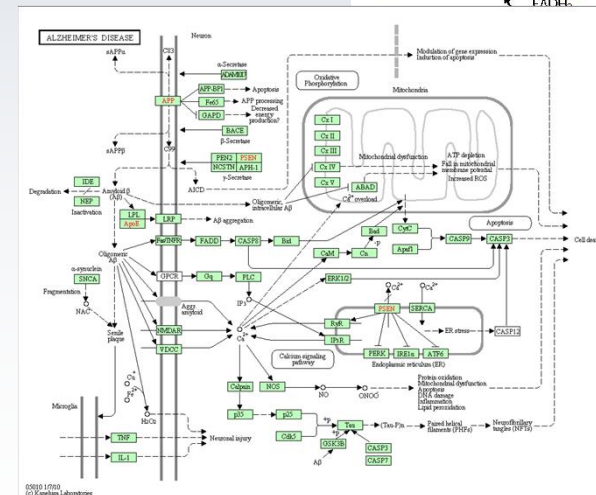
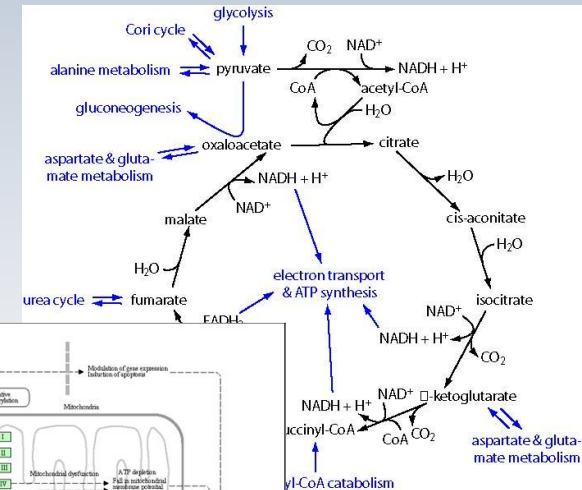


Systems Biology in Metabolomics

Maciej Lalowski
PhD, Adjunct Professor
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and
Folkhälsan Institute
of Genetics
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TrasMed Course 25.09.2014



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Dr. Xiaohua Li

Basic definitions:

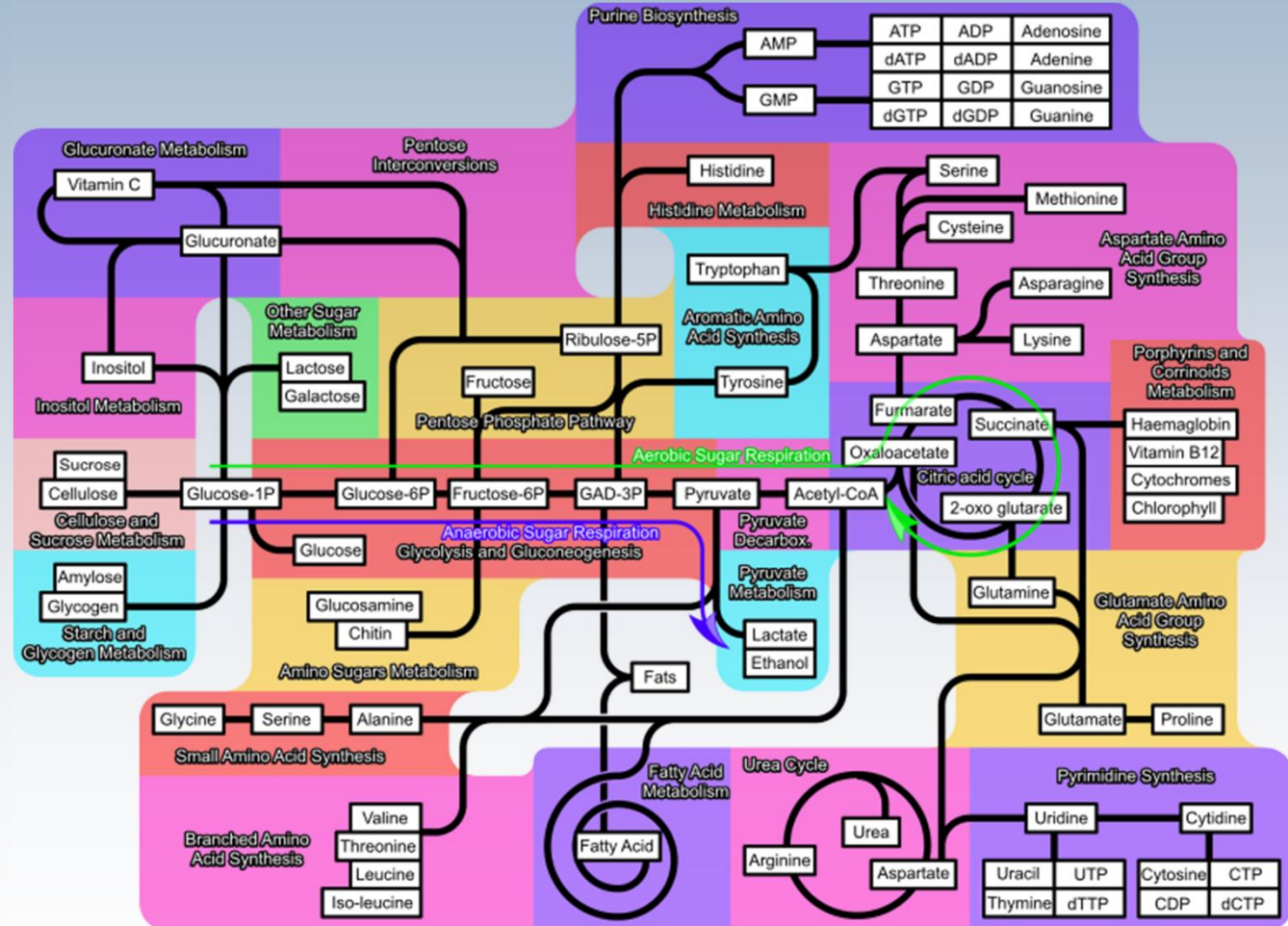
- **Metabolites** - are the intermediates and products of metabolism. The term *metabolite* is usually restricted to small molecules. A **primary metabolite** is directly involved in normal growth, development, and reproduction, e.g. alcohol. A **secondary metabolite** is not directly involved in those processes, but usually has an important ecological function. Examples include antibiotics and pigments. Some antibiotics use primary metabolites as precursors, e.g. actinomycin, a product of primary metabolite tryptophan.
- **Metabolome** - The metabolome forms a large network of metabolic reactions, where outputs from one **enzymatic chain reaction** are inputs to other chemical reactions. The metabolome represents the collection of all metabolites in a biological cell, tissue, organ or organism, which are the end products of cellular processes.
- **Metabolomics** - "systematic study of the unique chemical fingerprints that specific cellular processes leave behind", the study of their small-molecule metabolite profiles.
- **Metabolomic pathways** - are series of chemical reactions occurring within a cell. In each pathway, a principal chemical is modified by a series of chemical reactions. This collection of pathways is called the **metabolic network**. Pathways are important to the maintenance of **homeostasis** within an organism. **Catabolic (break-down)** and **anabolic (synthesis)** pathways often work interdependently to create new biomolecules as the final end-products.

Major metabolic pathways

A metabolic pathway involves the step-by-step modification of an initial molecule to form another product.

- 1) product is used immediately, as the **end-product** of a metabolic pathway
- 2) product initiates another metabolic pathway, called a **flux generating step**
- 3) product is **stored** by the cell.

A molecule called a **substrate** enters a metabolic pathway depending on the needs of the cell and the availability of the substrate. An increase in concentration of anabolic and catabolic intermediates and/or end-products may influence the metabolic rate for that particular pathway.



Entrez Gene: <http://www.ncbi.nlm.nih.gov/gene/>:

ACLY ATP citrate lyase [Homo sapiens] - Gene - NCBI - Mozilla Firefox

http://www.ncbi.nlm.nih.gov/gene/47

Gene

Display Settings: Full Report

ACLY ATP citrate lyase [Homo sapiens]
Gene ID: 47, updated on 1-Oct-2011

Summary

Official Symbol: [ACLY](#) provided by [HGNC](#)

Official Full Name: [ATP citrate lyase](#) provided by [HGNC](#)

Primary source: [HGNC:115](#)

See related: [Ensembl:ENS00000131473](#); [HPRD:00155](#); [MIM:108728](#)

Gene type: protein coding

RefSeq status: REVIEWED

Organism: [Homo sapiens](#)

Lineage: Eukaryota; Metazoa; Chordata; Craniata; Vertebrata; Euteleostomi; Mammalia; Eutheria; Euarchontoglires; Primates; Haplorhini; Catarrhini; Hominidae; Homo

Also known as: [ACL](#); [ATPCL](#); [CLATP](#)

Summary: ATP citrate lyase is the primary enzyme responsible for the synthesis of cytosolic acetyl-CoA in many tissues. The enzyme is a tetramer (relative molecular weight approximately 440,000) of apparently identical subunits. It catalyzes the formation of acetyl-CoA and oxaloacetate from citrate and CoA with a concomitant hydrolysis of ATP to ADP and phosphate. The product, acetyl-CoA, serves several important biosynthetic pathways, including lipogenesis and cholesterol synthesis. In nervous tissue, ATP citrate-lyase may be involved in the biosynthesis of acetylcholine. Two transcript variants encoding distinct isoforms have been identified for this gene. [provided by RefSeq, Jul 2008]

Genomic context

Location : 17q21.2

Sequence : Chromosome: 17; NC_000017.10 (40023179..40075272, complement)

[See ACLY in MapViewer](#)

Chromosome 17 - NC_000017.10

Table of contents

- Summary
- Genomic context
- Genomic regions, transcripts, and products
- Bibliography
- Interactions
- General gene info
- General protein info
- Reference sequences
- Related sequences
- Additional links

Links

- Order cDNA clone
- BioAssay, by Gene target
- BioProjects
- BioSystems
- CCDS
- Conserved Domains
- dbVar
- EST
- Full text in PMC
- Genome
- GEO Profiles
- HomoloGene

Entrez Gene: <http://www.ncbi.nlm.nih.gov/gene/>:

ACLY ATP citrate lyase [Homo sapiens] - Gene - NCBI - Mozilla Firefox

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http://www.ncbi.nlm.nih.gov/gene/47

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Figure 4 analyzes how mutations c Search Ask Facebook Amazon YouTube Weather BBC BBC News BBC Sports Options

ACLY ATP citrate lyase [Homo sapie... +

Homology

Homologs of the ACLY gene: The ACLY gene is conserved in chimpanzee, dog, cow, mouse, rat, chicken, zebrafish, fruit fly, mosquito, C.elegans, S.pombe, M.grisea, N.crassa, A.thaliana, and rice.
[Map Viewer](#) (Mouse, Rat)

Pathways from BioSystems

- [ChREBP activates metabolic gene expression, organism-specific biosystem](#) (from REACTOME)
- [Citrate cycle \(TCA cycle\), organism-specific biosystem](#) (from KEGG)
- * [Citrate cycle \(TCA cycle\), conserved biosystem](#) (from KEGG)
- * [Fatty Acid Biosynthesis, organism-specific biosystem](#) (from WikiPathways)
- * [Fatty Acyl-CoA Biosynthesis, organism-specific biosystem](#) (from REACTOME)
- * [Fatty acid, triacylglycerol, and ketone body metabolism, organism-specific biosystem](#) (from REACTOME)
- * [Integration of energy metabolism, organism-specific biosystem](#) (from REACTOME)
- [Metabolic pathways, organism-specific biosystem](#) (from KEGG)
- [Metabolism of lipids and lipoproteins, organism-specific biosystem](#) (from REACTOME)
- [Triglyceride Biosynthesis, organism-specific biosystem](#) (from REACTOME)

Gene Ontology [Provided by GOA](#)


Function	Evidence Code	Pubs
ATP binding	IEA	
ATP citrate synthase activity	IEA	
citrate (pro-3S)-lyase activity	TAS	
ligase activity	IEA	
metal ion binding	IEA	
nucleotide binding	IEA	
succinate-CoA ligase (ADP-forming) activity	IEA	
transferase activity	IEA	

http://www.ncbi.nlm.nih.gov/guide/all/

start ACLY ATP citrate lyas... TRANSMED Microsoft PowerPoint ... Links 14.59

KEGG <http://www.genome.jp/kegg/>

KEGG: Kyoto Encyclopedia of Genes and Genomes



» Japanese

KEGG Home
[Introduction](#)
[Overview](#)
[Release notes](#)
[Current statistics](#)

KEGG Identifiers
[Pathway maps](#)
[Brite hierarchies](#)

KEGG XML

KEGG API

KEGG FTP

KegTools

[GenomeNet](#)

[DBGET/UnkDB](#)

[Feedback](#)

KEGG: Kyoto Encyclopedia of Genes and Genomes

A grand challenge in the post-genomic era is a complete computer representation of the cell, the organism, the ecosystem, and the biosphere, which will enable computational prediction of higher-level complexity of cellular processes and organism behaviors from genomic and molecular information. Towards this end we have been developing a bioinformatics resource named KEGG as part of the research projects of the Kanehisa Laboratories in the Bioinformatics Center of Kyoto University and the Human Genome Center of the University of Tokyo.

- **Main entry point to the KEGG web service**
[KEGG2](#) [KEGG Table of Contents](#) [Update notes](#) [Help](#)
- **Data-oriented entry points**
 - **KEGG PATHWAY** [Pathway maps and pathway modules](#) [Pathway maps](#)
 - **KEGG BRITE** [Functional hierarchies and ontologies](#) [Brite hierarchies](#)
 - **KEGG DISEASE** [Human diseases](#) [Disease classification](#)
 - **KEGG DRUG** [Drugs](#) [ATC drug classification](#)
 - **KEGG ORTHOLOGY** [KO system and ortholog annotation](#) [KO system](#)
 - **KEGG GENES** [Genes and proteins](#)
 - **KEGG GENOME** [Genomes](#) [KEGG organisms](#)
 - **KEGG COMPOUND** [Chemical compounds](#) [Compound classification](#)
 - **KEGG GLYCAN** [Glycans](#)
 - **KEGG REACTION** [Reactions](#)
- **Organism-specific entry points**
[KEGG Organisms](#) Select (example) hsa
- **Analysis tools**
[KEGG Mapper](#) *New!* [KEGG PATHWAY](#) and [BRITE](#) mapping tools

KEGG <http://www.genome.jp/kegg/>

KEGG PATHWAY Database - Mozilla Firefox

File Edit View History Bookmarks Tools Help

<http://www.genome.jp/kegg/pathway.html>

Most Visited Customize Links

KEGG PATHWAY Database

KEGG2 PATHWAY BRITE DISEASE DRUG KO GENES GENOME LIGAND DBGET

Select prefix: map Organism Enter keywords: [] Go Help

Pathway Maps

KEGG PATHWAY is a collection of manually drawn pathway maps (see new maps, change history, and last updates) representing our knowledge on the molecular interaction and reaction networks for:

- 0. Global Map**
- 1. Metabolism**
- Carbohydrate Energy Lipid Nucleotide Amino acid Other amino acid Glycan Cofactor/vitamin Terpenoid/PK Other secondary metabolite Xenobiotics Overview
- 2. Genetic Information Processing**
- 3. Environmental Information Processing**
- 4. Cellular Processes**
- 5. Organismal Systems**
- 6. Human Diseases**

and also on the structure relationships (KEGG drug structure maps) in:

- 7. Drug Development**

KEGG Atlas may now be used to examine any of the KEGG pathway maps.

Pathway Entries and Pathway Modules

Pathway entries are text representation of pathway maps, containing descriptions (for a limited number of entries, at the moment). **Pathway modules** are specification of subnetworks that correspond to tighter functional units, each represented as a list of KO identifiers (K numbers).

Search Pathway entries for [] Go Clear

Pathway Mapping

Done

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KEGG <http://www.genome.jp/kegg/>

KEGG PATHWAY Database - Mozilla Firefox

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http://www.genome.jp/kegg/pathway.html#carbohydrate

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KEGG PATHWAY Database

Pathway Entries and Pathway Modules

Pathway entries are text representation of pathway maps, containing descriptions (for a limited number of entries, at the moment). **Pathway modules** are specification of subnetworks that correspond to tighter functional units, each represented as a list of KO identifiers (K numbers).

Search for

Pathway Mapping

KEGG PATHWAY mapping is the process to map molecular datasets, especially large-scale datasets in genomics, transcriptomics, proteomics, and metabolomics, to the KEGG pathway maps for biological interpretation of higher-level systemic functions.

- Search objects in KEGG pathways
- Color objects in KEGG pathways

0. Global Map

0.1 Metabolism

Metabolic pathways [zoom out] [Launch KEGG Atlas](#)
Biosynthesis of secondary metabolites [zoom out] [Launch KEGG Atlas](#)

1. Metabolism

1.1 Carbohydrate Metabolism

Glycolysis / Gluconeogenesis [Enzymes](#)
Citrate cycle (TCA cycle) [Compounds with biological roles](#)
Pentose phosphate pathway
Pentose and glucuronate interconversions
Fructose and mannose metabolism
Galactose metabolism
Ascorbate and aldarate metabolism
Starch and sucrose metabolism

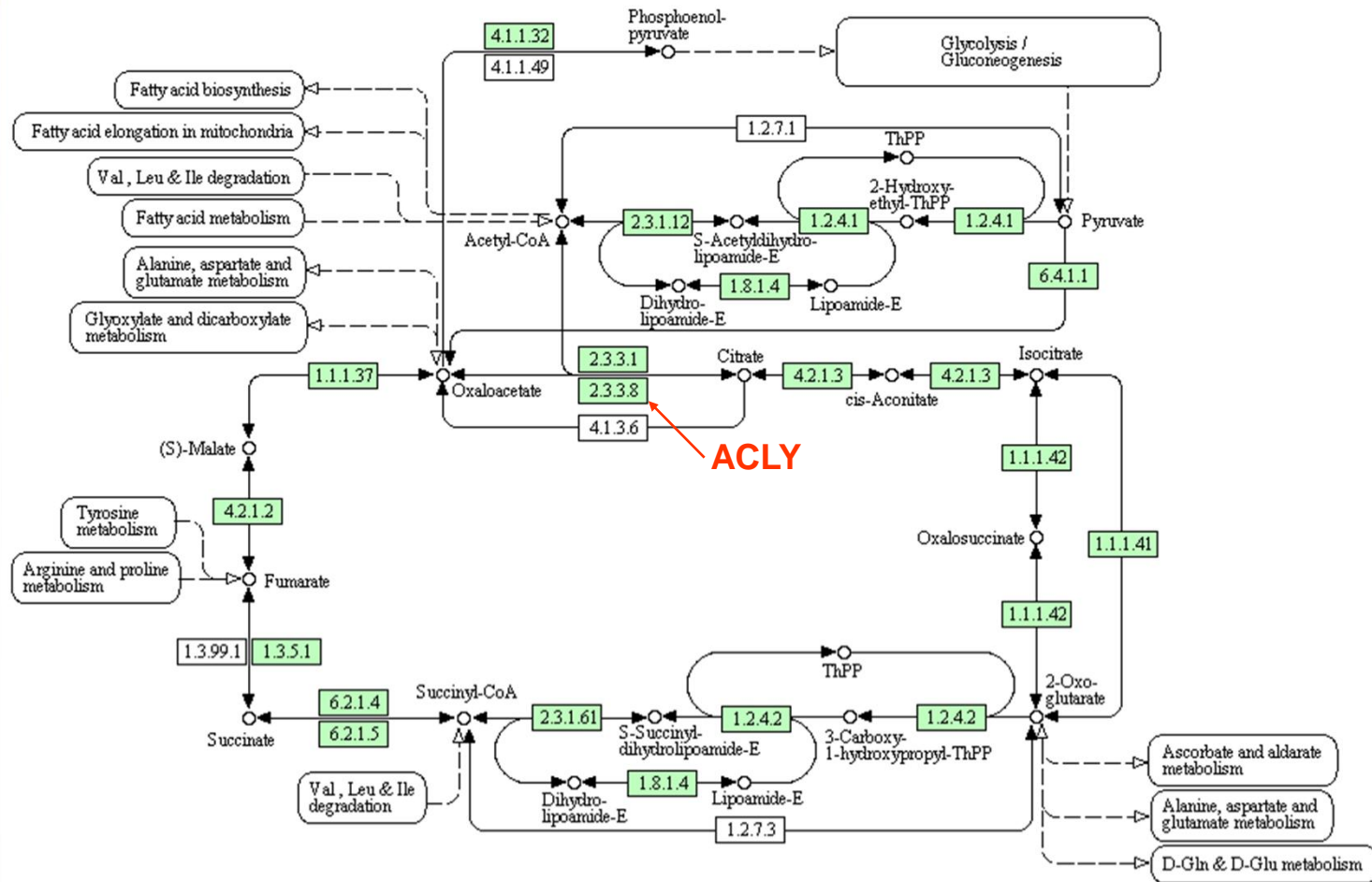
Done

start University of Helsinki... KEGG PATHWAY Data... Students_TRANSMED... Seminar_TRANSMED ... 17.17

KEGG <http://www.genome.jp/kegg/>

BSID: 82927 KEGG: hsa:00020

CITRATE CYCLE (TCA CYCLE)



<http://www.reactome.org/ReactomeGWT/entrypoint.html>

Reactome - Mozilla Firefox

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http://www.reactome.org/ReactomeGWT/entrypoint.html

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REACTOME

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Search

Pathway Browser

Pathway Analysis

Species Comparison

Expression Analysis

If you would prefer to use our old website, click here.

About Reactome

Reactome is an open-source, open access, manually curated and peer-reviewed pathway database. Pathway annotations are authored by expert biologists, in collaboration with Reactome editorial staff and cross-referenced to many bioinformatics databases. These include NCBI Entrez Gene, Ensembl and UniProt databases, the UCSC and HapMap Genome Browsers, the KEGG Compound and ChEBI small molecule databases, PubMed, and Gene Ontology... [more]

Reactome Milestone

Reactome has achieved its milestone of curating reactions and pathways involving at least 5000 distinct human proteins... [more]

Download

The following links allow you to download Reactome data in various formats:

- BioPax
- SBML
- Textbook

Tutorial

Reactome Introduction Us...

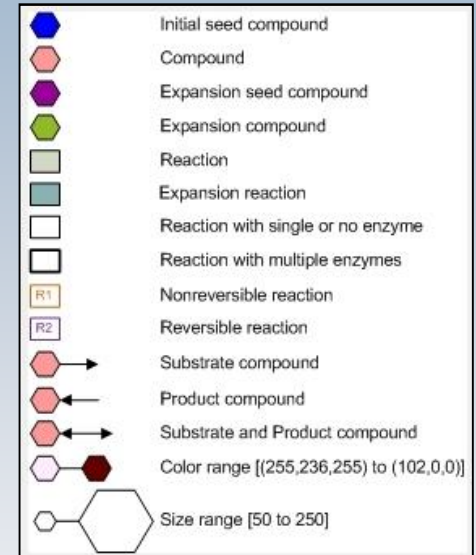
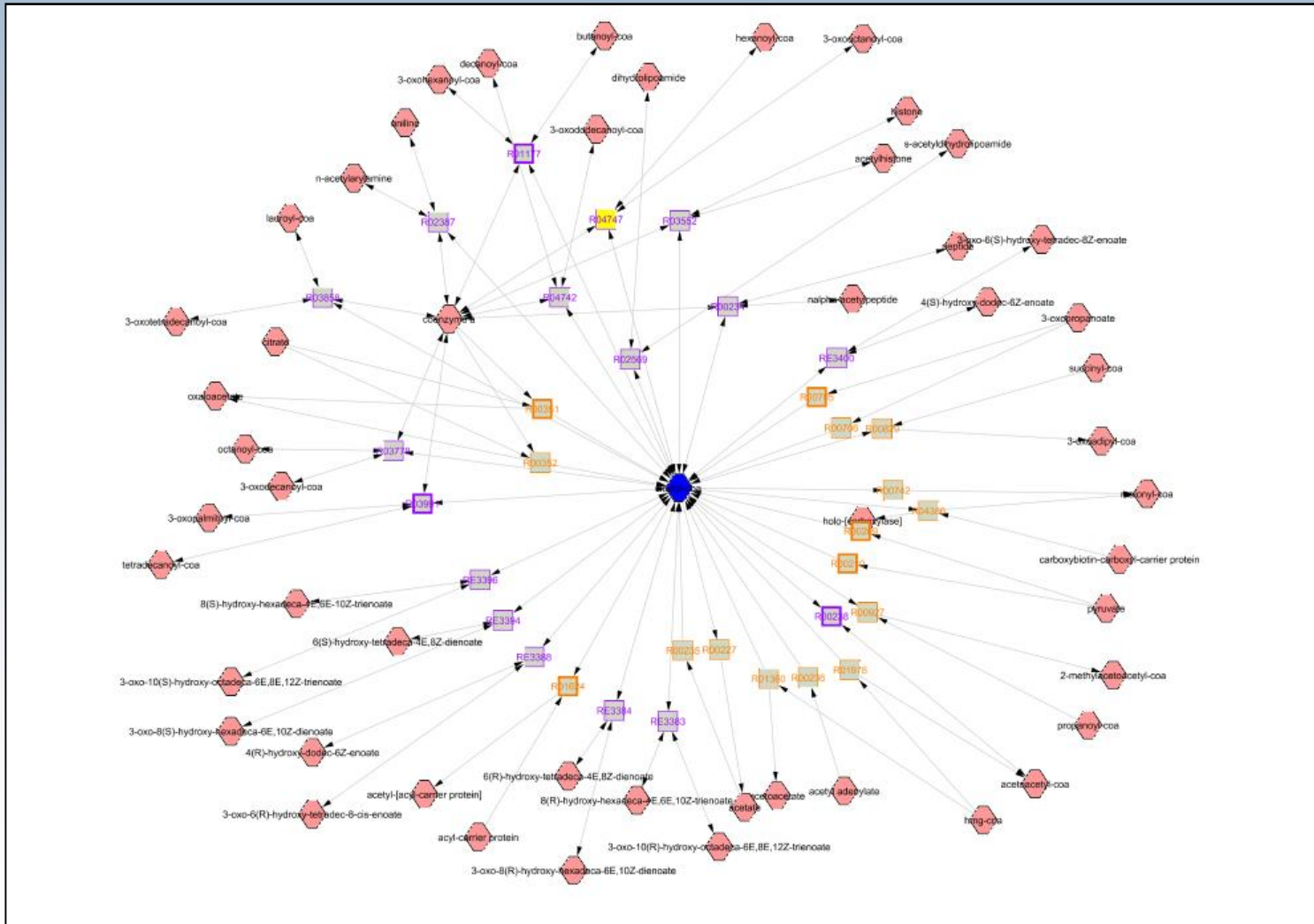
Pathway of the Month: G2/M DNA damage checkpoint

DNA Damage → kinase → Cyclin A/B Cdc 2 (Cdk 1) → pT14Y15

Read it. yting.com

start Reactome - Mozilla Fir... Seminar_TRANSMED... 17.00

Acetyl-CoA (C00024) network (view in MetScape)



C00024

Compound

Primary Name:
acetyl-coa

Synonyms:
acetyl coenzyme a

Formula:
C23H38N7O17P8S

Mass:
809.0

CAS:
72-89-9

SMILES:
CC(=O)SCCNC(=O)CCNC(=O)CC(C)COP(=O)(O)OP(=O)(O)CC(C)C(O)NCC(=O)CNC(=O)CNC(=O)OP(=O)(O)O

Links:
[PubML \[C00024\]](#)
[KEGG \[C00024\]](#)
[PubChem \[6302\]](#)
[BioCyc \[ACETYL_COA\]](#)
[ChEBI \[13331\]](#)
[HMDB \[HMDB01206\]](#)

KEGG 2D structure:


C00024

Lists of compound reactions

Reactions compound participates in (97 reactions found) - [show](#)/[hide](#)

97 reactions found, displaying page 1 of 5.
[First/Prev] 1, 2, 3, 4, 5 [Next/Last]

Id	Description	Reversible?	Equation
R00209	Pyruvate metabolism	false	pyruvate + coenzyme a + nad = acetyl-coa + carbon dioxide + nadh2
R00210	Glycolysis / Gluconeogenesis	false	pyruvate + coenzyme a + nadh = acetyl-coa + carbon dioxide + nadh2
R00227	Pyruvate metabolism	false	acetyl-coa + water = coenzyme a + acetate
R00234		true	acetyl-coa + peptide = coenzyme a + alpha-acetylpeptide
R00235	Glycolysis / Gluconeogenesis	false	adenosine 5'-triphosphate + acetate + coenzyme a = adenosine 5'-monophosphate + pyrophosphate + acetyl-coa
R00236	Pyruvate metabolism	false	acetyl adenyate + coenzyme a = adenosine 5'-monophosphate + acetyl-coa
R00238	Fatty acid metabolism	true	2 acetyl-coa = coenzyme a + acetoacetyl-coa
R00259	Urea cycle and metabolism of amino groups	false	acetyl-coa + glutamic acid = coenzyme a + n-acetyl-l-glutamate
R00351	Citrate cycle (TCA cycle)	false	citrate + coenzyme a = acetyl-coa + water + oxaloacetate
R00352	Citrate cycle (TCA cycle)	false	adenosine 5'-triphosphate + citrate + coenzyme a = adenosine 5'-diphosphate + orthophosphate + acetyl-coa
R00371	Glycine, serine and threonine metabolism	false	acetyl-coa + glycine = coenzyme a + l-2-amino-3-oxobutanoate
R00705	Inositol metabolism	false	3-oxopropanoate + coenzyme a + nad = acetyl-coa + carbon dioxide + nadh2 + h+
R00706	Inositol metabolism	false	3-oxopropanoate + coenzyme a + nadh = acetyl-coa + carbon dioxide + nadh2 + h+
R00742	Tetracycline biosynthesis	false	adenosine 5'-triphosphate + acetyl-coa + hco3-icarbonate = adenosine 5'-diphosphate + orthophosphate
R00829	Benzoate degradation via hydroxylation	false	succinyl-coa + acetyl-coa = coenzyme a + 3-oxoadipyl-coa
R00927	Valine, leucine and isoleucine degradation	false	propanoyl-coa + acetyl-coa = coenzyme a + 2-methylacetoacetyl-coa

MICHIGAN MOLECULAR INTERACTIONS 

Free Text Search | List Search | Query Interactions | MIMI | Help

Reaction Details

Reaction Description:
Fatty acid metabolism

ReactionID:
R00238 [View Reaction in KEGG](#)

Reversible:
true

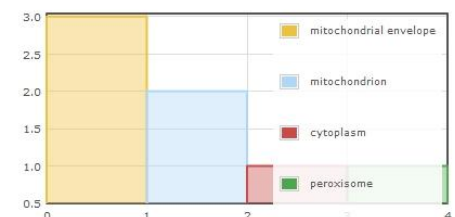
Reaction Text:
2 C00024=C00010+C00332

Equation:
2 Acetyl-CoA=CoA+Acetoacetyl-CoA

Enzymes for Reaction:
2.3.1.16 2.3.1.9

Genes for Reaction:
[ACAA1](#) [HADHB](#) [ACAA2](#) [ACAT1](#) [ACAT2](#)

Subcellular Locations:



Compounds in reaction (3 compounds found) - [show](#)/[hide](#)

AmiGO: <http://geneontology.org>

AmiGO: Gene Product Search Results - Mozilla Firefox

http://amigo.geneontology.org/cgi-bin/amigo/search.cgi?session_id=8648amigo1317651794&search_query=ACLY

Search GO GO terms genes or proteins exact match

Gene Product Search Results

12 results for **ACLY** in genes or proteins fields **symbol, full name(s) and synonyms**

▼ Filter search results ?

Filter Gene Products			Filter Gene Products by Associations	
Gene Product Type	Data source	Species	Ontology	Evidence Code
All	All	All	All	All
complex	ASAP	Arabidopsis thaliana	biological process	IBA
gene	AspGD	Aspergillus fumig...	cellular component	IBD
gene product	CGD	Aspergillus niger	molecular function	IKR

Results are sorted by **relevance**. To change the sort order, click on the column headers.

Select all Clear all Perform an action with this page's selected gene products... Go!

rel ↓	Symbol, full name	Species
<input type="checkbox"/>	ACLY	24 associations protein from <i>Mus musculus</i>

Done

start AmiGO: Gene Product... Seminar_TRANSMED... 17.24

Gene Ontology annotation: <http://www.ebi.ac.uk/GOA/>

Gene Ontology: component

ACLY Homo sapiens P53396 - Mozilla Firefox

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http://www.ebi.ac.uk/QuickGO/GProtein?ac=P53396

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University of Helsinki_ Research Progra... ACLY ATP citrate lyase [Homo sapiens] ... ACLY Homo sapiens P53396

UniProtKB	Accession	Gene	GO ID	Term	Evidence	Method	Database	Accession	Score	Source
UniProtKB P53396	ACLY	ACLY	GO:0046912	alkyl on transferase activity, transferring acyl groups, acyl groups converted into alkyl on transfer	F	IEA	InterPro2GO	InterPro:IPR016143	9606	20111001 InterPro
UniProtKB P53396	ACLY	ACLY	GO:0005634	nucleus	C	IDA	PMID:18029348		9606	20101115 HPA
UniProtKB P53396	ACLY	ACLY	GO:0005737	cytoplasm	C	IEA	InterPro2GO	InterPro:IPR014608	9606	20111001 InterPro
UniProtKB P53396	ACLY	ACLY	GO:0005737	cytoplasm	C	IEA	Swiss-Prot	SP_KW:KW-0963	9606	20111001 UniProtKB
UniProtKB P53396	ACLY	ACLY	GO:0005737	cytoplasm	C	IEA	Subcellular Location2GO	SP_SL:SL-0086	9606	20111001 UniProtKB
UniProtKB P53396	ACLY	ACLY	GO:0005737	cytoplasm	C	IDA	PMID:18029348		9606	20101115 HPA
UniProtKB P53396	ACLY	ACLY	GO:0005739	mitochondrion	C	IEA	Compara	Ensembl:ENSMUSP00000103012	9606	20111001 ENSEMBL
UniProtKB P53396	ACLY	ACLY	GO:0005829	cytosol	C	TAS	Reactome:REACT_1141		9606	20040609 Reactome
UniProtKB P53396	ACLY	ACLY	GO:0005829	cytosol	C	TAS	Reactome:REACT_1577		9606	20040609 Reactome
UniProtKB P53396	ACLY	ACLY	GO:0009346	citrate lyase complex	C	TAS	PMID:1371749		9606	20030904 PINC
UniProtKB P53396	ACLY	NOT	GO:0005730	nucleolus	C	IDA	PMID:18029348		9606	20101115 HPA

Please send comments, suggestions or bug reports to goa@ebi.ac.uk. Click [here](#) for details of how to cite UniProtKB-GOA and QuickGO.

Javascript: ON OFF

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Gene Ontology annotation: <http://www.ebi.ac.uk/GOA/>

Gene Ontology: process

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http://www.ebi.ac.uk/QuickGO/GProtein?ac=P53396

Results: 1 to 48 of 48 Page size: 25 (Show All) Additional filters: None Bookmarkable link

Database	Gene Product ID	Symbol	Qualifier	GO Identifier	GO Term Name	Aspect	Evidence	Reference	With	Taxon	Date	Assigned By	Pro Fo ID
Process													
UniProtKB	P53396	ACLY		GO:0006101	citrate metabolic process	P	TAS	PMID:1371749		9606	20030904	PINC	
UniProtKB	P53396	ACLY		GO:0006112	energy reserve metabolic process	P	TAS	Reactome:REACT_1505		9606	20110610	Reactome	
UniProtKB	P53396	ACLY		GO:0006200	ATP catabolic process	P	TAS	PMID:1371749		9606	20030904	PINC	
UniProtKB	P53396	ACLY		GO:0008152	metabolic process	P	IEA	InterPro2GO	InterPro:IPR005810	9606	20111001	InterPro	
UniProtKB	P53396	ACLY		GO:0008152	metabolic process	P	IEA	InterPro2GO	InterPro:IPR005811	9606	20111001	InterPro	
UniProtKB	P53396	ACLY		GO:0008152	metabolic process	P	IEA	InterPro2GO	InterPro:IPR017440	9606	20111001	InterPro	
UniProtKB	P53396	ACLY		GO:0008610	lipid biosynthetic process	P	IEA	Swiss-Prot Keywords2GO	SP_KW:KW-0444	9606	20111001	UniProtKB	
UniProtKB	P53396	ACLY		GO:0015936	coenzyme A metabolic process	P	TAS	PMID:1371749		9606	20030904	PINC	
UniProtKB	P53396	ACLY		GO:0019432	triglyceride biosynthetic process	P	TAS	Reactome:REACT_1190		9606	20040609	Reactome	
UniProtKB	P53396	ACLY		GO:0031325	positive regulation of	P	TAS	Reactome:REACT_2122		9606	20110610	Reactome	

Done

start | ACLY Homo sapiens P... | Seminar_TRANSMED_... | 17.17

Gene Cards: <http://www.genecards.org/>

GeneCards V3 - Human Genes | Gene Database | Gene Search - Mozilla Firefox

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http://www.genecards.org/

GeneCards V3 - Human Genes | Gen...

Version 3
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Search by **keyword(s)** for **ACL1** [Advanced Search](#) [About V3 Search](#)

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- GeneLoc Gene Location
- GeneNote Gene Microarray Expression
- GeneAnnot Mastering Gene Annotation

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About GeneCards®: GeneCards is a searchable, integrated, database of human genes that provides concise genomic related information, on all known and predicted human genes. [more...](#)

Extract information for many genes at once: [Hot genes](#) [Disease genes](#)

View Sample Gene

ABL1
c-abl oncogene 1, non-receptor tyrosine kinase

GeneCards Sections

Aliases	Drugs	Genome view	Pathways	Publications
Databases	Expression	Interactions	Paralogs	Summaries
Disorders	External search	IP/Patents	Products	Transcripts
Domains	Function	Orthologs	Proteins	Variants

View Random Gene

Category **SERPINA12**
(GIFTS: 54)

News and Views

[Version 3 features](#)
New [search engine](#):

- Speedy output
- Unlimited hits
- Field-specific input
- Better [minicards](#)
- [Relational database](#)

[What's New](#)
[User comments](#)
[Xenex PR](#)
[Site Map](#)

Version 3.06
19 June 2011
Revision 3.06.070

[Previous V3 site](#)

Done

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Gene Cards: aliases and descriptions

ACLY Gene - GeneCards | ACLY Protein | ACLY Antibody - Mozilla Firefox

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ACLY Gene - GeneCards | ACLY Prote...

Jump to Section...

Aliases & Descriptions for ACLY gene

(According to ¹HGNC, ²Entrez Gene, ³UniProtKB/Swiss-Prot, ⁴UniProtKB/TrEMBL, ⁵OMIM, ⁶GeneLoc, ⁷Ensembl, ⁸DME, and/or ⁹miRBase)

[About This Section](#)

Aliases & Descriptions

ATP citrate lyase ^{1,2}	ATP-citrate (pro-S-)-lyase ^{2,3}
ACL ^{1,2,3}	EC 2.3.3.8 ^{3,8}
ATPCL ^{1,2}	OTTHUMP00000164773 ²
CLATP ^{1,2}	ATP citrate synthase ²
Citrate cleavage enzyme ^{2,3}	ATP-citrate synthase ²

External Ids: HGNC: 115¹ Entrez Gene: 47² Ensembl: ENSG00000131473¹ UniProtKB: P53396³

[Export aliases for ACLY gene to outside databases](#)

Previous GC identifiers: GC17M039579 GC17M042174 GC17M039931 GC17M040396 GC17M037276 GC17M035785

Jump to Section...

Summaries for ACLY gene

(According to [Entrez Gene](#), [Toocris Bioscience](#), [Wikipedia's Gene Wiki](#), [UniProtKB/Swiss-Prot](#), and/or [UniProtKB/TrEMBL](#))

[About This Section](#)

Entrez Gene summary for ACLY:

ATP citrate lyase is the primary enzyme responsible for the synthesis of cytosolic acetyl-CoA in many tissues. The enzyme is a tetramer (relative molecular weight approximately 440,000) of apparently identical subunits. It catalyzes the formation of acetyl-CoA and oxaloacetate from citrate and CoA with a concomitant hydrolysis of ATP to ADP and phosphate. The product, acetyl-CoA, serves several important biosynthetic pathways, including lipogenesis and cholesterologenesis. In nervous tissue, ATP citrate-lyase may be involved in the biosynthesis of acetylcholine. Two transcript variants encoding distinct isoforms have been identified for this gene. (provided by RefSeq)

UniProtKB/Swiss-Prot: [ACLY_HUMAN, P53396](#)

Function: ATP citrate-lyase is the primary enzyme responsible for the synthesis of cytosolic acetyl-CoA in many tissues. Has a central role in de novo lipid synthesis. In nervous tissue it may be involved in the biosynthesis of acetylcholine

Done

start ACLY Gene - GeneCa... TRANSMED Microsoft PowerPoint ... Links 10.01

Gene Cards: compounds for ACLY

ACLY Gene - GeneCards | ACLY Protein | ACLY Antibody - Mozilla Firefox

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http://www.genecards.org/cgi-bin/carddisp.pl?gene=ACLY&search=ACLY

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ACLY Gene - GeneCards | ACLY Prote...

Aldrich, Tocris Bioscience, HMDB, and/or Novoseek and Drugs according to DrugBank, Enzo Life Sciences PharmGKB, and/or TarThera) [About This Section](#)

7 HMDB Compounds for ACLY NEW

Compound	Synonyms	CAS #	PubMed Ids
ADP	adenosindiphosphorsaeure (see all 8)	58-64-0	--
Acetyl-CoA	S-Acetyl coenzyme A (see all 13)	72-89-9	--
Adenosine triphosphate	5'(tetrahydrogen triphosphate) Adenosine (see all 24)	56-65-5	--
Citric acid	2-Hydroxy-1,2,3-propanetricarboxylate (see all 20)	77-92-9	--
Coenzyme A	Acetoacetyl coenzyme A sodium salt (see all 21)	85-61-0	--
Oxalacetic acid	2-Ketosuccinate (see all 20)	328-42-7	--
Phosphate	NFB Orthophosphate (see all 13)	14265-44-2	--

[About this table](#)

n|s

10/28 Novoseek chemical compound relationships for ACLY gene ([see all 28](#))

Compound	-log (P-Val)	Hits	PubMed IDs for Articles with Shared Sentences (# sentences)
hydroxycitrate	91	4	17476502 (1), 11319829 (1), 20372858 (1)
(-)-hydroxycitrate	89.1	3	2176080 (1), 11101469 (1)
acetyl-coa	84	26	14681844 (2), 8207683 (1), 7911658 (1), 11171136 (1) (see all 21)
citrate	77.7	31	17928289 (2), 1765100 (2), 8207683 (1), 9820262 (1) (see all 21)
oxaloacetate	69.9	7	7669753 (2), 11171137 (1), 1675605 (1), 18922930 (1)
phosphohistidine	69.2	2	1371749 (1)
pyruvate	62.2	14	8999918 (3), 17928289 (2), 11171136 (1), 7616129 (1) (see all 10)
fatty acid	62.1	26	10410463 (3), 8999918 (3), 15869874 (1), 17476502 (1) (see all 15)
6-phosphogluconate	60.9	2	14605988 (1), 8355562 (1)
3-hydroxy-3-methylglutaryl-coa	57.8	7	8999918 (2), 18774944 (1), 19389950 (1)

[About this table](#)

Done

start ACLY Gene - GeneCa... TRANSMED Microsoft PowerPoint ... 10.03

Gene Cards: expression in tissues and disease



OMIM: www.ncbi.nlm.nih.gov/omim

MIM ID *108728
ATP CITRATE LYASE; ACLY

Alternative titles; symbols
CLATP
ATPCL
ACL

Gene map locus: [17q21.1](#)

Description

ATP citrate lyase is the primary enzyme responsible for the synthesis of cytosolic acetyl-CoA in many tissues. The enzyme is a tetramer (relative molecular weight approximately 440,000) of apparently identical subunits. It catalyzes the formation of acetyl-CoA and oxaloacetate from citrate and CoA with a concomitant hydrolysis of ATP to ADP and phosphate. The product, acetyl-CoA, serves several important biosynthetic pathways, including lipogenesis and cholesterolgenesis. In nervous tissue, ATP citrate-lyase may be involved in the biosynthesis of acetylcholine.

Cloning

Cloning of cDNAs has been reported for murine (Sul et al., 1984), rat (Elshourbagy et al., 1990), and human (Elshourbagy et al., 1992) ATP citrate lyase. Elshourbagy et al. (1992) found that the subunits of the enzyme have 1,105 amino acids and a calculated molecular mass of 121,419 Da. The human and rat ATPCL cDNAs showed 96.3% amino acid identity.

Gene Function

Table of Contents

- MIM *108728
- Description
- Cloning
- Gene Function
- Mapping
- References
- Contributors
- Creation Date
- Edit History

Links

Selected Gene Related Links

- G Entrez Gene
- N Nomenclature
- R RefSeq
- G GenBank
- P Protein
- U UniGene

Other NCBI Links

- BioSystems
- GEO Profiles
- Gene
- Gene Genotype
- GeneView in dbSNP
- HomoloGene

ChEBI: Chemical Entities of Biological Interest

www.ebi.ac.uk/chebi/

Chemical Entities of Biological Interest (ChEBI) - Mozilla Firefox

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http://www.ebi.ac.uk/chebi/advancedSearchFT.do?searchString=ACLY&queryBean.starts=3&queryBean.star...

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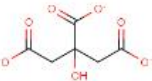
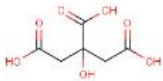
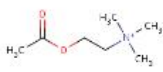
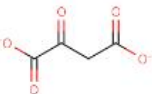
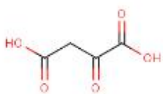
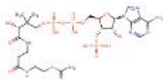
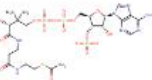
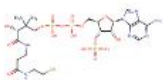
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Chemical Entities of Biological I... Mining metabolites: extracting the ye... Mining metabolites: extracting the ye... Mail :: Inbox

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ACLY search Download your search results: [Tab-delimited](#), [XML](#), [SDF](#)

46 entries found, displaying 1 to 15. << < 1 2 3 4 >>

CHEBI:50744 citrate salt		
	CHEBI:16947 citrate(3-)	CHEBI:30769 citric acid
		
CHEBI:15355 acetylcholine	CHEBI:16452 oxaloacetate(2-)	CHEBI:30744 oxaloacetic acid
		
CHEBI:15351 acetyl-CoA	CHEBI:57288 acetyl-CoA(4-)	CHEBI:15346 coenzyme A

Done

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HMDB: Human Metabolome Database

Metabolomics Toolbox

MetaboLIMS

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Human Metabolome Database Version 3.0

Search:

Search type: Metabolites

[\[Advanced\]](#)



The Human Metabolome Database (HMDB) is a freely available electronic database containing detailed information about small molecule metabolites found in the human body. It is intended to be used for applications in metabolomics, clinical chemistry, biomarker discovery and general education. The database is designed to contain or link three kinds of data: 1) chemical data, 2) clinical data, and 3) molecular biology/biochemistry data. The database (version 3.0) contains 40160 metabolite entries including both water-soluble and lipid soluble metabolites as well as metabolites that would be regarded as either abundant (> 1 uM) or relatively rare (< 1 nM). Additionally, 5716 protein (and DNA) sequences are linked to these metabolite entries. Each MetaboCard entry contains more than 110 data fields with 2/3 of the information being devoted to chemical/clinical data and the other 1/3 devoted to enzymatic or biochemical data. Many data fields are hyperlinked to other databases (KEGG, PubChem, MetaCyc, ChEBI, PDB, Swiss-Prot, and GenBank) and a variety of structure and pathway viewing applets. The HMDB database supports extensive text, sequence, chemical structure and relational query searches. Four additional databases, [DrugBank](#), [T3DB](#), [SMPDB](#) and [FooDB](#) are also part of the HMDB suite of databases. [DrugBank](#) contains equivalent information on ~1600 drug and drug metabolites, [T3DB](#) contains information on 3100 common toxins and environmental pollutants, [SMPDB](#) contains pathway diagrams for 440 human metabolic and disease pathways, while [FooDB](#) contains equivalent information on ~28,000 food components and food additives.

HMDB is supported by [David Wishart](#), Departments of [Computing Science](#) & [Biological Sciences](#), [University of Alberta](#).

HMDB is also supported by [The Metabolomics Innovation Centre](#), a Genome Canada-funded core facility serving the scientific community and industry with world-class expertise and cutting-edge technologies in metabolomics.

What's New?

Latest

September 15, 2012

- The [release notes](#) for version 3.0 of the Human Metabolome Database are now available. Additionally, version 2.5 of the HMDB downloads have been [archived](#).

[News archive](#)

Citing the HMDB


www.hmdb.ca/

HMDB: Human Metabolome Database

Metabolomics Toolbox MetaboLIMS

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Human Metabolome Database Version 3.0



Search: ACLY Search type: Proteins [Search](#) [\[Advanced\]](#)

Search Results



Proteins search for "ACLY" returned 2 results

Filter metabolites by status: Detected and quantified Detected and not quantified Expected and not quantified [Apply](#) [Clear Filter](#)

Uniprot ID	Gene Name <small>Locus</small>	Name	Type	Metabolites
P53396 EnzymeCard	ACLY 17q21.2	ATP-citrate synthase	Enzyme	<div style="border: 1px solid red; padding: 2px;"> Acetyl-CoA </div> Oxalacetic acid Citric acid Coenzyme A Adenosine triphosphate ADP Phosphate
P53396 EnzymeCard	ACLY 17q21.2	ATP-citrate synthase	Enzyme	

This project is supported by [Genome Alberta](#) & [Genome Canada](#), a not-for-profit organization that is leading Canada's national genomics strategy with \$600 million in funding from the federal government.

HMDB Version: 3.0 — [Contact us](#) | ©2005-2012 [Genome Alberta](#)

HMDB: Human Metabolome Database

Showing metabocard for Acetyl-CoA (HMDB01206)

Legend: metabolite field enzyme field

[Show XML](#) [Show Similar Structure](#)

Record Information

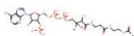
Version	3.0
Creation Date	2005-11-16 08:48:42 -0700
Update Date	2009-05-05 14:58:35 -0600
Accession Number	HMDB01206
Secondary Accession Numbers	None

Metabolite Identification

Common Name **Acetyl-CoA**

Description The main function of coenzyme A is to carry acyl groups (such as the acetyl group) or thioesters. Acetyl-CoA is an important molecule itself. It is the precursor to HMG CoA, which is a vital component in cholesterol and ketone synthesis. (wikipedia) acetyl CoA participates in the biosynthesis of fatty acids and sterols, in the oxidation of fatty acids and in the metabolism of many amino acids. It also acts as a biological acetylating agent.

Structure



Download: [MOL](#) | [SDF](#) | [SMILES](#) | [InChI](#)
Display: [2D Structure](#) | [3D Structure](#)

Synonyms

1. S-Acetyl coenzyme A
2. S-acetate CoA
3. S-acetate Coenzyme A
4. ac-CoA
5. ac-Coenzyme A
6. ac-S-CoA
7. ac-S-Coenzyme A
8. acetyl coenzyme-A
9. acetyl-CoA
10. acetyl-Coenzyme A
11. acetyl-S-CoA
12. acetyl-S-Coenzyme A
13. acetylcoenzyme-A

Chemical Formula $C_{23}H_{38}N_7O_{17}P_3S$

InChI Key InChIKey=ZSLZBFDCINBPY-ZSJKINUSA-N

Chemical Taxonomy

Kingdom Organic Compounds
Super Class Lipids
Class Fatty Acid Esters
Sub Class Acyl CoAs

Other Descriptors
Aromatic Heteropolycyclic Compounds
acyl-CoA(ChEBI)

1 Phosphoribosyl Imidazole
Aminopyrimidine
Carboxamide Group
Carboxylic Thioester
Coenzyme A
Glycosyl Compound
Imidazole
Imidazopyrimidine
Monosaccharide Phosphate
N Glycosyl Compound
Organic Hypophosphite
Organic Phosphite
Organic Pyrophosphate
Oxolane
Pentose Monosaccharide
Phosphoric Acid Ester
Purine
Purine Ribonucleoside 3',5' Bisphosphate
Pyrimidine
Saccharide
Secondary Alcohol
Secondary Carboxylic Acid Amide
Thiocarboxylic Acid Ester

Direct Parent Acyl CoAs

Ontology

Status Detected and not quantified

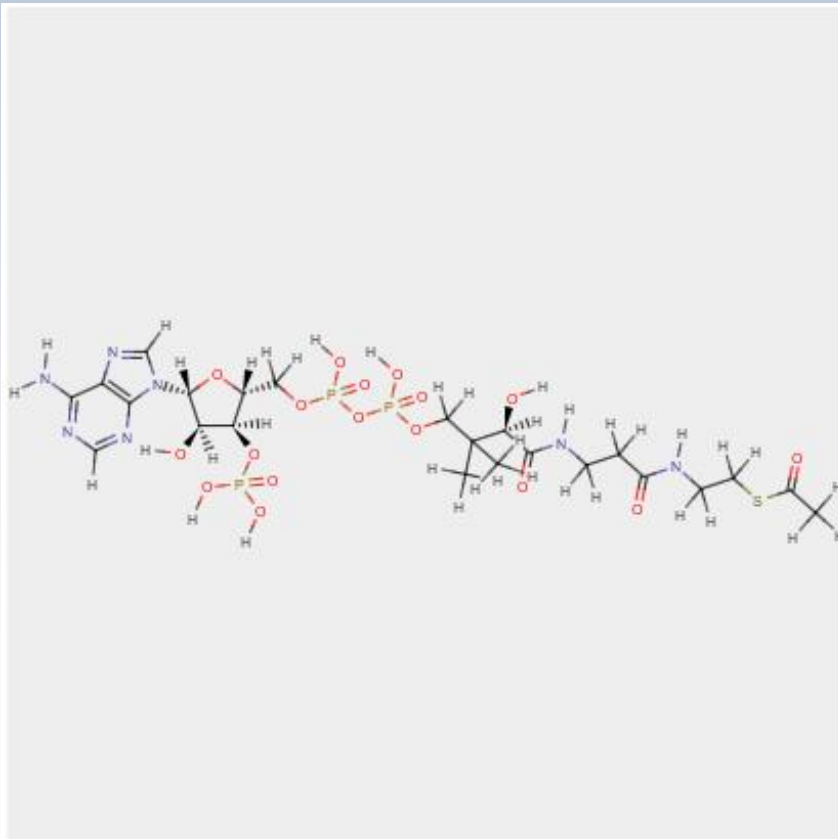
Origin Endogenous
Food

Cell signaling

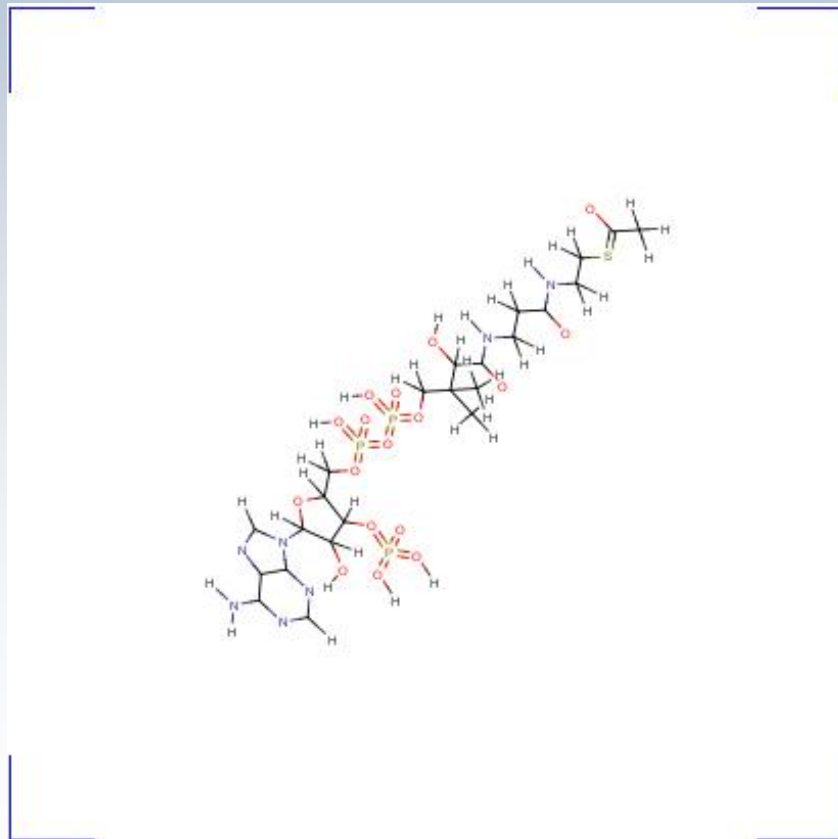
Component of Alanine and acetate metabolism

HMDB: Human Metabolome Database

2D-structure of Acetyl CoA



3D-structure of Acetyl CoA



HMDB: Human Metabolome Database

	nucleus		
	peroxisome		
Biofluid Locations	Not Available		
Tissue Location	Adipose Tissue		
	Brain		
	Muscle		
	Platelet		
	Prostate		
	Skeletal Muscle		
	Spleen		
Pathways	Name	SMPDB Link	KEGG Link
	Amino Sugar Metabolism	SMP00045	map00520
	Beta Oxidation of Very Long Chain Fatty Acids	SMP00052	map01040
	Beta-Alanine Metabolism	SMP00007	map00410
	Butyrate Metabolism	SMP00073	map00650
	Citric Acid Cycle	SMP00057	map00020
	Ethanol Degradation	SMP00449	Not Available
	Fatty Acid Biosynthesis	SMP00456	Not Available
	Fatty acid Metabolism	SMP00051	map00071
	Glycine and Serine Metabolism	SMP00004	map00260
	Ketone Body Metabolism	SMP00071	map00072
	Lysine Degradation	SMP00037	map00310
	Mitochondrial Beta-Oxidation of Long Chain Saturated Fatty Acids	SMP00482	Not Available
	Mitochondrial Beta-Oxidation of Medium Chain Saturated Fatty Acids	SMP00481	Not Available
	Mitochondrial Beta-Oxidation of Short Chain Saturated Fatty Acids	SMP00480	Not Available
	Oxidation of Branched Chain Fatty Acids	SMP00030	Not Available
	Phytanic Acid Peroxisomal Oxidation	SMP00450	Not Available
	Propanoate Metabolism	SMP00016	map00640
	Pyruvate Metabolism	SMP00060	map00620
	Steroid Biosynthesis	SMP00023	map00100
	Transfer of Acetyl Groups into Mitochondria	SMP00466	Not Available
Valine, Leucine and Isoleucine Degradation	SMP00032	map00280	
Normal Concentrations			
	Not Available		
Abnormal Concentrations			
	Not Available		
Associated Disorders and Diseases			
	..		

BioCyc Database collection

www.biocyc.org

Collection of **3563**
Pathway/Genome
databases.

Each database
describes the
genome and
pathways of a
single organism.

Tier 1: literature-
based curation
Tier 2 and Tier 3:
computational

HumanCyc:

250 pathways

MetaCyc:

2202 pathways
from 2063
organisms

Pathway Tools
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Sept 19, 2014

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Enter a gene, protein, metabolite or pathway... Quick Search Gene Search
Searching *Escherichia coli* K-12 substr. MG1655 change organism database

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BioCyc is a collection of **3563** Pathway/Genome Databases (PGDBs), with tools for understanding their data.

Getting Started

New to BioCyc? Typical usage is:

- Select one or more databases (genomes) to search. To do so, click "change organism database" in the box in the top right of every page. By default, BioCyc searches *Escherichia coli* K-12 substr. MG1655.
- Search for a gene or pathway using the Quick Search, or see the Search menu for more options.

[New User Guide >>](#)

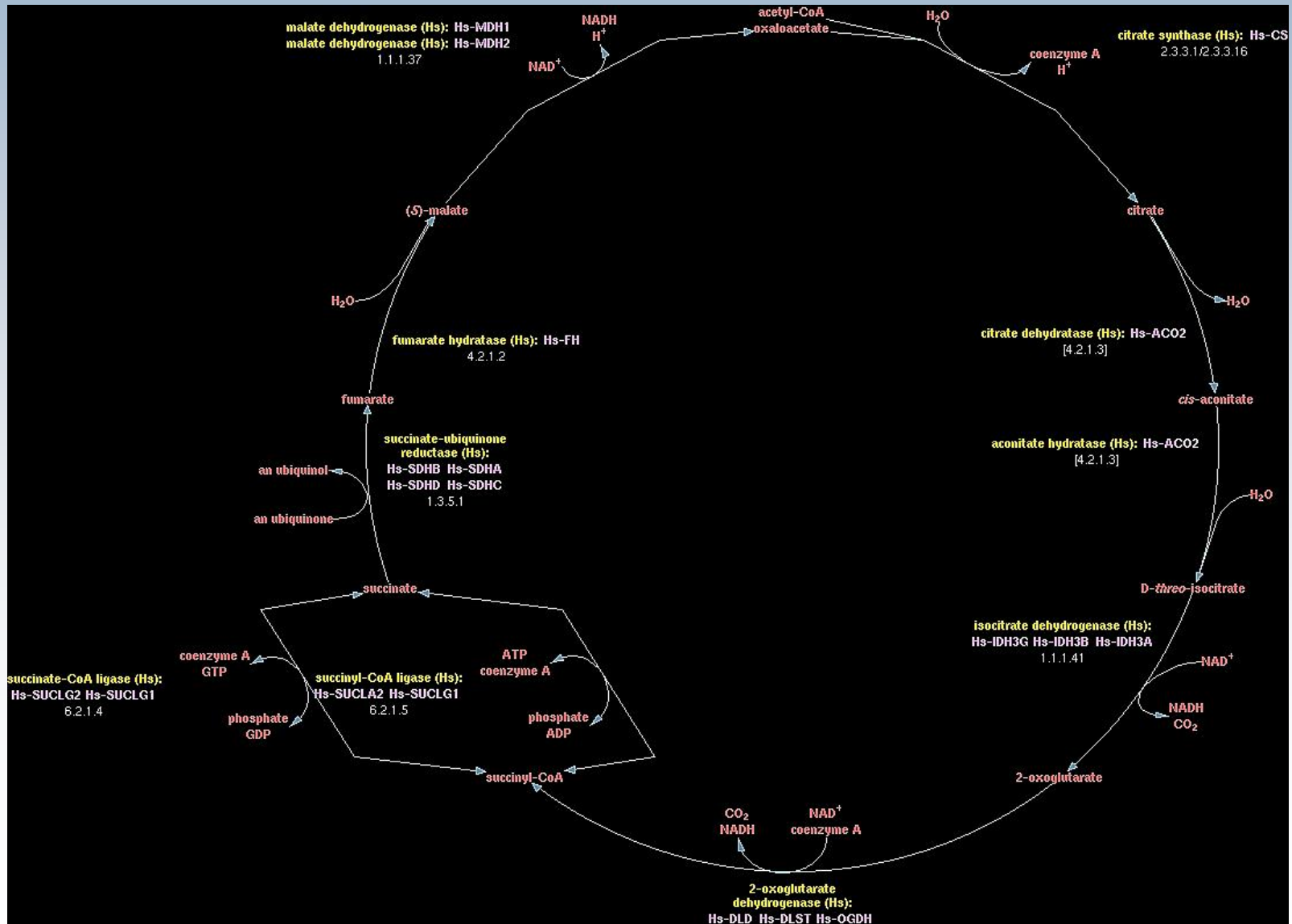
Install Pathway Tools Locally to Analyze Sequenced Genomes

Install SRI's Pathway Tools software locally to predict metabolic pathways from sequenced genomes, generate metabolic models, and analyze omics data.

[Learn More](#)

1 2 3 4 5 6 7 8 9 10 11

BioCyc Database collection: example TCA (human)



ChemSpider: the free chemical database

<http://www.chemspider.com/>

ChemSpider | Citrate | C6H5O7 - Mozilla Firefox

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ChemSpider
The free chemical database

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About More Searches Web APIs Help eg. Pyridine Search

Search term: Citrate (Found by approved synonym)

Citrate

ChemSpider ID: **29081**

Molecular Formula: C₆H₅O₇

Monoisotopic mass: 189.005 Da

▼ Systematic name
2-hydroxypropane-1,2,3-tricarboxylate

▶ SMILES and InChIs

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ChemSpider: the free chemical database

<http://www.chemspider.com/>

ChemSpider | Citrate | C6H5O7 - Mozilla Firefox

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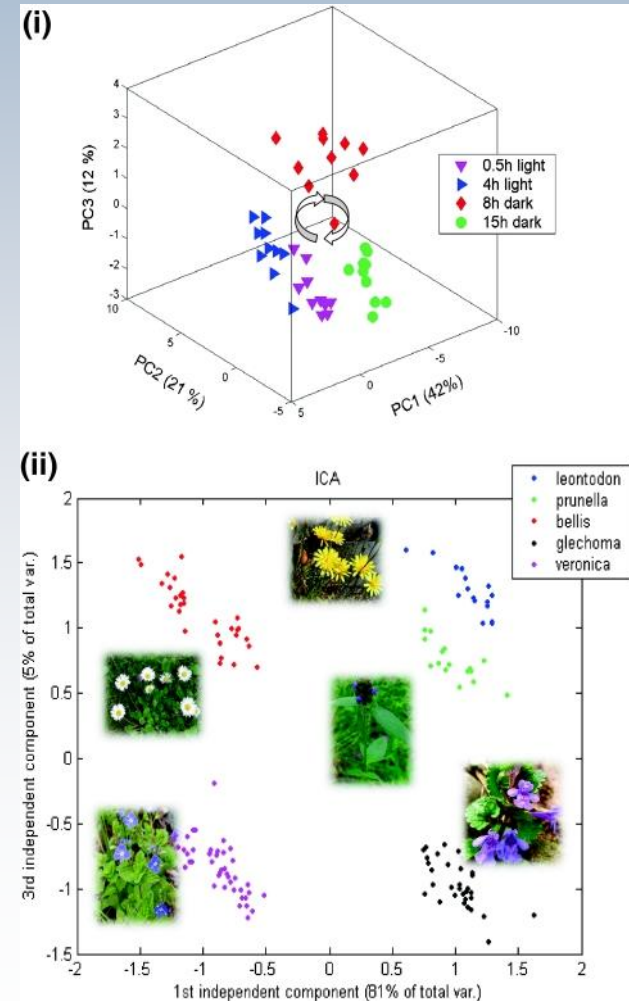
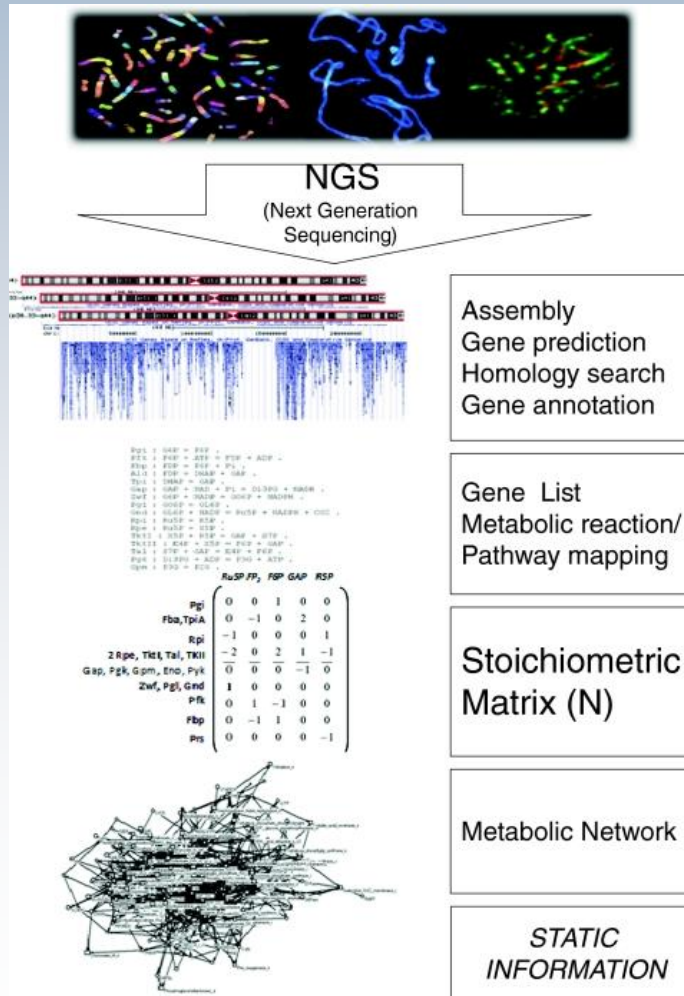
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Looking for Leads

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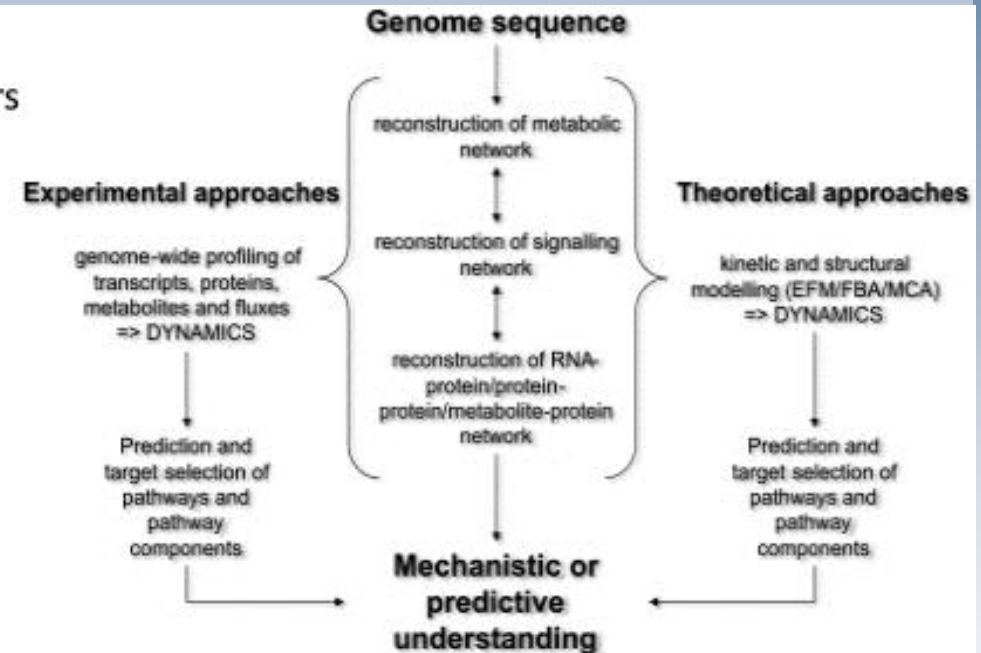
Unpredictability of metabolism--the key role of metabolomics science in combination with next-generation genome sequencing



Unpredictability of metabolism--the key role of metabolomics science in combination with next-generation genome sequencing

Metabolomics experiment

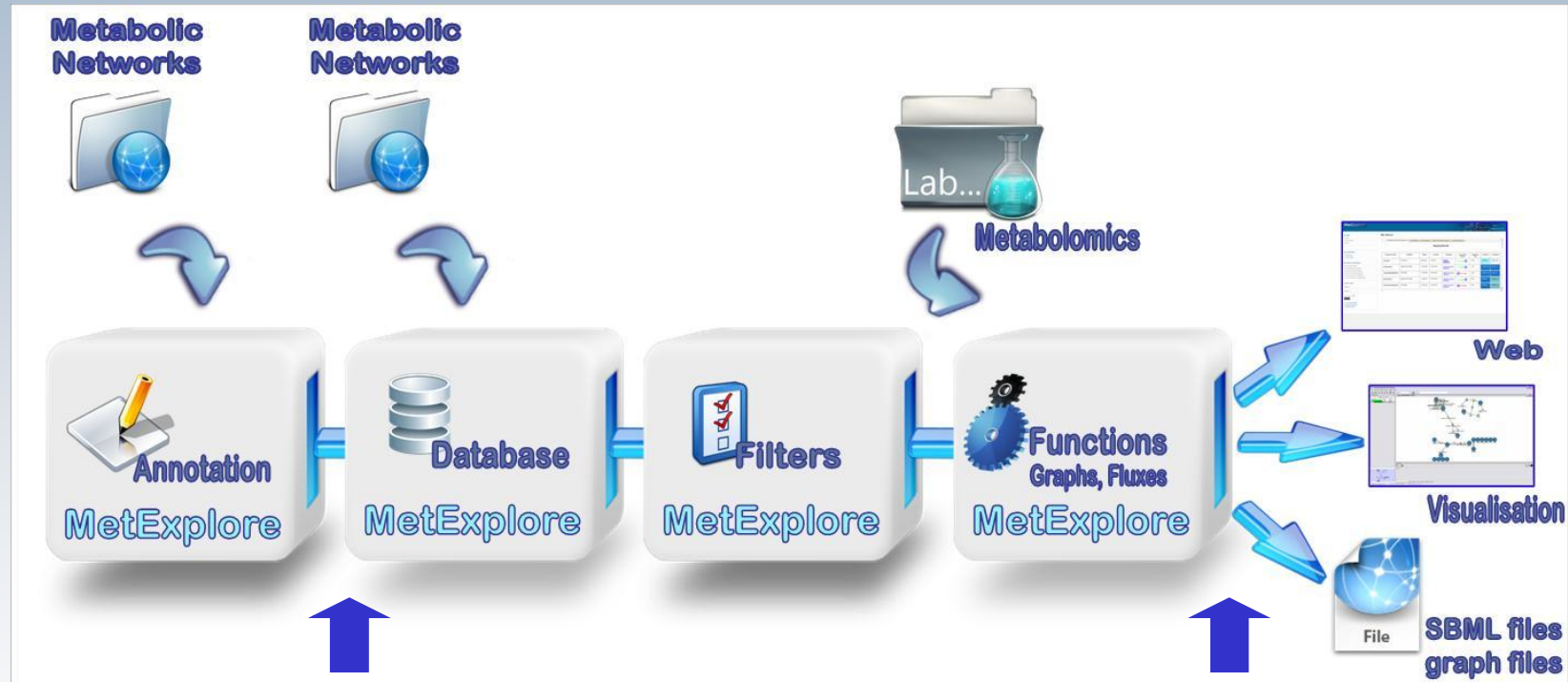
Metabolite profiling, biomedical diagnostics, physiological markers



Overall strategy combining full-scan mass spectrometry analyses of metabolites and targeted analysis. Physiological markers are identified in HTP-manner with MRM MS technology.

Integrative approach combining genome sequencing, dynamic modeling and *omics* analysis. EFM-elementary flux models, FBA- flux balance analysis MCA-metabolic control analysis.

MetExplore: a web server to link metabolomic experiments and genome-scale metabolic networks

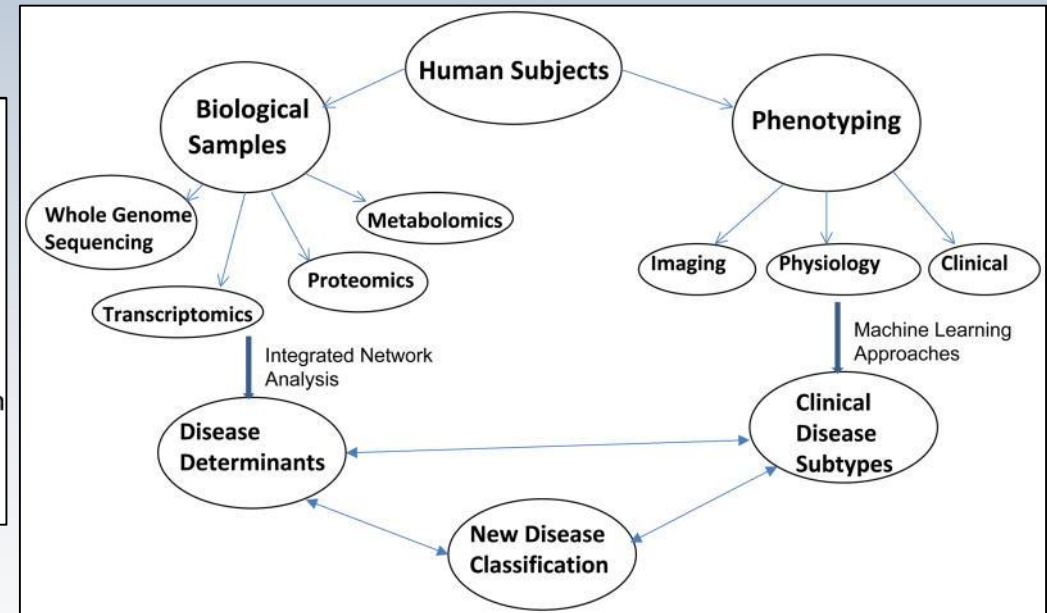
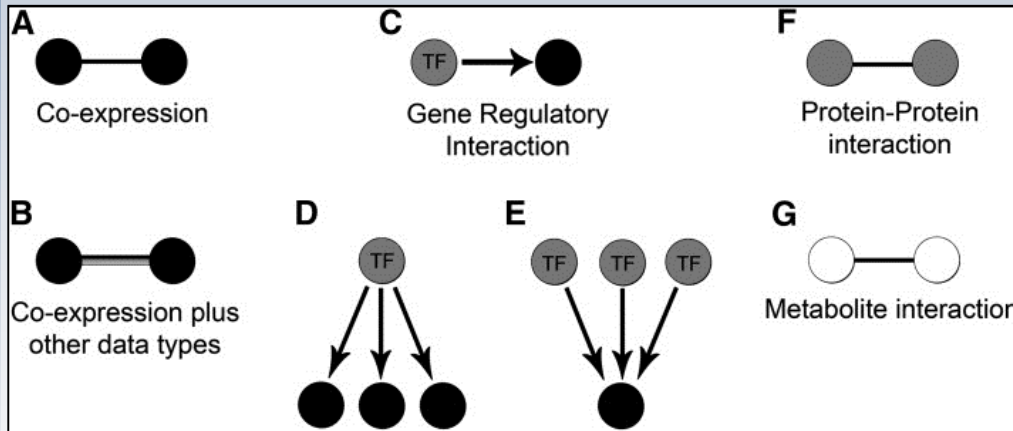


Metabolic networks from ~200 organisms

<http://metexplore.toulouse.inra.fr>

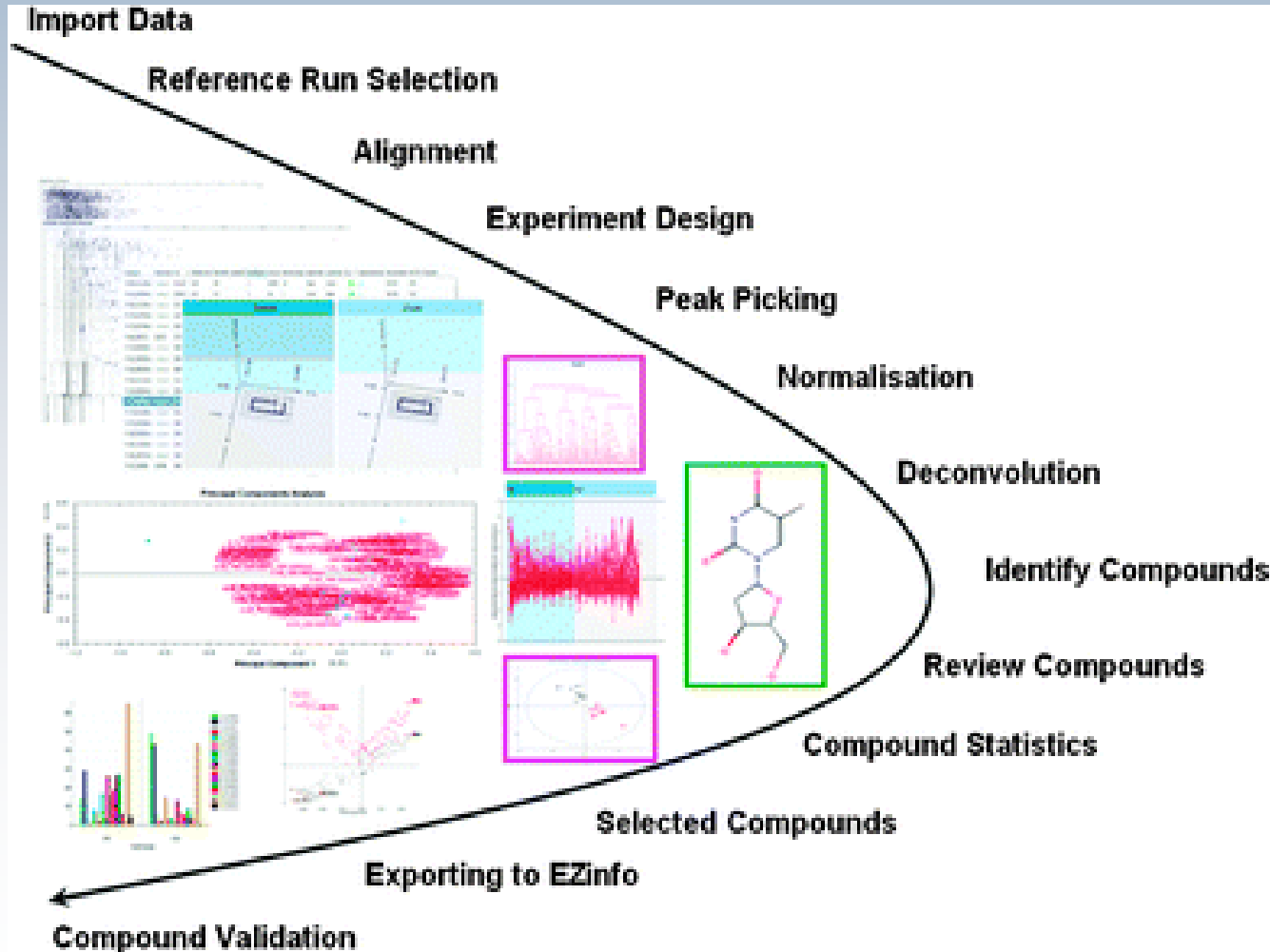
- Maps lists of metabolites to genome-inferred metabolic networks
- Provides computational functions that allow investigation of features, e.g. potential drug targets

Network medicine approaches to the genetics of complex diseases



<http://www.youtube.com/watch?v=6EbWdWa2rF0>

Rapidly improved determination of metabolites from biological data sets using the high-efficient TransOmics software tool



Detailed analysis workflow
of TransOmics
informatics
for metabolomics
(Waters/Nonlinear)

The detailed information for identification of metabolites by TransOmics software online

A

Compound	Neutral mass	m/z	z	Retention time	Peak Width	Accepted ID	Identifications	Anova (p)	Max fold change	Highest mean	Lowest mean	Tag	Isotope distribution	Max Abundance	Min CV%	Description
4.86_191.1145m/z	<unknown>	191.1145	1	4.86	0.08		1	0.00296	2.6	Model	Control	●		647.2017	45.74	
4.91_220.0010m/z	<unknown>	220.0010	1	4.91	0.10		1	0.41	1	Control	Model	●		966.7981	51.82	
5.09_215.1187m/z	<unknown>	215.1187	1	5.09	0.07		1	0.677	1.07	Control	Model	●		294.0438	28.65	
4.79_231.0754m/z	<unknown>	231.0754	1	4.79	0.08		1	0.193	6.31	Model	Control	●		403.8447	31.41	
4.79_203.0794m/z	<unknown>	203.0794	1	4.79	0.08		1	0.675	9.94	Model	Control	●		241.9278	48.81	
4.84_254.0571n	254.0571	277.0469	1	4.84	0.10		1	0.39	1.16	Control	Model	●		2378.6927	23.17	
5.18_268.0694m/z	<unknown>	268.0694	1	5.18	0.15		1	6.3E-05	3.18	Control	Model	●		2662.4642	36.48	
5.81_238.0083m/z	<unknown>	238.0083	1	5.81	0.04		1	0.352	1.24	Model	Control	●		238.0212	50.46	
5.84_288.0626m/z	<unknown>	288.0626	1	5.84	0.06		1	0.348	1.24	Control	Model	●		678.9418	44.36	
5.94_313.1112m/z	<unknown>	313.1112	1	5.94	0.09		1	0.148	1.96	Model	Control	●		993.7521	36.32	
5.26_300.0834m/z	<unknown>	300.0834	1	5.26	0.08		1	0.274	1.66	Control	Model	●		640.7929	39.32	
5.77_243.0989m/z	<unknown>	243.0989	1	5.77	0.15		1	0.0293	3.42	Model	Control	●		2342.7042	58.72	
5.78_291.1306m/z	<unknown>	291.1306	1	5.78	0.06		1	0.000858	1.44	Control	Model	●		565.3010	16.54	
4.78_220.0106m/z	<unknown>	220.0106	1	4.78	0.13		1	4.46E-05	6.42	Control	Model	●		2608.7112	59.02	
3.88_258.0839m/z	<unknown>	258.0839	1	3.88	0.04		1	0.0252	1.92	Model	Control	●		219.1541	30.12	
3.90_121.0323m/z	<unknown>	121.0323	1	3.90	0.12		1	0.218	1.2	Model	Control	●		967.6142	23.88	
3.98_128.0715m/z	<unknown>	128.0715	1	3.98	0.05		1	0.016	2.66	Model	Control	●		82.4211	75.98	
3.67_163.0664n	163.0664	164.0742	1	3.67	0.21		1	0.0399	1.53	Model	Control	●		3439.5021	27.60	

B

Compound 5.77_243.0989m/z

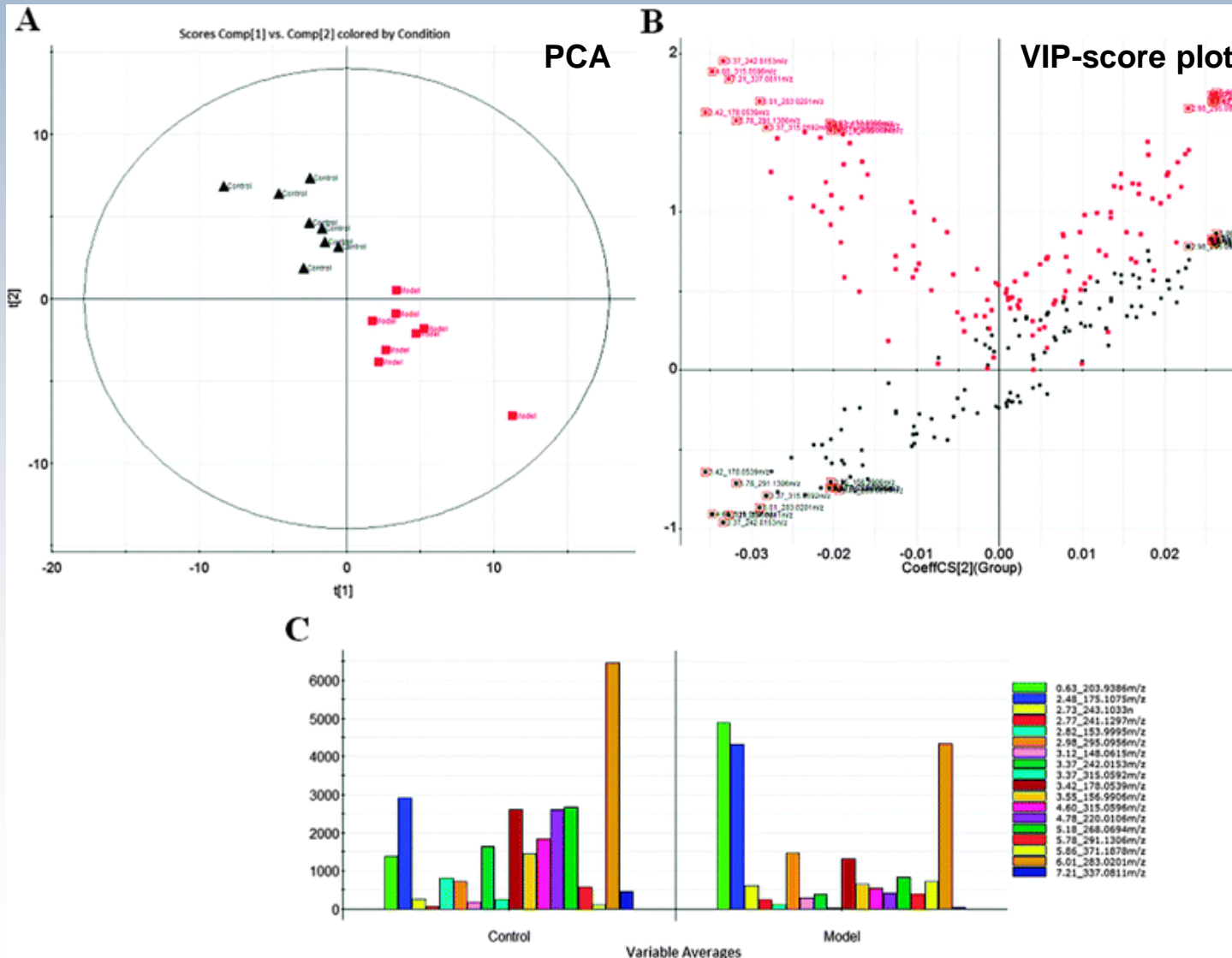
Compound abundance Possible identifications (1) 3D Montage

Compound ID	Description	Adducts	Formula	Retention time	Score	Mass error (ppm)	Isotope similarity	Link
HMD000273	Thymidine	M+H	C ₁₁ H ₁₄ N ₂ O ₅	63.9	3.24	95.41		ncmlms

Control

Model

Compound statistics (EZinfo)



Ezinfo software for compound statistics (PCA) and Orthogonal Projections to Latent Square Discriminant Analysis (OPLS-DA), correlation analysis and compound validation

Orthogonal partial least square discriminant analysis finds a linear regression model by projecting the predicted variables and the observable variables to a new space OPLS-DA (2002) works best with discrete variables in classification and biomarker studies

**Assigned:
17 features in 14 KEGG pathways**

Procedures of Reconstruction of Signal Flow in the Trans-Omic Network of Acute Insulin Action (< 60 minutes)

FAO cells

Simultaneous measurement of 304 metabolites, 7,277 P-sites on 3,458 proteins 19,778 RNA probes

