LIPID MAPS Bioinformatics

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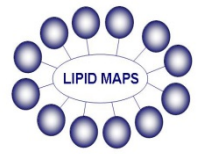
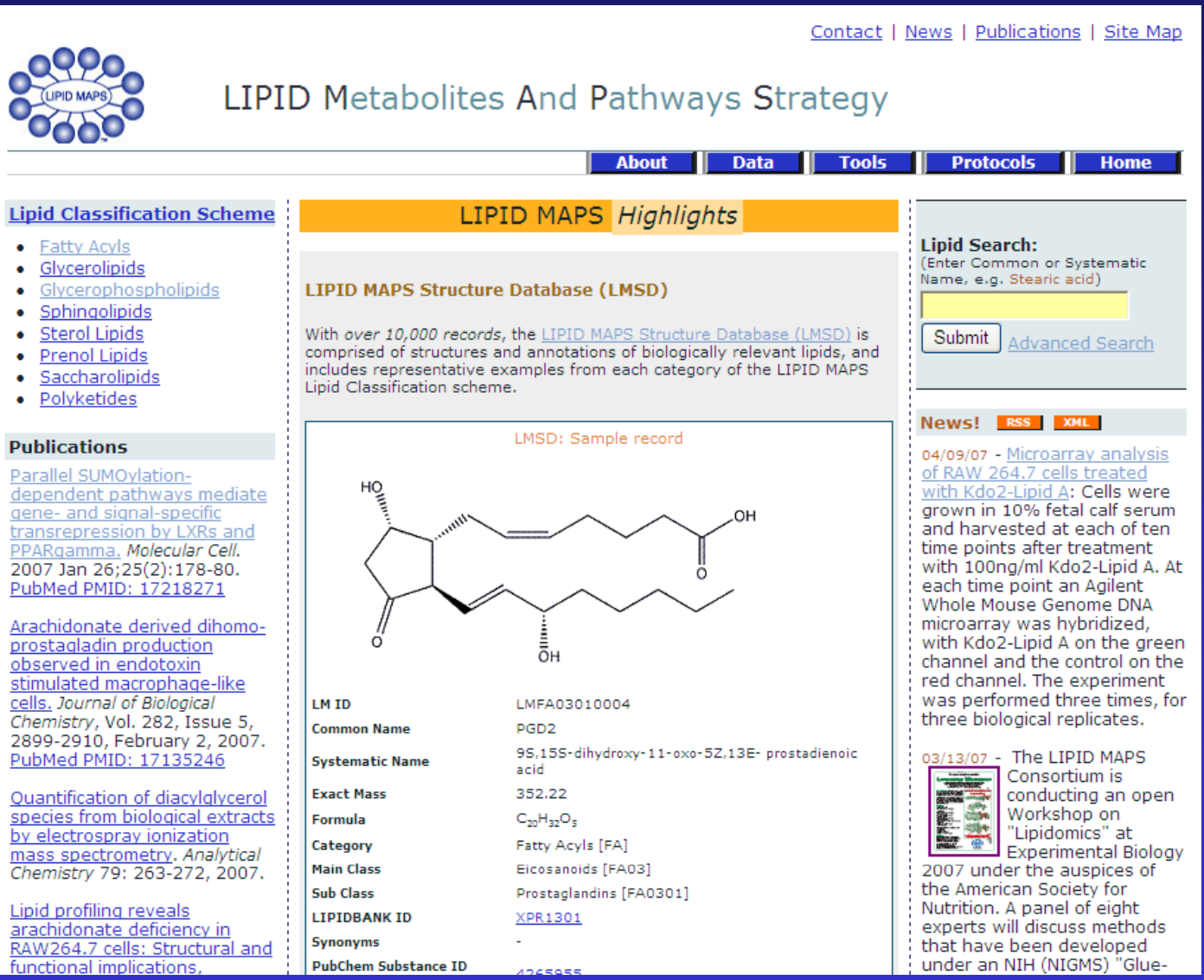
LIPID MAPS Bioinformatics Overview

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/



LIPID MAPS Classification System

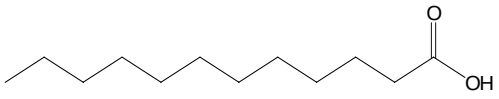
Categories and Examples

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

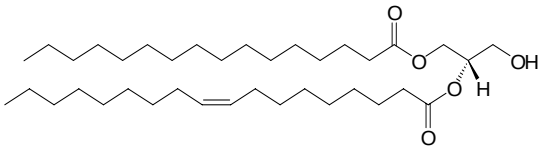
LIPID MAPS: Recommendations for drawing structures

Consistent structure representation across classes

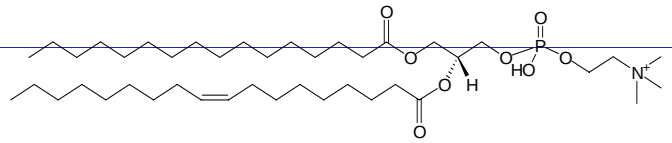
Fatty Acyls(FA)



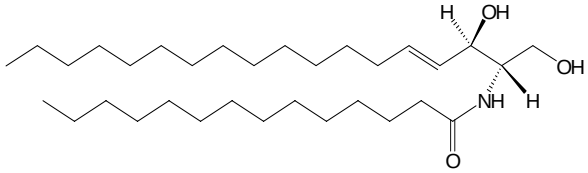
Glycerolipids (GL)



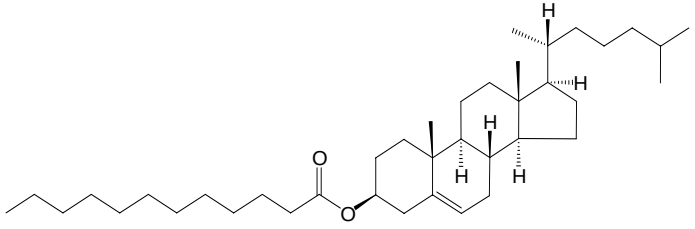
Glycerophospholipids (GP)



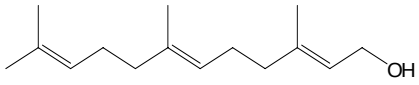
Sphingolipids (SP)



Sterol Lipids (ST)

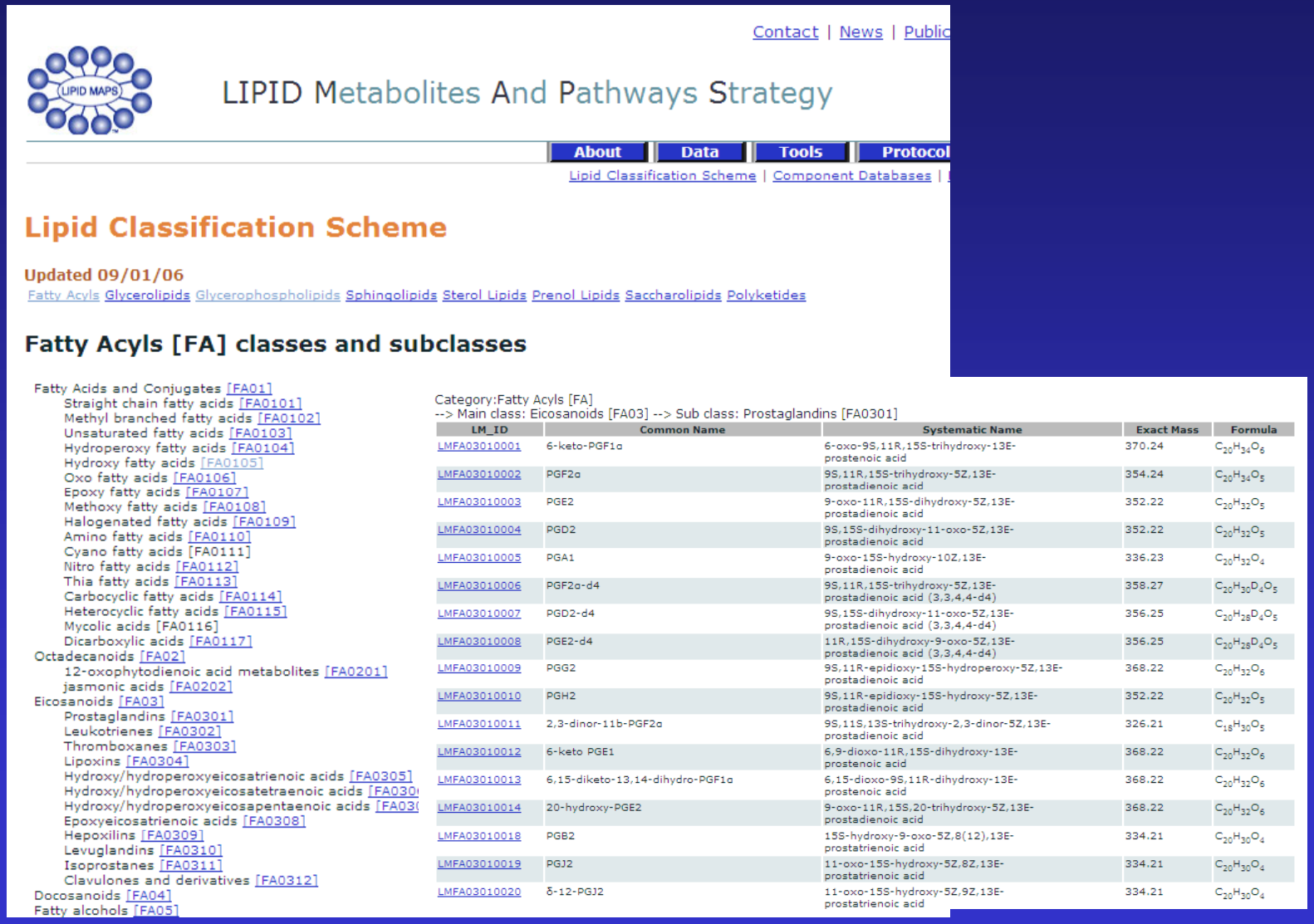


Prenol Lipids (PR)



LIPID MAPS Online Classification System

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



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LIPID Metabolites And Pathways Strategy

About | Data | Tools | Protocol

Lipid Classification Scheme | Component Databases |

Lipid Classification Scheme

Updated 09/01/06

Fatty Acyls Glycerolipids Glycerophospholipids Sphingolipids Sterol Lipids Prenol Lipids Saccharolipids Polyketides

Fatty Acyls [FA] classes and subclasses

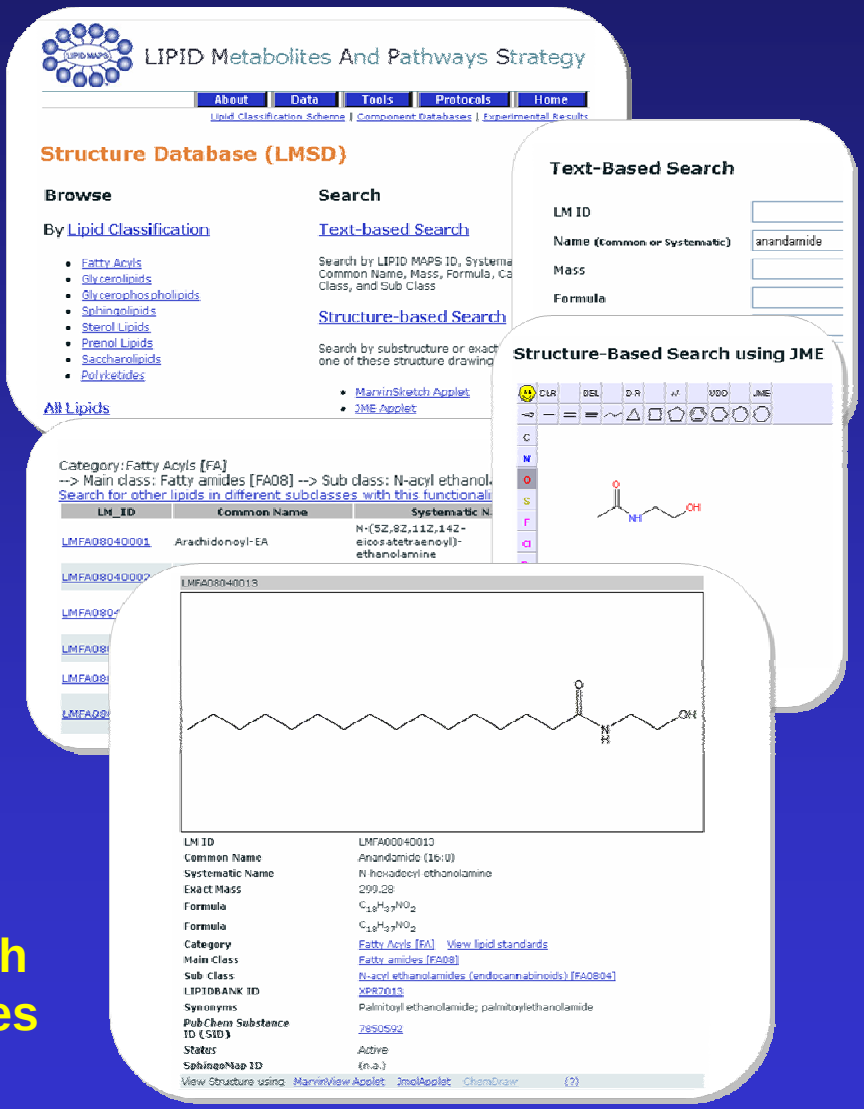
- Fatty Acids and Conjugates [FA01]
  - Straight chain fatty acids [FA0101]
  - Methyl branched fatty acids [FA0102]
  - Unsaturated fatty acids [FA0103]
  - Hydroperoxy fatty acids [FA0104]
  - Hydroxy fatty acids [FA0105]
  - Oxo fatty acids [FA0106]
  - Epoxy fatty acids [FA0107]
  - Methoxy fatty 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: Prostaglandins [FA0301]

LM_ID	Common Name	Systematic Name	Exact Mass	Formula
LMFA03010001	6-keto-PGF1α	6-oxo-9S,11R,15S-trihydroxy-13E-prostenoic acid	370.24	$C_{20}H_{34}O_6$
LMFA03010002	PGF2α	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	PGF2α-d4	9S,11R,15S-trihydroxy-5Z,13E-prostadienoic acid (3,3,4,4-d4)	358.27	$C_{20}H_{30}D_4O_5$
LMFA03010007	PGD2-d4	9S,15S-dihydroxy-11-oxo-5Z,13E-prostadienoic acid (3,3,4,4-d4)	356.25	$C_{20}H_{28}D_4O_5$
LMFA03010008	PGE2-d4	11R,15S-dihydroxy-9-oxo-5Z,13E-prostadienoic acid (3,3,4,4-d4)	356.25	$C_{20}H_{28}D_4O_5$
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	$C_{20}H_{30}O_4$

LIPID MAPS Structure Database (LMSD)

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



Online features:

Browse

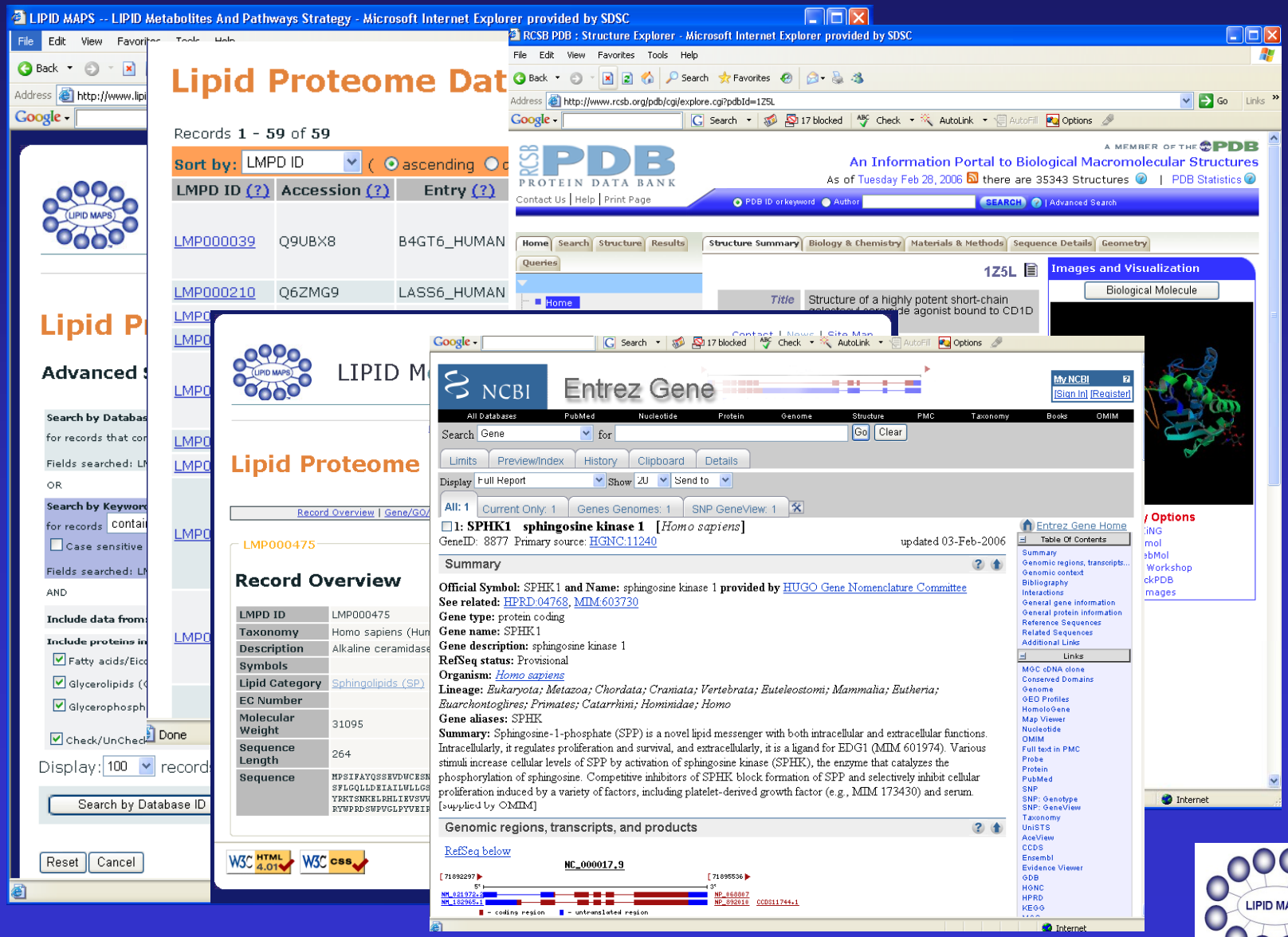
Text search

Substructure search

Download structures

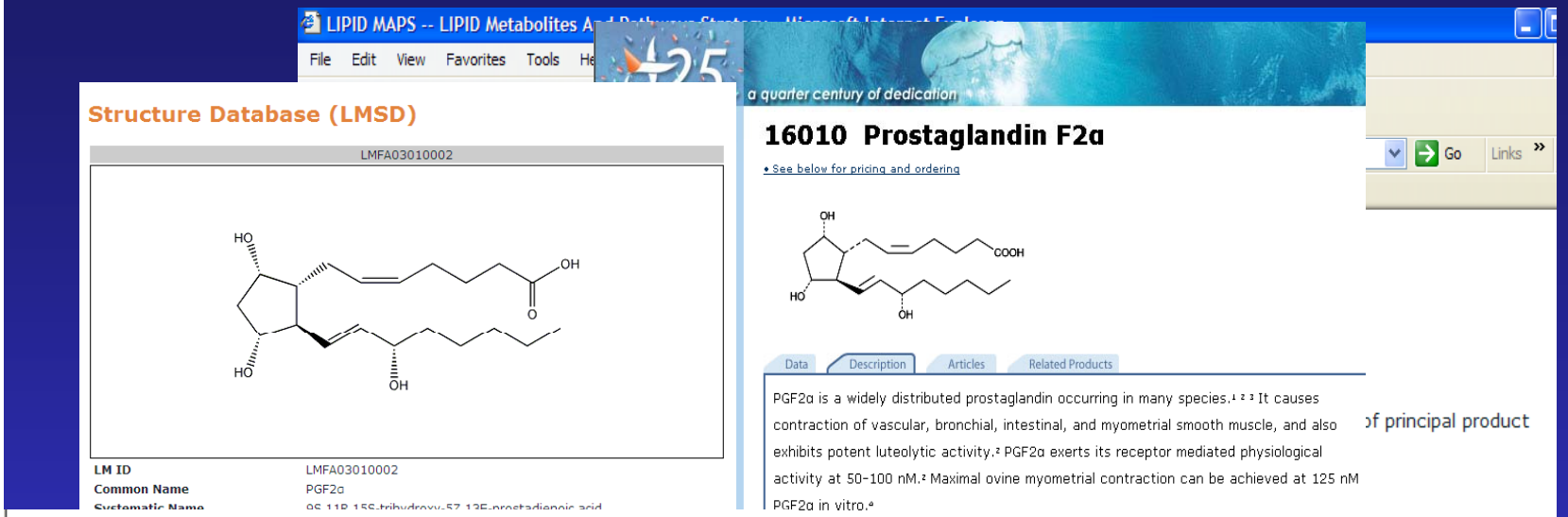
Lipid Proteome Database (LMPD)

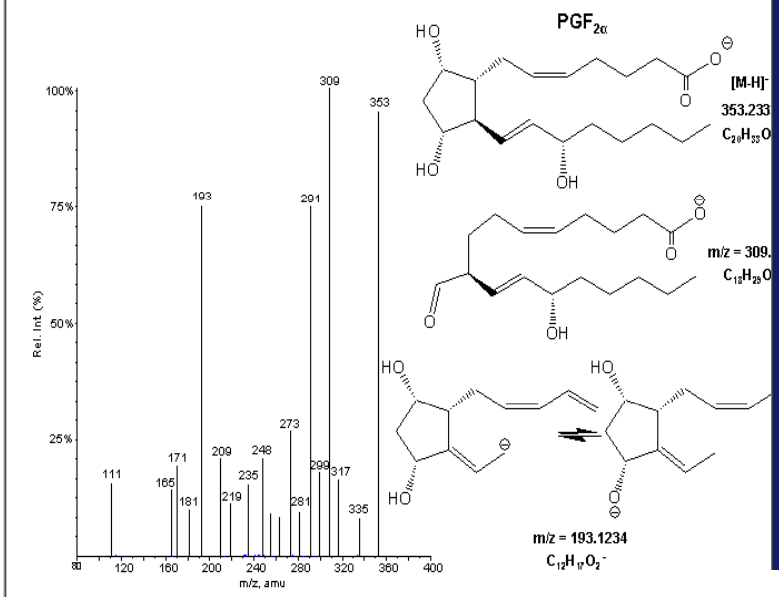
http://www.lipidmaps.org/data/proteome/

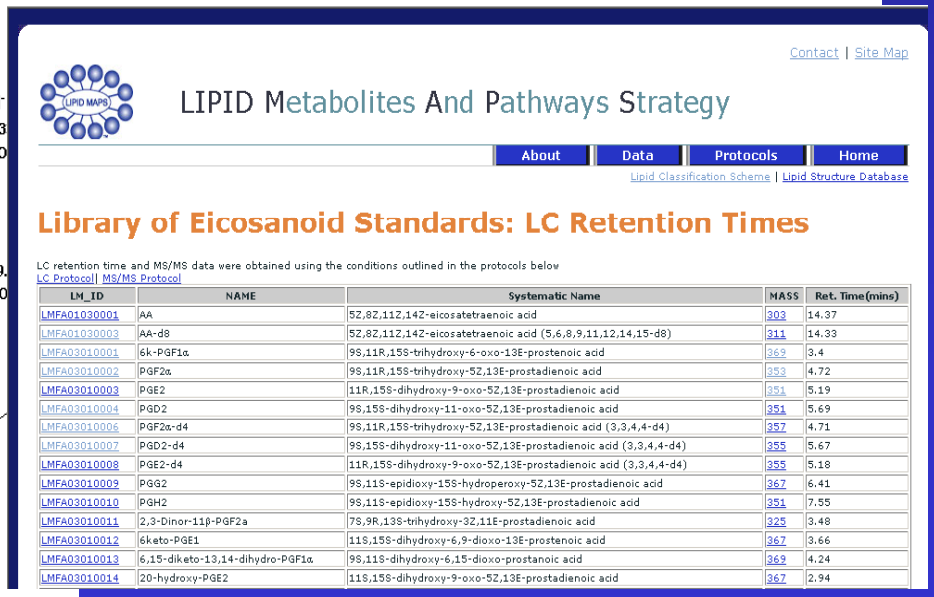


Lipidomics Data Display : MS Standards library

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



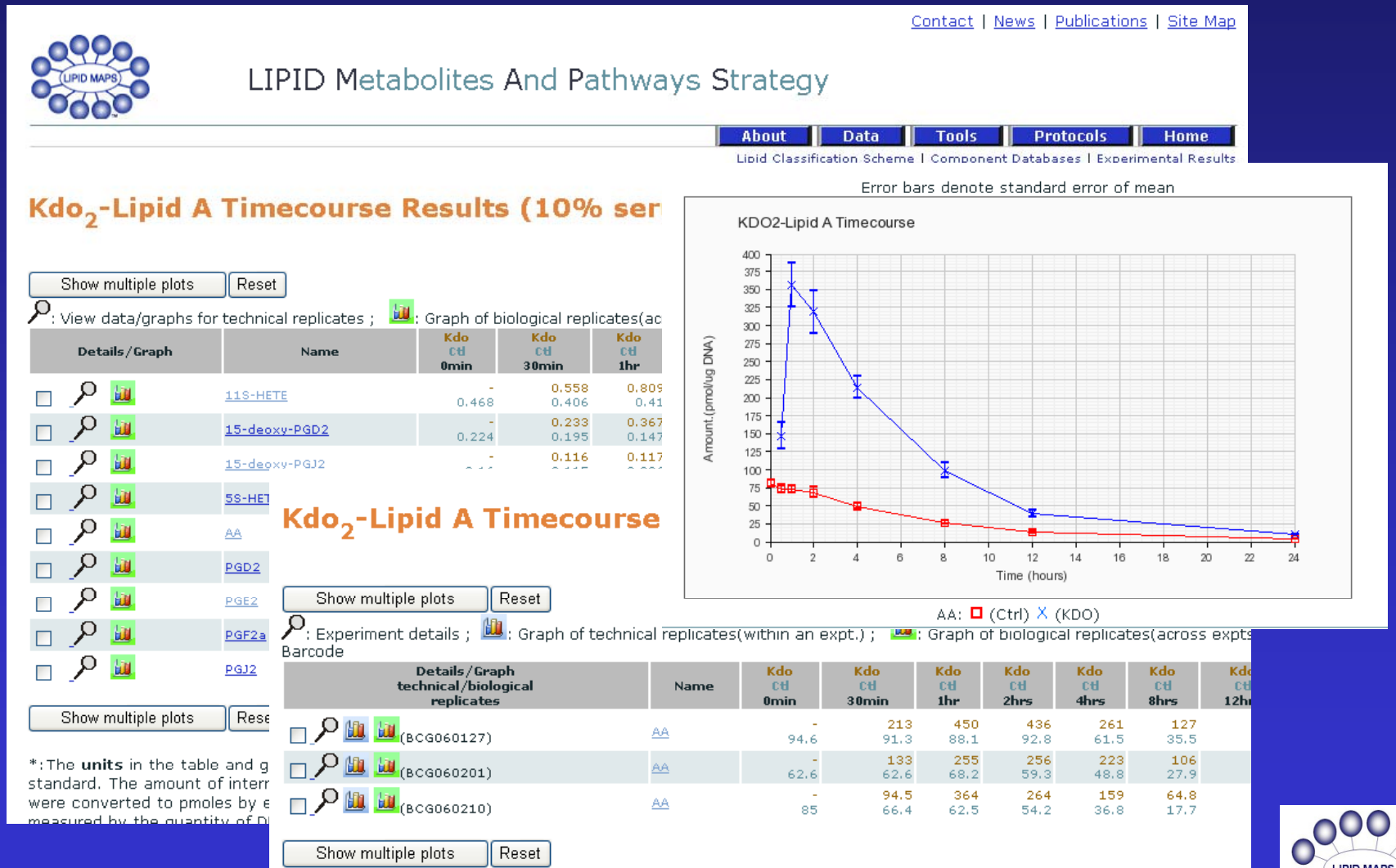




LM_ID	NAME	Systematic Name	MASS	Ret. Time(mins)
LMFA01030001	AA	5Z,8Z,11Z,14Z-eicosatetraenoic acid	303	14.37
LMFA01030003	AA-d8	5Z,8Z,11Z,14Z-eicosatetraenoic acid (5,6,8,9,11,12,14,15-d8)	311	14.33
LMFA03010001	6k-PGF1α	9S,11R,15S-trihydroxy-6-oxo-13E-prostenoic acid	369	3.4
LMFA03010002	PGF2α	9S,11R,15S-trihydroxy-5Z,13E-prostadienoic 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

Lipidomics Data Display : MS Experimental results

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

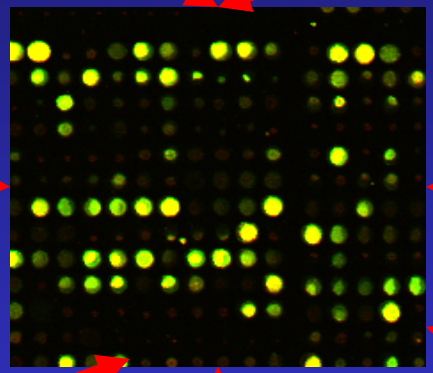


Lipidomics Data Display : Gene array data

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

LIPID MAPS

Lipidomics Data Display : Gene array-search by pathway

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

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LIPID Metabolites And Pathways Strategy

About | Data | Tools | Protocols | Home

Lipid Classification Scheme | Component Databases | Experimental Results

Microarray analysis of RAW 264.7 cells treat

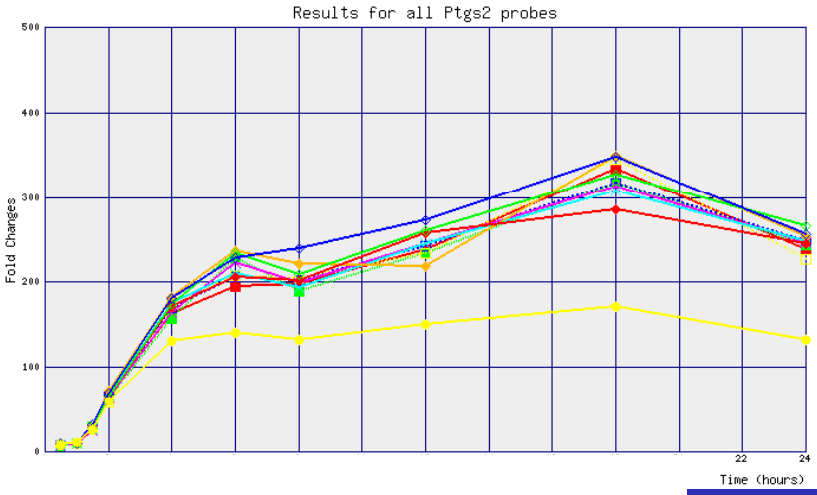
Introduction | Browse by lipid category | Search by gene annotation | Advanced search by KEGG pathway | Search by Biocarta pathway | VAMPIRE Analysis | GOby Analysis

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) degrada
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	Amino
mmu00440	mmu00440	Amino
mmu00530	mmu00530	Amino
mmu05030	mmu05030	Amyo
mmu00150	mmu00150	Andro

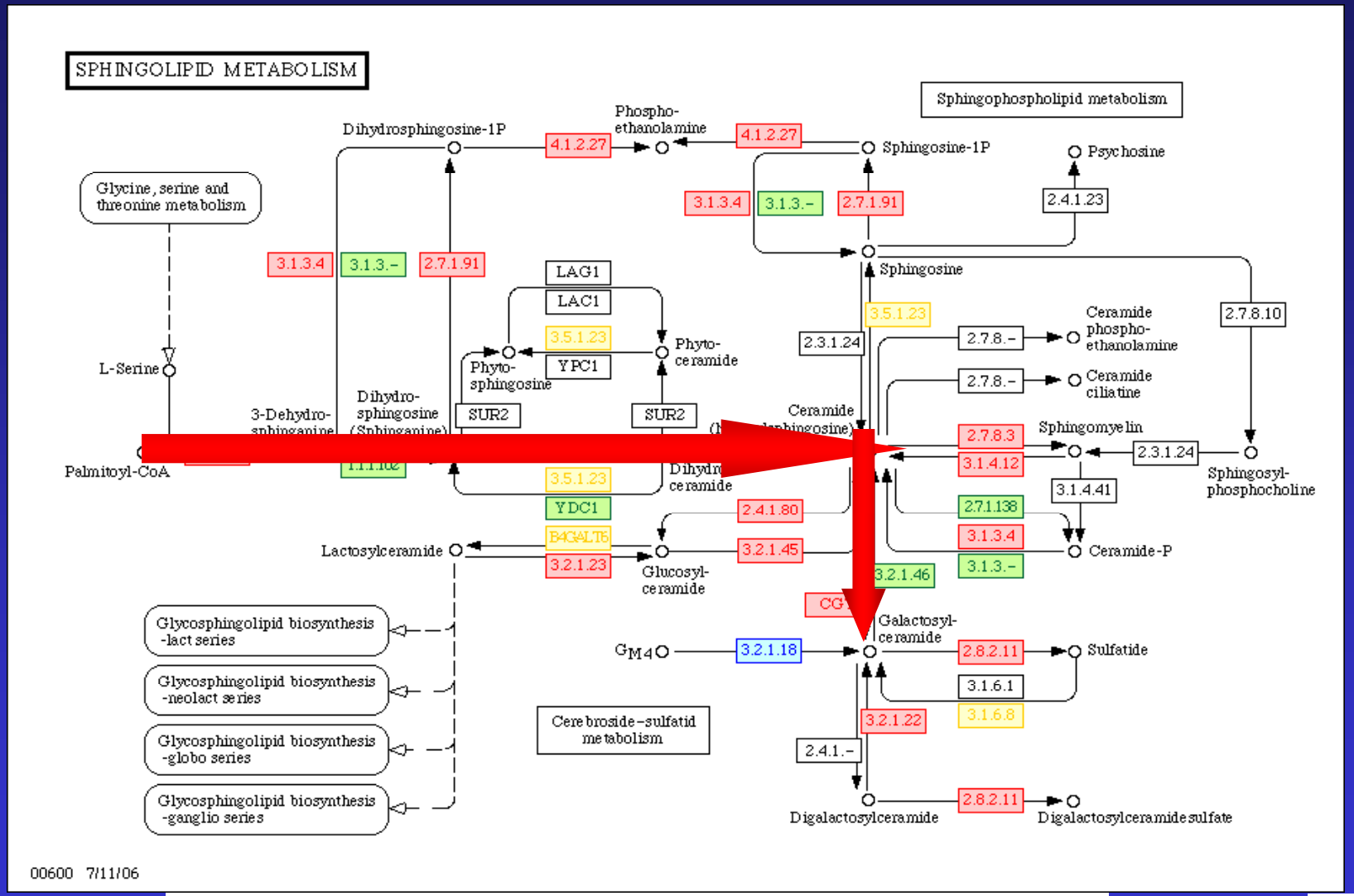


Results Summary

		repression ← (Fold changes: Treatment with Kdo_2-lipid A versus Control) → induction									
GENESYMBOL	GENENAME	KC30	KC60	KC90	KC2H	KC4H	KC6H	KC8H	KC12H	KC18H	KC24H
Ptgds	prostaglandin D2 synthase (brain)	.95	1.09	1.05	1.06	1.12	1.21	1.07	1.00	.87	.88
Ptgds2	prostaglandin D2 synthase 2, hematopoietic	.95	.73	.63	.53	.47	.61	.51	.61	1.10	1.02
Ptges	prostaglandin E synthase	1.37	2.52	3.00	3.19	5.12	6.22	5.04	6.16	10.19	11.24
Ptges2	prostaglandin E synthase 2	1.11	1.08	1.05	.96	.77	.72	.78	.82	.98	.99
Ptgis	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	244.08
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	171.90	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

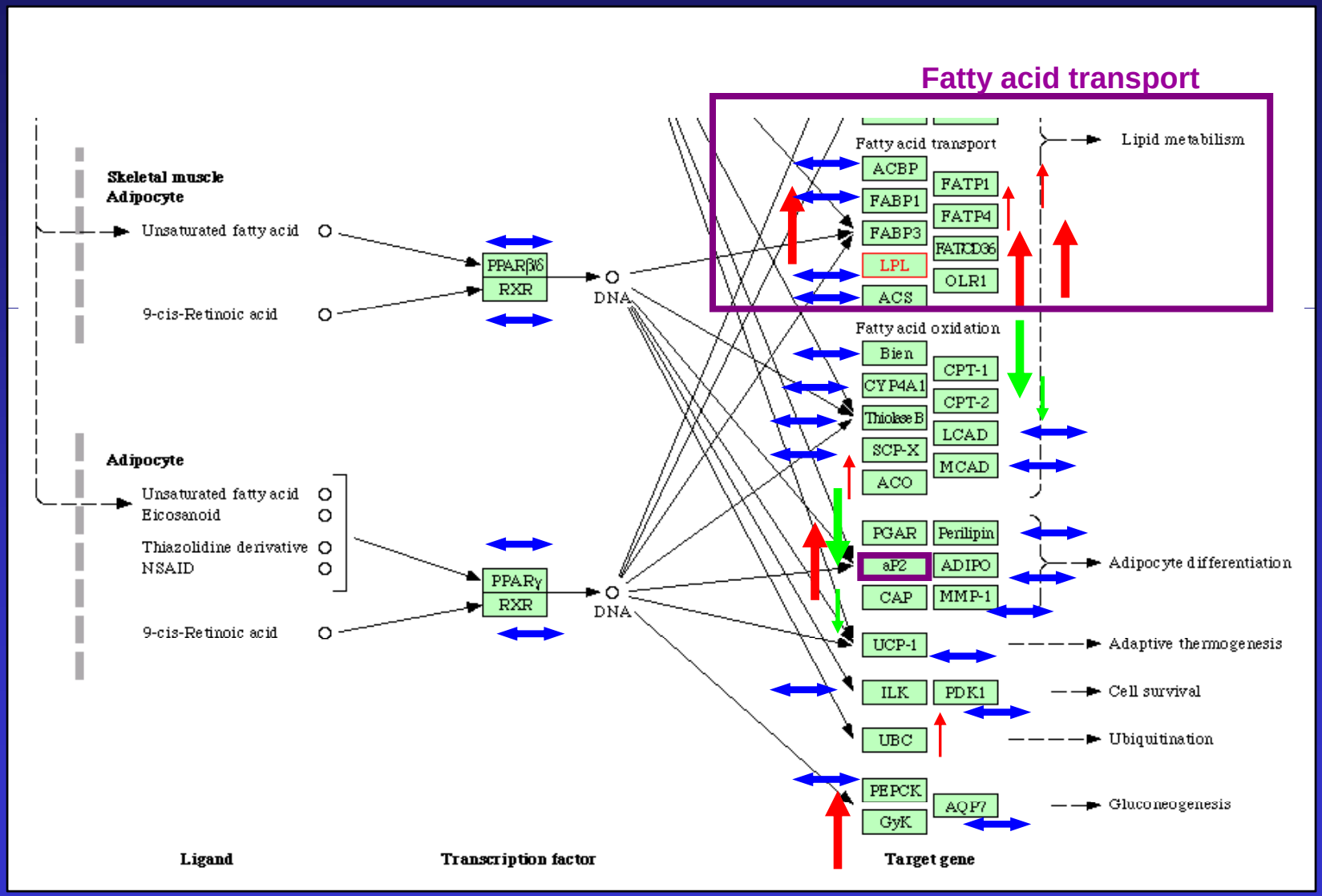
Sphingolipid pathway(KEGG)



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

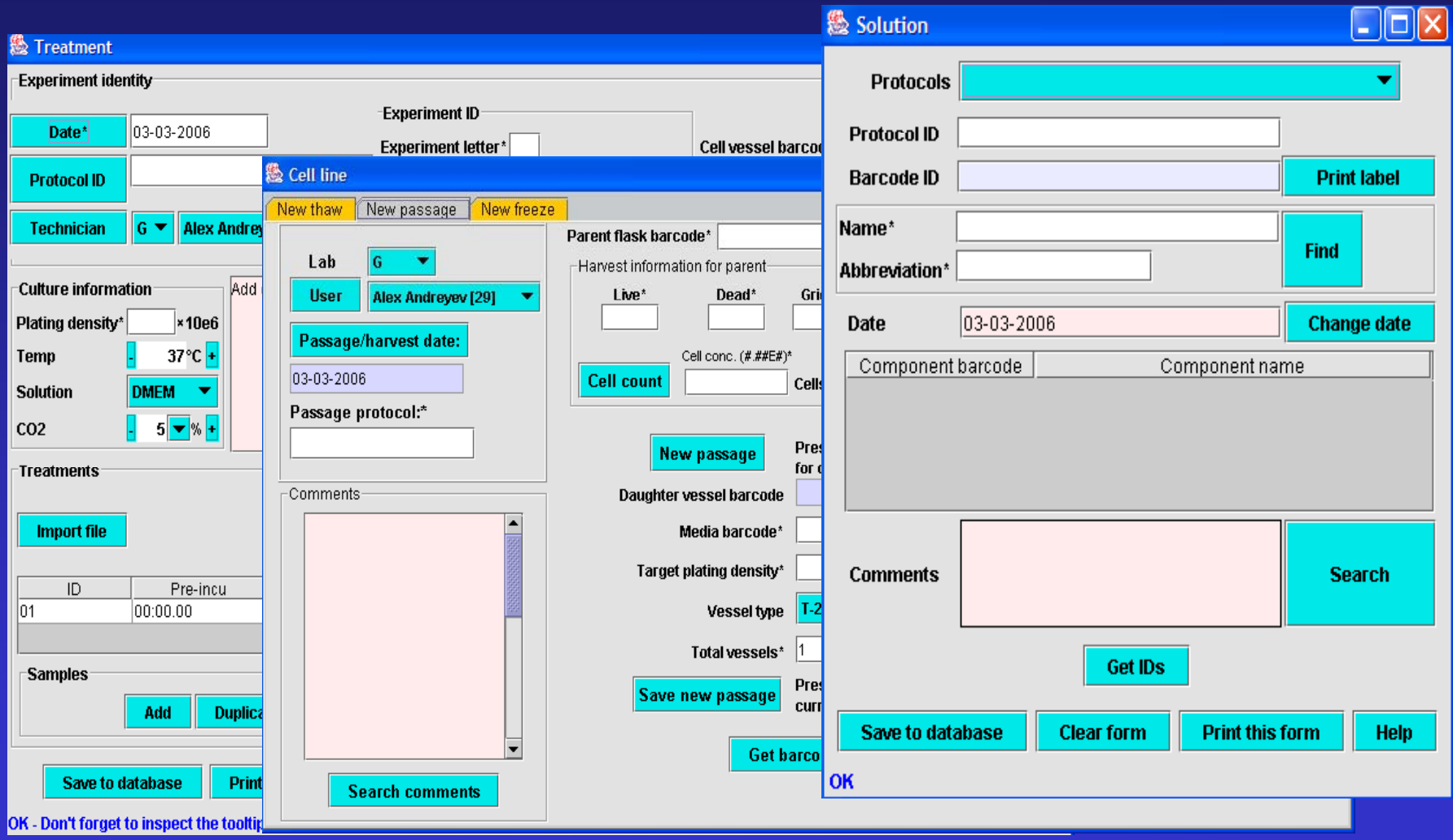
Lipidomics Data Display : Gene array data

Ppar-γ signaling pathway(KEGG)



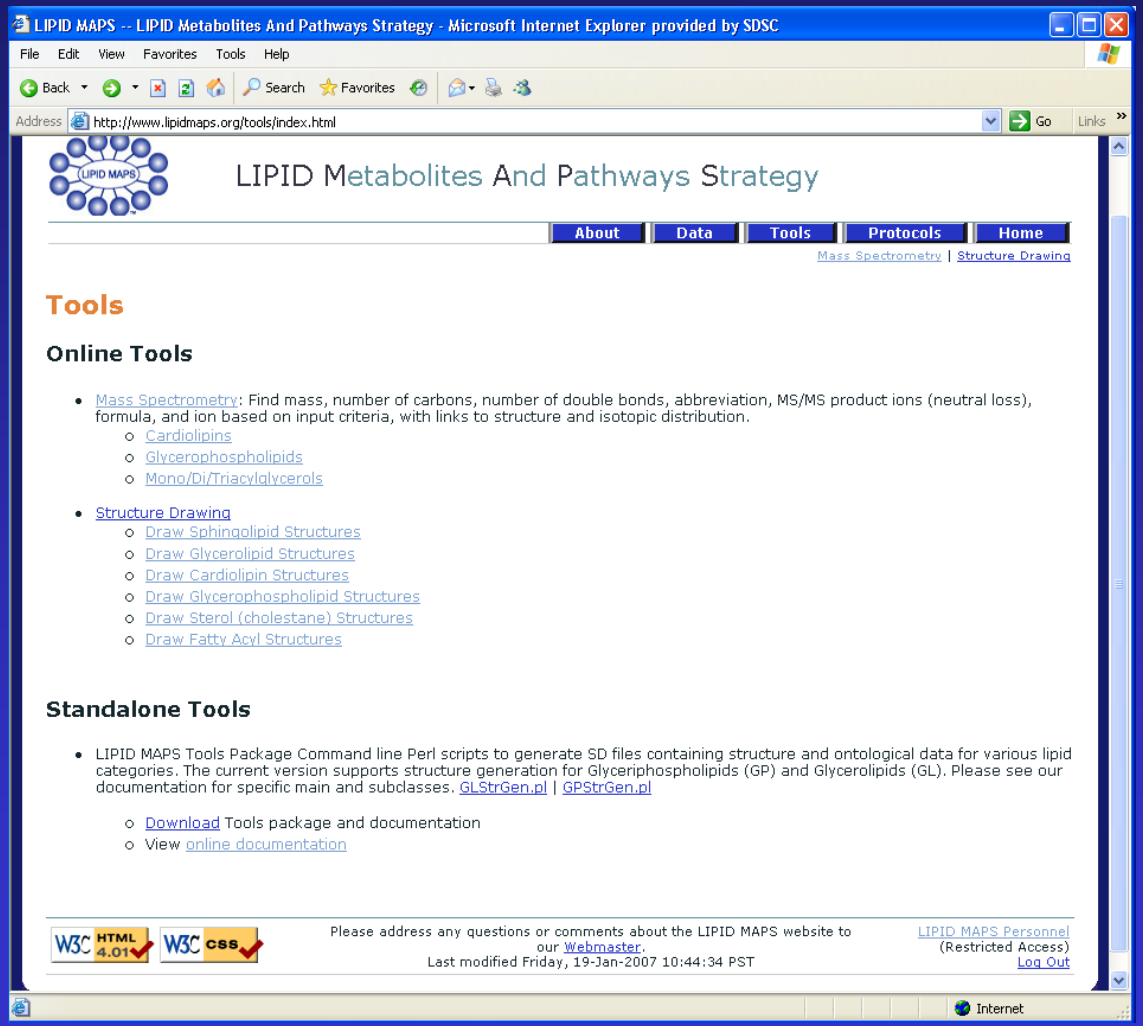
Capturing the Metadata: LIMS Data Input GUI's

(WebStart Java application communicates with Oracle database)



Bioinformatics tools for lipidomics

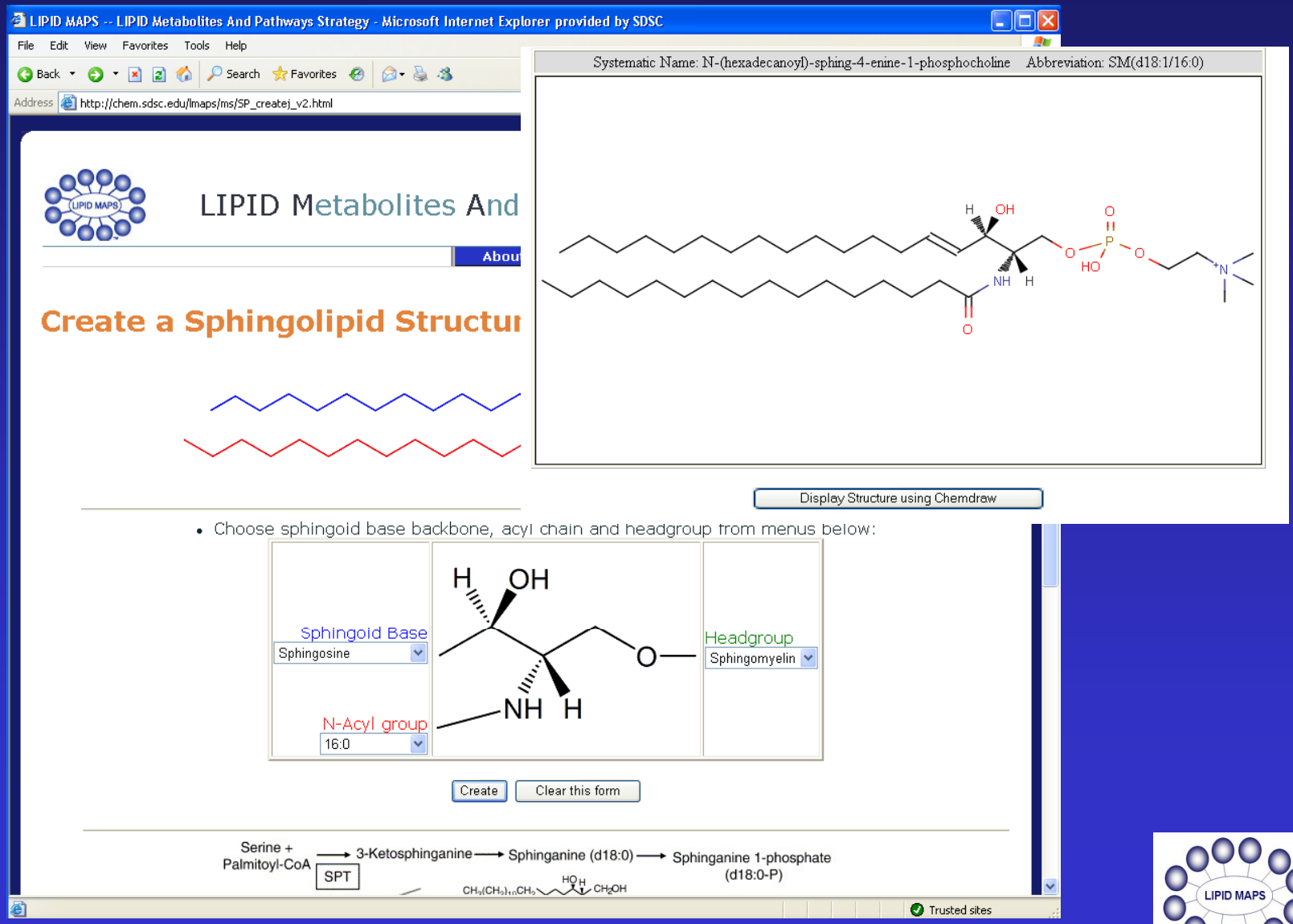
http://www.lipidmaps.org/data/tools/



LIPID MAPS

Bioinformatics tools : Automated structure drawing

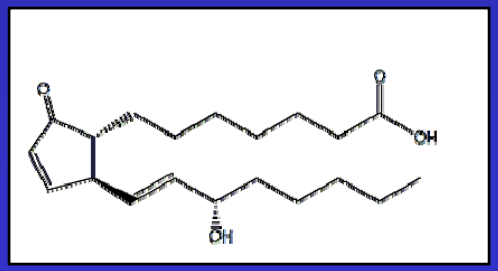
http://www.lipidmaps.org/data/tools/



Using abbreviations to automate structure, nomenclature and ontology generation

LIPID MAPS Abbreviation

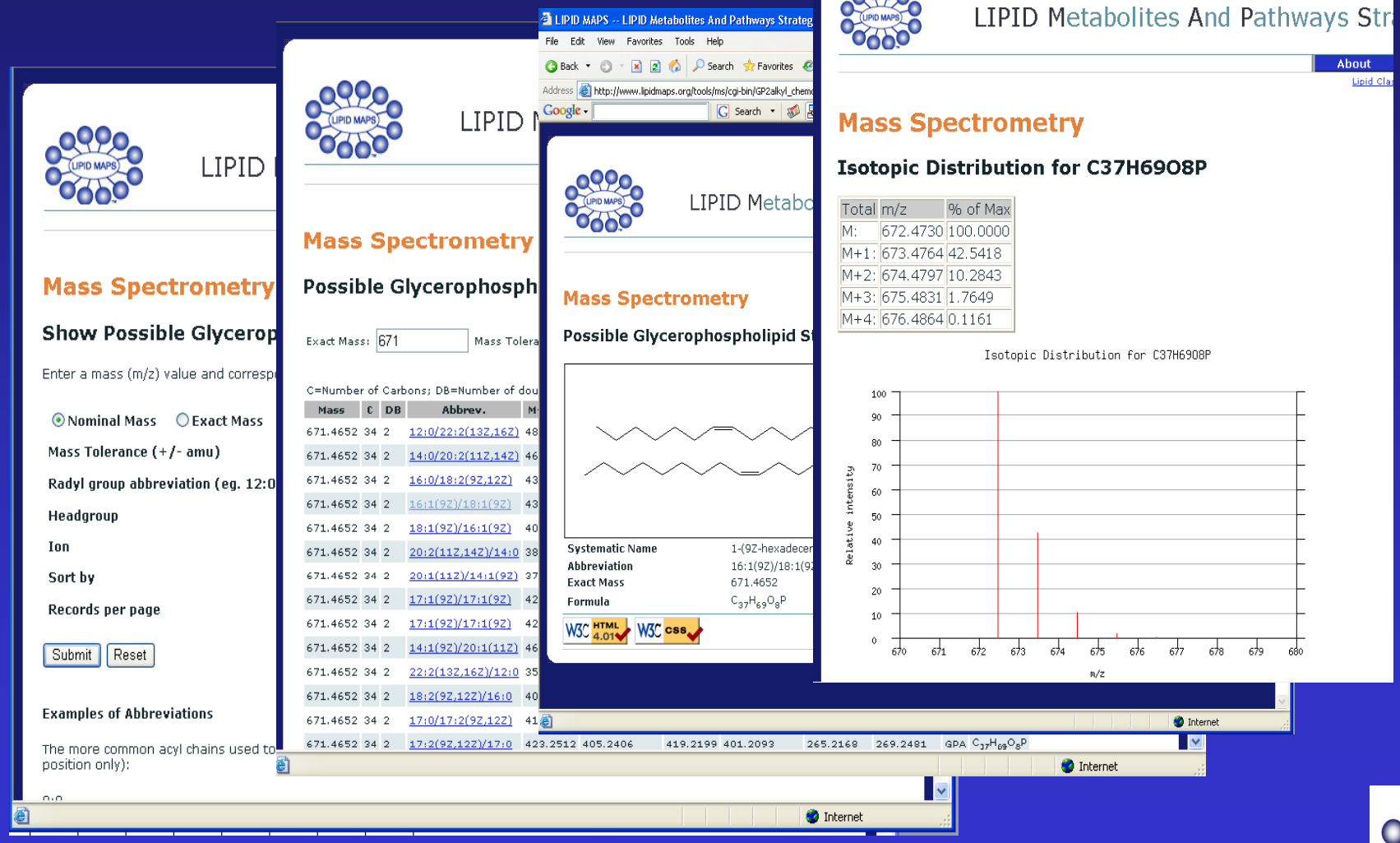
20:2(10Z,13E)(9Ke,15OH[S]){8a,12b}

Structures	Systematic names	Classification	Ontologies
	**9-oxo-15S-hydroxy-10Z,13E-prostadienoic acid**	**Fatty Acyls [FA]** **Eicosanoids [FA03]** **Prostaglandins [FA0301]**	**•Mol weight** **•Formula** **•# hydroxyls** **•# double bonds** **•#rings**

PGA_2

Bioinformatics tools :MS prediction

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



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

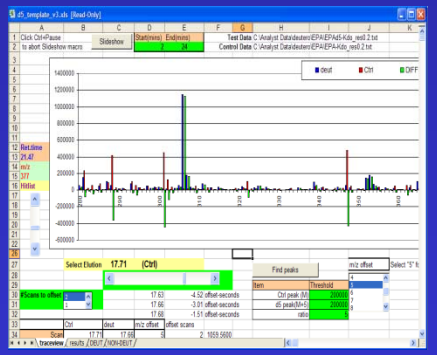
Processed file

Web application

Viewers

Excel template

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

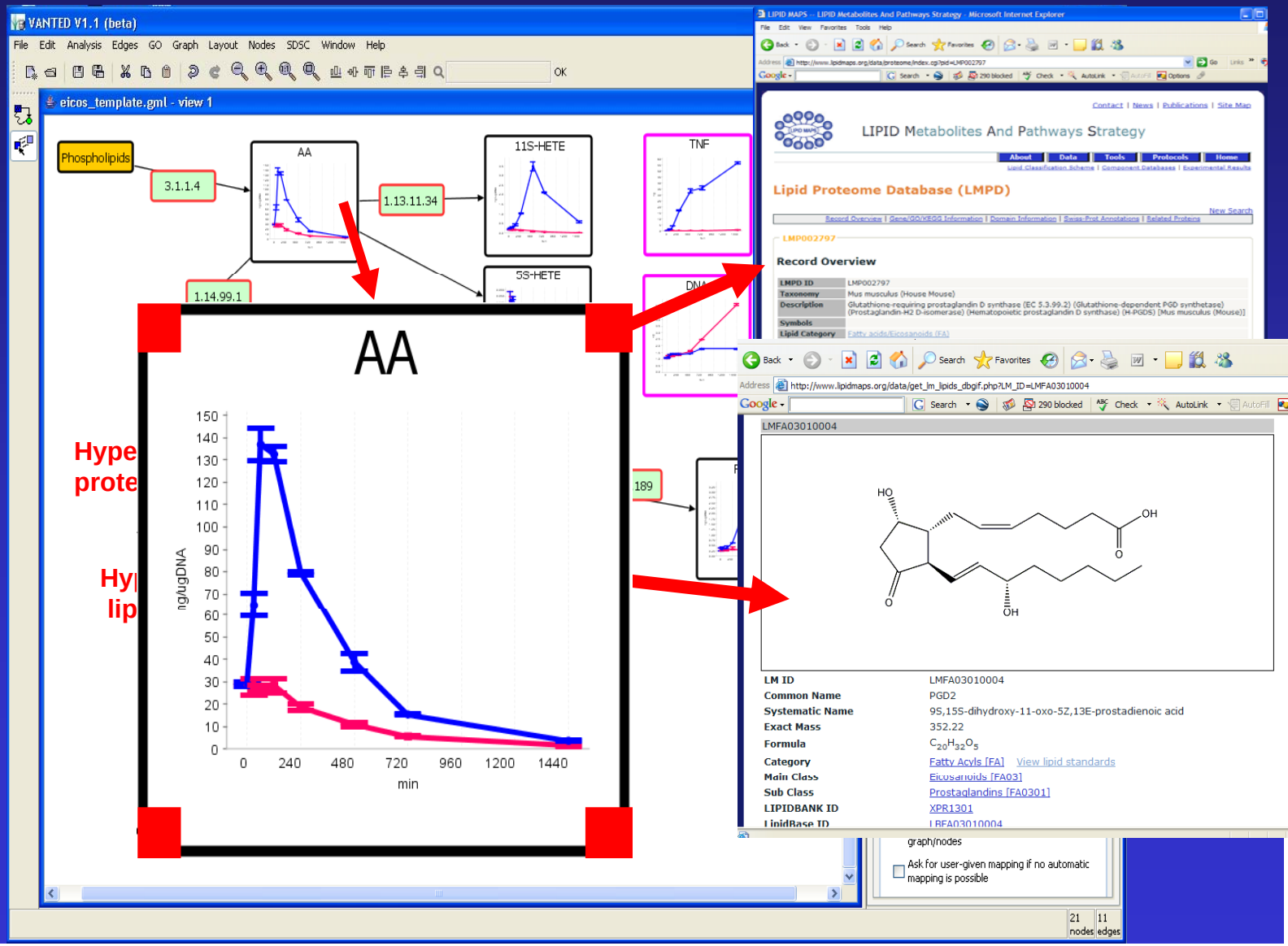


LIPID MAPS

Lipid Pathways and Networks:Visualization tools

VANTED: Displaying lipidomic timecourse data

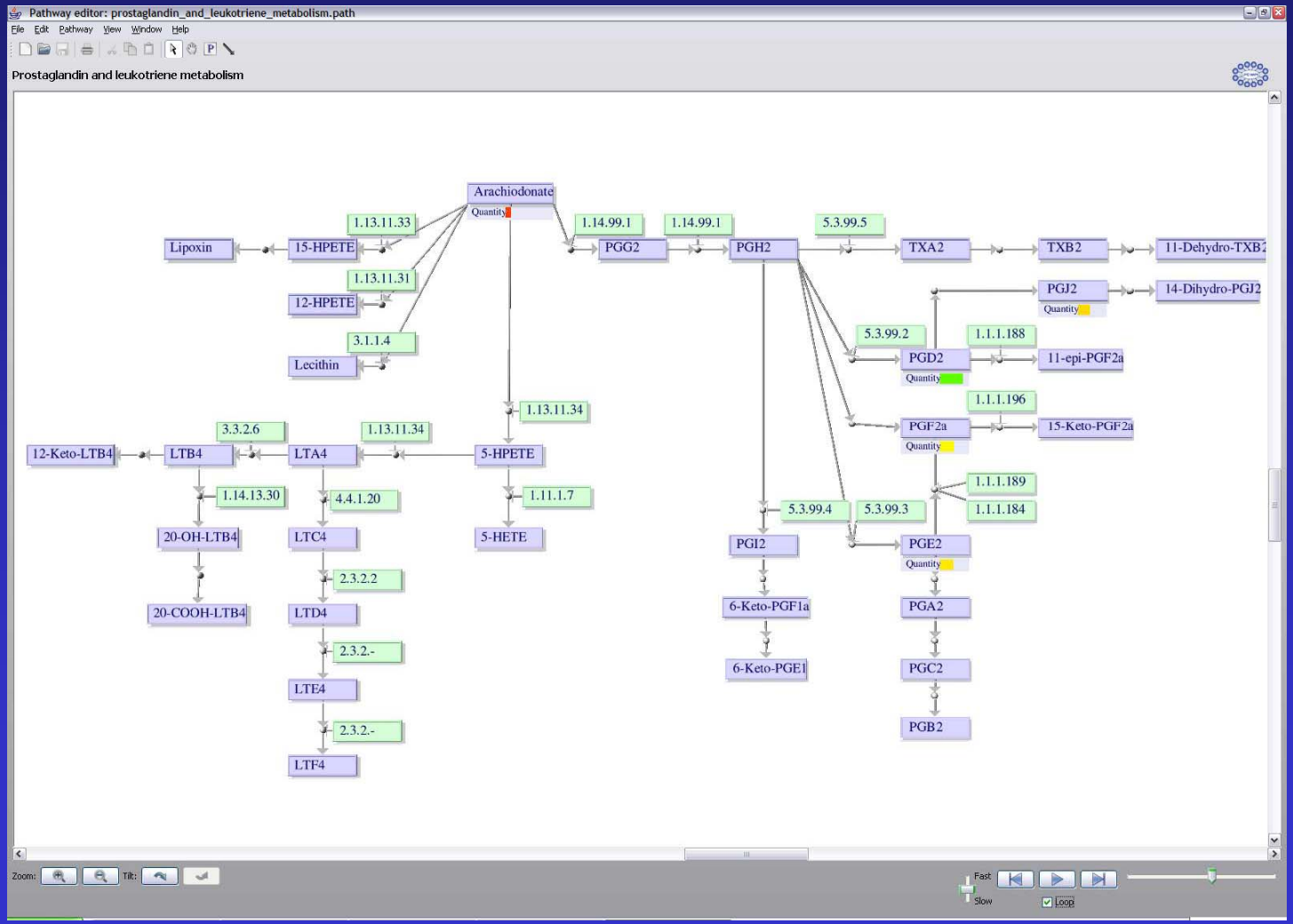
http://vanted.ipk-gatersleben.de/



Lipid Pathways and Networks:Visualization tools

Pathway Editor: Biopathways Workbench

http://www.BiopathwaysWorkbench.org



LIPID MAPS

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