

O. Rahman, S. P. Cummings, D. J. Harrington and I. C. Sutcliffe
World Journal of Microbiology and Biotechnology 24(11):2377-2382 (2008)

<http://bioinformatics.biol.uoa.gr/PRED-LIPO/>

PRED-LIPO
 PRED-LIPO

Prediction of Lipoprotein and Secretory Signal Peptides in Gram-positive Bacteria with Hidden Markov Models

We present a Hidden Markov Model method for the prediction of lipoprotein signal peptides of Gram-positive bacteria, trained on a set of 67 experimentally verified lipoproteins.

The method outperforms LipoP and the methods based on regular expression patterns, in various data sets containing experimentally characterized lipoproteins, secretory proteins, proteins with an N-terminal TM segment and cytoplasmic proteins.

The method is also very sensitive and specific in the detection of secretory signal peptides and in terms of overall accuracy outperforms even SignalP, which is the top-scoring method for the prediction of signal peptides.

Proceed with PRED-LIPO

Abstract Bacterial lipoproteins are a diverse and functionally important group of proteins that are amenable to bioinformatic analyses because of their unique signal peptide features. Here we have used a dataset of sequences of experimentally verified lipoproteins of Gram-positive bacteria to refine our previously described lipoprotein recognition pattern (G+LPP). Sequenced bacterial genomes can be screened for putative lipoproteins using the G+LPP pattern. The sequences identified can then be validated using online tools for lipoprotein sequence identification. We have used our protein sequence datasets to evaluate six online tools for efficacy of lipoprotein sequence identification. Our analyses demonstrate that LipoP (<http://www.cbs.dtu.dk/services/LipoP/>) performs best individually but that a consensus approach, incorporating outputs from predictors of general signal peptide properties, is most informative.

Proteiny

Glykoproteiny

Proteoglykany

Sacharidy

Lipoproteiny

Proteolipidy

Glykolipidy

Liposacharidy

Lipidy

Všechno souvisí se vším...

