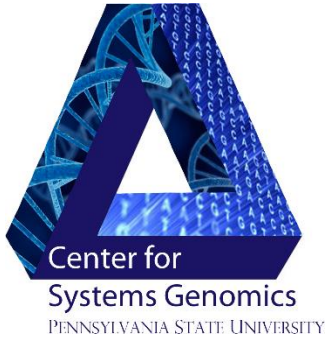
All things protein…

Marylyn D Ritchie, PhD
Professor, Biochemistry and Molecular Biology
Director, Center for Systems Genomics
The Pennsylvania State University



Amino Acid Sequence

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Nucleotide Sequence

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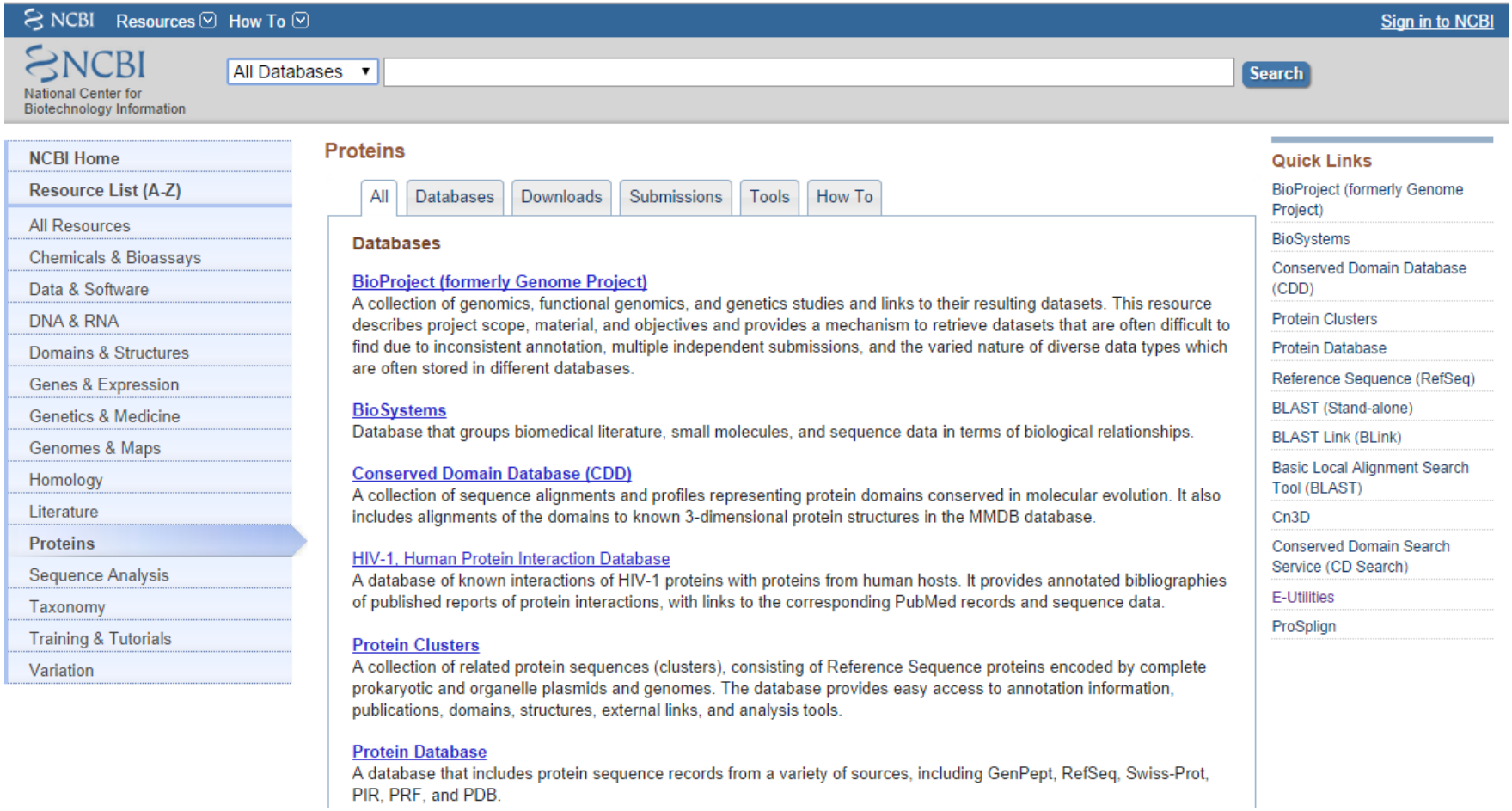
NCBI Protein Tools



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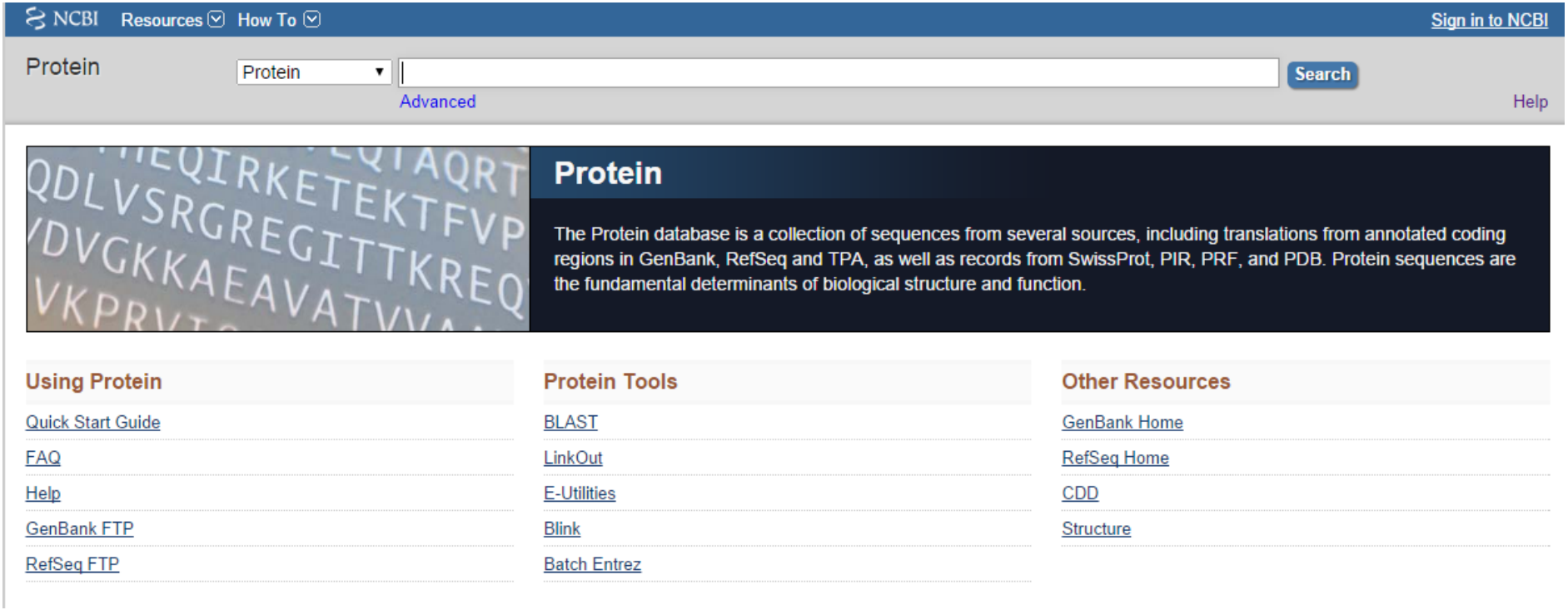

NCBI Protein Tools

NCBI Resources How To Sign in to NCBI

Protein Protein Search

Advanced Help

Display Settings: GenPept Send to:

SCN5A protein [Homo sapiens]

GenBank: AAI44622.1

FASTA Graphics

Go to:

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            Scheetz,T.E., Brownstein,M.J., Usdin,T.B., Toshiyuki,S.,
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Change region shown

Customize view

Analyze this sequence

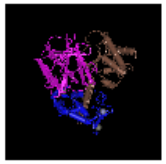
Run BLAST

Identify Conserved Domains

Highlight Sequence Features

Find in this Sequence

Protein 3D Structure



Voltage-gated Sodium Channel 1.5 C-terminal Domain In Complex With

PDB: 4JQ0

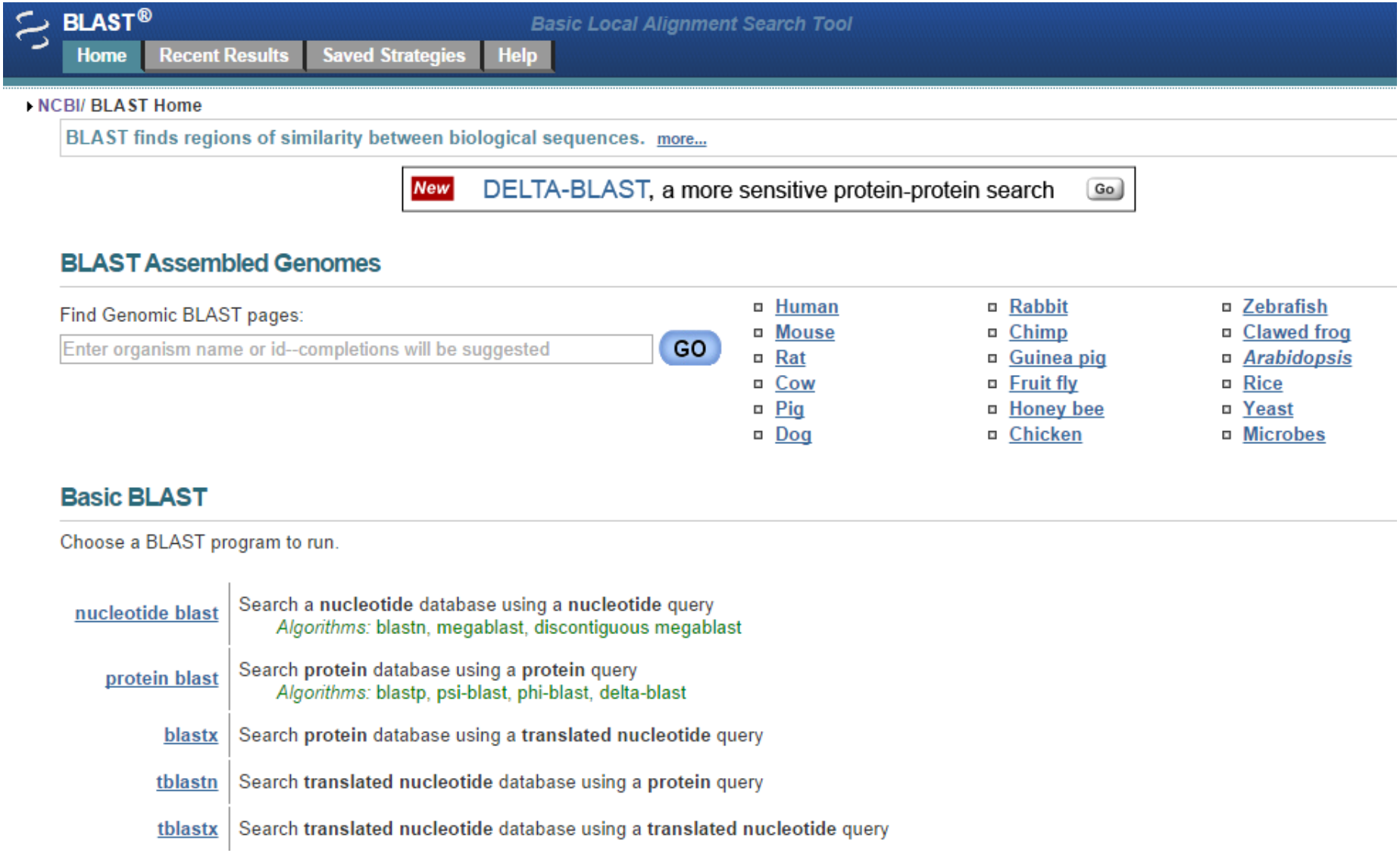
Source: Homo sapiens

Method: X-Ray Diffraction

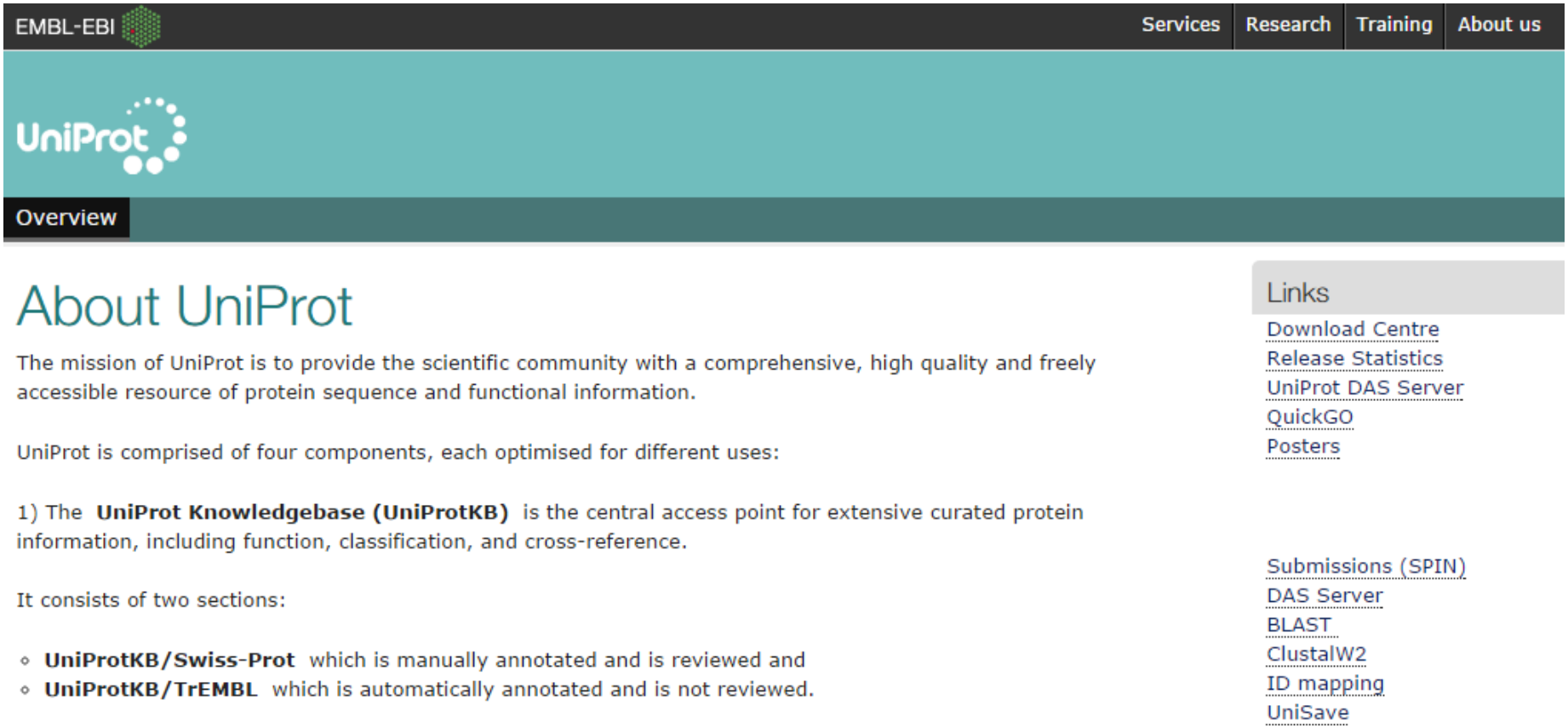
Resolution: 3.84 Å

See all 4 structures...

NCBI Protein Tools



Uniprot



http://www.ebi.ac.uk/uniprot

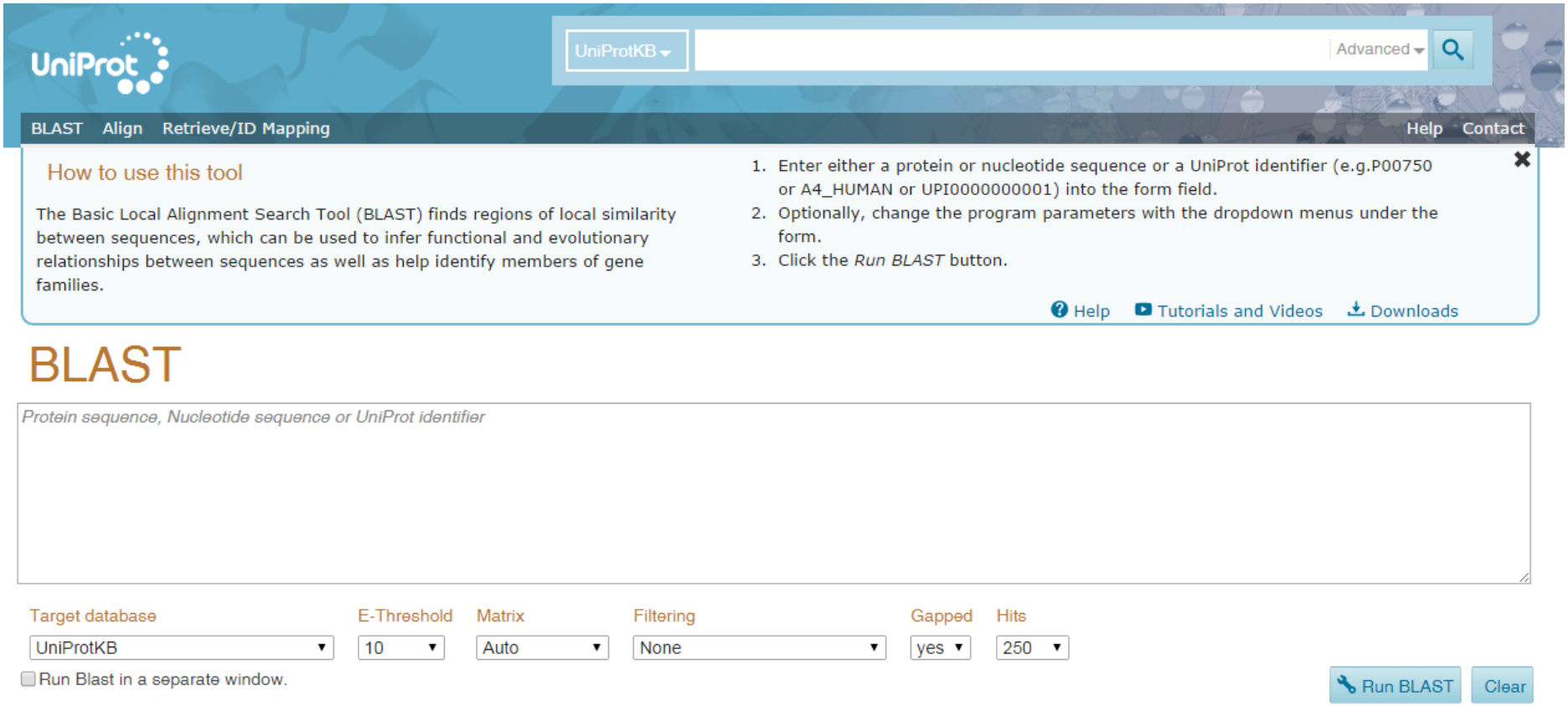
Uniprot

- Mission of UniProt is to provide comprehensive, high quality and freely accessible resource of protein sequence and functional information
- UniProt Knowledgebase (UniProtKB)
  - central access point for extensive curated protein information, including function, classification, and cross-reference
    - UniProtKB/Swiss-Prot which is manually annotated and is reviewed
    - UniProtKB/TrEMBL which is automatically annotated and is not reviewed

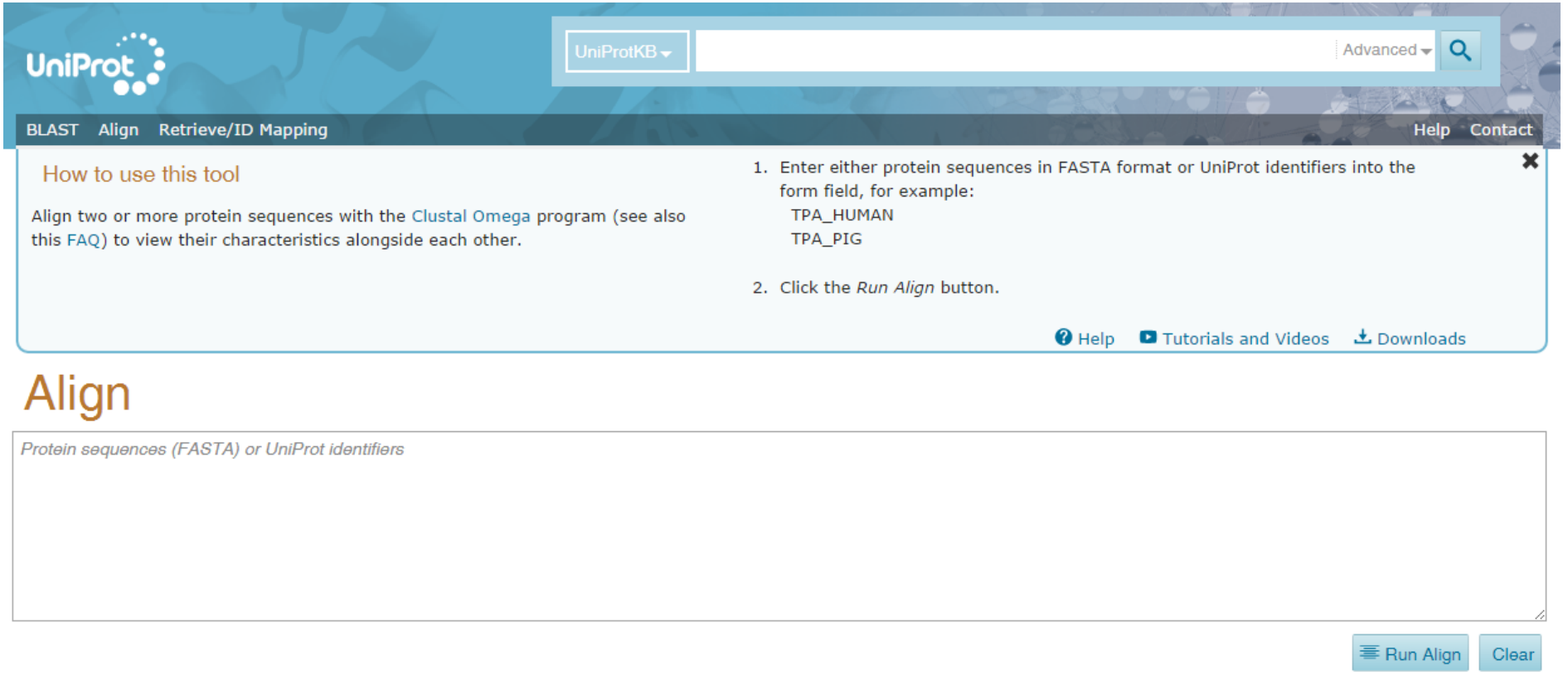
Uniprot

- UniProt Reference Clusters (UniRef) databases
  - clustered sets of sequences from the UniProtKB and selected UniProt Archive records to obtain complete coverage of sequence space at several resolutions while hiding redundant sequences
- UniProt Archive (UniParc)
  - comprehensive repository, used to keep track of sequences and their identifiers
- UniProt Metagenomic and Environmental Sequences (UniMES)
  - repository specifically developed for metagenomic and environmental data.

Uniprot


UniProt
UniProtKB
Advanced
BLAST
Align
Retrieve/ID Mapping
Help
Contact
How to use this tool
The Basic Local Alignment Search Tool (BLAST) finds regions of local similarity between sequences, which can be used to infer functional and evolutionary relationships between sequences as well as help identify members of gene families.
1. Enter either a protein or nucleotide sequence or a UniProt identifier (e.g.P00750 or A4_HUMAN or UPI0000000001) into the form field.
2. Optionally, change the program parameters with the dropdown menus under the form.
3. Click the Run BLAST button.
Help
Tutorials and Videos
Downloads
BLAST
Protein sequence, Nucleotide sequence or UniProt identifier
Target database
E-Threshold
Matrix
Filtering
Gapped
Hits
UniProtKB
10
Auto
None
yes
250
Run Blast in a separate window.
Run BLAST
Clear

Uniprot


UniProt
UniProtKB
Advanced
BLAST
Align
Retrieve/ID Mapping
Help
Contact
How to use this tool
Align two or more protein sequences with the Clustal Omega program (see also this FAQ) to view their characteristics alongside each other.
1. Enter either protein sequences in FASTA format or UniProt identifiers into the form field, for example:
TPA_HUMAN
TPA_PIG
2. Click the Run Align button.
Help
Tutorials and Videos
Downloads
Align
Protein sequences (FASTA) or UniProt identifiers
Run Align
Clear

Aligning multiple sequences

- Highlights areas of similarity which may be associated with specific features that have been more highly conserved than other regions
  - These regions in turn can help classify sequences or to inform experiment design
- important step for phylogenetic analysis, which aims to model the substitutions that have occurred over evolution and derive the evolutionary relationships between sequences
- Clustal Omega improves on ClustalW in a number of ways - alignment accuracy and improved scaling to many sequences are the main results

PDB

- Single worldwide repository of information about the 3D structures of large biological molecules, including proteins and nucleic acids
- Understanding the shape of a molecule helps to understand how it works
- Can be used to help deduce a structure's role in human health and disease, and in drug development
- Structures in the archive range from tiny proteins and bits of DNA to complex molecular machines like the ribosome
- PDB archive is available at no cost to users
- PDB archive is updated each week at the target time of Wednesday 00:00 UTC (Coordinated Universal Time)
- Most recent release is timestamped and linked on every page in the top right header.

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RCSB PDB PROTEIN DATA BANK → PDB-101

A MEMBER OF THE PDB | EMDataBank

An Information Portal to Biological Macromolecular Structures

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Everything | Author | Macromolecule | Sequence | Ligand

e.g., PDB ID, molecule name, author

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Biological Macromolecular Resource

Full Description

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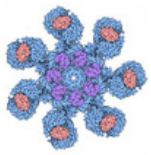
Structural View of Biology

List View of Archive By: Title | Date | Category



Molecule of the Month

Apoptosomes

"To be, or not to be"--that question is continually being asked by each of your cells. Your cells are preprogrammed to die on command. This is essential during development of large organisms like ourselves, where cells work together, growing and dying to shape our complicated bodies. It is also essential throughout our adult lives, to remove damaged or infected or cancerous cells. The machinery for cell death is always silently present in cells, but can be instantly mobilized if the choice is made to die.

Full Article

Protein Structure Initiative Featured System

Peptidyl-carrier Proteins

Bacteria are creative chemists, constantly discovering new ways to build unusualmolecules for exploiting natural resources and fighting

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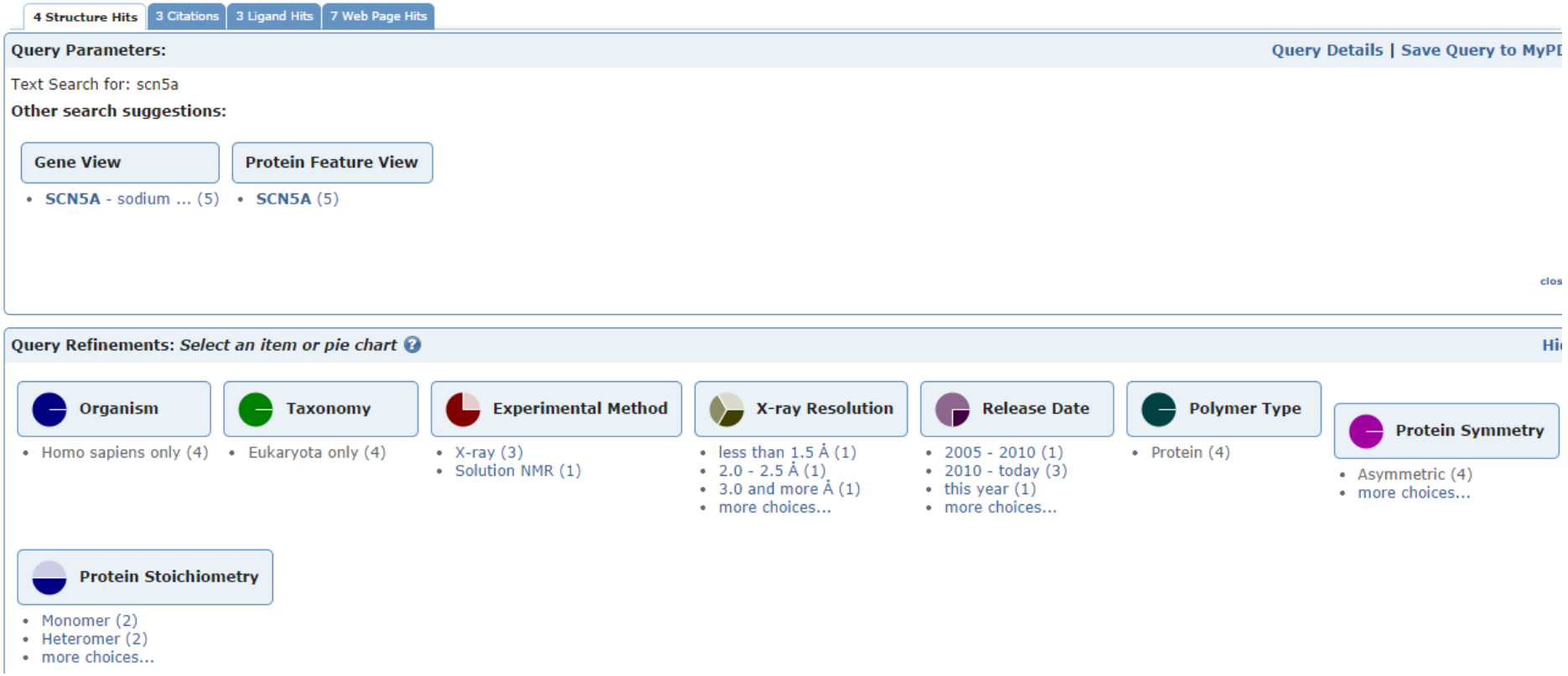
PDB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3 Ligand Hits
7 Web Page Hits
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Other search suggestions:
Gene View
Protein Feature View
SCN5A - sodium ... (5)
SCN5A (5)
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Organism
Homo sapiens only (4)
Taxonomy
Eukaryota only (4)
Experimental Method
X-ray (3)
Solution NMR (1)
X-ray Resolution
less than 1.5 Å (1)
2.0 - 2.5 Å (1)
3.0 and more Å (1)
more choices...
Release Date
2005 - 2010 (1)
2010 - today (3)
this year (1)
more choices...
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more choices...
Protein Stoichiometry
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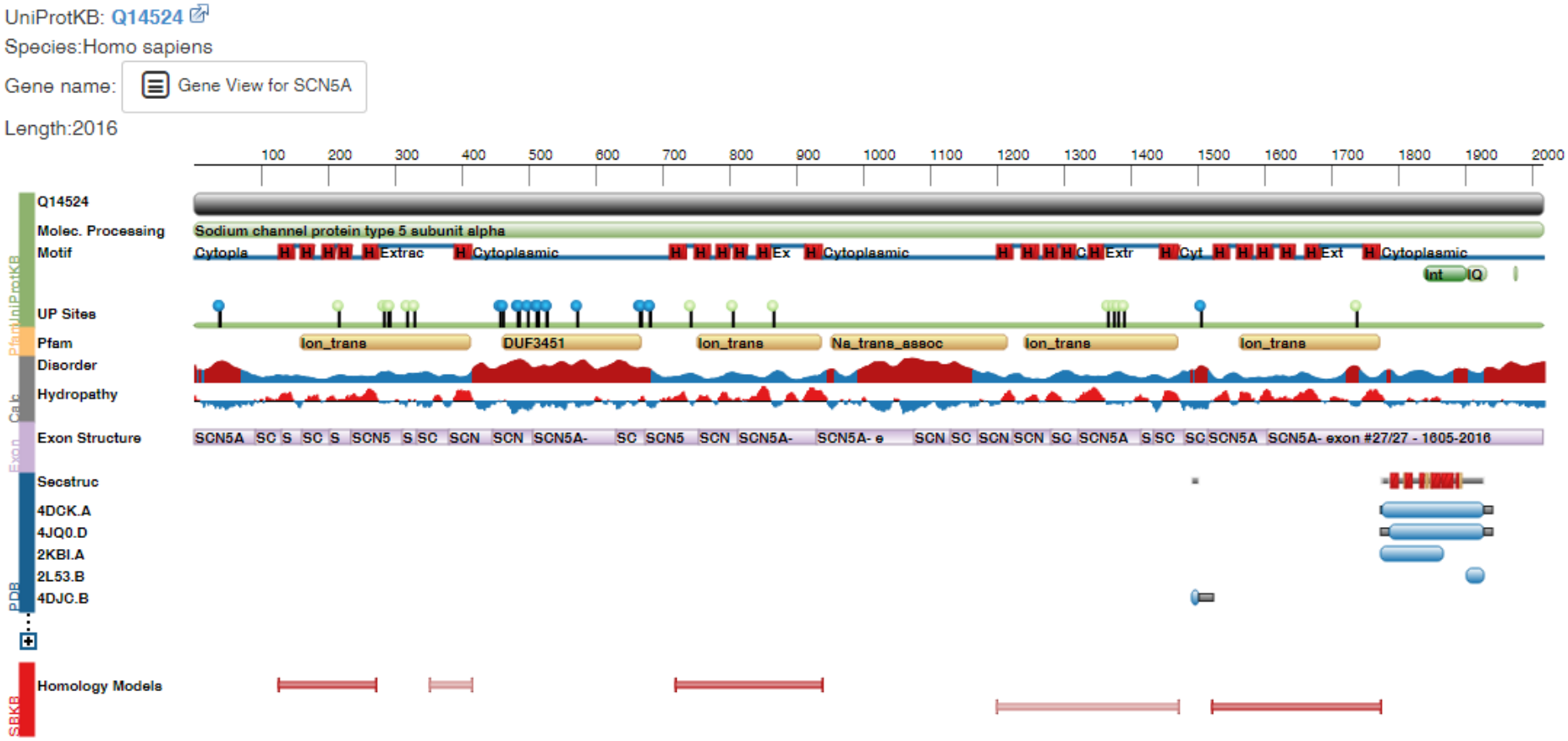
Heteromer (2)
more choices...

PDB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4DJC.B
Homology Models
PfamUniProtKB
Cath
Exon
PDB
SRKB

PDB

38340 Structure Hits | 14104 Citations | 5605 Ligand Hits

Query Parameters: Query Details | Save Quer

TaxonomyTree Search for Bacteria (eubacteria)

Query Refinements: *Select an item or pie chart*

Organism
- Escherichia coli (4888)
- Escherichia coli K-12 (2076)
- Bacillus subtilis (1037)
- Thermus thermophilus HB8 (995)
- Mycobacterium tuberculosis (925)
- Staphylococcus aureus (798)
- Pseudomonas aeruginosa (677)
- Other (27135)

Taxonomy
- Bacteria only (37229)
- Bacteria/Eukaryota (770)
- Bacteria/Other (182)
- Bacteria/Viruses (87)
- Bacteria/Archaea (32)
- Bacteria/Eukaryota/Viruses (14)
- Bacteria/Eukaryota/Other (12)
- Other (14)

Experimental Method
- X-ray (36100)
- Solution NMR (1907)
- Electron Microscopy (270)
- Hybrid (28)
- Solid-State NMR (19)
- Neutron Diffraction (9)
- Electron Crystallography (6)
- Fiber Diffraction (1)

X-ray Resolution
- less than 1.5 Å (2857)
- 1.5 - 2.0 Å (12776)
- 2.0 - 2.5 Å (12172)
- 2.5 - 3.0 Å (5737)
- 3.0 and more Å (2569)
- more choices...

Release Date
- before 2000 (3123)
- 2000 - 2005 (6451)
- 2005 - 2010 (12673)
- 2010 - today (16093)
- this year (2752)
- this month (84)
- more choices...

Polymer Type
- Protein (36115)
- Mixed (2102)
- RNA (120)

Enzyme Classification
- 3: Hydrolases (7032)
- 2: Transferases (5586)
- 1: Oxidoreductases (4683)
- 4: Lyases (2077)
- 5: Isomerases (1313)
- 6: Ligases (960)

SCOP Classification
- Alpha and beta proteins (a/b) (6190)
- Alpha and beta proteins (a+b) (4077)
- All beta proteins (3250)
- All alpha proteins (2485)
- Multi-domain proteins (alpha an ... (569)
- Small proteins (379)
- Membrane and cell surface prote ... (377)
- Other (338)

Protein Symmetry
- Asymmetric (18125)
- Cyclic (14374)
- Dihedral (4600)
- Tetrahedral (225)
- Octahedral (76)
- Helical (46)
- Icosahedral (12)
- more choices...

Protein Stoichiometry
- Homomer (18766)
- Monomer (15804)
- Heteromer (2888)
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Membrane Proteins
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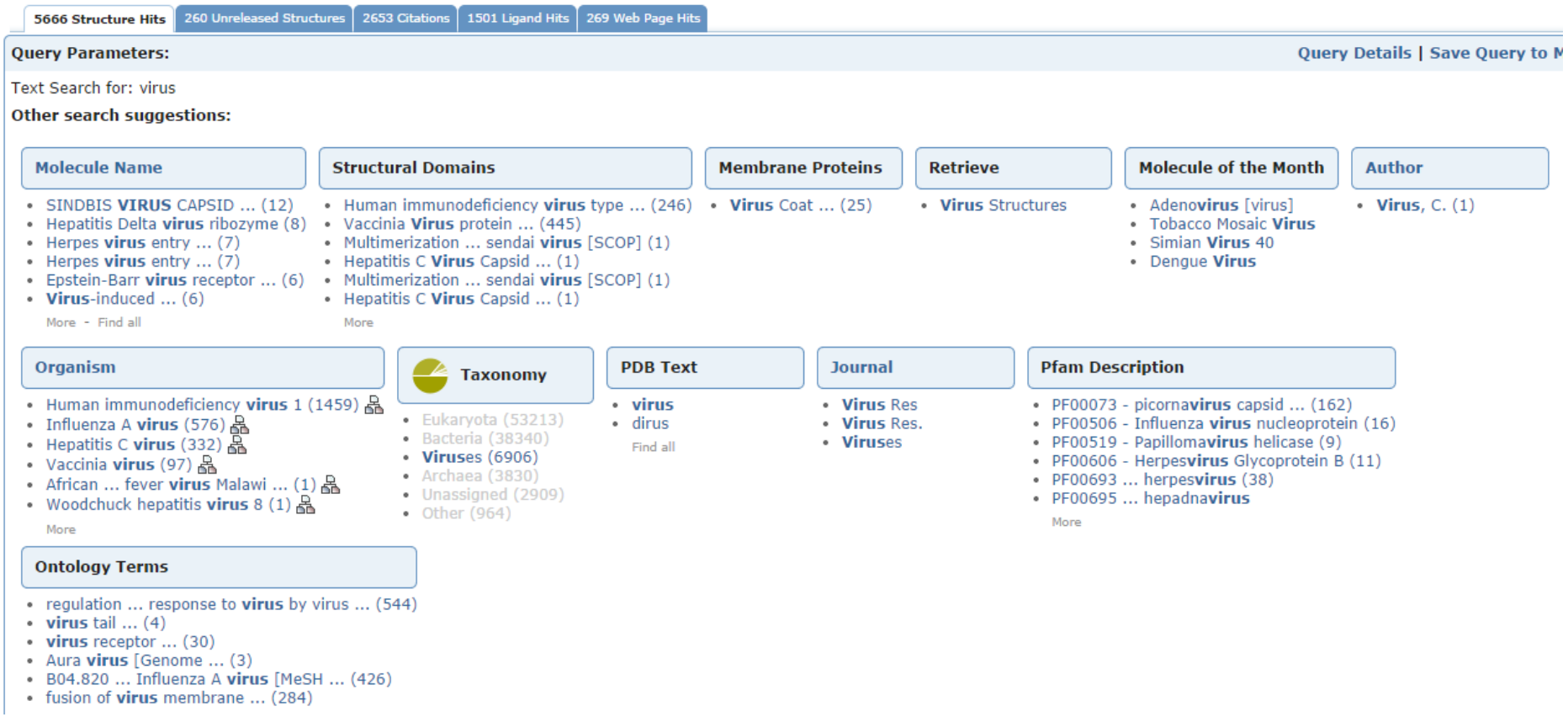
- BETA-BARREL (331)
- MONOTOPIC MEMBRANE PROTEINS (84)

PDB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2653 Citations
1501 Ligand Hits
269 Web Page Hits
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Query Details | Save Query to M
Text Search for: virus
Other search suggestions:
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Hepatitis Delta virus ribozyme (8)
Herpes virus entry ... (7)
Herpes virus entry ... (7)
Epstein-Barr virus receptor ... (6)
Virus-induced ... (6)
More - Find all
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Vaccinia Virus protein ... (445)
Multimerization ... sendai virus [SCOP] (1)
Hepatitis C Virus Capsid ... (1)
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Hepatitis C Virus Capsid ... (1)
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Molecule of the Month
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Tobacco Mosaic Virus
Simian Virus 40
Dengue Virus
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Virus, C. (1)
Organism
Human immunodeficiency virus 1 (1459)
Influenza A virus (576)
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Vaccinia virus (97)
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Woodchuck hepatitis virus 8 (1)
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Bacteria (38340)
Viruses (6906)
Archaea (3830)
Unassigned (2909)
Other (964)
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Find all
Journal
Virus Res
Virus Res.
Viruses
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PF00519 - Papillomavirus helicase (9)
PF00606 - Herpesvirus Glycoprotein B (11)
PF00693 ... herpesvirus (38)
PF00695 ... hepadnavirus
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regulation ... response to virus by virus ... (544)
virus tail ... (4)
virus receptor ... (30)
Aura virus [Genome ... (3)
B04.820 ... Influenza A virus [MeSH ... (426)
fusion of virus membrane ... (284)

Pfam

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Pfam 27.0 (March 2013, 14831 families)

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VIEW A CLAN	See groups of related families
VIEW A SEQUENCE	Look at the domain organisation of a protein sequence
VIEW A STRUCTURE	Find the domains on a PDB structure
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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

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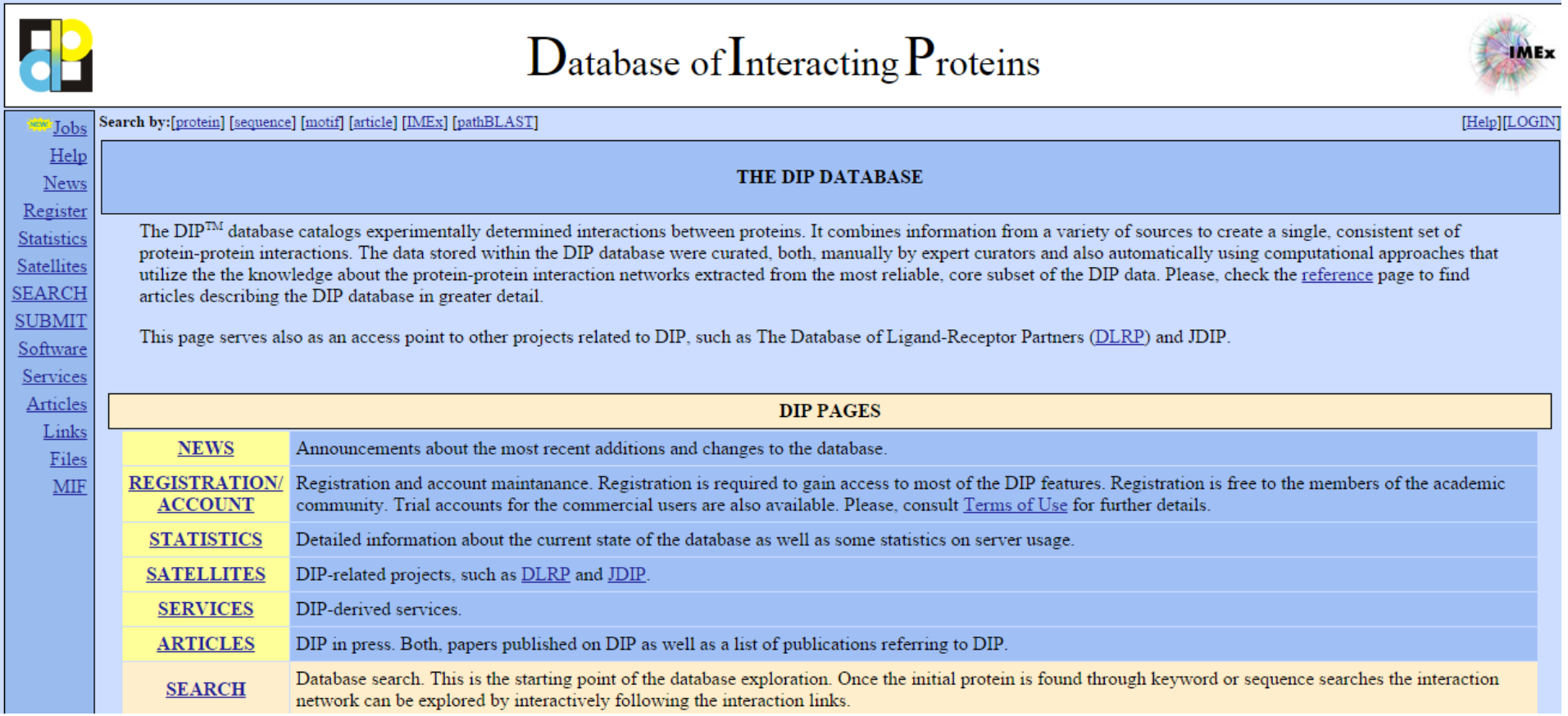
Moving to xfam.org (posted 1 May 2014)

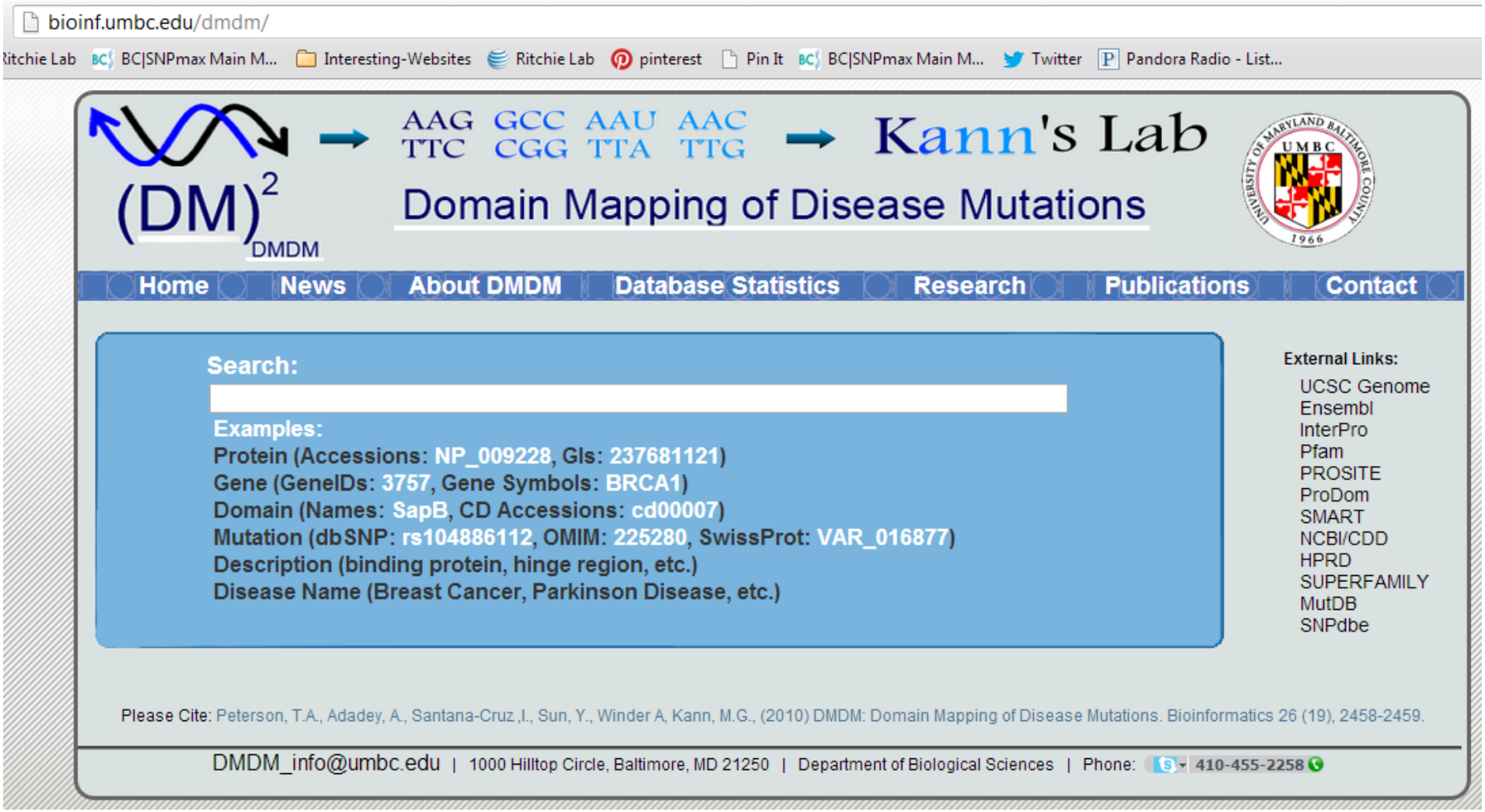
http://pfam.xfam.org/

DIP



http://dip.doe-mbi.ucla.edu/dip/Main.cgi

DM^2


bioinf.umbc.edu/dmdm/
Ritchie Lab
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DMDM
AAG GCC AAU AAC
TTC CGG TTA TTG
Kann's Lab
Domain Mapping of Disease Mutations
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Examples:
Protein (Accessions: NP_009228, GIs: 237681121)
Gene (GeneIDs: 3757, Gene Symbols: BRCA1)
Domain (Names: SapB, CD Accessions: cd00007)
Mutation (dbSNP: rs104886112, OMIM: 225280, SwissProt: VAR_016877)
Description (binding protein, hinge region, etc.)
Disease Name (Breast Cancer, Parkinson Disease, etc.)
External Links:
UCSC Genome
Ensembl
InterPro
Pfam
PROSITE
ProDom
SMART
NCBI/CDD
HPRD
SUPERFAMILY
MutDB
SNPdbe
Please Cite: Peterson, T.A., Adadey, A., Santana-Cruz ,I., Sun, Y., Winder A, Kann, M.G., (2010) DMDM: Domain Mapping of Disease Mutations. Bioinformatics 26 (19), 2458-2459.
DMDM_info@umbc.edu | 1000 Hilltop Circle, Baltimore, MD 21250 | Department of Biological Sciences | Phone: 410-455-2258

Worldwide PDB

Access the PDB FTP:
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Archive Download
Chemical Component Dictionary
Biologically Interesting Molecule Reference Dictionary (BIRD)
New Deposition and Annotation System
Tutorial
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The Worldwide Protein Data Bank (wwPDB) consists of organizations that act as deposition, data processing and distribution centers for PDB data.[1] Members are: RCSB PDB (USA), PDBe (Europe) and PDBj (Japan), and BMRB (USA). The wwPDB's mission is to maintain a single PDB archive of macromolecular structural data that is freely and publicly available to the global community.

18-September-2014

Inclusion of Large Structures in the Main PDB Archive

The wwPDB recently combined entries that represent large structures (such as ribosomes) across multiple PDB files (SPLIT entries) into single files. These combined structures have been issued new PDB IDs and are represented in the archive in both PDBx/mmCIF and PDBML formats.

more

FULL NEWS

Questions? info@wwpdb.org

1. H.M. Berman, K. Henrick, H. Nakamura (2003): **Announcing the worldwide Protein Data Bank.** Nature Structural Biology 10 (12), p. 980

RCSB PDB PROTEIN DATA BANK PDBe Protein Data Bank in Europe PDBj Protein Data Bank Japan BMRB

Questions???