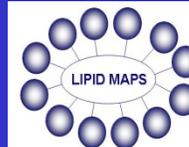


**LIPID MAPS
Bioinformatics**

EB2007 Apr 28,2007

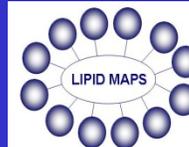
Eoin Fahy

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/>

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Lipid Classification Scheme

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

Publications

[Parallel SUMOylation-dependent pathways mediate gene- and signal-specific transrepression by LXRs and PPARgamma](#). *Molecular Cell*. 2007 Jan 26;25(2):178-80. PubMed PMID: 17218271

[Arachidonate derived dihomo-prostaglandin production observed in endotoxin stimulated macrophage-like cells](#). *Journal of Biological Chemistry*, Vol. 282, Issue 5, 2899-2910, February 2, 2007. PubMed PMID: 17135246

[Quantification of diacylglycerol species from biological extracts by electrospray ionization mass spectrometry](#). *Analytical Chemistry* 79: 263-272, 2007.

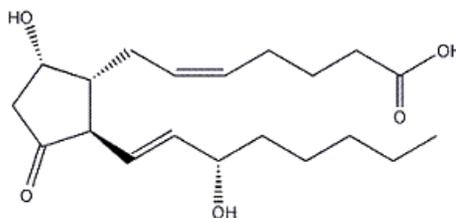
[Lipid profiling reveals arachidonate deficiency in RAW264.7 cells: Structural and functional implications](#).

LIPID MAPS Highlights

LIPID MAPS Structure Database (LMSD)

With over 10,000 records, 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 scheme.

LMSD: Sample record



LM ID	LMFA03010004
Common Name	PGD2
Systematic Name	9S,15S-dihydroxy-11-oxo-5Z,13E-prostadienoic acid
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
Synonyms	-
PubChem Substance ID	4265855

Lipid Search:

(Enter Common or Systematic Name, e.g. [Stearic acid](#))

[Advanced Search](#)

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

04/09/07 - [Microarray analysis of RAW 264.7 cells treated with Kdo2-Lipid A](#): Cells were grown in 10% fetal calf serum and harvested at each of ten time points after treatment with 100ng/ml Kdo2-Lipid A. At each time point an Agilent Whole Mouse Genome DNA microarray was hybridized, with Kdo2-Lipid A on the green channel and the control on the red channel. The experiment was performed three times, for three biological replicates.

03/13/07 - The LIPID MAPS Consortium is conducting an open Workshop on "Lipidomics" at Experimental Biology 2007 under the auspices of the American Society for Nutrition. A panel of eight experts will discuss methods that have been developed under an NIH (NIGMS) "Glue-



LIPID MAPS Classification System

Categories and Examples

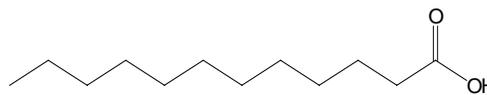
Category	Abbrev	Example
Fatty Acyls	FA	dodecanoic acid
Glycerolipids	GL	1-hexadecanoyl-2-(9Z-octadecenoyl)-sn-glycerol
Glycerophospholipids	GP	1-hexadecanoyl-2-(9Z-octadecenoyl)-sn-glycero-3-phosphocholine
Sphingolipids	SP	N-(tetradecanoyl)-sphing-4-enine
Sterol Lipids	ST	cholest-5-en-3 β -ol
Prenol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



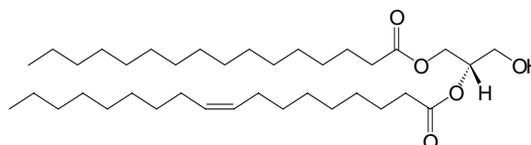
LIPID MAPS: Recommendations for drawing structures

Consistent structure representation across classes

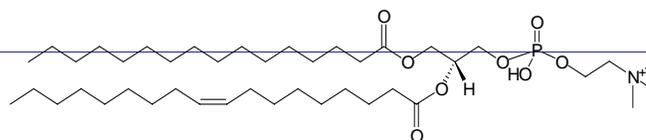
Fatty Acyls(FA)



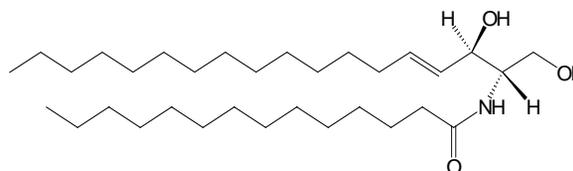
Glycerolipids (GL)



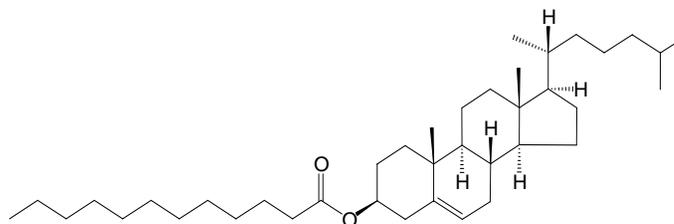
Glycerophospholipids (GP)



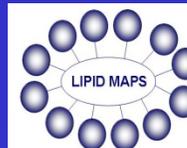
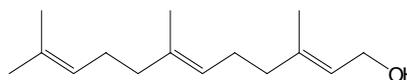
Sphingolipids (SP)



Sterol Lipids (ST)



Prenol Lipids (PR)



LIPID MAPS Online Classification System



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



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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](#)]

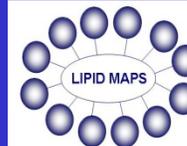
Docosanoids [[FA04](#)]

Fatty alcohols [[FA05](#)]

Category:Fatty Acyls [FA]

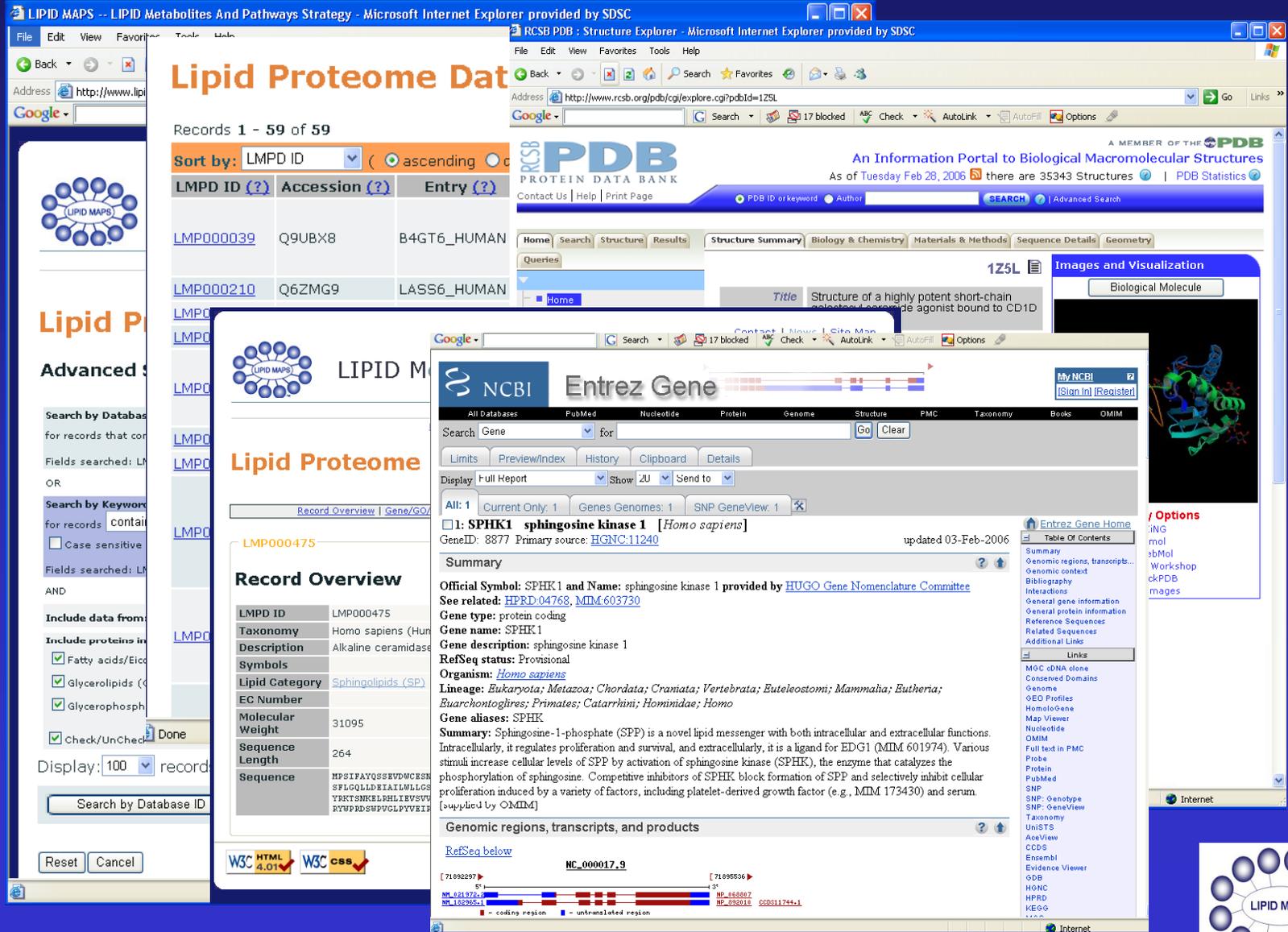
--> Main class: Eicosanoids [FA03] --> Sub class: Prostaglandins [FA0301]

LM_ID	Common Name	Systematic Name	Exact Mass	Formula
LMFA03010001	6-keto-PGF1 α	6-oxo-9S,11R,15S-trihydroxy-13E-prostenoic acid	370.24	C ₂₀ H ₃₄ O ₆
LMFA03010002	PGF2 α	9S,11R,15S-trihydroxy-5Z,13E-prostadienoic acid	354.24	C ₂₀ H ₃₄ O ₅
LMFA03010003	PGE2	9-oxo-11R,15S-dihydroxy-5Z,13E-prostadienoic acid	352.22	C ₂₀ H ₃₂ O ₅
LMFA03010004	PGD2	9S,15S-dihydroxy-11-oxo-5Z,13E-prostadienoic acid	352.22	C ₂₀ H ₃₂ O ₅
LMFA03010005	PGA1	9-oxo-15S-hydroxy-10Z,13E-prostadienoic acid	336.23	C ₂₀ H ₃₂ O ₄
LMFA03010006	PGF2 α -d4	9S,11R,15S-trihydroxy-5Z,13E-prostadienoic acid (3,3,4,4-d4)	358.27	C ₂₀ H ₃₀ D ₄ O ₅
LMFA03010007	PGD2-d4	9S,15S-dihydroxy-11-oxo-5Z,13E-prostadienoic acid (3,3,4,4-d4)	356.25	C ₂₀ H ₂₈ D ₄ O ₅
LMFA03010008	PGE2-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
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-PGF2 α	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-PGF1 α	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



Lipid Proteome Database (LMPD)

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



The screenshot displays the LMPD website interface, which is a member of the RSCB PDB Protein Data Bank. The main content area shows a list of records with columns for LMPD ID, Accession, and Entry. The records listed are:

LMPD ID	Accession	Entry
LMP00039	Q9UBX8	B4GT6_HUMAN
LMP000210	Q6ZMG9	LASS6_HUMAN

Below the list, there is a detailed record overview for LMP000475. The record information includes:

- LMPD ID:** LMP000475
- Taxonomy:** Homo sapiens (Human)
- Description:** Alkaline ceramidase
- Symbols:** SPHK1
- Lipid Category:** Sphingolipids (SP)
- EC Number:** 3.1.1.5
- Molecular Weight:** 31095
- Sequence Length:** 264
- Sequence:** NPSIFAYOSSEVDMCRSN SFLGQLLDEIALLNLLGS YPKTSMKELRHLLEVSIV RYVPRDSUPVGLPYVEIV

The record overview also includes a summary of the gene, SPHK1 (sphingosine kinase 1), and a genomic map showing the gene structure and associated features.



Lipidomics Data Display : MS Standards library



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

LIPID MAPS -- LIPID Metabolites And Pathways Strategy

File Edit View Favorites Tools Help

Structure Database (LMSD)

LMFA03010002

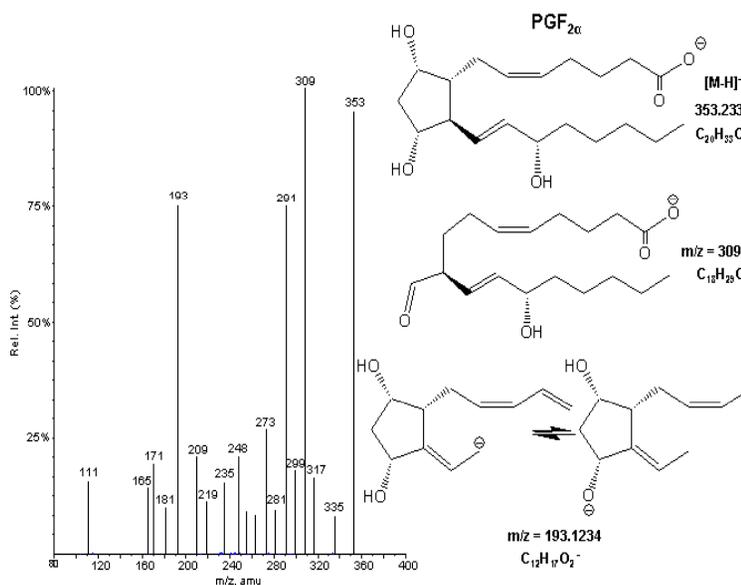
16010 Prostaglandin F2α

• 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

LM ID: LMFA03010002
 Common Name: PGF2α
 Systematic Name: 6S,11R,15S-trihydroxy-5Z,13E-prostadienoic acid



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Library of Eicosanoid Standards: LC Retention Times

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

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	363	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	362	4.24
LMFA03010014	20-hydroxy-PGE2	11S,15S-dihydroxy-9-oxo-5Z,13E-prostadienoic acid	367	2.94

Lipidomics Data Display : MS Experimental results



<http://www.lipidmaps.org/data/results/raw2647/kdo2lipidatimecourse/>

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Kdo₂-Lipid A Timecourse Results (10% ser

Show multiple plots Reset

: View data/graphs for technical replicates ;
 : Graph of biological replicates(ac

Details/Graph	Name	Kdo ctd 0min	Kdo ctd 30min	Kdo ctd 1hr
<input type="checkbox"/>	11S-HETE	-	0.558	0.805
<input type="checkbox"/>	15-deoxy-PGD2	0.468	0.406	0.41
<input type="checkbox"/>	15-deoxy-PGJ2	-	0.233	0.367
<input type="checkbox"/>	15-deoxy-PGJ2	-	0.195	0.147
<input type="checkbox"/>	5S-HET	-	0.116	0.117
<input type="checkbox"/>	AA	-	-	-
<input type="checkbox"/>	PGD2	-	-	-
<input type="checkbox"/>	PGE2	-	-	-
<input type="checkbox"/>	PGF2a	-	-	-
<input type="checkbox"/>	PGJ2	-	-	-

Kdo₂-Lipid A Timecourse

Show multiple plots Reset

: Experiment details ;
 : Graph of technical replicates(within an expt.) ;
 : Graph of biological replicates(across expts)

Barcode

Details/Graph technical/biological replicates	Name	Kdo ctd 0min	Kdo ctd 30min	Kdo ctd 1hr	Kdo ctd 2hrs	Kdo ctd 4hrs	Kdo ctd 8hrs	Kdo ctd 12hr
<input type="checkbox"/> (BCG060127)	AA	-	213	450	436	261	127	
<input type="checkbox"/> (BCG060201)	AA	94.6	91.3	88.1	92.8	61.5	35.5	
<input type="checkbox"/> (BCG060210)	AA	62.6	133	255	256	223	106	
<input type="checkbox"/> (BCG060210)	AA	85	62.6	68.2	59.3	48.8	27.9	
<input type="checkbox"/> (BCG060210)	AA	-	94.5	364	264	159	64.8	
<input type="checkbox"/> (BCG060210)	AA	-	85	66.4	62.5	54.2	36.8	17.7

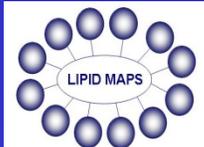
Show multiple plots Reset

*: The **units** in the table and g standard. The amount of inter were converted to pmoles by e measured by the quantity of D

Error bars denote standard error of mean



AA: ■ (Ctrl) × (KDO)



Lipidomics Data Display : Gene array data

 <http://www.lipidmaps.org/data/results/raw2647/microarray/>

Search by:
Name,Symbol,Gene_ID

Search by:
Kdo/Ctrl ratio at
any/all timepoints

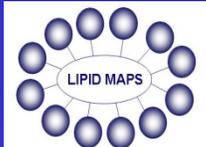
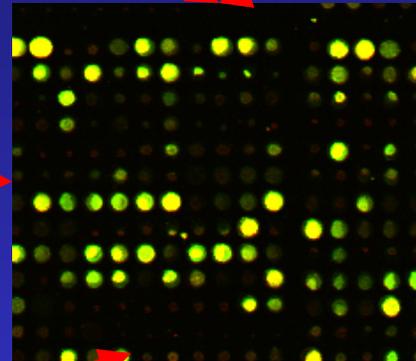
Search by:
KEGG Pathway

Search by:
BIOCARTA Pathway

Search by:
Gene Ontology term

Search by:
Lipid category

Search by:
Correlation coefficient



Lipidomics Data Display : Gene array-search by pathway



<http://www.lipidmaps.org/data/results/raw2647/microarray/>



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Microarray analysis of RAW 264.7 cells treat

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Mouse-over the above links for more information

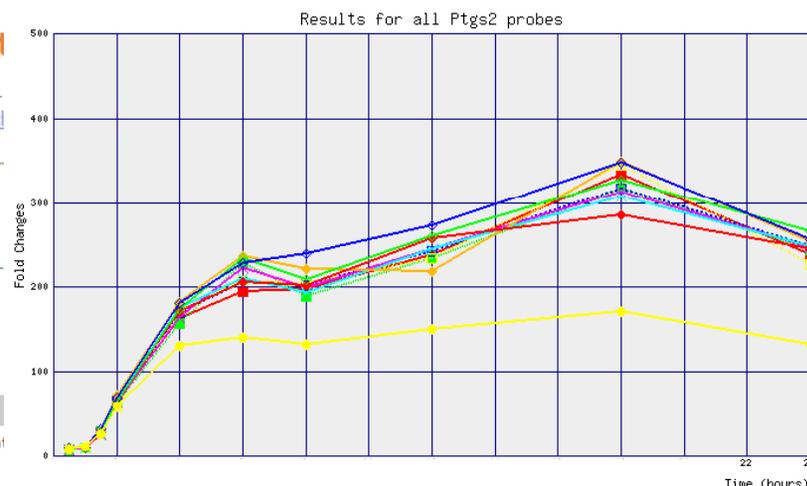
View results by KEGG pathway

Select a pathway to view fold change data for genes found in that pathway

View Array data	View KEGG Map	Description
mmu00351	mmu00351	1,1,1-Trichloro-2,2-bis(4-chlorophenyl)ethane (DDT) degradat
mmu00624	mmu00624	1- an
mmu00623	mmu00623	2,4-D
mmu02010	mmu02010	ABC t
mmu04520	mmu04520	Adher
mmu04920	mmu04920	Adipo
mmu00252	mmu00252	Alanir
mmu00950	mmu00950	Alkalc
mmu00960	mmu00960	Alkalc
mmu05010	mmu05010	Alzhe
mmu00970	mmu00970	Aminc
mmu00440	mmu00440	Aminc
mmu00530	mmu00530	Aminc
mmu05030	mmu05030	Amyo
mmu00150	mmu00150	Andro

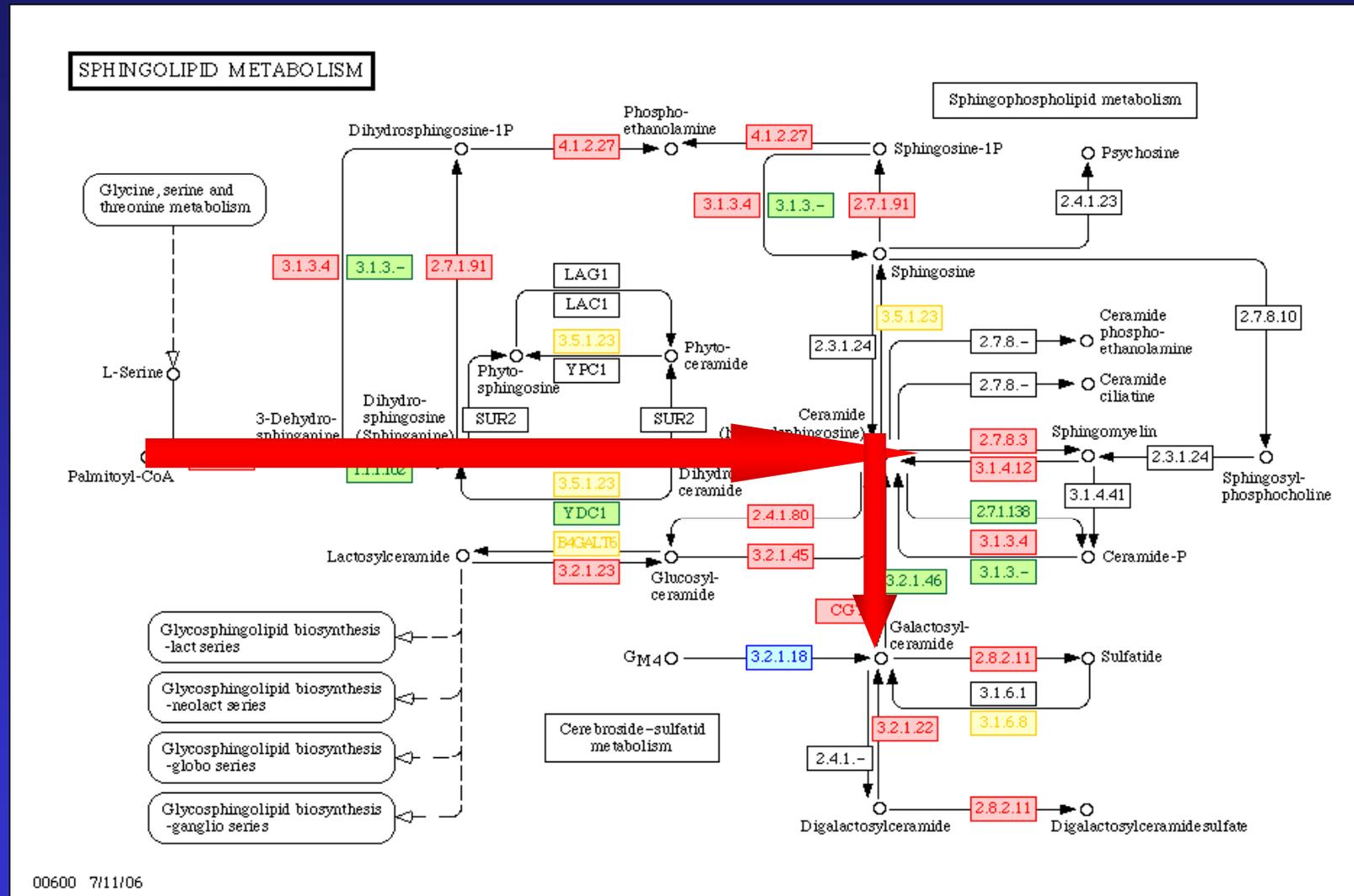
Results Summary

		repression ← (Fold changes: Treatment with Kdo ₂ -lipid A versus Control) → induction									
GENESYMBOL	GENENAME	KC30	KC60	KC90	KC2H	KC4H	KC6H	KC8H	KC12H	KC18H	KC24H
Ptgs2	prostaglandin D2 synthase (brain)	.95	1.09	1.05	1.06	1.12	1.21	1.07	1.00	.87	.88
Ptgs2	prostaglandin D2 synthase 2, hematopoietic	.95	.73	.63	.53	.47	.61	.51	.61	1.10	1.02
Ptgs2	prostaglandin E synthase	1.37	2.52	3.00	3.19	5.12	6.22	5.04	6.16	10.19	11.24
Ptgs2	prostaglandin E synthase 2	1.11	1.08	1.05	.96	.77	.72	.78	.82	.98	.99
Ptgs2	prostaglandin I2 (prostacyclin) synthase	1.13	1.16	1.02	1.06	1.01	1.10	1.23	1.06	1.22	1.23
Ptgs1	prostaglandin-endoperoxide synthase 1	2.14	1.99	2.05	2.07	.94	.66	.47	.75	2.49	2.78
Ptgs2	prostaglandin-endoperoxide synthase 2	8.00	9.17	25.91	65.44	163.62	194.80	197.20	238.19	333.71	238.73
Ptgs2	prostaglandin-endoperoxide synthase 2	7.49	9.38	28.63	63.35	157.06	228.02	189.29	233.62	317.64	244.00
Ptgs2	prostaglandin-endoperoxide synthase 2	8.00	10.32	26.58	65.40	169.73	205.76	202.15	242.02	317.13	248.11
Ptgs2	prostaglandin-endoperoxide synthase 2	8.57	10.55	28.89	71.75	182.89	236.19	221.56	218.21	349.52	253.89
Ptgs2	prostaglandin-endoperoxide synthase 2	8.53	10.31	27.16	65.40	174.31	233.34	209.23	260.71	327.74	265.53
Ptgs2	prostaglandin-endoperoxide synthase 2	9.92	9.98	31.37	70.26	181.38	228.12	239.17	273.42	347.74	256.57
Ptgs2	prostaglandin-endoperoxide synthase 2	7.91	9.11	26.35	65.92	171.96	206.32	202.61	257.37	286.04	244.60
Ptgs2	prostaglandin-endoperoxide synthase 2	7.96	10.23	25.99	66.45	175.43	210.55	194.11	245.12	308.32	247.40
Ptgs2	prostaglandin-endoperoxide synthase 2	8.56	9.33	27.07	57.82	176.25	206.86	204.67	234.58	345.94	227.48
Ptgs2	prostaglandin-endoperoxide synthase 2	7.57	10.38	25.14	64.58	164.18	222.94	199.13	244.51	314.00	246.63
Ptgs2	prostaglandin-endoperoxide synthase 2	8.48	10.92	26.77	60.34	131.34	140.33	131.83	150.13	171.86	132.82
Tbxas1	thromboxane A synthase 1, platelet	1.15	1.18	1.16	.92	1.23	1.05	1.27	1.02	.73	.69
Tbxas1	thromboxane A synthase 1, platelet	1.21	1.20	1.09	1.12	1.38	1.13	1.36	1.17	.86	.78
Tbxas1	thromboxane A synthase 1, platelet	.92	1.03	.97	.93	1.06	1.03	1.06	.95	1.15	.95

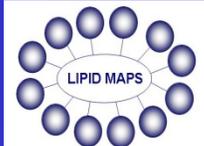


Lipidomics Data Display : Gene array data

Spingolipid pathway(KEGG)

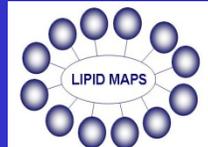
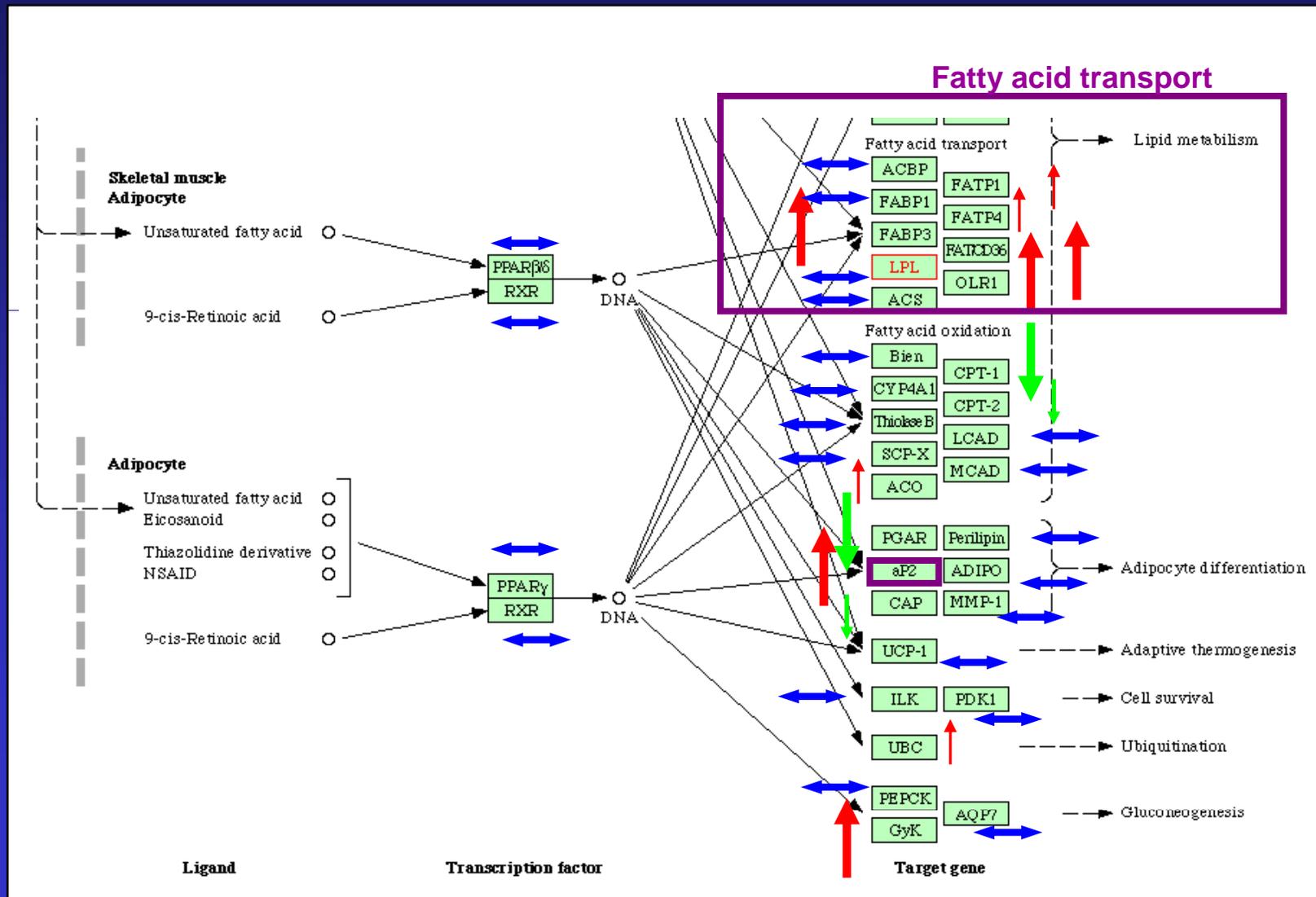


Red: up-regulated; **Green:** down-regulated;
Blue: up/down; **Yellow:** p > 0.01



Lipidomics Data Display : Gene array data

Ppar- γ signaling pathway(KEGG)



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

The screenshot displays two overlapping windows from a LIMS application. The 'Treatment' window (left) contains the following sections:

- Experiment identity:** Date* (03-03-2006), Experiment ID, Experiment letter*, Cell vessel barcode.
- Protocol ID:** Text input field.
- Technician:** G, Alex Andrejev.
- Culture information:** Plating density* (x10e6), Temp (37°C), Solution (DMEM), CO2 (5%).
- Treatments:** Import file button, table with columns ID and Pre-incu (row 01, 00:00.00).
- Samples:** Add, Duplicate buttons.
- Buttons:** Save to database, Print.

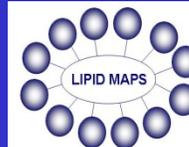
The 'Cell line' window (middle) contains:

- Lab:** G.
- User:** Alex Andreyev [29].
- Passage/harvest date:** 03-03-2006.
- Passage protocol:*** Text input field.
- Comments:** Text area with Search comments button.
- Buttons:** New thaw, New passage, New freeze, New passage, Save new passage.

The 'Solution' window (right) contains:

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

At the bottom left, a tooltip reads: "OK - Don't forget to inspect the tooltip".



Bioinformatics tools for lipidomics



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

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

File Edit View Favorites Tools Help

Back Forward Stop Home Search Favorites

Address <http://www.lipidmaps.org/tools/index.html> Go Links

 LIPID Metabolites And Pathways Strategy

[About](#) [Data](#) [Tools](#) [Protocols](#) [Home](#)

[Mass Spectrometry](#) | [Structure Drawing](#)

Tools

Online Tools

- [Mass Spectrometry](#): Find mass, number of carbons, number of double bonds, abbreviation, MS/MS product ions (neutral loss), formula, and ion based on input criteria, with links to structure and isotopic distribution.
 - [Cardiolipins](#)
 - [Glycerophospholipids](#)
 - [Mono/Di/Triacylglycerols](#)
- [Structure Drawing](#)
 - [Draw Sphingolipid Structures](#)
 - [Draw Glycerolipid Structures](#)
 - [Draw Cardiolipin Structures](#)
 - [Draw Glycerophospholipid Structures](#)
 - [Draw Sterol \(cholestane\) Structures](#)
 - [Draw Fatty Acyl Structures](#)

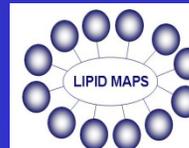
Standalone Tools

- 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 structure generation for Glycerophospholipids (GP) and Glycerolipids (GL). Please see our documentation for specific main and subclasses. [GLStrGen.pl](#) | [GPStrGen.pl](#)
 - [Download](#) Tools package and documentation
 - View [online documentation](#)

  Please address any questions or comments about the LIPID MAPS website to our [Webmaster](#). [LIPID MAPS Personnel](#) (Restricted Access) [Log Out](#)

Last modified Friday, 19-Jan-2007 10:44:34 PST

Internet



Bioinformatics tools : Automated structure drawing



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

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

File Edit View Favorites Tools Help

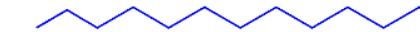
Back Forward Stop Home Search Favorites

Address http://chem.sdsc.edu/maps/ms/SP_create_v2.html

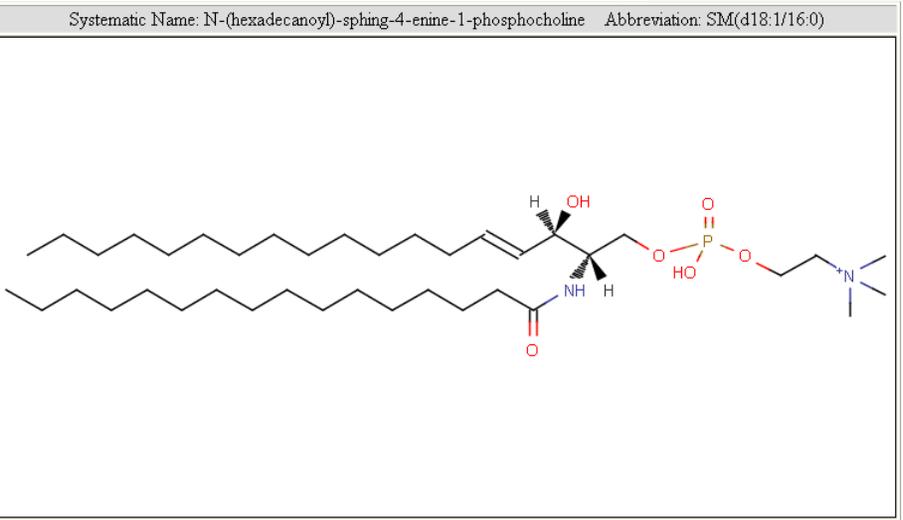
 LIPID Metabolites And Pathways Strategy

About

Create a Sphingolipid Structure




Systematic Name: N-(hexadecanoyl)-sphing-4-ene-1-phosphocholine Abbreviation: SM(d18:1/16:0)



Display Structure using Chemdraw

- Choose sphingoid base backbone, acyl chain and headgroup from menus below:

Sphingoid Base: Sphingosine

N-Acyl group: 16:0

Headgroup: Sphingomyelin

Create Clear this form

Serine + Palmitoyl-CoA $\xrightarrow{\text{SPT}}$ 3-Ketosphinganine \rightarrow Sphinganine (d18:0) \rightarrow Sphinganine 1-phosphate (d18:0-P)



Trusted sites

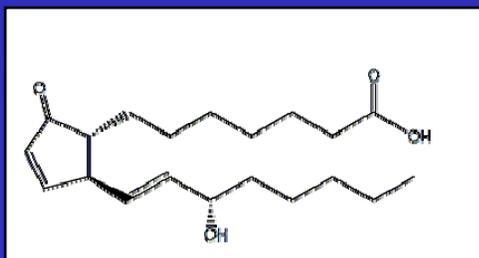


Using abbreviations to automate structure, nomenclature and ontology generation

LIPID MAPS Abbreviation

20:2(10Z,13E)(9Ke,15OH[S]){8a,12b}

Structures



Systematic names

9-oxo-15S-hydroxy-
10Z,13E-prostadienoic acid

Classification

Fatty Acyls [FA]
Eicosanoids [FA03]
Prostaglandins [FA0301]

Ontologies

- Mol weight
- Formula
- # hydroxyls
- # double bonds
- #rings

PGA₂



Bioinformatics tools :MS prediction



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

LIPID MAPS

Mass Spectrometry

Show Possible Glycerophospholipid

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 date (in order of increasing position only):

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	42

Exact Mass: Mass Tolerance:

Mass Spectrometry

Possible Glycerophospholipid Structure

Systematic Name: 1-(9Z)-hexadecenyl-3'-phosphatidylglycerol
Abbreviation: 16:1(9Z)/18:1(9Z)
Exact Mass: 671.4652
Formula: C₃₇H₆₉O₈P

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



Lipidomic profiling tools using stable isotopes

Comparative analysis using deuterated precursors

SCIEX/ABI
.wiff file

(Proprietary format)

MzStar
conversion

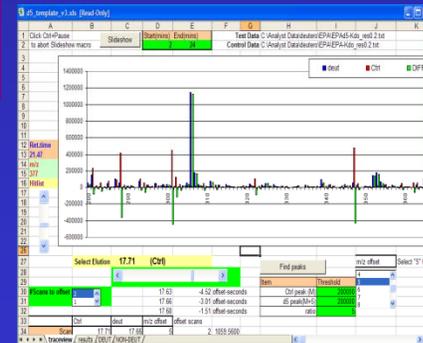
mzXML file

(Open-source format)

Peak extraction
Peak integration
File formatting

Processed file

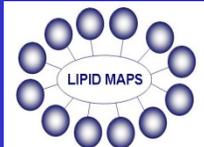
Harkewicz, R.
et al.
J. Biol. Chem.
(2007) 282(5),
2899-2910



Web application

Viewers

Excel template



Lipid Pathways and Networks: Visualization tools

VANTED: Displaying lipidomic timecourse data



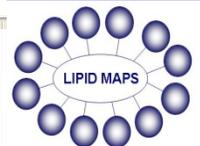
<http://vanted.ipk-gatersleben.de/>

The screenshot displays the VANTED V1.1 (beta) interface. The main window shows a network diagram with nodes for Phospholipids, AA, 11S-HETE, 5S-HETE, TNF, and DNA. A large graph shows the concentration of AA (ng/ugDNA) over time (min) for two conditions: 'Hype prote' (blue line) and 'Hylip' (red line). The 'Hype prote' condition shows a sharp peak at approximately 120 minutes, while the 'Hylip' condition shows a much lower, broader peak. Red arrows indicate the flow of information from the network diagram to the main graph and from the graph to the LIPID MAPS database.

The LIPID MAPS database entry for LMFA03010004 (PGD2) is shown, including its chemical structure and associated metadata:

LM ID	LMFA03010004
Common Name	PGD2
Systematic Name	9S,15S-dihydroxy-11-oxo-5Z,13E-prostadienoic acid
Exact Mass	352.22
Formula	C ₂₀ H ₃₂ O ₅
Category	Fatty Acids [FA] View lipid standards
Main Class	Eicosanoids [FA03]
Sub Class	Prostaglandins [FA0301]
LIPIDBANK ID	XPR1301
inidBase ID	1RFA03010004

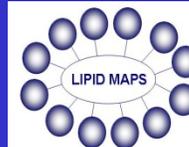
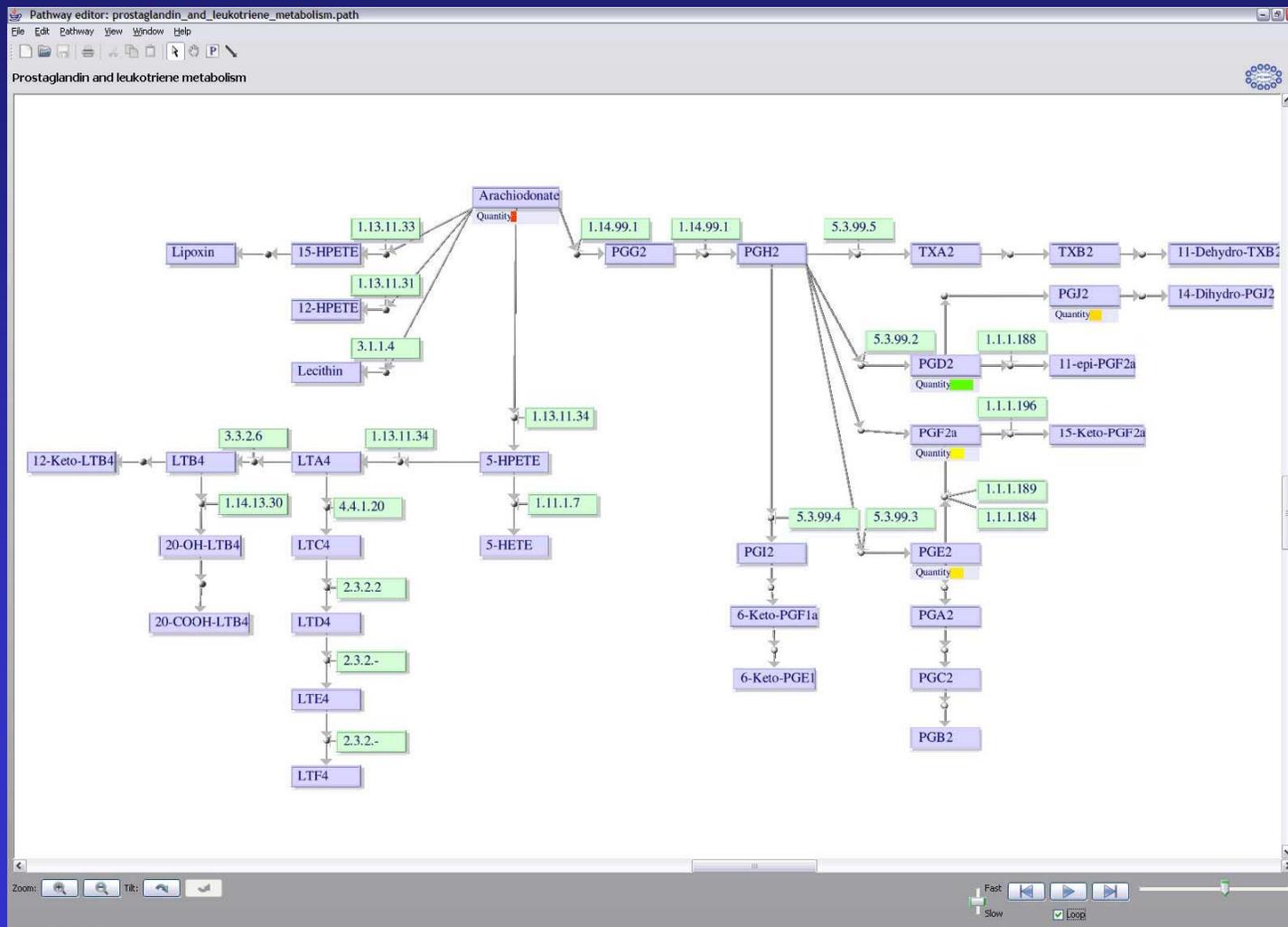
Additional information from the LIPID MAPS entry includes the taxonomic classification (Mus musculus) and the description (Glutathione-requiring prostaglandin D synthase). The interface also shows a search bar and a 'graph/nodes' section with a checkbox for 'Ask for user-given mapping if no automatic mapping is possible'.



Lipid Pathways and Networks: Visualization tools

Pathway Editor: Biopathways Workbench

 <http://www.BiopathwaysWorkbench.org>



Acknowledgements

- ❖ **Shankar Subramaniam (PI)**
- ❖ Robert Byrnes
- ❖ Dawn Cotter
- ❖ Andreia Maer
- ❖ David Nadeau
- ❖ Manish Sud
- ❖ Yihua Zhao
- ❖ **NIH/NIGMS Glue Grant GM69338**

