

UGC SPONSORED NATIONAL WORKSHOP ON BIOINFORMATICS AND GENOME ANALYSIS FOR COLLEGE TEACHERS



LECTURE TOPIC: PROTEIN DATABASE

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TOPICS COVERED

- Protein Terms & Definitions Computational biology aspect of protein
- ExPASy SIB Bioinformatics Resource Portal (http://www.expasy.org)
- UniProt Swiss-Prot A comprehensive, non-redundant, expert manually annotated protein sequence database (http://www.uniprot.org/)
 - NERE /PIR A comprehensive, non-redundant, expertly manually annotated, fully classified and extensively cross-referenced protein sequence database (http://pir.georgetown.edu/)
 - PDB A single worldwide repository of information about the 3D structures of large biological molecules, including proteins and nucleic acids (http://rcsb.org/pdb)
 - SCOP Knowledge-based expert analysis and classification of proteins that are structurally characterized and deposited in the Protein Data Bank (http://scop2.mrc-lmb.cam.ac.uk/)
 - CATH A hierarchical domain classification of protein structures in the Protein Data Bank (http://www.cathdb.info/)
 - MUTTE Finds sequence motifs in a query sequence, also provides functional and genomic information of the found motifs using DBGET and LinkDB as the hyperlinked annotations (http://www.genome.jp/tools/motif/)
 - Pram Database of protein HMM profiles that define domain families (http://pfam.xfam.org/)
 - Database of protein motifs expressed as patterns or profiles (http://prosite.expasy.org/)

PROTEIN TERMS & DEFINITIONS

- Protein Sequence 20 a.a. characters [A, C, D, E, F, G, H, I, K, L, M, N, P, Q, R, S, T, V, W, Y] sequence
- Protein Structure 3D of atomic co-ordinates [x-axis, y-axis, z-axis]
- Types of Biological Databases [Raw Database = Plain text, Object-oriented Database = Table (Records), Relational Database = Table of tables]
- 3D Atom Model [Sphere = Atom, Cylinder = Bond, Dotted Line = Bond Interaction]
- Sequence Alignment [Match = Similar Character, Mismatch = Dissimilar Character, Gap = No Substitute Character, Word = Sub-string, Sequence = Super-string, Score = Rating, Identity = Similar in function]
- Motif Short, conserved sequence associated with a distinct function.
- Domain Evolutionarily conserved sequence region that corresponds to a structurally independent 3D unit associated with a particular functional role. <u>It is usually much larger than a</u> <u>motif</u>.
- Pattern Sequence with symbol representation for a expression. Example: N{P}[ST]{P}
- Regular Expression Representation format for a sequence motif, which includes positional information for conserved and partly conserved residues. <u>Similar to Pattern, but applies to MSA.</u>
- Profile Scoring matrix that represents a multiple sequence alignment. It contains probability or

EXPASY

 ExPASy (Expert Protein Analysis System) is a bioinformatics resource portal operated by the Swiss Institute of Bioinformatics (SIB).

- ExPASy was the first website of the life sciences.
- Extensible and integrative portal for accessing many scientific resources, databases and software tools.
- Wide range of resources in many different domains, such as proteomics, genomics, phylogeny/evolution, systems biology, population genetics, transcriptomics, etc.
- Proteomics server to analyze protein sequences and structures and 2D Page gel electrophoresis.
- Databases, online and offline software tools are hosted by different groups of the SIB and partner institutions. --- CFSSP
- ExPASy references the provision of the provi

ARCHITECTURE OF UNIPROT/SWISS-PROT

- Universal Protein Resource (UniProt) is a comprehensive resource for protein sequence and annotation data
- The UniProt databases are the UniProt Knowledgebase (UniProt KB), the UniProt Reference Clusters (UniRef), and the UniProt Archive (UniParc)
- UniProt Metagenomic and Environmental Sequences (UniMES) database is a repository specifically develored for the transformed and increased and the second sec



BACKGROUND OF UNIPROT/SWISS-PROT

- UniProt is a collaboration between the European Bioinformatics Institute (EMIBL-EBI), the Swiss
 Institute of Bioinformatics (SIB) and the Protein Information Resource (PIR)
- EMBL-EBI and SIB together used to produce Swiss-Prot and TrEMIBL, while PIR produced the Protein Sequence Database (PIR-PSD)
- Translated EMBL Nucleotide Sequence Data Library (THENTEL) was originally created because sequence data was being generated at a pace that exceeded Swiss-Prot's ability to keep up
- PIR maintained the PIR-PSD and related databases, including iProClass, a database of protein sequences and curated families

UniProt

http://www.uniprot.org/

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WELCOME

Search

Protein Knowledgebase (UniProtKB)

UniProt

Search in

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.

•

Align

Query

serpin

Retrieve

ID Mapping

Blast

What we provide

UniProtKB	Protein knowledgebase, consists of two sections:
	☆ 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)



TRY THE NEW UNIPROT WEBSITE

UniProt BETA

NEWS

UniProt release 2014_07 - Jul 9, 2014

Lark or owl? PER3 is the answer | Cross-references to CCDS and GeneReviews | UniParc cross-references with protein and gene names

 Statistics for UniProtKB: Swiss-Prot · TrEMBL
 Forthcoming changes

> News archives

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SITE TOUR



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

PROTEIN SPOTLIGHT

it did it its way July 2014

Temperatures can get cold. And living organisms have to find ways of keeping themselves warm. Humans use clothes. Polar bears grow fur. Whales are lined with blubber. And many animals avoid the cold by migrating to warmer parts of the planet...

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	P05120	PAI2_HUMAN	*	Plasminogen activator inhibitor 2	SERPINB2 PAI2 PLANH	2	Drosophila melanogaster (Fruit fly) Homo sapiens (Human)	44
	Q5I2A0	PAI2_HUMAN SPA3G_MOUSE	*	Plasminogen activator inhibitor 2 Serine protease inhibitor A3G	Serpina3g Spi2A	2	Drosophila melanogaster (Fruit fly) Homo sapiens (Human) Mus musculus (Mouse)	44 41 44
	Q5I2A0 Q8IW75	PAI2_HUMAN SPA3G_MOUSE SPA12_HUMAN	*	Plasminogen activator inhibitor 2 Serine protease inhibitor A3G Serpin A12	SERPINB2 PAI2 PLANH Serpina3g Spi2A SERPINA12	2	Drosophila melanogaster (Fruit fly) Homo sapiens (Human) Mus musculus (Mouse) Homo sapiens (Human)	44 41 44 41
	Q5I2A0 Q8IW75 Q9UIV8	PAI2_HUMAN SPA3G_MOUSE SPA12_HUMAN SPB13_HUMAN	* * * *	Plasminogen activator inhibitor 2 Serine protease inhibitor A3G Serpin A12 Serpin B13	SERPINB2 PAI2 PLANH Serpina3g Spi2A SERPINA12 SERPINB13 PI13	2	Drosophila melanogaster (Fruit fly) Homo sapiens (Human) Mus musculus (Mouse) Homo sapiens (Human) Homo sapiens (Human)	44 41 44 41 39
	Q5I2A0 Q8IW75 Q9UIV8 Q9S7T8	PAI2_HUMAN SPA3G_MOUSE SPA12_HUMAN SPB13_HUMAN SPZX_ARATH	* * * * *	Plasminogen activator inhibitor 2 Serine protease inhibitor A3G Serpin A12 Serpin B13 Serpin-ZX	SERPINB2 PAI2 PLANH Serpina3g Spi2A SERPINA12 SERPINB13 PI13 At1g47710 F16N3.3 T2E0	5.22	Drosophila melanogaster (Fruit fly) Homo sapiens (Human) Mus musculus (Mouse) Homo sapiens (Human) Homo sapiens (Human) Arabidopsis thaliana (Mouse-ear cress)	44 41 44 41 39 39
	2512A0 Q512A0 Q8IW75 Q9UIV8 Q9S7T8 D6WWC4	PAI2_HUMAN SPA3G_MOUSE SPA12_HUMAN SPB13_HUMAN SPZX_ARATH D6WWC4_TRICA	* * * *	Plasminogen activator inhibitor 2 Serine protease inhibitor A3G Serpin A12 Serpin B13 Serpin-ZX Serpin peptidase inhibitor 23	SERPINB2 PAI2 PLANH Serpina3g Spi2A SERPINA12 SERPINB13 PI13 At1g47710 F16N3.3 T2E0 serpin23 TcasGA2_TC00	2 5.22 15771	Drosophila melanogaster (Fruit fly) Homo sapiens (Human) Mus musculus (Mouse) Homo sapiens (Human) Homo sapiens (Human) Arabidopsis thaliana (Mouse-ear cress) Tribolium castaneum (Rec Pour beetle)	44 41 44 41 39 39 1 38

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UNIPROT/SWISS-PROT FILE FORMAT

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Line code	Content	Occurrence in an entry
ID	Identification	Once; starts the entry
AC	Accession number(s)	Once or more
DT	Date	Three times
DE	Description	Once or more
GN	Gene name(s)	Optional
OS	Organism species	Once or more
OG	Organelle	Optional
OC	Organism classification	Once or more
OX	Taxonomy cross-reference	Once
OH	Organism host	Optional
RN	Reference number	Once or more
RP	Reference position	Once or more
RC	Reference comment(s)	Optional
RX	Reference cross-reference(s)	Optional
RG	Reference group	Once or more (Optional if RA line)
RA	Reference authors	Once or more (Optional if RG line)
RT	Reference title	Optional
RL	Reference location	Once or more
CC	Comments or notes	Optional
DR	Database cross-references	Optional
PE	Protein existence	Once
KW	Keywords	Optional
FT	Feature table data	Once or more in Swiss-Prot, optional in TrEMBL
SQ	Sequence header	Once
(blanks)	Sequence data	Once or more
11	Termination line	Onco: and the ontry



NBRF/PIR

- The Protein Information Resource (PIR) was established in 1984 by the National Biomedical Research Foundation (NERE) as a resource to assist researchers in the identification and interpretation of protein sequence information.
- In 2002 PIR, along with its international partners, EBI and SIB, were awarded a grant from NIH to create UniProt, by unifying the PIR-PSD, Swiss-Prot, and TrEMBL databases.
- As of 2010, PIR offers a wide variety of resources mainly oriented to assist the propagation and standardization of protein annotation: PRO, iProClass, iProLINK.





	About PIR	Resources Sear	ch/Analys	is Download	Support		
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	Protein AC/ID	Protein Name	Length	Organism Name	PRO ID	PIRSF ID	UniRef50
	F7VJQ1/APRIO_HUMAN /ProClass UniProtKB/Swiss-Prot	Alternative prion protein	<u>73</u>	<u>Homo sapiens</u> <u>(Human)</u>			UniRef50 F7VJQ1
	O15394/NCAM2_HUMAN /ProClass UniProtKB/Swiss-Prot	Neural cell adhesion molecule 2 precursor	<u>837</u>	<u>Homo sapiens</u> <u>(Human)</u>	PR:000011018; PR:015394	PIRSF002507; PIRSF501037	<u>UniRef50 015394</u>
	O43414/ERI3_HUMAN /ProClass UniProtKB/Swiss-Prot	ERI1 exoribonuclease 3	337	<u>Homo sapiens</u> <u>(Human)</u>	PR:000013260; PR:043414		UniRef50 043414
	P00441/SODC_HUMAN /ProClass UniProtKB/Swiss-Prot	Superoxide dismutase [Cu-Zn]	<u>154</u>	<u>Homo sapiens</u> (<u>Human)</u>	PR:000015399; PR:P00441	PIRSF000348	<u>UniRef50_P00441</u>
	P01031/CO5_HUMAN /ProClass UniProtKB/Swiss-Prot	Complement C5 precursor	<u>1676</u>	<u>Homo sapiens</u> <u>(Human)</u>	PR:000004904; PR:P01031	PIRSF001635	UniRef50 P01031
	P01583/IL1A_HUMAN /ProClass UniProtKB/Swiss-Prot	Interleukin-1 alpha precursor	<u>271</u>	<u>Homo sapiens</u> <u>(Human)</u>	PR:000001135; PR:P01583	PIRSF001937	UniRef50 P01583
	P01584/IL1B_HUMAN /ProClass UniProtKB/Swiss-Prot	Interleukin-1 beta precursor	<u>269</u>	<u>Homo sapiens</u> <u>(Human)</u>	PR:000001136; PR:P01584	PIRSF001937	UniRef50 P01584
	P02745/C1QA_HUMAN ProClass UniProtKB/Swiss-Prot	Complement C1q subcomponent subunit A precursor	<u>245</u>	<u>Homo sapiens</u> (Human)	PR:000004875; PR:P02745	PIRSF002477	UniRef50 P02745
	P02746/C1QB_HUMAN /ProClass UniProtKB/Swiss-Prot	Complement C1q subcomponent subunit B precursor	253	<u>Homo sapiens</u> (Human)	PR:000004876; PR:P02746	PIRSF002477	UniRef50 P02746
	P02747/C1QC_HUMAN /ProClass UniProtKB/Swiss-Prot	Complement C1q subcomponent subunit C	245	<u>Homo sapiens</u> (Human)	PR:000004878; PR:P02747	PIRSF002477	<u>UniRef50 P02747</u>

3015 proteins | 302 pages | 10 / page | K « < 1 | 2 | 3 | 4 | 5 > » >



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ProClass Summary Report for UniProtKB Entry: F7VJQ1

GENERAL INFORMATION UniProtKB ID UniProtKB Accession Protein Name APRIO HUMAN Alternative prion protein F7VJQ1 Protein Name and ID RefSeq: <u>NP 001258490.1</u> GenPept: <u>DAA34790.1</u> IPI: <u>IPI01026282</u> Source Organism: Homo sapiens (Human) Taxon Group: Euk/mammal NCBI Taxon: <u>9606</u> Lineage: Eukaryota; Metazoa; Chordata; Craniata; Vertebrata; Euteleostomi; Mammalia; Eutheria; Euarchontoglires; Primates; Haplorrhini; Catarrhini; Hominidae; Taxonomy Homo. Keywords complete proteome; membrane; mitochondrion; mitochondrion outer membrane; reference proteome; transmembrane; transmembrane helix Function Involved in the secretion of alkaline protease. Tissue Specificity Detected in brain homogenate, primary neurons, and peripheral blood mononuclear cells (at protein level).

CROSS-REFERENCES	
Bibliography	View Bibliography Information Annotated references: PMID: 11120052; 11220650; 11244488; 11559357; 11584448; 11593450; 11684342; 11704923; 11756421; 11775001; 11787070; 11833672; 11840201; 11961239; 11986958; 12070046; 12084159; 12161431; 12186633; 12205650 [GeneRIF] More Other references: PMID: 16004966; 2180366; 16294306; 7913755; 10970892; 1683708; 8105771; 1736177; 1357663; 12679034; 2564168; 12514748; 12356908; 17500595; 11438138; 18051367; 1351748; 9786248; 10988071; 1363802; More
DNA Sequence	EMBL: AL133396; BK007887 DDB1: AL133396; BK007887 GenBank: AL133396; BK007887
Genome/Gene	Gene Name: PRNP; prion protein Locus Tag: RP5-1068H6.2; Synonyms: ASCR; AltPrP; CD230; CJD; GSS; KURU; PRIP; PrP; PrP27-30; PrP33-35C; PrPc; p27-30; Map Location: 20p13 Entrez Gene: <u>15621</u> UniGene: <u>Hs.472010; Hs.610285; Hs.721670</u> RefSeq: NM 000311.3 NP 001073592.1 [Map Viewer]; NM 001080121.1 NP 001073590.1 [Map Viewer]; NM 001080122.1 NP 001073591.1 [Map Viewer]; NM 001080123.1 NP 001073592.1 [Map Viewer]; NM 001271561.1 NP 001258490.1 [Map Viewer]; NM 183079.2 NP 898902.1 [Map Viewer] UCSC: <u>ucD02wtkw.4</u> human KEGG: <u>hsa:5621</u>
Gene Expression	GEO
Ontology	Gene Ontology: Cellular Component G0:0005739:mitochondrion [GO_REF:0000037; evidence:IEA] G0:0005741:mitochondrial outer membrane [GO_REF:0000037; evidence:IEA][GO_REF:0000039; evidence:IEA][PMID:21478263; evidence:IDA] G0:0016021:integral component of membrane [GO_REF:0000037; evidence:IEA] G0:0016020:membrane [GO_REF:0000037; evidence:IEA]
Structure	ProteinModelPortal: <u>F7VJQ1</u>
Other Databases	neXtProt: <u>NX_F7VJ01</u> NextBio: <u>35510517</u> CTD: <u>5621</u> GenomeRNAi: <u>5621</u> GeneWiki: <u>PRNP</u>

FAMILY CLASSIFICATION		
UniRef	UniRef100 F7VJQ1; UniRef90 F7VJQ1; UniRef50 F7VJQ1	
Other Classification	KO: <u>K05634</u>	

FEATURE & SEQUENCE DISPLAY	
Length = 73 F7VIQ1 1 61	Click on a bar to show its sequence; to copy and paste it, press ctl c then ctl v. 73 74 75 75 76 77 MEHWGQPIPGAGQPURQPLPTSGRUWLGAASUWULGAASUWULGAAPUWULGTASUWULG



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Georgetown University Medical Center 3300 Whitehaven Street, NW, Suite 1200 Washington, DC 20007, USA







SEQUENCE RETRIEVED FROM NBRF/PIR IN FASTA FILE FORMAT

>F7VJQ1 APRIO_HUMAN Alternative prion protein [Homo sapiens] MEHWGQPIPGAGQPWRQPLPTSGRWWLGAASWWWLGAASWWWLGAAPWWWLGTASWWWL G

SRRWHPQSVEQAE

PDB

- The Protein Data Bank (PDB) archive is the single worldwide repository of information about the 3D structures of large biological molecules, including proteins and nucleic acids.
- The PDB was established in 1971 at Brookhaven National Laboratory (**HNL**) under the leadership of Walter Hamilton and originally contained 7 structures.
- In 1998, the Research Collaboratory for Structural Bioinformatics (**RCSB**) became responsible for the management of the PDB.
- In 2003, the wwPDB was formed to maintain a single PDB archive of macromolecular structural data that is freely and publicly available to the global community.
- The RCSB PDB supports a website where visitors can perform simple and complex queries on the data, analyze, and visualize the results.

W_O R L D W I D

Data Bank Japan

• Members of wwPDB are: **ICSB PDB** (USA), **PDBe** (Europe) and **PDB** (Japan), and Biological Magnetic Resonance Data Bank **EVIRB** (USA).

http://rcsb.org/pdb/



© RCSB Protein Data Bank



A MEMBER OF THE PDB EMDataBank An Information Portal to Biological Macromolecular Structures As of Tuesday Jul 29, 2014 at 5 PM PDT there are 102158 Structures | PDB Statistics | 🖾 🖸 🚔





SECTION	DESCRIPTION	RECORD TYPE	
Title	Summary descriptive remarks	HEADER, OBSLTE, TITLE, SPLIT, CAVEAT, COMPND, SOURCE, KEYWDS, EXPDTA, NUMMDL, MDLTYP, AUTHOR, REVDAT, SPRSDE, JRNL	
Remark Annotations	Various comments about entry in more depth than standard records	REMARKs 0-999	
Primary structure	Peptide and/or nucleotide sequence and the relationship between the PDB sequence and that found in the sequence database(s)	DBREF, SEQADV, SEQRES MODRES	
Heterogen	Description of non-standard groups	HET, HETNAM, HETSYN, FORMUL	
Secondary structure	Description of secondary structure	HELIX, SHEET	
Connectivity annotation	Chemical connectivity	SSBOND, LINK, CISPEP	
Miscellaneous features	Features within the macromolecule	SITE	
Crystallographic	Description of the crystallographic cell	CRYST1	
Coordinate transformation	Coordinate transformation operators	ORIGXn, SCALEn, MTRIXn,	
Coordinate	Atomic coordinate data	MODEL, ATOM, ANISOU, TER, HETATM, ENDMDL	
Connectivity	Chemical connectivity	CONECT	01
Bookkeeping	Summary information, end-of-file marker	MASTER, END	

SCOP

• The Structural Classification of Proteins (SCOP) database is a largely manual classification of protein structural domains based on similarities of their structures and amino acid sequences.

- A motivation for this classification is to determine the evolutionary relationship between proteins.
- Proteins with the same shapes but having little sequence or functional similarity are placed in different "superfamilies", and are assumed to have only a very distant common ancestor.
- Proteins having the same shape and some similarity of sequence and/or function are placed in "families", and are assumed to have a closer common ancestor.
- SCOP has been discontinued and the last official version of SCOP is 1.75. <u>SCOP1.75</u> is also known as <u>SCOP2</u>.
- SCOP2 offers two different ways for accessing data: SCOP2-browser, and SCOP2-graph.
- SCOP2-browser allows navigation in a traditional way by browsing pages displaying the node information.
- SCOP2-graph is a graph-based web tool for display and navigation.
- The source of protein structures is the Protein Data Bank.

HIERARCHICAL STRUCTURE OF SCOP

• The unit of classification of structure in SCOP is the protein domain.

- The levels of SCOP are as follows.
 - **1. Class**: Types of folds, e.g., all α , all β , α/β , $\alpha+\beta$, $\alpha\&\beta$, etc.
 - 2. Fold: The different shapes of domains within a class, e.g., 2 helices; antiparallel hairpin, left-handed twist, etc.
 - **3. Superfamily**: The domains in a fold are grouped into superfamilies, which have at least a distant common ancestor.
 - **4. Family**: The domains in a superfamily are grouped into families, which have more recent common ancestor.
 - **5. Protein domain**: The domains in families are grouped into protein domains, which are essentially the same protein.
 - 6. Species: The domains in "protein domains" are grouped according to species.
 - **7. Domain**: It is part of a protein. For simple proteins, <u>it can be the entire protein</u>.

http://scop2.mrc-lmb.cam.ac.uk/





News

November,2013

During the development of SCOP2, we have identified a new, previously unrecognised type of alpha-alpha superhelic. Unlike other alpha-alpha superhelices... More...

January,2014

SCOP2 article in NAR is published More...

January, 2014

The structure of the month More...

Welcome to SCOP2!

Citation

Antonina Andreeva, Dave Howorth, Cyrus Chothia, Eugene Kulesha, Alexey Murzin, SCOP2 prototype: a new approach to protein structure mining (2014) Nucl. Acid Res., 42 (D1): D310-D314. [PDF]

Description of the SCOP2 database

SCOP2 is a successor of Structural classification of proteins (SCOP). Similarly to SCOP, the main focus of SCOP2 is on proteins that are structurally characterized and deposited in the PDB. Proteins are organized according to their structural and evolutionary relationships, but, in contrast to SCOP, instead of a simple tree-like hierarchy these relationships form a complex network of nodes. Each node represents a relationship of a particular type and is exemplified by a region of protein structure and sequence.

In SCOP2, we try to put in use the knowledge we acquired over the past years and the lessons we have learned during the classification of protein structures. We believe that there are many peculiarities of proteins and their structures that have been missed due to the constraints of the original SCOP hierarchical schema. We hope that our users will find the new resource useful and that it could open new avenues for protein analysis and research.

Quick introduction on how to browse, search and download

SCOP2 offers two different ways for accessing data: SCOP2-browser, that allows navigation through the SCOP2 classification in a traditional way by browsing pages displaying the node information, and SCOP2-graph, which is a graph-based web tool for display and navigation through the SCOP2 classification. Both tools provide search of SCOP2 data by free text, node names, IDs, tags and keywords, as well as external identifiers associated with them, e.g. PDB and UniProt. SCOP2 data can also be retrieved via REST interface or downloaded from the SCOP2 Download page. For more information visit the About page.

Web browser compatibility check

To test whether your web browser and its settings are suitable to view SCOP2-graph and to visualize protein structures using Jmol applet click here.

Information about the release

This is a beta release and contains a fraction of protein structure data. We wish to introduce the new database to our users and seek for a comprehensive feedback that would guide us for the future database development and expansion. We plan to regularly update the site with new classification data.

Search Browser

invertase Search

Add an asterisk to search free text (e.g. serine*)

Search Graph

Search

Add an asterisk to search free text (e.g. protein*domain)

OUTPUT OF SCOP



Structural Classification of Proteins



Family: Plant invertase/pectin methylesterase inhibitor

<u>Pfam 04043</u>

Lineage:

- 1. Root: scop
- 2. Class: All alpha proteins [46456]
- 3. Fold: Bromodomain-like [47363]
 - 4 helices; bundle; minor mirror variant of up-and-down topology
- 4. Superfamily: <u>Plant invertase/pectin methylesterase inhibitor</u> [101148] contains a short alpha-hairpin at the N-terminal extension S<u>uperfamily</u>
- 5. Family: <u>Plant invertase/pectin methylesterase inhibitor</u> [101149] <u>Pfam 04043</u>

Protein Domains:

- 1. Invertase inhibitor [101150]
 - 1. Common tobacco (Nicotiana tabacum) [TaxId: 4097] [101151] (9) 🔤
- Pectin methylesterase inhibitor 1, PMEI1 [116887] forms dimers and trimers by swapping the extra N-terminal hairpins
 - <u>Thale cress (Arabidopsis thaliana) [TaxId: 3702]</u> [116888] (3) SQ <u>Q9LNF2</u> 28-176

Enter search key:

Search



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CATH

- The CATH (Class, Architecture, Topology, and Homologous superfamily) is a semiautomatic, hierarchical classification of protein domains.
- CATH shares many broad features with its principal rival, SCOP.
- The four main levels of the CATH hierarchy are as follows:
 - Class: the overall secondary-structure content of the domain. e.g., all α , all β , α/β , $\alpha+\beta$, $\alpha\&\beta$, etc.
 - Architecture: high structural similarity but **no evidence of homology**. Equivalent to a fold in SCOP.
 - **Topology:** a large-scale grouping of topologies which share particular structural features
 - **Homologous superfamily:** indicative of a demonstrable evolutionary relationship. Equivalent to the superfamily level of SCOP.

CATH

http://www.cathdb.info/

Latest Release Statistics

Gene3D v12 released March 18, 2012

CATH v4.0 based on PDB dated March 26, 2013

CATH Domains

CATH Superfamilies

Annotated PDBs

Cellular Genomes

Protein Sequences

CATH Domain Predictions

CATH / Gene3D

26 million protein domains classified into 2,738 superfamilies



277,687

2,738

69,058

6,131

21,662,155

25,615,754

What is CATH?

CATH is a classification of protein structures downloaded from the Protein Data Bank. We group protein domains into superfamilies when there is sufficient evidence they have diverged from a common ancestor.

- Search CATH by text, ID or keyword
- <u>Search CATH by protein</u> sequence (FASTA)
- Search CATH by PDB structure

Example pages

- PDB "2bop"
- Domain "1cukA01"
- Relatives of "1cukA01"
- Superfamily "HUPs"
- Search for "enolase"
 Superfamily Comparison

Functional Family

FunFam Alignment

Browse CATH Hierarchy

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Citing CATH

If you find this resource useful, please consider citing the reference that describes this work:

New functional families (FunFams) in CATH to improve the mapping of conserved functional sites to 3D structures. Sillitoe I, Cuff AL, Dessailly BH, Dawson NL, Furnham N, Lee D, Lees JG, Lewis TE, Studer RA, Rentzsch R, Yeats C, Thornton JM, Orengo CA Nucleic Acids Res. 2013 Jan Pubmed: 23203873

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CATH

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degranulation polymer polypeptide(I) positive regulation of i-kappab kinase/nf-kappab signaling positive regulation of nf-kappab transcription factor activity positive regulation of cell proliferation positive regulation of transcription from rna polymerase ii promoter stress-activated mapk cascade tetrameric toll-like receptor 1 signaling pathway toll-like receptor 2 signaling pathway toll-like receptor 3 signaling pathway toll-like receptor 4 signaling pathway trimeric vascular endothelial growth factor receptor signaling pathway Water zinc ion binding

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MOTIF

- Motif is a search service provided by GenomeNet to search with a protein query
 sequence against Motif Libraries.
- Supports several motif databases such as Prosite, BLOCKS, ProDom, Pfam, and PRINTS.
- Allows you to search protein sequence libraries with your patterns.
 - Each residue must be separated with (minus sign).
 - x represents any amino acids.
 - [DE] means either D or E.
 - {FWY} means any amino acids except for F, W and Y
 - A(2,3) means that A appears 2 to 3 times consecutively.
 - The pattern string must be terminated with . (period).
 For example, C-x-{C}-[DN]-x(2)-C-x(5)-C-C.
- Generates a profile from a set of multiple aligned sequences using PFMake or HMM.genome.jp/tools/motif/









MATCHING MOTIF HITS

Your Query Sequence:

MTKMGGNLAVMLLSLFLSALATGNGNSIPTTTTPQGVFETRTDKLPGGAASVPSGAGIYD DIDTFVPFRSDSHDPFSWHLLKTVLQNETADKNVIISPFSVKLVLALLAEAAGAGTQTQV ELANTQTDIRSQNNVREFYRKTLNSFKKENQLHETLSVRTKLFTDSFIETQQKFTATLKH FYDSEVEALDFTNPEAAADAINAWAANITQGRLQQLVAPDNVRSSVMLLTNLIYFNGLWR RQFATTFQGSFFRSKDDQSRAEFMEQTDYFYYTTSEKLKAQILRLPYKGKNSLFVLLPYA LNGIHDLVKNLENDELKSAQWAMEEVKVKVTLPKFHFDYQQNLKETLRSLGVREIFEDSA SLPGLTRGADVAGKVKVSNILQKAGINVNEKGTEAYAATVVEIENKFGGSTAIEEFNVNR PFVFFIEEESTGNILFAGKVHSPTTQN

Number of found motifs: 1

PROSITE PATTERN

Found Motif	Position	PROSITE	Description	Related Sequences	Related Structures
SERPIN	416426 Detail	PS00284	Serpins signature.	232	<u>127</u>

PATTERN OF MATCHING MOTIF HITS

Motif SERPIN in your sequence

Prosite ID:

SERPIN (PS00284)

Description:

Serpins signature.

Pattern:

[LIVMFY]-{G}-[LIVMFYAC]-[DNQ]-[RKHQS]-[PST]-F-[LIVMFY]-[LIVMFYC]-x-[LIVMFAH].

Appearance:

Position	Found Motif	
416426	FNVNRPFVFFI	

Sequence:

MTKMGGNLAVMLLSLFLSALATGNGNSIPTTTTPQGVFETRTDKLPGGAASVPSGAGIYD DIDTFVPFRSDSHDPFSWHLLKTVLQNETADKNVIISPFSVKLVLALLAEAAGAGTQTQV ELANTQTDIRSQNNVREFYRKTLNSFKKENQLHETLSVRTKLFTDSFIETQQKFTATLKH FYDSEVEALDFTNPEAAADAINAWAANITQGRLQQLVAPDNVRSSVMLLTNLIYFNGLWR RQFATTFQGSFFRSKDDQSRAEFMEQTDYFYYTTSEKLKAQILRLPYKGKNSLFVLLPYA LNGIHDLVKNLENDELKSAQWAMEEVKVKVTLPKFHFDYQQNLKETLRSLGVREIFEDSA SLPGLTRGADVAGKVKVSNILQKAGINVNEKGTEAYAATVVEIENKFGGSTAIEEFNVNR PFVFFIEEESTGNILFAGKVHSPTTQN

PFAM

- The Pfam database is a large collection of protein families, each represented by multiple sequence alignments and hidden Markov models (HMMs).
- Pfam version 27.0 was produced at the European Bioinformatics Institute using a sequence database called **Pfamseq**, which is based on UniProt.
- The descriptions of Pfam families are managed by the general public using Wikipedia.
- The Pfam database contains information about protein domains and families.
- Pfam-A is the manually curated portion of the database that contains over 10,000 entries.
- Pfam-B contains a large number of small families derived from clusters produced by an algorithm called ADDA (for automatic generation).

htp://pointanfiliesoca/ be useful when no Pfam-A families are found (but low pfam quality).



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Pfam 27.0 (March 2013, 14831 families)

The Pfam database is a large collection of protein families, each represented by **multiple sequence alignments** and **hidden Markov models (HMMs)**. <u>More...</u>

YOU CAN FIND DATA IN PFAM IN VARIOUS WAYS			
Analyze your protein sequence for Pfam matches			
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See groups of related families			
Look at the domain organisation of a protein sequence			
Find the domains on a PDB structure			
Query Pfam by keywords			
Insulin Enter any type of accession or ID to jump to the page for a Pfam family or clan, UniProt sequence, PDB structure, etc.			

Or view the help pages for more information

Citing Pfam

If you find Pfam useful, please consider citing the reference that describes this work:

<u>The Pfam protein families database</u> R.D. Finn, A. Bateman, J. Clements, P. Coggill, R.Y. Eberhardt, S.R. Eddy, A. Heger, K. Hetherington, L. Holm, J. Mistry, E.L.L. Sonnhammer, J. Tate, M. Punta **Nucleic Acids Research** (2014) Database Issue 42:D222-D230

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Comments or questions on the site? Send a mail to pfam-help@ebi.ac.uk. European Molecular Biology Laboratory





0

Family: Insulin (PF00049)

6 architectures 1447 sequences 3 interactions 340 species 923 structures

Summary	Summary: Insulin/IGF/Relaxin family					
Domain organisation	Pfam includes annotations and additional family information from a range of different sources. These sources can be accessed via the tabs below.					
Clan						
Alignments	Wikipedia: Insulin/IGF/Relaxin family Pfam InterPro					
HMM logo	This tab holds the annotation information that is stored in the Pfam database. As we move to using Wikipedia as our main source of annotation, the contents of this tab will be gradually replaced by the Wikipedia tab.					
Trees						
Curation & model	Insulin/IGF/Relaxin family Provide feedback					
Species	Superfamily includes insulins; relaxins; insulin-like growth factor; and bombyxin. All are					
Interactions	secreted regulatory hormones. Disulfide rich, all-alpha fold. Alignment includes B chain, linker (which is processed out of the final product), and A chain.					
Structures						
Jump to 🌵	External database links					
enter ID/acc Go	HOMSTRAD: ins 답					
	PANDIT: PF00049 대	•				
	PRINTS: PR00276 ₫	•				
	PROSITE: PDOC00235 di	Example structure				
	Pseudotam: PF00049 G	PDB entry 2QIU: Structure of Human				
	SCOP: Icplier	Arg-Insulin View a different structure:				
		2QIU V				

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PROSITE

• PROSITE, a protein domain database for functional characterization and annotation.

- PROSITE consists of entries describing the protein families, domains and functional sites as well as amino acid patterns and profiles in them.
 - PROSITE is manually curated by a team of the Swiss Institute of Bioinformatics and tightly integrated into Swiss-Prot protein annotation.
 - PROSITE is complemented by ProRule, a collection of rules based on profiles and patterns.
 - The rules contain information about biologically meaningful residues, like active sites, substrate- or co-factor-binding sites, posttranslational modification sites or disulfide bonds, to help function determination.

http://prosite.expasy.org/



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Database of protein domains, families and functional sites

PROSITE consists of documentation entries describing protein domains, families and functional sites as well as associated patterns and profiles to identify them [More... / References / Commercial users].

PROSITE is complemented by ProRule, a collection of rules based on profiles and patterns, which increases the discriminatory power of profiles and patterns by providing additional information about functionally and/or structurally critical amino acids [More...].

Forthcoming changes to the profile format



Release 20.104 of 06-Jul-2014 contains 1703 documentation entries, 1308 patterns, 1087 profiles and 1076 ProRule.



found: 13 hits in 1 sequence

sp-P98073-ENTK HUMAN (1019 aa)

MGSKRGISSRHHSLSSYEIMFAALFAILVVLCAGLIAVSCLTIKESQRGAALGQSHEARATFKITS GVTYNPNLQDKLSVDFKVLAFDLQQMIDEIFLSSNLKNEYKNSRVLQFENGSIIVVFDLFFAQWVS DENVKEELIQGLEANKSSQLVTFHIDLNSVDILDKLTTTSHLATPGNVSIECLPGSSPCTDALTCI KADLFCDGEVNCPDGSDEDNKMCATVCDGRFLLTGSSGSFQATHYPKPSETSVVCQWIIRVNQGLS IKLSFDDFNTYYTDILDIYEGVGSSKILRASIWETNPGTIRIFSNQVTATFLIESDESDYVGFNAT YTAFNSSELNNYEKINCNFEDGFCFWVQDLNDDNEWERIQGSTFSPFTGPNFDHTFGNASGFYIST PTGPGGRQERVGLLSLPLDPTLEPACLSFWYHMYGENVHKLSINISNDQNMEKTVFQKEGNYGDNW NYGQVTLNETVKFKVAFNAFKNKILSDIALDDISLTYGICNG</mark>SLYPEPTLVPTPPPELPTDCGGPF ELWEPNTTFSSTNFPNSYPNLAFCVWILNAQKGKNIQLHFQEFDLENINDVVEIRDGEEADSLLLA VYTGPGPVKDVFSTTNRMTVLLITNDVLARGGFKANFTTGYHLGIPEPCKADHFQCKNGECVPLVN LCDGHLHCEDGSDEADCVRFFNGTTNNNGLVRFRIQSIWHTACAENWTTQISNDVCQLLGLGSGNS SKPIFPTDGGPFVKLNTAPDGHLILTPSQQCLQDSLIRLQCNHKSCGKKLAAQDITPKIVGGSNAK EGAWPWVVGLYYGGRLLCGASLVSSDWLVSAAHCVYGRNLEPSKWTAILGLHMKSNLTSPQTVPRL IDEIVINPHYNRRRKDNDIAMMHLEFKVNYTDYIQPICLPEENQVFPPGRNCSIAGWGTVVYQGTT ANILQEADVPLLSNERCQQQMPEYNITENMICAGYEEGGIDSCQGDSGGPLMCQENNRWFLAGVTS FGYKCALPNRPGVYARVSRFTEWIQSFLH





Please note that the graphical representations of domains displayed hereafter are for illustrative purposes only, and that their colors and shapes are not intended to indicate homology or shared function.

For more information about how these graphical representations are constructed, go to http://prosite.expasy.org/mydomains/.

hits by profiles: [8 hits (by 6 distinct profiles) on 1 sequence]

Upper case represents match positions, lower case insert positions, and the '-' symbol represents deletions relative to the matching profile.





hits by patterns: [5 hits (by 4 distinct patterns) on 1 sequence]



THANK YOU