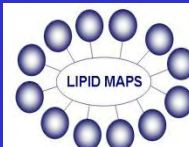


LIPID MAPS
Bioinformatics

EB2009 Apr 18,2009

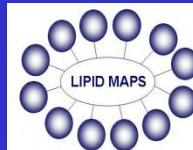
Eoin Fahy

University Of California San Diego



LIPID MAPS Bioinformatics Overview

- 1. Lipid classification, nomenclature and structure representation**
- 2. Lipid Molecular Databases**
- 3. Lipid-associated Protein/Gene databases**
- 4. Lipidomic Experimental Data Display**
- 5. Laboratory information management systems (LIMS)**
- 6. Bioinformatics tools for lipidomics**
- 7. Lipid-associated Pathways and Networks**



LIPID MAPS Website



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

LIPID MAPS -- LIPID Metabolites And Pathways Strategy - Microsoft Internet Explorer provided by SDSC

File Edit View Favorites Tools Help

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

Google

LIPID MAPS -- LIPID ... x http://chem.sdsc.edu/a... La Costa Canyon High S... 2009 LCC Track and Fiel...

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 **LIPID Metabolites And Pathways Strategy**

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[Guided Tour of the LIPID MAPS Website](#)

[Lipid Classification Scheme](#)

- [Fatty Acyls](#)
- [Glycerolipids](#)
- [Glycerophospholipids](#)
- [Sphingolipids](#)
- [Sterol Lipids](#)
- [Prenol Lipids](#)
- [Saccharolipids](#)
- [Polyketides](#)

[Classification Updates](#)

LIPID MAPS Annual Meeting 2009
Lipidomics Impact on Cell Biology, Structural Biochemistry and Immunopathology

Lipid recognition in the immune system * Eicosanoid signaling * Membrane proteins and specific lipid interactions * Advances in lipidomics * Macrophage lipidomics * Sphingolipid signaling * Macrophages and disease, systems biology implications

May 6-7, 2009 * UCSD * LA JOLLA, CA

Lipid Search
(Enter Common or Systematic Name, e.g. Stearic acid)

[Submit](#) [Advanced Search](#)

News! [RSS](#) [XML](#)

Lipidomics Meetings

Apr 18-22, 2009 - [Lipidomics Workshop](#) at Experimental Biology 2009, New Orleans, LA.

May 6-8, 2009 - [LIPID MAPS Annual Meeting 2009: Lipidomics Impact on Cell Biology, Structural Biochemistry and Immunopathology](#), CA.

May 10-13, 2009 - [Frontier Lipidology: Lipidomics in Health and Disease](#) Gothenburg, Sweden.

Effective May 1, 2009, the LIPID MAPS web site will become a Nature Lipidomics Gateway. The appearance of the site will change, but the same LIPID MAPS generated tools and data will be available on the new web site.

09 - LIPID MAPS Annual Meeting 2009 Registration is open for our 6th annual meeting: Lipidomics Impact on Cell Biology, Structural Biochemistry and Immunopathology. May 6-7, La Jolla, CA.

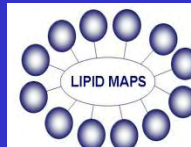
02/09/09 - [EB 2009 Lipidomics Workshop](#) The LIPID MAPS Consortium is conducting an open Workshop on Lipidomics and Experimental Biology 2009, LA, CA.

10/13/08 - [Lipidomics Studies on Macrophages: RAW 264.7 cells treated with Compactin + Kdo2-Lipid A](#) Browse averages of biological replicates and treatment:control ratios by analyte category, or search by ANOVA p-value.

10/13/08 - [Subcellular fractionation studies: RAW 264.7 cells treated with Kdo2-](#)

Garrett, T. A., Guan, Z., and Raetz, C. R. (2007) Analysis of ubiquinones, dolichols and dolichol diphosphate-oligosaccharides by liquid chromatography-electrospray ionization mass spectrometry. In Meth. Enzymol., Academic Press, 432, 117-142.

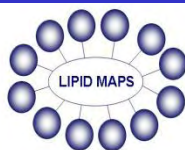
Ivanova, P., Milne, S., Byrne, M. O., Xiang, Y., and Brown, H. A. (2007)



Definition of a lipid*

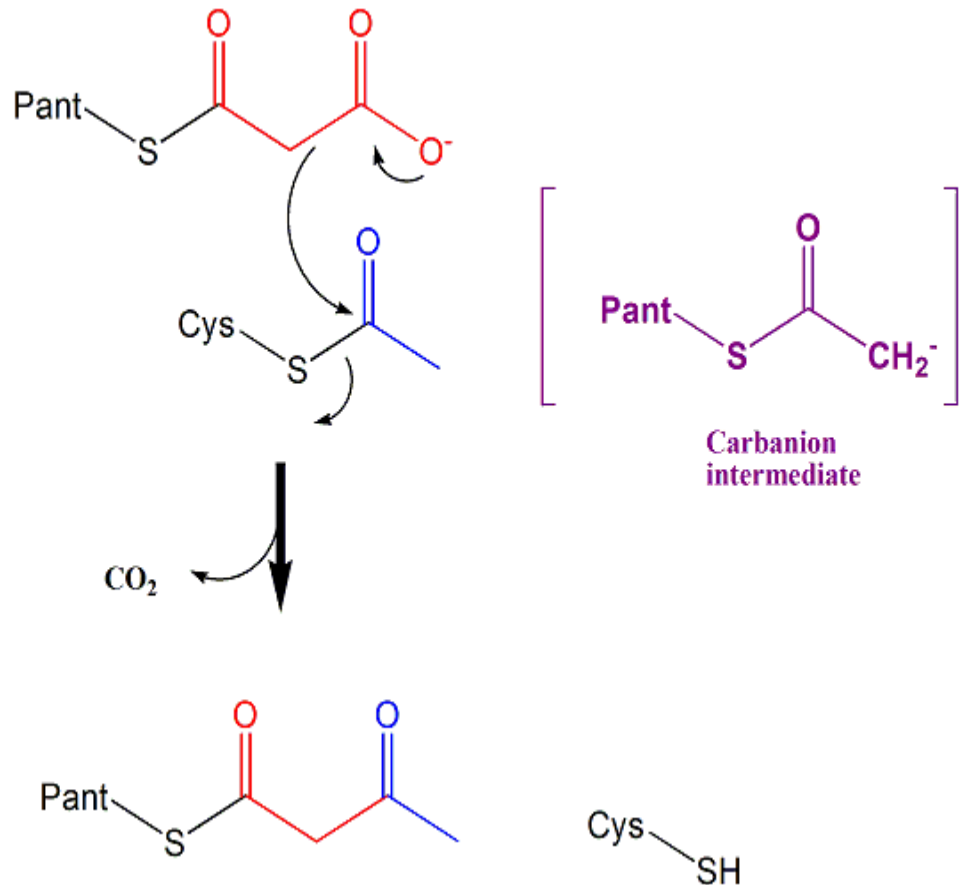
Lipids may be broadly defined as hydrophobic or amphiphilic small molecules that originate entirely or in part from **two distinct types of biochemical subunits or "building blocks": ketoacyl and isoprene groups**. Using this approach, lipids may be divided into **eight categories** : fatty acyls, glycerolipids, ,glycerophospholipids, sphingolipids, saccharolipids and polyketides (derived from condensation of ketoacyl subunits); and sterol lipids and prenol lipids (derived from condensation of isoprene subunits).

* Fahy,E. *et al*, Journal of Lipid Research, Vol. 46, 839-862, May 2005



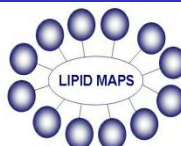
Lipid classification: biosynthetic routes

1: Carbanion-based condensation



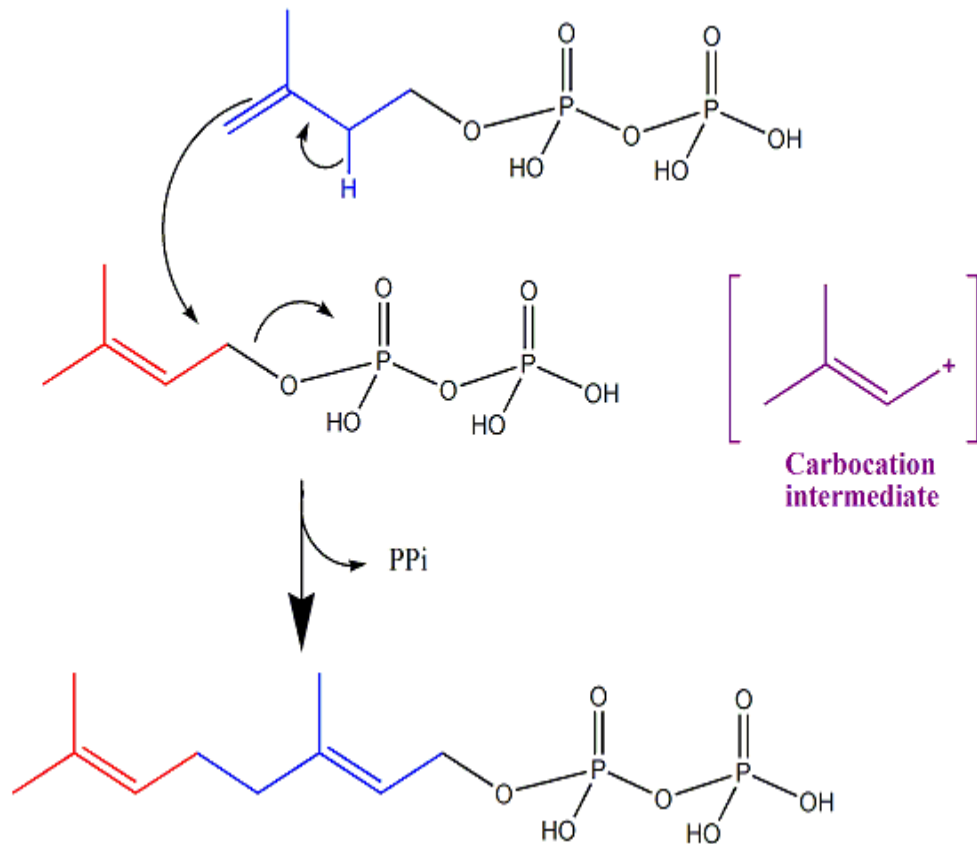
CATEGORIES

Fatty Acyls
Glycerolipids
Glycerophospholipids
Sphingolipids
Saccharolipids
Polyketides



Lipid classification: biosynthetic routes

2: Carbocation-based condensation



CATEGORIES

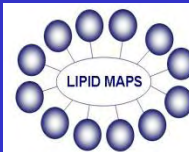
Sterol lipids

Prenol lipids

LIPID MAPS Classification System

Categories and Examples

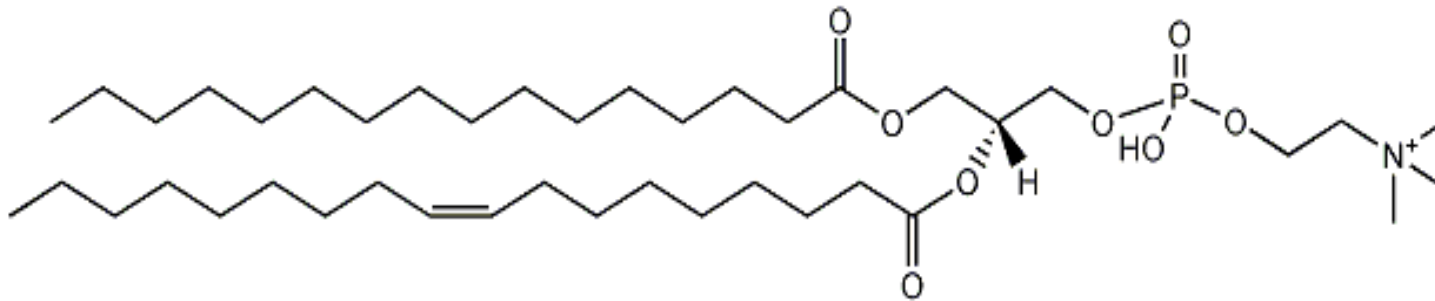
Category	Abbreviation	Example
Fatty acyls	FA	Dodecanoic acid
Glycerolipids	GL	1-hexadecanoyl-2-(9Z-octadecenoyl)-sn-glycerol
Glycerophospholipids	GP	1-hexadecanoyl-2-(9Z-octadecenoyl)-sn-glycero-3-phosphocholine
Sphingolipids	SP	N-(tetradecanoyl)-sphing-4-enine
Sterol lipids	ST	Cholest-5-en-3 β -ol
Prenol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



LIPID MAPS: Compound ID

- **LIPID MAPS compound ID**

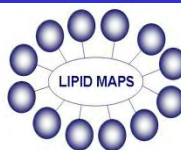
- **LMGP01010005**



1-hexadecanoyl-2-(9Z-octadecenoyl)-sn-glycero-3-phosphocholine

- **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**



J. Lipid Res. : Classification publications

Journal of Lipid Research, Vol. 46, 839-862, May 2005

Journal of Lipid Research, 50th anniversary edition, May 2009

A comprehensive classification system for lipids -- Fahy et al., 10.1194/jlr.E400004-JLR200 -- Microsoft Internet Explorer

Update of the LIPID MAPS comprehensive classification system for lipids -- Fahy et al., 10.1194 - Microsoft Internet Explorer p

http://www.jlr.org/cgi/content/abstract/R800095-JLR200v1

Address http://www.jlr.org

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Institution: Univ of California

A more recent version

Papers In Press, published online ahead of print December 19, 2008
J. Lipid Res., doi:10.1194/jlr.R800095-JLR200

Submitted on November 25, 2008
Revised on December 19, 2008
Accepted on December 19, 2008

Update of the LIPID MAPS comprehensive classification system for lipids

Eoin Fahy, Shankar Subramaniam, Robert C. Murphy, Masahiro Nishijima, Christian R.H. Raetz, Takao Shimizu, Friedrich Spener, Gerrit van Meer, Michael J.O. Wakelam, and Edward A. Dennis

Chemistry and Biochemistry, University of California, San Diego, La Jolla, CA 92093

Corresponding Author: edennis@ucsd.edu

In 2005, the International Lipid Classification and Nomenclature Committee (ILCNC) under the sponsorship of the LIPID MAPS Consortium developed and established a "Comprehensive Classification System for Lipids" based on well-defined chemical and biochemical principles, and using an ontology that is extensible, flexible and scalable. This classification system which is compatible with contemporary databasing and informatics needs has now been accepted internationally and widely adopted. In response to considerable attention and requests from lipid researchers from around the globe and in a variety of fields, the comprehensive classification system has undergone significant revisions over the last few years to more fully represent lipid structures from a wider variety of sources and to provide additional levels of detail as necessary. The details of this classification system are reviewed and updated and are presented here, along with revisions to its suggested nomenclature and structure-drawing recommendations for lipids.

Department of Chemistry
92037-0601

Corresponding Author

Lipids are produced, binding proteins and context of genomics a

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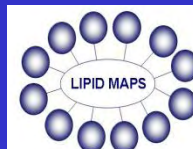
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LIPID MAPS Online Classification System



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



LIPID Metabolites And Pathways Strategy

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Structure database (LMSD)

Lipid Classification Scheme

Updated 09/01/06

[Fatty Acyls](#) [Glycerolipids](#) [Glycerophospholipids](#) [Sphingolipids](#) [Sterol Lipids](#) [Prenol Lipids](#) [Saccharolipids](#) [Polyketides](#)

Fatty Acyls [FA] classes and subclasses

Fatty Acids and Conjugates [\[FA01\]](#)

Straight chain fatty acids [\[FA0101\]](#)
Methyl branched fatty acids [\[FA0102\]](#)
Unsaturated fatty acids [\[FA0103\]](#)
Hydroperoxy fatty acids [\[FA0104\]](#)
Hydroxy fatty acids [\[FA0105\]](#)
Oxo fatty acids [\[FA0106\]](#)
Epoxy fatty acids [\[FA0107\]](#)
Methoxy fatty acids [\[FA0108\]](#)
Halogenated fatty acids [\[FA0109\]](#)
Amino fatty acids [\[FA0110\]](#)
Cyano fatty acids [\[FA0111\]](#)
Nitro fatty acids [\[FA0112\]](#)
Thia fatty acids [\[FA0113\]](#)
Carbocyclic fatty acids [\[FA0114\]](#)
Heterocyclic fatty acids [\[FA0115\]](#)
Mycolic acids [\[FA0116\]](#)
Dicarboxylic acids [\[FA0117\]](#)

Octadecanoids [\[FA02\]](#)
12-oxophytodienoic acid metabolites [\[FA0201\]](#)
jasmonic acids [\[FA0202\]](#)

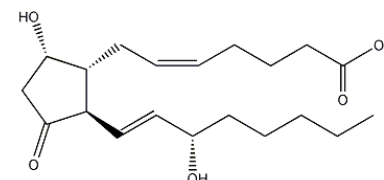
Eicosanoids [\[FA03\]](#)

Prostaglandins [\[FA0301\]](#)
Leukotrienes [\[FA0302\]](#)
Thromboxanes [\[FA0303\]](#)
Lipoxins [\[FA0304\]](#)
Hydroxy/hydroperoxyeicosatrienoic acids [\[FA0305\]](#)
Hydroxy/hydroperoxyeicosatetraenoic acids [\[FA0306\]](#)
Hydroxy/hydroperoxyeicosapentaenoic acids [\[FA0307\]](#)
Epoxyeicosatrienoic acids [\[FA0308\]](#)
Hepoxilins [\[FA0309\]](#)
Levuglandins [\[FA0310\]](#)
Isoprostanes [\[FA0311\]](#)
Clavulones and derivatives [\[FA0312\]](#)
Docosanoids [\[FA04\]](#)
Fatty alcohols [\[FA05\]](#)

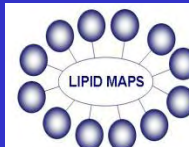
Category:Fatty Acyls [FA]

--> Main class: Eicosanoids [FA03] --> Sub class: Prostaglandin

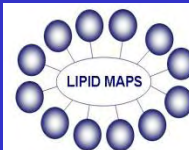
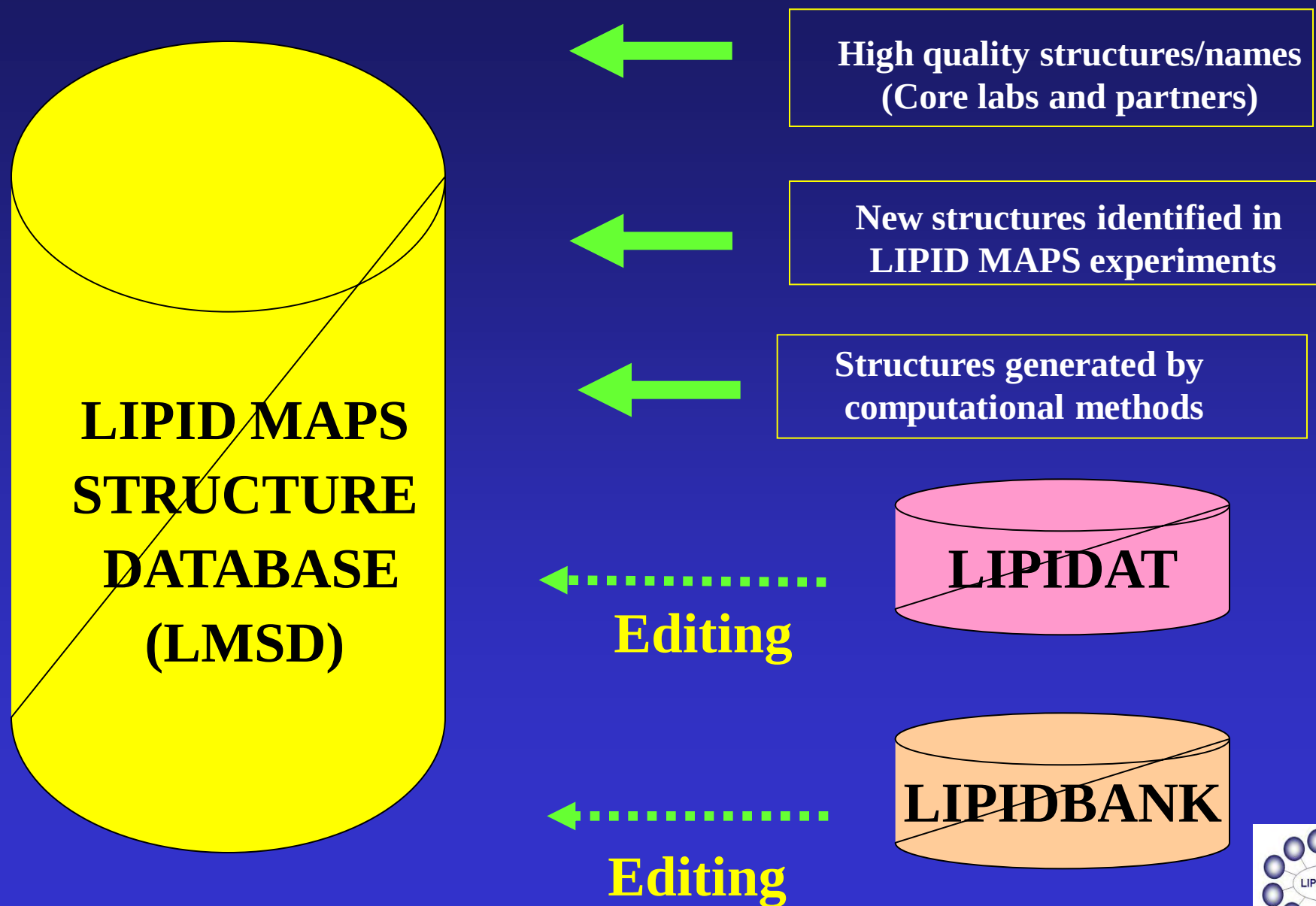
LM ID	Common Name	
LMFA03010001	6-keto-PGF1 α	6
LMFA03010002	PGF2 α	9
LMFA03010003	PGE2	9
LMFA03010004	PGD2	9
LMFA03010005	PGA1	9
LMFA03010006	PGF2 α -d4	9
LMFA03010007	PGD2-d4	9
LMFA03010008	PGE2-d4	9
LMFA03010009	PGG2	9
LMFA03010010	PGH2	9
LMFA03010011	2,3-dinor-11 β -PGF2 α	9
LMFA03010012	6-keto PGE1	9
LMFA03010013	6,15-diketo-13,14-dihydro-PGF1 α	9
LMFA03010014	20-hydroxy-PGE2	9
LMFA03010018	PGB2	9
LMFA03010019	PGJ2	9
LMFA03010020	δ -12-PGJ2	9



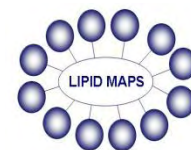
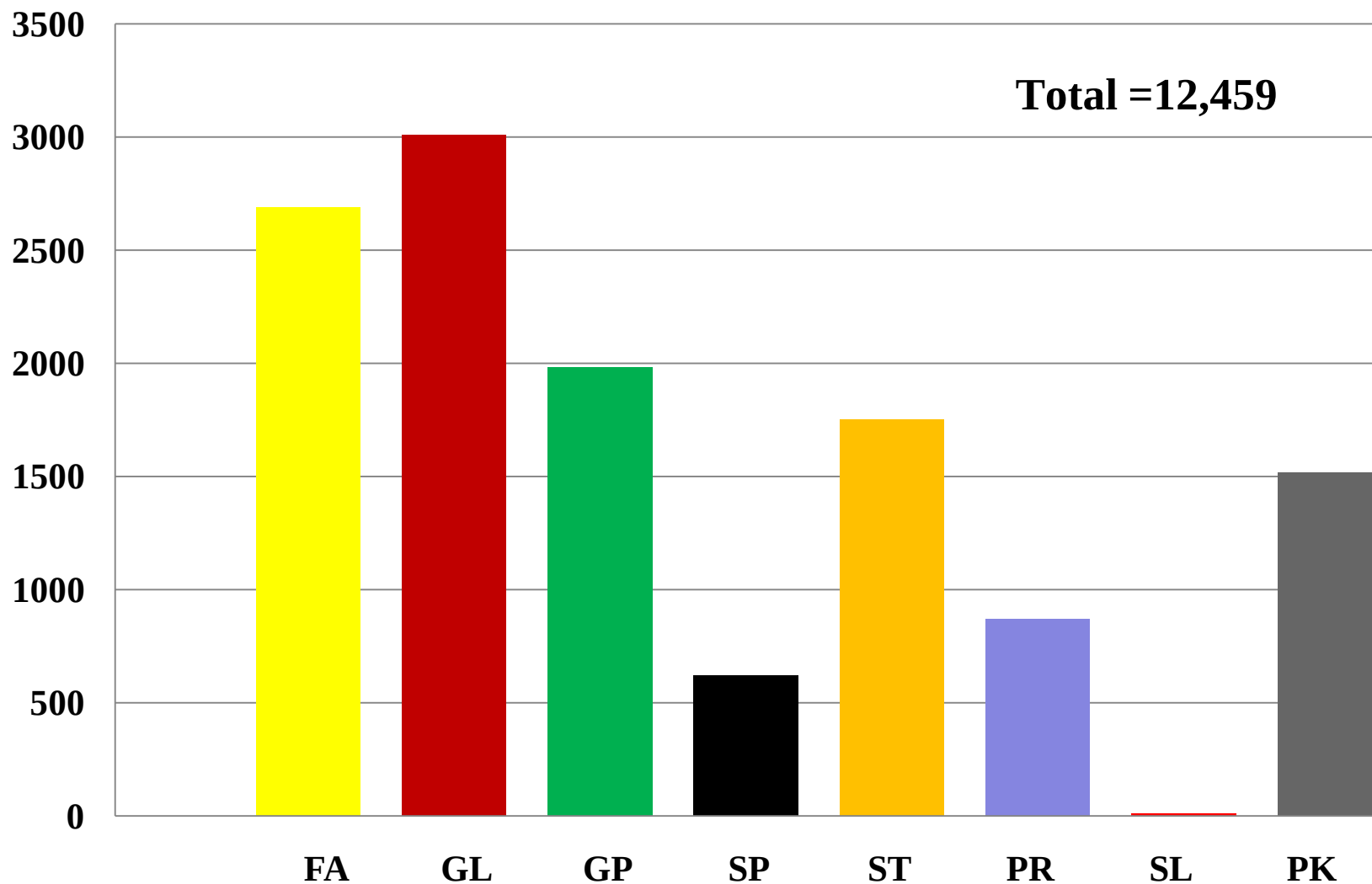
LM ID	LMFA03010004		
Common Name	PGD2 (W)		
Systematic Name	9S,15S-dihydroxy-11-oxo-5Z,13E-prostadienoic acid		
Synonyms	-		
Exact Mass	352.22		
Formula	C ₂₀ H ₃₂ O ₅		
Category	Fatty Acyls [FA]		
Main Class	Eicosanoids [FA03]		
Sub Class	Prostaglandins [FA0301]		
LIPIDBANK ID	XPR1301		
PubChem Substance ID (SID)	4265955		
KEGG ID	C00696		
prostadienoic acid (3,3,4,4-d4)			
11R,15S-dihydroxy-9-oxo-5Z,13E-prostadienoic acid (3,3,4,4-d4)	356.25	C ₂₀ H ₂₈ D ₄ O ₅	
9S,11R-epidioxo-15S-hydroperoxy-5Z,13E-prostadienoic acid	368.22	C ₂₀ H ₃₂ O ₆	
9S,11R-epidioxo-15S-hydroxy-5Z,13E-prostadienoic acid	352.22	C ₂₀ H ₃₂ O ₅	
9S,11S,13S-trihydroxy-2,3-dinor-5Z,13E-prostadienoic acid	326.21	C ₁₈ H ₃₀ O ₅	
6,9-dioxo-11R,15S-dihydroxy-13E-prostenoic acid	368.22	C ₂₀ H ₃₂ O ₆	
6,15-dioxo-9S,11R-dihydroxy-13E-prostenoic acid	368.22	C ₂₀ H ₃₂ O ₆	
9-oxo-11R,15S,20-trihydroxy-5Z,13E-prostadienoic acid	368.22	C ₂₀ H ₃₂ O ₆	
15S-hydroxy-9-oxo-5Z,8(12),13E-prostatrienoic acid	334.21	C ₂₀ H ₃₀ O ₄	
11-oxo-15S-hydroxy-5Z,8Z,13E-prostatrienoic acid	334.21	C ₂₀ H ₃₀ O ₄	
11-oxo-15S-hydroxy-5Z,9Z,13E-prostatrienoic acid	334.21	C ₂₀ H ₃₀ O ₄	



LIPID MAPS Structure Database



Lipids per category in LMSD (4/1/09)



Web-based Lipid Structure Registration tool

LIPID Metabolites And Pathways Strategy

About Lipid Classification Standards Experimental Data Databases Pathways Tools

2-oxo-dodecanoic acid

Common Name:

Systematic Name:

Synonyms:

Category:

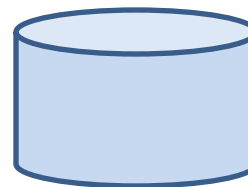
Mainclass:

Subclass:

Classification:

Submit Reset

User data entry form



Temporary database table

Review:
Check for duplicates
Check structure format
Check classification
Check systematic name

LIPID Metabolites And Pathways Strategy

About Lipid Classification Standards Experimental Data Databases Pa

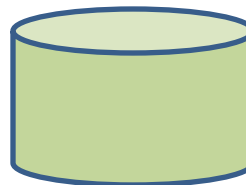
LMSD: Lipid classification search results

Fatty Acids [FA] (W) --> Fatty Acids and Conjugates [FA01] --> Oxo fatty acids [FA0106]

Search for other lipids in different subclasses with this functionality

LM_ID	Common Name	Systematic Name
LMFA01060001	2-oxo capric acid	2-oxo-decanoic acid
LMFA01060002	3-methyl pyruvic acid	2-oxo-butanolic acid
LMFA01060003	Acetoacetic acid (W)	3-oxo-butanolic acid
LMFA01060004	2-keto valeric acid	2-oxo-pentanoic acid
LMFA01060005	3-keto valeric acid	3-oxo-pentanoic acid
LMFA01060006	Levulinic acid (W)	4-oxo-pentanoic acid
LMFA01060007	2-keto-n-caproic acid	2-oxo-heptanoic acid
LMFA01060008	3-keto-n-caproic acid	3-oxo-heptanoic acid
LMFA01060009	4-keto-n-caproic acid	4-oxo-heptanoic acid
LMFA01060010	5-keto-n-caproic acid	5-oxo-heptanoic acid
LMFA01060011	2-Keto-n-heptylic acid	2-oxo-octanoic acid
LMFA01060012	n-valeryl acetic acid	2-oxo-octanoic acid

www.lipidmaps.org



LIPID MAPS structure database

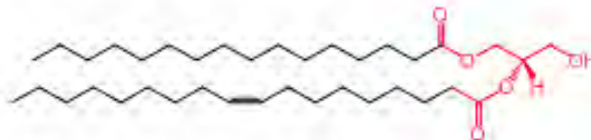
LIPID MAPS: Recommendations for drawing structures

Consistent structure representation across classes

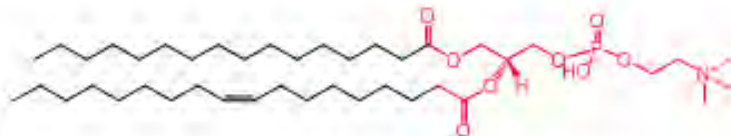
Fatty Acyls(FA)



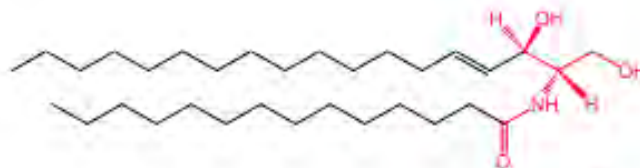
Glycerolipids (GL)



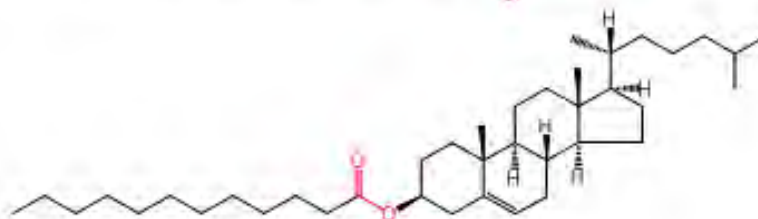
Glycerophospholipids (GP)



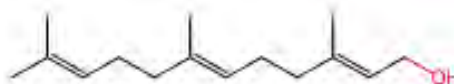
Sphingolipids (SP)



Sterol Lipids (ST)



Prenol Lipids (PR)



LIPID MAPS Structure Database (LMSD)



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

Structure Database (LMSD)

Browse

By Lipid Classification

- [Fatty Acyls](#)
- [Glycerolipids](#)
- [Glycerophospholipids](#)
- [Sphingolipids](#)
- [Sterol Lipids](#)
- [Prenol Lipids](#)
- [Saccharolipids](#)
- [Polyketides](#)

Search

Text-based Search

Search by LIPID MAPS ID, Systematic or Common Name, Mass, For Category, Main Class, and Sub Class

Text/ontology-based Search

Search by Ontology (# of functional groups), LIPID MAPS ID, Systematic or Common Name, Mass, Formula, Category, Main Class, and Sub Class

Structure-based Search

Search by substructure or exact match using one of these structure drawing tools:

- [MarvinSketch Applet](#)
- [JME Applet](#)
- [ChemDrawPro](#)

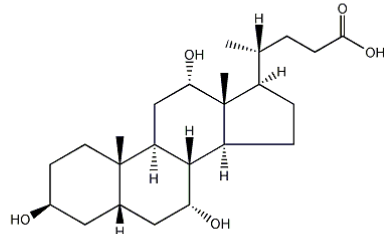
LMSD: Structure-based search results

Modify Search

LM_ID	Common Name	Systematic Name	Formula	Mass	
LMST04010086	-	3β,7α,12α-Trihydroxy-5β-cholan-24-oic Acid	C ₂₄ H ₄₀ O ₅	408.29	Bile acids and derivatives [ST04]
LMST04010089	-	3α,7β,12β-Trihydroxy-5β-cholan-24-oic Acid	C ₂₄ H ₄₀ O ₅	408.29	Bile acids and derivatives [ST04]
LMST04010094	-	3β,7α,12α-Trihydroxy-5α-cholan-24-oic Acid	C ₂₄ H ₄₀ O ₅	408.29	Bile acids and derivatives [ST04]
LMST04010097	-	3α,7β,12β-Trihydroxy-5α-cholan-24-oic Acid	C ₂₄ H ₄₀ O ₅	408.29	Bile acids and derivatives [ST04]
LMST04010117	-	3β,4β,7α,12α-Tetrahydroxy-5β-cholan-24-oic Acid	C ₂₄ H ₄₀ O ₆	424.28	Bile acids and derivatives [ST04]
LMST04010123	-	3α,6β,7β,12β-Tetrahydroxy-5β-cholan-24-oic Acid	C ₂₄ H ₄₀ O ₆	424.28	Bile acids and derivatives [ST04]
LMST04030009	-	5α-Cholestane-3β,7α,12α,26,27-pentol	C ₂₇ H ₄₈ O ₅	452.35	Bile acids and derivatives [ST04]

Structure database (LMSD)

LMST04010086



LM ID	LMST04010086
Common Name	-
Systematic Name	3β,7α,12α-Trihydroxy-5β-cholan-24-oic Acid
Synonyms	-
Exact Mass	408.29
Formula	C ₂₄ H ₄₀ O ₅
Category	Sterol Lipids [ST]
Main Class	Bile acids and derivatives [ST04]
Sub Class	C24 bile acids, alcohols, and derivatives [ST0401]
LIPIDBANK ID	BBA0086
PubChem Substance ID (SID)	7850973

Structure Database (LMSD)

Text-based search

LM ID

Name(Common or Systematic)

Mass +/- 0.5

Formula

Category

Main class

Sub class

Records per page

Sort by

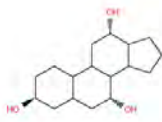
Structure Database (LMSD)

Structure-based search using MarvinSketch

File Edit View Insert Tools Help

H C N O F React Select Erase Paste Undo Zoom

More Dr I



Search type

LM ID

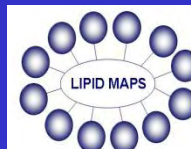
Name(Common or Systematic)

Records per page

Sort by

Online features:

- Browse
- Text search
- Substructure search
- Download structures



Lipid Proteome Database (LMPD)

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

LIPID MAPS -- LIPID Metabolites And Pathways Strategy - Microsoft Internet Explorer provided by SDSL

File Edit View Favorites Tools

http://www.lipidmaps.org

LIPID MAPS -- LIPID

LIPID MAPS

LIPID Metabolites And Pathways Strategy

Contact | Discussion | News | Publications | Site Map

About | Lipid Classification | Standards | Experimental Data | Databases | Pathways | Tools | Protocols | Home

Proteome Database (LMPD)

Introduction | Browse by lipid | Mouse-over the above |

About

Proteome Database (LMPD)

Introduction | Browse by lipid | Mouse-over the above |

Browse by lipid

Search for proteins as

Include data from:

Display: 100 records

Submit Cancel Reset

W3C HTML 4.01 CSS

LIPID MAPS

Lipid Proteome

Record Overview | Gene/GO

LMPD000475

Record Overview

LMPD ID	LMPD000475
Taxonomy	Homo sapiens (Human)
Description	Alkaline ceramidase
Symbols	
Lipid Category	Sphingolipids (SP)
EC Number	
Molecular Weight	31095
Sequence Length	264
Sequence	NPSTFAYOSSEVDWDCSN SFLQQLDDEIATLWLLGS YKTSMKELRLHLEVSUV RYWPRDSWVPLPVVRI

Summary

Official Symbol: SPHK1 and **Name:** sphingosine kinase 1 provided by **HUGO Gene Nomenclature Committee**

See related: [HPRD:04768](#), [MIM:603730](#)

Gene type: protein coding

Gene name: SPHK1

Gene description: sphingosine kinase 1

RefSeq status: Provisional

Organism: [Homo sapiens](#)

Lineage: *Eukaryota; Metazoa; Chordata; Craniata; Vertebrata; Euteleostomi; Mammalia; Eutheria; Euarchontoglires; Primates; Catarrhini; Homimidae; Homo*

Gene aliases: SPHK

Summary: Sphingosine-1-phosphate (SPP) is a novel lipid messenger with both intracellular and extracellular functions. Intracellularly, it regulates proliferation and survival, and extracellularly, it is a ligand for EDG1 (MIM 601974). Various stimuli increase cellular levels of SPP by activation of sphingosine kinase (SPHK), the enzyme that catalyzes the phosphorylation of sphingosine. Competitive inhibitors of SPHK block formation of SPP and selectively inhibit cellular proliferation induced by a variety of factors, including platelet-derived growth factor (e.g., MIM 173430) and serum. [supplied by OMIM]

Genomic regions, transcripts, and products

RefSeq below

NC_000017.9

[71692287] [71695536]

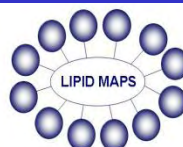
NP_058887
NP_058887
NP_058887

■ coding region ■ untranslated region

Entrez Gene Home

Table Of Contents

- Summary
- Genomic regions, transcripts...
- Genomic context
- Bibliography
- Interactions
- General gene information
- General protein information
- Reference Sequences
- Related Sequences
- Additional Links
- Links
- MGC cDNA clone
- Conserved Domains
- Genome
- GEO Profiles
- HomoloGene
- Map Viewer
- Nucleotide
- OMIM
- Full text in PMC
- Probe
- Protein
- PubMed
- SNP
- SNP: Genotype
- SNP: GeneView
- Taxonomy
- UniSTS
- AcView
- CCDS
- Ensembl
- Evidence Viewer
- GDB
- HGNC
- HPD
- KEGG

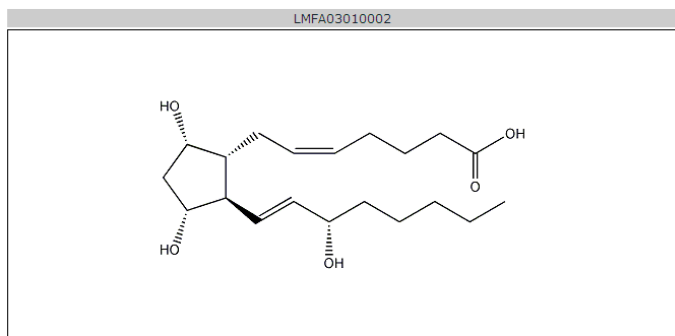


Lipidomics Data Display : MS Standards library



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

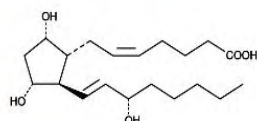
Structure Database (LMSD)



LM ID LMFA03010002
Common Name PGF2α
Systematic Name (S)-11β,15α-trihydroxy-5Z,13E-prostadienoic acid

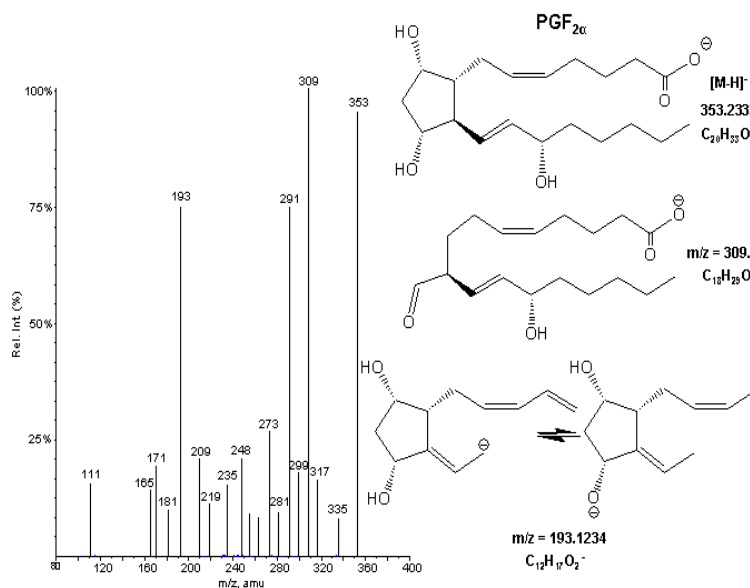
16010 Prostaglandin F2α

See below for pricing and ordering



Data Description Articles Related Products

PGF2α is a widely distributed prostaglandin occurring in many species.^{1,2,3} It causes contraction of vascular, bronchial, intestinal, and myometrial smooth muscle, and also exhibits potent luteolytic activity.² PGF2α exerts its receptor mediated physiological activity at 50-100 nM.² Maximal ovine myometrial contraction can be achieved at 125 nM PGF2α in vitro.⁴



LIPID Metabolites And Pathways Strategy

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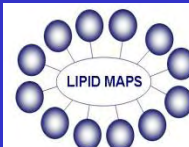
About Data Protocols Home

Lipid Classification Scheme | Lipid Structure Database

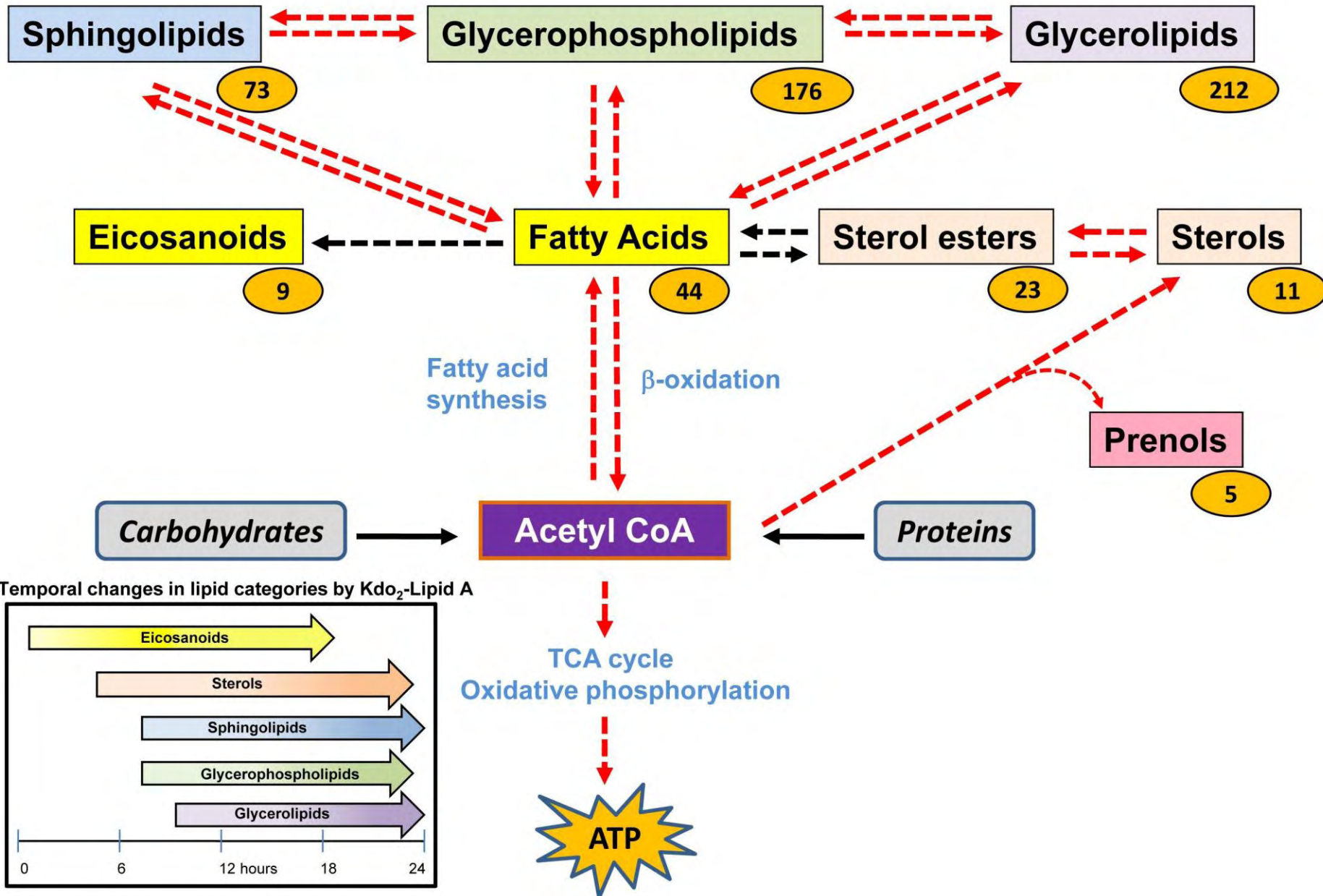
Library of Eicosanoid Standards: LC Retention Times

LC retention time and MS/MS data were obtained using the conditions outlined in the protocols below
LC Protocol | MS/MS Protocol

LM_ID	NAME	Systematic Name	MASS	Ret. Time(mins)
LMFA01030001	AA	5Z,8Z,11Z,14Z-eicosatetraenoic acid	303	14.37
LMFA01030003	AA-d8	5Z,8Z,11Z,14Z-eicosatetraenoic acid (5,6,8,9,11,12,14,15-d8)	311	14.33
LMFA03010001	6k-PGF1α	6k,11R,15S-trihydroxy-6-oxo-13E-prostenoic acid	369	3.4
LMFA03010002	PGF2α	9S,11R,15S-trihydroxy-5Z,13E-prostadienoic acid	353	4.72
LMFA03010003	PGE2	11R,15S-dihydroxy-9-oxo-5Z,13E-prostadienoic acid	351	5.19
LMFA03010004	PGD2	9S,15S-dihydroxy-11-oxo-5Z,13E-prostadienoic acid	351	5.69
LMFA03010006	PGF2α-d4	9S,11R,15S-trihydroxy-5Z,13E-prostadienoic acid (3,3,4,4-d4)	357	4.71
LMFA03010007	PGD2-d4	9S,15S-dihydroxy-11-oxo-5Z,13E-prostadienoic acid (3,3,4,4-d4)	355	5.67
LMFA03010008	PGE2-d4	11R,15S-dihydroxy-9-oxo-5Z,13E-prostadienoic acid (3,3,4,4-d4)	355	5.18
LMFA03010009	PGG2	9S,11S-epidixy-15S-hydroperoxy-5Z,13E-prostadienoic acid	367	6.41
LMFA03010010	PGH2	9S,11S-epidixy-15S-hydroxy-5Z,13E-prostadienoic acid	351	7.55
LMFA03010011	2,3-Dinor-11β-PGF2α	7S,9R,13S-trihydroxy-3Z,11E-prostadienoic acid	325	3.48
LMFA03010012	6keto-PGE1	11S,15S-dihydroxy-6,9-dioxo-13E-prostenoic acid	367	3.66
LMFA03010013	6,15-diketo-13,14-dihydro-PGF1α	9S,11S-dihydroxy-6,15-dioxo-prostanoic acid	369	4.24
LMFA03010014	20-hydroxy-PGE2	11S,15S-dihydroxy-9-oxo-5Z,13E-prostadienoic acid	367	2.94

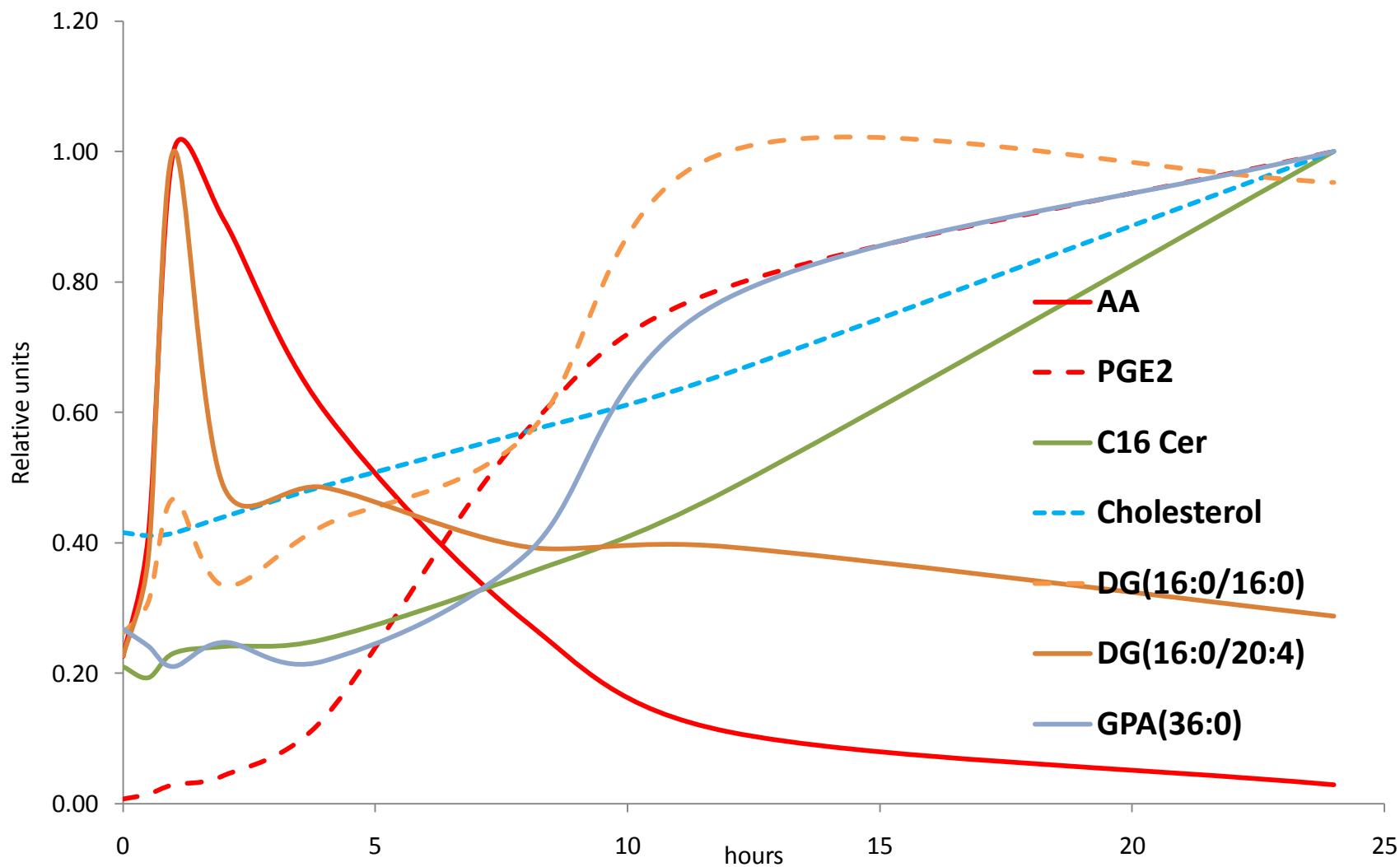


MACROPHAGE LIPID METABOLISM

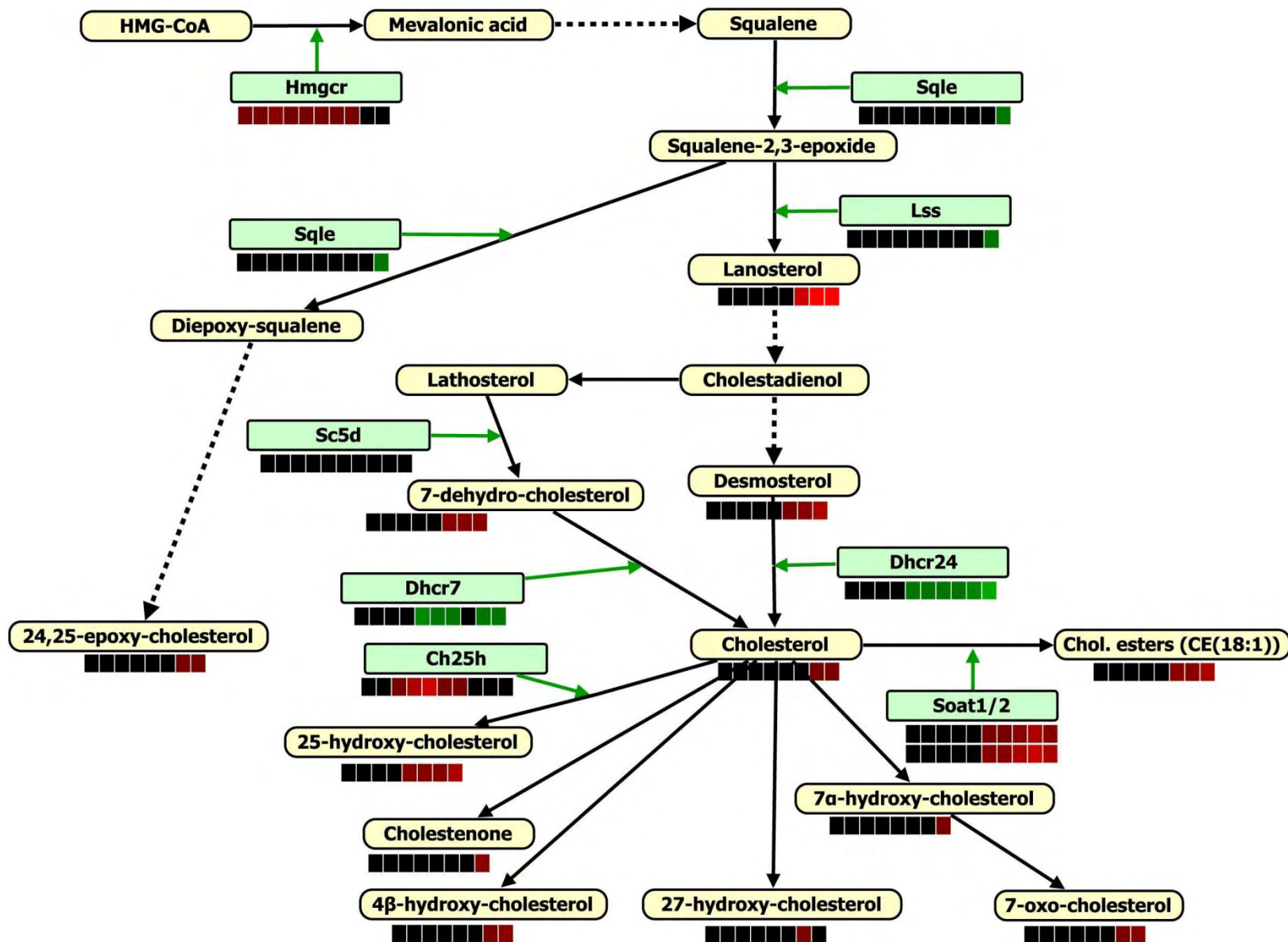


Genes

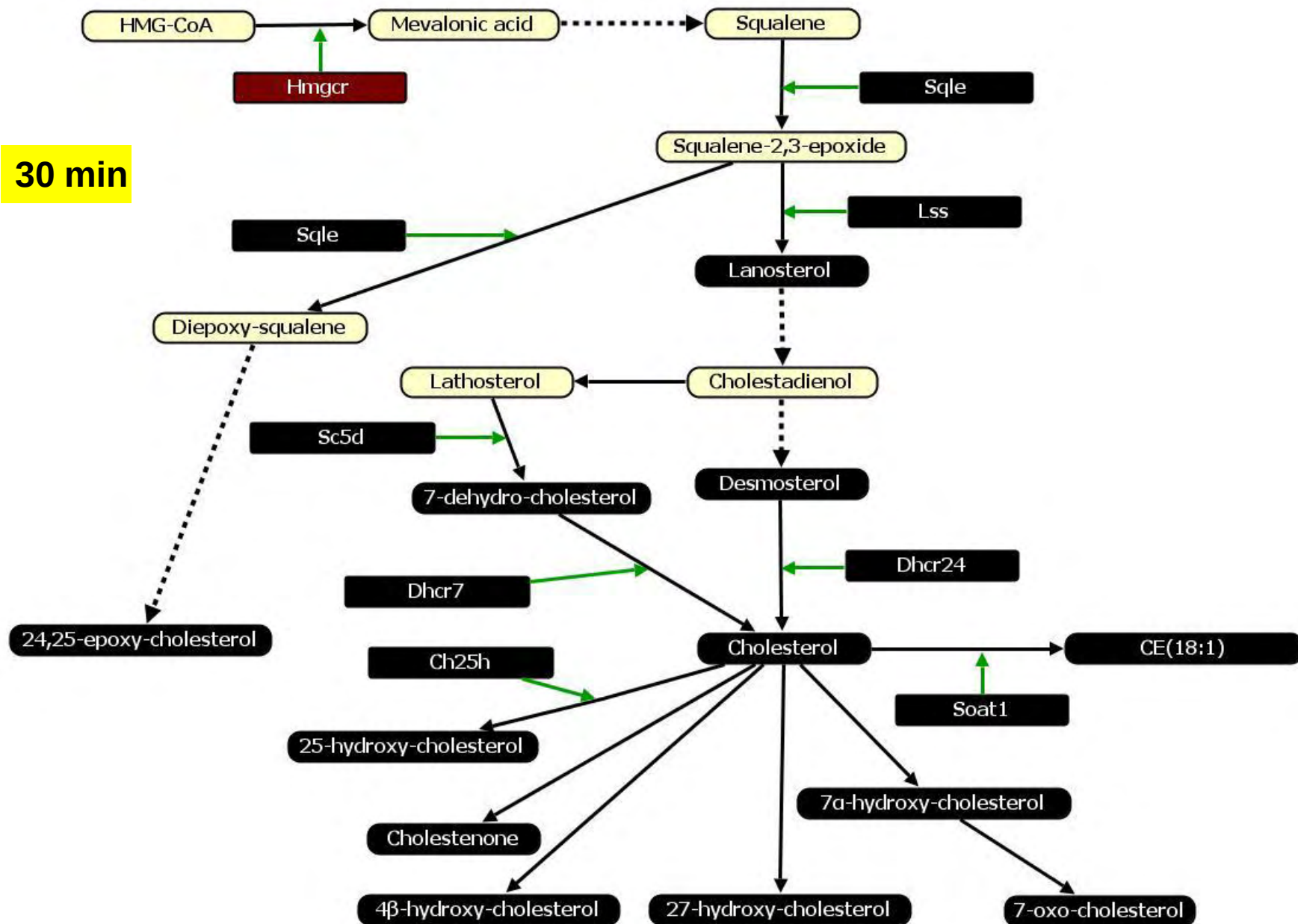
Kdo Timecourse Data: Examples of different profiles with time



Cholesterol Biosynthesis



30 min

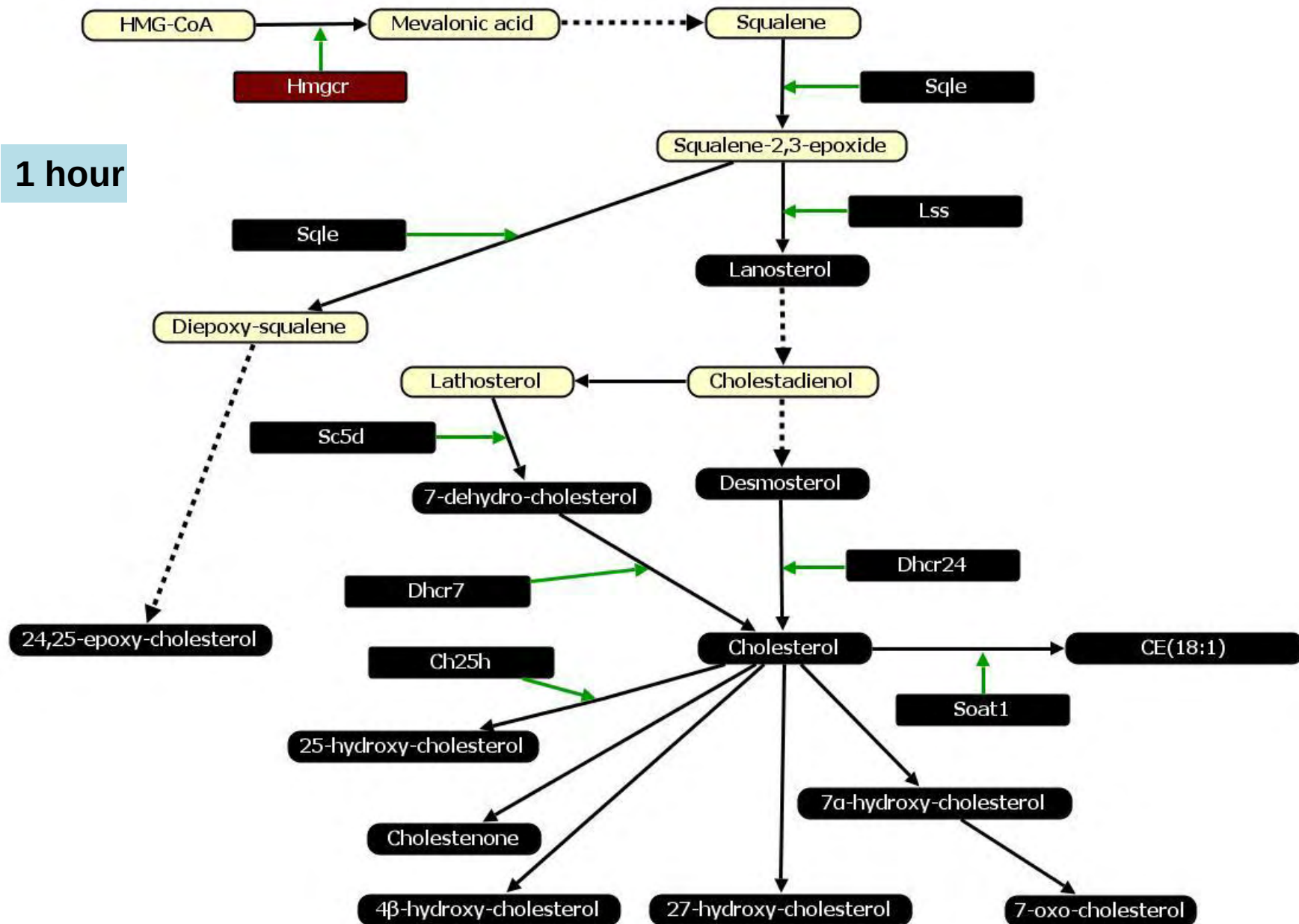


>10 >5 >4 >3 >2 >1.5 --- <0.67 <0.5 <0.33 <0.25 <0.2 <0.1



Kdo/Ctrl ratio

1 hour

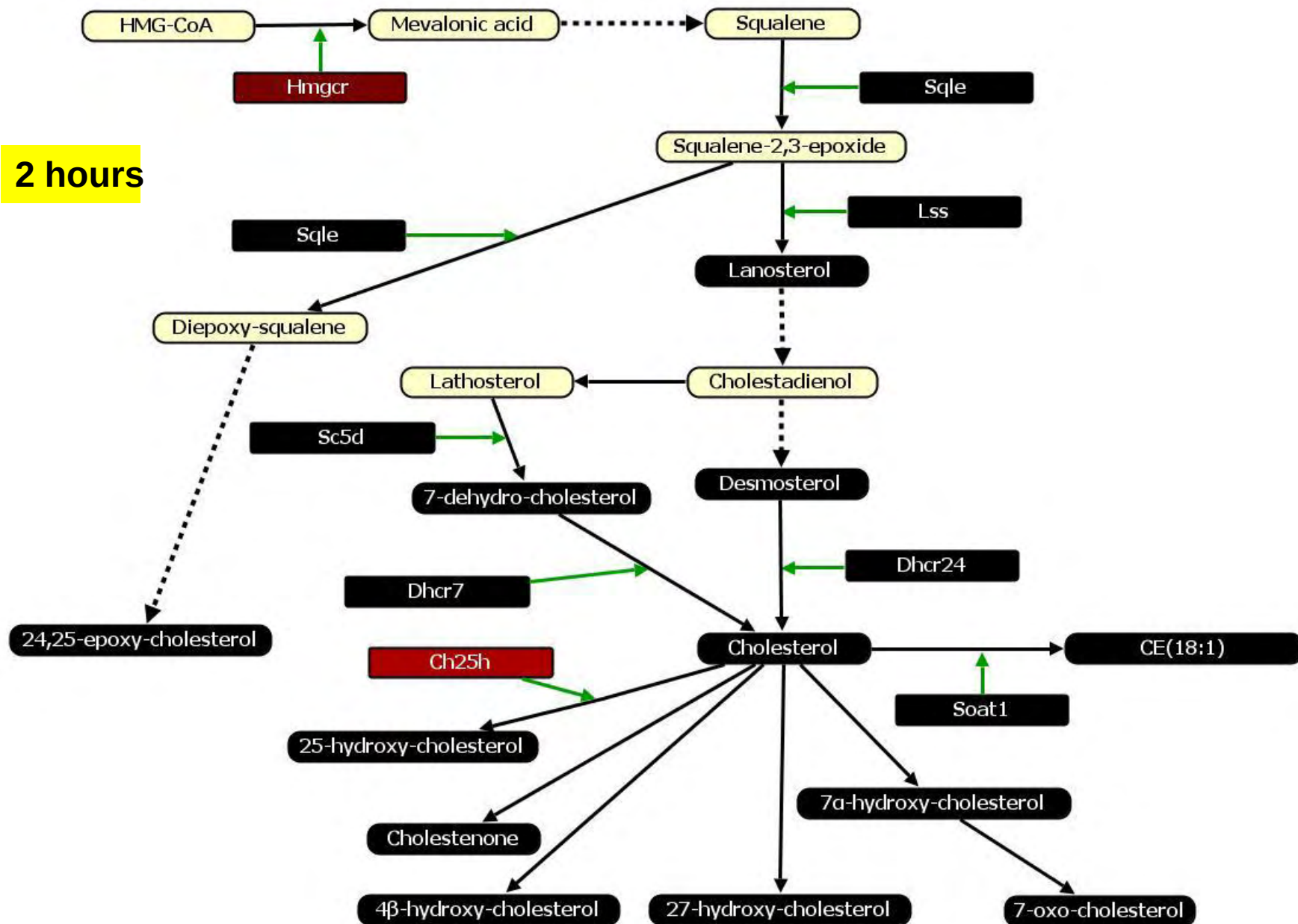


>10 >5 >4 >3 >2 >1.5 --- <0.67 <0.5 <0.33 <0.25 <0.2 <0.1



Kdo/Ctrl ratio

2 hours

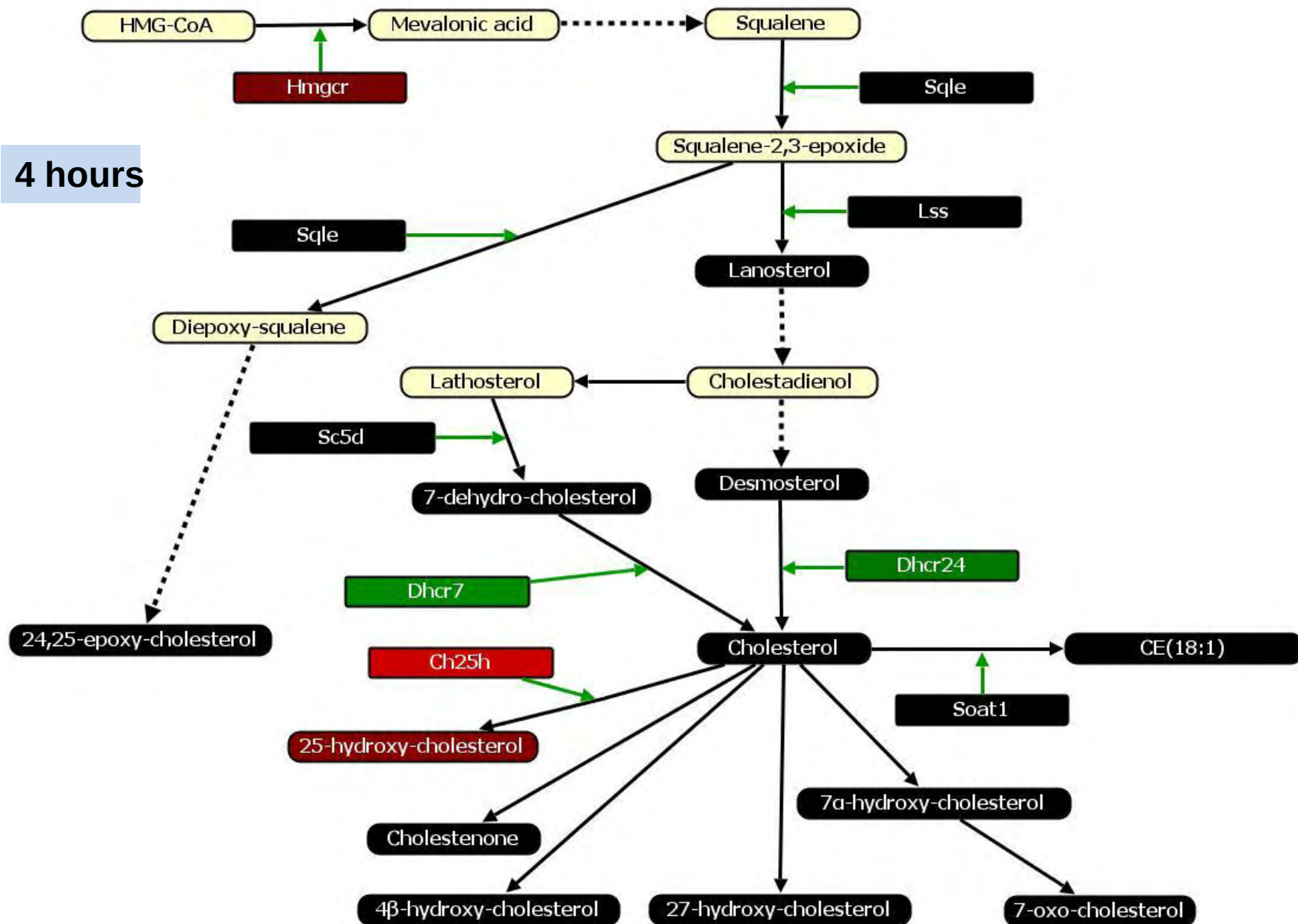


>10 >5 >4 >3 >2 >1.5 --- <0.67 <0.5 <0.33 <0.25 <0.2 <0.1



Kdo/Ctrl ratio

4 hours

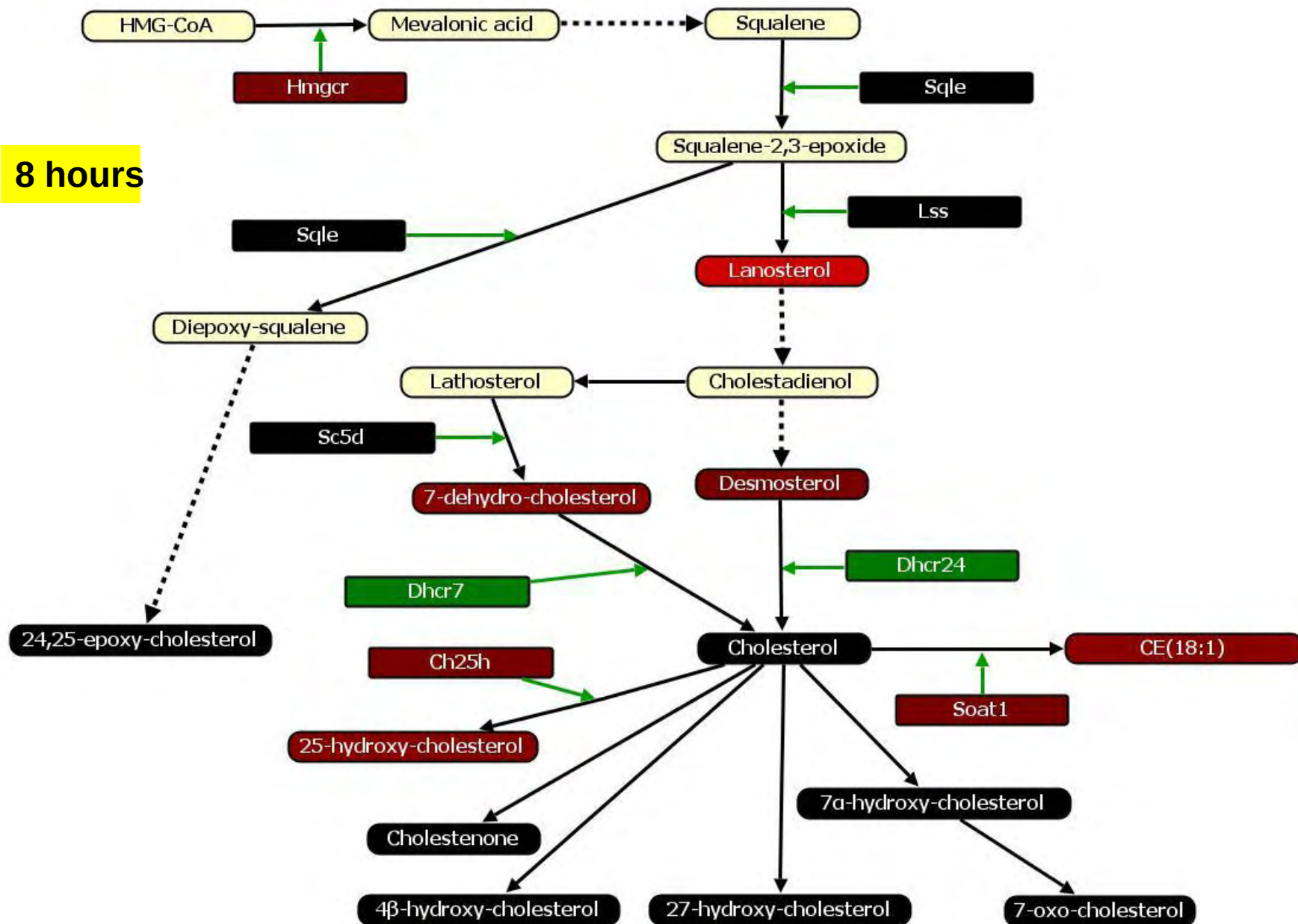


>10 >5 >4 >3 >2 >1.5 --- <0.67 <0.5 <0.33 <0.25 <0.2 <0.1



Kdo/Ctrl ratio

8 hours

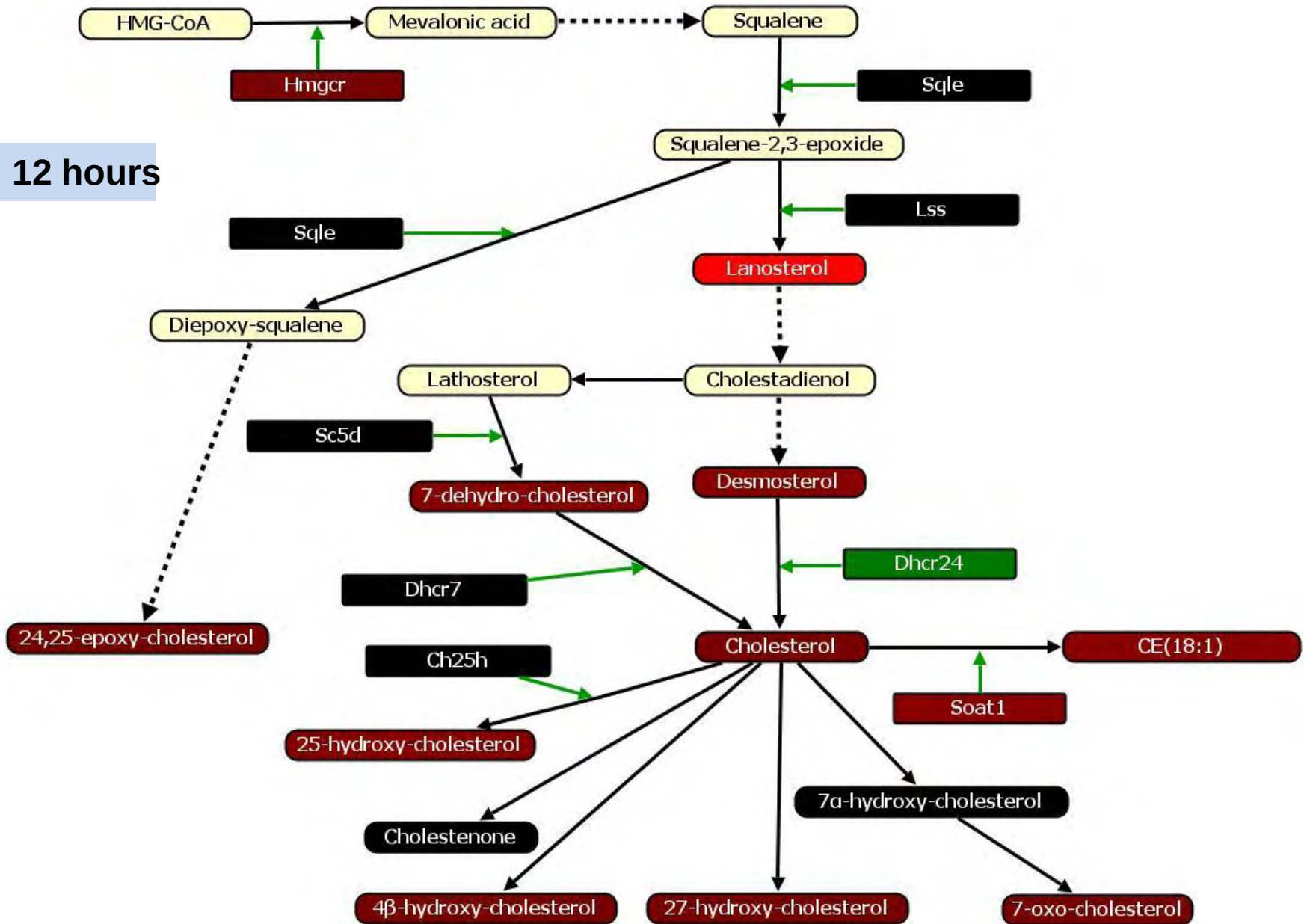


>10 >5 >4 >3 >2 >1.5 --- <0.67 <0.5 <0.33 <0.25 <0.2 <0.1



Kdo/Ctrl ratio

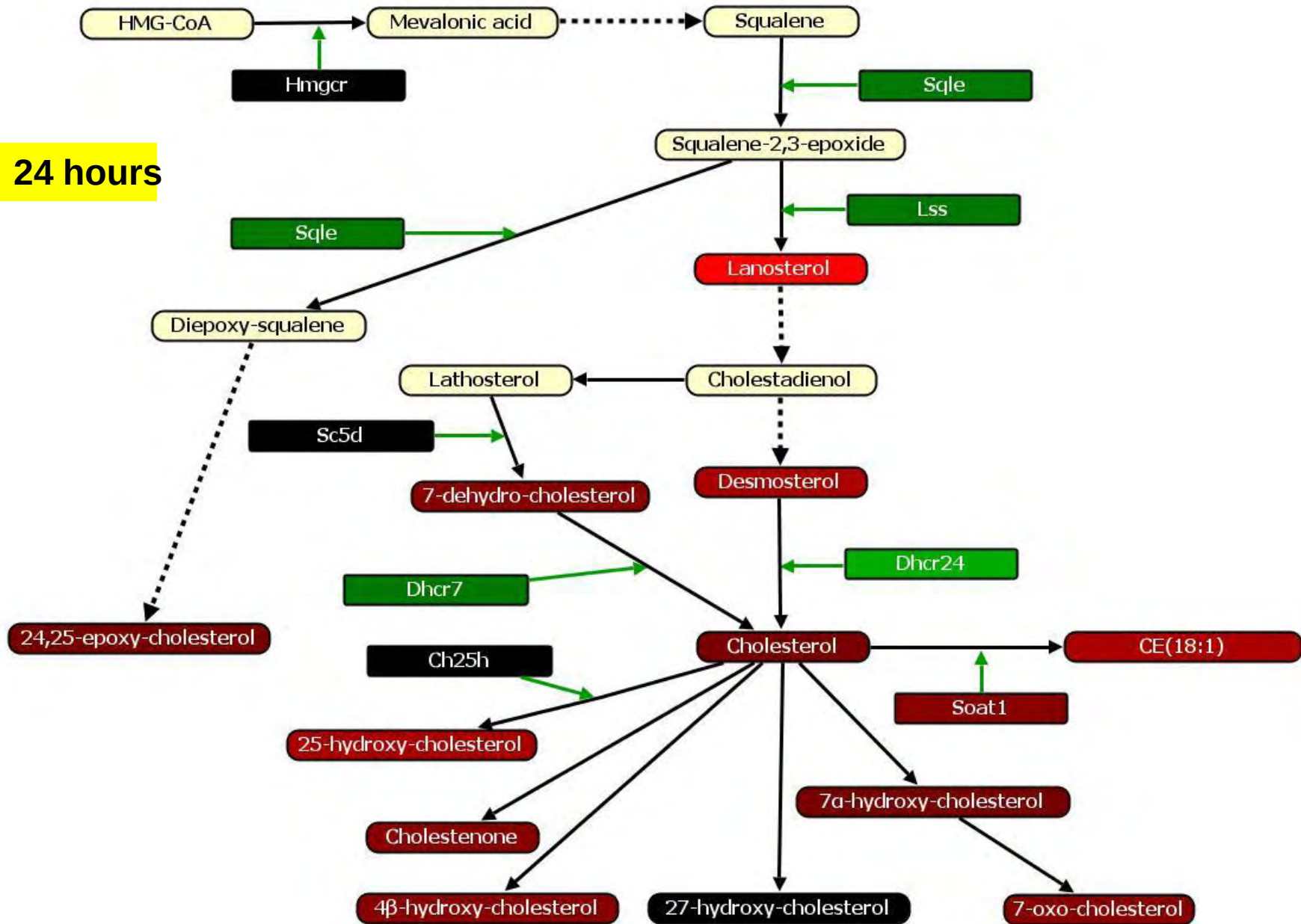
12 hours



>10 >5 >4 >3 >2 >1.5 --- <0.67 <0.5 <0.33 <0.25 <0.2 <0.1



Kdo/Ctrl ratio



Capturing the **Metadata**: LIMS Data Input GUI's (WebStart Java application communicates with Oracle database)

The image displays two overlapping Java WebStart application windows for a Laboratory Information Management System (LIMS). The 'Treatment' window is in the background, and the 'Solution' window is in the foreground.

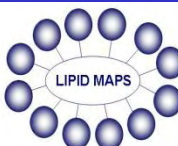
Treatment Window:

- Experiment identity:** Date* (03-03-2006), Experiment ID, Experiment letter*.
- Protocol ID:** Text field.
- Technician:** G, Alex Andrejev.
- Culture information:** Plating density* (x10e6), Temp (37°C), Solution (DMEM), CO2 (5%).
- Treatments:** Import file button, table with ID and Pre-incu columns.
- Samples:** Add, Duplicate buttons.
- Cell line:** New thaw, New passage, New freeze buttons. Lab (G), User (Alex Andrejev [29]), Passage/harvest date (03-03-2006), Passage protocol.*.
- Comments:** Text area with Search comments button.
- Parent flask barcode*:** Text field.
- Harvest information for parent:** Live*, Dead*, Grid* checkboxes.
- Cell count:** Text field.
- Cell conc. (#.##E#)*:** Text field.
- New passage:** Button.
- Daughter vessel barcode:** Text field.
- Media barcode*:** Text field.
- Target plating density*:** Text field.
- Vessel type:** T-2.
- Total vessels*:** 1.
- Save new passage:** Button.
- Get barcode:** Button.
- Save to database:** Button.
- Print:** Button.

Solution Window:

- Protocols:** Dropdown menu.
- Protocol ID:** Text field.
- Barcode ID:** Text field.
- Print label:** Button.
- Name*:** Text field.
- Abbreviation*:** Text field.
- Find:** Button.
- Date:** 03-03-2006.
- Change date:** Button.
- Component barcode:** Text field.
- Component name:** Text field.
- Comments:** Text area.
- Search:** Button.
- Get IDs:** Button.
- Save to database:** Button.
- Clear form:** Button.
- Print this form:** Button.
- Help:** Button.
- OK:** Button.

OK - Don't forget to inspect the tooltip



Bioinformatics tools for lipidomics



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



LIPID Metabolites And Pathways Strategy

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[About](#) | [Lipid Classification](#) | [Standards](#) | [Experimental Data](#) | [Databases](#) | [Pathways](#) | [Tools](#) | [Protocols](#)

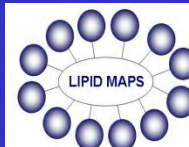
Tools

Online Tools

- Mass Spectrometry: Find mass, number of carbons, number of double bonds, abbreviation, MS/MS product ions (neutral loss), formula, and ion base peak. Input criteria, with links to structure and isotopic distribution.
 - [Cardiolipins](#)
 - [Glycerophospholipids](#)
 - [Mono/Di/Triacylglycerols](#)
 - [Glycerophospholipid analysis in batch mode](#)
 - [Glycerolipid analysis in batch mode](#)
 - [Sphingolipid analysis in batch mode](#)
 - [Fatty acid analysis in batch mode \(based on structures in the LIPID MAPS database\)](#)
 - [Fatty acid analysis in batch mode \(based on computationally generated structures\)](#)
 - [Cholesteryl ester analysis in batch mode \(based on fatty acid structures in the LIPID MAPS database\)](#)
 - [Cholesteryl ester analysis in batch mode \(based on computationally generated structures\)](#)
 - [Search a database of MS/MS spectra of Eicosanoids for precursor and product ions \(neg. ion mode\)](#)
- Structure Drawing
 - [Draw Fatty Acyl Structures](#)
 - [Draw Glycerolipid Structures](#)
 - [Draw Glycerophospholipid Structures](#)
 - [Draw Cardiolipin Structures](#)
 - [Draw Sphingolipid Structures](#)
 - [Draw Sterol \(cholestane, ergostane, campestane and stigmastane\) Structures](#)
 - [Draw Glycan structures \(attached to either an R group or ceramide\)](#)

Stand-alone Tools

- **LIPID MAPS Tools Package**
Command line Perl scripts to generate SD files containing structure and ontological data for various lipid categories. The current version supports generation for Fatty acyls (FA), Glycerolipids (GL), Glycerophospholipids (GP), Cardiolipins (CL), Sphingolipids (SP) and Sterols (ST). Please see our documentation for specific main and subclasses. [FAStrGen.pl](#) | [GLStrGen.pl](#) | [GPStrGen.pl](#) | [CLStrGen.pl](#) | [SPStrGen.pl](#) | [STStrGen.pl](#)
 - Download Tools package and documentation: [lipidmapstools.tar.gz \(366 KB\)](#) or [lipidmapstools.zip \(555 KB\)](#)
 - View [online documentation](#)



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



Glycan structure drawing: Glycosphingolipid example

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LIPID Metabolites And Pathways Strategy

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[Experimental Data](#)

[Databases](#)

[Pat](#)

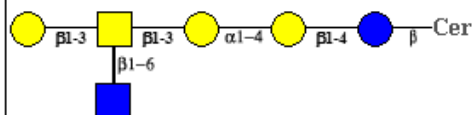
Structure database (LMSD)

LM_ID:LMSP0502AF00

Gal β 1-3(GlcNAc β 1-6)GalNAc β 1-3Gal α 1-4Gal β 1-4Glc β -Cer

Symbol Nomenclature

Click on sugar icons to display chemical structure



LM ID	LMSP0502AF00
Common Name	-
Systematic Name	Galβ1-3(GlcNAcβ1-6)GalNAcβ1-3Galα1-4Galβ1-4Glcβ-Cer
Synonyms	-
Exact Mass	-
Formula	-
Category	Sphingolipids [SP]
Main Class	Neutral glycosphingolipids [SP05]
Sub Class	GalNAc β 1-3Gal α 1-4Gal β 1-4Glc- (Globo series) [SP0502]
LIPIDBANK ID	GSG1429
PubChem Substance ID (SID)	14714508
KEGG ID	-
Status	Active
SphingoMap ID	22

[Add additional information for LMSP0502AF00](#) (Restricted Access)

Download file

CSV

Click on name
hyperlink to
display structure
in full
chemical format

Glycan structure drawing: Glycosphingolipid example

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LIPID Metabolites And Pathways Strategy

[About](#)

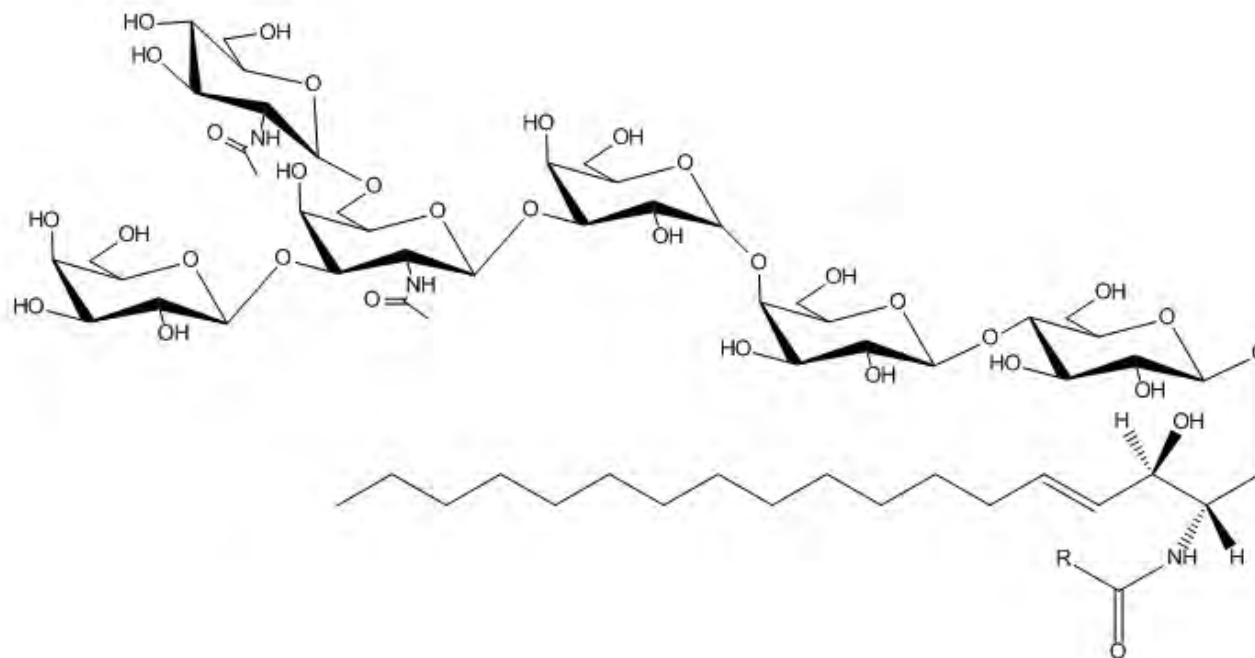
[Lipid Classification](#)

[Standards](#)

[Experimental Data](#)

[Databases](#)

[Pathway](#)



[Display in Marvin format\(Java must be enabled\)](#)

Bioinformatics tools :MS prediction



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



LIPID

Mass Spectrometry

Show Possible Glycerophospholipids

Enter a mass (m/z) value and corresponding mass tolerance (amu):

☒ Nominal Mass ☐ Exact Mass

Mass Tolerance (+/- amu):

Radyl group abbreviation (eg. 12:0):

Headgroup:

Ion:

Sort by:

Records per page:

Examples of Abbreviations

The more common acyl chains used to position only):



LIPID

Mass Spectrometry

Possible Glycerophospholipids

Exact Mass: Mass Tolerance:

C=Number of Carbons; DB=Number of double bonds

Mass	C	DB	Abbrev.	M
671.4652	34	2	12:0/22:2(132,162)	48
671.4652	34	2	14:0/20:2(112,142)	46
671.4652	34	2	16:0/18:2(92,122)	43
671.4652	34	2	16:1(92)/18:1(92)	43
671.4652	34	2	18:1(92)/16:1(92)	40
671.4652	34	2	20:2(112,142)/14:0	38
671.4652	34	2	20:1(112)/14:1(92)	37
671.4652	34	2	17:1(92)/17:1(92)	42
671.4652	34	2	17:1(92)/17:1(92)	42
671.4652	34	2	14:1(92)/20:1(112)	46
671.4652	34	2	22:2(132,162)/12:0	35
671.4652	34	2	18:2(92,122)/16:0	40
671.4652	34	2	17:0/17:2(92,122)	41
671.4652	34	2	17:2(92,122)/17:0	423.2512 405.2406 419.2199 401.2093 265.2168 269.2481 GPA C ₃₇ H ₆₉ O ₈ P



LIPID Metabolites And Pathways Strategy

Mass Spectrometry

Possible Glycerophospholipids

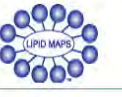
Systematic Name: 1-(9Z)-hexadecenyl 16:1(9Z)/18:1(9Z)

Abbreviation: 16:1(9Z)/18:1(9Z)

Exact Mass: 671.4652

Formula: C₃₇H₆₉O₈P

W3C HTML 4.01 W3C CSS



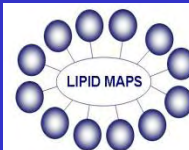
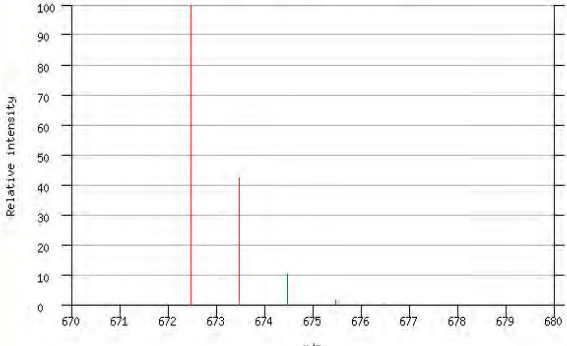
LIPID Metabolites And Pathways Strategy

Mass Spectrometry

Isotopic Distribution for C₃₇H₆₉O₈P

Total	m/z	% of Max
M:	672.4730	100.0000
M+1:	673.4764	42.5418
M+2:	674.4797	10.2843
M+3:	675.4831	1.7649
M+4:	676.4864	0.1161

Isotopic Distribution for C₃₇H₆₉O₈P



Bioinformatics tools : Standalone MS prediction application

Lipid MS Predictor

Menu Help

Lipid Mass Spec. Prediction

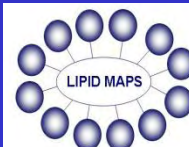


Glycerophospholipids | Glycerolipids | Cardiolipins | Sphingolipids | Fatty acids | Chol. esters | Calculate Mass

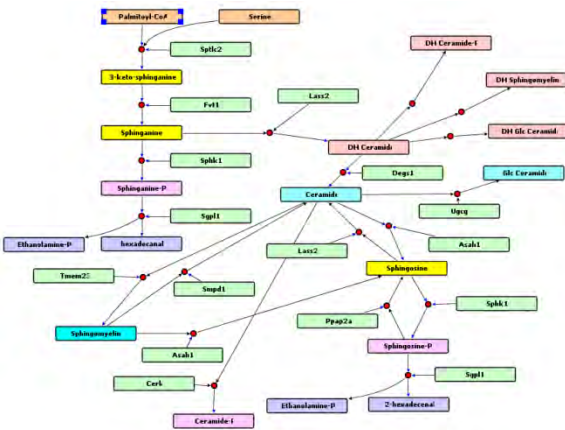
Mass: Mass tolerance: Headgroup: Ion:

Mass format
☐ Nominal ☒ Exact

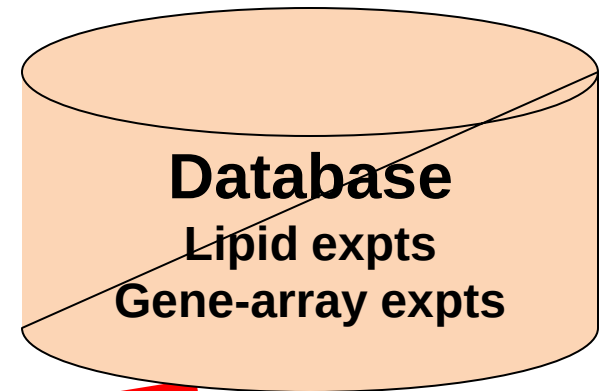
	Abbrev	Radyl carbons	Double bonds	Exact mass	Delta(m/z)	Formula(neutral)
▶	GPA(12:0/22:0)	34	0	677.5116	0.4884	C37H73O8P
	GPA(13:0/21:0)	34	0	677.5116	0.4884	C37H73O8P
	GPA(14:0/20:0)	34	0	677.5116	0.4884	C37H73O8P
	GPA(15:0/19:0)	34	0	677.5116	0.4884	C37H73O8P
	GPA(16:0/18:0)	34	0	677.5116	0.4884	C37H73O8P
	GPA(0-16:0/19:0)	35	0	677.5480	0.4520	C38H77O7P
	GPA(17:0/17:0)	34	0	677.5116	0.4884	C37H73O8P
	GPA(0-18:0/17:0)	35	0	677.5480	0.4520	C38H77O7P
	GPA(18:0/16:0)	34	0	677.5116	0.4884	C37H73O8P
	GPA(19:0/15:0)	34	0	677.5116	0.4884	C37H73O8P
	GPA(20:0/14:0)	34	0	677.5116	0.4884	C37H73O8P
	GPA(21:0/13:0)	34	0	677.5116	0.4884	C37H73O8P
	GPA(22:0/12:0)	34	0	677.5116	0.4884	C37H73O8P
	GPCho(6:0/22:0)	28	0	678.5068	0.5068	C36H72N08P
	GPCho(8:0/20:0)	28	0	678.5068	0.5068	C36H72N08P



Lipid Pathways and Networks: Visualization VANTED

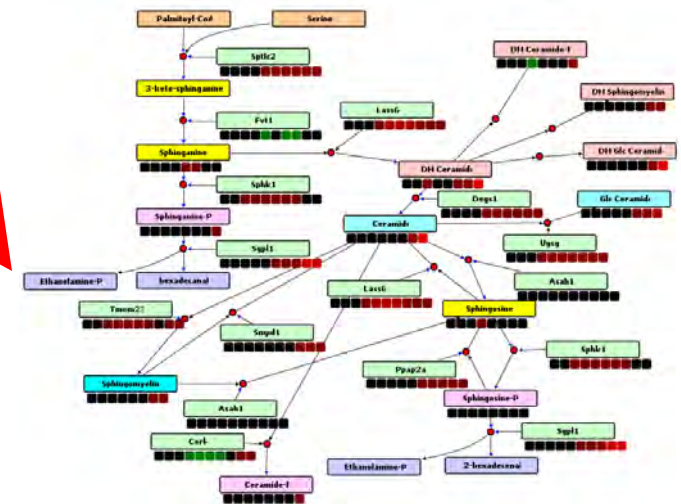


Pathway template
Created with
VANTED



Program

STEPS:
Import pathway template
Add lipid data
Add gene-array data
Output pathway with heatmaps



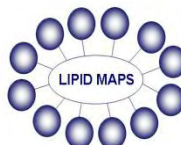
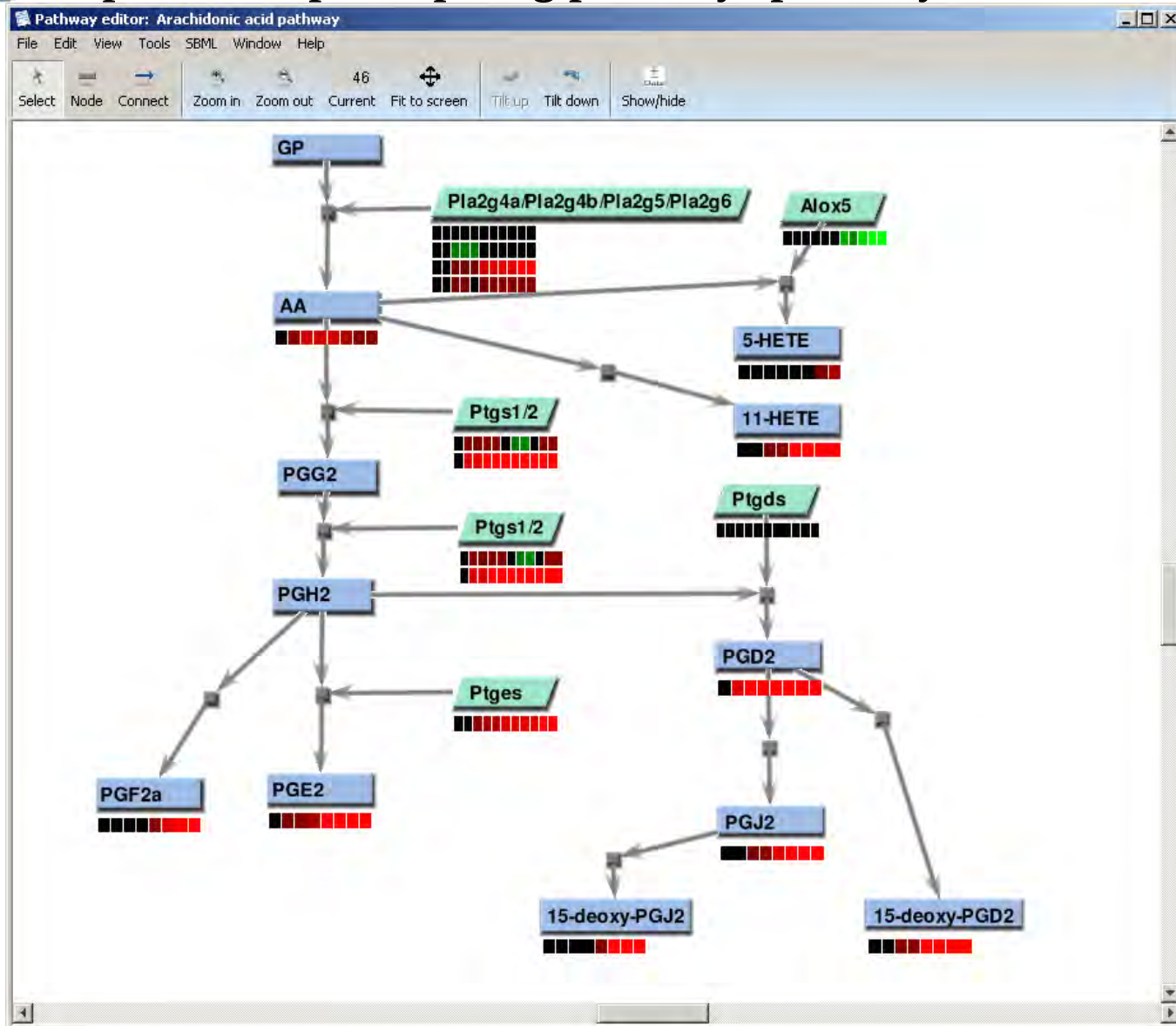
Pathway with heatmap

Lipid Pathways and Networks: Visualization tools

Biopathways Workbench-Pathway Editor



<http://www.lipidmaps.org/pathways/pathwayeditor.html>



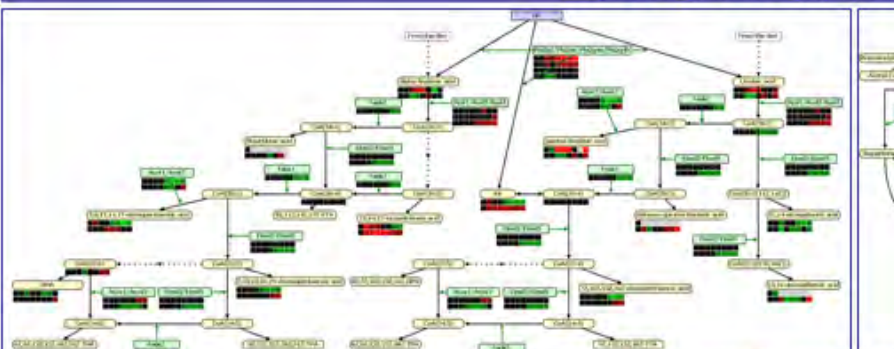


Integrated lipids, genes, and pathways data across timecourse experiments for RAW 264.7 cells treated with Kdo₂-lipid A

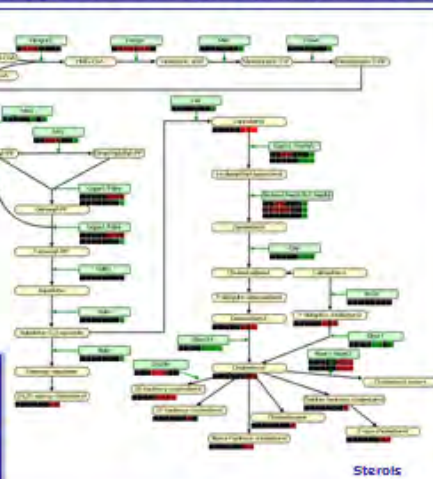


LIPID MAPS funded by Glue Grant from: www.nigms.nih.gov

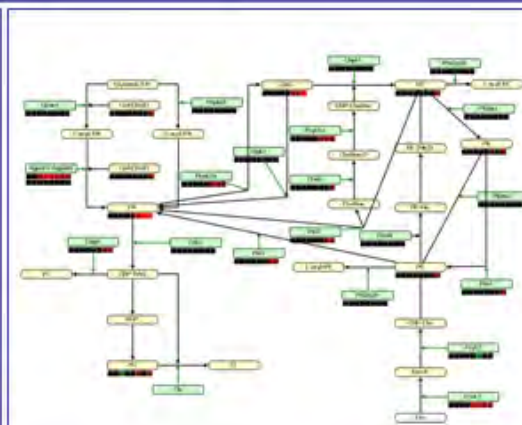
Manish Sud*, Eoin Fahy*, Yihua Zhao*, Dawn Cotter*, Robert Byrne*, Shakti Gupta*, Sean Li*, Manu Maurya*, Shankar Subramaniam^{1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17,18,19,20,21,22,23,24,25,26,27,28,29,30,31,32,33,34,35,36,37,38,39,40,41,42,43,44,45,46,47,48,49,50,51,52,53,54,55,56,57,58,59,60,61,62,63,64,65,66,67,68,69,70,71,72,73,74,75,76,77,78,79,80,81,82,83,84,85,86,87,88,89,90,91,92,93,94,95,96,97,98,99,100}, H. Alex Brown*, Christopher K. Glass*, Alfred H. Merrill, Jr*, Robert C. Murphy*, Christian R.H. Raetz*, David W. Russell*, Edward A. Dennis*



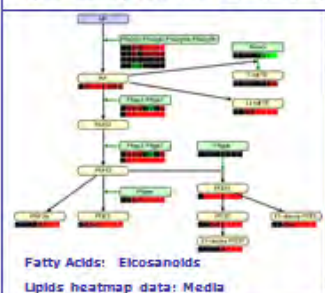
Fatty Acids: Omega-3 and Omega-6 polyunsaturated fatty acids
Lipids heatmap data: First line - Cells; Second line - Media



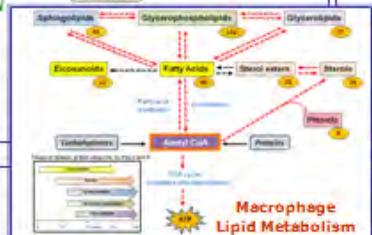
Steroids



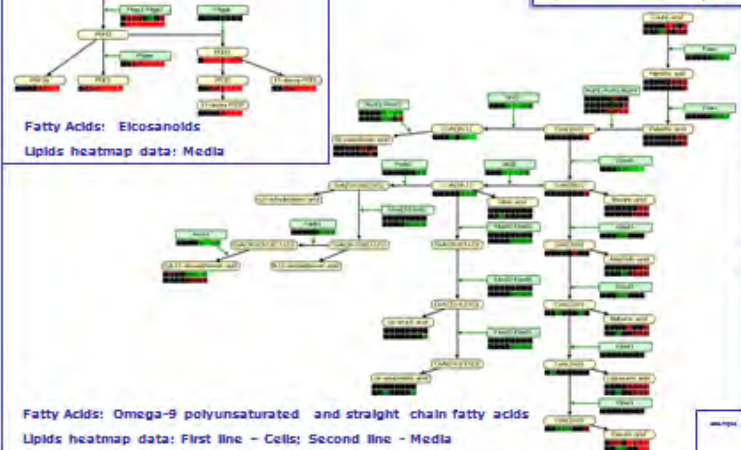
Glycerophospholipids
Lipids heatmap data: C32:0 acyl chains



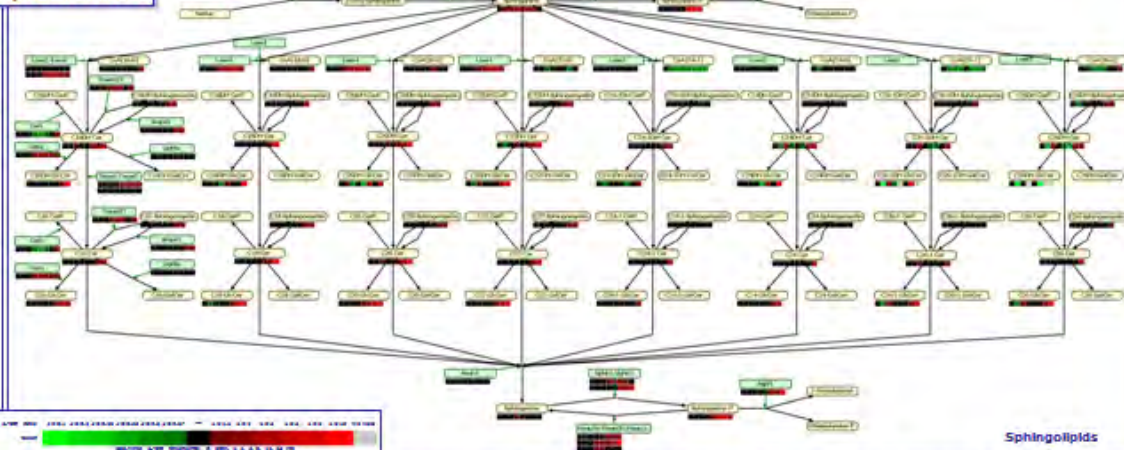
Fatty Acids: Elcosanoids
Lipids heatmap data: Media



Macrophage Lipid Metabolism



Fatty Acids: Omega-9 polyunsaturated and straight chain fatty acids
Lipids heatmap data: First line - Cells; Second line - Media



Sphingolipids

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LIPID MAPS: Educating the public:

Top hit on Google search on “lipid” or “lipidomics”



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Lipid

From Wikipedia, the free encyclopedia

Lipids are broadly defined as any fat-soluble (lipophilic), naturally-occurring

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Lipidomics

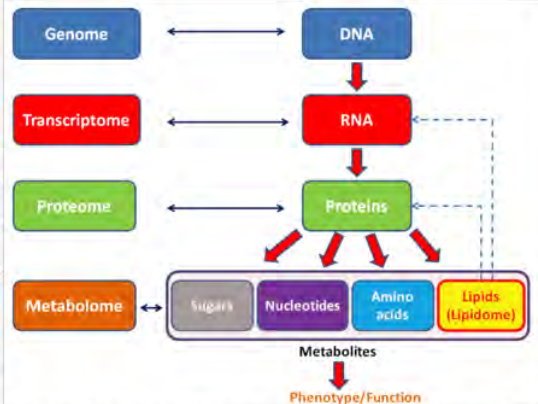
From Wikipedia, the free encyclopedia

Lipidomics may be defined as the large-scale study of pathways and networks of cellular lipids in biological systems [1] [2]. The word "lipidome" is used to describe the complete lipid profile within a cell, tissue or organism and is a subset of the "metabolome" which also includes the three other major classes of biological molecules: proteins/amino-acids, sugars and nucleic acids. Lipidomics is a relatively recent research field that has been driven by rapid advances in technologies such as mass spectrometry (MS), nuclear magnetic resonance (NMR) spectroscopy, fluorescence spectroscopy and computational methods, coupled with the recognition of the role of lipids in many metabolic diseases such as obesity, atherosclerosis, stroke, hypertension and diabetes. This rapidly expanding field [3] complements the huge progress made in genomics and proteomics, all of which constitute the family of systems biology.

Lipidomics research involves the identification and quantitation of the thousands of cellular lipid molecular species and their interactions with other lipids, proteins, and other metabolites. Investigators in lipidomics examine the structures, functions, interactions, and dynamics of cellular lipids and the changes that occur during perturbation of the system.

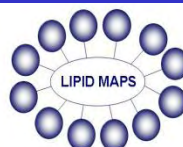
Han and Gross [4] first defined the field of lipidomics through integrating the specific chemical properties inherent in lipid molecular species with a comprehensive mass spectrometric approach. Although lipidomics is under the umbrella of the more general field of "metabolomics", lipidomics is itself a distinct discipline due to the uniqueness and functional specificity of lipids relative to other metabolites.

In lipidomic research, a vast amount of information quantitatively describing the spatial and temporal alterations in the content and composition of different lipid molecular species is accrued after perturbation of a cell through changes in its physiological or pathological state. Information obtained from these studies facilitates mechanistic insights into changes in cellular function. Therefore, lipidomic studies play an essential role in defining the biochemical mechanisms of lipid-related disease processes through identifying alterations in cellular lipid metabolism, trafficking and homeostasis. The growing attention on lipid research is also seen from the initiatives underway of the LIPID Metabolites And Pathways Strategy (LIPID MAPS Consortium), [5] and The European Lipidomics Initiative (ELiFi) [6].



General schema showing the relationships of the lipidome to the genome, transcriptome, proteome and metabolome. Lipids also regulate protein function and gene transcription as part of a dynamic "interactome" within the cell.

Contents [show]



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