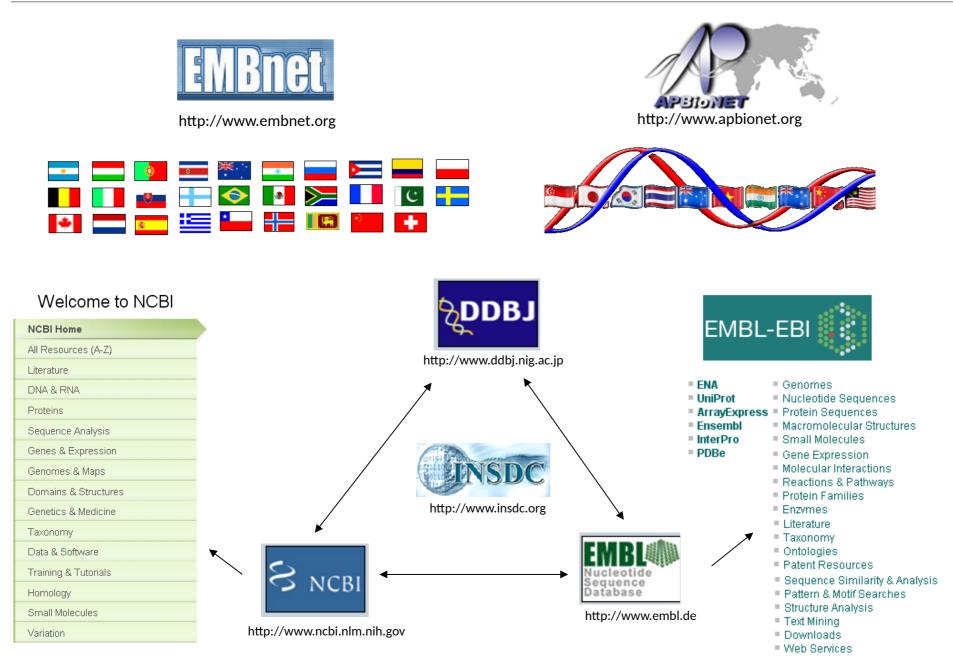
# Biological data banks: a guided survey

prof. Matteo Ram

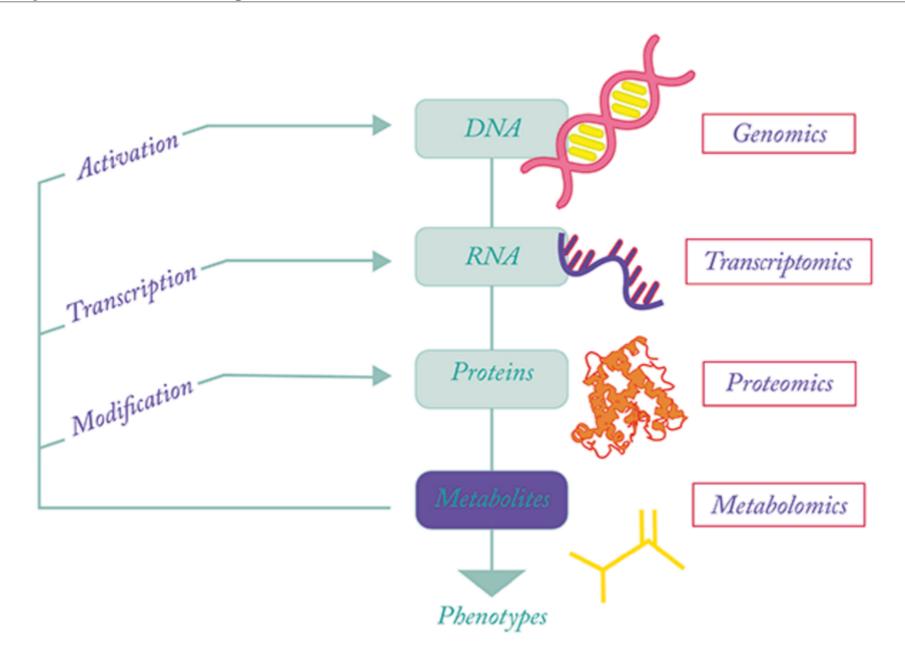
EMBL-Bank equence Read Archive

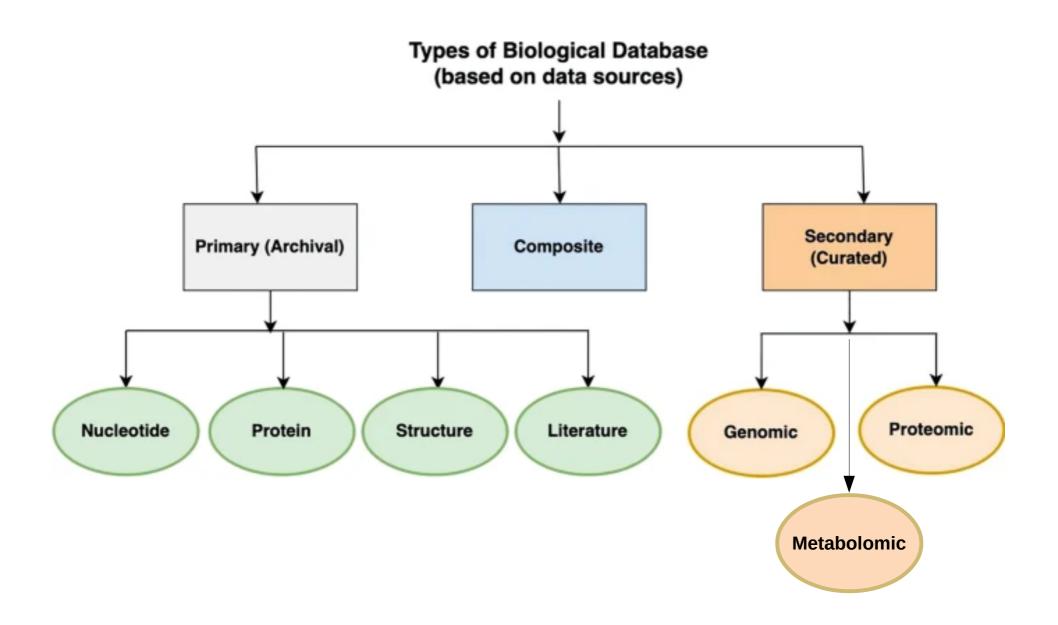
prof. Matteo Ramazzotti, PhD

## Data banks: the infrastructure

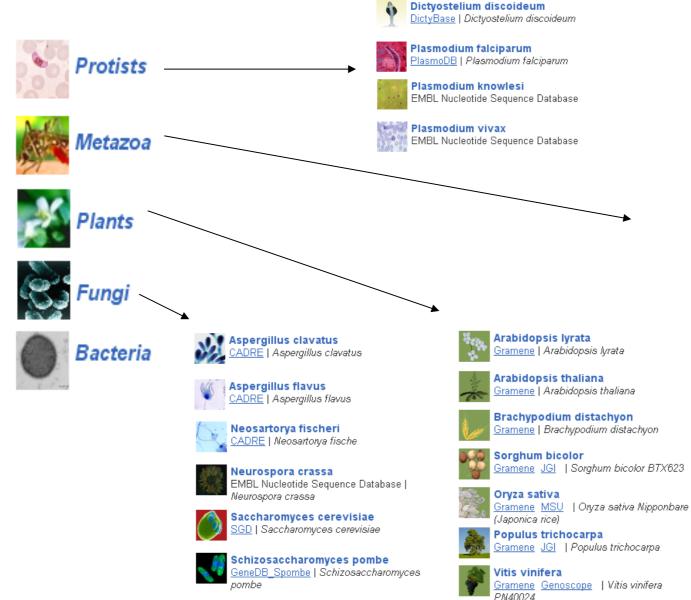


## Why we need biological databases









Aedes aegypti
<u>VectorBase</u> | Aedes aegypti



Anopheles gambiae VectorBase | Anopheles gambiae

Culex quinquefasciatus
<u>VectorBase</u> | Culex quinquefasciatus



Caenorhabditis elegans WormBase | Caenorhabditis elegans N2

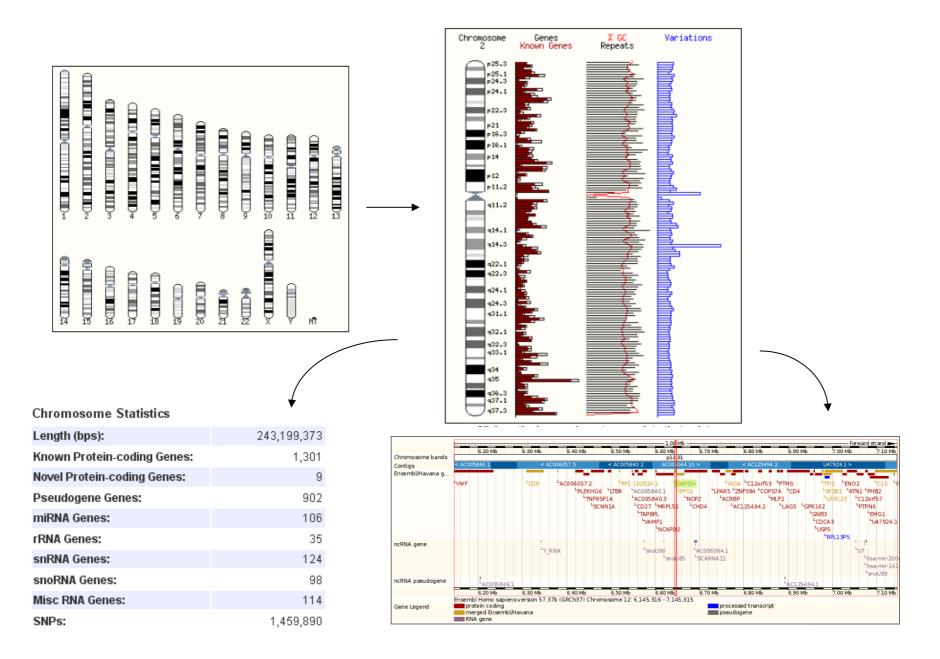
	Dr
The C	<u>Fly</u>

Drosophila melanogaster <u>ElyBase</u> | Drosophila melanogaster

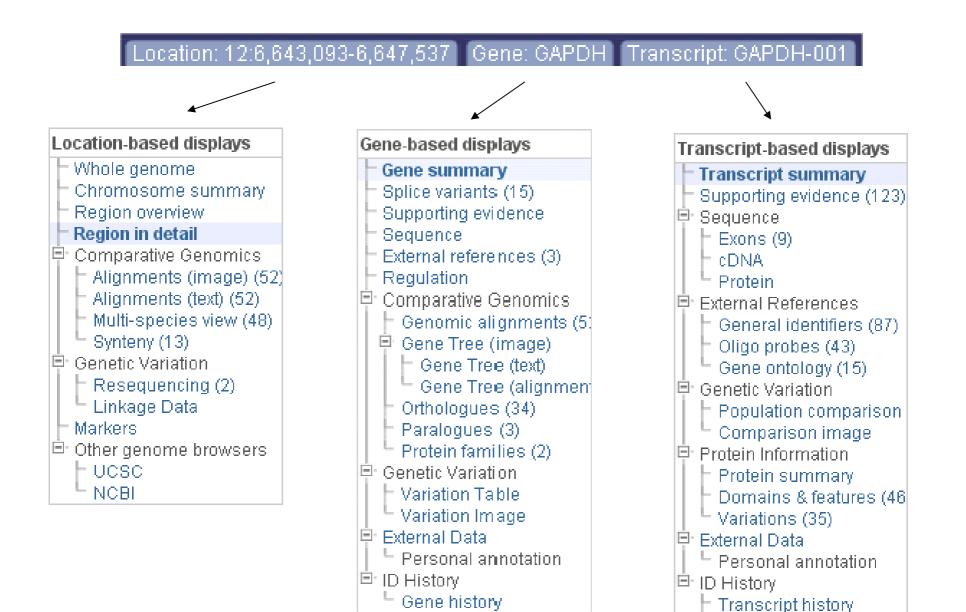
- de

Ixodes scapularis VectorBase | Ixodes scapularis Wikel









7/52

Protein history



## Click to go to the browser

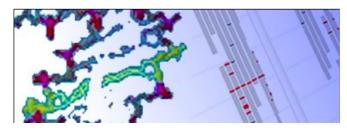


```
bio
```

BioMart is very useful for creating sub-databases of a main database. It expose all the features that can be extracted from a databank and allows to set filters to exclude part of the records.

	Dat	tasets → Filters →	output ಿ Restar	rt • Previous	Results »		
SUMMARY Database Ensembl 73 Genes (WTSI, UK)	<> view XML						
Datasets Homo sapiens genes (GRCh37.p12)		Main da	ataset				
Filters Gene type: protein_coding	8	Selection	n filters				
Status (gene): KNOWN	8						
Status (transcript): KNOWN	8				V		
Source: ensembl	8				_		
Attributes		Bookma	ark	SPARQL 2 Java	± Download data	• Back	
Ensembl Gene ID	8	Ensembl	Gene ID 🔹 Ensembl Prote	ein ID 🔹 % GC content 🤅	GO Term Accession +	ArrayExpress +	Interpro ID 🗢
Associated Gene Name	8		000099977 ENSP000003			ENSG00000099977	IPR001398
Ensembl Protein ID	8		000099977 ENSP000003			ENSG0000099977	IPR001398
% GC content	8		000099977 ENSP000003				IPR001398
GO Term Accession	8					ENSG0000099977	
ArrayExpress	8		000099977 S ENSP000003			ENSG00000099977	IPR001398
Interpro ID	8	ENSG000	000099977 ENSP000003	381386 54.24	GO:0042438	ENSG0000099977	IPR014347
		ENSG000	000099977 ENSP000003	381386 54.24	GO:0005737	ENSG00000099977	IPR014347
		ENSG000	000099977 ENSP000003	381386 54.24	GO:0004167	ENSG0000099977	IPR014347
		ENSG000	000099977 ENSP00000	381386 54.24	GO:0033981	ENSG0000099977	IPR014347

## **Genome Wide Association Studies: databases**



https://www.ncbi.nlm.nih.gov/snp/

NCBI main repository of information about polymorphisms and their penetrance, possible molecular effects and functional role.



www.ncbi.nlm.nih.gov/gap



# GWAS Catalog

The NHGRI-EBI Catalog of published genome-wide association studies

www.ebi.ac.uk/gwas/

"The database of Genotypes and Phenotypes (dbGaP) was developed to archive and distribute the results of studies that have investigated the interaction of genotype and phenotype".

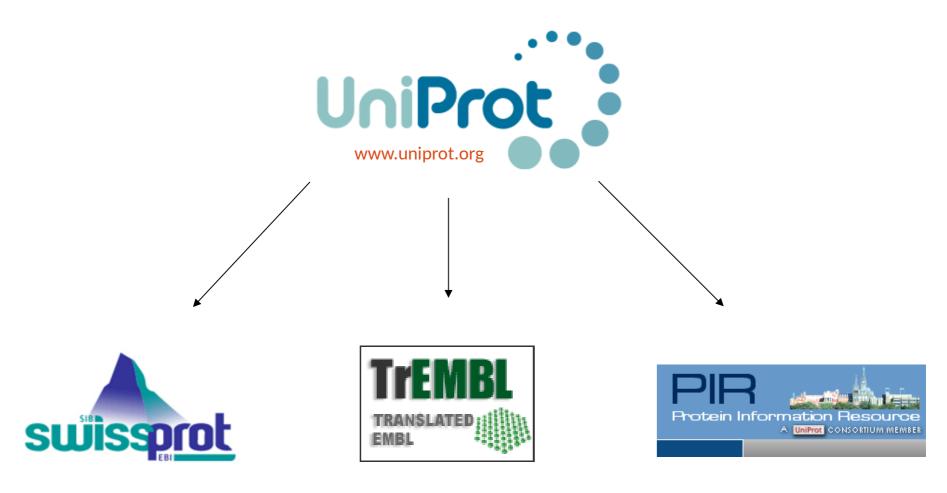
The catalog of Published Genome-Wide Association Studies of the NIH National Human Genome Research Institute (NHGRI)



www.gwascentral.org

GWAS Central provides a centralized compilation of summary level findings from genetic association studies, both large and small.

## **UniProt: the reference protein database**



Highly accurate and detailed, with manual annotations about function, structure, PTM and much more.

Contains *in silico* translation of each coding sequence in the EMBL primary database. Huge but inaccurate. The direct descendent of the Dayhoff Protein Atlas, the best protein database available.

Click to go to the browser



## **UniProt: the reference protein database**

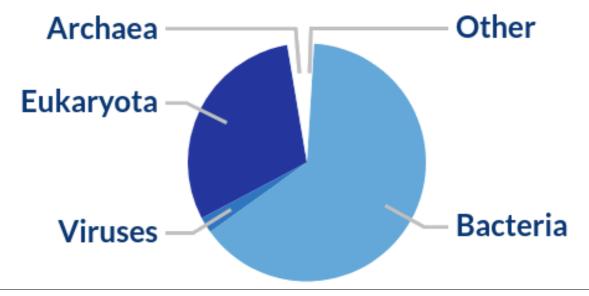
Total
-------

Section	Number of entries in total
UniProtKB	250,322,721
Reviewed (Swiss- Prot)	570,830
Unreviewed (TrEMBL)	249,751,891

# Human UniProtKB 204,052 results

Reviewed (Swiss-Prot) (20,433)

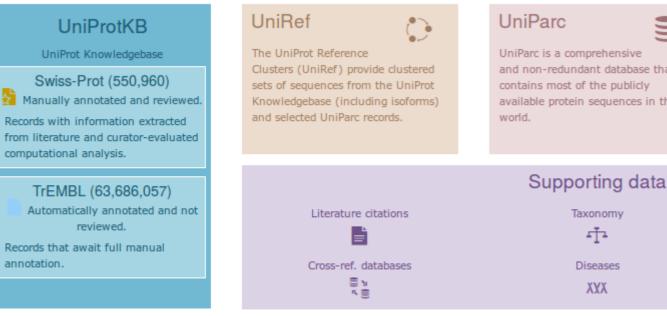
Unreviewed (TrEMBL) (183,619)



## **UniProt: the reference protein database**

UniProtKB collects and join Swiss-Prot and TrEMBL and is an interface and a data bank that integrate annotations coming from a huge variety of sources in an integrated framework.

The possibility of having a common interface to look at proteins makes UniProtKB the reference source for protein records.



Provide clustered sets of sequences in order to obtain complete coverage of the sequence space at several resolutions

UniRef 100: identical and sequences subfragments are merged.

UniRef 90: clustered if they share >90% identity.

UniRef 50: clustered if they share >50% identity.

Is a collection organized by proteins sequence of coming from databases all over the world.

1 sequence => many IDs and annotations.

The entry is classified with and unique stable а identifier (UPI), that is never removed or changed.

Searching in uniparc is like searching in many DBs.

UniParc is a comprehensive and non-redundant database that contains most of the publicly available protein sequences in the A proteome is the set of proteins thought to be expressed by an organism.

The set of proteins that constitute the proteome is classified usina the proteome identifier (UPID), consisting in of the characters 'UP' followed by 9 diaits.

UPIDs are stable across releases.

## Proteomes 💥 /

A proteome is the set of proteins thought to be expressed by an organism. UniProt provides proteomes for species with completely sequenced genomes.

Subcellular locations Keywords ĿA

The concept of "signature" is of paramaount importance in bioinformatics: a pattern of residues that is found in a protein can describe many of its properties and may lead to automatic functional / structural classification.

InterPro allows to automatically scan a protein against several signature data banks, searchign for signatures, domain (functional or structural) or patterns.

Download Soft	ware				
				RESULTS	YOUR EMAIL
				interactive 💌	
	APPLICAT	IONS TO RUN	I 🔘 Clear all 🤇	🕑 Check all	
🗷 BlastProDom	🗹 FPrintScan	MMMPIR	🗹 HMMPfam	🗹 HMMSmart	
HMMTigr	🗹 ProfileScan	🗹 HAMAP	🗹 patternScar	🛛 🗹 SuperFamily	🗹 SignalPHMM
🗹 ТМНММ	MMPanther	🗹 Gene3D			
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	· ·			2PHIQWIKHVEKNG	· · ·
NHTYHLDVVERS: YGPDGLPYLKVL:	PHRPILQAGLPA KAAGVNTTDKEI	NASTVVGGD EVLYIRNVT	VEFVCKVYSDA( FEDAGEYTCLA(	GNSIGISFHSAWLI	SK VL
NHTYHLDVVERS: YGPDGLPYLKVL: PAPGREKEITAS:	PHRPILQAGLPA KAAGVNTTDKEI PDYLEIAIYCIG	NASTVVGGD EVLYIRNVT VFLIACMVV	VEFVCKVYSDAG FEDAGEYTCLAG TVILCRMKNTTF	SNSIGISFHSAWLT KKPDFSSQPAVHKL	SK TVL TK
NHTYHLDVVERS: YGPDGLPYLKVL PAPGREKEITAS: RIPLRRQVTVSA:	PHRPILQAGLPA KAAGVNTTDKEI PDYLEIAIYCIG ESSSSMNSNTPL	NASTVVGGD EVLYIRNVT VFLIACMVV VRITTRLSS	VEFVCKVYSDAQ FEDAGEYTCLAQ TVILCRMKNTTF TADTPMLAGVSE	GNSIGISFHSAWLI	SSK TVL .TK RDK
YGPDGLPYLKVL PAPGREKEITAS RIPLRRQVTVSA LTLGKPLGEGCF IGKHKNIINLLG	PHRPILQAGLPA KAAGVNTTDKEI PDYLEIAIYCIG ESSSSMNSNTPL GQVVMAEAVGID ACTQDGPLYVIV	NASTVVGGD EVLYIRNVT VFLIACMVV VRITTRLSS KDKPKEAVT EYASKGNLR	VEFVCKVYSDAG FEDAGEYTCLAG TVILCRMKNTTF TADTPMLAGVSF VAVKMLKDDATF EYLRARRPPGMF	GNSIGISFHSAWLT KKPDFSSQPAVHKL CYELPEDPKWEFPF CKDLSDLVSEMEMM CYSYDINRVPEEQM	SK VL .TK QDK IKM ITF
NHTYHLDVVERS: YGPDGLPYLKVL PAPGREKEITAS: RIPLRRQVTVSA LTLGKPLGEGCF IGKHKNIINLLG. KDLVSCTYQLAR	PHRPILQAGLPA KAAGVNTTDKEI PDYLEIAIYCIG ESSSSMNSNTPL GQVVMAEAVGID ACTQDGPLYVIV GMEYLASQKCIH	NASTVVGGD EVLYIRNVT VFLIACMVV VRITTRLSS KDKPKEAVT EYASKGNLR RDLAARNVL	VEFVCKVYSDAG FEDAGEYTCLAG TVILCRMKNTTF TADTPMLAGVSF VAVKMLKDDATF EYLRARRPPGMF VTENNVMKIADF	NSIGISFHSAWLT KKPDFSSQPAVHKL YELPEDPKWEFPF KKDLSDLVSEMEMM YSYDINRVPEEQM FGLARDINNIDYYF	SK VL TK QDK IKM ITF KT
NHTYHLDVVERS YGPDGLPYLKVL PAPGREKEITAS RIPLRRQVTVSA LTLGKPLGEGCF IGKHKNIINLLG KDLVSCTYQLAR INGRLPVKWMAP	PHRPILQAGLPA KAAGVNTTDKEI PDYLEIAIYCIG ESSSSMNSNTPL GQVVMAEAVGID ACTQDGPLYVIV GMEYLASQKCIH EALFDRVYTHQS	NASTVVGGD EVLYIRNVT VFLIACMVV VRITTRLSS KDKPKEAVT EYASKGNLR RDLAARNVL DVWSFGVLM	VEFVCKVYSDAG FEDAGEYTCLAG TVILCRMKNTTF TADTPMLAGVSF VAVKMLKDDATF EYLRARRPPGMF VTENNVMKIADF WEIFTLGGSPYF	GNSIGISFHSAWLT KKPDFSSQPAVHKL CYELPEDPKWEFPF CKDLSDLVSEMEMM CYSYDINRVPEEQM	SSK VUL DTK DDK LIKM LITF CGH



## InterPro: many hits make a result...

Table View	Raw C	Output	XML Output	Original Seque	nces	SUBMIT ANOTHE	RJOB		
	s	SEQUENCE	FGFR2 HUMAN	<u>1</u> CRC64: 6CD500	1C960ED	82F LENGTH: 821 (	aa 🔍 G	l	
InterPro	Protein kina	nase, cataly	tic domain						PS: ProSite
Domain	PS50011	EIN_KINASE_DOM	P5. Prosile						
InterPro	Serine-thre	eonine/tyro	osine-protein kii	nase					PF: Pfam
Domain	PF07714							e_Tyr	
InterPro IPR003598	Immunogio	obulin subt	type 2						
Domain	SM00408						- IGc2		SM: SMART
InterPro IPR007110	Immunogio	obulin-like							PS: ProSite
Domain	PS50835						— IG_LIK	E	15.110510
InterPro	Protein kina	nase-like de	omain						SSF: SuperFamily
Domain	SSF56112					•	Proteir	n kinase-like (PK-like)	sorrouperrunniy
InterPro IPR013783	Immunoglo	obulin-like	fold						G3DSA: Gene 3D
Domain	G3DSA:2.60.	0.40.10						no description	GobsA. Gene SD
InterPro	Tyrosine-pr	protein kina	ise						PTHR: Panther
Region	PTHR23256						TYRO	SINE PROTEIN KINASE	
noIPR unintegrated	unintegrate	ed							
aninicgrateu	SignalP	•						signal-peptide	Topology predictors
	tmhmm				•	•		transmembrane_regions	

It is a 820 AA residue long protein with an Ig domain (so, extracellular), with a transmembrane region and a protein kinase domain, with several phoshporylation sites and a signal peptide typic of ER produced proteins: definitely a receptor.

## **NCBI Taxonomy – collector, indexer and accessor**



- Hominoidea (apes) Click on organism name to get more information.
  - Hominidae (great apes)
    - O Homininae
      - <u>Gorilla</u>
      - Homo
      - Pan (chimpanzees)
    - Ponginae
      - Pongo
  - Hylobatidae (gibbons)
    - O Bunopithecus
      - <u>Bunopithecus hoolock</u> (Hoolock gibbon)
    - Hylobates
      - Hylobates agilis (agile gibbon)
      - Hylobates alibarbis (Bornean white-bearded gibbon)
      - Hylobates klossii (Kloss's gibbon)
      - Hylobates lar (common gibbon)
      - Hylobates moloch (silvery gibbon)
      - Hylohates muelleri (Mueller's Borneo oibbon)

#### Homo

Taxonomy ID: 9605

Inherited blast name: primates Rank: genus Genetic code: <u>Translation table 1 (Standard)</u> Mitochondrial genetic code: Translation table 2 (Vertebrate Mitochondrial)

#### <u>Lineage(</u>full)

<u>cellular organisms; Eukaryota; Fungi/Metazoa group; Metazoa; Eumetazoa; Bilateria; Coelomata;</u> Deuterostomia; Chordata; Craniata; Vertebrata; Gnathostomata; Teleostomi; Euteleostomi; Sarcopterygii; Tetrapoda; Amniota; Mammalia; Theria; Simiiformes; Catarrhini; Hominoidea; Hominidae; Homininae Eutheria; Euarchontoglires; Primates; Haplorrhini;

Entrez records					
Database name	Subtree links	Direct links			
Nucleotide	16,329,633	1			
Nucleotide EST	8,301,205	-			
Nucleotide GSS	1,291,174	-			
Protein	<u>517,003</u>	_			
Structure	<u>15,087</u>	-			
Genome Sequences	<u>75</u>	-			
Genome Projects	<u>32</u>	_			
Popset	21,577	20,352			
SNP	25,003,333	_			
3D Domains	<u>59,719</u>	-			
Domains	8	-			
GEO Datasets	<u>8,886</u>	_			
GEO Expressions	17,689,684	_			
UniGene	123,267	-			
UniSTS	327,286	_			
PubMed Central	<u>8,543</u>	<u>1,493</u>			
Gene	45,510	-			
HomoloGene	<u>18,876</u>	_			
SRA Experiments	7,283	_			
Taxonomy	3	<u>1</u>			



#### Homininae

Taxonomy ID: 207598

Entrez records					
Database name	Subtree links	Direct links			
Nucleotide	13,513,288	-			
Nucleotide EST	8,722,459	-			
Nucleotide GSS	<u>1,929,671</u>	-			
Protein	1,202,463	-			
Structure	29,915	-			
Genome	5	-			
Popset	24,135	20,870			
SNP	163,116,552	-			
Domains	26	1			
GEO Datasets	1,064,407	-			
UniGene	132,468	-			
PubMed Central	22,689	54			
Gene	<u>341,776</u>	-			
HomoloGene	19,739	-			
SRA Experiments	449,610	1			
Probe	27,382,680	-			
Assembly	<u>95</u>	-			
Bio Project	27,567	1			
Bio Sample	1,834,762	<u>1</u>			
Bio Systems	4,644	-			
Clone DB	19,133,161	-			
dbVar	3,527,044	-			
Epigenomics	5,110	-			
GEO Profiles	52,194,103	-			
PubChem BioAssay	260,659	-			
Protein Clusters	<u>13</u>	-			
Taxonomy	23	1			

#### Homo

#### Taxonomy ID: 9605

Entrez records						
Database name	Subtree links	Direct links				
Nucleotide	12,866,193	<u>3</u>				
Nucleotide EST	<u>8,705,079</u>	-				
Nucleotide GSS	<u>1,729,196</u>	_				
Protein	1,005,297	-				
Structure	29,901	-				
Genome	2	-				
Popset	23,337	20,389				
SNP	161,456,298	-				
Domains	25	-				
GEO Datasets	<u>1,063,551</u>	-				
UniGene	<u>130,056</u>	-				
PubMed Central	20,617	20,614				
Gene	215,981	-				
HomoloGene	18,713	-				
SRA Experiments	448,306	<u>12</u>				
Probe	27,382,448	_				
Assembly	77	-				
Bio Project	27,508	1				
Bio Sample	1,833,465	<u>12</u>				
Bio Systems	<u>3,171</u>	-				
Clone DB	17,567,165	-				
dbVar	3,526,684	-				
Epigenomics	<u>5,110</u>	-				
GEO Profiles	52,194,103	-				
PubChem BioAssay	260,526	-				
Protein Clusters	<u>13</u>	-				
Taxonomy	<u>5</u>	1				

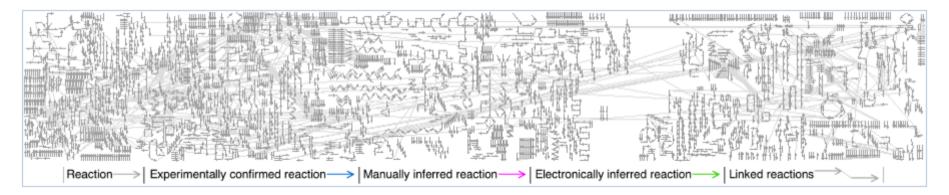
#### Homo sapiens

#### Taxonomy ID: 9606

Entrez records					
Database name	Subtree links	Direct links			
Nucleotide	12,866,188	12,866,152			
Nucleotide EST	<u>8,705,079</u>	<u>8,705,079</u>			
Nucleotide GSS	<u>1,729,196</u>	<u>1,727,870</u>			
Protein	1,005,271	1,005,083			
Structure	29,901	<u>29,901</u>			
Genome	1	1			
Popset	23,337	23,337			
SNP	161,456,298	161,456,298			
Domains	25	25			
GEO Datasets	<u>1,063,551</u>	<u>1,063,551</u>			
UniGene	<u>130,056</u>	<u>130,056</u>			
PubMed Central	17,608	17,588			
Gene	215,944	<u>215,871</u>			
HomoloGene	18,713	<u>18,713</u>			
SRA Experiments	448,285	448,065			
Probe	27,382,448	27,382,448			
Assembly	77	77			
Bio Project	27,506	27,496			
Bio Sample	1,833,448	<u>1,833,319</u>			
Bio Systems	<u>3,171</u>	<u>3,171</u>			
Clone DB	17,567,165	17,567,165			
dbVar	3,526,684	3,526,684			
Epigenomics	5,110	<u>5,110</u>			
GEO Profiles	52,194,103	52,194,103			
PubChem BioAssay	260,526	<u>260,518</u>			
Protein Clusters	<u>13</u>	<u>13</u>			
Taxonomy	<u>3</u>	<u>1</u>			

#### The Reactome pathway database





			Sear	ch for:		in	Homo sapiens	•	
changed. In 1972 k <i>ist changed</i> : 2010-0 <b>Pathway</b> : Regu regulated balance b	Pathways (49) tosis (Homo s t form of cell deat (err et al introduct (3-03 07:51:00 tlation of Apopt etween cell survi , neurodegenera	Reactions (69) apiens) th that is functionall ed the concept of a tosis (Homo sap ival and apoptosis i	Proteins (209) y and morphologica poptosis as a distir iiens) is essential for norr	Others (134) ally different from not form of "cell-o mal developmen	Show In mic reticulum, a leath", and the mech t and homeostasis o h is one of the major	anc an	All species Arabidopsis thal Caenorhabditis Cryptococcus ne Cyanidioschyzor Dictyostelium dis Drosophila mela Entamoeba histo Escherichia coli Gallus gallus Homo sapiens Methanocaldoco Mus musculus Mycobacterium ti Neurospora cras Oryza sativa Plasmodium falo	iana elegans eoforman n merolae scoideum anogaster olytica ccus jan ubercul ssa	
ŵ					۲		Rattus norvegicu Saccharomyces Schizosaccharor	cerevisiae	~
2,673		15,046	11,392		2,120		1,046	37,933	

Small Molecules

Proteins

matteo.ramazzotti@unifi.it

Human Pathways

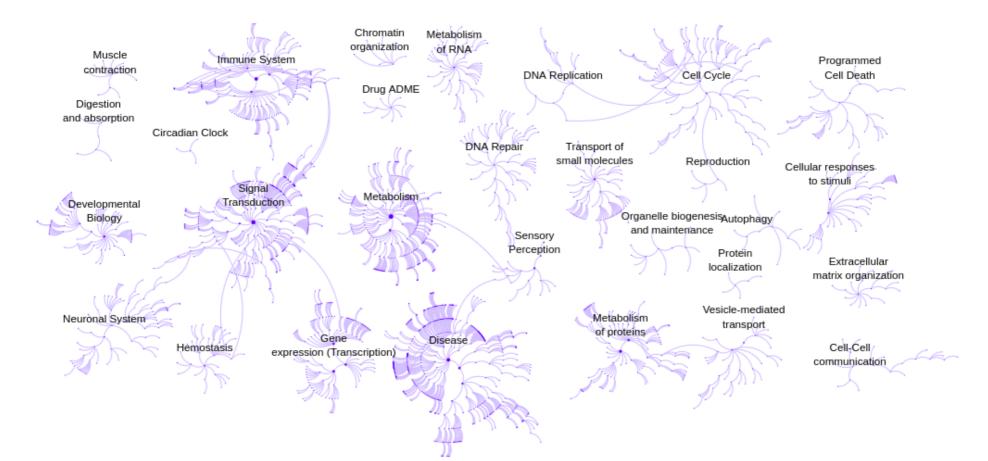
Reactions

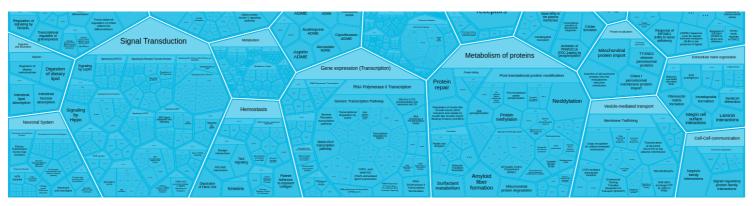
Literature References

Drugs

## The Reactome pathway database







#### operito stektse event jobed a0 doce ରା 🏾

#### 

- Extrinsic Pathway for Apoptosis
  - 🚊 🖾 🖾 Death Receptor Signalling
    - i ∰ ⊈ FasL/ CD95L signaling
    - 🚊 🛫 TNF signaling
    - 💼 🖾 TRAIL signaling
  - 💼 🖾 Caspase-8 is formed from procaspase-8
- i → Intrinsic Pathway for Apoptosis

  - □-- I Activation of BH3-only proteins

    - ⊡ ∴ ¥ Activation of PUMA and translocation to
  - 🗄 🖾 🗸 BH3-only proteins associate with and inac
  - 💼 🖾 Activation, translocation and oligomerizatio
  - □ ↓ Activation and oligomerization of BAK prote
  - # Permeabilization of mitochondria
  - En T Release of apoptotic factors from the mito
  - 💼 🖾 Apoptotic factor-mediated response
- 😅 Activation of Effector Caspases
- ⊡ ↓ Regulation of Apoptosis

Extrinsic Pathway for Apoptosis						
DOI	10.3180/REACT_1059.1					
Stable identifier	REACT_1059.1					
Authored	Gillespie, ME, 2004-08-1(					
Reviewed	Vaux, D, 2010-03-02					

Plasma membrane

Procaspase-3

\*

TRENDS in Cell Biology Vol.11 No.12 Decemb

Active

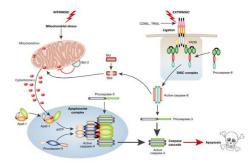
caspase-8

Active

caspase-3

FADD

Procaspase-8



Apoptosis and disease: a life or death decision EMBO Rep. 2004 Jul;5(7):674-8. Epub 2004 Jun 25.

FasL/CD95L signaling	
Stable identifier	REACT_900.1
Authored	Gillespie, ME, 2004-08-18
Reviewed Vaux, D, 2010-03-02	
Your feedback	Let us know what you think of this article (click here)

The Fas family of cell surface receptors initiate the apototic pathway through interaction with the external ligand, FasL. The cytoplasmic domain of Fas interacts with a number of molecules in the transduction of the external signal to the cytoplasmic side of the cell membrane. The most notable cytoplasmic domain is the Death Domain (DD) that is involved in recruiting the FAS-associating death domaincontaining protein (FADD). This interaction drives downstream events. [Itoh et al 1991, Yonehara et al 1989, Chinnaiyan et al 1995]

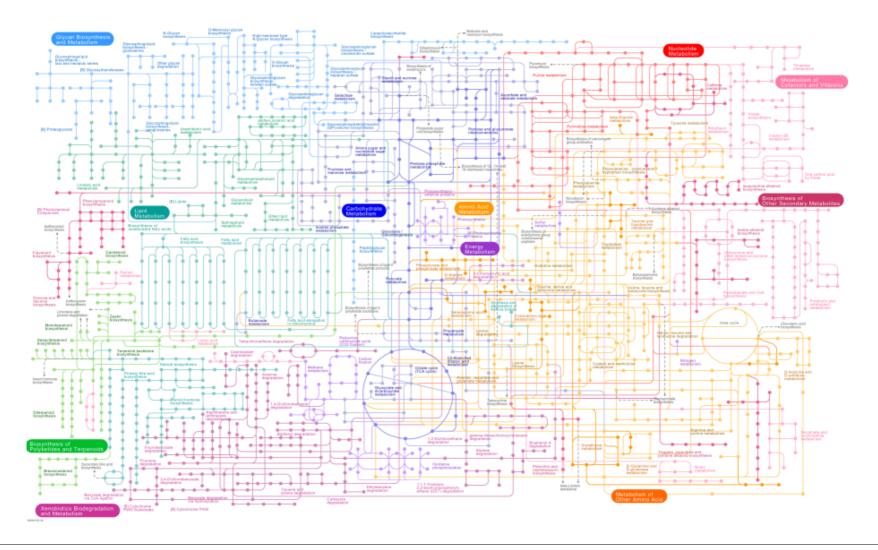
Drganism	Homo sapiens
Cellular compartment	cell <mark>GO</mark>
References	
Hengartner, MO <i>The</i>	biochemistry of apoptosis. 2000 Nature PubMed
Represents GO biological process	induction of apoptosis by extracellular signals $\overline{50}$
Equivalent event(s) n other organism(s)	FasL/ CD95L signaling [Mus musculus] FasL/ CD95L signaling [Rattus norvegicus] FasL/ CD95L signaling [Gallus gallus]
Participating molecu	lles
	recursor (plasma membrane) <mark>UKEG</mark> BCd <mark>OORHUR</mark> ecursor (cvtosol) <b>UKEG</b> BCd <b>OORRHHURR</b> PPPPPDDDDDD

- FADD [cytosol] UKEGBCdORHURPPPDDDDD
- FAS Receptor [plasma membrane] UKEGBCdOORHURPPDD
- FASL [extracellular region] UKEGBCdOORHURPD





KEGG Pathways offers the possibility of looking at the complexity of the network in cell signaling or metabolism using predefined sets of images (maps) that are cross-connected through proteins or metabolites. The interactive maps are shared across organisms, so that organism specificity can be fully understood.



#### 1. Metabolism

- 1.1 Carbohydrate Metabolism
- 1.2 Energy Metabolism
- 1.3 Lipid Metabolism
- 1.4 Nucleotide Metabolism
- 1.5 Amino Acid Metabolism
- 1.6 Metabolism of Other Amino Acids
- 1.7 Glycan Biosynthesis and Metabolism
- 1.8 Metabolism of Cofactors and Vitamins
- 1.9 Biosynthesis of Polyketides and Terpenoids
- 1.10 Biosynthesis of Other Secondary Metabolites
- 1.11 Xenobiotics Biodegradation and Metabolism
- 1.12 Overview

#### 2. Genetic Information Processing

- 2.1 Transcription
- 2.2 Translation
- 2.3 Folding, Sorting and Degradation
- 2.4 Replication and Repair

#### 3. Environmental Information Processing

- 3.1 Membrane Transport
- 3.2 Signal Transduction
- 3.3 Signaling Molecules and Interaction

#### 4. Cellular Processes

- 4.1 Transport and Catabolism
- 4.2 Cell Motility
- 4.3 Cell Growth and Death
- 4.4 Cell Communication

#### 5. Organismal Systems

- 5.1 Immune System
- 5.2 Endocrine System
- 5.3 Circulatory System
- 5.4 Excretory System
- 5.5 Nervous System
- 5.6 Sensory System
- 5.7 Development
- 5.8 Environmental Adaptation

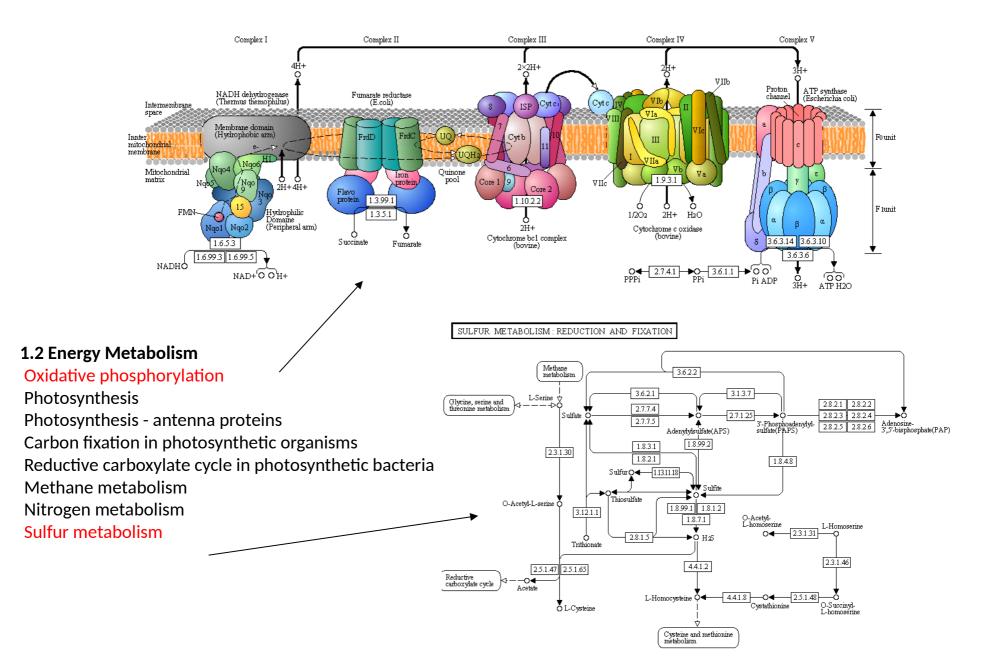
#### 6. Human Diseases

- 6.1 Cancers
- 6.2 Immune System Diseases
- 6.3 Neurodegenerative Diseases
- 6.4 Cardiovascular Diseases
- 6.5 Metabolic Diseases
- 6.6 Infectious Diseases
- 7. Drug Development
- 7.1 Chronology: Antibiotics
- 7.2 Chronology: Antineoplastics
- 7.3 Chronology: Nervous System Agents
- 7.4 Chronology: Other Drugs
- 7.5 Target Based Classification
- 7.6 Structure Based Classification
- 7.7 Skeleton Based Classification

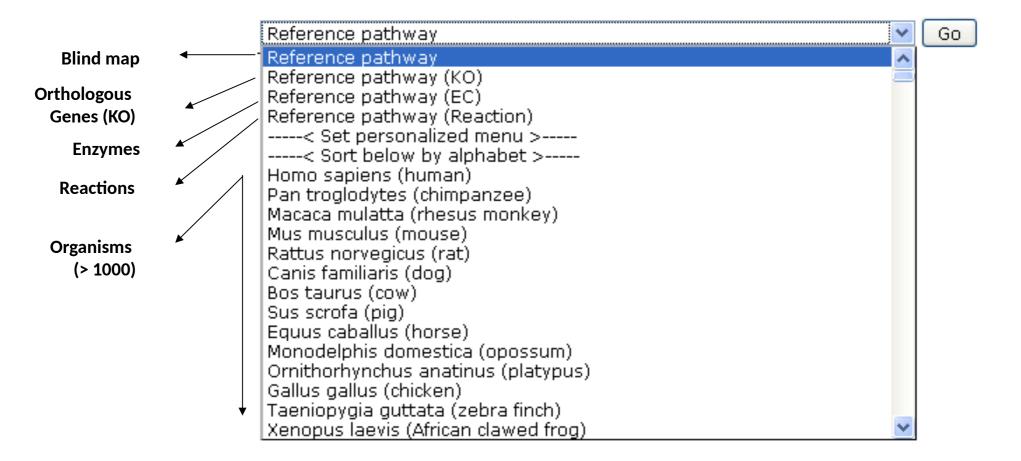


## Schemes and interactive maps and diagrams



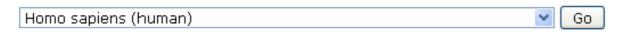




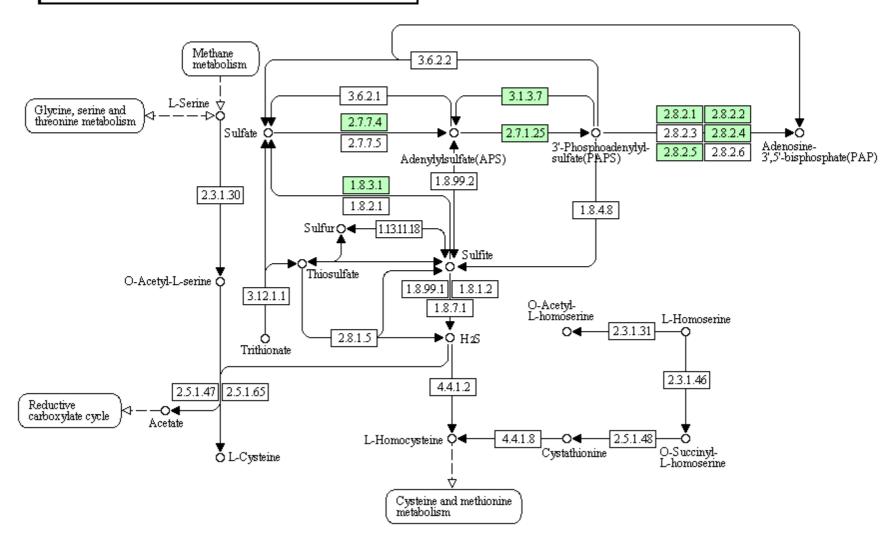


## **Reference maps get colors according to selections**







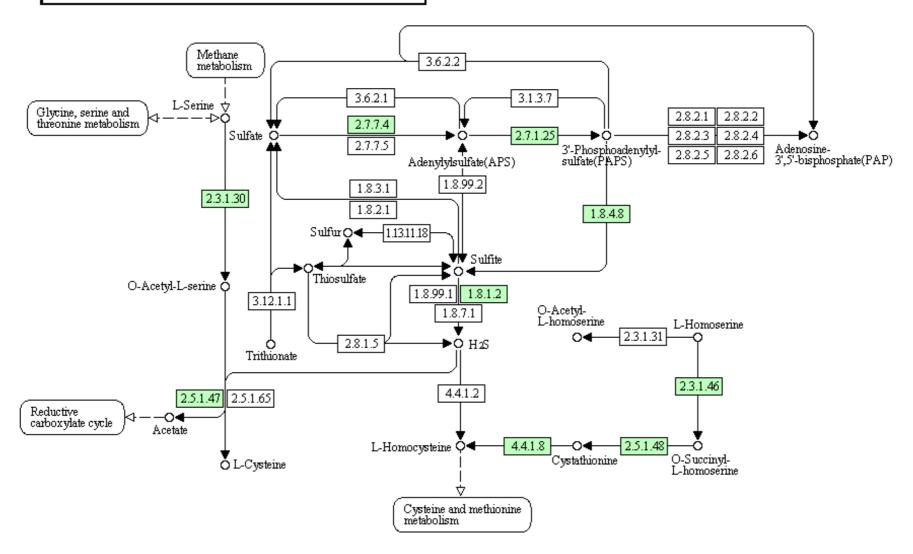


## **Reference maps get colors according to selections**



Escherichia coli K-12 MG1655

SULFUR METABOLISM: REDUCTION AND FIXATION



Go

¥



# KFaa

#### Homo sapiens (human): 9060

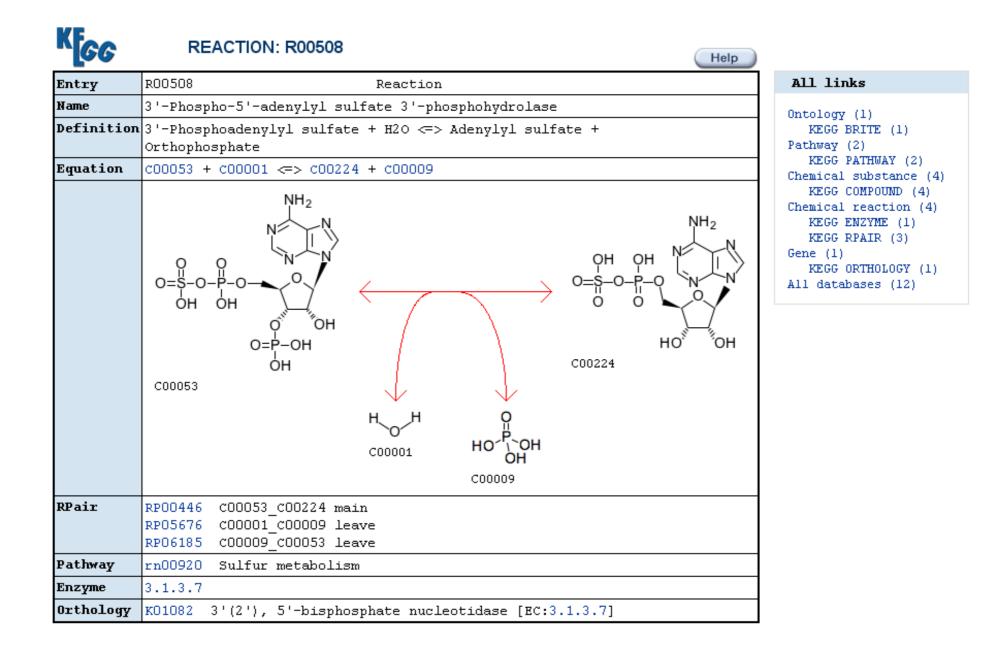
<b>~[</b> 66	Homo sapiens (human): 9060	)
Entry	9060 CDS H.sapiens	All links
Gene name Definition	PAPSS2 3'-phosphoadenosine 5'-phosphosulfate synthase 2 (EC:2.7.1.25 2.7.7.4)	Pathway (4) KEGG PATHWAY (4) Disease (2)
Orthology	KOO860 adenylylsulfate kinase [EC:2.7.1.25] KOO958 sulfate adenylyltransferase [EC:2.7.7.4]	OMIM (2) Chemical reaction (2) KEGG ENZYME (2)
Pathway	hsa00230 Purine metabolism hsa00450 Selenoamino acid metabolism hsa00920 Sulfur metabolism hsa01100 Metabolic pathways	Genome (1) KEGG GENOME (1) Gene (15) KEGG ORTHOLOGY (2) NCBI-Gene (1)
Class	Metabolism; Energy Metabolism; Sulfur metabolism [PATH:hsa00920] Metabolism; Nucleotide Metabolism; Purine metabolism [PATH:hsa00230] Metabolism; Metabolism of Other Amino Acids; Selenoamino acid metabolism [PATH:hsa00450] BRITE hierarchy	NCBI-GI (8) UniGene (1) HGNC (1) HPRD (1) ENSEMBL-HSA (1) Protein sequence (7)
SSDB	Ortholog Paralog Gene cluster GFIT	UniProt (1) RefSeq(pep) (2)
Motif	Pfam: ATP-sulfurylase APS_kinase DUF74 Motif	IPI (4) DNA sequence (24) RefSeq(nuc) (2)
Other DBs	NCBI-GI: 62912492 NCBI-GeneID: 9060 OMIM: 603005 HGNC: 8604 HPRD: 04303 Ensembl: ENSG00000198682 UniProt: 095340	GenBank (11) EMBL (11) 3D Structure (1) PDB (1) Protein domain (3) Pfam (3) All databases (59)
Structure	PDB: 2AX4 Thumbnails Jmol	

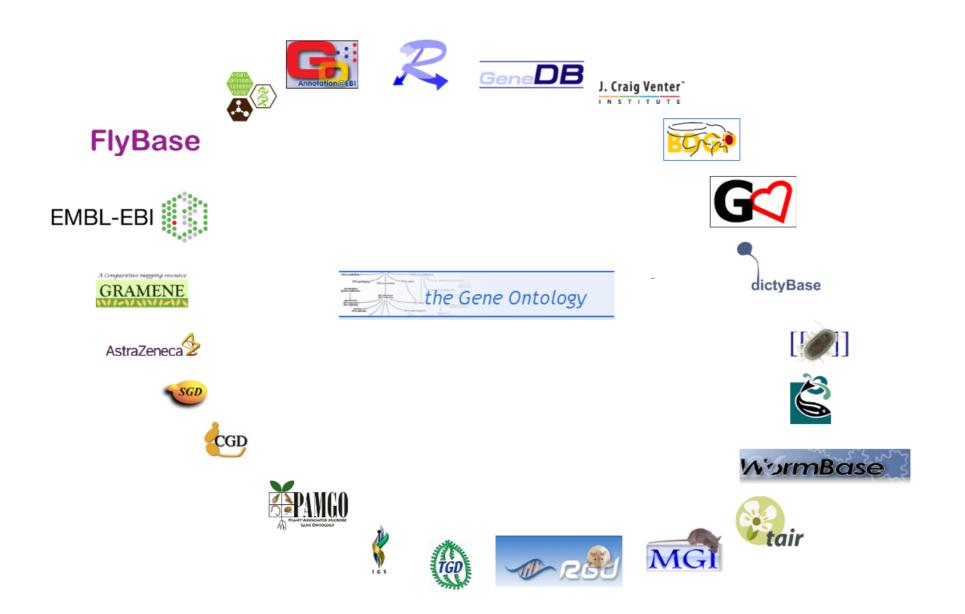
## **Reference maps allow access to cross-annotations**



COMP	OUND: C00224			Help	
C00224	c	Compound			All links
Adenosine 5 APS;	'-phosphosulfate;				Pathway (3520) KEGG PATHWAY (3519) KEGG MODULE (1) Chemical substance (7)
c10H14N5010	PS				PubChem (1)
427.0199					ChEBI (1) 3DMET (1)
	но он	mol			HMDB (1) KNApSAcK (1) NIKKAJI (1) PDB-CCD (1) Chemical reaction (29) KEGG ENZYME (10) KEGG REACTION (11) KEGG RPAIR (8) All databases (3556)
		00531 R00860 RC	)1618 R01619		
ko00920 Su	lfur metabolism				
1.8.4.9 2.7.7.4 3.1.3.7	1.8.4.10 2.7.7.5 3.6.2.1	1.8.99.2 2.7.7.51	2.7.1.25 2.7.7.53		
PubChem: 35 ChEBI: 1770 KNApSAcK: C PDB-CCD: AD 3DMET: B011	24 9 00007445 X 94				
	C00224 Adenylyl su Adenosine 5 APS; 5'-Adenylyl C10H14N5010 427.0199 OH OH O=S-O-P- U O C00224 Mol file K R00508 R005 R05717 R071 ko00230 Pu ko00920 Su ko01100 Me 1.8.4.9 2.7.7.4 3.1.3.7 CAS: 485-84 PubChem: 35 ChEBI: 1770 KNApSACK: C PDB-CCD: AD 3DMET: B011	Adenylyl sulfate; Adenosine 5'-phosphosulfate; APS; 5'-Adenylyl sulfate C10H14N5010PS 427.0199 427.0199 OH OH O	COO224 Compound Adenylyl sulfate; Adenosine 5'-phosphosulfate; APS; 5'-Adenylyl sulfate C10H14N5010PS 427.0199	C00224 Compound Adenylyl sulfate; Adenosine 5'-phosphosulfate; APS; 5'-Adenylyl sulfate C10H14N5010PS 427.0199	Help       C00224     Compound       Adenosine 5'-phosphosulfate;     APS;       S'-Adenylyl sulfate     C10H14N5010PS       427.0199     Image: Compound image: Comp

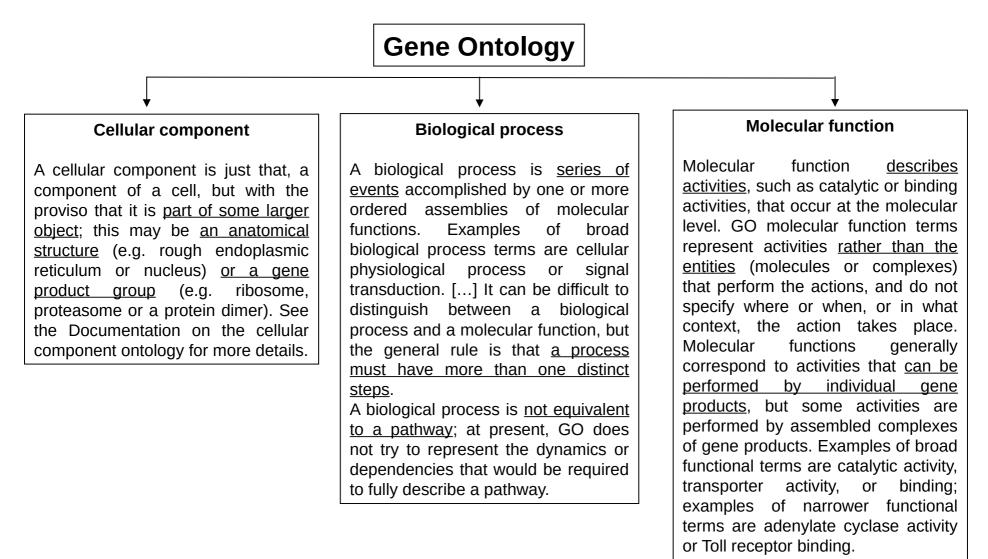
#### **Reference maps allow access to cross-annotations**





#### The Gene Ontology Database (GO)

In informatics the term "ontology" refers to a controlled vocabulary of terms and definitions that can be used to describe objects and relationships among them. GO is an accurate and complete collection of definitions used to describe genes.



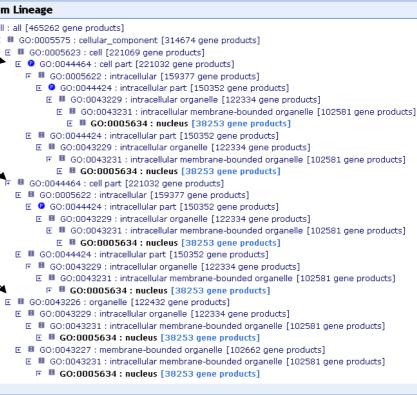
the	Gene
Onto	ology

Term Info	Term Information		
Accession	GO:0005634		
Ontology	cellular component		
Synonyms	exact: cell nucleus		
Definition	A membrane-bounded organelle of eukaryotic cells in which chromosomes are housed and replicated. In most cells, the nucleus contains all of the cell's chromosomes except the organellar chromosomes, and is the site of RNA synthesis and processing. In some species, or in specialized cell types, RNA metabolism or DNA replication may be absent. [source: GOC:go_curators]		

Here is how GO define the term "nucleus". If I refer to the nucleus as "GO:0005634", al ambiguities are removed.

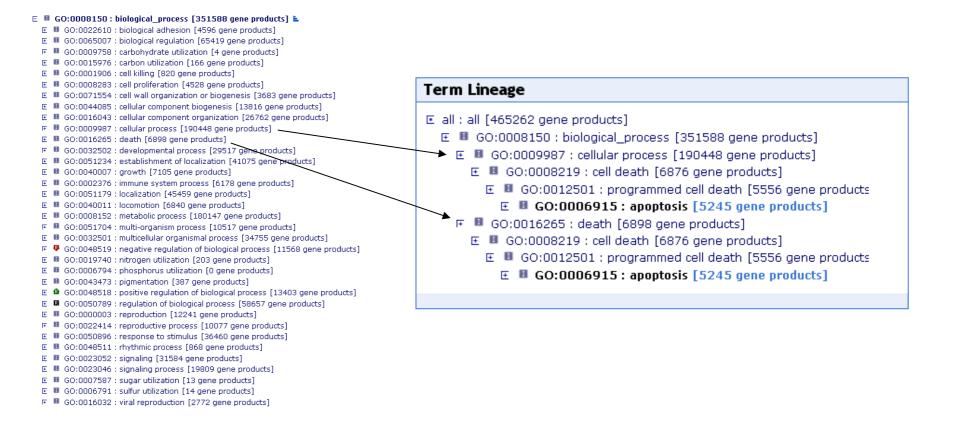
E 🔲 GO:0005575 : cellular_component [314674 gene products] 💺	
F GO:0005623 : cell [221069 gene products]	Term Lineage
<ul> <li>Go:0003023 : cell [221039 gene products]</li> <li>Go:00044464 : cell part [221032 gene products]</li> <li>Go:0005576 : extracellular region [15221 gene products]</li> <li>GO:0044421 : extracellular region part [5481 gene products]</li> <li>GO:0032991 : macromolecular complex [45131 gene products]</li> <li>GO:0031974 : membrane-enclosed lumen [10295 gene products]</li> <li>GO:0043226 : organelle [122432 gene products]</li> <li>GO:0044422 : organelle part [38500 gene products]</li> <li>GO:0055044 : symplast [15 gene products]</li> <li>GO:0044456 : synapse part [1620 gene products]</li> <li>GO:0019012 : virion [2890 gene products]</li> <li>GO:0044423 : virion part [2557 gene products]</li> </ul>	<ul> <li>F all : all [465262 gene products]</li> <li>E ■ G0:0005575 : cellular_component</li> <li>E ■ G0:0005623 : cell [221069 gen</li> <li>E ■ G0:0005623 : cell part [2211</li> <li>F ■ G0:0005622 : intracellular</li> <li>E ■ G0:004424 : intracellular</li> <li>E ■ G0:0043229 : intracellular</li> <li>E ■ G0:0043229 : intracellular</li> <li>E ■ G0:0043229 : intracellular</li> <li>E ■ G0:004424 : intracellular</li> <li>E ■ G0:0043229 : intracellular</li> <li>E ■ G0:0043229 : intracellular</li> <li>E ■ G0:0043231 : intracellular</li> <li>E ■ G0:0043231 : intracellular</li> <li>E ■ G0:0045634 : nu</li> <li>F ■ G0:0044464 : cell part [221033</li> <li>E ■ G0:0044424 : intracellular [2</li> <li>E ■ G0:0044424 : intracellular</li> <li>E ■ G0:004424 : intracellular</li> <li>E ■ G0:004424 : intracellular</li> <li>E ■ G0:004424 : intracellular</li> </ul>
Clearly, the nucleus is contained in $\searrow$	E 🖪 GO:0005634 : nu E 🖪 GO:0044424 : intracellular pa
other cell structures (components)	F B GO:0043229 : intracellular E B GO:0043231 : intracellu F B GO:0005634 : nucle
that will have an appropriate GO term	<ul> <li>E ■ GO:0043226 : organelle [1224:</li> <li>E ■ GO:0043229 : intracellular or</li> </ul>
and code.	

A hierarchical structure forms, that exemplify the reasoning behind GO.



Term Info	Term Information		
Accession	GO:0006915		
Ontology	biological process		
Synonyms	exact: apoptotic cell death exact: apoptotic programmed cell death exact: programmed cell death by apoptosis		
Definition	A form of programmed cell death that begins when a cell receives internal or external signals that trigger the activity of proteolytic caspases, proceeds through a series of characteristic stages typically including rounding-up of the cell, retraction of pseudopodes, reduction of cellular volume (pyknosis), chromatin condensation, nuclear fragmentation (karyorrhexis), and plasma membrane blebbing (but maintenance of its integrity until the final stages of the process), and ends with the death of the cell. [source: GOC:go_curators, <u>ISBN:0198506732</u> , <u>PMID:18846107</u> ]		

Here the definition of apoptosis (GO:000915): different criteria have to be used for a biological process, but the same hierarchical structure is presented.



E II GO:0045182 : translation regulator activity [146 gene products]
 E II GO:0005215 : transporter activity [22077 gene products]

## **GO Molecular Function (MF)**

Note that each lemma in the "molecular function" class end with the term "activity". We are not talking about specific gene or proteins, they are abstract cathegories.

Term Information	
Accession GO:0004784	
Ontology	molecular function
Synonyms exact: superoxide:superoxide oxidoreductase activity	
Definition	Catalysis of the reaction: 2 superoxide + 2 H+ = O2 + H2O2. [source: $EC:1.15.1.1$ ]

Molecular function: now go defines how molecules or complexes acts. This is the deinition of superoxide dismutase activity (GO:0004784)

E 📕 GO:0003674 : molecular\_function [374617 gene products] 🛓 GO:0016209 : antioxidant activity [2318 gene products] + + GO:0005488 : binding [171007 gene products] Term Lineage 🗉 📕 GO:0003824 : catalytic activity [147372 gene products]. Image: all [465262 gene products] 🗉 🗉 GO:0016247 : channel regulator activity [489 gene products E B GO:0003674 : molecular function [374617 gene products] 🗉 📕 GO:0042056 : chemoattractant activity [50 gene products] 🏝 🗉 GO:0016209 : antioxidant activity [2318 gene products] GO:0045499 : chemorepellent activity [20 gene products] E 📕 GO:0009055 : electron carrier activity [6056 gene products] GO:0004784 : superoxide dismutase activity [477 gene products] E E GO:0030234 : enzyme regulator activity [7175 gene products] GO:0003824 : catalytic activity [147372 gene products] **F** GO:0016530 : metallochaperone activity [76 gene products] + E E GO:0016491 : oxidoreductase activity [27992 gene products] 👎 📕 GO:0060089 : molecular transducer activity [21025 gene products] 👎 📱 GO:0016721 : oxidoreductase activity, acting on superoxide radicals as acceptor GO:0045735 : nutrient reservoir activity [222 gene products] . [488 gene products] GO:0010860 : proteasome regulator activity [70 gene products] + ■ GO:0004784 : superoxide dismutase activity [477 gene products] E B GO:0031386 : protein tag [43 gene products] + GO:0005198 : structural molecule activity [17315 gene products] E E GO:0030528 : transcription regulator activity [19229 gene products]

#### **Tree Browser**

🔻 Filter tree view 🕯	2		
Filter by ontology	Filter Gene Product Co	unts	View Options
Ontology	Data source	Species	Tree view 💿 Full 🔘 Compact
All 📃 🔨	All 🔼	All 🔼	
biological process	ASAP	🛛 Arabidopsis thaliana 📃	Set filters
cellular component molecular function 🐸	AspGD CGD	Bacillus anthraci Bacillus subtilis	
			Remove all filters

📧 all : all [465262 gene products] 💺

E ■ GO:0008150 : biological\_process [351588 gene products]

👎 📕 GO:0005575 : cellular\_component [314674 gene products]

E 📕 GO:0003674 : molecular\_function [374617 gene products]

Search Browse BLAST More Tools Help	Current filters
Search GO Wiquitin 💿 terms 🔘 genes or proteins 🗹 exact	Species:
Term Search Results	Filter tree view      Filter Gene Product Counts     Filter by ontology     Filter Gene Product Counts     Ontology     Data source     Species     Tree view     Options
113 results for ubiquitin in terms fields term accession, term name and synonyms	Ontology Data source Species All All Geobacillus stear
Filter search results	biological process AAAP Geobacter sulfurr Set filters
Ontology Set filters All biological process cellular component	cellular component molecular function     AspGD CGD     Haloarcula marism       Homo sapiens     Remove all filters
molecular function	🖻 all : all [18242 gene products] 💺
Results are sorted by <b>relevance</b> . To change the sort order, click on the column headers.	E 📕 GO:0008150 : biological_process [14766 gene products]
1 2 3 View all results	🗉 📕 GO:0005575 : cellular_component [36757 gane preducts]
	E 📕 GO:0003674 : molecular_function [15769 gene products]
Select all Clear all Perform an action with this page's selected terms	temin
rel , <u>Accession</u> , <u>Term</u>	Onto Logy
G0:0016579 : <u>protein de<b>ubiquitin</b>ation</u> <u>(show def)</u> Query matches synonyms "de <b>ubiquitin</b> ation" [exact synonym], <u>and 1 more</u>	231 gene products biological process view in tree
GO:0043130 : ubiguitin binding [show def]	188 gene products molecular fun tige 7 7 7
GO:0010992 : ubiquitin homeostasis [show def]	4 gene products biological process view in tree
GO:0031593 : polyubiquitin binding [show def]	<u>64 gene products molecular function</u>
GO:0016574 : histone ubiquitination [show def]	95 gene products biological process view in tree
GO:0016567 : protein ubiquitin ation [show def]	1293 gene products biological process view in tree
GO:0000151: ubiquitin ligase complex [show def]	949 gene products cellular component view in tree
GO:0031625 : ubiquitin protein ligase binding [show def]	231 gene products molecular function
Query matches synonym " <b>ubiquitin</b> ligase binding" [exact synonym]	view in tree
G0:0004842 : <b>ubiquitin</b> -protein ligase activity (show def)	1303 gene products molecular function

## **EBI ArrayExpress**

It is one of the most important transcriptomics repository. The International journals nowadays force authors of high throughput data to expose them into specialized data banks.

	PRESS			Æ
The ArrayExpress Archive is a database collected to MIAME and MINSEQE standar queried for individual gene expression und	ds. Gene Expression Atlas	contains a subset of curated		
Experiments Archive 11318 experiments, 314001 assays		Gene Expressio		ditions
Experiment, citation, sample and factor ar	notations	Genes		Conditions
			up/down in 🛛 🔽	
Browse experiments Advanced query interface	Query	Any species	~	Query
		Gene Expression Atlas H	ome	
🔎 Submitter/reviewer login	left ArrayExpress Query Help			

This is the the true data bank, that stores, collects and organizes experiments according to rigid submission protocols. All the experimental details, sample descriptions, and statistical procedures are also stored.

This is a gene centric version of the data bank where the measurement for a given gene is normalized across experiments to allow comparison.

# **MIAME - Minimum Information About a Microarray Experiment**

nent <del>(</del>

The submission of microarray data (not only) follows a strict check: the MIAME standard ensure that all deposited experiment is correct and clearly understandable (and reproducible, in principle) by every user of the data bank...

The six most critical elements contributing towards MIAME are:

- 1. The raw data for each hybridisation (e.g., CEL or GPR files)
- 2. The final processed (normalised) data for the set of hybridisations in the experiment (study) (e.g., the gene expression data matrix used to draw the conclusions from the study)
- 3. The essential sample annotation including experimental factors and their values (e.g., compound and dose in a dose response experiment)
- The experimental design including sample data relationships (e.g., which raw data file relates to which sample, which hybridisations are technical, which are biological replicates)
- Sufficient annotation of the array (e.g., gene identifiers, genomic coordinates, probe oligonucleotide sequences or reference commercial array catalog number)
- 6. The essential laboratory and data processing protocols (e.g., what normalisation method has been used to obtain the final processed data)

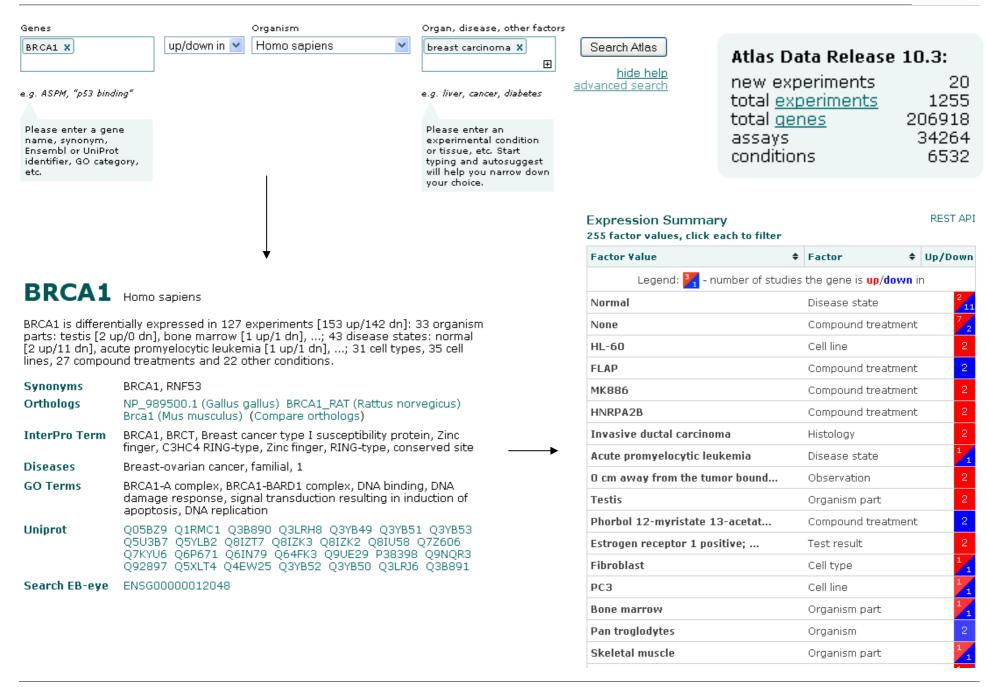
For more details, see MIAME 2.0.

Raw data Preprocessed data Ontology driven annotations Experiment design Array specifications Experimental and informatic protocols

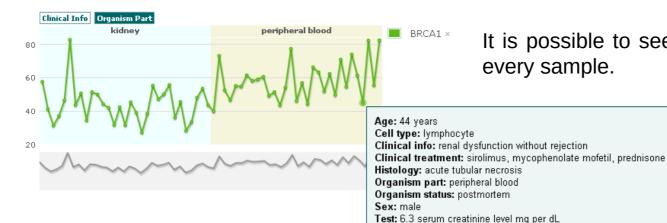
Experiment, citation, sample and factor annotations [clear]	Filter on [reset]	
	Homo sapiens	*
Expand search using Experimental Factor Ontology	All arrays	*
🔑 Submitter/reviewer login	DNA assay 🖌 by Array	*

ID	Title		
⊟ E-GEOD-18347	CREB ChIP-chip and HaloCHIP-chip experim	ments	
Description	interactions. In this study we finely map the subset of these binding events using high-ti fusion protein, and also high-throughput pri	for normal development and cellular growth. Transcriptional ev e genome-wide targets of the CREB protein across all known ar chroughput reporter assays. To measure CREB binding, we used omoter-luciferase reporter assays, which provide rapid and qua tes. HaloCHIP-chip three biological replicates with and without f	nd pre 1 Halo antitat
MIAME score	Array designs Protocols Factors Proce	essed data Raw data	
Contact	Danette Hartzell <danette.hartzell@promeg< td=""><td>ga.com&gt;</td><td></td></danette.hartzell@promeg<>	ga.com>	
Citations	A functional analysis of the CREB signaling PubMed 19860899	pathway using HaloCHIP-chip and high throughput reporter as	says.
Links	GEO - GSE18347 Array design A-GEOD-9325 - NimbleGen Ho Experimental protocols ArrayExpress Advanced Interface	uman 385K custom array	
Files	Data Archives Sample and Data Relationship Investigation Description Experiment Design Images Array Design Browse all available files	E-GEOD-18347.processed.1.zip, E-GEOD-18347.raw.1.zip E-GEOD-18347.sdrf.txt E-GEOD-18347.idf.txt E-GEOD-18347.biosamples.png, E-GEOD-18347.biosample A-GEOD-9325.adf.txt	
Experiment type	ChIP-chip by tiling array		
Sample attributes	Attribute name antibody cell line genome/variation Organism	<b>Attribute values</b> CREB, none HeLa cells HaloTag-CREB fusion construct Homo sapiens	

### **ArrayExpress: the gene expression atlas**



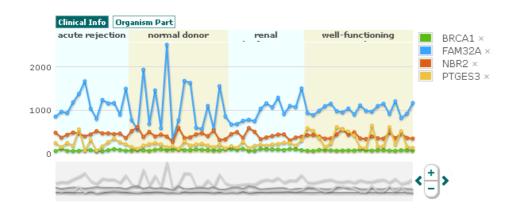
## **ArrayExpress: gene expression atlas**



It is possible to see the gene expresion profiles of every sample.

Using the menus, it is possible to add the profiles of other genes selected by:

- Name
- Similar expression profile
- Top variable genea in the sample



Display genes matching by name or attribute
 Find genes (all genes) Search
 Display genes with similar expression profiles
 Show ten genes similar (Pearson correlation) to BRCA1 Search

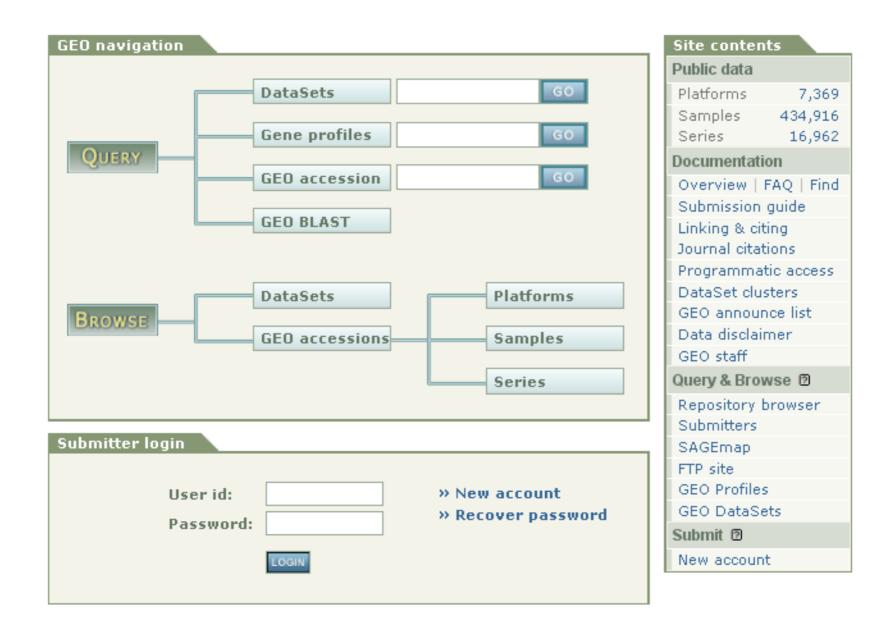
Experimental data can be

easily accessed.

Choose from top ten differentially expressed genes

Gene	Organism	Condition	Expression
M FAM32	A Homo sapiens	peripheral blood	↑ 2,48E-9
🗛 C16orf:	3 Homo sapiens	peripheral blood	↑ 1,8E-7
M DNASE	1 Homo sapiens	peripheral blood	↓ 3,09E-7
NBR2	Homo sapiens	peripheral blood	↓ 4,82E-6
📈 OR2F2	Homo sapiens	peripheral blood	↑1,13E-3
🗸 CEP170	) Homo sapiens	peripheral blood	↑1,14E-3
V PSG3	Homo sapiens	renal dysfunction without rejection	↑8,62E-3
M SH2D7	Homo sapiens	peripheral blood	↓ 2,04E-2
M PTGES:	Homo sapiens	well-functioning transplant	↑ 2,95E-2
CEBPD	Homo sapiens	peripheral blood	↑ 4,98E-2





## **Gene Expression Omnibus (GEO)**





GEO data are very clearly organized: platforms (GPL, types of chip) where samples (GPS) have been hybridized in series (GSE, the experiments).

table of processed

data columns)

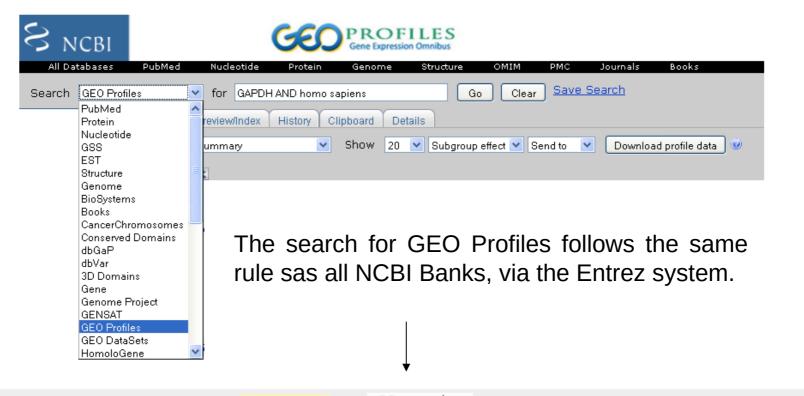
hybridization result (may optionally include raw

Original raw data file

Text description of the overall experiment

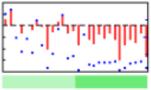


GEO curators continuously check the GSE series in order to verify wheter they can be combined (due to experimetal and technical reasons) into <u>dataset</u> (GDS), the heart of the GEO gene **profiles**, i.e. the expression level of genes across different conditions.



<b>1:</b> GDS1562 record   GPL2011 3797	[ Homo sapiens ]	] 28 samples	Profile Neighbors, Chromosome Neighbors, Sequence Neighbors, Homologs,

Annotation:	GAPDH: glyceraldehyde-3-phosphate dehydrogenase G3PD, GAPD, MGC88685



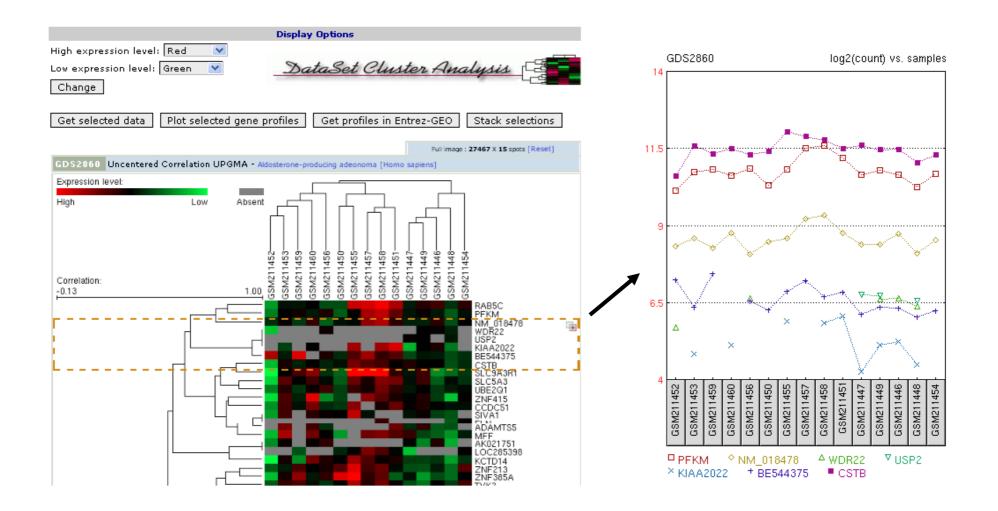
Reporter:

NM 002046

# **GEO: cluster analysis**

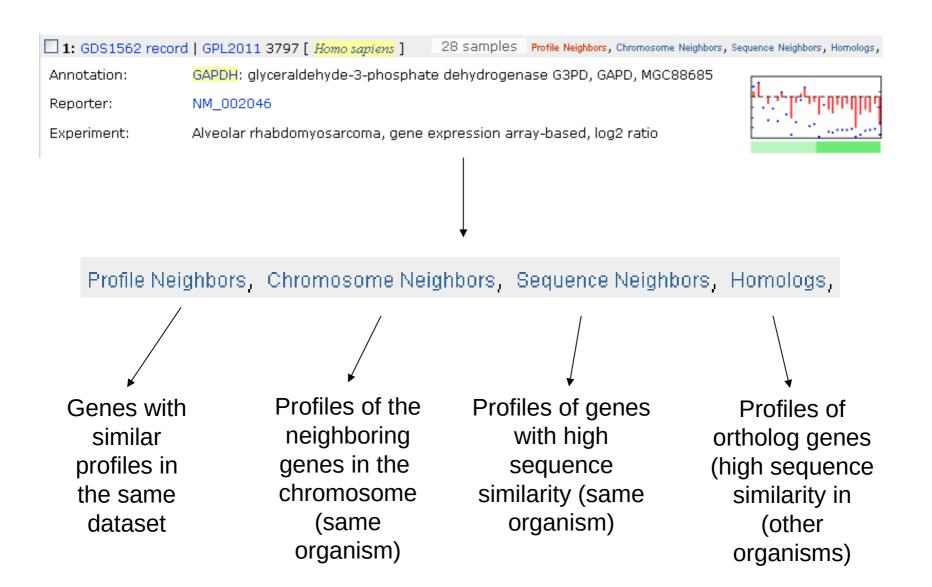


Microarray data, after background correction and normalization, can be analyzed in several multivariate ways, among which cluster analysis. Genes with similar profiles are precomputed in GEO.





The GEO systesm also extends the gene-based analysis by searching for **neighbours** in term of profile, sequence or position in the chromosome.



# **PRIDE: PRoteomics IDEntifications database**

This is the central repository for shotgun proteomics. Experiments are archived as in ArrayExpress and can be searched using filters and then download as raw or processd files.

#### PXD001874

#### 29 Search results + 2 filters

#### Filter your results

Current active filters

Remove all

#### Species:

Homo sapiens (Human)

Tissues:

liver

Human Hepatocyte Proteome Species: Homo sapiens (Human) Project description: Here we report a comprehensive proteomic analysis of purified hu <u>(More)</u> Tissues: <mark>liver</mark> Made public: 2016-01-26

🤉 Biological Dataset

## Project PXD001874

PRIDE ASSIGNED TAGS: @ Biological Dataset

NED TAGS. O Biological

### Summary

#### Title

X

**X** 

Human Hepatocyte Proteome

#### Description

Here we report a comprehensive proteomic analysis of purified human hepatocytes and a human hepatoma cell line HepG2. The complete dataset comprises 9,400 proteins and provides quantitative depiction of the proteomes of hepatocytes and HepG2 cells at the protein titer and copy number dimensions.

#### Sample Processing Protocol

Filter aided sample preparation (FASP), Strom anion exchemge (SAX), LC-MS/MS on QExactive mass spectrometers

#### Data Processing Protocol

Data analysis was performed using MaxQuant version 1.2.6.20 using Anromeda search engine.



4175 projects
58096 assays

Name	Size	HTTP Download
20120814_EXQ4_JRW_SA_B21_0_L1.raw	2,713.674 MB	速 Download
20120814_EXQ4_JRW_SA_B21_0_L2.raw	2,074.9 MB	🖄 Download
20120814_EXQ4_JRW_SA_B21_0_L3.raw	2,273.445 MB	🗄 Download
20120814_EXQ4_JRW_SA_B21_0_L4.raw	2,479.706 MB	🖄 Download
20120814_EXQ4_JRW_SA_B21_0_T1.raw	2,468.011 MB	🗄 Download
20120814_EXQ4_JRW_SA_B21_0_T2.raw	2,059.587 MB	🗄 Download
20120814_EXQ4_JRW_SA_B21_1_L1.raw	2,577.641 MB	🖄 Download
20120814_EXQ4_JRW_SA_B21_1_L2.raw	2,117.355 MB	🖄 Download
20120814_EXQ4_JRW_SA_B21_1_L3.raw	2,186.073 MB	🗄 Download
20120814_EXQ4_JRW_SA_B21_1_L4.raw	2,431.84 MB	🖄 Download
20120814_EXQ4_JRW_SA_B21_1_T1.raw	2,332.173 MB	速 Download
20120814_EXQ4_JRW_SA_B21_1_T2.raw	2,116.427 MB	🗄 Download

### Protein view

Page	e 1 2 3 4 5 .	2170		Show	ving 1-10 of 21698 results
#	Submitted Id	Assay	Curated Id	Cross Refs	Protein Description
▶ 1	1433B_HUMAN 🕎	34867	1433B_HUMAN	💭 <b>e</b>	14-3-3 protein beta/alpha (Protein 1054) (Protein kinase C inhibitor protein 1) (KCIP-1) More
2	2AAA_HUMAN 🕎	34867	2AAA_HUMAN	) <i>e</i>	Serine/threonine-protein phosphatase 2A 65 kDa regulatory subunit A alpha isoform More
3	A1AT_HUMAN	34867	A1AT_HUMAN	💭 <b>e</b>	Alpha-1-antitrypsin (Alpha-1 protease inhibitor) (Alpha-1-antiproteinase) (Serpin More
♦ 4	A1CF_HUMAN	34867	A1CF_HUMAN	)) <i>e</i> l	APOBEC1 complementation factor (APOBEC1- stimulating protein)
5	AAAS_HUMAN	34867	AAAS_HUMAN	)) <i>e</i> !	Aladin (Adracalin)
6	ABCD3_HUMAN	34867	ABCD3_HUMAN	) <i>e</i>	ATP-binding cassette sub-family D member 3 (70 kDa peroxisomal membrane protein) More
7	ABCE1_HUMAN	34867	ABCE1_HUMAN	💭 <b>e</b>	ATP-binding cassette sub-family E member 1 (2'-5'-oligoadenylate-binding protein) More
8	ABH15_HUMAN 🔝	34867	ABH15_HUMAN	)) <i>e</i> l	Abhydrolase domain-containing protein 15 (EC 3.1.1)
9	ACAD9_HUMAN	34867	ACAD9_HUMAN	i) e	Acyl-CoA dehydrogenase family member 9, mitochondrial (ACAD-9) (EC 1.3.99)
▶ 10	ACADV_HUMAN	34867	ACADV_HUMAN	) <i>e</i>	Very long-chain specific acyl-CoA dehydrogenase, mitochondrial (VLCAD) (EC More

Experiments can be accessed as raw machine files (gigabytes of data, actually) or in processed forms, displaying the assignment (e.g. via Mascot) of peptides and the corresponding proteins, as the result of a mass fingerprint.

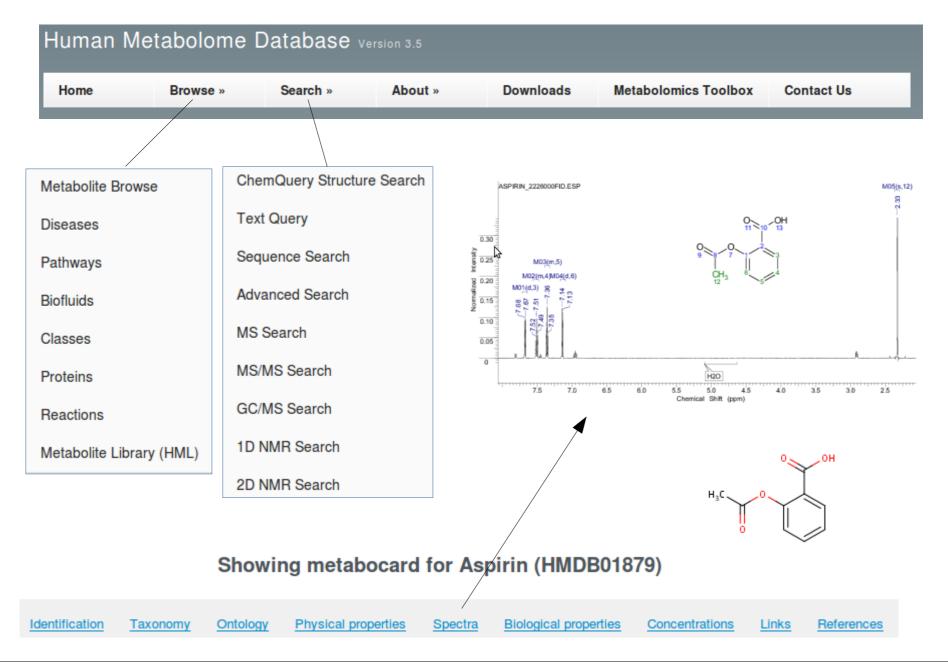
### Peptide view

Page	e 1 2 3 4 5 22	254	Sho	wing 1 - 10 of 222531	results
#	Peptide Sequence	Submitted Id	Assay	Search Engine Score	Experimental m/z
▶ 1	ETGVDLTK	GRP75_HUMAN	34843	<ul> <li>Mascot score 46.0</li> </ul>	431.72641
▶ 2	ETGVDLTK	GRP75_HUMAN	34843	<ul> <li>Mascot score 44.1</li> </ul>	431.72723
▶ 3	LFEMAYK	GRP75_HUMAN	34843	Mascot score 33.82	459.222
▶ 4	LFEMAYK	GRP75_HUMAN	34843	o Mascot score 35.05	459.22402
▶ 5	VLENAEGAR	GRP75_HUMAN	34843	<ul> <li>Mascot score 55.8</li> </ul>	479.74793
▶ 6	VLENAEGAR	GRP75_HUMAN	34843	Mascot score 55.75	479.74931
▶ 7	DDIENMVK	GRP75_HUMAN	34843	Mascot score 33.52	482.22351
▶ 8	VLENAEGAR	GRP75_HUMAN	34843	Mascot score 79.16	482.75868
▶ 9	VLENAEGAR	GRP75_HUMAN	34843	Mascot score 73.2	482.75954
▶ 10	VLENAEGAR	GRP75_HUMAN	34843	• Mascot score 74.75	484.75259

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## **MetaboLights**

MetaboLights is a general purpose, open access repository for metabolomics studies, their raw experimental data and associated metadata. As all EBI repositories, it is highly interactive and allow to browse data by

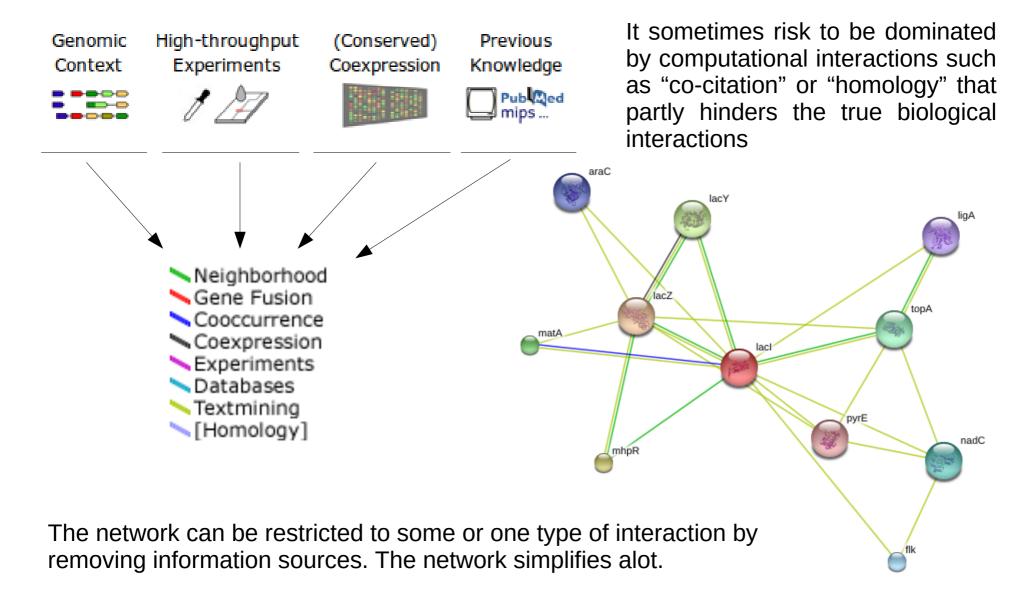
### Data in MetaboLights

Total number of studies	279
- Public	154
- in Review	16
- in Curation	16
- in Submission	93
Different organisms	2056
Reference compounds	18509
Total study size (TB)	3.87
<ul> <li>Max study size (GB)</li> </ul>	712.33
<ul> <li>Average study size (GB)</li> </ul>	13.86
<ul> <li>Median study size (GB)</li> </ul>	1.15

Browse Studies	Browse Compounds	Browse Species

Filter your results	31 results, showing 1 to 10	<pre>« &lt; Page 1 of 4 &gt; &gt;&gt;</pre>	
Туре	Automated Label-free Quantification of Metabolites from Liquid Chromatography-Mass Spectrometry Data (Plasma)		
Study	Validations Status: 🔘 🖉 🖲		
compound	Release date: 16-Dec-2015		
Technology	Organism		
mass spectrometry	<ul> <li>Homo sapiens</li> </ul>		
NMR spectroscopy	Study Factors	Study identifier: MTBLS234	
Organism	<ul> <li>spike-in concentration</li> <li>replicate</li> </ul>	Total Study size: 2.45GB Submitted by	
Find your Organism		Erhan Kenar	
🥑 Homo sapiens	8		

The interactions include direct (physical) and indirect (functional) associations and are derived from four several experimental or computational sources.



STRING