LIPID MAPS Bioinformatics

EB2009 Apr 18,2009

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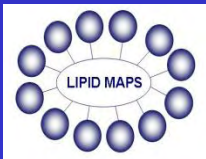
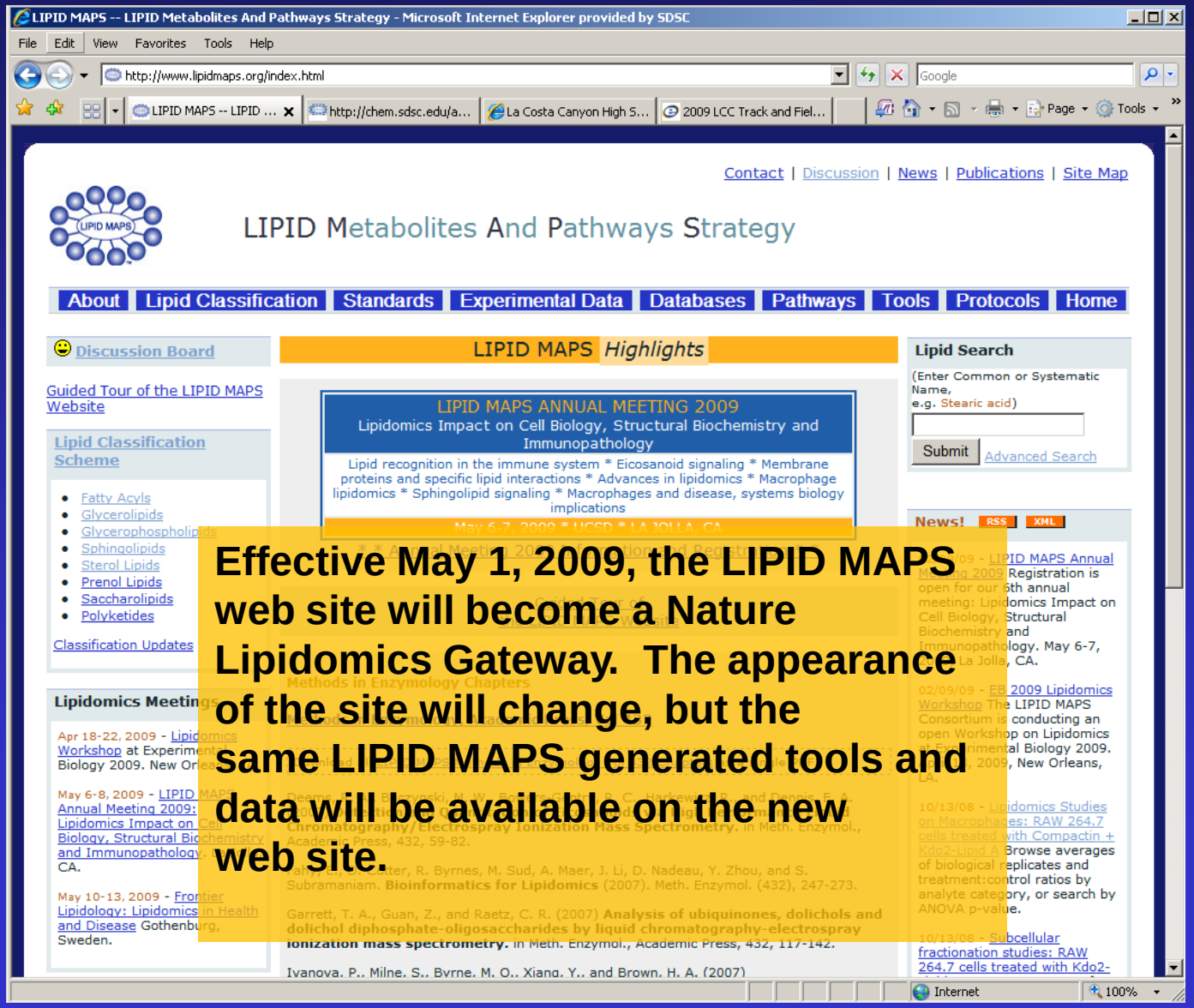
LIPID MAPS Bioinformatics Overview

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/



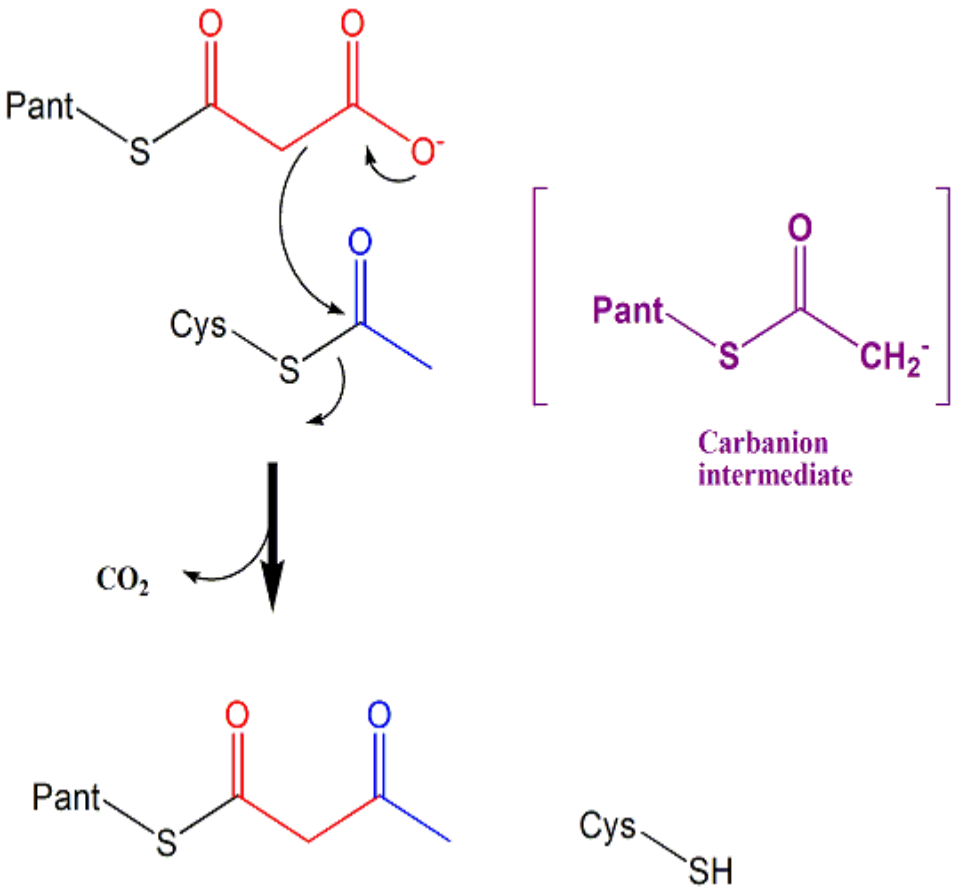
Definition of a lipid*

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

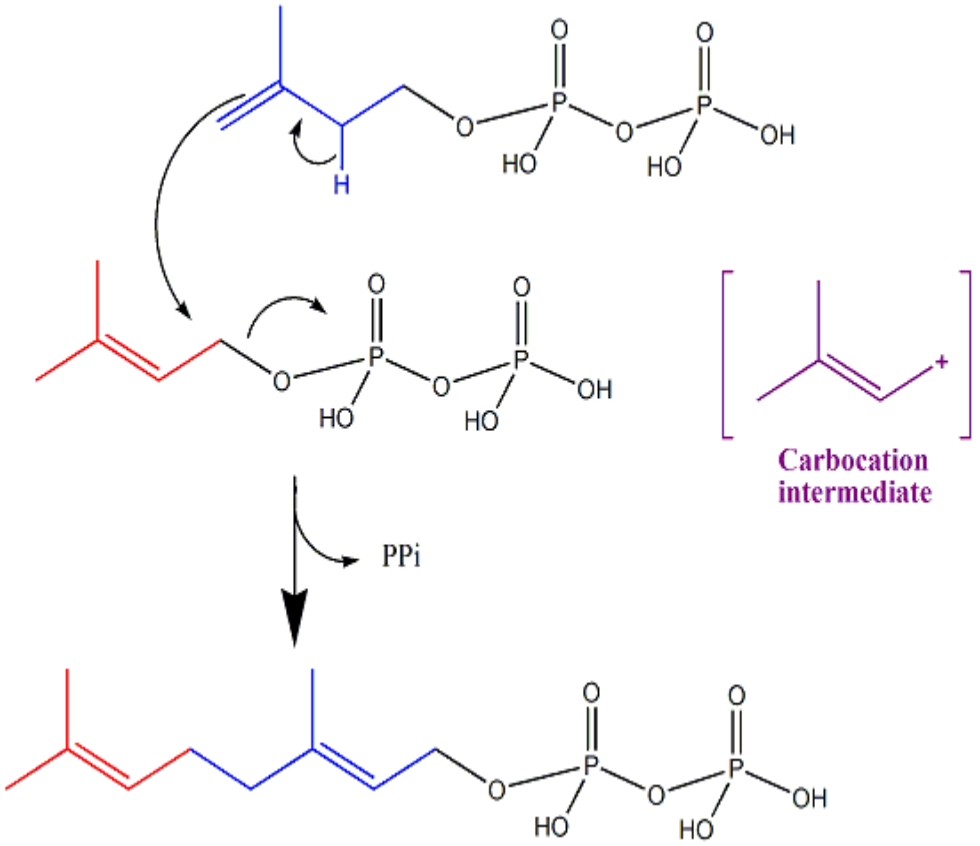
1: Carbanion-based condensation



CATEGORIES

Fatty Acyls
Glycerolipids
Glycerophospholipids
Sphingolipids
Saccharolipids
Polyketides

Lipid classification: biosynthetic routes
2: Carbocation-based condensation



CATEGORIES

Sterol lipids

Prenol lipids

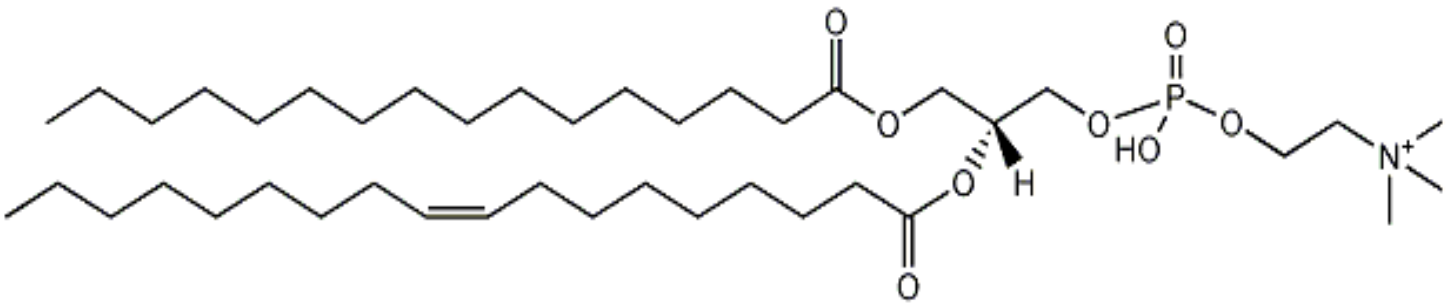
LIPID MAPS Classification System

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-3β-ol
Prenol lipids	PR	2E,6E-farnesol
Saccharolipids	SL	UDP-3-O-(3R-hydroxy-tetradecanoyl)-αD-N-acetylglucosamine
Polyketides	PK	Aflatoxin B_1

LIPID MAPS: Compound ID

- **LIPID MAPS compound ID**
  - **LMGP01010005**

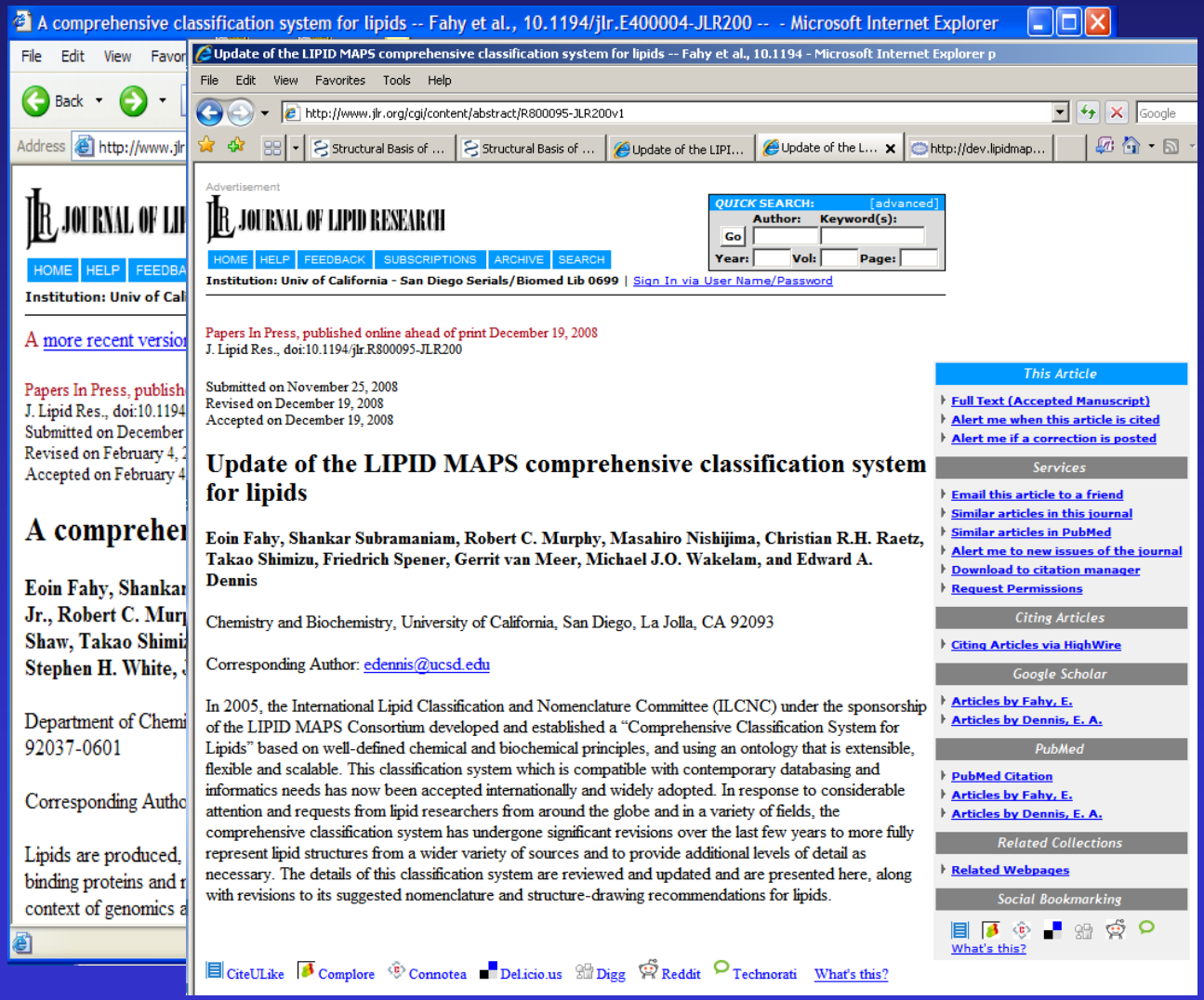


1-hexadecanoyl-2-(9Z-octadecenoyl)-sn-glycero-3-phosphocholine

- **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



LIPID MAPS Online Classification System

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

Contact | News | Public

LIPID Metabolites And Pathways Strategy

About | Data | Tools

Lipid Classification Scheme | Compon

Lipid Classification Scheme

Updated 09/01/06

Fatty Acyls | Glycerolipids | Glycerophospholipids | Sphingolipids | Sterol Lipids | Prenol Lipids | Saccharolipids | Polyketides

Fatty Acyls [FA] classes and subclasses

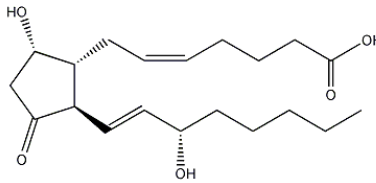
- Fatty Acids and Conjugates [FA01]
  - Straight chain fatty acids [FA0101]
  - Methyl branched fatty acids [FA0102]
  - Unsaturated fatty acids [FA0103]
  - Hydroperoxy fatty acids [FA0104]
  - Hydroxy fatty acids [FA0105]
  - Oxo fatty acids [FA0106]
  - Epoxy fatty acids [FA0107]
  - Methoxy fatty 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 [FA030
  - Hydroxy/hydroperoxyeicosapentaenoic acids [FA03
  - 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-PGF1α	6 p	
LMFA03010002	PGF2α	9 p	
LMFA03010003	PGE2	9 p	
LMFA03010004	PGD2	9 p	
LMFA03010005	PGA1	9 p	
LMFA03010006	PGF2α-d4	9 p	
LMFA03010007	PGD2-d4	9 prostadienoic acid (3,3,4,4-d4)	
LMFA03010008	PGE2-d4	11R,15S-dihydroxy-9-oxo-5Z,13E-prostadienoic acid (3,3,4,4-d4)	356.25	$C_{20}H_{28}D_4O_5$
LMFA03010009	PGG2	9S,11R-epidioxy-15S-hydroperoxy-5Z,13E-prostadienoic acid	368.22	$C_{20}H_{32}O_6$
LMFA03010010	PGH2	9S,11R-epidioxy-15S-hydroxy-5Z,13E-prostadienoic acid	352.22	$C_{20}H_{32}O_5$
LMFA03010011	2,3-dinor-11b-PGF2α	9S,11S,13S-trihydroxy-2,3-dinor-5Z,13E-prostadienoic acid	326.21	$C_{18}H_{30}O_5$
LMFA03010012	6-keto PGE1	6,9-dioxo-11R,15S-dihydroxy-13E-prostenoic acid	368.22	$C_{20}H_{32}O_6$
LMFA03010013	6,15-diketo-13,14-dihydro-PGF1α	6,15-dioxo-9S,11R-dihydroxy-13E-prostenoic acid	368.22	$C_{20}H_{32}O_6$
LMFA03010014	20-hydroxy-PGE2	9-oxo-11R,15S,20-trihydroxy-5Z,13E-prostadienoic acid	368.22	$C_{20}H_{32}O_6$
LMFA03010018	PGB2	15S-hydroxy-9-oxo-5Z,8(12),13E-prostatrienoic acid	334.21	$C_{20}H_{30}O_4$
LMFA03010019	PGJ2	11-oxo-15S-hydroxy-5Z,8Z,13E-prostatrienoic acid	334.21	$C_{20}H_{30}O_4$
LMFA03010020	δ-12-PGJ2	11-oxo-15S-hydroxy-5Z,9Z,13E-prostatrienoic acid	334.21	$C_{20}H_{30}O_4$

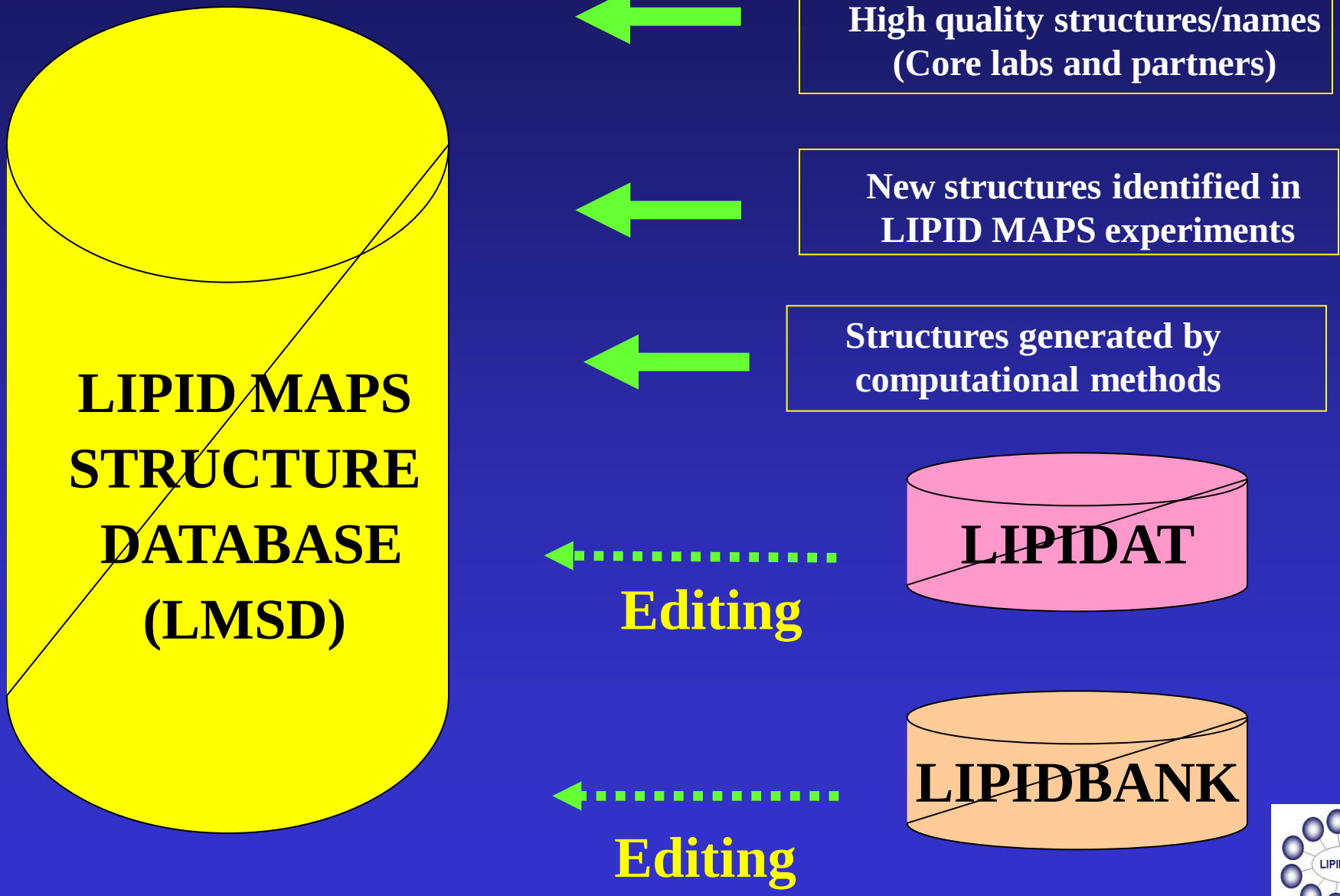
Structure database (LMSD)

LMFA03010004

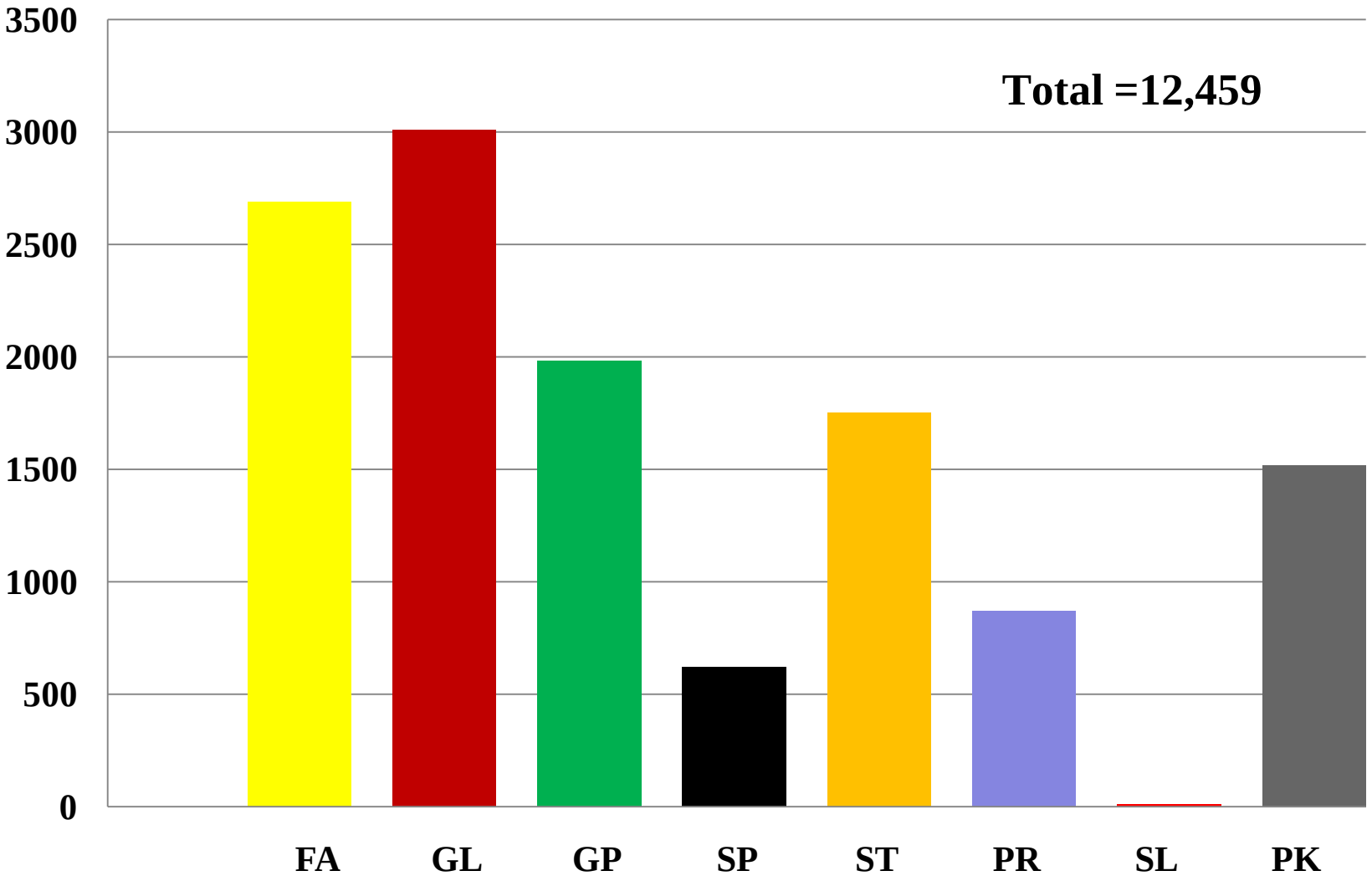


LM ID	LMFA03010004
Common Name	PGD2 (W)
Systematic Name	9S,15S-dihydroxy-11-oxo-5Z,13E-prostadienoic acid
Synonyms	-
Exact Mass	352.22
Formula	$C_{20}H_{32}O_5$
Category	Fatty Acyls [FA]
Main Class	Eicosanoids [FA03]
Sub Class	Prostaglandins [FA0301]
LIPIDBANK ID	XPR1301
PubChem Substance ID (SID)	4265955
KEGG ID	C00696

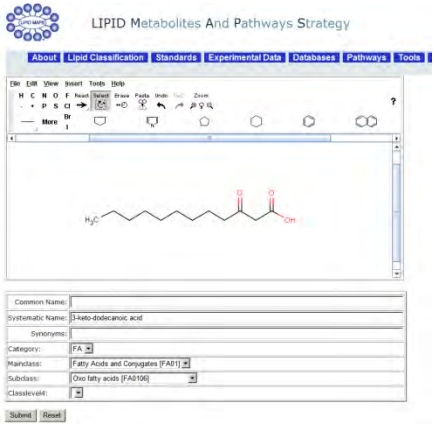
LIPID MAPS Structure Database



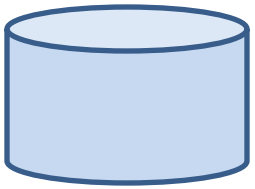
Lipids per category in LMSD (4/1/09)



Web-based Lipid Structure Registration tool



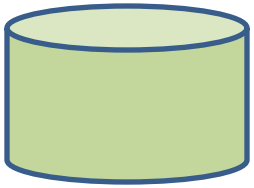
User data entry form



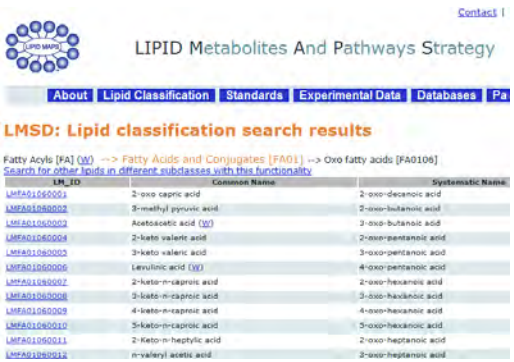
Temporary database table

Review:

Check for duplicates
Check structure format
Check classification
Check systematic name



LIPID MAPS structure database

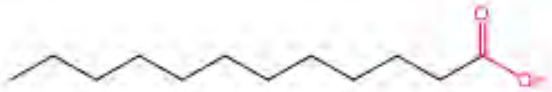


www.lipidmaps.org

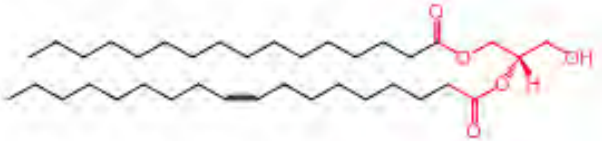
LIPID MAPS: Recommendations for drawing structures

Consistent structure representation across classes

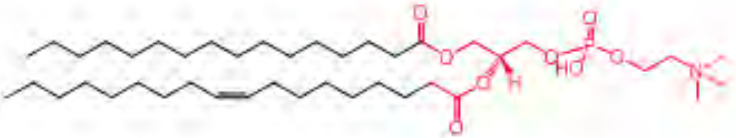
Fatty Acyls(FA)



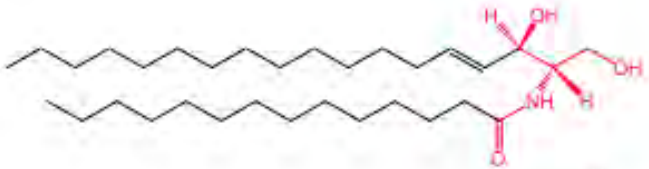
Glycerolipids (GL)



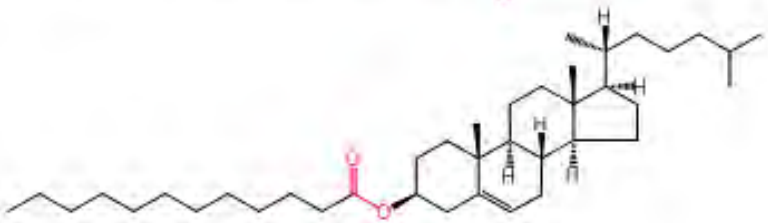
Glycerophospholipids (GP)



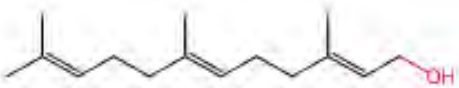
Sphingolipids (SP)



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, Syste
or Common Name, Mass, Formula, Category, Main Class, and Sub

Structure-based Search

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

- MarvinSketch Applet
- JME Applet
- * ChemDrawPro

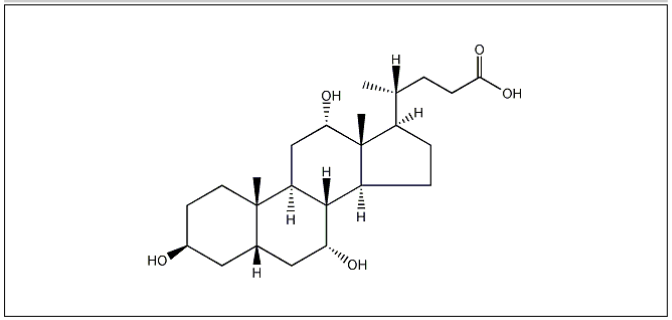
LMSD: Structure-based search results

Modify Search

LM_ID	Common Name	Systematic Name	Formula	Mass	
LMST04010086	-	3β7α,12α-Trihydroxy-5β-cholan-24-oic Acid	$C_{24}H_{40}O_5$	408.29	Bile acids and de
LMST04010089	-	3α,7β,12β-Trihydroxy-5β-cholan-24-oic Acid	$C_{24}H_{40}O_5$	408.29	Bile acids and de
LMST04010094	-	3β,7α,12α-Trihydroxy-5α-cholan-24-oic Acid	$C_{24}H_{40}O_5$	408.29	Bile acids and de
LMST04010097	-	3α,7β,12β-Trihydroxy-5α-cholan-24-oic Acid	$C_{24}H_{40}O_5$	408.29	Bile acids and de
LMST04010117	-	3β,4β,7α,12α-Tetrahydroxy-5β-cholan-24-oic Acid	$C_{24}H_{40}O_6$	424.28	Bile acids and de
LMST04010123	-	3α,6β,7β,12β-Tetrahydroxy-5β-cholan-24-oic Acid	$C_{24}H_{40}O_6$	424.28	Bile acids and de
LMST04030009	-	5α-Cholestane-3β,7α,12α,26,27-pentol	$C_{27}H_{48}O_5$	452.35	Bile acids and de
LMST04030012	-				
LMST04030046	-				
LMST04030063	-				
LMST04030103	-				

Structure database (LMSD)

LMST04010086



LM ID	LMST04010086
Common Name	-
Systematic Name	3β7α,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)

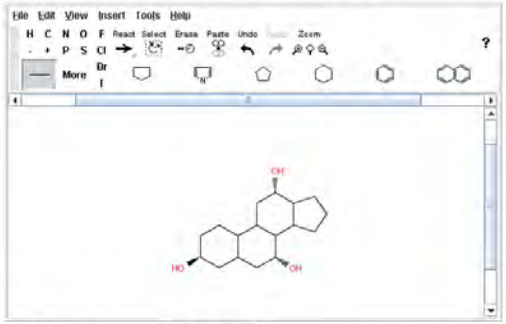
Text-based search

LM ID	
Name(Common or Systematic)	cholan-24-oic Acid
Mass	+/- 0.5
Formula	
Category	
Main class	
Sub class	
Records per page	50
Sort by	LM_ID

Submit Reset

Structure Database (LMSD)

Structure-based search using MarvinSketch



Search type	Substructure
LM ID	
Name(Common or Systematic)	
Records per page	50
Sort by	LM_ID

Online features:

Browse

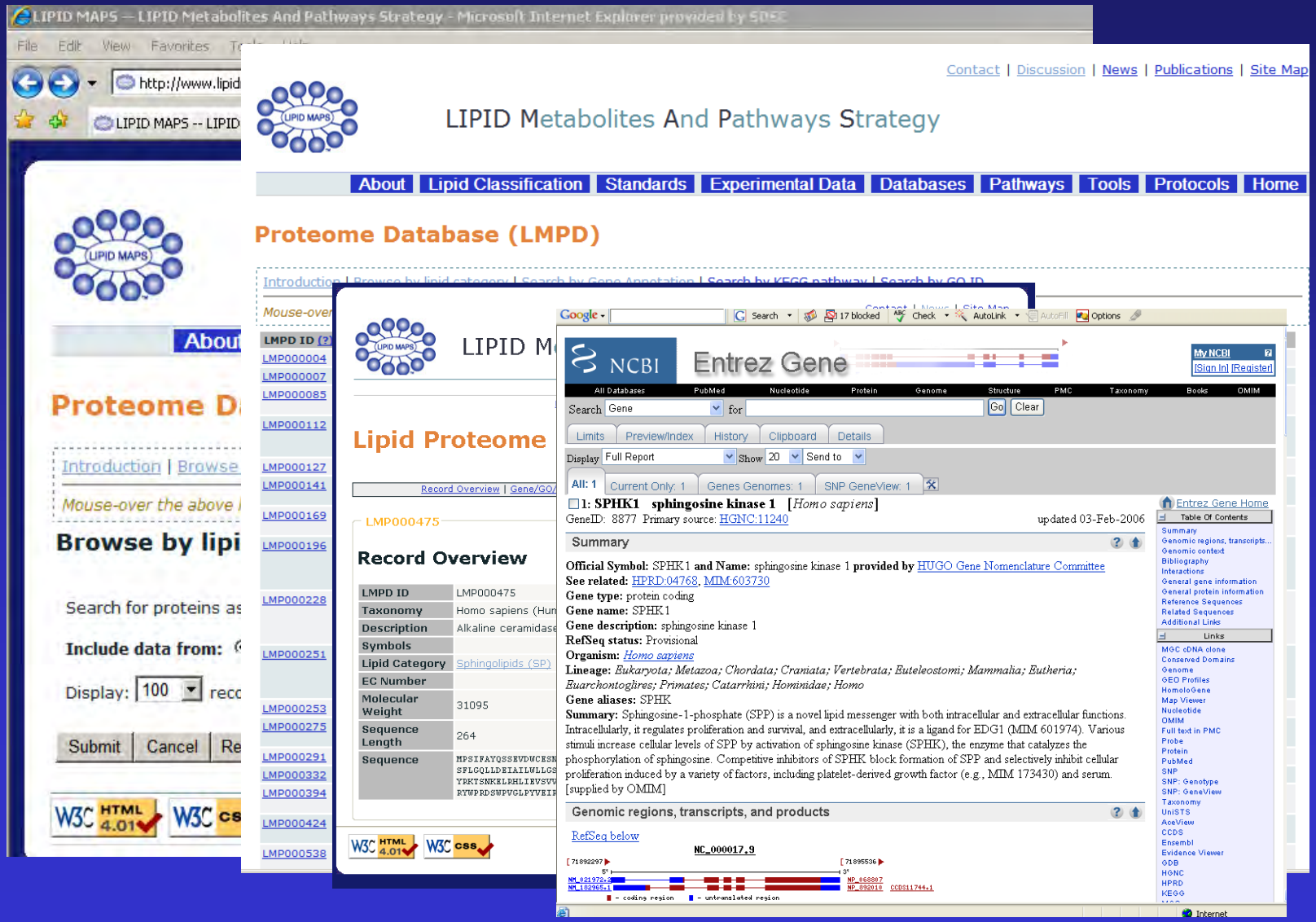
Text search

Substructure search

Download structures

Lipid Proteome Database (LMPD)

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

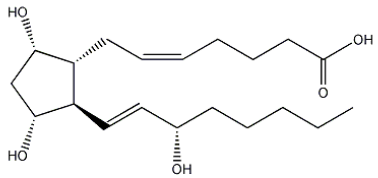


Lipidomics Data Display : MS Standards library

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

Structure Database (LMSD)

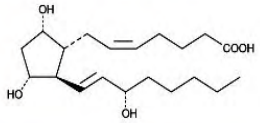
LMFA03010002



LM ID	LMFA03010002
Common Name	PGF2α
Systematic Name	9S,11R,15S-trihydroxy-5Z,13E-prostadienoic acid

16010 Prostaglandin F2α

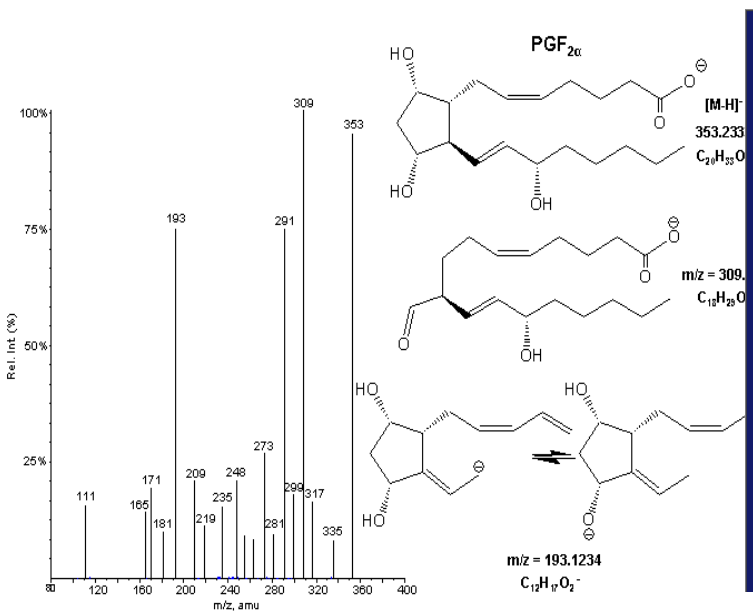
• See below for pricing and ordering



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]

of principal product



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LIPID Metabolites And Pathways Strategy

About | Data | Protocols | Home

Lipid Classification Scheme | Lipid Structure Database

Library of Eicosanoid Standards: LC Retention Times

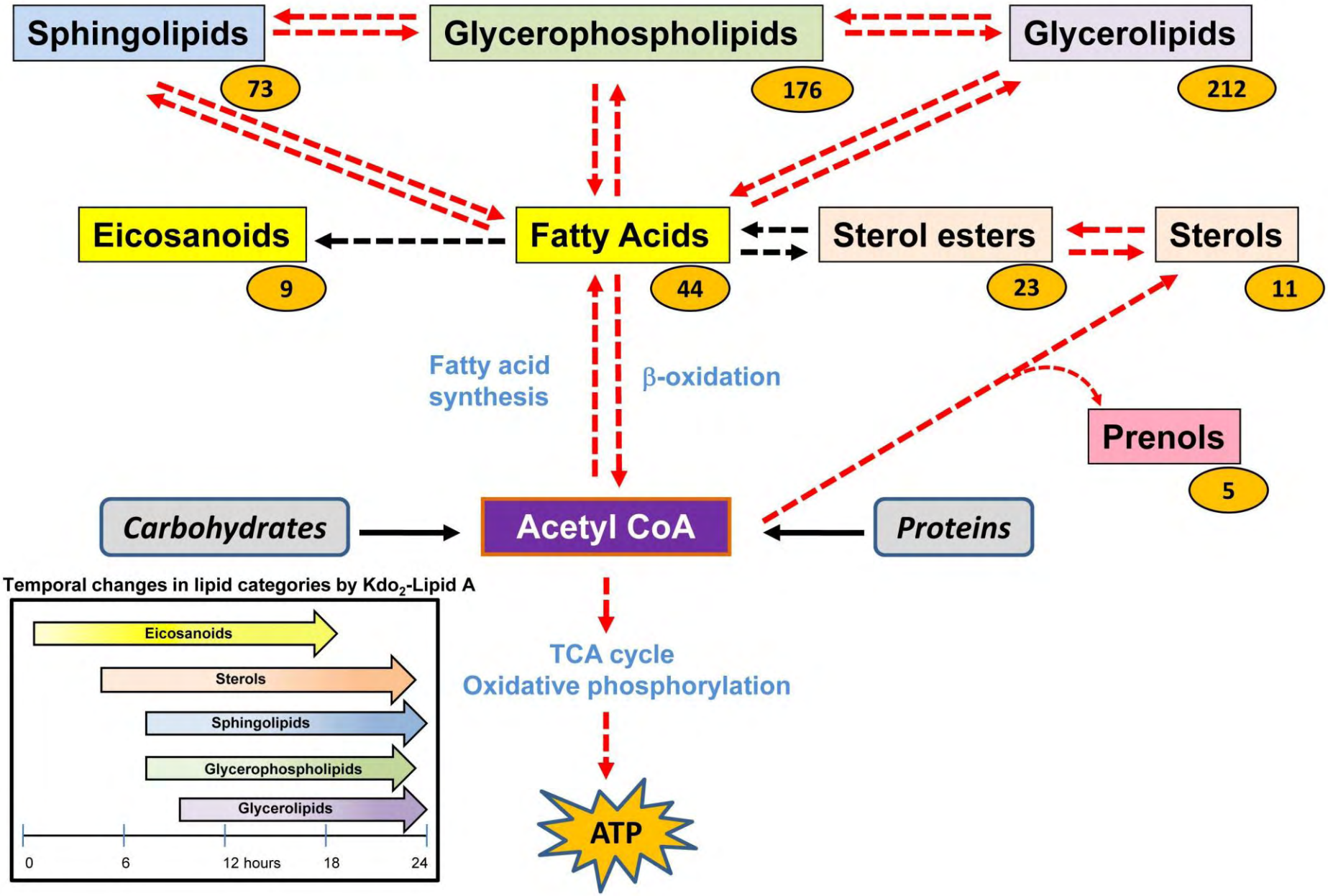
LC retention time and MS/MS data were obtained using the conditions outlined in the protocols below

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	9S,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-epidioxy-15S-hydroperoxy-5Z,13E-prostadienoic acid	367	6.41
LMFA03010010	PGH2	9S,11S-epidioxy-15S-hydroxy-5Z,13E-prostadienoic acid	351	7.55
LMFA03010011	2,3-Dinor-11β-PGF2a	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

LIPID MAPS

MACROPHAGE LIPID METABOLISM

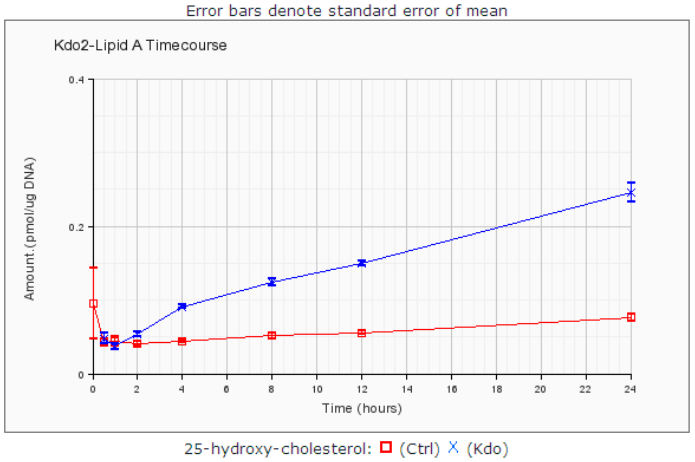


Data presentation formats

Tabular:

Details/Graph	Name	Kdo Ctl 0min	Kdo Ctl 30min	Kdo Ctl 1hr	Kdo Ctl 2hrs	Kdo Ctl 4hrs	Kdo Ctl 8hrs	Kdo Ctl 12hrs	Kdo Ctl 24hrs	Units
	11-HETE	- 0.468	0.558 0.406	0.809 0.41	1.02 0.378	3.07 0.298	6.99 0.189	4.74 0.102	1.37 0.017	pmol/ug DNA
	15-deoxy-PGD2	- 0.224	0.233 0.195	0.367 0.147	0.481 0.162	2.36 0.175	18.3 0.153	37.2 0.166	72.7 0.111	pmol/ug DNA
	15-deoxy-PGJ2	- 0.16	0.116 0.115	0.117 0.096	0.13 0.109	0.26 0.104	2.03 0.084	7.16 0.067	23.5 0.055	pmol/ug DNA
	5-HETE	- 0.107	0.102 0.092	0.123 0.098	0.096 0.089	0.068 0.066	0.044 0.038	0.029 0.019	0.02 0.006	pmol/ug DNA
	AA	- 80.7	147 73.4	357 72.9	319 68.8	214 49	99.2 27	39.4 14.1	10.5 3.89	pmol/ug DNA
	PGD2	- 0.702	4.43 0.612	8.98 0.652	14.1 0.788	70.3 0.594	193 0.485	160 0.382	82.2 0.17	pmol/ug DNA
	PGE2	- 0.173	0.344 0.219	0.671 0.233	0.991 0.251	3.01 0.24	12.9 0.164	17.9 0.136	22.6 0.078	pmol/ug DNA
	PGF2a	- 0.815	0.9 0.703	0.813 0.846	1.03 0.785	1.59 0.749	4.05 0.579	4.54 0.38	6.89 0.158	pmol/ug DNA
	PGJ2	- 0.491	0.492 0.422	0.805 0.426	1.23 0.514	5.22 0.556	37.1 0.494	66.2 0.467	109 0.333	pmol/ug DNA
	DNA	- 1.22	1.35 1.35	1.33 1.42	1.58 1.44	1.65 1.6	1.81 2.14	2.13 3	2.15 6.21	ug
	TNF	- 0.07	0.117 0.082	1.52 0.089	5.77 0.13	21.8 0.165	40.6 0.175	50.4 0.256	65 0.453	ng

Graphical:



Heatmap:

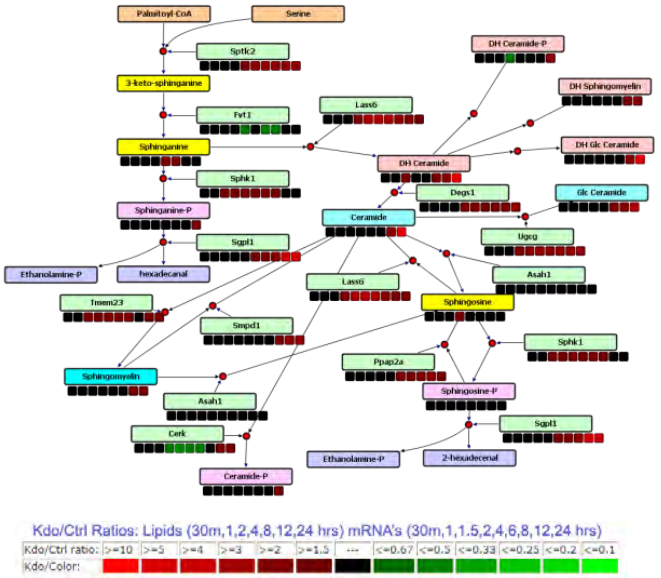
Heatmap of Kdo timecourse data for lipid category ST,PR (Ratio Kdo/ctrl values)

Clicking on Analyte column displays data and graphs for timecourse experiment.

ANALYTE	30	1	2	4	8	12	24
24,25-epoxy-cholesterol	1.10	1.05	1.10	1.17	1.41	1.93	1.97
25-hydroxy-cholesterol	1.12	0.84	1.32	2.07	2.43	2.68	3.22
27-hydroxy-cholesterol	1.13	0.86	1.34	1.06	1.43	1.50	1.19
4beta-hydroxy-cholesterol	0.98	1.15	1.06	1.07	1.30	1.69	2.36
7-dehydro-cholesterol	1.04	1.06	1.10	1.41	2.37	2.87	2.15
7-oxo-hydroxy-cholesterol	0.98	1.18	1.37	1.10	1.32	1.33	1.91
7alpha-hydroxy-cholesterol	1.09	1.05	1.08	1.10	1.32	1.68	2.22
Cholestenone	1.09	1.13	1.04	0.94	1.17	1.46	2.14
Cholesterol	1.04	1.04	1.06	1.15	1.31	1.56	1.82
Desmosterol	1.02	1.01	1.11	1.19	1.75	2.71	3.14
Lanosterol	1.05	0.97	0.95	1.24	4.53	14.90	31.10
Coenzyme Q10	1.05	1.16	1.02	1.24	1.09	0.98	1.10
Coenzyme Q9	0.97	1.19	1.07	1.24	1.22	1.02	1.04
Dolichol-18	0.74	1.03	0.68	0.94	0.91	1.22	1.31
Dolichol-19	0.84	1.27	0.94	1.14	1.04	1.35	1.49
Dolichol-20	1.21	1.48	1.12	1.55	1.30	1.57	1.72

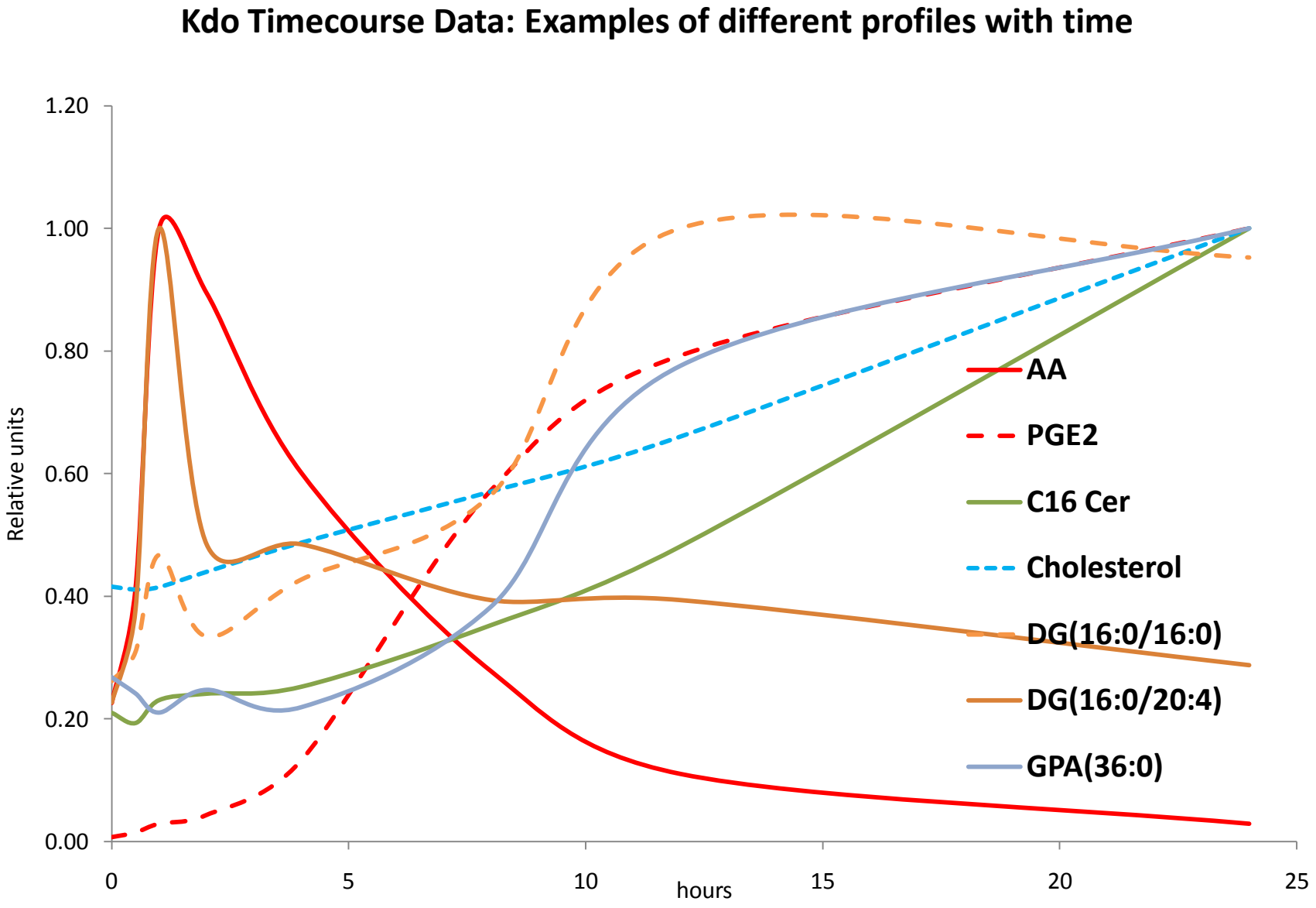
SYMBOL	GENENAME	30	1	1.5	2	4	6	8	12	18	24
Cyp27b1	cytochrome P450, family 27, subfamily b, polypeptide 1	0.94	0.89	0.96	0.97	0.94	0.92	0.89	0.91	0.92	0.86
Dhcr7	7-dehydrocholesterol reductase	1.08	1.01	0.91	0.70	0.41	0.55	0.53	0.70	0.60	0.56
Ebp	phenylalkylamine Ca2+ antagonist (emopamil) binding protein	0.88	0.89	0.89	0.83	0.68	0.68	0.63	0.63	0.63	0.63
Fdft1	farnesyl diphosphate farnesyl transferase 1	1.09	1.14	1.16	1.16	1.05	0.92	1.03	1.05	0.91	0.79
Fdps	farnesyl diphosphate synthetase	1.13	0.87	0.83	0.81	0.74	0.70	0.72	0.70	0.55	0.44
Ggps1	geranylgeranyl diphosphate synthase 1	0.90	0.94	0.99	1.02	1.32	1.67	1.58	1.61	1.48	1.58
Hmgcr	3-hydroxy-3-methylglutaryl-Coenzyme A reductase	1.55	1.94	2.04	1.87	1.76	1.72	1.65	1.69	1.40	1.05
Idi1	isopentenyl-diphosphate delta isomerase	1.46	1.72	1.86	1.77	1.60	1.11	1.10	0.90	0.48	0.34
Lss	lanosterol synthase	1.05	1.11	1.07	1.00	0.97	0.91	0.94	1.05	0.83	0.62
Mvd	mevalonate (diphospho) decarboxylase	1.04	0.96	1.09	0.92	0.75	0.67	0.67	0.69	0.62	0.51
Mvk	mevalonate kinase	1.16	1.14	1.14	1.00	0.88	0.91	0.80	0.89	0.80	0.67
Nqo1	NAD(P)H dehydrogenase, quinone 1	1.51	1.44	1.34	1.58	1.37	1.01	1.09	1.26	2.30	2.78
Pmvk	phosphomevalonate kinase	1.16	1.31	1.22	1.19	1.02	0.99	0.89	0.94	0.75	0.54
Sc5d	sterol-C5-desaturase (fungal ERG3, delta-5-desaturase) homolog (S. cerevisae)	1.33	1.13	1.10	1.03	0.89	0.87	0.83	0.80	0.83	0.70
Sqle	squalene epoxidase	1.07	1.11	1.18	1.07	0.74	0.77	1.07	0.89	0.72	0.64
Vkorc1	vitamin K epoxide reductase complex, subunit 1	1.02	1.00	0.99	0.93	0.81	0.61	0.62	0.52	0.44	0.39
Fdft1	farnesyl diphosphate farnesyl transferase 1	1.09	1.14	1.16	1.16	1.05	0.92	1.03	1.05	0.91	0.79
Fdps	farnesyl diphosphate synthetase	1.13	0.87	0.83	0.81	0.74	0.70	0.72	0.70	0.55	0.44
Ggps1	geranylgeranyl diphosphate synthase 1	0.90	0.94	0.99	1.02	1.32	1.67	1.58	1.61	1.48	1.58
Idi1	isopentenyl-diphosphate delta isomerase	1.46	1.72	1.86	1.77	1.60	1.11	1.10	0.90	0.48	0.34
Sqle	squalene epoxidase	1.07	1.11	1.18	1.07	0.74	0.77	1.07	0.89	0.72	0.64

Integrated pathway/heatmap:

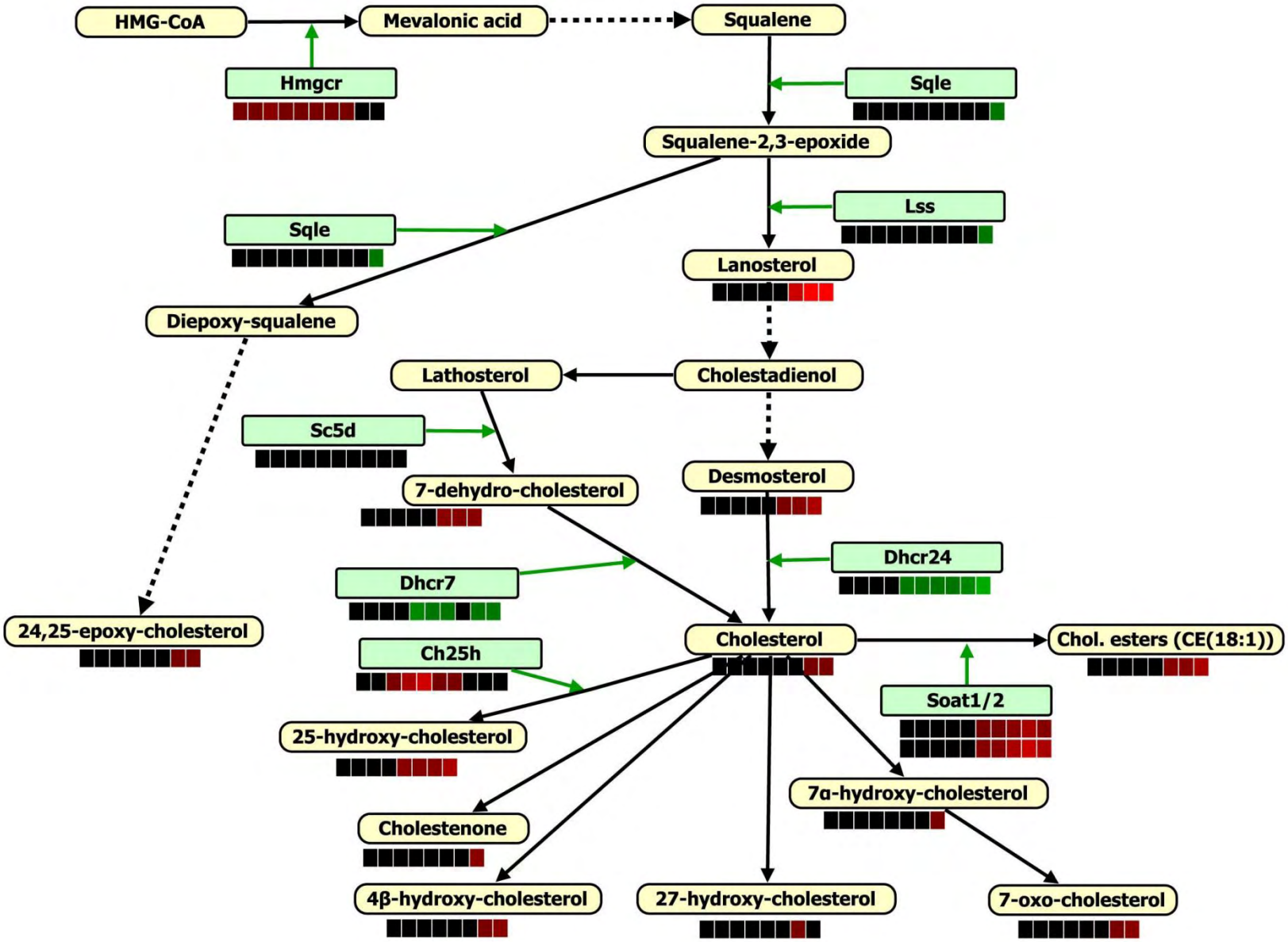


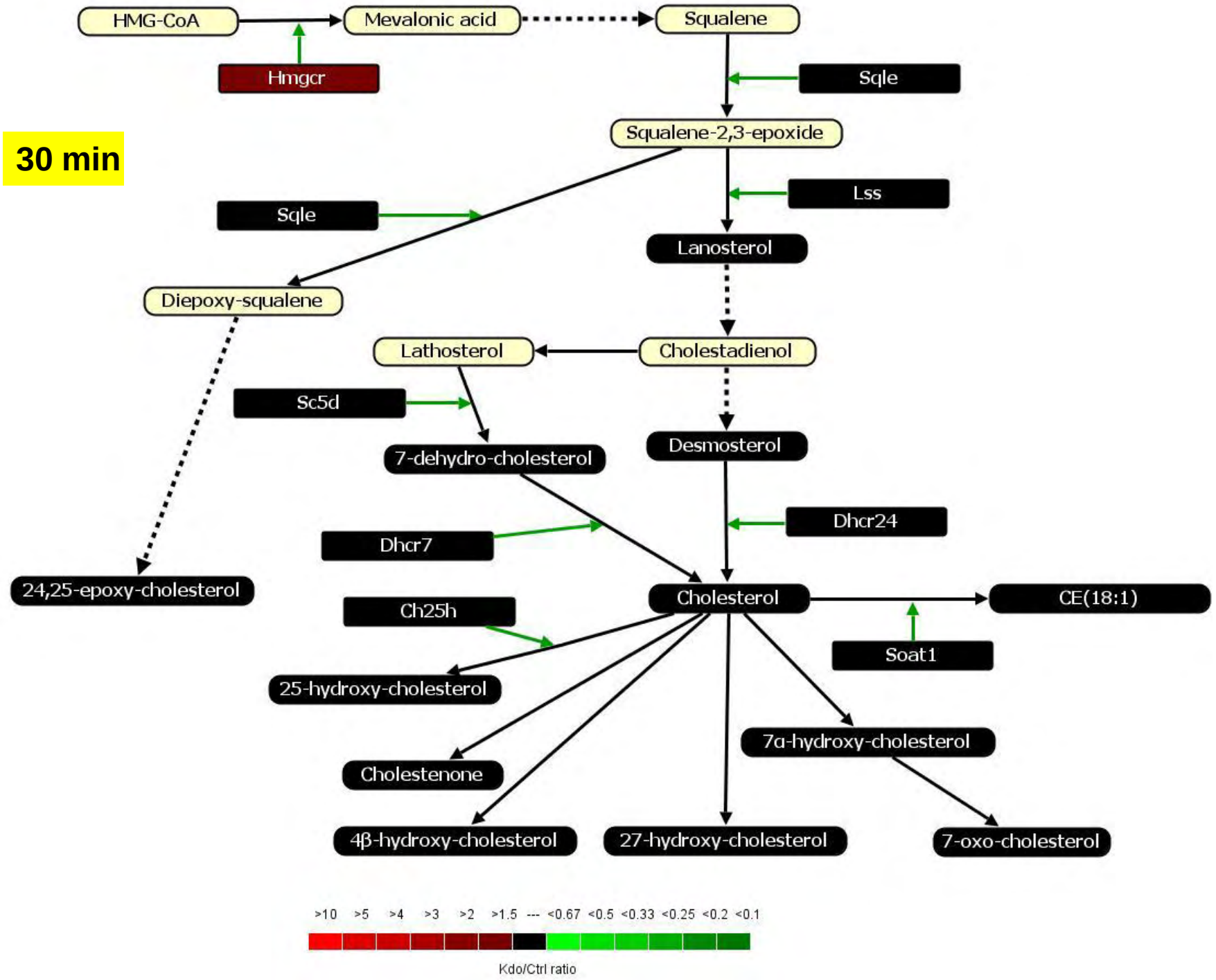
Lipids

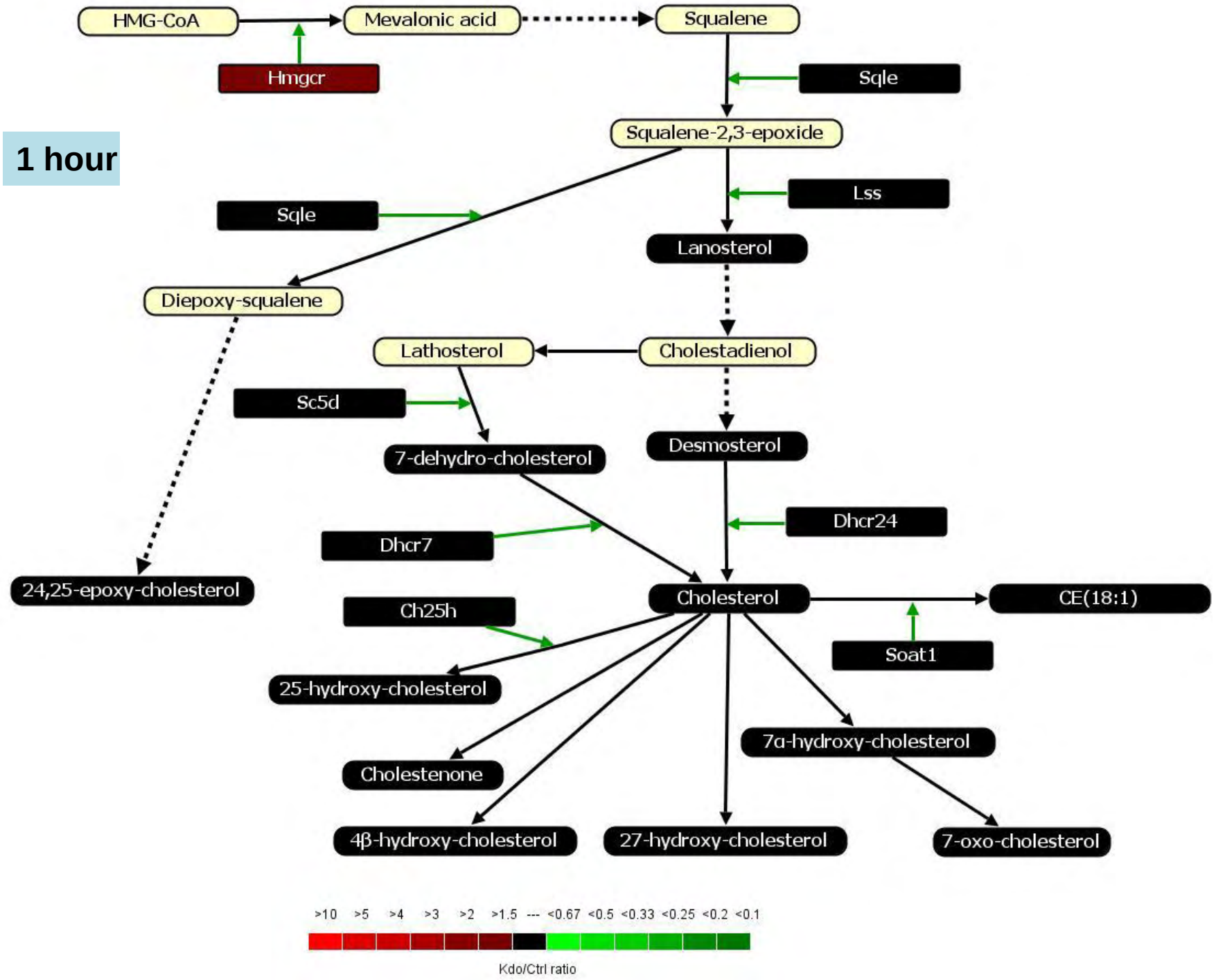
Genes

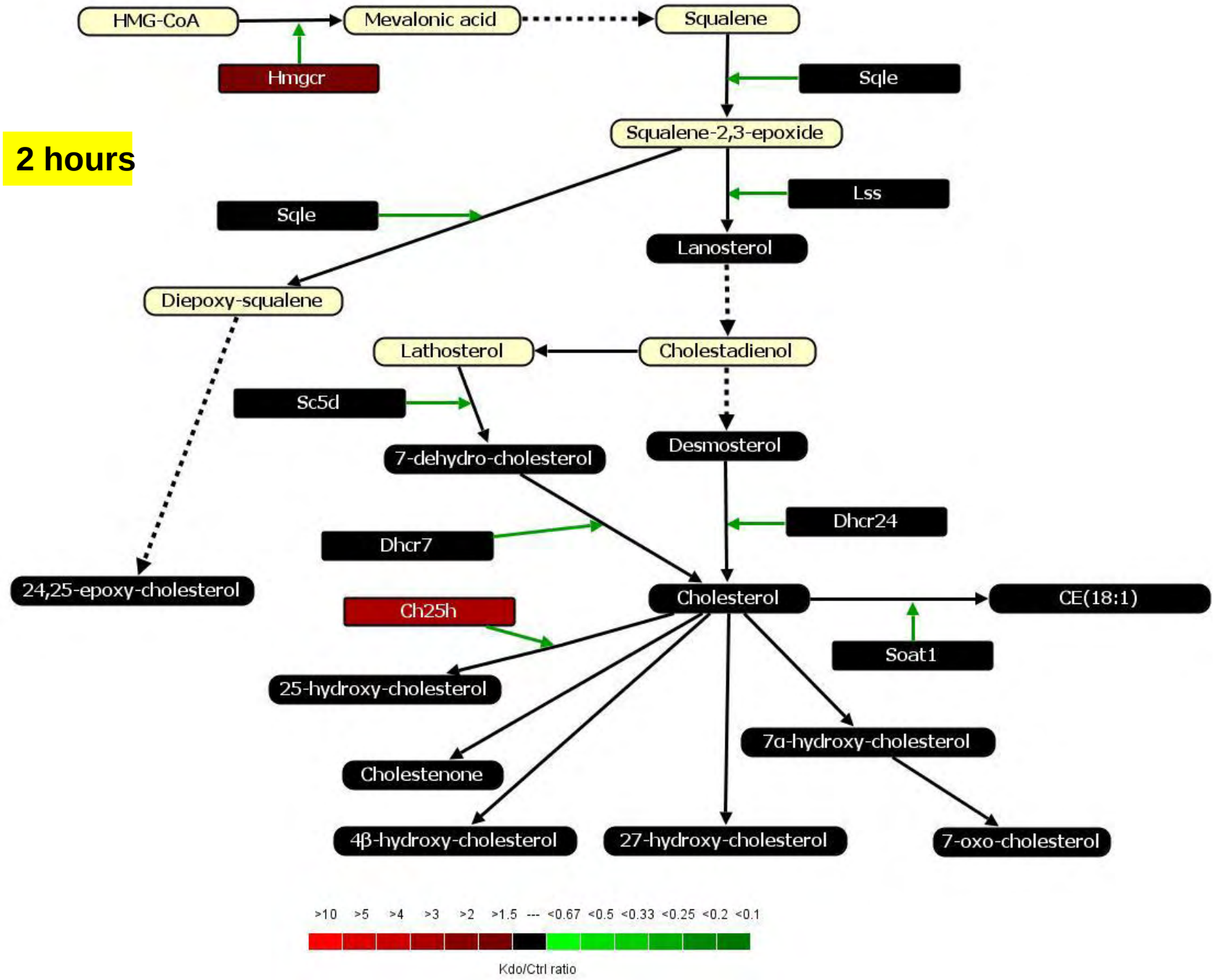

Kdo Timecourse Data: Examples of different profiles with time
Relative units
1.20
1.00
0.80
0.60
0.40
0.20
0.00
0
5
10
15
20
25
hours
AA
PGE2
C16 Cer
Cholesterol
DG(16:0/16:0)
DG(16:0/20:4)
GPA(36:0)

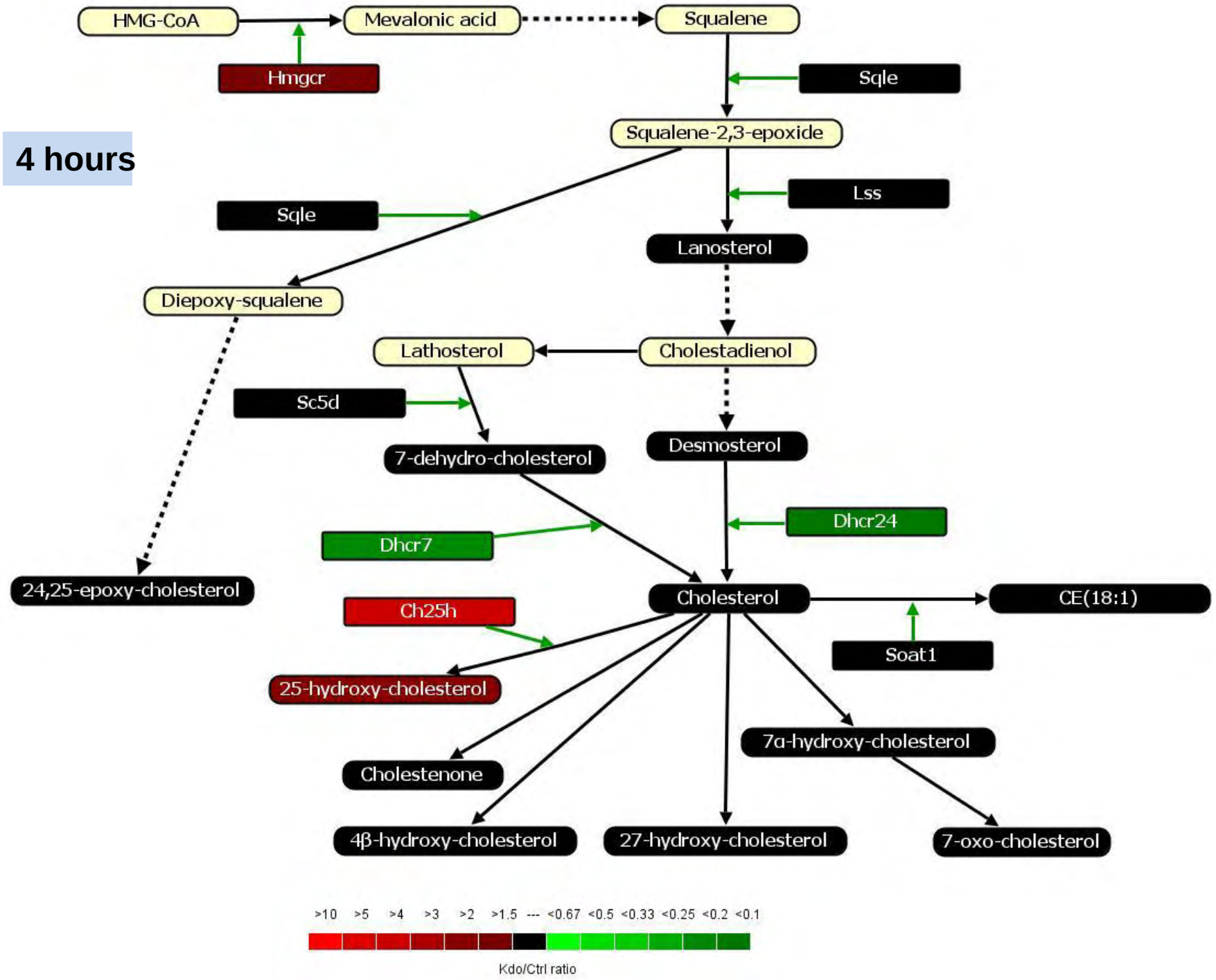
Cholesterol Biosynthesis

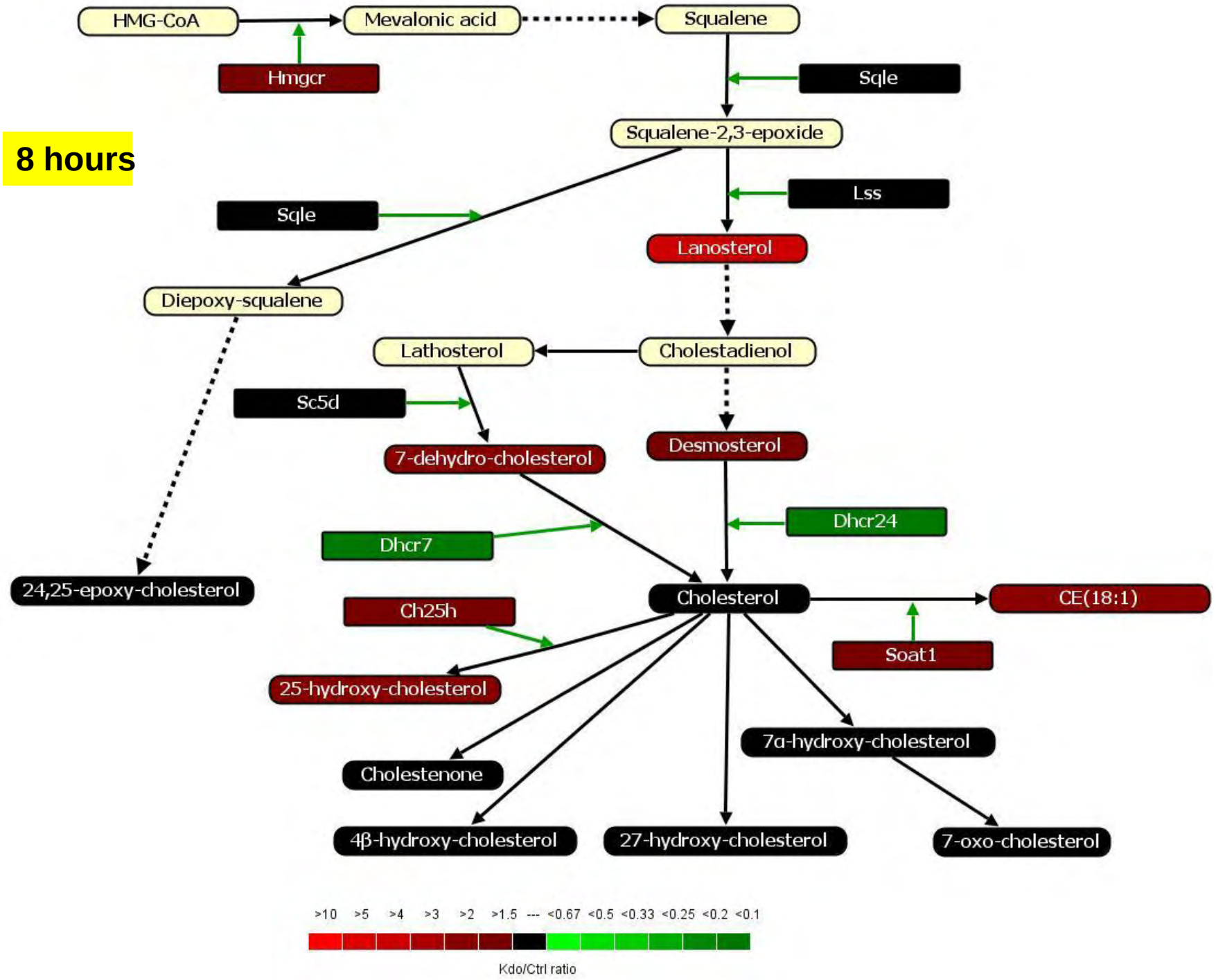


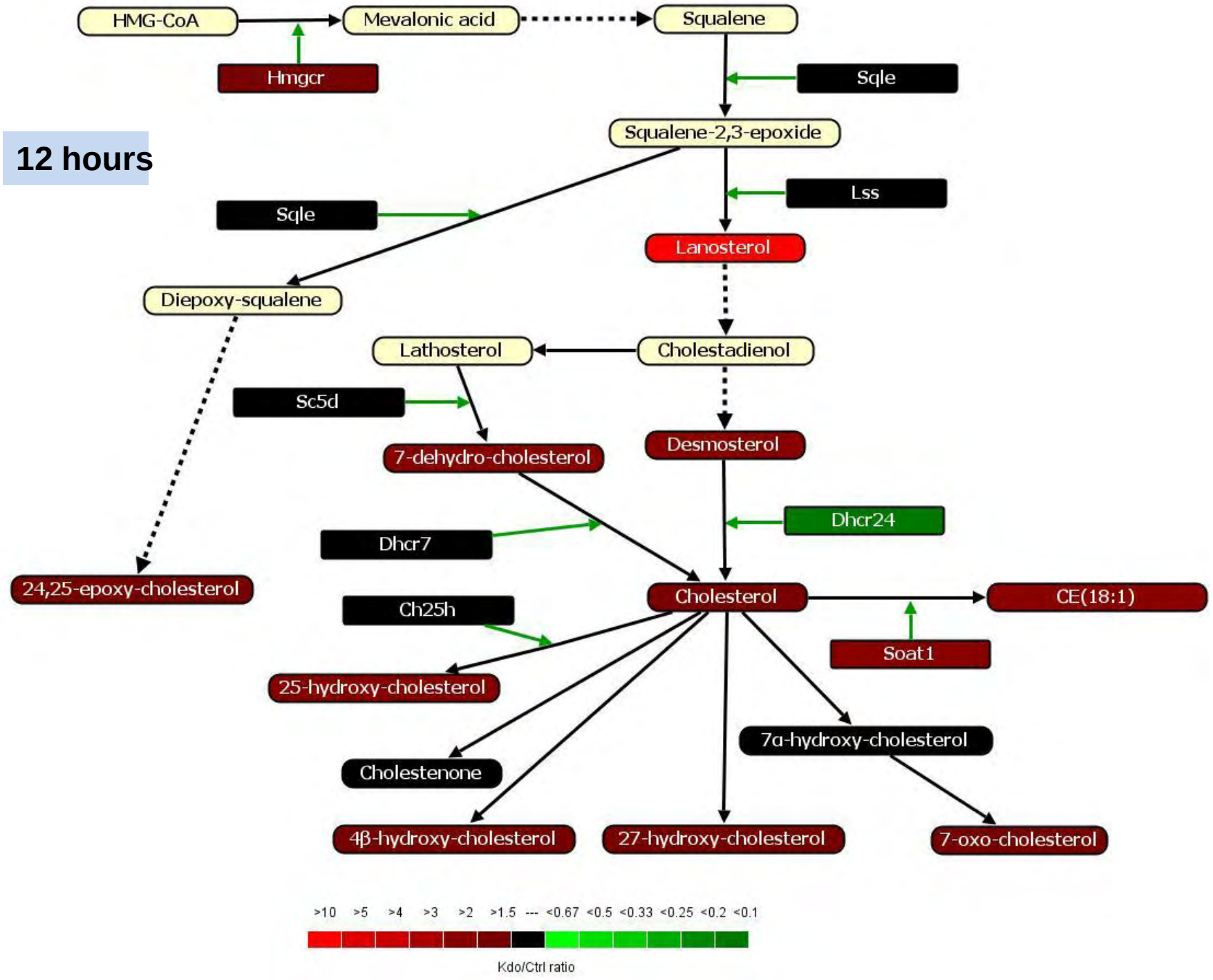

30 min
HMG-CoA
Mevalonic acid
Squalene
Hmgcr
Sqle
Squalene-2,3-epoxide
Lss
Sqle
Lanosterol
Diepoxy-squalene
Lathosterol
Cholestadienol
Sc5d
7-dehydro-cholesterol
Desmosterol
Dhcr24
Dhcr7
24,25-epoxy-cholesterol
Cholesterol
CE(18:1)
Ch25h
Soat1
25-hydroxy-cholesterol
7α-hydroxy-cholesterol
Cholestenone
4β-hydroxy-cholesterol
27-hydroxy-cholesterol
7-oxo-cholesterol
>10 >5 >4 >3 >2 >1.5 --- <0.67 <0.5 <0.33 <0.25 <0.2 <0.1
Kdo/Ctrl ratio

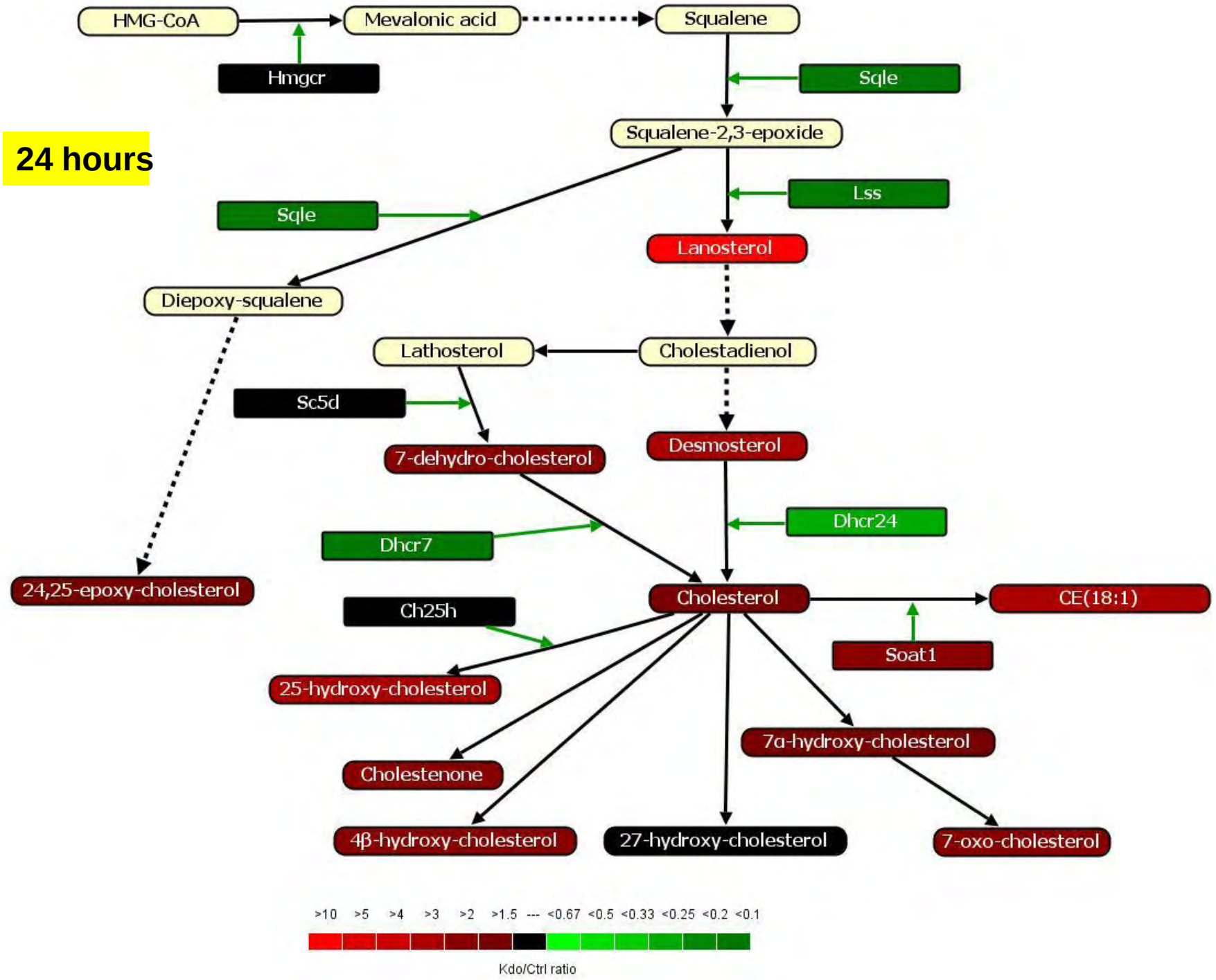

1 hour
HMG-CoA
Mevalonic acid
Squalene
Hmgcr
Sqle
Squalene-2,3-epoxide
Lss
Sqle
Lanosterol
Diepoxy-squalene
Lathosterol
Cholestadienol
Sc5d
Desmosterol
7-dehydro-cholesterol
Dhcr24
Dhcr7
24,25-epoxy-cholesterol
Cholesterol
CE(18:1)
Ch25h
Soat1
25-hydroxy-cholesterol
7α-hydroxy-cholesterol
Cholestenone
4β-hydroxy-cholesterol
27-hydroxy-cholesterol
7-oxo-cholesterol
>10 >5 >4 >3 >2 >1.5 --- <0.67 <0.5 <0.33 <0.25 <0.2 <0.1
Kdo/Ctrl ratio


2 hours
HMG-CoA
Mevalonic acid
Squalene
Hmgcr
Sqle
Squalene-2,3-epoxide
Lss
Sqle
Lanosterol
Diepoxy-squalene
Lathosterol
Cholestadienol
Sc5d
Desmosterol
7-dehydro-cholesterol
Dhcr24
Dhcr7
24,25-epoxy-cholesterol
Cholesterol
CE(18:1)
Ch25h
Soat1
25-hydroxy-cholesterol
7α-hydroxy-cholesterol
Cholestenone
4β-hydroxy-cholesterol
27-hydroxy-cholesterol
7-oxo-cholesterol
>10 >5 >4 >3 >2 >1.5 --- <0.67 <0.5 <0.33 <0.25 <0.2 <0.1
Kdo/Ctrl ratio


4 hours
HMG-CoA
Mevalonic acid
Squalene
Hmgcr
Sqle
Squalene-2,3-epoxide
Lss
Sqle
Lanosterol
Diepoxy-squalene
Lathosterol
Cholestadienol
Sc5d
Desmosterol
7-dehydro-cholesterol
Dhcr24
Dhcr7
24,25-epoxy-cholesterol
Cholesterol
CE(18:1)
Ch25h
Soat1
25-hydroxy-cholesterol
7α-hydroxy-cholesterol
Cholestenone
4β-hydroxy-cholesterol
27-hydroxy-cholesterol
7-oxo-cholesterol
>10 >5 >4 >3 >2 >1.5 --- <0.67 <0.5 <0.33 <0.25 <0.2 <0.1
Kdo/Ctrl ratio

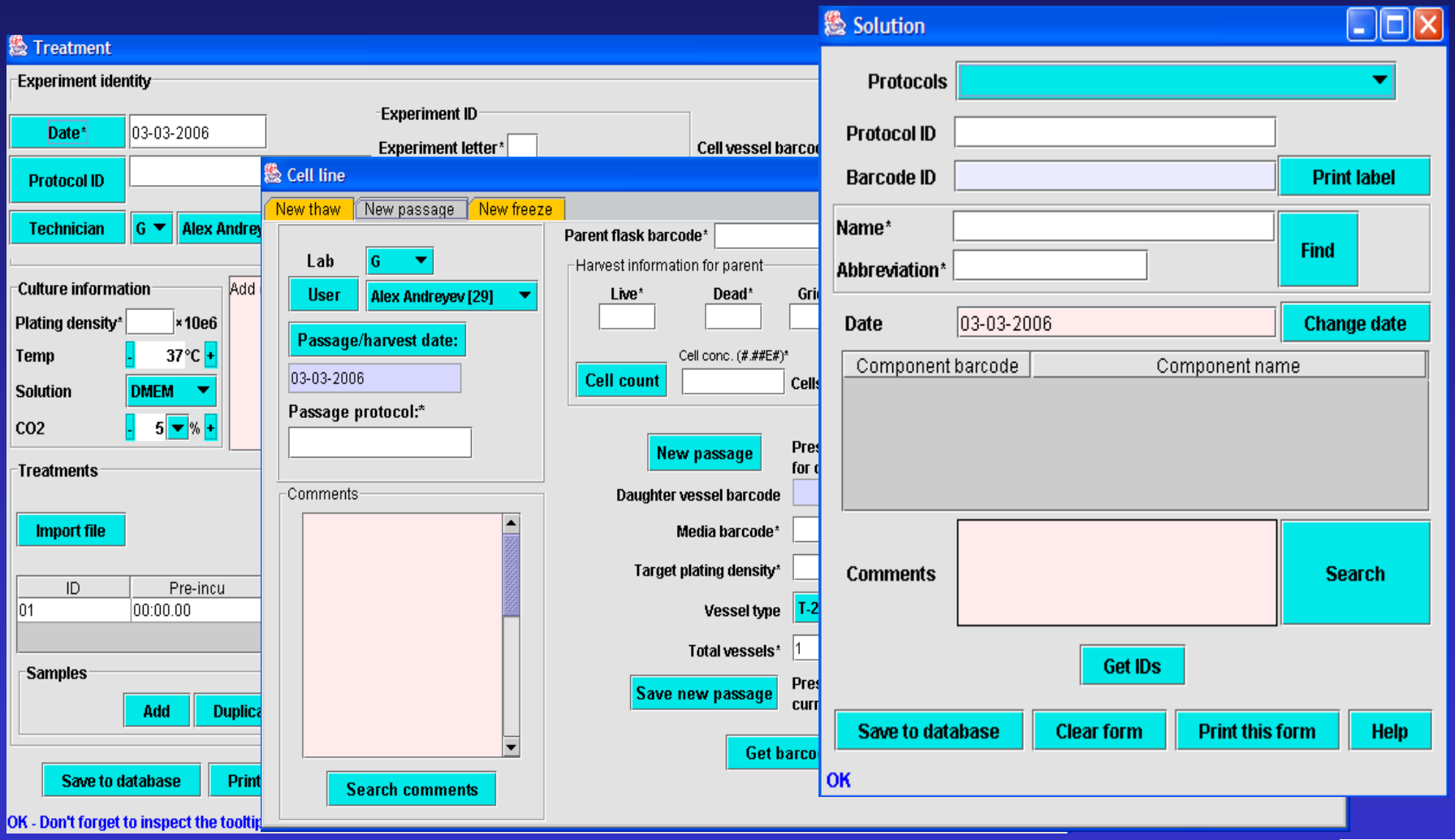

8 hours
HMG-CoA
Mevalonic acid
Squalene
Hmgcr
Sqle
Squalene-2,3-epoxide
Lss
Sqle
Lanosterol
Diepoxy-squalene
Lathosterol
Cholestadienol
Sc5d
Desmosterol
7-dehydro-cholesterol
Dhcr24
Dhcr7
24,25-epoxy-cholesterol
Cholesterol
CE(18:1)
Ch25h
Soat1
25-hydroxy-cholesterol
7α-hydroxy-cholesterol
Cholestenone
4β-hydroxy-cholesterol
27-hydroxy-cholesterol
7-oxo-cholesterol
>10 >5 >4 >3 >2 >1.5 --- <0.67 <0.5 <0.33 <0.25 <0.2 <0.1
Kdo/Ctrl ratio


12 hours
HMG-CoA
Mevalonic acid
Squalene
Hmgcr
Sqle
Squalene-2,3-epoxide
Lss
Sqle
Lanosterol
Diepoxy-squalene
Lathosterol
Cholestadienol
Sc5d
Desmosterol
7-dehydro-cholesterol
Dhcr24
Dhcr7
24,25-epoxy-cholesterol
Cholesterol
CE(18:1)
Ch25h
Soat1
25-hydroxy-cholesterol
7α-hydroxy-cholesterol
Cholestenone
4β-hydroxy-cholesterol
27-hydroxy-cholesterol
7-oxo-cholesterol
>10 >5 >4 >3 >2 >1.5 --- <0.67 <0.5 <0.33 <0.25 <0.2 <0.1
Kdo/Ctrl ratio


24 hours
HMG-CoA
Mevalonic acid
Squalene
Hmgcr
Sqle
Squalene-2,3-epoxide
Lss
Sqle
Lanosterol
Diepoxy-squalene
Lathosterol
Cholestadienol
Sc5d
Desmosterol
7-dehydro-cholesterol
Dhcr24
Dhcr7
24,25-epoxy-cholesterol
Cholesterol
CE(18:1)
Ch25h
Soat1
25-hydroxy-cholesterol
7α-hydroxy-cholesterol
Cholestenone
4β-hydroxy-cholesterol
27-hydroxy-cholesterol
7-oxo-cholesterol
>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

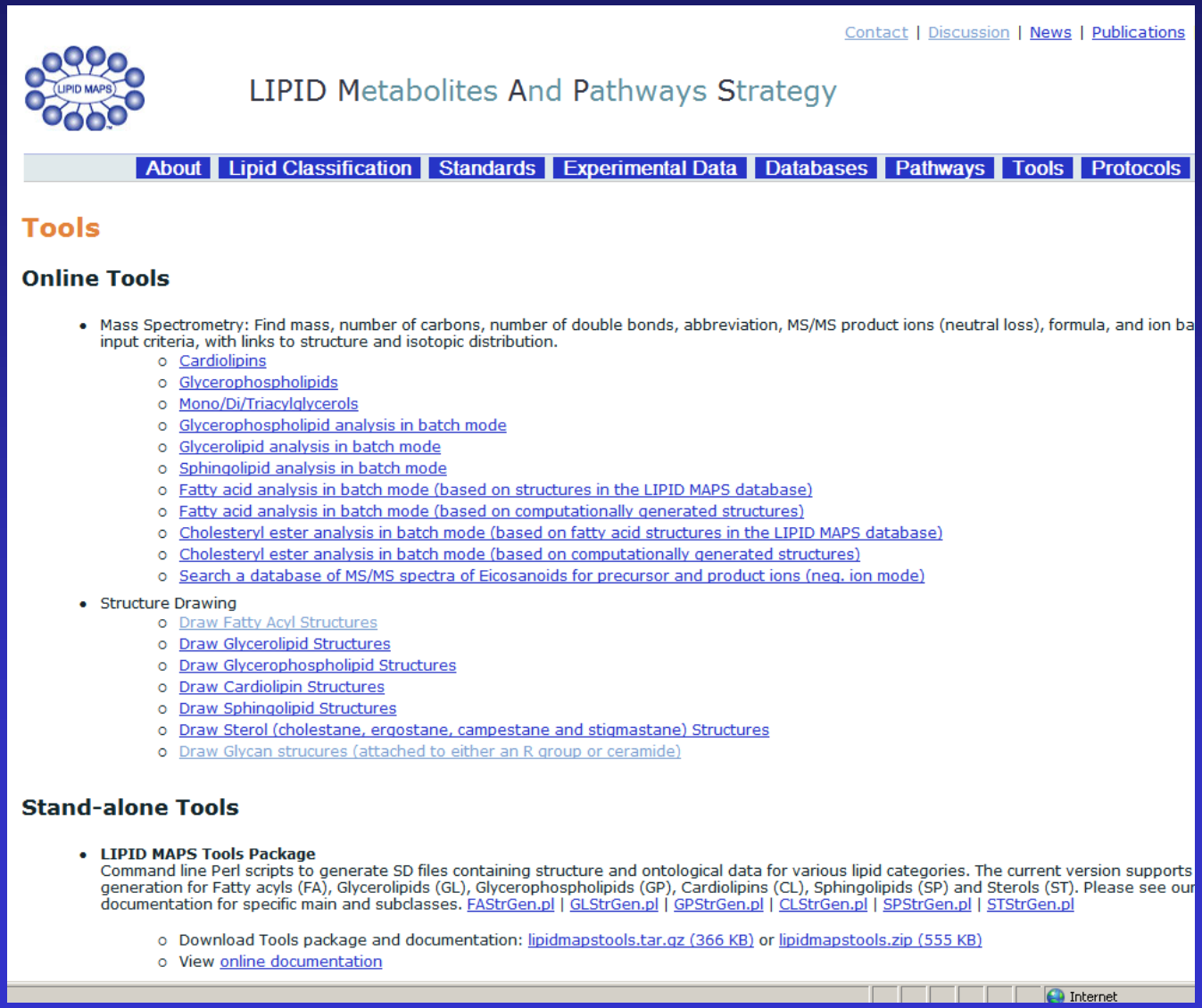
(WebStart Java application communicates with Oracle database)



LIPID MAPS

Bioinformatics tools for lipidomics

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



Contact | Discussion | News | Publications

LIPID Metabolites And Pathways Strategy

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 ba 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 strucures (attached to either an R group or ceramide)

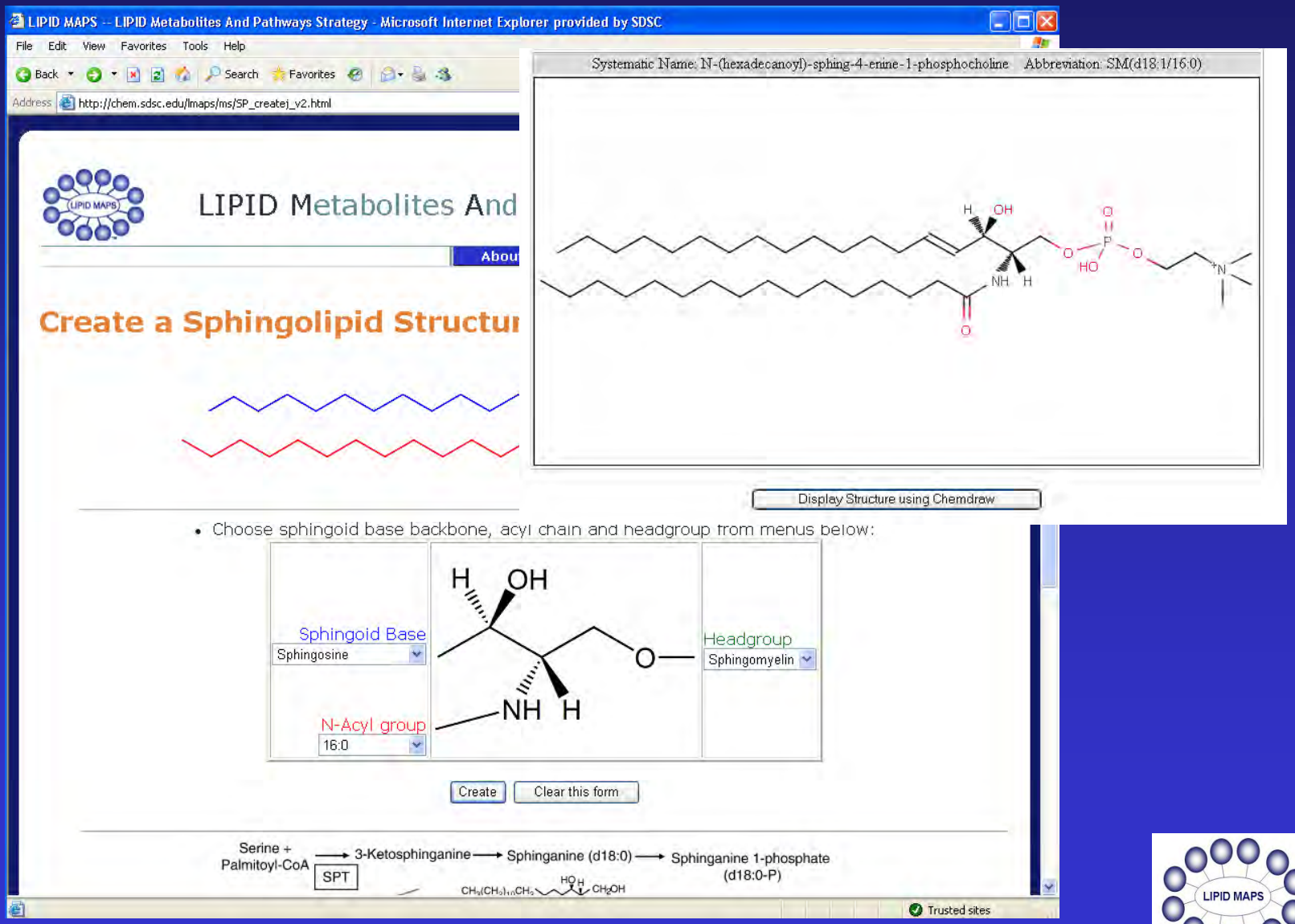
Stand-alone Tools

- **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

Internet

Bioinformatics tools : Automated structure drawing

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

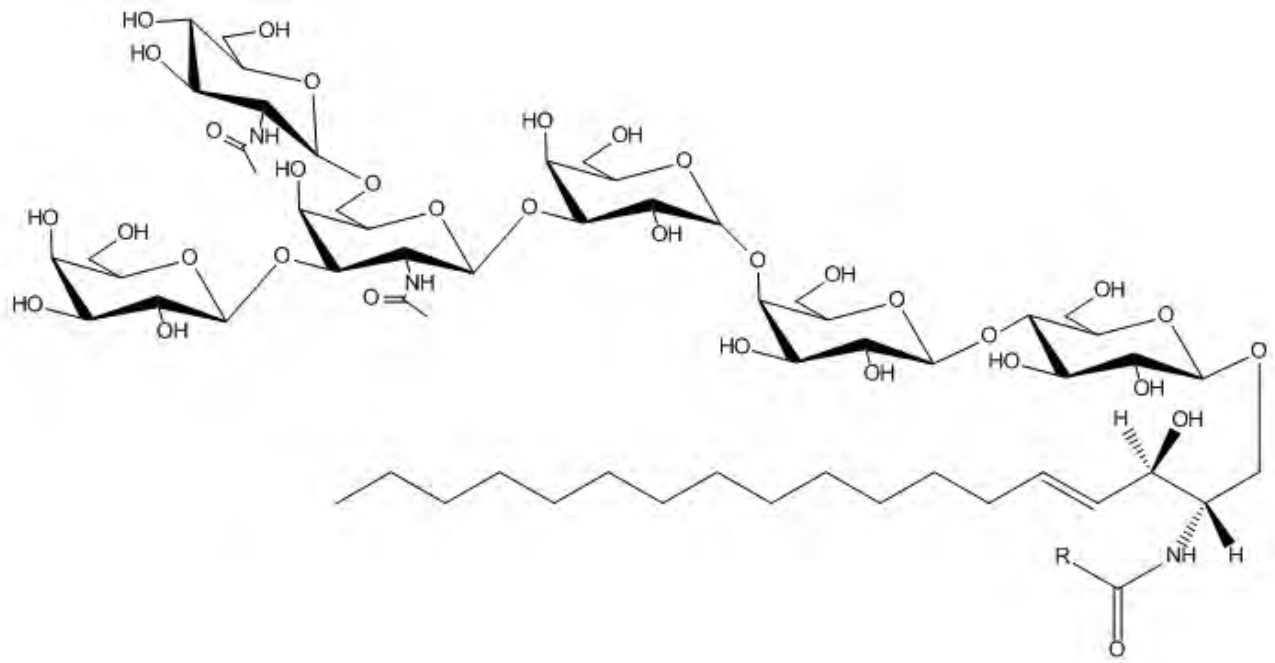


Glycan structure drawing: Glycosphingolipid example

Click on name hyperlink to display structure in full chemical format

Glycan structure drawing: Glycosphingolipid example

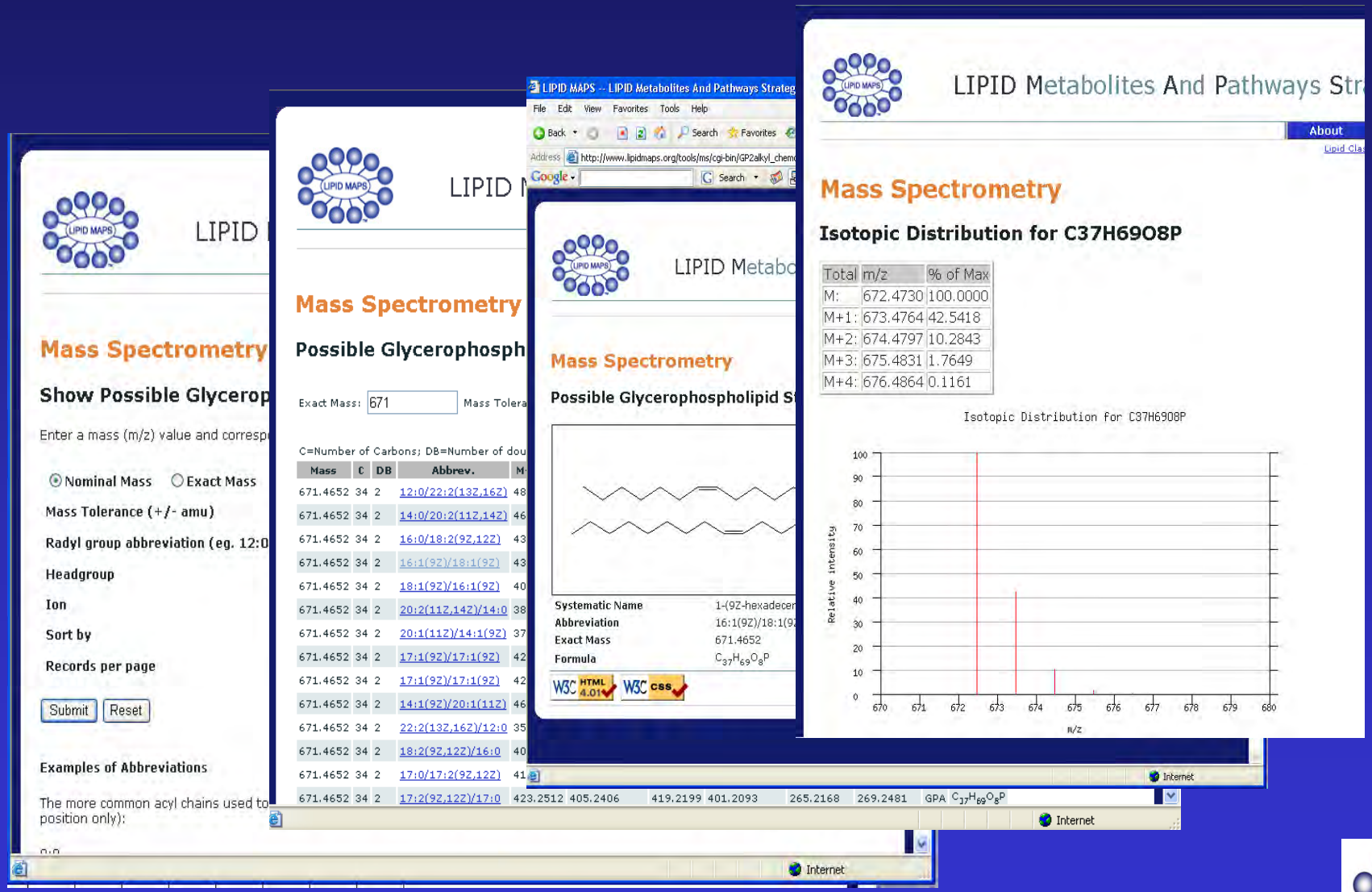
LIPID Metabolites And Pathways Strategy



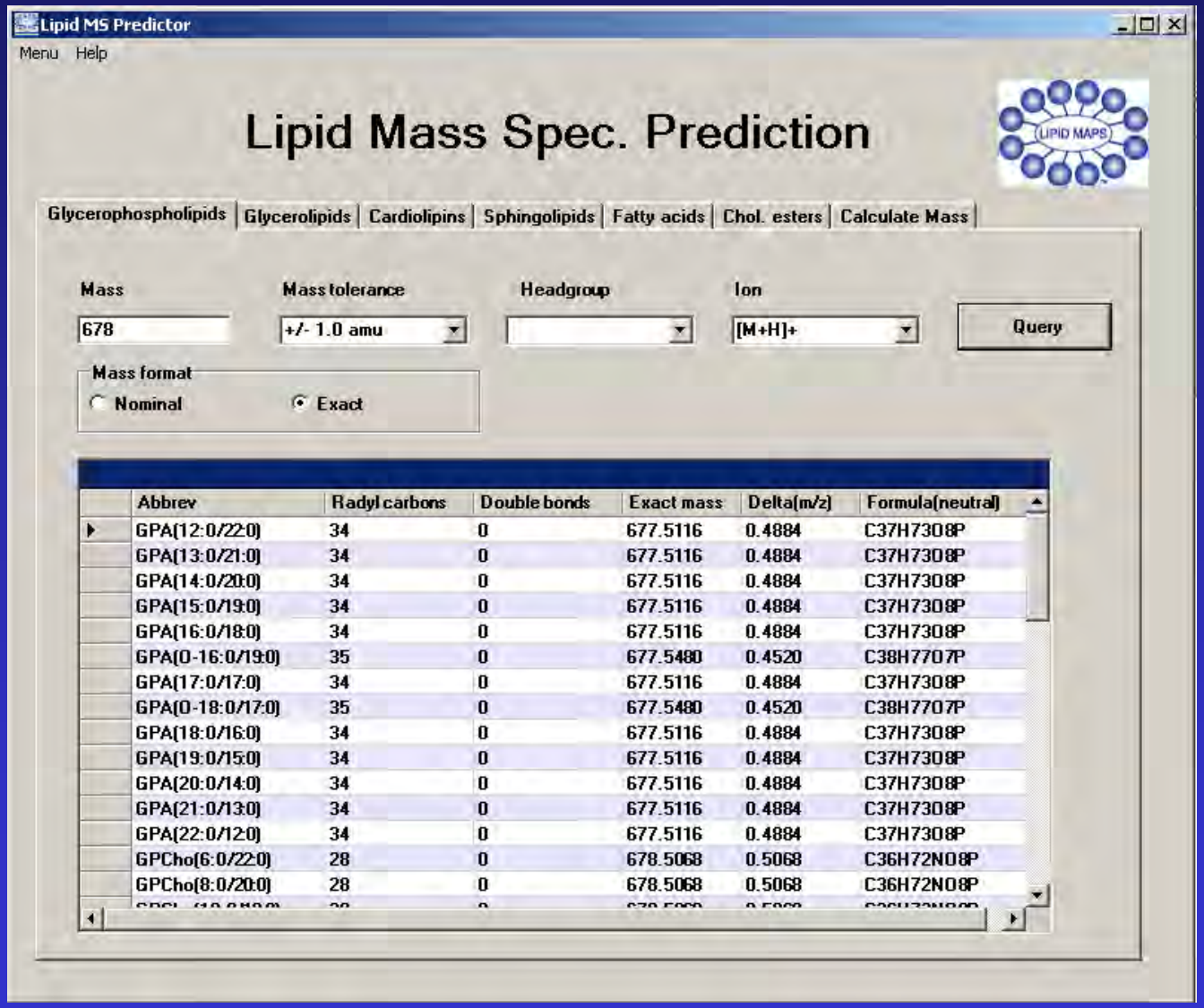
Display in Marvin format(Java must be enabled)

Bioinformatics tools :MS prediction

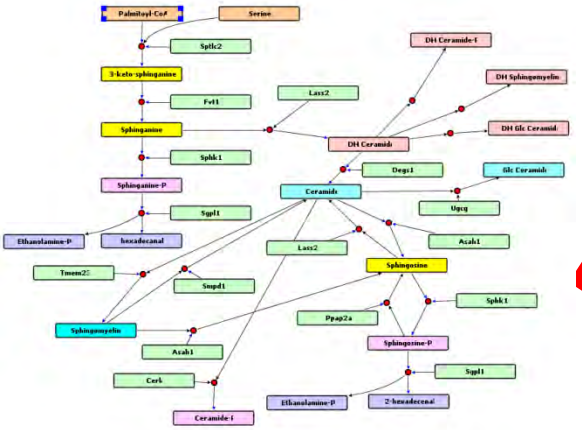
http://www.lipidmaps.org/data/tools/



Bioinformatics tools : Standalone MS prediction application



Lipid Pathways and Networks:Visualization VANTED

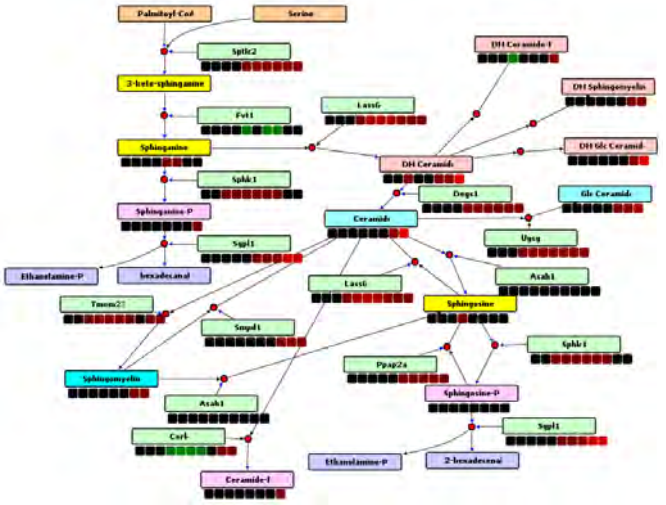


Pathway template Created with VANTED

Database
Lipid expts
Gene-array expts

Program

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

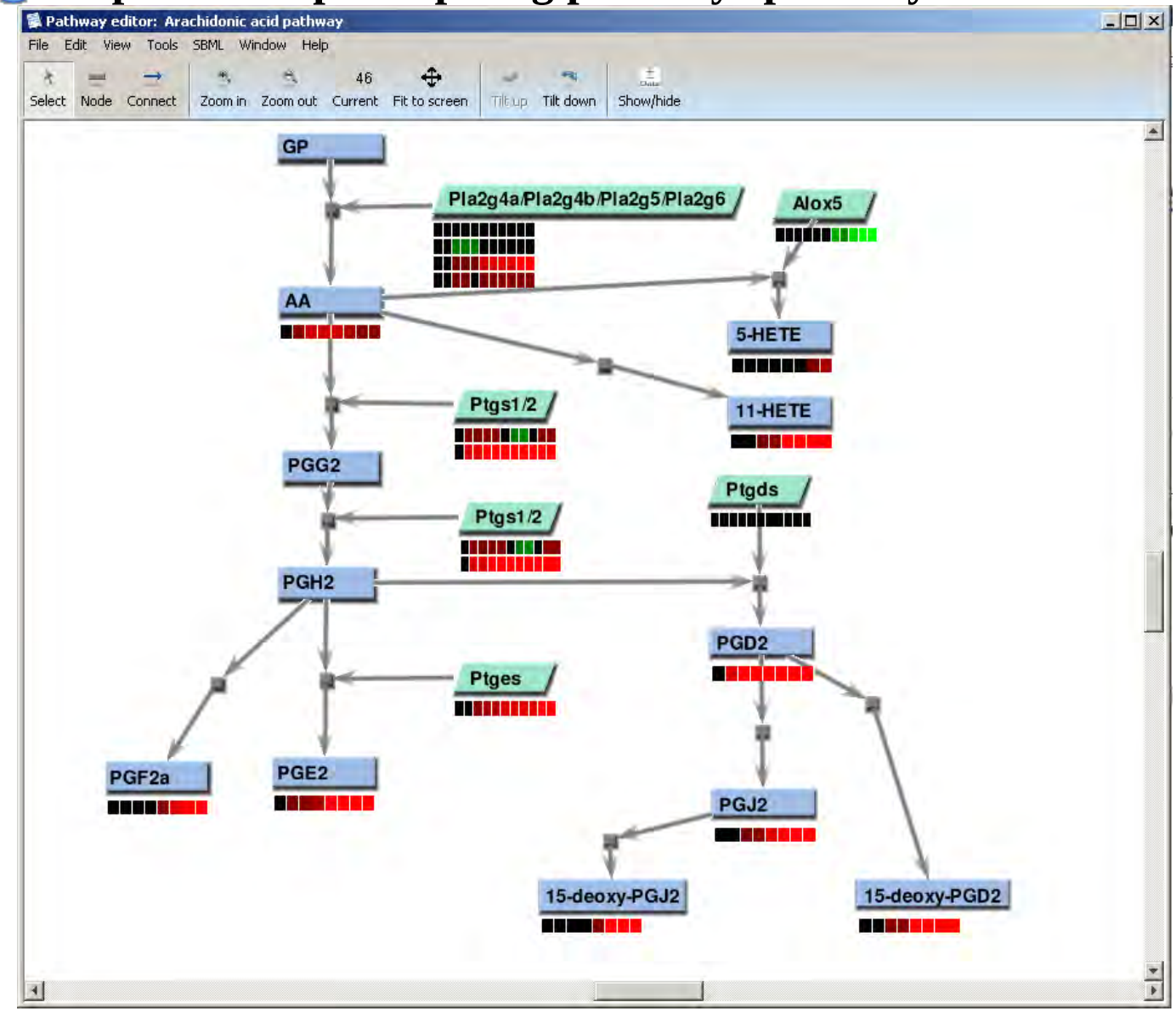


Pathway with heatmap

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 Kdo_2-lipid A

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www.lipidmaps.org

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

Fatty Acids: Omega-3 and Omega-6 polyunsaturated fatty acids

Lipids heatmap data: First line – Cells; Second line - Media

Macrophage Lipid Metabolism

Sterols

Glycerophospholipids

Lipids heatmap data: C32:0 acyl chains

Fatty Acids: Eicosanoids

Lipids heatmap data: Media

Fatty Acids: Omega-9 polyunsaturated and straight chain fatty acids

Lipids heatmap data: First line – Cells; Second line - Media

Sphingolipids

LIPID MAPS Bioinformatics Core*, SDSC, UCSD, 9500 Gilman Dr, La Jolla, CA 92093; Department of Bioengineering¶, UCSD, 9500, Gilman Dr, La Jolla, CA, 92093; Department of Pharmacology†, Vanderbilt University Medical Center, Nashville, TN 37232; Department of Cellular and Molecular Medicine‡, UCSD, 9500 Gilman Dr, La Jolla, CA 92093; School of Biology¶, Georgia Institute of Technology, Atlanta, GA 30332; University of Colorado Health Sciences Center†, Aurora, CO 80045; Department of Biochemistry‡, Duke University Medical Center, Durham, NC 27710; Department of Molecular Genetics¶, University of Texas Southwestern Medical Center, Dallas, Texas 75390; Department of Chemistry and Biochemistry, and Department of Pharmacology†, UCSD, La Jolla, CA 92093.

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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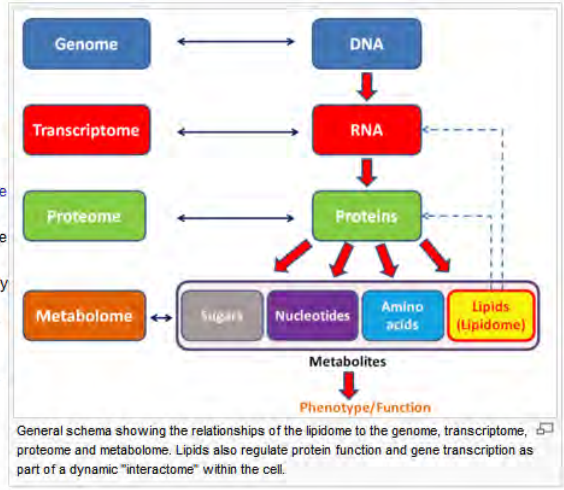
Lipidomics

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.



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.

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 (ELIfe)[6].

Contents [show]

LIPID MAPS

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