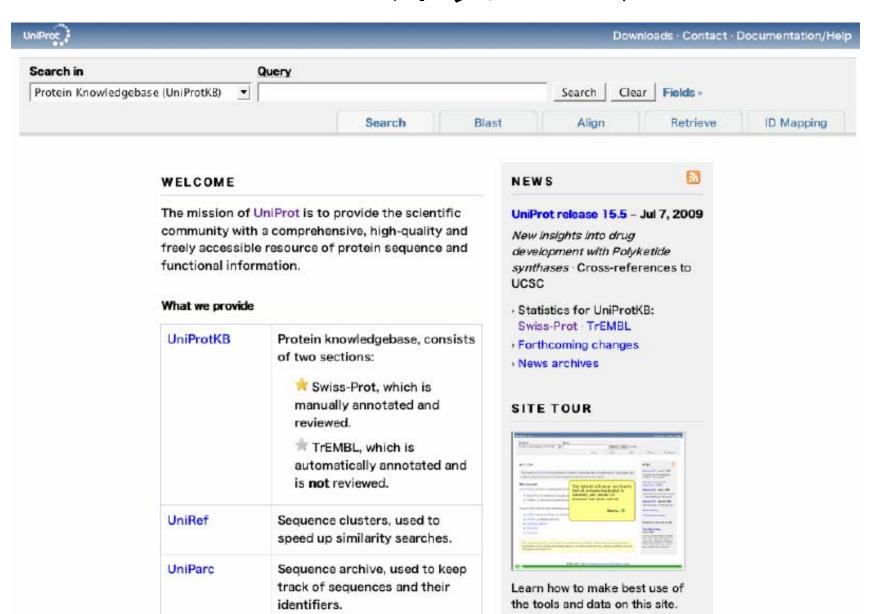
タンパク質配列のデータベース

UniProt http://www.uniprot.org/

InterPro http://www.ebi.ac.uk/interpro/

UniProtのトップページ



UniProt

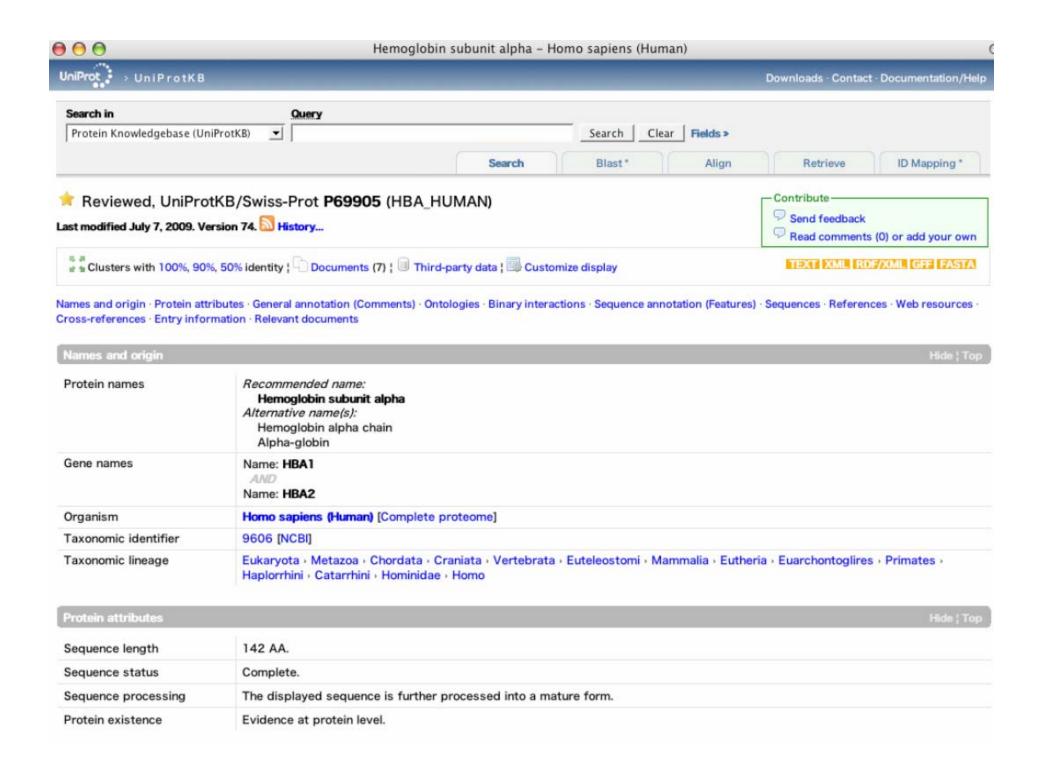
タンパク質の配列と機能に関する網羅的で高精度の情報を、無料で提供するデータベース。3つのデータベースで構成されている。

- UniProtKB (UniProt Knowledgebase)
- -Swiss-Prot: マニュアル(手動)でアノテーションを行い、 レビュー(チェック+修正)されたデータ。
- -TrEMBL: 計算機を使って自動でアノテーションされた データ。レビューを受けていない。
- UniRef

配列のクラスター。相同性検索の対象データベース等に用いるために、膨大な量のデータを圧縮してある。

UniParc

配列データとデータIDのアーカイブ。



UniProtのデータ例(ヒトのヘモグロビンA)

```
ID HBA HUMAN
                      Reviewed:
                                   142 AA.
AC P69905; P01922; Q1HDT5; Q3MIF5; Q53F97; Q96KF1; Q9NYR7; Q9UCM0;
DT 21-JUL-1986, integrated into UniProtKB/Swiss-Prot.
DT 23-JAN-2007, sequence version 2.
DT 07-JUL-2009, entry version 74.
DE RecName: Full=Hemoglobin subunit alpha;
                                               アクセッション番号は、
DE AltName: Full=Hemoglobin alpha chain;
                                               統合などのため別名が複数ある
DE AltName: Full=Alpha-globin;
GN Name=HBA1;
GN and
GN Name=HBA2;
OS Homo sapiens (Human).
OC Eukaryota; Metazoa; Chordata; Craniata; Vertebrata; Euteleostomi;
OC Mam malia; Eutheria; Euarchontoglires; Primates; Haplorrhini;
OC Catarrhini; Hominidae; Homo.
OX NCBI TaxID=9606;
RN [1]
RP NUCLEOTIDE SEQUENCE [GENOMIC DNA] (HBA1).
RX MEDLINE=81088339; PubMed=7448866; DOI=10.1016/0092-8674 (80) 90347-5;
RA Michelson A.M., Orkin S.H.;
RT "The 3' untranslated regions of the duplicated human alpha-globin
   genes are unexpectedly divergent.";
RL Cell 22:371-377(1980).
SO SEQUENCE 142 AA; 15258 MW; 15E13666573BBBAE CRC64;
   MVLSPADKTN VKAAWGKVGA HAGEYGAEAL ERMFLSFPTT KTYFPHFDLS HGSAQVKGHG
   KKVADALTNA VAHVDDMPNA LSALSDLHAH KLRVDPVNFK LLSHCLLVTL AAHLPAEFTP
   AVHASLDKFL ASVSTVLTSK YR
```

UniProtのデータ構造

ID データ識別名

AC アクセッション番号

DT 公開日

DE タンパク質名

GN 遺伝子名

OC 生物種の分類

R* 引用文献(reference)

CC コメント

DR 外部データベースの対応データ

KW キーワード

FT タンパク質の特徴(feature)

SQ アミノ酸配列

InterPro

- InterProは、(1)タンパク質のファミリー分類、(2)ドメイン、(3)リピート、(4)機能サイト、に関する記述を集めた統合データベースである。
- ●タンパク質の特徴を集めた複数のデータベースから、ひとつのデータベースを構築した。
- ●合計18,843のエントリー(Release 22.0)

InterPro; http://www.ebi.ac.uk/interpro/

InterProのメンバーデータベース(1)



The UniProt (Universal Protein Resource) is the world's most comprehensive catalog of information on proteins. It is a central repository of protein sequence and function created by joining the information contained in Swiss-Prot, TrEMBL, and PIR.



PROSITE is a database of protein families and domains. It consists of biologically significant sites, patterns and profiles that help to reliably identify to which known protein family (if any) a new sequence belongs.



HAMAP, stands for High-quality Automated and Manual Annotation of microbial Proteomes. HAMAP profiles are manually created by expert curators they identify proteins that are part of well-conserved bacterial, archaeal and plastid-encoded (i.e. chloroplasts, cyanelles, apicoplasts, non-photosynthetic plastids) proteins families or subfamilies.



Pfam is a large collection of multiple sequence alignments and hidden Markov models covering many common protein domains.



PRINTS is a compendium of protein fingerprints. A fingerprint is a group of conserved motifs PRINTIS used to characterise a protein family, its diagnostic power is refined by iterative scanning of UniProt. Usually the motifs do not overlap, but are separated along a sequence, though they may be contiguous in 3D-space. Fingerprints can encode protein folds and functionalities more flexibly and powerfully than can single motifs, their full diagnostic potency deriving from the mutual context afforded by motif neighbours.



The ProDom protein domain database consists of an automatic compilation of homologous domains. Current versions of ProDom are built using a novel procedure based on recursive PSI-BLAST searches (Altschul SF, Madden TL, Schaffer AA, Zhang J, Zhang Z, Miller W & Lipman DJ, 1997, Nucleic Acids Res., 25:3389-3402; Gouzy J., Corpet F. & Kahn D., 1999, Computers and Chemistry 23:333-340.) Large families are much better processed with this new procedure than with the former DOMAINER program (Sonnhammer, E.L.L. & Kahn, D., 1994, Protein Sci., 3:482-492).



SMART (a Simple Modular Architecture Research Tool) allows the identification and annotation of genetically mobile domains and the analysis of domain architectures. More than 500 domain families found in signalling, extracellular and chromatin-associated proteins are detectable. These domains are extensively annotated with respect to phyletic distributions, functional class, tertiary structures and functionally important residues. Each domain found in a non-redundant protein database as well as search parameters and taxonomic information are stored in a relational database system. User interfaces to this database allow searches for proteins containing specific combinations of domains in defined taxa.

InterProのメンバーデータベース(2)



<u>TIGRFAMs</u> is a collection of protein families, featuring curated multiple sequence alignments, hidden Markov models (HMMs) and annotation, which provides a tool for identifying functionally related proteins based on sequence homology. Those entries which are "equivalogs" group homologous proteins which are conserved with respect to function.



<u>PIRSF</u> The PIRSF protein classification system is a network with multiple levels of sequence diversity from superfamilies to subfamilies that reflects the evolutionary relationship of full-length proteins and domains. The primary PIRSF classification unit is the homeomorphic family, whose members are both homologous (evolved from a common ancestor) and homeomorphic (sharing full-length sequence similarity and a common domain architecture).



SUPERFAMILY is a library of profile hidden Markov models that represent all proteins of known structure. The library is based on the SCOP classification of proteins: each model corresponds to a SCOP domain and aims to represent the entire SCOP superfamily that the domain belongs to. SUPERFAMILY has been used to carry out structural assignments to all completely sequenced genomes. The results and analysis are available from the SUPERFAMILY website.



Gene3D database describes protein families and domain architectures in complete genomes. Protein families are formed using a Markov clustering algorithm, followed by multi-linkage clustering according to sequence identity. Mapping of predicted structure and sequence domains is undertaken using hidden Markov models libraries representing CATH and Pfam domains. Functional annotation is provided to proteins from multiple resources. Functional prediction and analysis of domain architectures is available from the Gene3D website.



PANTHER is a large collection of protein families that have been subdivided into functionally related subfamilies, using human expertise. These subfamilies model the divergence of specific functions within protein families, allowing more accurate association with function (human-curated molecular function and biological process classifications and pathway diagrams), as well as inference of amino acids important for functional specificity. Hidden Markov models (HMMs) are built for each family and subfamily for classifying additional protein sequences. PANTHER is publicly available without restriction.

InterProを用いた配列解析ツール: InterProScan

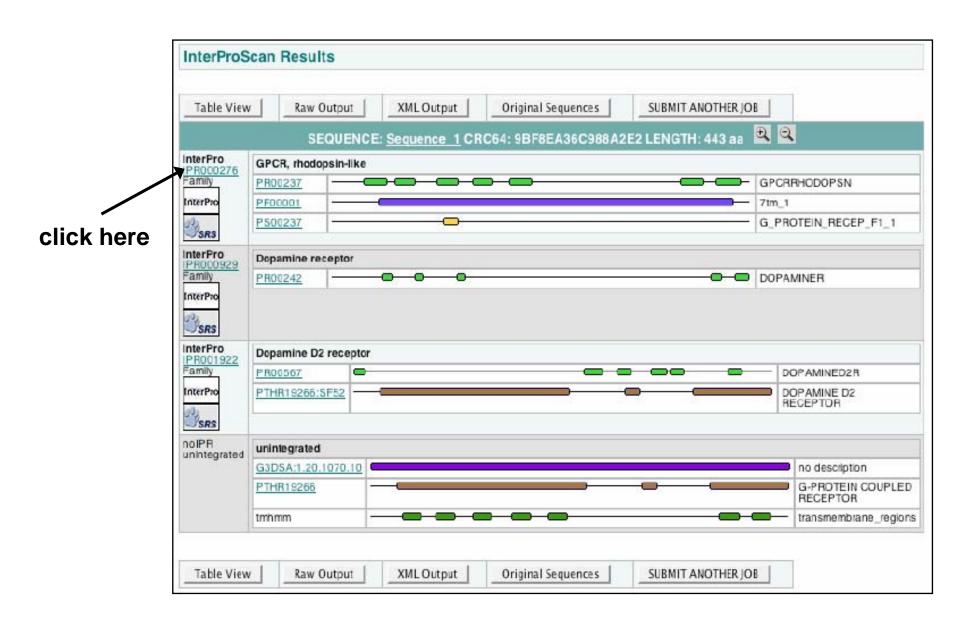
InterProScanは、ウェブサーバーで提供されるツールで、InterProに登録されている各種の機能ドメイン・構造ドメインを検索したり、ユーザーが入力した機能未知の配列を解析して特徴を発見することができるツールである。

http://www.ebi.ac.uk/Tools/InterProScan/

InterProScanの使い方

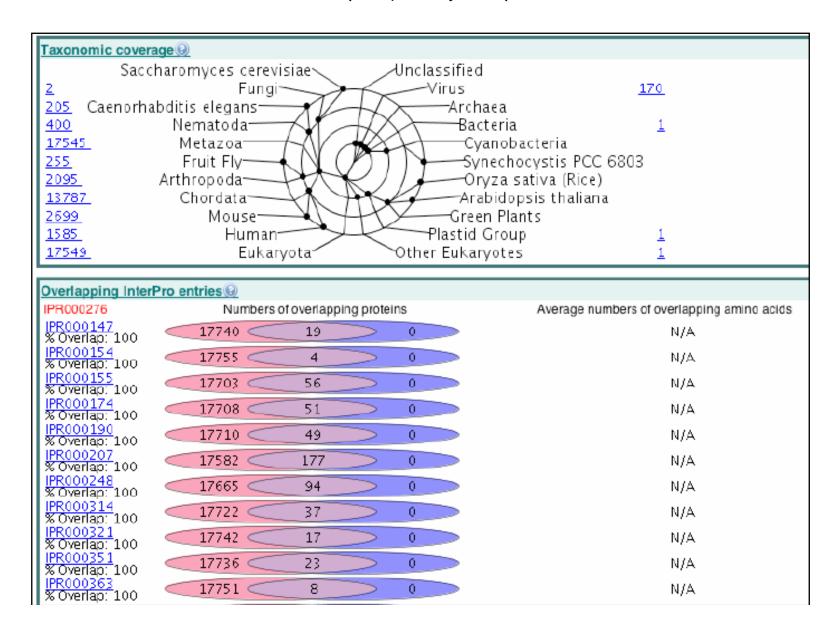


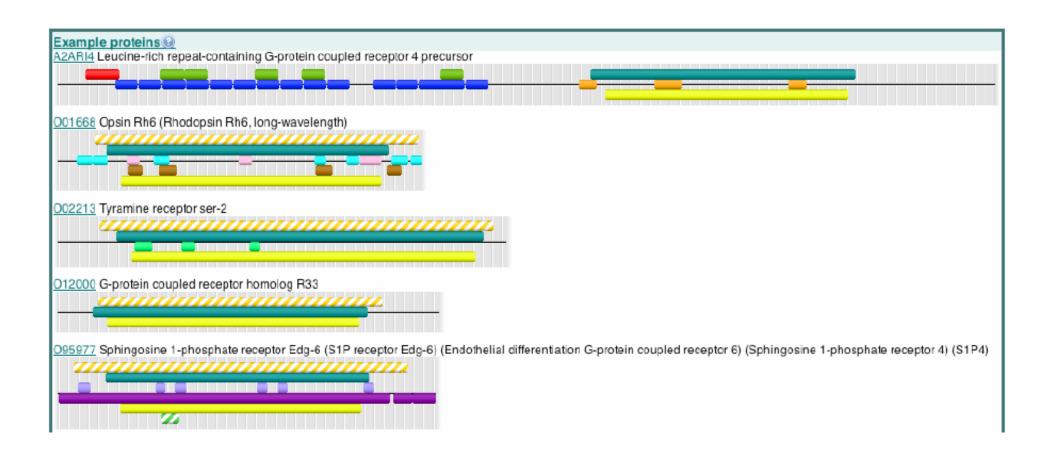
結果画面



Protein matches (9)								
UniProtKB Matches: 17759 proteins	Overview: Detailed: Table:	sorted by AC sorted by AC For all match		sorted by name, sorted by name, of known structu	of known structure	proteins with splice variants proteins with splice variants		
	Architectures Accession List							
Accession (i)	IPR000276 GPCR_Rhodpsn							
Secondary (9)	IPR002356							
Type 😡	Family							
Signatures 😡	Database	ID	Name		Proteins			
	<u>Pfam</u>	PF00001	7tm_1		17497			
	PRINTS	PR00237	GPCRRHO	DOPSN	15184			
	PROSITE patte	m PS00237	G_PROTEIN	N_RECEP_F1_1	15124			

GO Term annotation (i)						
Process	GO:0007186 G-protein coupled receptor protein signaling pathway					
Function	GO:0001584 rhodopsin-like receptor activity					
Component	GO:0016021 integral to membrane					
InterPro annotation						
Abstract @	G-protein-coupled receptors, GPCRs, constitute a vast protein family that encompasses a wide range of functions (including various autocrine, paracrine and endocrine processes). They show considerable diversity at the sequence level, on the basis of which they can be separated into distinct groups. We use the term clan to describe the GPCRs, as they embrace a group of families for which there are indications of evolutionary relationship, but between which there is no statistically significant similarity in sequence [1]. The currently known clan members include the rhodopsin-like GPCRs, the secretin-like GPCRs, the cAMP receptors, the fungal mating pheromone receptors, and the metabotropic glutamate receptor family. There is a specialised database for GPCRs: http://www.gpcr.org/7tm/. The rhodopsin-like GPCRs themselves represent a widespread protein family that includes hormone, neurotransmitter and light receptors, all of which transduce extracellular signals through interaction with guanine nucleotide-binding (G) proteins. Although their activating ligands vary widely in structure and character, the amino acid sequences of the receptors are very similar and are believed to adopt a common structural framework comprising 7 transmembrane (TM) helices [2, 3, 4].					
Structural links (2)	CATH: 1.20.1070.10.6 SCOP: f.13.1.2 , j.101.1.1 , j.35.1.1 , j.94.1.1 PDB - click here					
Batalana Kala (S)	PANDIT: <u>PF00001</u> PROSITE doc: <u>PD0C00210</u> MSDsite: <u>PS00237</u> <u>Ptam Clan: CL0192.5</u>					





InterProScanの出力結果は4つのタイプに分類される

Type defines the entry as a Family, Domain, Repeat or PTM (Post-translational modification).

An InterPro family is a group of evolutionarily related proteins, that share one or more domains/repeats in common. A InterPro entry of type=family may contain a signature for a small conserved region that is representative of the family, and need therefore not necessarily cover the whole protein.

An InterPro domain is an independent structural unit which can be found alone or in conjunction with other domains or repeats. Domains are evolutionarily related. An InterPro entry of the type=domain is diagnostic for a domain but not necessarily define domain boundaries exactly.

An InterPro repeat is a region that is not expected to fold into a globular domain on its own. For example 6-8 copies of the WD40 repeat are needed to form a single globular domain. There also many other short repeat motifs that probably do not form a globular fold that have type=repeat.

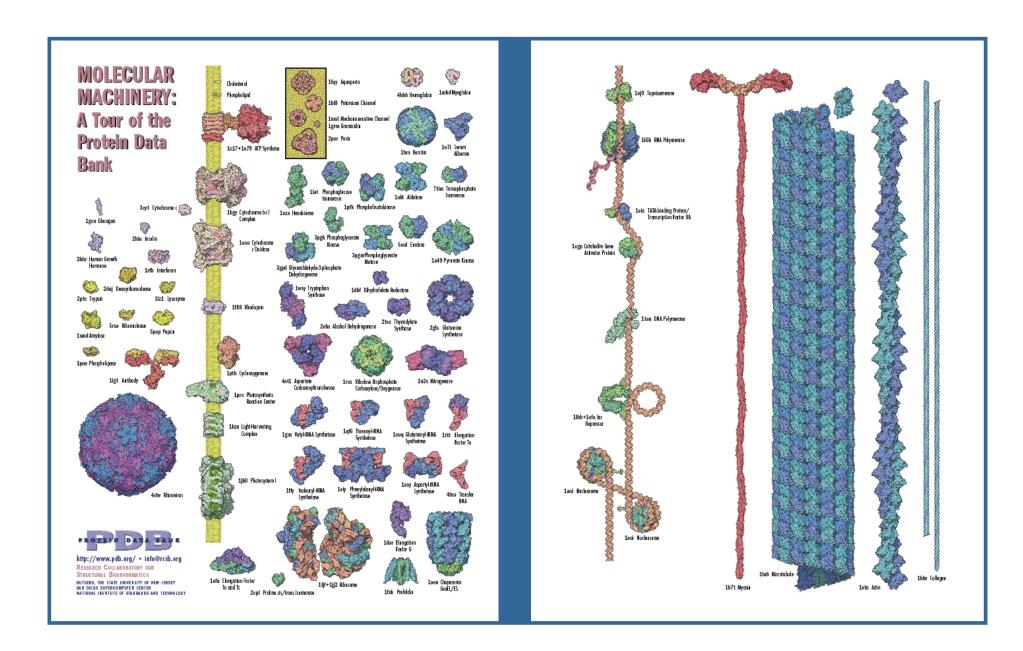
A post-translational modification includes for example, an N glycosylation site. The sequence motif is defined by the molecular recognition of this region in a cell. This may group together proteins that need not be evolutionarily related.

タンパク質立体構造の データベース

Protein Data Bank (PDB)

PDBとは

- Protein Data Bank (PDB)は、タンパク質と核酸の3次元構造データのデータベース
- 3次元構造データは、X線結晶解析法、NMR法 (核磁気共鳴法) などによって実験的に決定されたデータ
- Worldwide Protein Data Bank (wwPDB)
 - PDBのデータの登録、処理、配布を行う
 - 以下の組織による共同組織
 - Research Collaboratory for Structural Bioinformatics (RCSB PDB), USA
 - the Protein Databank in Europe (PDBe), Europe
 - 日本蛋白質構造データバンク (PDBj), Japan
 - Biological Magnetic Resonance Data Bank (BMRB), USA







Access the PDB FTP:

RCSB PDB | PDBe | PDBj

Archive Download

Chemical Component Dictionary

Deposit Data to the PDB:

RCSB PDB | PDBe

PDBj | BMRB

Search for Structures:

RCSB PDB | PDBe

PDBj | BMRB

PDB Archive Snapshots:

RCSB PDB | PDBj

Instructions to Journals

Documentation

Format

Annotation

Workshops

X-ray Validation

wwPDBAC

Home wwPDB Agreement Statistics FAQ News Contact Us

The Worldwide Protein Data Bank (wwPDB) consists of organizations that act as deposition, data processing and distribution centers for PDB data. The founding members are RCSB PDB (USA), PDBe (Europe) and PDBj (Japan)¹. The BMRB (USA) group joined the wwPDB in 2006. The mission of the wwPDB is to maintain a single Protein Data Bank Archive of macromolecular structural data that is freely and publicly available to the global community.

This site provides information about services provided by the individual member organizations and about projects undertaken by the wwPDB.

Please note: ftp://ftp.rcsb.org is no longer updated. Please access the PDB archive using one of the FTP sites listed in the left menu.

30-June-2009

wwPDB News: Gerard Kleywegt to head Protein Data Bank Europe

Starting July 1, 2009, Gerard Kleywegt will lead the Protein Data Bank Europe (PDBe) project at the European Bioinformatics Institute (Hinxton, UK). During the last 17 years he has been working in Uppsala, Sweden, a center of excellence for biomolecular crystallography and has developed many tools that are widely used by structural biologists worldwide. He has an extensive publication record and has served on the PDBe Scientific Advisory Board for the last few years. He has also been one of the European representatives on the wwPDB advisory committee. He has a very strong international reputation and is well respected in the structural biology community.

Gerard will be replacing Kim Henrick, who has been the team leader of the PDBe since 2001. During his tenure at the EBI, Kim has made enormous contributions to the PDBe at the EBI, by establishing and leading a strong team that has developed a wide variety of services. Kim was a strong advocate for the formation of the wwPDB in 2003. He has played a key role in developing the standards for representing all the data in the archive from small melecules to

www.wwpdb.org

日本タンパク質構造データベース PDBj http://www.pdbj.org/



反応経路のデータベース

Reactome KEGG

Reactome http://reactome.org

- Reactomeは、ヒトの主要反応経路(pathway)や生化学反応(reaction)の精査されたデータベース
- ヒト以外のデータも格納している(23種)
- タンパク質間相互作用データもある
- 外部へリンクしているDBとしては、NCBI Entrez Gene, Ensembl and UniProt databases, the UCSC や HapMap のゲノムブラウザ, the KEGG Compound や ChEBI の低分子DB, PubMed, GO などがある
- Cold Spring Harbor Laboratory, EBI, GOコンソーシアムによる開発

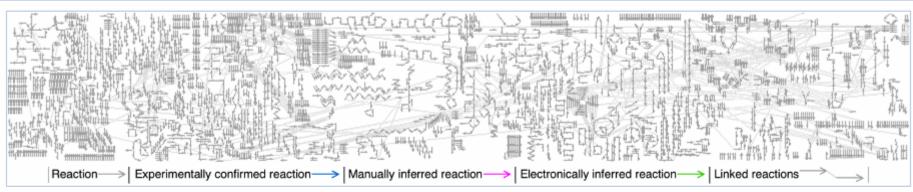
Try out Beta version of Reactome's new web user interface. We would greatly appreciate your comments, suggestions and bug reports.

Home About Content Documentation Tools Download Help Announcements

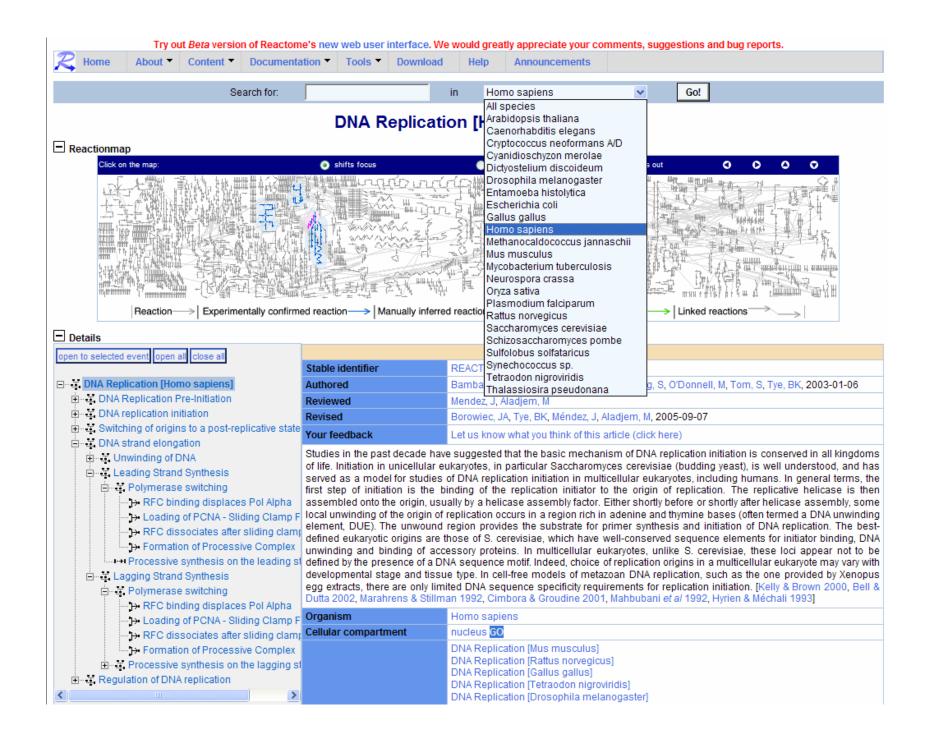
Search for: in Homo sapiens Go!

Reactome - a curated knowledgebase of biological pathways

The data displayed is for Homo sapiens Use the menu to change the species. Check for cross-species comparison.



Apoptosis	Axon guidance	Biological oxidations	Botulinum neurotoxicity
Cell Cycle Checkpoints	Cell Cycle, Mitotic	DNA Repair	DNA Replication
Diabetes pathways	Electron Transport Chain	Gap junction trafficking and regulation	Gene Expression
HIV Infection	Hemostasis	Influenza Infection	Integration of energy metabolism
Integrin cell surface interactions	Metabolism of lipids and lipoproteins	Membrane Trafficking	Metabolism of amino acids
Metabolism of carbohydrates	Metabolism of nitric oxide	Metabolism of non-coding RNA	Metabolism of polyamines
Metabolism of proteins	Metabolism of vitamins and cofactors	Muscle contraction	Metablism of nucleotides
Metabolism of porphyrins	Pyruvate metabolism and TCA cycle	Regulation of beta-cell development	Regulatory RNA pathways
Signaling by BMP	Signaling by EGFR	Signaling by FGFR	Signaling by GPCR
Signaling by PDGF	Signaling in Immune system	Signaling by Insulin receptor	Signalling by NGF
Signaling by Notch	Opioid Signalling	Signaling by Rho GTPases	Signaling by TGF beta
Signaling by VEGF	Signaling by Wnt	Synaptic Transmission	Telomere Maintenance
Transcription	Transmembrane transport of small molecules	mRNA Processing	



KEGG: Kyoto Encyclopedia of Genes and Genomes http://www.genome.jp/ja/gn_kegg_ja.html



分子相互作用を扱う KEGG pathway が有 名だが、それ以外にも 化合物を扱うKEGG LIGANDなど、多くの データがある

多型データベース

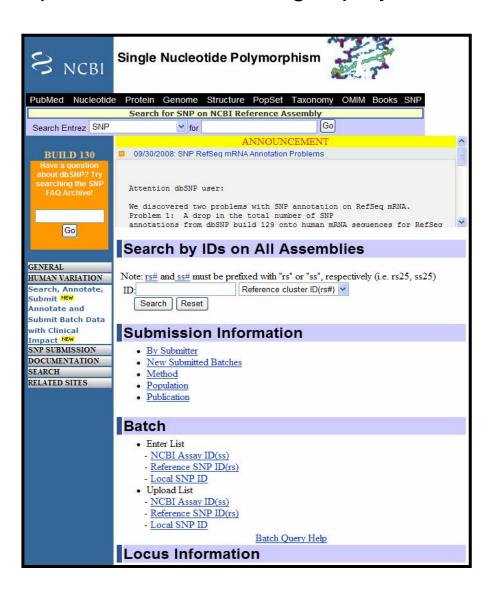
dbSNP

SNP

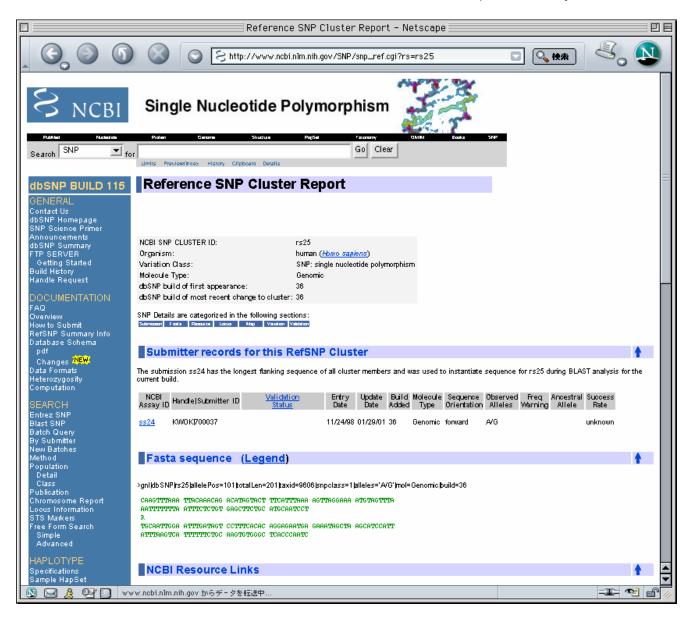
- 1塩基多型(single nucleotide polymorphisms, SNPs)
 は、最も共通な変異
- ゲノム中に、100から300塩基に1つの割合で存在する
- ゲノムと表現型をつなぐ基礎データ
- dbSNP(NCBI)は、置換だけでなく、挿入・欠失のSNPを 含む

NCBIのdbSNP (トップ画面)

http://www.ncbi.nlm.nih.gov/projects/SNP/



NCBIのdbSNPのデータ



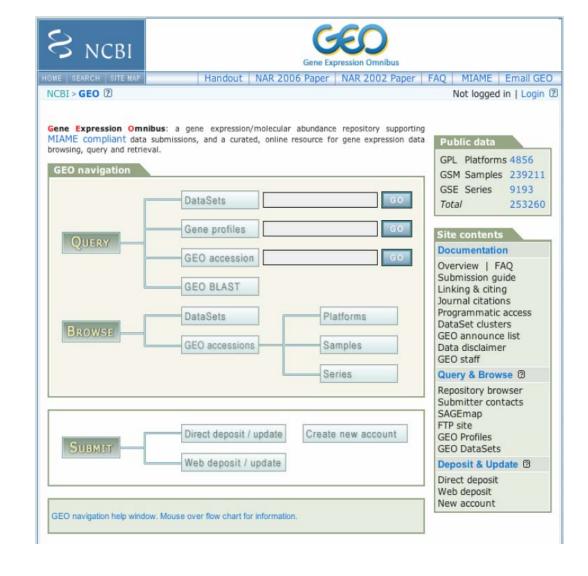
遺伝子発現データベース

GEO (NCBI)
ArrayExpress (EBI)
CIBEX (DDBJ)

Gene Expression Omnibus (GEO)

http://www.ncbi.nlm.nih.gov/geo/

GEOは、
 MIAMEに準拠した遺伝子発現である。
 データのリポジトリ(倉庫)



GEO and MIAME (Minimum Information About a Microarray Experiment)

- MIAME:マイクロアレイ実験を記述する上で最低限の情報を規定したガイドライン
- データの形式や手段ではなく、中身を規定する
- 中身の例:生データ、生物種、どの臓器の試料か、 実験デザイン、プローブ配列、データ処理プロトコール等

http://www.ncbi.nlm.nih.gov/geo/info/MIAME.html

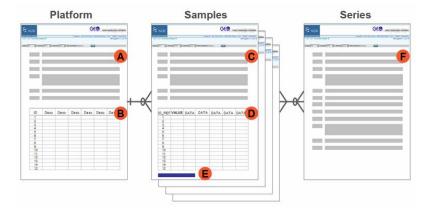
GEO基本データ構造

• Platform (GPLxxxx): アレイタイプ、プローブリスト等

Sample (GSMxxxx): 実験条件、測定値。Platformは1つだけ。
 多くのSeriesに属しうる。

Series (GSExxxx): 登録者が関連するサンプル(GSM)を

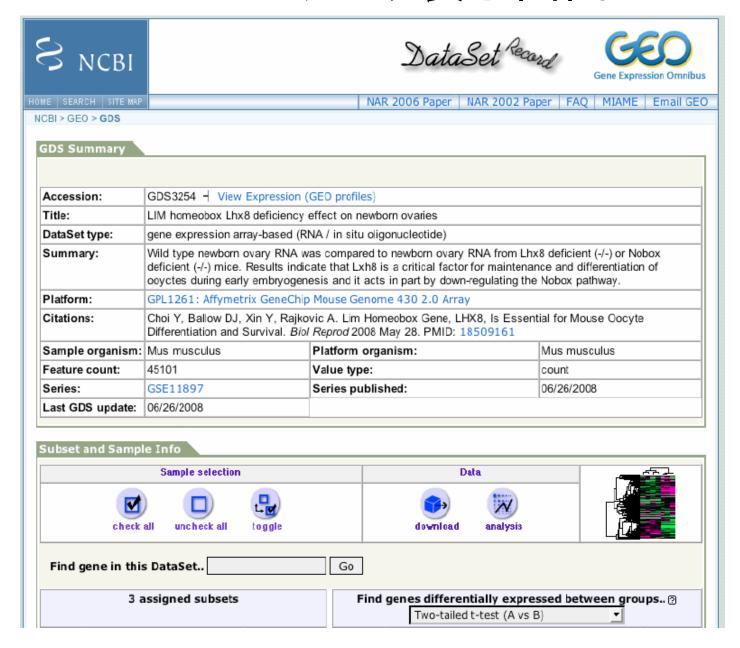
グループ化したもの



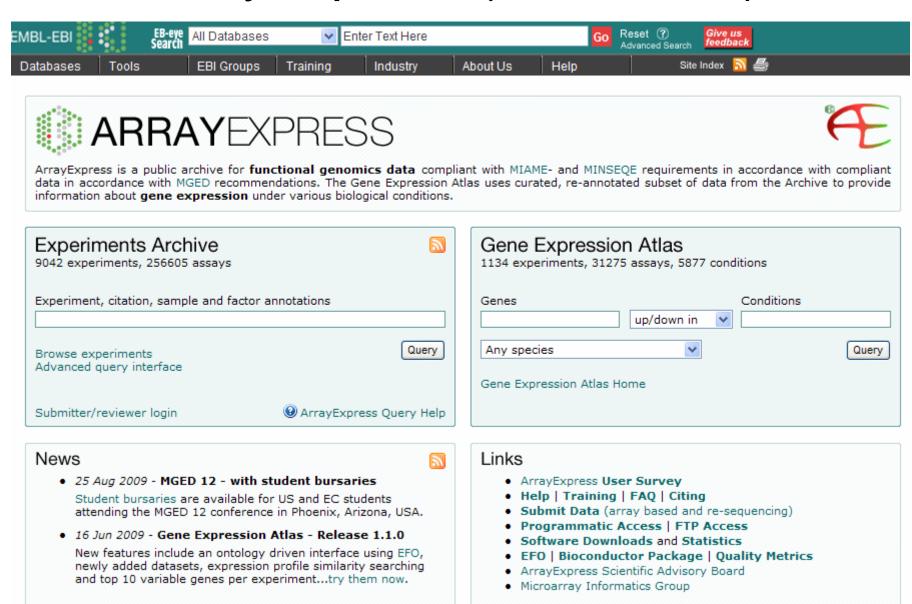
- DataSets (GDSxxxx): 統計的に比較可能なGSMをGEOが独自に再編成したもの
 - すぐ解析に使えて便利

http://www.ncbi.nlm.nih.gov/projects/geo/info/overview.html

GEOのデータ表示画面



ArrayExpress (EMBL-EBI)



CIBEX (DDBJ)

CIBE	Center for	Information	iology ge	ne EXpr	ression databas	se
Top Sea	rch Exper	iment List	Array Li	ist	Submission	Contact
CIBEX is a public storing MIAME-co recommendations	mpliant data in a				CIE	• • • • • • • • • • • • • • • • • • •
Search		Browse			Link	
Experiment Accession Title Authors advanced search Array Accession Model Name Provider advanced search	GO	Show summary lisarrays in CIBEX. Experiment L Array List Statistics Experiments Arrays Hybridizations	ist :	59 102 1850		Databases ess
our site certifica	o submit your mic	roarray data. icate authority appe	eared, please	e accept	Submission If you want to sub microarray data, psubmission site of bex Grant Support The construction is supported by "(Publication of Sci Results" from JSF	olease visit our r contact us at ci t of this database Grant-in-Aid for entific Research

If you have any trouble or question, please contact us at cibex@ddbj.nig.ac.jp

オントロジー

Gene Ontology (GO)

Gene Ontology (GO)

- Gene Ontology Project とは、生物種やDBを超えて、遺伝子・遺伝子産物に関する表現(用語)を標準化するプロジェクト
- [効果]異なるDBの結合、比較が可能になる
- Gene Ontology Consortiumが主催するプロジェクト。
- 主なゲノム・バイオインフォマティクス研究機関が 参加(Sanger, TIGR, EBIなど)。
- マウス、ショウジョウバエ、酵母などが対象。
- EC番号、MIPSの分類、InterPro、 UniprotKB/Swiss-Protなどとの対応づけがある。

GO termの構造

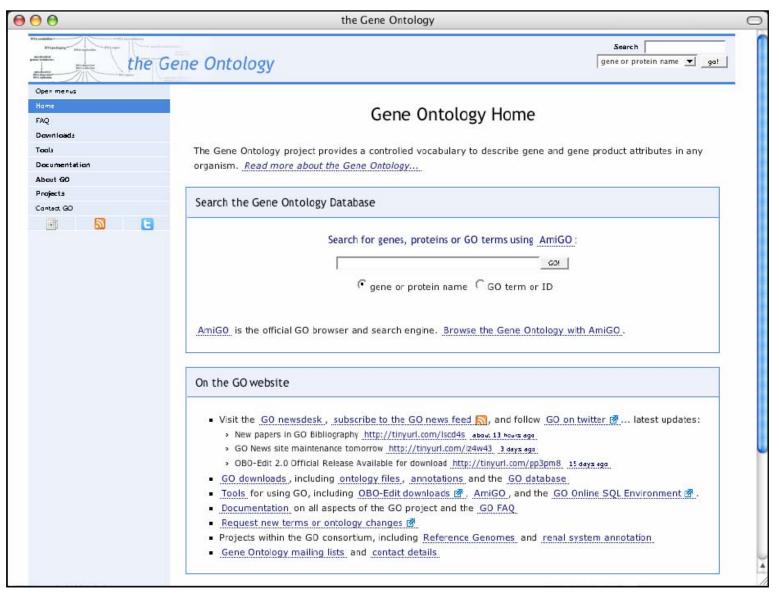
- 用語全体は階層構造を持つ
- 第1階層は3つ
 - 1. 分子機能(molecular function)
 - 2. 生体内における役割(biological process)
 - 3. 細胞内構造や分布(cellular component)

GO termの例

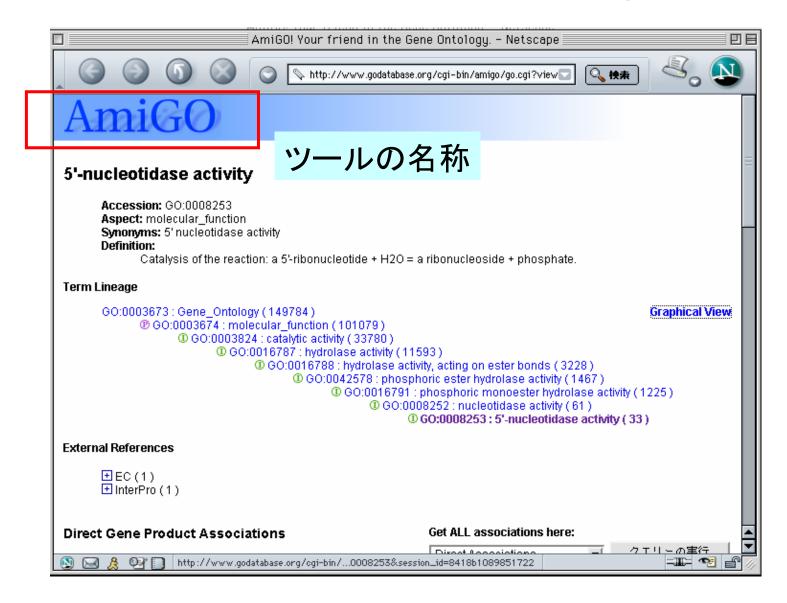
ID: GO:nnnnn

Name: cell, fibroblast growth factor receptor binding

http://www.geneontology.org/

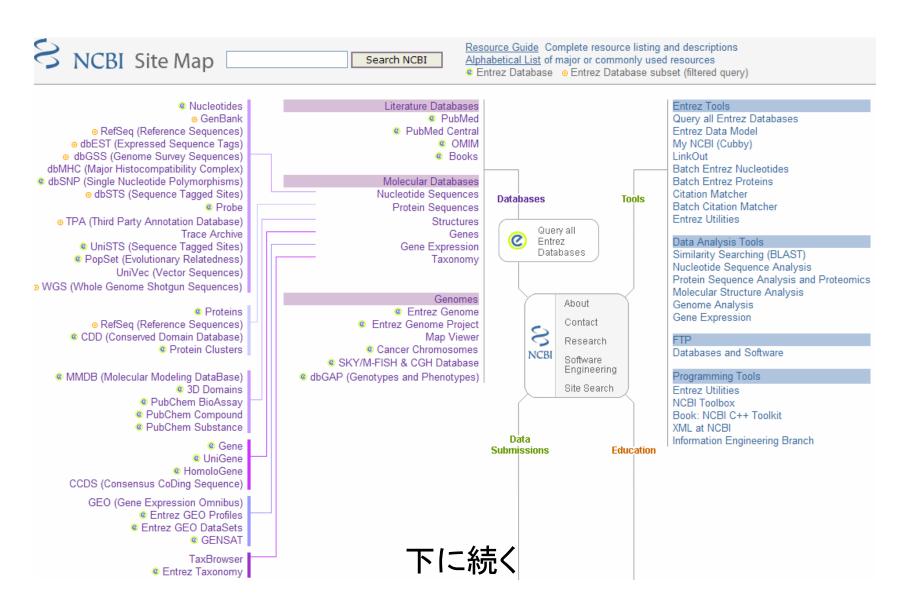


Molecular functionの例



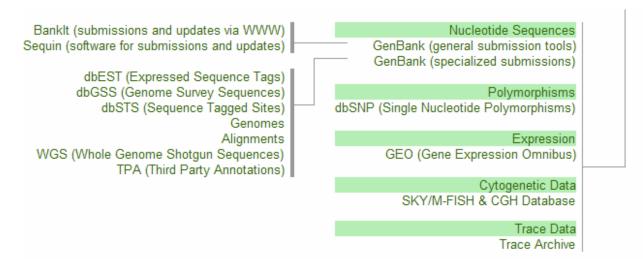
NCBI その他

NCBI site map (1)



NCBI site map (2)

データ提出



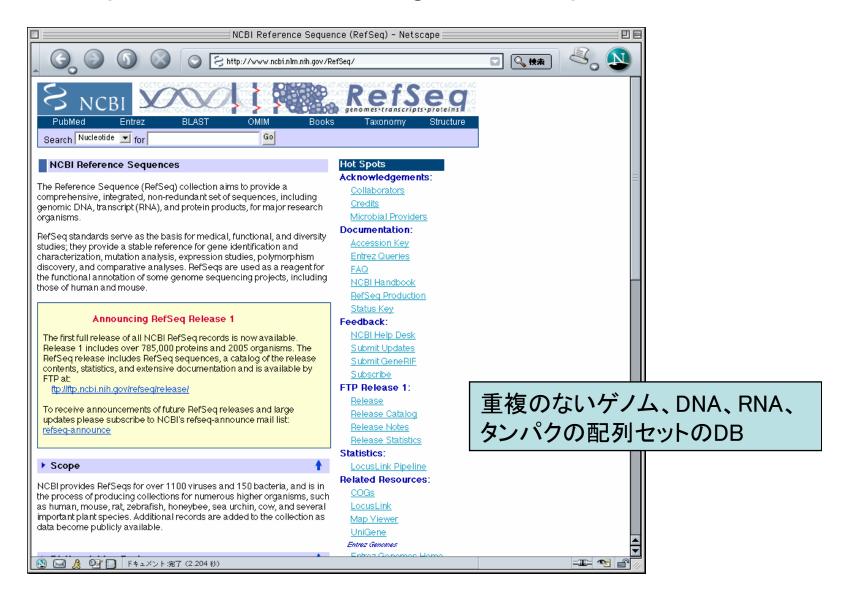
教育

News
NCBI News
What's New
Announcement Mailing Lists
RSS Feeds
Bookshelf
Coffee Break
Genes and Disease
NCBI Handbook

Resources
Tutorials, Courses, and more

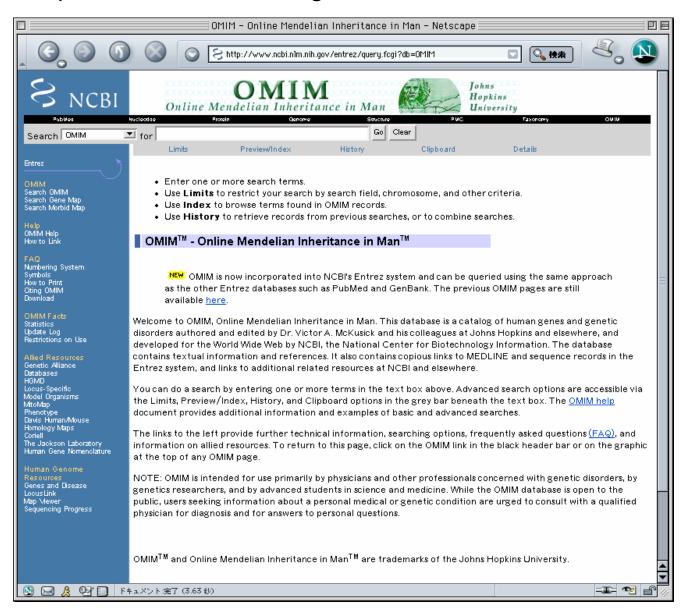
NCBIORefSeq

http://www.ncbi.nlm.nih.gov/RefSeq/



NCBIのOMIM(遺伝性疾患情報)

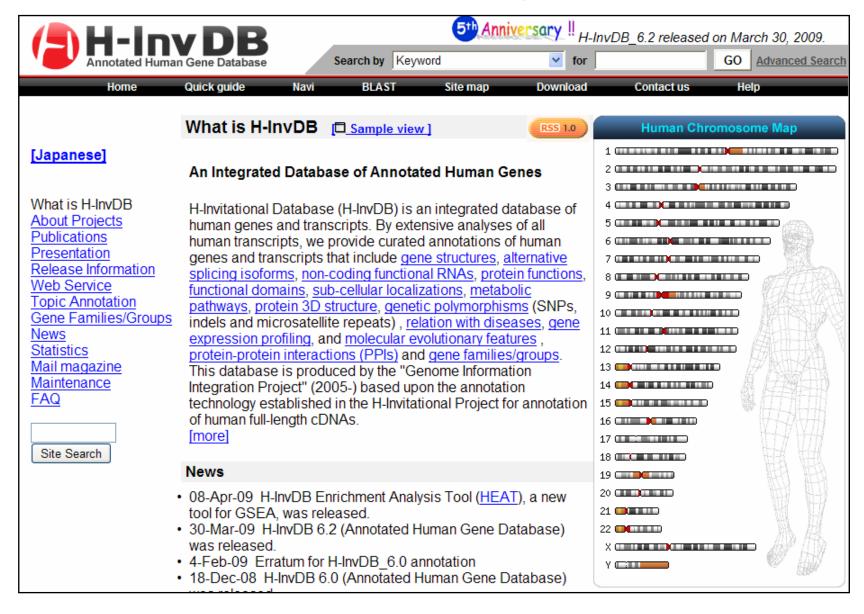
http://www.ncbi.nlm.nih.gov/sites/entrez?db=omim



その他

ヒト遺伝子統合データベース: H-InvDB

http://h-invitational.jp/



日本の統合データベースプロジェクト



その他の情報リソース

- Nucleic Acids Research(NAR) のDB issue
 - 1993から現在まで、毎年1月に特集号
 - 1,170個の運用中DB (2009まで)
 - 繰り返し(1, 2年ごと)載るDBもある
 - 2009年は、179個のうち84個(47%)がupdate版
- Wikipedia、特に英語版
- Google scholar(文献の引用、論文本体)
- ISI Web of knowledge, SCOPUS(文献引用)

バイオデータベース参考書

• JSTのサイトにある参考図書

http://www.jsbi.org/modules/jsbi/index.php/nintei/index.html

- バイオリソース&データベース活用術—Webでキャッチ!!実験材料・インフォマティクス (細胞工学 別冊) (大型本)
 - ナショナルバイオリソースプロジェクト情報運営委員会
 - 4830円
- バイオデータベースとウェブツールの手とり足とり活用法 遺伝子の配列・機能解析、タンパク質解析、プロテオミクス、文献検索、検索エンジン...etc.真に役立つサイトを使い倒す!
 - 中村保一(編集),石川淳(編集),礒合敦(編集),平川美夏(編集),坊農秀雅(編集)
 - 4410円





バイオデータベース参考書

- バイオデータベースとソフトウェア最前線—DNA解析からRNA・タンパク質の機能解明、エピジェネティクス研究、システム生物学と誰もが使う文献検索の新機能(実験医学増刊 Vol. 26-7)
 - 森下 真一 (編集), 阿久津達也 (編集)
 - 5670円

