

Web-based Bioinformatics Applications

Joint Lecture GBS 722 and BMG 744

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February 1, 2012

Philosophical underpinnings ...

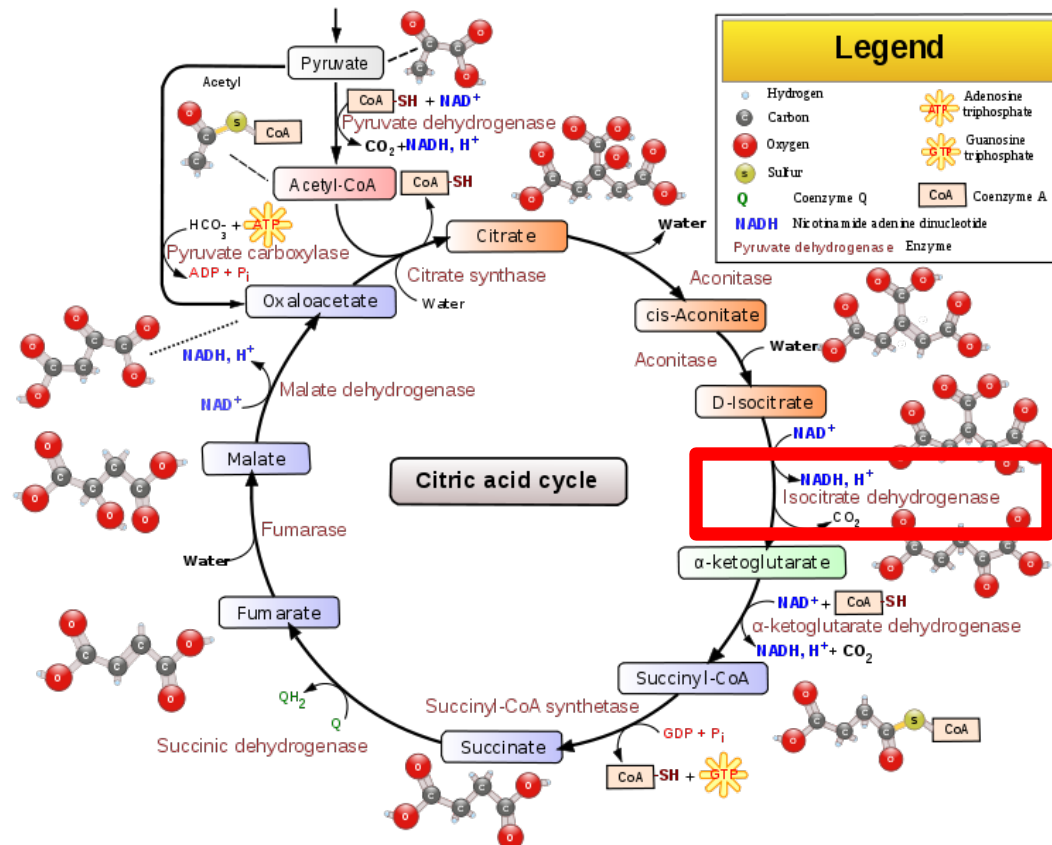
- Bioinformatics is here to stay—simply because computers are part of everyday life. This is not going to change in the near or distant future
- Students, researchers, etc., will be better served embracing bioinformatics ideas even if they do not necessarily want to pursue bioinformatics-driven careers, and opt to be “bench” scientists
- There is significant tool development that will allow scientists to access these to enhance their research (data-analysis, information dissemination, etc.) without having to recourse to collaborations with bioinformatics specialists—unless if specific tools have to be developed
- One should not ignore the intellectualism that goes into conceptualizing and developing tools
- It makes sense then to be able to access and understand how to use these tools

Interoperability & Database Accessibility

- **Interoperability:** the ability of systems to interoperate, that is exchange information in meaningful ways without having to reproduce information
- **Database Accessibility:** Access relevant information that is stored within the database architecture ONCE, but accessed and presented from different sources

Theme of the today's class—web-based proteomics applications

- **Isocitrate dehydrogenase** ([EC 1.1.1.42](#)) and ([EC 1.1.1.41](#)), also known as **IDH**, is an enzyme that participates in the citric acid cycle. It catalyzes the third step of the cycle: the oxidative decarboxylation of isocitrate, producing alpha-ketoglutarate (α -ketoglutarate) and CO_2 while converting NAD^+ to NADH .



NCBI (National Center for Biotechnology Information)

<http://www.ncbi.nlm.nih.gov/>

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Biotechnology Information

Search

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Site Map (A-Z)

All Resources

Chemicals & Bioassays

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DNA & RNA

Domains & Structures

Genes & Expression

Genetics & Medicine

Genomes & Maps

Homology

Literature

Proteins

Sequence Analysis

Taxonomy

Training & Tutorials

Variation

Welcome to NCBI

The National Center for Biotechnology Information advances science and health by providing access to biomedical and genomic information.

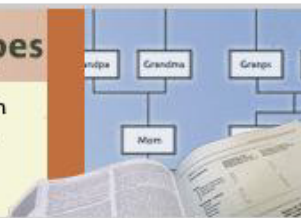
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- [Downloads](#): Get NCBI data or software
- [How-To's](#): Learn how to accomplish specific tasks at NCBI
- [Submissions](#): Submit data to GenBank or other NCBI databases

Genotypes and Phenotypes

Data from Genome Wide Association studies that link genes and diseases. See study variables, protocols, and analysis.



1 2 3 4

Popular Resources

- [BLAST](#)
- [Bookshelf](#)
- [Gene](#)
- [Genome](#)
- [Nucleotide](#)
- [OMIM](#)
- [Protein](#)
- [PubChem](#)
- [PubMed](#)
- [PubMed Central](#)
- [SNP](#)

NCBI News

[NCBI Discovery Workshop: A Practical Hands-On Course](#)

18 Jan 2011

February 15-16, 2011 @ NLM:
Space is still available in the 2-day

[NAR's 2011 Database Issue is out with 9 NCBI-Authored Papers](#)

05 Jan 2011

New articles are available
describing the new Epigenomics

[More...](#)

Selected Applications through NCBI

- GenBank—resource for genes
- BioSystems
- BLAST
- Pubmed
- Computational Resources from NCBI's Structure Group
- Conserved Domain Database (CDD)
- Peptidome
- Protein Clusters
- Protein Database
- Structure (Molecular Modeling Database)

Genbank (Search Nucleotide)

The image shows a screenshot of the NCBI GenBank Overview page. At the top left is the NCBI logo. To its right is the title 'GenBank Overview'. Below this is a navigation bar with links for PubMed, Entrez, BLAST, OMIM, Books, Taxonomy, and Structure. A search bar is present with a dropdown menu set to 'Nucleotide', a text input field containing 'isocitrate dehydrogenase', and a 'Go' button. On the left side, there is a vertical menu with links: NCBI Home, NCBI Site Map, Submit to GenBank, Submit an update, Search GenBank, GenBank and RefSeq: a comparison, and BLAST. The main content area has a heading 'What is GenBank?' followed by a paragraph describing the database's scope and a link to release notes. Below that is another paragraph about the International Nucleotide Sequence Database Collaboration. A third paragraph provides an example of a GenBank record. A section titled 'In The News: 2009 H1N1 Flu Virus (Swine Flu)' follows, with a paragraph about the CDC and other health officials tracking the virus. At the bottom, there is a section 'NLN/NCBI 2009 H1N1 Flu Resources:' with a bulleted list of links. To the right of this list is a 'FLU.GOV' widget with a 'VISIT FLU.GOV' button and a 'SHARE THIS WIDGET' link.

NCBI

GenBank Overview

PubMed Entrez BLAST OMIM Books Taxonomy Structure

Search Nucleotide for isocitrate dehydrogenase Go

NCBI Home
NCBI Site Map
Submit to GenBank
Submit an update
Search GenBank
GenBank and RefSeq:
a comparison
BLAST

What is GenBank?

GenBank[®] is the NIH genetic sequence database, an annotated collection of all publicly available DNA sequences (*Nucleic Acids Research*, 2008 Jan;36(Database issue):D25-30). There are approximately 106,533,156,756 bases in 108,431,692 sequence records in the traditional GenBank divisions and 148,165,117,763 bases in 48,443,067 sequence records in the WGS division as of August 2009.

The complete [release notes](#) for the current version of GenBank are available on the NCBI ftp site. A new release is made every two months. GenBank is part of the [International Nucleotide Sequence Database Collaboration](#), which comprises the DNA DataBank of Japan (DDBJ), the European Molecular Biology Laboratory (EMBL), and GenBank at NCBI. These three organizations exchange data on a daily basis.

An example of a GenBank [record](#) may be viewed for a *Saccharomyces cerevisiae* gene.

In The News: 2009 H1N1 Flu Virus (Swine Flu)

The Centers for Disease Control and Prevention and other health officials are actively tracking the recent emergence of human cases of swine influenza A (H1N1) virus infection. Influenza A virus sequences from patients affected by this strain are being submitted to GenBank and can be accessed through the [NCBI Flu Resource](#)

NLM/NCBI 2009 H1N1 Flu Resources:

- Newest [2009 H1N1 influenza A sequences](#)
- Citations [recently added](#) to PubMed
- [MedlinePlus \(consumer health information\)](#)
- [Enviro-Health Links](#)

FLU.GOV
Know what to do about the flu.
VISIT FLU.GOV
SHARE THIS WIDGET

Nucleotide-Genbank's gene repository

NCBI Resources How To My NCBI Sign In

Nucleotide Alphabet of Life

Search: Nucleotide

Save search Limits Advanced search Help

isocitrate dehydrogenase and Human Search Clear

Display Settings: Summary, 20 per page, Sorted by Default order Send to:

Found 1702 nucleotide sequences. Nucleotide (1227) EST (475)

Gene Information

This search in Gene shows 36 results, including:

- [IDH3B](#) (*Homo sapiens*): isocitrate dehydrogenase 3 (NAD+) beta
- [IDH1](#) (*Homo sapiens*): isocitrate dehydrogenase 1 (NADP+), soluble
- [IDH2](#) (*Homo sapiens*): isocitrate dehydrogenase 2 (NADP+), mitochondrial

Gene

Filter your results:

All (1227)

[Bacteria \(801\)](#)

[INSDC \(GenBank\) \(696\)](#)

[mRNA \(159\)](#)

[RefSeq \(531\)](#)

[Manage Filters](#)

Top Organisms [Tree]

[Homo sapiens \(133\)](#)

[Coxiella burnetii \(27\)](#)

[Mus musculus \(20\)](#)

[Leishmania infantum \(18\)](#)

[synthetic construct \(18\)](#)

[All other taxa \(1012\)](#)

[More...](#)

Results: 1 to 20 of 1227

<< First < Prev Page 1 of 62 Next > Last >>

- [Streptococcus anginosus 1_2_62CV genomic scaffold supercont1.1, whole genome shotgun sequence](#)
 - 1,137,758 bp linear DNA
GL636615.1 GI:320042214
[GenBank](#) [FASTA](#) [Graphics](#)
- [Coprobacillus sp. 29_1 genomic scaffold supercont1.1, whole genome shotgun sequence](#)
 - 953,248 bp linear DNA
GL636577.1 GI:320042207
[GenBank](#) [FASTA](#) [Graphics](#)
- [Mus musculus lactate dehydrogenase A \(Ldha\), transcript variant 2, mRNA](#)
 - 1,854 bp linear mRNA
NM_001136069.2 GI:257743038
[GenBank](#) [FASTA](#) [Graphics](#) [Related Sequences](#)
- [Homo sapiens isocitrate dehydrogenase 2 \(NADP+\), mitochondrial \(IDH2\), nuclear gene encoding mitochondrial protein, mRNA](#)
 - 1,740 bp linear mRNA
NM_002168.2 GI:28178831
[GenBank](#) [FASTA](#) [Graphics](#) [Related Sequences](#)

Find related data

Database: Select

[Find items](#)

Search details

```
isocitrate dehydrogenase[All  
Fields] AND ("Homo sapiens"  
[Organism] OR Human[All Fields])
```

Accession Number

A Nucleotide Entry in Genbank

NCBI Resources Help How To

Nucleotide

Alphabet of Life

Search Nucleotide Limits Advanced search Help

Search Clear

Display Settings: GenBank

Send

Homo sapiens isocitrate dehydrogenase 2 (NADP+), mitochondrial (IDH2), nuclear gene encoding mitochondrial protein, mRNA

NCBI Reference Sequence: NM_002168.2

FASTA Graphics

Go to

LOCUS NM_002168 1740 bp mRNA linear PRI 23-JAN-2011

DEFINITION Homo sapiens isocitrate dehydrogenase 2 (NADP+), mitochondrial (IDH2), nuclear gene encoding mitochondrial protein, mRNA.

ACCESSION NM_002168

VERSION NM_002168.2 GI:28178831

KEYWORDS

SOURCE Homo sapiens (human)

ORGANISM [Homo sapiens](#)
Eukaryota; Metazoa; Chordata; Craniata; Vertebrata; Euteleostomi; Mammalia; Eutheria; Euarchontoglires; Primates; Haplorhini; Catarrhini; Hominoidea; Homo.

REFERENCE 1 (bases 1 to 1740)

AUTHORS Patel,K.P., Ravandi,F., Mo,D., Paidugala,A., Barkob,B.A., Medeiros,L.J. and Luthra,R.

TITLE Acute myeloid leukemia with IDH1 or IDH2 mutation: frequency and clinicopathologic features

JOURNAL Pubmed 21173122

REMARK **COMMENT:** We conclude that IDH1 (R) (1) (3) (2) and IDH2 (R) (1) (2) mutations occur most often in cytogenetically normal acute myeloid leukemia cases with an overall frequency of approximately 11.8%.

REFERENCE 2 (bases 1 to 1740)

AUTHORS Figueroa,M.E., Abdel-Wahab,O., Lu,C., Ward,P.S., Patel,J., Shih,A., Li,Y., Bhagwat,N., Vasanthakumari,A., Fernandez,H.F., Tallman,M.S., Sun,Z., Wolniak,K., Peeters,J.K., Liu,W., Choe,S.E., Pantin,V.R., Fausch,S., Lowenberg,B., Licht,J.D., Godley,L.A., Delwel,W., Valk,A.J., Thompson,C.B., Levine,R.L. and Melnick,A.

TITLE Leukemic IDH1 and IDH2 mutations result in a hypermethylation phenotype, disrupt TET2 function, and impair hematopoietic differentiation

JOURNAL Pubmed 21130701

REMARK **GENE:** Leukemic IDH1 and IDH2 mutations result in a hypermethylation phenotype, disrupt TET2 function, and impair hematopoietic differentiation.

REFERENCE 3 (bases 1 to 1740)

AUTHORS Metelitsa,P., Coulibaly,S., Colin,C., de Paula,A.M., Vasiljevic,A., Taiab,D., Farlier,A., Boisselier,S., Mokhtari,K., Wang,Y.H., Loundou,A., Chapon,F., Pineau,S., Ouaif,K.L., Chinot,O. and Figarilli-Bauger,D.

TITLE Absence of IDH mutation identifies a novel radiologic and molecular subtype of WHO grade II gliomas with dismal prognosis

JOURNAL Pubmed 21080178

REMARK **GENE:** Observational study of gene-disease association. (BioRx Nov14/2011)

DIFFFSPM/4 (bases 1 to 1740)

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RQ"
```

Protein Sequence

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1621 ggcaggagca gtcgctttta cctcagccag tcagtatggt ttatcactag taatttatat  
1681 tgcctttgga acacatgggt ccatatttag ctactaaaaa gctcttccca aaaaaaaaaa  
//
```

Links to Pubmed

Gene Sequence

Protein Sequence in Genbank (isocitrate dehydrogenase)

NCBI Resources How To

Protein
Translations of Life

Search: Protein

Save search Limits Advanced search Help

isocitrate dehydrogenase and Human

Search Clear

Display Settings: Summary, 20 per page, Sorted by Default order

Send to:

Gene Information

This search in Gene shows 36 results, including:

- [IDH3B](#) (*Homo sapiens*): isocitrate dehydrogenase 3 (NAD+) beta
- [IDH1](#) (*Homo sapiens*): isocitrate dehydrogenase 1 (NADP+), soluble
- [IDH2](#) (*Homo sapiens*): isocitrate dehydrogenase 2 (NADP+), mitochondrial

Gene

Results: 1 to 20 of 603

<< First < Prev Page 1 of 31 Next > Last >>

- [isocitrate dehydrogenase \[Homo sapiens\]](#)
1. 419 aa protein
AAC50455.1 GI:1277203
[GenPept](#) [FASTA](#) [Graphics](#) [Related Sequences](#) [Identical Proteins](#)
- [isocitrate dehydrogenase \[Corynebacterium jeikeium K411\]](#)
2. 742 aa protein
YP_251488.1 GI:68536783
[GenPept](#) [FASTA](#) [Graphics](#) [Related Sequences](#) [Identical Proteins](#)
- [isocitrate dehydrogenase \[Francisella tularensis subsp. holarctica OSU18\]](#)
3. 747 aa protein
YP_763190.1 GI:115314467
[GenPept](#) [FASTA](#) [Graphics](#) [Related Sequences](#) [Identical Proteins](#)
- [isocitrate dehydrogenase \[Corynebacterium jeikeium K411\]](#)
4. 742 aa protein
CAI37870.1 GI:68264382
[GenPept](#) [FASTA](#) [Graphics](#) [Related Sequences](#) [Identical Proteins](#)

NCBI Resources How To

Protein
Translations of Life

Search: Protein

Limits Advanced search Help

Search Clear

Display Settings: GenPept

Send to:

isocitrate dehydrogenase [Homo sapiens]

GenBank: AAC50455.1

[FASTA](#) [Graphics](#)

Go to:

LOCUS AAC50455 419 aa linear PRI 25-APR-1996

DEFINITION isocitrate dehydrogenase [Homo sapiens].

ACCESSION AAC50455

VERSION AAC50455.1 GI:1277203

DBSOURCE locus HSU52144 accession [US2144.1](#)

KEYWORDS .

SOURCE Homo sapiens (human)

ORGANISM [Homo sapiens](#)
Eukaryota; Metazoa; Chordata; Craniata; Vertebrata; Euteleostomi; Mammalia; Eutheria; Euarchontoglires; Primates; Haplorrhini; Catarrhini; Hominidae; Homo.

REFERENCE 1 (residues 1 to 419)
Luo, H., Shan, X. and Wu, J.
TITLE Expression of human mitochondrial NADP-dependent isocitrate dehydrogenase during lymphocyte activation
J. Cell. Biochem. 60 (4), 495-507 (1996)
PUBMED [8707889](#)

REFERENCE 2 (residues 1 to 419)
Wu, J.
TITLE Direct Submission
Submitted (22-MAR-1996) Jiangping Wu, Notre-Dame Hospital Research Center, University of Montreal, 1560 Sherbrooke East, Montreal, Quebec H2L 4M1, Canada

COMMENT Method: conceptual translation.

FEATURES
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121 ckniprlypg wkyptcigrh shdqykatcd fvadragtjk nvrtpkdgsg vkesevynfp
181 agvgvgnvyn tesisgfhah scfgyalqkk uplymetknt ilkaydrkk difqefidkh
241 ykdfdknki vyehlidda vaqrlkassg fvwacknydg dvqsdilagg fsglimgtvs
301 lvcpgdkttie aaahgtvtr hyrehgkgrp tstnpiasif avtrglehrg kidgnqdir
361 faqplekvcv evtesgamtk dlagcibgis nvklnehfln ttdflditiks nidraigrq
//

Note that the protein sequence and the rest of the entries are formatted similar to that of the nucleotide sequences in Genbank. This is a database architecture issue.

BioSystems

BioSystems

BioSystems

Limits Advanced

Display Settings: Abstract

Send to:

[Citric acid cycle \(TCA cycle\)](#)

In the citric acid or tricarboxylic acid (TCA) cycle, the acetyl group of acetyl CoA (derived primarily from oxidative decarboxylation of pyruvate, beta-oxidation of long-chain fatty acids, and catabolism of ketone bodies and several amino acids) can be completely oxidized to CO₂ in reactions that also yield one high-energy phosphate bond (as GTP or ATP) and four reducing equivalents (three NADH + H⁺, and one FADH₂). The NADH and FADH₂ are then oxidized by the electron transport chain to yield nine more high-energy phosphate bonds (as ATP). All reactions of the **citric acid cycle** take place in the mitochondrion. Eight canonical reactions mediate the synthesis of citrate from acetyl-CoA and oxaloacetate and the metabolism of citrate to re-form oxaloacetate. Six additional reactions are included here. Three reversible reactions, the interconversions of citrate and isocitrate, of fumarate and malate, and of malate and oxaloacetate are annotated in both their canonical (forward) and reverse directions. The synthesis of succinate from succinyl-CoA can be coupled to the phosphorylation of either GDP (the canonical reaction) or ADP; both reactions are annotated. Two mitochondrial isocitrate dehydrogenase isozymes catalyze the oxidative decarboxylation of isocitrate to form alpha-ketoglutarate (2-oxoglutarate): IDH3 catalyzes the canonical reaction coupled to the reduction of NAD⁺, while IDH2 catalyzes the same reaction coupled to reduction of NADP⁺, a reaction whose normal physiological function is unclear. Both reactions are annotated. Finally, a reaction is annotated in which reducing equivalents are transferred from NADPH to NAD⁺ coupled to proton import across the inner mitochondrial membrane. The cyclical nature of the reactions responsible for the oxidation of acetate was first suggested by Hans Krebs, from biochemical studies of pigeon breast muscle (Krebs et al. 1938; Krebs and Eggleston 1940). Many of the molecular details of individual reactions were worked out by Ochoa and colleagues, largely through studies of enzymes purified from pig heart (Ochoa 1980). While the human homologues of these enzymes have all been identified, their biochemical characterization has in general been limited and many molecular details of the human reactions are inferred from those worked out in studies of the model systems.

Type: pathway Taxonomic scope: organism-specific biosystem Organism: [Homo sapiens](#)

BSID: 105919 [REACTOME: REACT_1785](#)

Diagram not available [?](#)

Genes	Proteins	Small Molecules	Related BioSystems	Citations	Comments
View or save all or selected records in Entrez Gene Clear Selections ?					
<input type="checkbox"/>	Gene ID	Gene Symbol	External ID	Name	
<input type="checkbox"/>	50	ACO2	49554	aconitase 2, mitochondrial	
<input type="checkbox"/>	1431	CS	52130	citrate synthase	
<input type="checkbox"/>	1738	DLD	53720	dihydropyrimidine dehydrogenase	
<input type="checkbox"/>	1743	DLST	60870	dihydropyrimidine S-succinyltransferase (E2 component of 2-oxo-glutarate complex)	
<input type="checkbox"/>	2271	FH	55030	fumarate hydratase	
<input type="checkbox"/>	3418	IDH2	57070	isocitrate dehydrogenase 2 (NADP+), mitochondrial	
<input type="checkbox"/>	3419	IDH3A	57062	isocitrate dehydrogenase 3 (NAD+) alpha	
<input type="checkbox"/>	3420	IDH3B	57064	isocitrate dehydrogenase 3 (NAD+) beta	

BLAST Results

NCBI/BLAST/blastp suite/Formatting Results - JH7C44JT016

[Edit and Resubmit](#) [Save Search Strategies](#) [Formatting options](#) [Download](#)

gi|47938312|gb|AAH71828.1| Isocitrate dehydrogenase

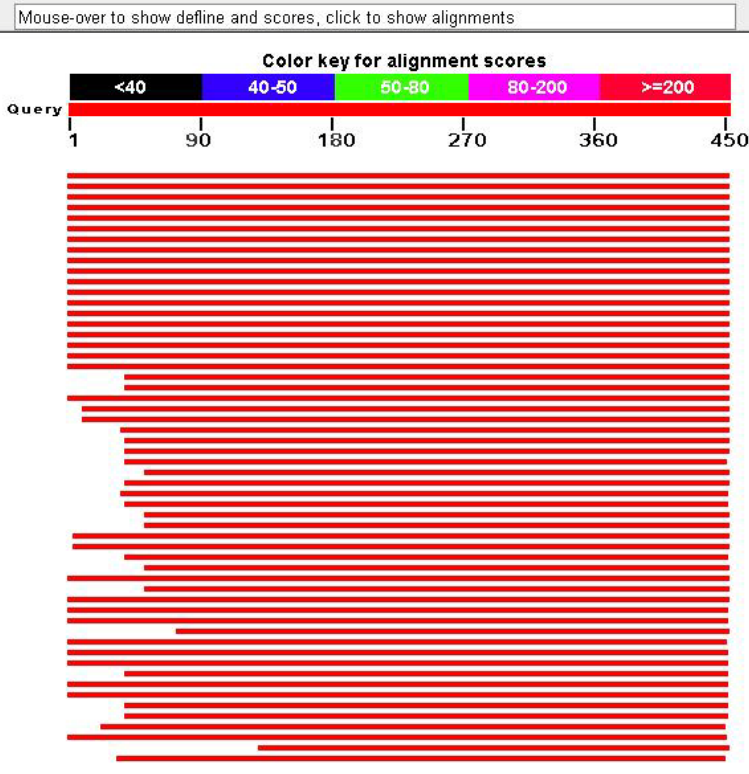
Query ID lc|46523
Description gi|47938312|gb|AAH71828.1| Isocitrate dehydrogenase 2 (NADP+), mitochondrial [Homo sapiens]
Molecule type amino acid
Query Length 452

Database Name nr
Description All non-redundant GenBank CDS translations+PDB+SwissProt+PIR+PRF excluding environmental samples from WGS projects
Program BLASTP 2.2.26+ [Citation](#)

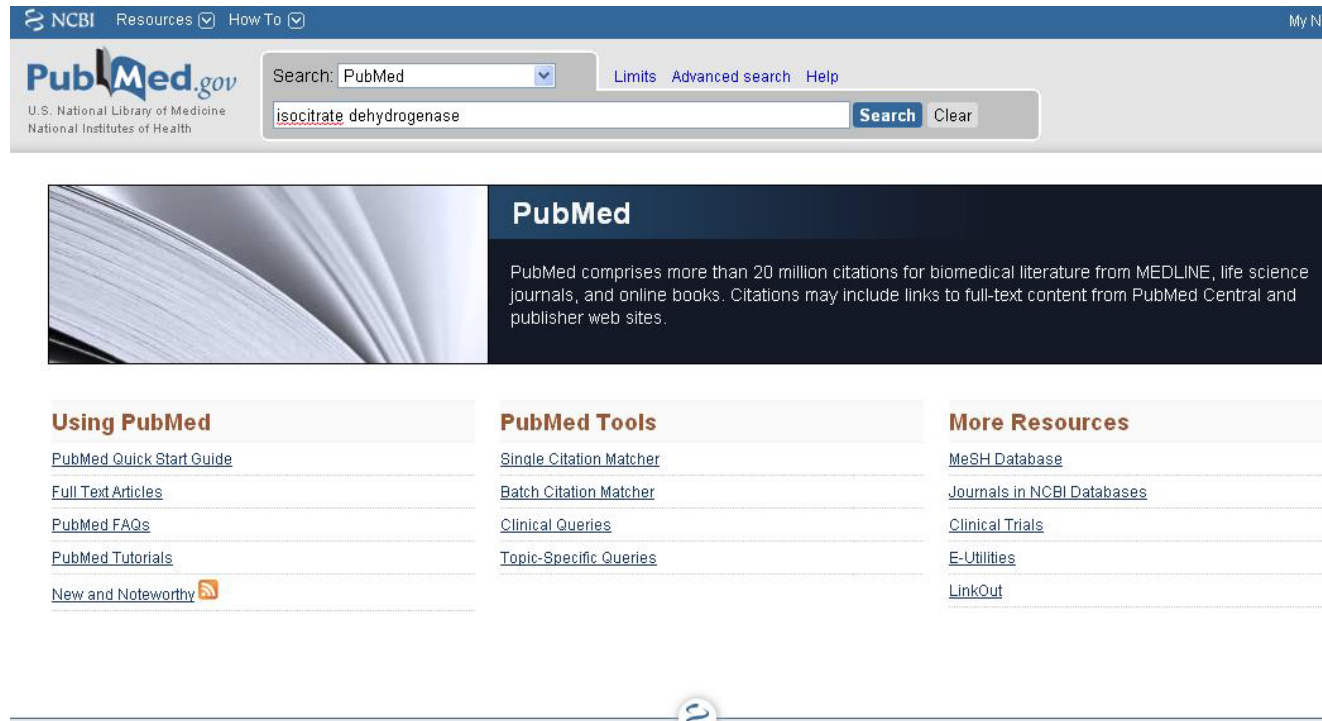
Other reports: [Search Summary](#) [Taxonomy reports](#) [Distance tree of results](#) [Related Structures](#) [Multiple alignment](#)

Graphic Summary

Distribution of 100 Blast Hits on the Query Sequence



Pubmed—repository of biomedical abstracts



The screenshot shows the PubMed.gov website interface. At the top, there is a navigation bar with "NCBI Resources" and "How To" menus. The main header features the PubMed.gov logo and the text "U.S. National Library of Medicine National Institutes of Health". A search bar is prominently displayed with the text "isocitrate dehydrogenase" entered. To the right of the search bar are links for "Limits", "Advanced search", and "Help". Below the search bar, there is a "Search" button and a "Clear" button. A large banner image of a book is on the left, and a dark blue box on the right contains the text: "PubMed comprises more than 20 million citations for biomedical literature from MEDLINE, life science journals, and online books. Citations may include links to full-text content from PubMed Central and publisher web sites." Below this banner, there are three columns of links: "Using PubMed" (PubMed Quick Start Guide, Full Text Articles, PubMed FAQs, PubMed Tutorials, New and Noteworthy), "PubMed Tools" (Single Citation Matcher, Batch Citation Matcher, Clinical Queries, Topic-Specific Queries), and "More Resources" (MeSH Database, Journals in NCBI Databases, Clinical Trials, E-Utilities, LinkOut).

Information in Pubmed is available in several formats.

Abstracts can be downloaded 500 at a time

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NCBI has made several utility tools available to automatically download abstracts

A single Abstract in Pubmed

NCBI Resources How To

PubMed.gov
U.S. National Library of Medicine
National Institutes of Health

Search: PubMed

Limits Advanced search Help

isocitrate dehydrogenase Search Clear

Display Settings: Abstract

Send to:

Biochem Biophys Res Commun. 2011 Jan 22. [Epub ahead of print]

Ataxia telangiectasia mutated influences cytochrome c oxidase activity.

Patel AY, Macdonald TM, Spears LD, Ching JK, Fisher JS.

Department of Biology, Saint Louis University, St. Louis, MO 63103, USA.

Abstract

Cells lacking ataxia telangiectasia mutated (ATM) have impaired mitochondrial function. Furthermore, mammalian cells lacking ATM have increased levels of reactive oxygen species (ROS) as well as mitochondrial DNA (mtDNA) deletions in the region encoding for cytochrome c oxidase (COX). We hypothesized that ATM specifically influences COX activity in skeletal muscle. COX activity was ~40% lower in tibialis anterior from ATM-deficient mice than for wild-type mice ($P < 0.01$, $n = 9/\text{group}$). However, there were no ATM-related differences in activity of succinate dehydrogenase, isocitrate dehydrogenase, alpha-ketoglutarate dehydrogenase, mitochondrial glycerol 3-phosphate dehydrogenase, or complex III. Incubation of wild-type extensor digitorum longus muscles for 1 h with the ATM inhibitor KU55933 caused a ~50% reduction ($P < 0.05$, $n = 5/\text{group}$) in COX activity compared to muscles incubated with vehicle alone. Among the control muscles and muscles treated with the ATM inhibitor, COX activity was correlated ($r = 0.61$, $P < 0.05$) with activity of glucose 6-phosphate dehydrogenase, a key determinant of antioxidant defense through production of NADPH. Overall, the findings suggest that ATM has a protective role for COX activity.




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PMID: 21266166 [PubMed - as supplied by publisher]

Computational Resources from NCBI's Structure Group

<http://www.ncbi.nlm.nih.gov/Structure/index.shtml>

Three-dimensional structure views in Genbank-- STRUCTURE

All Databases PubMed Nucleotide Protein Genome Structure OMIM PMC Journals

Search Structure for [Save Search](#)

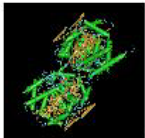

Display Summary Show 20 Sort By Send to

Links: [Literature](#), [Domains](#), [Chemicals](#), [Other Links](#)

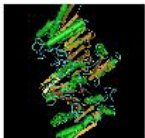

All: 98 NMR: 0 X-ray: 98

Items 1 - 20 of 98 of 5 Next

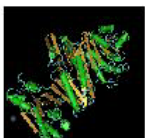

2Y42 [Domains](#), [Chemicals](#)

1:   Structure Of Isopropylmalate Dehydrogenase From Thermus Thermophilus - Complex With Nadh And Mn [Oxidoreductase, EC: 1.1.1.85]
Taxonomy: [Thermus thermophilus](#)
Proteins: 4; Chemicals: 3
modified: 2011/01/20; MMDB ID: 87988

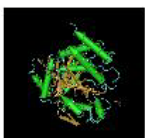

2Y41 [Domains](#), [Chemicals](#)

2:   Structure Of Isopropylmalate Dehydrogenase From Thermus Thermophilus - Complex With lpm And Mn [Oxidoreductase, EC: 1.1.1.85]
Taxonomy: [Thermus thermophilus](#)
Proteins: 2; Chemicals: 3
modified: 2011/01/20; MMDB ID: 87987

2Y40 [Domains](#), [Chemicals](#)

3:   Structure Of Isopropylmalate Dehydrogenase From Thermus Thermophilus - Complex With Mn [Oxidoreductase, EC: 1.1.1.85]
Taxonomy: [Thermus thermophilus](#)
Proteins: 2; Chemicals: 2
modified: 2011/01/20; MMDB ID: 87986

2Y3Z [Domains](#), [Chemicals](#)

4:   Structure Of Isopropylmalate Dehydrogenase From Thermus Thermophilus - Apo Enzyme [Oxidoreductase, EC: 1.1.1.85]
Taxonomy: [Thermus thermophilus](#)
Proteins: 1; Chemicals: 4
modified: 2011/01/20; MMDB ID: 87985

Structure of Actin—Genbank Structure View

Structure Summary
MMDDB

NCBI

HOME SEARCH SITE MAP Entrez Structure Protein CDD PubMed Taxonomy PubChem Help Cn3D

MMDB ID: 86995 PDB ID: 2CMJ Search PDB or MMDB ID

Description Crystal Structure Of Mouse Cytosolic Isocitrate Dehydrogenase.

Deposition: Cho HJ, Kim KJ, Huh SL, Kang BS, 2006/5/10

Taxonomy: Mus musculus

Related Structure: VAST

Structure View in Cn3D Structure View in RasMol ?

Tasks: Display Drawing: All Atoms

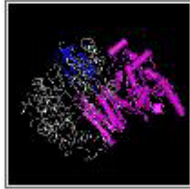
Download Cn3D View Cn3D Tutorial

Molecular components in the MMDB structure are listed below and may include macromolecular chains, 3D domains, protein classifications (domain families), and ligands, as available. Mouse over each icon for more information on the component.

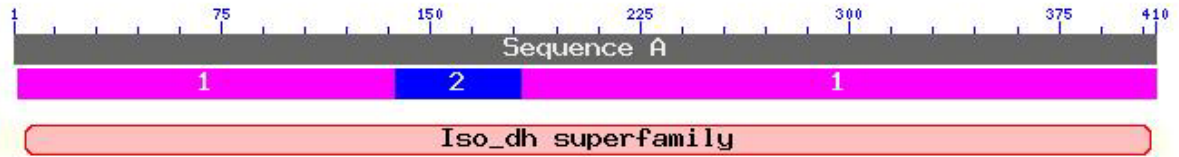
Link to Protein Databank

Visualization software

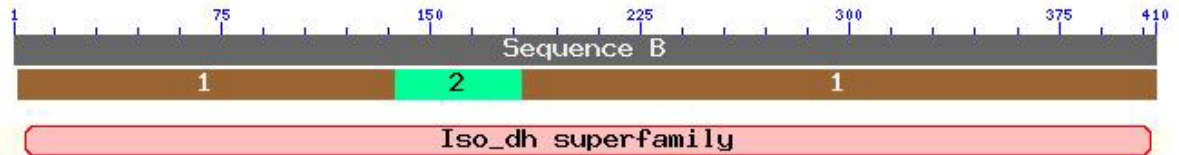
Structure of Domains in Genbank



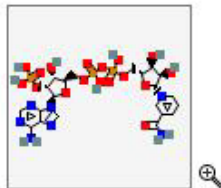
Protein
[3d Domains](#)
[Domain Families](#)
[Super Families](#)



Protein
[3d Domains](#)
[Domain Families](#)
[Super Families](#)



Chemical



NADP

2 occurrences

List of domains related to
or associated with
Isocitrate Dehydrogenase

Conserved domain database (CDD) in Genbank

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All Databases PubMed Gene HomoloGene Protein Protein Clusters Structure PubChem BioSys.

Search for

Limits Preview/Index History Clipboard Details

Conserved Domains Database RESOURCES SEARCH METHODS HOW TO HELP NEWS FTP PUBLICATIONS DISCOVER

Hints on Finding a Conserved Domain

- This page is used for searching by text term (other [search methods](#) allow queries by protein sequence)
- Enter one or more [search terms](#) (e.g., chloride channel)
- Use [search fields](#) to narrow your search ([tips](#))
- [Advanced search options](#) are available in the [Limits](#), [Preview/Index](#), and [History](#) folder tabs
- [Boolean operators](#) AND, OR, NOT must be in upper case
- Use [quotes](#) to force a phrase search (e.g., "voltage gated")
- Use a [wildcard](#) (e.g., glycol*[title]) to search for a word stem
- Search results and conserved domain records are described in the [help document](#).

About the Database



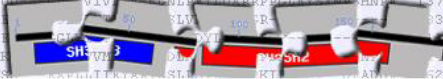
Conserved domains are functional units within a protein that have been used as building blocks in molecular evolution and recombined in various arrangements to make proteins with different functions.

The Conserved Domain Database (CDD) brings together several [collections](#) of multiple sequence alignments representing conserved domains, including [NCBI-curated domains](#), which use 3D-structure information to explicitly to define domain boundaries and provide insights into [sequence/structure/function relationships](#), as well as domain models imported from a number of [external source databases](#) (Pfam, SMART, COG, PRK, TIGRFAM).

The data are then used for putative functional annotation of [protein query](#) sequences based on matches to [specific hits](#) ([illustrated example](#)) or [superfamilies](#), identification of proteins with similar domain [architectures](#), and protein [classification](#). The Conserved Domains and Protein Classification overview page provides more information about the [resources](#) available and how they can be used.

What is a conserved domain?


CDD ...

All Databases PubMed Gene HomoloGene Protein Protein Clusters Structure PubChem

Search **Conserved Domains** for [Save Search](#)


Display **Summary** Show Sort By Send to

Links: [Related CDs](#), [Literature](#), [Sequence](#), [Structure](#), [BioSystems](#), [Other Links](#) 


All: 24 NCBI-curated: 0 families: 22 imported: 17 superfamilies: 3

Items 1 - 20 of 24 of 2 [Next](#)


[cl01891](#) [Related CDs](#), [Literature](#), [Sequence](#), [Structure](#), [Other Links](#)

1:
 AceK: Isocitrate dehydrogenase kinase/phosphatase (AceK)
This family consists of several bacterial isocitrate dehydrogenase kinase/phosphatase (AceK) proteins (EC:2.7.1.116). [186492]


[pfam06315](#) [Related CDs](#), [Literature](#), [Sequence](#), [Structure](#), [Other Links](#)

2:
 AceK: Isocitrate dehydrogenase kinase/phosphatase (AceK)
This family consists of several bacterial isocitrate dehydrogenase kinase/phosphatase (AceK) proteins (EC:2.7.1.116). [148119]

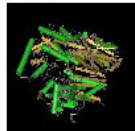
[pfam03971](#) [Literature](#), [Sequence](#), [Structure](#), [Other Links](#)

3:
 IDH: Monomeric isocitrate dehydrogenase
NADP(+)-dependent isocitrate dehydrogenase (ICD) is an important enzyme of the intermediary metabolism, as it controls the carbon flux within the citric acid cycle and supplies the cell with 2-oxoglutarate EC:1.1.1.42 and NADPH for biosynthetic purposes. [112770]

[TIGR02924](#) [Sequence](#), [Structure](#), [Other Links](#)

4:
 ICDH_alpha: isocitrate dehydrogenase
This family of mainly alphaproteobacterial enzymes is a member of the isocitrate/isopropylmalate dehydrogenase superfamily described by pfam00180. Every member of the seed of this model appears to have a TCA cycle lacking only a determined isocitrate dehydrogenase. The precise identity of the cofactor (NADH -- 1.1.1.41 vs. NADPH -- 1.1.1.42) is unclear. [163075]

[TIGR00178](#) [Literature](#), [Sequence](#), [Structure](#), [Other Links](#)

5:
 monomer_idh: isocitrate dehydrogenase, NADP-dependent, monomeric type
The monomeric type of isocitrate dehydrogenase has been found so far in a small number of species, including *Azotobacter vinelandii*, *Corynebacterium glutamicum*, *Rhodocrobium vannielii*, and *Neisseria meningitidis*. It is NADP-specific. [129282]

[TIGR00183](#) [Related CDs](#), [Sequence](#), [Structure](#), [Other Links](#)

CDD...



Conserved Domains



HOME SEARCH SITE MAP Entrez CDD Structure Protein Help

TIGR02924: ICDH_alpha

isocitrate dehydrogenase

This family of mainly alphaproteobacterial enzymes is a member of the isocitrate/isopropylmalate dehydrogenase superfamily described by pfam00180. Every member of the seed of this model appears to have a TCA cycle lacking only a determined isocitrate dehydrogenase. The precise identity of the cofactor (NADH -- 1.1.1.41 vs. NADPH -- 1.1.1.42) is unclear.

Links ?

Statistics ?

Structure ?

TIGR02924 is classified as a model that may span more than one domain.

TIGR02924 is not assigned to any domain superfamily.

Sequence Alignment

Reformat Format: Hypertext Row Display: All 6 rows Color Bits: 2.0 bit Type Selection: top listed sequences

	10	20	30	40	50	60	70	80
gi 58418940	3	TPITVAYGDGIGPEIMEAVLSMLREAEAKISIDVIEIGERVYNKEWSYGISPSGWESIERTKVLLKSPPTTSQGGHKSL	82					
gi 67004940	13	TPITVAYGDGIGPEIMEAVLYILRKAEARIRLETIEVGEKLYKKHYTSGISEESWESIQTGII LKAPITTPQGGGYSKL	92					
gi 46401058	7	IPITVAEGDGIPEIMDATLRILKAAGAPLDIKNVEIGEKVYLSGQPTGIENSTWDLIRQSKALLKAPITTPQGGGPKSL	86					
gi 68171798	3	IPITVAYGDGIGPEIMEAVLLILSEAESGLVVTIEVGHNLVYKKEWSSGIAPSSWDSIYRTKVLLKSPMTMPQGRGHKSL	82					
gi 88606810	3	VPITVAYGDGIGPEIMEAVLLILKEAQAQDI AVETAEIGHAQYKRDWPCGIAPSSWASIRRTKVLLKSPMTMPQGGGHSKL	82					
gi 88607979	2	PKLTVAYGDGVGPEIMTSVLEIIFEAGAELIQIDTIEIGQKIYKGVHSGISDSGWETLKRNVLLKAPITTPRGGGVRSL	81					
	90	100	110	120	130	140	150	160
gi 58418940	83	NVALRKSGLYANIRPCTSYHPVIENKFRDFDIVVIRENEEDVYTGIEHRLTGNSYQCTKIITRSGSEKICRYAFNYAKR	162					
gi 67004940	93	NVTIRKTLQLFANIRPSVSFHPFTMLHPLHMLTI IRENEEDLYAGIEYRQTHMMYESIKLISHTGCEKIIRYAFYAVK	172					
gi 46401058	87	NVTIRTTLGLYANVRPCVAYYFPVETKYPGMVVIVRENEEDLYTGIEYRQTPDVYEALKLITRPGCEKIIRYAFYAAQI	166					
gi 68171798	83	NVTLRKRLLGLYANIRPCISYHPVIKTRYPNLMVIVRENEEDTYTGIEHRLTNDTYQCSKVITRSGSERICDYAFHYAKV	162					
gi 88606810	83	NVALRKSGLYANVRPCVYTSPIIDTGSTNLDIVVIRENEEDTYCGVEYRISQDASVCDKITTASERLCAYAFRYARS	162					
gi 88607979	82	NVTLRKKLGLFANIRPCKSH---LEWQSPKMDIV IIRENEEDLYSGTEYRQTLDTYVCTKVITESTSERICRYAFYARK	158					
	170	180	190	200	210	220	230	240
gi 58418940	163	HNRKRVTCCLKDNIKMTDGI FHTAFDSIAKEYPD IKAHEYIVDIGMARVATEPENFDVIVTENLYGDIISDVAAQTSGS	242					
gi 67004940	173	MNRKRVTCCLKDNIKMTDGI FSDGVFHKIFNEIAKEYPQINNEHYIIDIGTARLATKPEIFDVI VTSNLYGDIISDVAAEISGS	252					
gi 46401058	167	YHRKRVTCCLKDNIKMTDGI FHLFHKIFDEIGAEYYPQIEKEHWIVDIGAAKLADTPTAFDVI VMPNLYGDIISDVAAQIAGS	246					
gi 68171798	163	HNRKRVTCCLKDNIKMTDGI FHKSFSKIAENYPD IESDHYIVDIGMARVASNPENFVDIVTTNLYGDIISDVAAEISGS	242					
gi 88606810	163	HNRKRVTCCLKDNIKMTDGI FFRSAFQKIAAMYPD ISSEYCIDVIGMARIAAHPEEYDVVVTPNLYGDIISDVVAVASGS	242					
gi 88607979	159	NGRKRVTVMVKDNIMKLTGDI FHKLFKVALEYPD IESSENYIIDIGAAARIAKNPEKFDVIVTTLNLYGDIISDIAAEISGS	238					

Clustering Proteins in terms of Sequence Similarities--Genbank

The screenshot shows the NCBI Protein Clusters website. At the top left is the NCBI logo. The main header features the text "Protein Clusters" in a large, stylized font, with a colorful sequence logo behind it. To the right of the header is a "My NCBI" box with "Sign In" and "Register" links. Below the header is a navigation bar with tabs for "All Databases", "PubMed", "PMC", "Genome", "Nucleotide", "Gene", "Protein", "Structure", and "CDD". A search bar is present with the text "Search Protein Clusters for" and "Go" and "Clear" buttons. Below the search bar are buttons for "Limits", "Preview/Index", "History", "Clipboard", and "Details".

Protein Clusters

About the Database

Welcome to Entrez Protein Clusters. This collection of related protein sequences (clusters) consists of Reference Sequence proteins encoded by complete genomes. This database contains both curated and non-curated clusters. For release-specific information check the [stats page](#).

The Protein Clusters database provides easy access to annotation information, publications, domains, structures, and external links and analysis tools including multiple alignments, phylogenetic trees, and genomic neighborhoods ([ProtMap](#)).

Protein Clusters can be searched like any other Entrez database. For more information on how to use Entrez please examine the [Entrez Help](#) Document.

A specialized BLAST service is accessible ([Concise Protein BLAST](#)).

Data is available for download via [Protein Clusters FTP](#)

Example Searches

all clusters with ribosomal protein as the curated name
["ribosomal protein"\[Protein Name\]](#)
all clusters that are encoded by chloroplasts
["source_chloroplast"\[All Fields\]](#)

Check the [limits page](#) and the [help document](#) for more information.

Left Sidebar:

- NCBI
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- Entrez Protein Clusters
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- Help
- FTP
- Statistics
- NCBI Resources
- Concise BLAST search clusters sliced at genera with BLAST
- CD-Search search against PSSMs with RPS-BLAST
- Microbial Genomes browse microbial resources at NCBI
- Plasmids browse complete plasmids at NCBI
- Organelles browse organelle genome resources
- ProtMap examine genome neighborhoods
- Related Resources
- ACLAME A Classification of genetic Mobile Elements

Clustering Proteins in terms of Sequence Similarities--Genbank

PTZ00435

isocitrate dehydrogenase

Gene name: **None**

(Curated - Provisional)

▼ Cluster Info

ID : 2743117
 Total proteins : **31**
 Conserved in : **Eukaryota**
 Total genera : 12
 Total organisms : 29
 Putative Paralogs : 0
 Publications : **20**

▼ Cluster Tools

Show detailed alignment

Build tree

▼ Cross references

EC Number : [1.1.1.42](#)
 KEGG KO : [K00031](#)
 InterPro : [3](#)
 TIGRFAM : [TIGR00127](#)
 Domain(s) : [cl00445\(Iso_dh\)](#)

► Entrez Links

Catalyzes the oxidative decarboxylation of isocitrate into alpha-ketoglutarate; dependent on NADP+. Cytoplasmic localization.

Domain description: **Isocitrate/isopropylmalate dehydrogenase**

BRITE hierarchy:

Metabolism;Carbohydrate Metabolism;Citrate cycle (TCA cycle)
Energy Metabolism;Reductive carboxylate cycle (CO2 fixation)
Metabolism of Other Amino Acids;Glutathione metabolism

► Publications by categories (only one publication per category is shown)

[\(Show all 20\)](#)

- **Curated** [3] : [Influence of compartmental localization on the function of yeast NADP+-specific isocitrate dehydrogenases. Arch Biochem Biophys 2004 Mar 15 more...](#)
- **SwissProt** [2] : [Proteomics fingerprinting of phagosome maturation and evidence for the role of a Galpha during uptake. Mol Cell Proteomics 2006 Dec more...](#)
- **CDD** [15] : [The high-resolution Structure of LeuB \(Rv2995c\) from Mycobacterium tuberculosis. J Mol Biol 2005 Feb 11 more...](#)

Organism (Collapse)	Protein name	Prev. Cluster	Accession	Next Cluster	Locus_tag	Length	UniProt	BLink	Alignment
a.Eukaryota									
<input type="checkbox"/>	Babesia bovis T2Bo	isocitrate dehydrogenase, NADP-dependent family protein	CLS22434787 XP_001811855	CLS22434773	BBOV_III007260	446aa	A7AP03	◆	 All sequences have the same domain structure (Expand)
<input type="checkbox"/>	Cryptosporidium muris RN66	isocitrate dehydrogenase	CLS22429108 XP_002141313	CLS22435904	CMU_033490	412aa	B6AFH3	◆	
<input type="checkbox"/>	Dictyostelium discoideum AX4	isocitrate dehydrogenase (NADP+)	CLS22430407 XP_645283	PTZ00435	DDB_G0272208	412aa	Q75JR3	◆	
<input type="checkbox"/>	Dictyostelium discoideum AX4	isocitrate dehydrogenase (NADP+)	PTZ00435 XP_645284	PTZ00237	DDB_G0272210	428aa	Q75JR2	◆	
<input type="checkbox"/>	Leishmania braziliensis MHOM/BR/75/M2904	isocitrate dehydrogenase	CLS22455726 XP_001562802	CLS22455727	LbrM10_V2.0310	435aa	A4H812	◆	
<input type="checkbox"/>	Leishmania infantum JPCM6	isocitrate dehydrogenase	CLS22455726 XP_001463680	CLS22455727	LinJ10.0610	435aa	A4HUD9	◆	
<input type="checkbox"/>	Leishmania major strain Friedlin	isocitrate dehydrogenase	CLS22455726 XP_001881361	CLS22455727	LmIF10.0290	435aa	Q4QH17	◆	
<input type="checkbox"/>	Naegleria gruberi strain NEG-M	isocitrate dehydrogenase NADP-dependent	CLS22737184 XP_002673333	CLS22736598	NAEGRDRAFT_82731	330aa		◆	
<input type="checkbox"/>	Paramecium tetraurelia strain d4-2	hypothetical protein	CLS22448920 XP_001426548	CLS22448918	GSPATT00029781001	411aa	A0BK13	◆	

ENSEMBL—European version of Genbank—now focused exclusively on genome wide applications

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Home

Search: for

e.g. [human gene BRCA2](#) or [rat X:100000..200000](#) or [coronary heart disease](#)

Browse a Genome

The Ensembl project produces genome databases for vertebrates and other eukaryotic species, and makes this information freely available online.

Click on a link below to go to the species' home page.

Popular genomes ([Log in to customize this list](#))



Human
GRCh37



Mouse
NCBIM37



Zebrafish
Zv9

All genomes

-- Select a species --

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Other species are available in [Ensembl Pre!](#) and [EnsemblGenomes](#)



Ensembl is a joint project between [EMBL - EBI](#) and the [Wellcome Trust Sanger Institute](#) to develop a software system which produces and maintains automatic annotation on selected eukaryotic genomes.



Ensembl receives major funding from the Wellcome Trust. Our [acknowledgements page](#) includes a list of additional current and previous funding bodies.

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What's New in Release 60 (8 November 2010)

- **New species - Giant Panda** (Giant panda)
- **New zebrafish assembly** (Zebrafish)
- **New rabbit assembly** (Rabbit)
- **New Gene Ontology displays** (all species)
- **New navigation options on Region in Detail** (all species)

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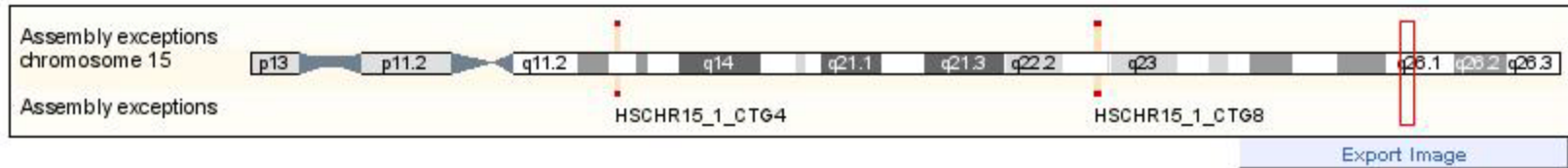
- 2011-01-18: [Ensembl Events in February 2011](#)
- 2011-01-19: [New Search - Lucene](#)
- 2011-01-13: [New Ensembl mirror in Asia](#)



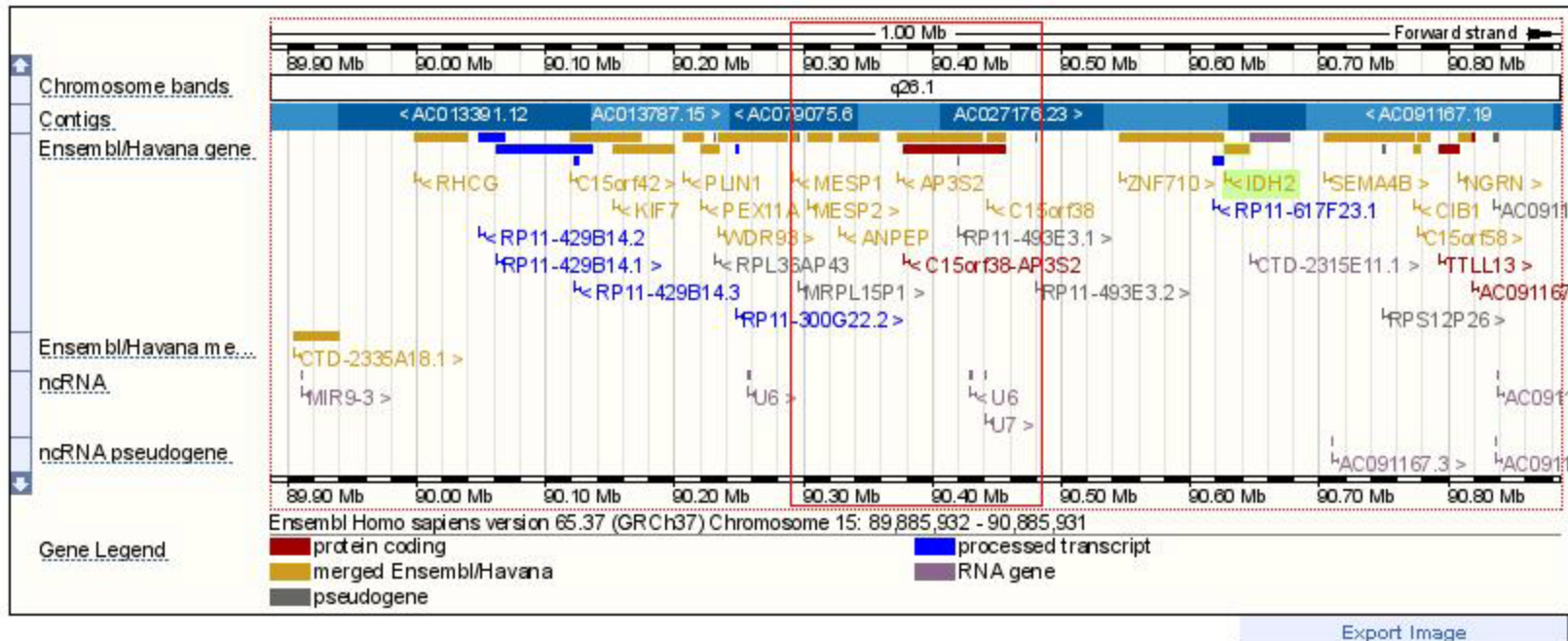
[Go to Ensembl blog →](#)

Sample Ensembl Result—Chromosomal location and other features for downloading information

Chromosome 15: 90,288,632-90,483,231



Region in detail [help](#)

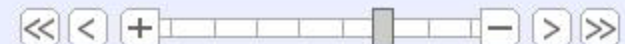


Location:

Go

Gene:

Go



ENSEMBL—Gene Summary

Description mesoderm posterior 1 homolog (mouse) [Source:HGNC Symbol;Acc:29658]

Location [Chromosome 15: 90,291,892-90,294,541](#) reverse strand.

Transcripts This gene has 2 transcripts

Show/hide columns		Filter				
Name	Transcript ID	Length (bp)	Protein ID	Length (aa)	Biotype	CCDS
MESP1-001	ENST00000300057	2369	ENSP00000300057	268	Protein coding	CCDS10355
MESP1-002	ENST00000559894	451	No protein product	-	Processed transcript	-

Transcript and Gene level displays

In Ensembl we provide displays at two levels:

- Transcript views which provide information specific to an individual transcript such as the cDNA and CDS sequences and protein domain annotation.
- Gene views which provide displays for data associated at the gene level such as orthologues, paralogues, regulatory regions and splice variants.

This view is a gene level view. To access the transcript level displays select a Transcript ID in the table above and then navigate to the information you want using the menu at the left hand side of the page. To return to viewing gene level information click on the Gene tab in the menu bar at the top of the page.

Gene summary [help](#)

Name [MESP1](#) (HGNC Symbol)

Synonyms bHLHc5, MGC10676 [To view all Ensembl genes linked to the name [click here](#).]

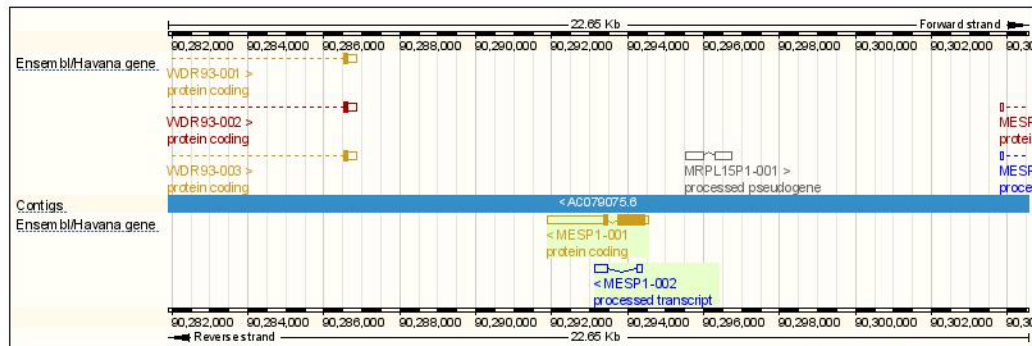
CCDS This gene is a member of the Human CCDS set: [CCDS10355](#)

Gene type Known protein coding

Prediction Method Annotation for this gene includes both automatic annotation from Ensembl and [Havana](#) manual curation, see [article](#).

Alternative genes **This gene corresponds to the following database identifiers:**

Havana gene: [Q1THUMG00000149810](#) (version 2) [[view all locations](#)]



[Export Image](#)

ENSEMBL—Protein

Transcript: MESP1-001 ENST00000300057

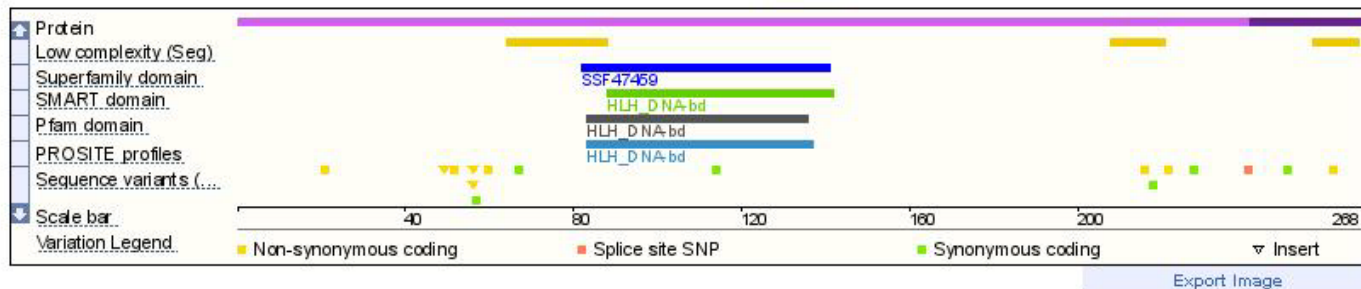
Description mesoderm posterior 1 homolog (mouse) [Source:HGNC Symbol;Acc:29658]
Location [Chromosome 15: 90,291,892-90,294,541](#) reverse strand.
Gene This transcript is a product of gene [ENSG00000166823](#) - This gene has 2 transcripts

Show/hide columns		Filter				
Name	Transcript ID	Length (bp)	Protein ID	Length (aa)	Biotype	CCDS
MESP1-001	ENST00000300057	2369	ENSP00000300057	268	Protein coding	CCDS10355
MESP1-002	ENST00000559894	451	No protein product	-	Processed transcript	-

i Transcript and Gene level displays ✕

Views in Ensembl are separated into gene based views and transcript based views according to which level the information is more appropriately associated with. This view is a transcript level view. To flip between the two sets of views you can click on the Gene and Transcript tabs in the menu bar at the top of the page.

Protein summary [help](#)



Statistics
Ave. residue weight: 106.348 g/mol
Charge: 8.0
Isoelectric point: 9.0165
Molecular weight: 28,501.38 g/mol
Number of residues: 268 aa

SWISSPROT--<http://www.expasy.ch/>

- UniProt combines SwissProt and TrEMBI

“UniProtKB/TrEMBL (unreviewed) contains protein sequences associated with computationally generated annotation and large-scale functional characterization. UniProtKB/Swiss-Prot (reviewed) is a high quality manually annotated and non-redundant protein sequence database, which brings together experimental results, computed features and scientific conclusions” --<http://www.uniprot.org/help/uniprotkb>

UniProt has replaced SwissProt

Mirror Sites

Switzerland: <http://www.expasy.org/> at [Swiss Institute of Bioinformatics, Geneva](#)

Australia: <http://au.expasy.org/> at [Australian Proteome Analysis Facility, Sydney](#)

Brazil: <http://br.expasy.org/> at [Laboratório Nacional de Computação Científica, Petrópolis](#)

Canada: <http://ca.expasy.org/> at [Canadian Bioinformatics Resource, Halifax](#)

China: <http://cn.expasy.org/> at [Peking University](#)

Korea: <http://kr.expasy.org/> at [Yonsei Proteome Research Center, Seoul](#)

UNIPROT SWISSPROT

UniProt Downloads Contact Documentation

Search Blast Align Retrieve ID Mapping

Search in Query

Protein Knowledgebase (UniProtKB)

WELCOME

The mission of UniProt is to provide the scientific community with a comprehensive, high-quality and freely accessible resource of protein sequence and functional information.

What we provide

UniProtKB	Protein knowledgebase, consists of two sections: <ul style="list-style-type: none">★ Swiss-Prot, which is manually annotated and reviewed.★ TrEMBL, which is automatically annotated and is not reviewed. Includes complete and reference proteome sets.
UniRef	Sequence clusters, used to speed up sequence similarity searches.
UniParc	Sequence archive, used to keep track of sequences and their identifiers.
Supporting data	Literature citations, taxonomy, keywords, subcellular locations, cross-referenced databases and more.

Getting started

- Text search
- Sequence similarity searches (BLAST)
- Sequence alignments
- Batch retrieval
- Database identifier mapping (ID Mapping)



NEWS

UniProt release 2012_01 - Jan 25, 2012

What's in a (species) name? | Clustal Omega

- > Statistics for UniProtKB
- Swiss-Prot - TrEMBL
- > Forthcoming changes
- > News archives

[Follow @uniprot](#) (195 followers)

SITE TOUR



Learn how to make best use of the tools and data on this site.

PROTEIN SPOTLIGHT

zips, necklaces and mobile telephones December 2011

I would hate to leave the house without the odd necklace hanging round my neck. But I happen to be fortunate. Millions of other people are not...



query UniProtKB [help](#)

Visual Guidance

Categories

- proteomics
- genomics
- structural bioinformatics
- systems biology
- phylogeny/evolution
- population genetics
- transcriptomics
- biophysics
- imaging
- IT infrastructure
- drug design

Resources A..Z

Links/Documentation

ExPASy is the new **SIB Bioinformatics Resource Portal** which provides access to scientific databases and software tools in different areas of life sciences including proteomics, genomics, phylogeny, systems biology, population genetics, transcriptomics etc. (see **Categories** in the left menu). On this portal you find resources from many different SIB groups as well as external institutions.

Featuring today

T-Coffee

Multiple alignments of DNA, RNA, protein sequences and structures
[\(details\)](#)

TCoffee



How to use this portal?

- New features
- New to ExPASy
- Experienced ExPASy users: what is different

SwissProt—search for Proteins

Search in Protein Knowledgebase (UniProtKB) [Advanced Search »](#)

- 25 of 8,133 results for **isocitrate** AND **dehydrogenase** in UniProtKB sorted by **score** descending

Browse by [taxonomy](#), [keyword](#), [gene ontology](#), [enzyme class](#) or [pathway](#) | Reduce sequence redundancy to [100%](#), [90%](#) or [50%](#) |

[Download](#)

Page 1 of 326 | [Next](#) »

Results [Customize](#)

- > Show only [reviewed \(555\)](#) ★ (UniProtKB/Swiss-Prot) or [unreviewed \(7,578\)](#) ★ (UniProtKB/TrEMBL) entries
- > Quote terms: "isocitrate dehydrogenase"
- > Restrict term "isocitrate" to [protein family \(6,747\)](#), [gene ontology \(4,102\)](#), [protein name \(4,818\)](#), [web resource \(1\)](#)
- > Restrict term "dehydrogenase" to [protein family \(2\)](#), [gene ontology \(6,887\)](#), [protein name \(7,752\)](#), [web resource \(1\)](#)
- > Restrict term "isocitrate" to [pathway](#)
- > Restrict term "dehydrogenase" to [pathway](#)

	Accession	Entry name	Status	Protein names	Gene names	Organism	Length
<input type="checkbox"/>	O75874	IDHC_HUMAN	★	Isocitrate dehydrogenase [NADP] cytoplasmic	IDH1 PICD	Homo sapiens (Human)	414
<input type="checkbox"/>	P08200	IDH_ECOLI	★	Isocitrate dehydrogenase [NADP]	icd icdA icdE b1136 JW1122	Escherichia coli (strain K12)	416
<input type="checkbox"/>	P0A9G6	ACEA_ECOLI	★	Isocitrate lyase	aceA icl b4015 JW3975	Escherichia coli (strain K12)	434
<input type="checkbox"/>	P28241	IDH2_YEAST	★	Isocitrate dehydrogenase [NAD] subunit 2, mit...	IDH2 YOR136W O3326 YOR3326W	Saccharomyces cerevisiae (Baker's yeast)	369
<input type="checkbox"/>	P11071	ACEK_ECOLI	★	Isocitrate dehydrogenase kinase/phosphatase	aceK b4016 JW3976	Escherichia coli (strain K12)	578
<input type="checkbox"/>	P33198	IDHP_PIG	★	Isocitrate dehydrogenase [NADP], mitochondria...	IDH2	Sus scrofa (Pig)	421
<input type="checkbox"/>	P28834	IDH1_YEAST	★	Isocitrate dehydrogenase [NAD] subunit 1, mit...	IDH1 YNL037C N2690	Saccharomyces cerevisiae (Baker's yeast)	360
<input type="checkbox"/>	P39126	IDH_BACSU	★	Isocitrate dehydrogenase [NADP]	icd citC BSU29130	Bacillus subtilis	423
<input type="checkbox"/>	Q8LFC0	IDH1_ARATH	★	Isocitrate dehydrogenase [NAD] regulatory sub...	IDH1 At4g35260 F23E12.180	Arabidopsis thaliana (Mouse-ear cress)	367
<input type="checkbox"/>	O43837	IDH3B_HUMAN	★	Isocitrate dehydrogenase [NAD] subunit beta, ...	IDH3B	Homo sapiens (Human)	385

EXPASY-Databases and Features

The image shows a screenshot of the EXPASY website's database and feature list, organized alphabetically by letter. Each entry is preceded by a small red icon of a folder with a document. A large blue arrow with the word 'Translate' inside points to the 'Translate' entry in the 't' section.

f

- FastEpistasis
- fastsimcoal
- FetchGWI / tagger
- FindMod
- FindPept

g

- Genome History
- GlycanMass
- GlycoMod
- GlycoSuiteDB
- GMM
- GPSDB

h

- HAMAP
- HamapScan
- HCD/CID spectra merger

i

- ImageMaster / Melanie
- ImmunoDB
- ISA
- IScan
- IsotopIdent

l

- Linear Classification

m

- MADAP
- Make2D-DB II
- MALDI PepQuant
- MAMOT
- MARA
- MARCOIL
- MassSearch
- MIAPEGelDB
- miROrtho
- MLtree
- MLTreeMap
- MOSAIC Software Repository
- MSight
- MyDomains
- MyHits
- Myristoylator

RandSeq

RAxML

s

- ScanProsite
- Selectome
- Sequence Similarity Maps (SSM)
- ShoRAH
- SIBsim4
- smimaDB
- Soaplab services
- SSA
- STRING
- SugarBind
- Sulfinator
- SuperTree
- SWISS-2DPAGE
- SWISS-MODEL Repository
- SWISS-MODEL Workspace
- Swiss-Pdb/Viewer
- SwissDock
- SwissParam
- SwissRegulon
- SwissVar

t

- T-Coffee
- TagIdent
- TagScan
- TCS
- The Systems Biology Search Tool
- TMPred
- Translate
- TreeGen
- TriFLe
- tromer

u

- UniPathway
- UniProtKB
- UniProtKB/Swiss-Prot

v

- Vertex Cover
- ViralZone
- Vital-IT

...

Swiss 2D-PAGE

SWISS-2DPAGE

Search by

[[accession number](#)]
[[description, ID or gene](#)] ▶
[[author names](#)]
[[spot ID / serial number](#)]
[[identification methods](#)]
[[pI / Mw range](#)]
[[combined fields](#)]

Maps

[[experimental info](#)]
[[protein list](#)]
[[graphical interface](#)]

Select Remote Interfaces

[All Interfaces]

World-2DPAGE Portal

World-2DPAGE Repository

Exclude local DBs
*has only effect if a remote
interface is selected*

SWISS-2DPAGE

Search by description (DE), entry name (ID), gene name (GN) or UniProtKB/Swiss-Prot keywords (KW)

Enter search keywords:

Limit to: All fields DE ID GN KW

Include external UniProtKB data in search

Sort by: Accession number Protein ID Gene name

Please enter a keyword. This may be any word or partial word appearing in the entry identifier (ID), the description (DE), the gene names (GN) or a UniProtKB/Swiss-Prot keyword (KW). For example, you may type *apoa1_human*, or just *apo*, or *APO* or *APOA1_HUMAN*.

If you give more than one keyword, entries having **any** keyword will be listed. Please do **NOT** use any boolean operators (and, or, etc.), nor quotes ("").



SWISS-2DPAGE

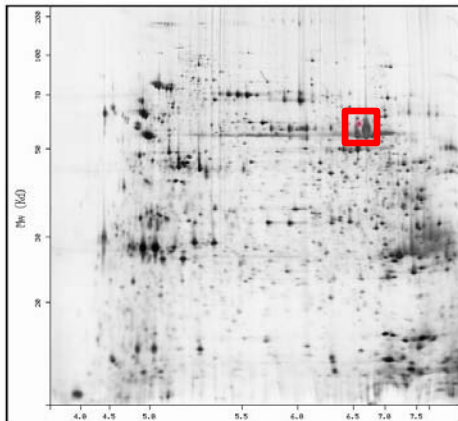
Swiss 2DPAGE –Isocitrate dehydrogenase

Searching in 'SWISS-2DPAGE' for entries matching any of the keywords:
 'isocitrate dehydrogenase'
 in their description (DE), entry name (ID), gene names (GN) or UniProtKB/Swiss-Prot keywords (KW).

Query Result: 99 matches

Accession number	ID	Description	Genes	Keywords	Species
008749	DLDH_MOUSE	Dihydropyridyl dehydrogenase, mitochondrial (EC 1.8.1.4) (Dihydropyridamide dehydrogenase)	{Name=Dld}	Acetylation; Direct protein sequencing; FAD; Flavoprotein; Mitochondrion; NAD; Oxidoreductase; Redox-active center; Transit peptide	Mus musculus (Mouse)
008756	HCD2_MOUSE	3-hydroxyacyl-CoA dehydrogenase type-2 (EC 1.1.1.35) (3-hydroxyacyl-CoA dehydrogenase type II) (Type II HADH) (3-hydroxy-2-methylbutyryl-CoA dehydrogenase) (EC 1.1.1.178) (Endoplasmic reticulum-associated amyloid beta-peptide-binding protein)	{Name=Hsd17b10; Synonyms=Erab, Hsdh2}	Acetylation; Direct protein sequencing; NAD; Oxidoreductase	Mus musculus (Mouse)
088844		<p>Switch to Gen: <input type="text" value="Mus musculus (Mouse) - ISLETS_MOUSE Pancreatic islet cells "/></p> <p>Rescale Gel from 100% to: <input type="text" value="100%"/> View: <input type="text" value="008749"/></p> <p><input type="button" value="Refresh"/> Display: <input checked="" type="checkbox"/> Identified spots</p> <p>Identified by: <input type="radio"/> show <input type="radio"/> hide</p> <p><input checked="" type="checkbox"/> PFM <input type="checkbox"/> Tandem MS (Peptide Sequencing) <input type="checkbox"/> AA Composition <input checked="" type="checkbox"/> Micro-Sequencing / Tagging <input checked="" type="checkbox"/> Gel Matching <input checked="" type="checkbox"/> Comigration <input checked="" type="checkbox"/> Immunoblotting</p>	3D-structure; Cytoplasm; protein sequencing; oxylate pass; nesium; ganese; l-binding; ADP; eductase; rboxylic d cycle	Mus musculus (Mouse)	

Get more information by dragging your mouse pointer over any spot, or click on a spot to access all its associated proteins [estimated location]



SWISS-2DPAGE: 008749

008749

General information about the entry

View entry in simple text format

Entry name **DLDH_MOUSE**
 Primary accession number **008749**
 integrated into SWISS-2DPAGE on April 1, 2000 (release 12)
 2D Annotations were last modified on March 31, 2004 (version 1)
 General Annotations were last modified on May 25, 2007 (version 7)

Name and origin of the protein

Description **Dihydropyridyl dehydrogenase, mitochondrial (EC 1.8.1.4) (Dihydropyridamide dehydrogenase).**
 Gene name **Name=Dld**
 Annotated species **Mus musculus (Mouse) [TaxID: 10090]**
 Taxonomy **Eukaryota; Metazoa; Chordata; Craniata; Vertebrata; Euteleostomi; Mammalia; Eutheria; Euarchontoglires; Glires; Rodentia; Sciurognathi; Muroidea; Muridae; Murinae; Mus.**

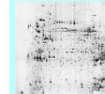
References

[1] MAPPING ON GEL
 PubMed=11690894; [NCBI, ExPASy, EBI, Israel, Japan]
 Sanchez J.-C., Chiappe D., Converset V., Hoogland C., Binz P.-A., Paesano S., Appel R.D., Wang S., Sennitt M., Nolan A., Cawthorne M.A., Hochstrasser D.F.
 "The mouse SWISS-2DPAGE database: a tool for proteomics study of diabetes and obesity"
 Proteomics 1.136-163(2001)

2D PAGE maps for identified proteins

How to interpret a protein

ISLETS_MOUSE (Pancreatic islet cells)
Mus musculus (Mouse)
 Tissue: Pancreatic islet



map experimental info
 protein estimated location

ISLETS_MOUSE

MAP LOCATIONS:
 • SPOT 2D-0018HS: pI=6.59; Mw=58739 [identification data]

MAPPING (identification):
 Peptide mass fingerprinting [1].

Copyright

This SWISS-2DPAGE entry is copyright the Swiss Institute of Bioinformatics. There are no restrictions on its use by non-profit institutions as long as its content is in no way modified and this statement is not removed. Usage by and for commercial entities requires a license agreement (See <http://www.expasy.org/ch2d/license.html> or send email to license@isb-sib.ch).

Cross-references

REPRODUCTION:2DPAGE 008749; DLDH_MOUSE.

Swiss PDB Model Repository



SWISS-MODEL Repository

Modelling

Tools

Repository

Documentation

[[Repository Query](#)] [[Full Text Query](#)]

Welcome to the SWISS-MODEL Repository

The SWISS-MODEL Repository is a database of annotated three-dimensional comparative protein structure models generated by the fully automated homology-modelling pipeline SWISS-MODEL.

Example Queries:

[P23298] [GLDA_ECOLI] [IP100743503] [NP_416402] [GI:26454606] [ENTREZ:54401] [Sequence]

```
P08200 -- isocitrate dehydrogenase Accession Number
```

SEARCH



The current release of the SWISSMODEL-Repository (10.2.2) consists of 3021'185 model entries for 2'244'854 unique sequences in the UniProt database.

NOTE: The SWISS-MODEL repository contains theoretically calculated models, which may contain significant errors.



Swiss Institute of
Bioinformatics

SwissModel Repository ...



SWISS-MODEL Repository

Modelling Tools Repository Documental

Summary Sequence Annotations Seq. Similarity 3D Similarity Literature Biol. & Chem. Methods Geometry Links

[Repository Query] [Full Text Query]

A four location model to explain the stereospecificity of proteins.

1PB1

Display Files
Download Files
Share this Page

DOI:10.2210/pdb1pb1/pdb

SWISS-MODEL Repository - Model Details

Model Overview [+/-]

Click on the bars to get more details about individual Models or experimental structures



Sequence [+/-]

UniProt P08200 Isocitrate dehydrogenase [NADP] (IDP)
Escherichia coli (strain K12)
Database: Swiss-Prot (Reviewed) ★

Domain [+/-]

no data available!

Model 3D Structure [+/-]



Based on structure: **1pb1** [SMTL] [RCSB] [PDBe] [SCOP] [CATH]
Sequence identity: 100%
Residue range: 1 to 416

Primary Citation

A new model for protein stereospecificity.

Mesecar, A.D., Koshland Jr., D.E.

Journal: (2000) Nature 403: 614-615

PubMed: 10688187

DOI: 10.1038/35001144

Search Related Articles in PubMed

PubMed Abstract:

No abstract available... [Read More & Search PubMed Abstracts]

Molecular Description

Classification: Oxidoreductase

Structure Weight: 46374.47

Molecule: Isocitrate dehydrogenase [NADP]

Polymer: 1 Type: polypeptide(L) Length: 416

Chains: A

EC#: 1.1.1.42

Other Details: wildtype

Source

Polymer: 1

Scientific Name: Escherichia coli

Taxonomy Expression System: Escherichia coli

Related PDB Entries

Id Details
1PB1F

Ligand Chemical Component

Identifier Formula Name Interactions

Biological Assembly

More Images...

View in Jmol SimpleViewer
Other Viewers Protein Workshop

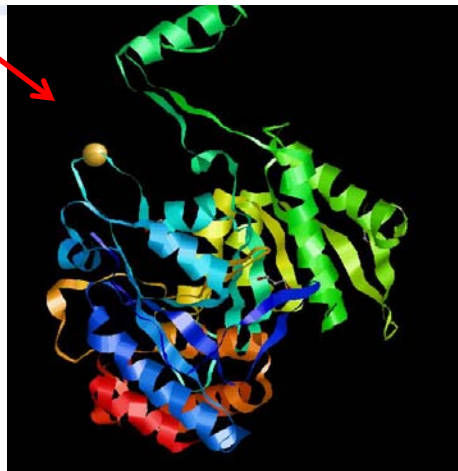
Biological assembly assigned by authors

MyPDB Personal Annotations

To save personal annotations, please login to your MyPDB account.

Deposition Summary

Authors: Mesecar, A.D., Koshland Jr., D.E.
Deposition: 2003-05-14
Release: 2003-06-17
Last Modified (REVDAT): 2009-02-24



Uniref—Clustering of Proteins

Cluster: Isocitrate dehydrogenase [NADP] (50%) ★

Published January 11, 2011

Built on seed sequence [A1WZE1](#) | List component clusters with 100% or 90% identity

[xml](#) [rdf/xml](#) [fasta](#) [tab](#)

Filter · Members · Sequence · [Customize order](#)

Page 1 of 46 | [Next](#) »

Filter

1 - 25 of 1,137 members from 837 organisms

Dataset

UniProt (1137) ▾

Taxonomy

... ▾

Filter

Reset

Members [Customize](#)

Member	Entry name	Status	Protein names	Organism	Component clusters	Length
<input type="checkbox"/> Q9ZN36	IDH_HELPJ	★	Isocitrate dehydrogenase [NADP]	Helicobacter pylori J99 (Campylobacter pylori J99)	UniRef100_Q9ZN36 UniRef90_Q9ZN36	425
<input type="checkbox"/> B2ZP83	B2ZP83_HELPY	★	Isocitrate dehydrogenase [NADP]	Helicobacter pylori (Campylobacter pylori)	UniRef100_B2ZP83 UniRef90_Q9ZN36	425
<input type="checkbox"/> B6JPC2	B6JPC2_HELP2	★	Isocitrate dehydrogenase [NADP]	Helicobacter pylori (strain P12)	UniRef100_B6JPC2 UniRef90_Q9ZN36	425
<input type="checkbox"/> B9XWT5	B9XWT5_HELPY	★	Isocitrate dehydrogenase [NADP]	Helicobacter pylori 98-10	UniRef100_B9XWT5 UniRef90_Q9ZN36	425
<input type="checkbox"/> E1Q800	E1Q800_HELP2	★	Isocitrate dehydrogenase [NADP]	Helicobacter pylori (strain Cuz20)	UniRef100_E1Q800 UniRef90_Q9ZN36	425
<input type="checkbox"/> Q1CV00	Q1CV00_HELPH	★	Isocitrate dehydrogenase [NADP]	Helicobacter pylori (strain HPAG1)	UniRef100_Q1CV00 UniRef90_Q9ZN36	425

KEGG (Kyoto Encyclopedia of Genes and Genomes)

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



Search KEGG

Get Entry

KEGG Home

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

KEGG Identifiers

[KGML](#)

[KEGG API](#)

[KEGG FTP](#)

[KegTools](#)

[Feedback](#)

[GenomeNet](#)

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, 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 Atlas](#) Global maps of cell/organism functions
[KEGG PATHWAY](#) Pathway maps and pathway modules
[KEGG BRITE](#) Functional hierarchies and ontologies
[KEGG ORTHOLOGY](#) KO system and ortholog annotation
[KEGG GENES](#) Genomes, genes, and proteins
[KEGG LIGAND](#) Chemical compounds, drugs, glycans, and reactions

● Organism-specific entry points

[KEGG Organisms](#) Select (example) hsa

● Subject-specific entry points

[KEGG DISEASE](#) Gene/molecule based disease information resource
[KEGG DRUG](#) Chemical structure based drug information resource
[KEGG GLYCAN](#) Glycome informatics resource
[KEGG COMPOUND](#) Knowledge base for biochemical compounds
[KEGG REACTION](#) Knowledge base for biochemical reactions
[KEGG PLANT](#) Knowledge base for plant natural products
[KAAS](#) KEGG automatic annotation server

Kegg Atlas

KEGG2 ATLAS PATHWAY BRITE KO GENES SSDB LIGAND DBGET

KEGG Atlas

KEGG Atlas is a new graphical interface to the KEGG suite of databases, especially to the systems information in the PATHWAY and BRITE databases. It currently consists of a global metabolism map with newly developed viewers and a cancer map with the traditional KEGG map viewer.

Metabolism map (version 0.1, to be phased out)

~~Metabolism map (version 0.2)~~

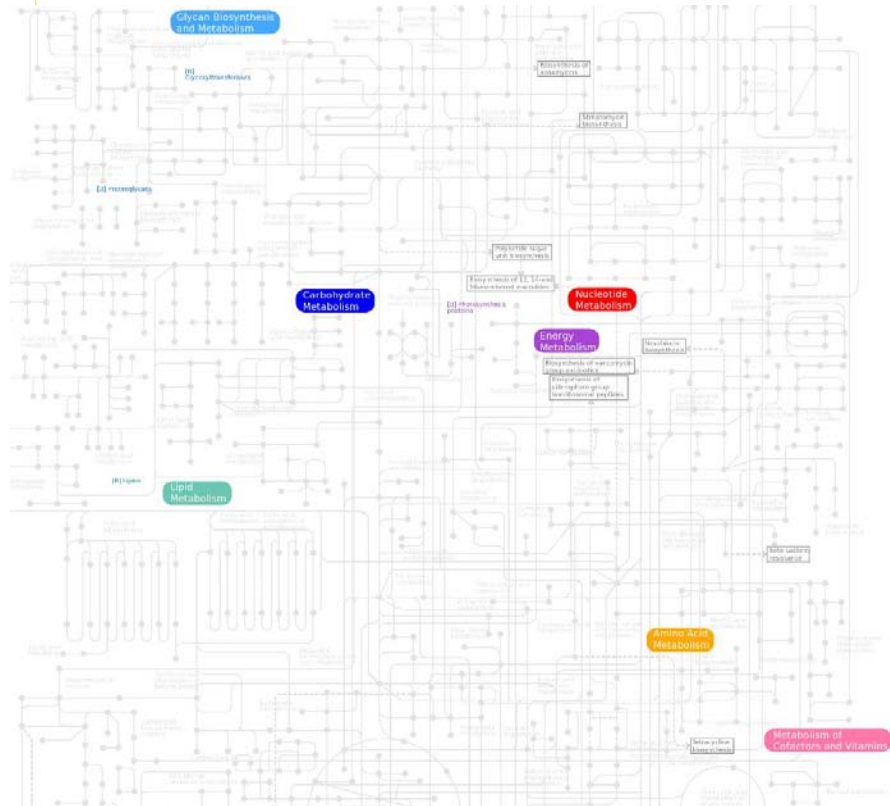
Plant secondary metabolism map

Cancer map

Other global maps are being developed or planned including:

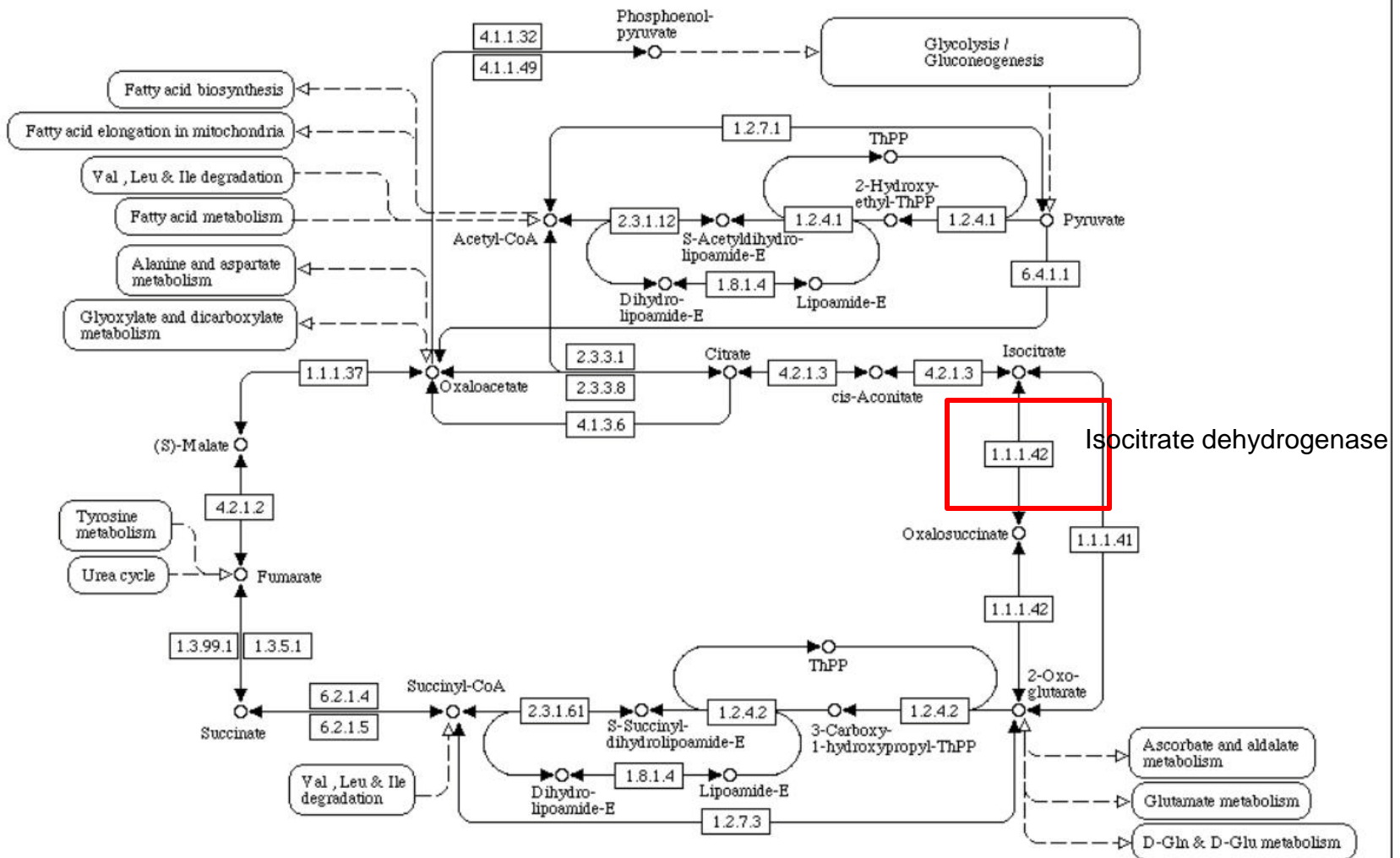
- Cell map
- Body map
- Brain map

The new **KEGG metabolism map** is created as an SVG file by manually combining about 120 existing metabolic pathway maps. Each node (circle) is a chemical compound identified by the C number. Each line (curved or straight) connecting two nodes is manually defined as a segment lacking branches in the existing maps, named NetElement, and identified by the N number. Each NetElement corresponds to one to several KO's (such as this) in the reference pathway view, or one to several genes (such as this) in an organism-specific view.




KEGG Pathway

CITRATE CYCLE (TCA CYCLE)



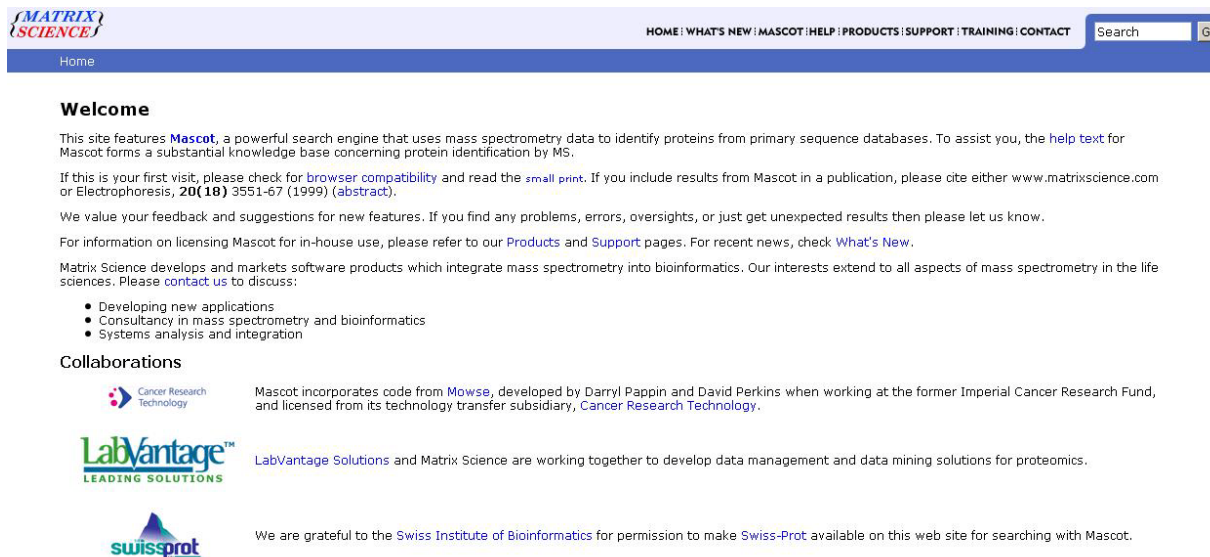
Isocitrate Dehydrogenase in KEGG

KEGG Homo sapiens (human): 3417 Help

Entry	3417 CDS H.sapiens
Gene name	IDH1, IDCD, IDH, IDP, IDPC, PICD
Definition	isocitrate dehydrogenase 1 (NADP+), soluble (EC:1.1.1.42)
Orthology	K00031 isocitrate dehydrogenase [EC:1.1.1.42]
Pathway	hsa00020 Citrate cycle (TCA cycle) hsa00480 Glutathione metabolism hsa01100 Metabolic pathways hsa04146 Peroxisome
Class	Metabolism; Carbohydrate Metabolism; Citrate cycle (TCA cycle) [PATH:hsa00020] Metabolism; Metabolism of Other Amino Acids; Glutathione metabolism [PATH:hsa00480] Cellular Processes; Transport and Catabolism; Peroxisome [PATH:hsa04146] BRITE hierarchy
SSDB	Ortholog Paralog GFIT
Motif	Pfam: Iso_dh PGA2 DUF505 PROSITE: IDH_IMDH Motif
Other DBs	NCBI-GI: 28178825 NCBI-GeneID: 3417 OMIM: 147700 HGNC: 5382 HPRD: 00984 Ensembl: ENSG00000138413 UniProt: O75874 Q6FHQ6
Structure	PDB: 3INM 1TOL 1T09 3MAP 3MAS 3MAR Thumbnails  Jmol
Position	2q33.3

MASCOT—Protein Identification from Mass Spectroscopy Data

- Peptide Mass Fingerprinting
- Sequence Query
- MS/MS Ion Search



The screenshot shows the Mascot website homepage. At the top left is the logo for Matrix Science, consisting of the word "MATRIX" in blue and "SCIENCE" in red, both in a stylized font. To the right of the logo is a navigation menu with links: HOME | WHAT'S NEW | MASCOT | HELP | PRODUCTS | SUPPORT | TRAINING | CONTACT. Further right is a search bar with the text "Search" and a "Go" button. Below the navigation bar is a blue header with the word "Home" on the left. The main content area starts with a "Welcome" section. The text in this section describes the Mascot search engine, provides contact information, and lists the services offered: developing new applications, consultancy in mass spectrometry and bioinformatics, and systems analysis and integration. Below the "Welcome" section is a "Collaborations" section. It features three logos: Cancer Research Technology, LabVantage (with the tagline "LEADING SOLUTIONS"), and swissprot. Each logo is accompanied by a short paragraph describing the collaboration.

WELCOME

This site features **Mascot**, a powerful search engine that uses mass spectrometry data to identify proteins from primary sequence databases. To assist you, the [help text](#) for Mascot forms a substantial knowledge base concerning protein identification by MS.

If this is your first visit, please check for [browser compatibility](#) and read the [small print](#). If you include results from Mascot in a publication, please cite either [www.matrixscience.com](#) or *Electrophoresis*, **20(18)** 3551-67 (1999) ([abstract](#)).


We value your feedback and suggestions for new features. If you find any problems, errors, oversights, or just get unexpected results then please let us know.


For information on licensing Mascot for in-house use, please refer to our [Products](#) and [Support](#) pages. For recent news, check [What's New](#).


Matrix Science develops and markets software products which integrate mass spectrometry into bioinformatics. Our interests extend to all aspects of mass spectrometry in the life sciences. Please [contact us](#) to discuss:

- Developing new applications
- Consultancy in mass spectrometry and bioinformatics
- Systems analysis and integration

Collaborations

 Cancer Research Technology Mascot incorporates code from [Mowse](#), developed by Darryl Pappin and David Perkins when working at the former Imperial Cancer Research Fund, and licensed from its technology transfer subsidiary, [Cancer Research Technology](#).

 LabVantage™ LEADING SOLUTIONS LabVantage Solutions and Matrix Science are working together to develop data management and data mining solutions for proteomics.

 swissprot We are grateful to the [Swiss Institute of Bioinformatics](#) for permission to make [Swiss-Prot](#) available on this web site for searching with Mascot.

MRM-Path

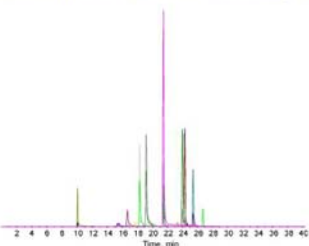
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Metabolomics &
Proteomics
Laboratory

MRMPath – software for studying protein pathways

Home MRMPath Useful Links

MRMPath - software for studying protein pathways



The quantitative study of proteins in biological pathways using mass spectrometry is rapidly replacing discovery proteomics. MRMPath is a web-based, platform-independent software that facilitates the identification of the peptides and their fragment ions for each protein in a metabolic or signaling pathway, or for the components of a protein complex that can be used for quantitative analysis using multiple reaction ion monitoring-mass spectrometry (MRM-MS).

MRMPath offers two ways to identify the peptides

1. To extract ions from previously obtained MSMS spectra to generate instrument-specific ion pair combinations
2. To predict the peptides from a protein sequence that would be most suitable for MRM-MS analysis

MRMPath takes into account peptide type, peptide size and peptide sequence, and the likelihood that the peptide(s) are unique and not found in other proteins.

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MRMPath – software for studying protein pathways

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MRMPath

- **Analysis of Protein Mass Fragments from Pathways: Metabolism, Genetic, Environmental, Cellular, Organismal, Human**

Presented here is a methodology that allows the user to select individual proteins from the pathways associated with a disease process in a given species. Once the sequence of the protein is recovered, it is subjected to in silico digestion with trypsin to determine peptides that are suited to multiple reaction ion monitoring. For each fragment, the m/z values of the ?b-? and ?y" ions are presented (only those with values greater than the doubly charged parent ion are included). For each tryptic peptide, an automated BLAST search is deployed, which results in a list of the highest similarity hits, each with the links to GENBANK. The resulting data can be exported to a comma-delimited file.

Analysis of Protein Mass Fragments from Pathways

None --Select here--

Trypsin Arg-C Lys-C Chymotrypsin Glu-C

- **Analysis of Protein Mass Fragments**

Presented here is a methodology that allows the user to select individual proteins and perform a tryptic digest in silico to determine peptides that are suited to multiple reaction ion monitoring. The only input required is the SWISSPROT Accession ID (or) a protein sequence. For each fragment, the m/z values of the ?b-? and ?y" ions are presented (only those with values greater than the doubly charged parent ion are included). For each tryptic peptide, an automated BLAST search is deployed, which results in a list of the highest similarity hits, each with the links to GENBANK. The resulting data can be exported to a comma-delimited file.

Protein ID

Protein ID (EXPASy): Trypsin Arg-C Lys-C Chymotrypsin Glu-C (Example: P63276)

Protein Sequence

Protein Sequence:

Glu-C Trypsin Arg-C Lys-C Chymotrypsin

(Example: MAKLTAVPLSALVDEPVHIQVTGLAPFQVVCQLQASLKDKEGNLFSQAFYRASEVGEVDL)

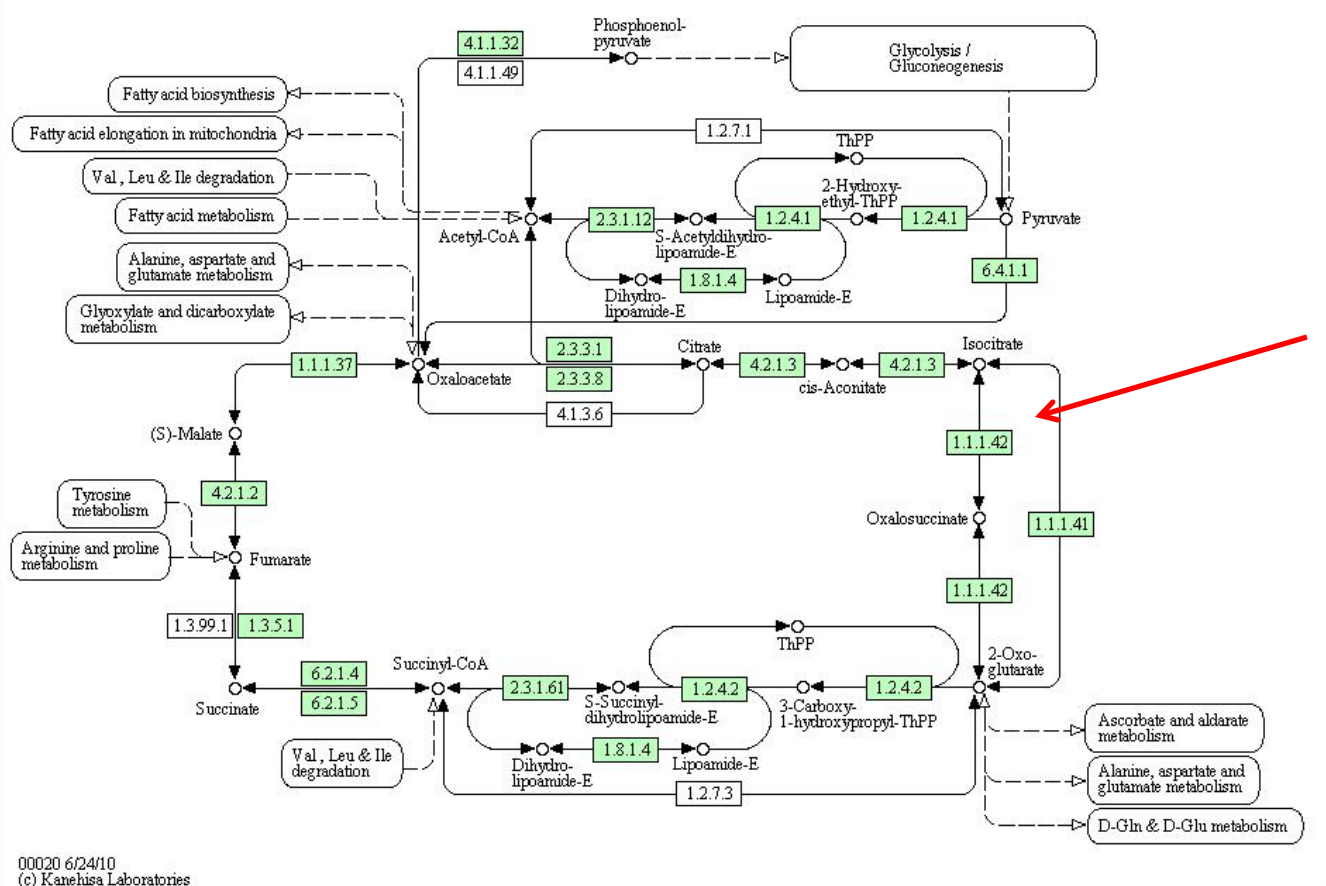
MRMPath ...

Homo sapiens (human)

Go

- = +

CITRATE CYCLE (TCA CYCLE)



Isocitrate dehydrogenase

MRMPPath results for isocitrate dehydrogenase

Click [here](#) to download this into an Excel sheet

NOTE: Please click on the 'YES' button if a warning appears when you try to open the excel sheet

hsa:3417 IDH1, IDCD, IDH, IDP, IDPC, PICD; isocitrate dehydrogenase 1 (NADP+), soluble (EC:1.1.1.42); K00031 isocitrate dehydrogenase [EC:1.1.1.42] (A)

BLAST ALL FRAGMENTS			
Sequence	m/z Parent Ion	B Ion Mass	Y > Parent Ions
BLAST IIWELIK	457.792	542.2979	801.4921
		655.3819	688.4080
		768.4660	502.3287
		896.5609	
BLAST LIFPYVELDLHSYDLGIENR	1203.6235	1203.6666	2293.1551
		1340.7256	2180.0710
		1427.7576	2033.0026
		1590.8209	1935.9499
		1705.8479	1772.8865
		1818.9320	1673.8181
		1875.9535	1544.7755
		1989.0376	1431.6915
		2118.0801	1316.6645
		2232.1231	
2388.2241			
BLAST DATNDQVTK	496.2411	517.1894	876.4474
		645.2480	805.4103
		744.3164	704.3626
		845.3641	590.3197
		973.4591	
BLAST DAAEAIK	359.1954	387.1516	602.3560
		458.1887	531.3189
		571.2728	460.2818
		699.3678	
BLAST SPNGTIR	372.7065	457.2047	657.3731
		570.2887	560.3204
		726.3898	446.2774
			389.2560

.....

MRM-Mutation


- **Analysis of Protein Mutations**

MRMutation is a methodology that allows the user to select individual proteins and determine whether they have known mutations. This is determined by examining the EXPaSY.org database. Each of the protein sequence is subjected to trypsin digestion in silico to determine whether these peptides with mutations are suited to multiple reaction ion monitoring. The input required is the UNIPROT Accession ID. The output spreadsheet contains the m/z values of the first three 'b' and 'y' ions (only those with values greater than the doubly charged parent ion are included), the start and end residues of the peptide with respect to the parent protein and the mutation.

Protein ID

Protein ID ([EXPASY](#)): (Example: P04632)



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MRMPath

 – software for studying protein pathways

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Protein Data Bank-PDB

- <http://www.rcsb.org/pdb/home/home.do>
- **“A Resource for Studying Biological Macromolecules**

The PDB archive contains information about experimentally-determined structures of proteins, nucleic acids, and complex assemblies. As a member of the [wwPDB](#), the RCSB PDB curates and annotates PDB data according to agreed upon standards.

The RCSB PDB also provides a variety of tools and resources. Users can perform simple and advanced searches based on annotations relating to sequence, structure and function. These molecules are visualized, downloaded, and analyzed by users who range from students to specialized scientists.”

Problems during Protein Identification

- No sequence in database --- nothing to correlate with
- Problems with entries in database: human errors in entering information (typographical errors and curation); sequencing errors; errors during transcription
- Modifications in large proteins: degradation, oxidation of methionine, deamidation of N and Q, remember glycosylations, phosphorylations, and acetylations

<http://www.unimod.org/> lists the possible modifications that can occur