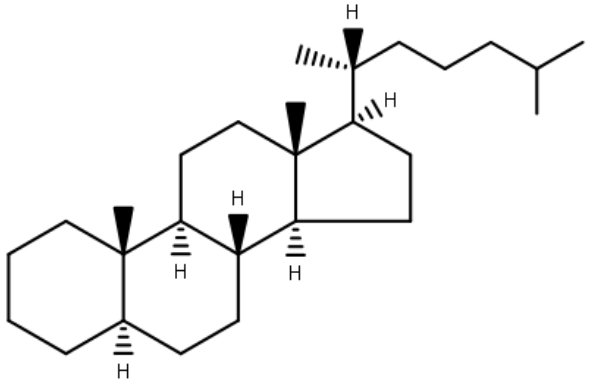
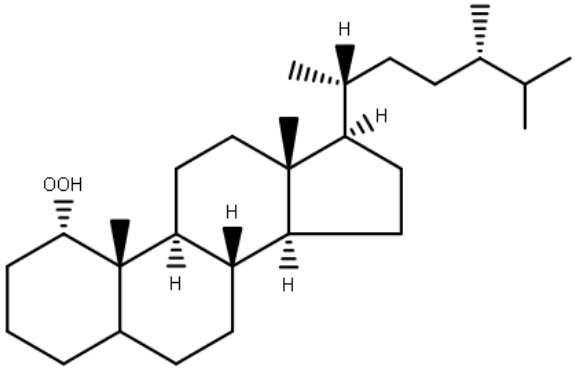
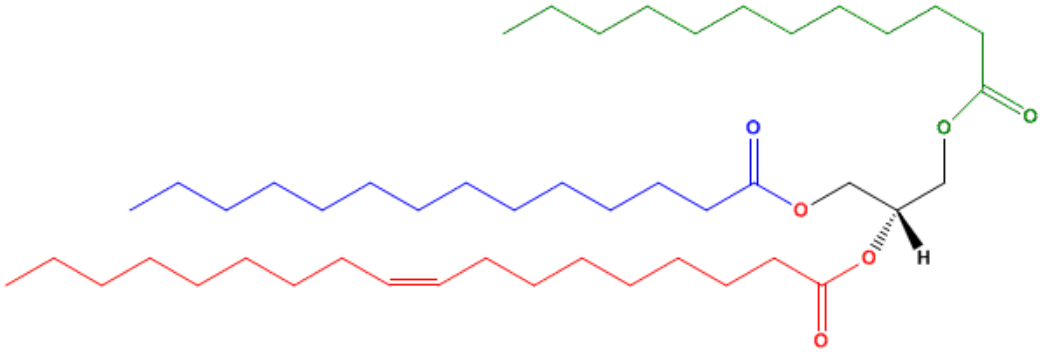
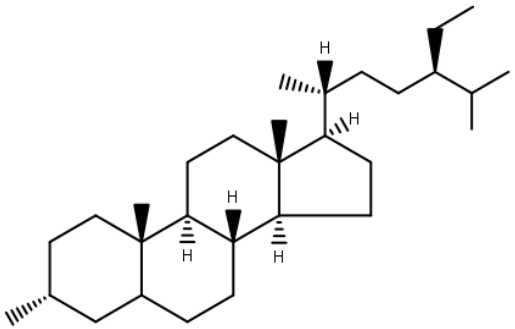




Lipidy a bioinformatika



Aplikovaná bioinformatika, Jaro 2014



LIPIDY

Lipidy jsou heterogenní skupina biomolekul nerozputných 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 Lipodomics and Imaging Mass Spectrometry.

Klasifikační systém zahrnující 8 hlavních tříd, každá je dále členěná

LIPID MAPS

http://www.lipidmaps.org/

Lipid Classification System

The LIPID MAPS Lipid Classification System is comprised of eight lipid categories, each with its own sublassification 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

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.

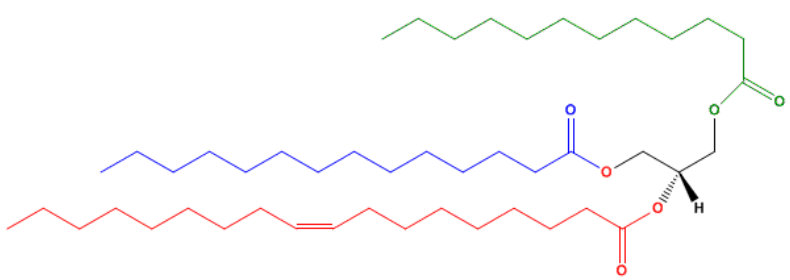
LIPID MAPS

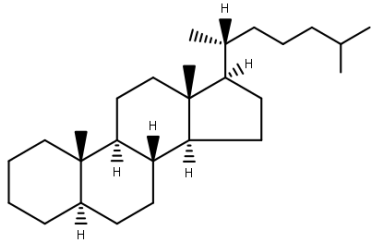
Nástroje pro MS analýzu lipidů

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

Haowei Song[1], **Jack Ladenson**[2], and **John Turk**[1,*]

Nástroje pro grafické znázornění lipidů





LipidBank

http://lipidbank.jp/

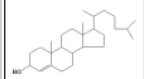
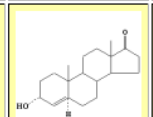
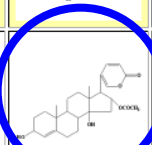
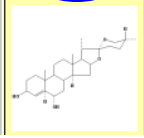
"LipidBank" is an open, publicly free database of natural lipids including fatty acids, glycerolipids, sphingolipids, steroids, and various vitamins.

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).

479 / 479 matched | 1-20 displayed (out of 479 matched) Next Page change

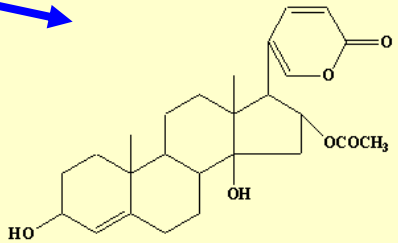
1		**Allocholesterol / Coprostenol / 4:5-Coprosten-3-ol** /Cholest-4-en-3b-ol (No = SST0001)
2		**Androsterone / Cis-androsterone / 3a-Hydroxy-17-androstanone / A 3(a)-Hydroxyetioallocholan-17-one / 3-Epihydroxyetioallocholan-17** (No = SST0002)
3		**Bufotalin** /16-(Acetyloxy)-3,14-dihydroxybufa-20,22-dienolide / 3b,14,16b 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-acetat

COMMON NAME : Bufotalin
SYMBOL :
FORMULA : $C_{26}H_{36}O_6$ **MOL.WT (average)** : 444.560



Download ChemDraw structure data

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?

ANALYSIS

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

LINKS

Cosmetics oil - eco Finance Export (cashew, h
Craig Byrdwell Lipid site - Mass analyses of vita
CREOL - Pilote d'études de graines d'oléagineux
CTIO-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 information
Fats of life - Information on fatty acids and nutr
Fats You Need -- Essential Fatty Acids
Fatty acids : list of composition and trivial name

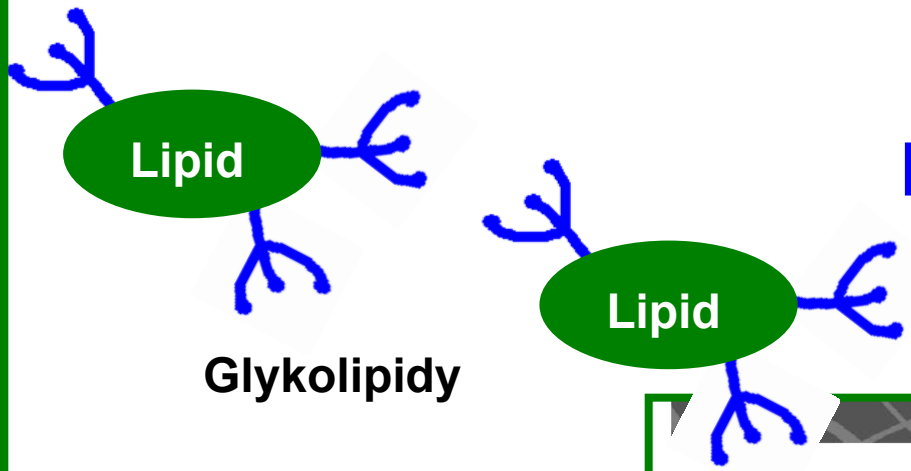
HISTORY

1783:
Fourcroy AF introduced alcohol to extract brain lipids.

CALENDAR

13-16 March 2014 - National Lipid Association, Spring Clinical Lipid Update - "Atheroprevention: Global Perspectives and Evolving Concepts", Maui, Hawaii.
For information contact : web site

LIPIDY + SACHARIDY



Glykolipidy

- 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.

Advanced article

Article Contents

doi: 10.1002/9780470015902.a0000706.pub2

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',

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 glycoglycerolipids (see below). **See also**: Glycolipids: distribution and biological function

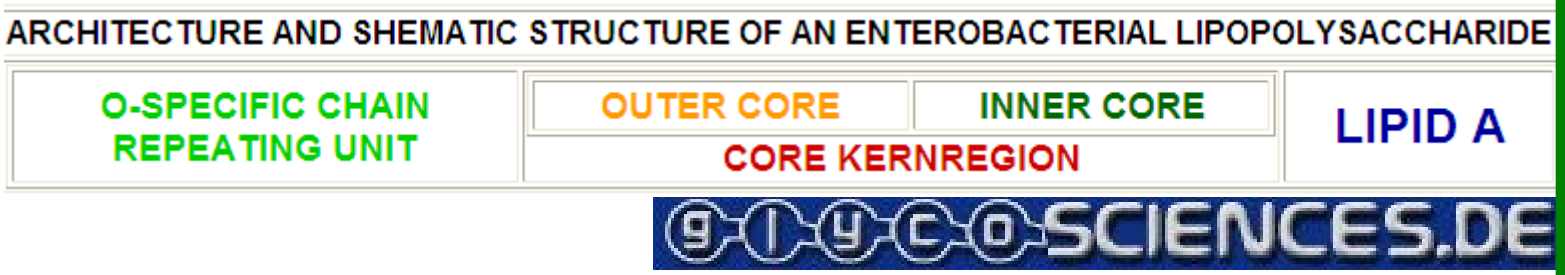
Structure

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 stigmastane) Structures
- Generate Glycan strucures (attached to either an R group or ceramide)
- Species-Specific lipidomes
  - Generate Mycobacterium tuberculosis strucures

http://www.lipidmaps.org/



- **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)

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.

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

PRED-LIPO

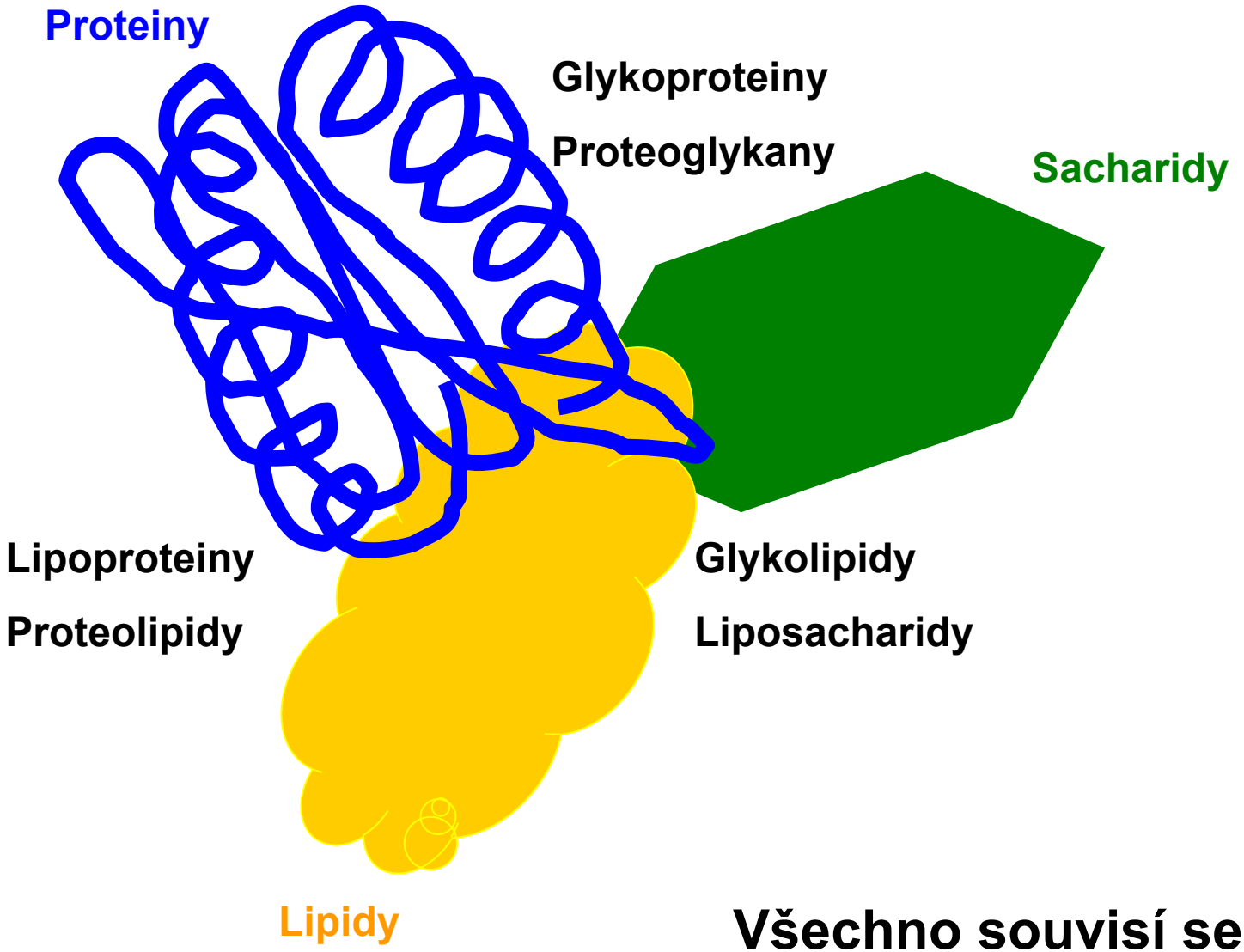
Prediction of Lipoprotein and Secretory Signal Peptides in Gram-positive Bacteria with Hidden Markov Models

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



Všechno souvisí se vším…