

# *Ontologies and ontology-based data analysis*

*Rob Hoehndorf and Paul Schofield*



Thanks to Michel Dumontier Mark Musen and Ian Horrocks for generous slide sharing

# *Overview*

- General introduction
- Ontologies and the semantic web
- Ontologeis and graphs
- Semantic similarity
- Machine learning and ontologies
- Applications

# *The problems with biological data*

- Recorded mainly in natural language. E.g. mutant phenotypes
  - Language uses symbols and rules (natural language) to communicate knowledge
  - Expressive
  - Semantically ambiguous
  - Hard to compute on
- Computational language
  - Precise
  - Less expressive
  - Allows grouping and data exploration
- Why do we need to compute?
  - Database searching, query extension
  - Data/Literature mining
  - Knowledge transfer between databases and analytical packages
  - Complex queries
  - Data integration
  - Reasoning
  - Machine learning

# *The naming of things...*

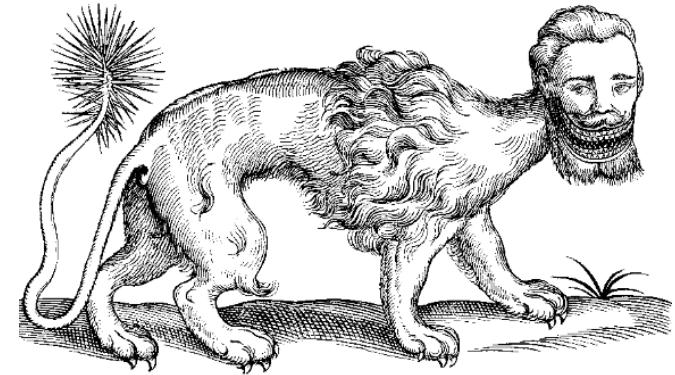
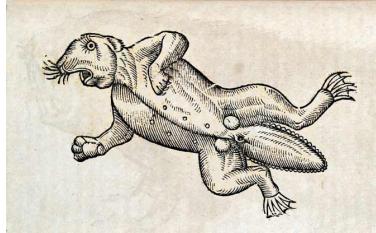
- Naming and classification are essential for the capture and use of knowledge about the world.
- Names (labels) are a common reference that can be used by everyone to refer to the same entity
- Labels can be attached to many things
  - Physical entities in the real world
  - Concepts
  - Processes
  - Qualities
  - Relationships



Now... *that* should clear up a few things around here

# Classification systems

1. those that belong to the Emperor,
2. embalmed ones,
3. those that are trained,
4. suckling pigs,
5. mermaids,
6. fabulous ones,
7. stray dogs,
8. those included in the present classification,
9. those that tremble as if they were mad,
10. innumerable ones,
11. those drawn with a very fine camelhair brush,
12. others,
13. those that have just broken a flower vase,
14. those that from a long way off look like flies.



*Do you mean what you say...or do you say what you mean?*

OMIM Query	# Records
"large bone"	785
"enlarged bone"	156
"big bone"	16
"huge bones"	4
"massive bones"	28
"hyperplastic bones"	12
"hyperplastic bone"	40
"bone hyperplasia"	134
"increased bone growth"	612



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An Online Catalog of Human Genes and Genetic Disorders  
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# *Lessons*

- Systematic, meaningful and unambiguous nomenclature is important in handling concepts
- The definitions of terms is as important, if not more so, than the terms themselves

# Applied Ontology

- Builds on philosophy, cognitive science, linguistics and logic with the purpose of understanding, clarifying, making explicit and communicating people's assumptions about the nature and structure of the world
- Orientation towards helping people understand each other
- Distinguishes applied ontology from philosophical ontology, and motivates its unavoidable interdisciplinary nature
- Ontological analysis: study of content (of these assumptions) as such (independently of their representation)

# *What is an ontology?*

- Gruber: “A specification of a conceptualization of a domain”
- Studer: An ontology is a formal, explicit specification of a shared conceptualization”
- Guarino: An ontology is a logical theory accounting for the intended meaning of a formal vocabulary, i.e. its ontological commitment to a particular conceptualization of the world. The intended models of a logical language using such a vocabulary are constrained by its ontological commitment. An ontology indirectly reflects this commitment (and the underlying conceptualization) by approximating these intended models.”
- Horrocks: an ontology [is] equivalent to a Description Logic knowledge base

# *What is a conceptualisation?*

- Formal structure of (a piece of) reality as perceived and organized by an agent, independently of:
  - the vocabulary used
  - the actual occurrence of a specific situation
- Different situations involving the same objects, described by different vocabularies, may share the same conceptualization
  - Language 1: Apple
  - Language 2: تفاحة



# *What is an ontology?*

- An ontology is a CS artefact consisting of:
  - A **vocabulary** used to describe (a particular view of) some domain
  - An **explicit specification** of the **intended meaning** of the vocabulary.
    - Often includes classification-based information
  - Contains **categories and relations** describing the nature and structure of a domain of discourse
  - Logical constraints capturing **background knowledge** about the domain
    - Adult\_Elephants weigh at least 2,000 kg
    - All Elephants are either African\_Elephants or Indian\_Elephants
    - No individual can be both a Herbivore and a Carnivore
- Ideally, an ontology should:
  - Capture a **shared understanding** of a domain of discourse
  - Provide a **formal and machine-manipulatable** model

# *Ontologies vs classifications*

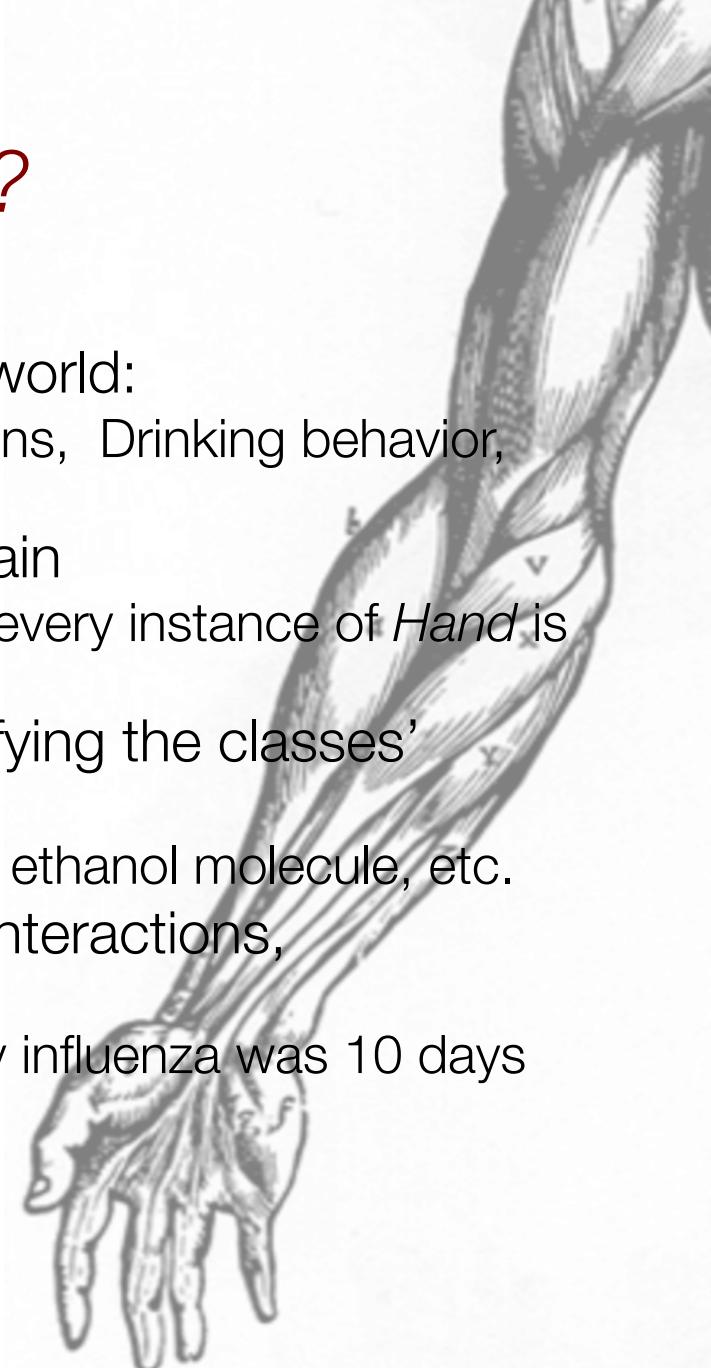
- **Classifications** focus on:
  - access, based on pre-determined criteria (encoded by syntactic keys)
- **Ontologies** focus on:
  - meaning of terms
  - nature and structure of a domain



Now... *that* should clear up a few things around here

# *What do ontologies comprise?*

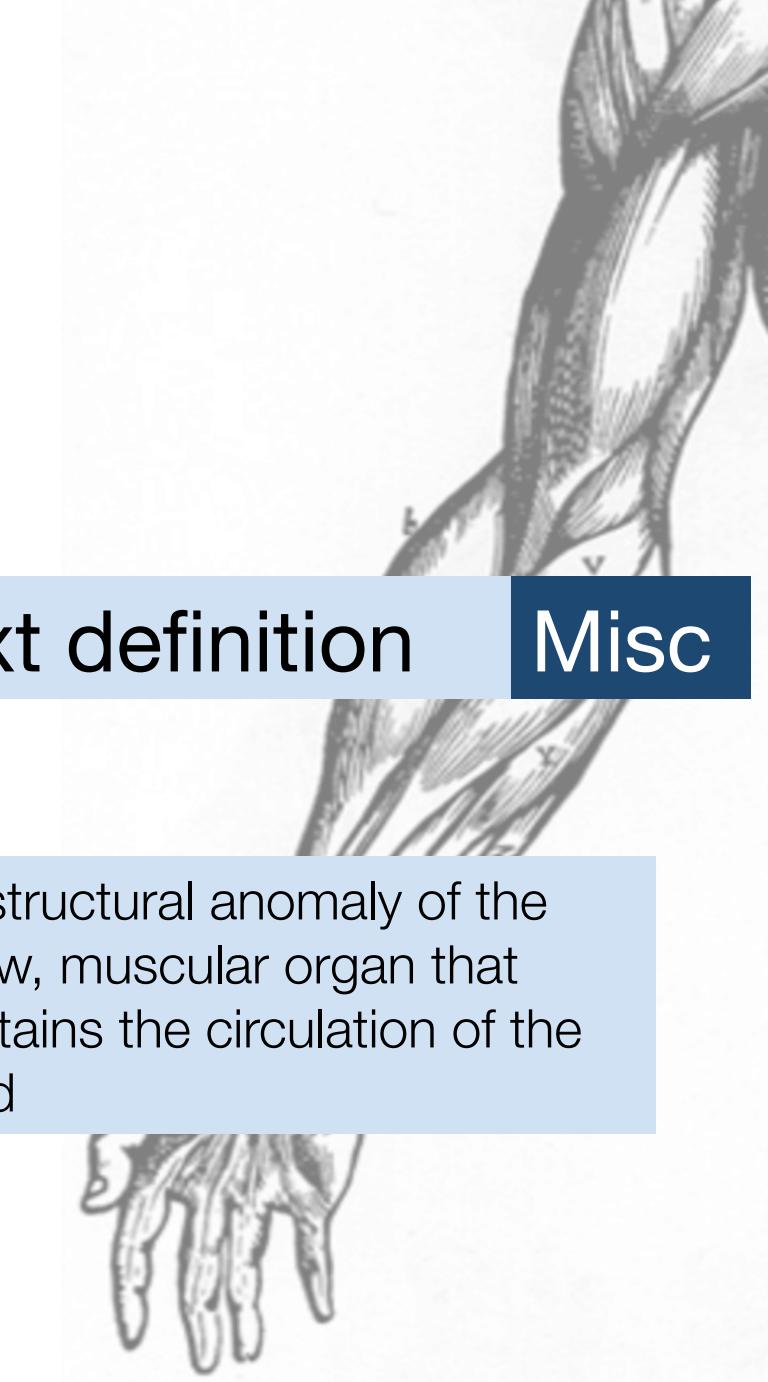
- **Classes** represent kinds of things in the world:
  - Arm, Apoptosis, Influenza, Homo sapiens, Drinking behavior, Membrane
- **Axioms** specify our knowledge of a domain
  - ie statements considered to be true. eg. every instance of *Hand* is a *part\_of* an instance of an *arm*
- **Instances of classes** are individuals satisfying the classes' intension
  - my arm, the influenza I had last year, one ethanol molecule, etc.
- Relations between instances arise from interactions, configurations, etc., of individuals
  - my arm is *part\_of* me, the *duration\_of* my influenza was 10 days



# *Specification of a class*

Class Label	Class ID	Text definition	Misc
Abnormal heart morphology	MP: 0000266	any structural anomaly of the hollow, muscular organ that maintains the circulation of the blood	

Namespace



# Ontologies as graphs

Ontology  $\mathcal{O}$

Graph  $G = (V, E)$

$V := \text{classes}(\mathcal{O})$

If class  $C_1$  SubClassOf  $C_2$ , create edge  $\text{isa}(C_1, C_2)$

How about other edges?

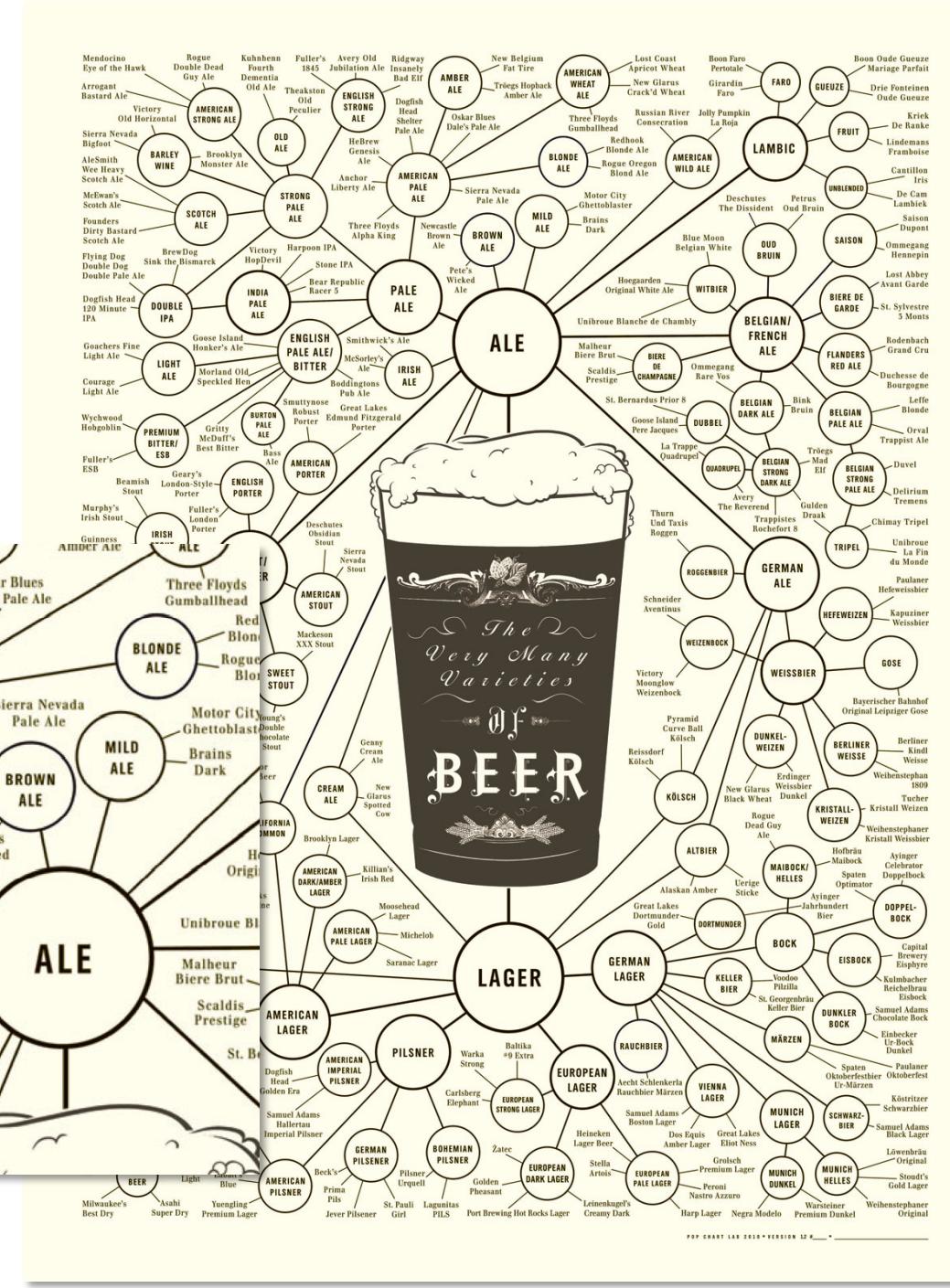
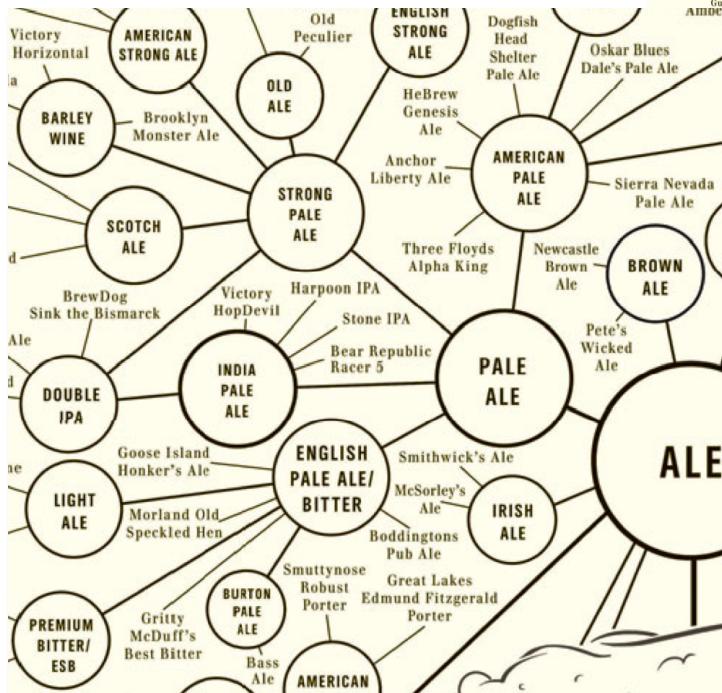
OBO Relation Ontology: relations are patterns

- PartOf:  $\text{PartOf}(X, Y) \iff X \text{SubClassOf} : \text{partOfsome}Y$

Generate an edge labeled  $R$  between  $X$  and  $Y$  iff

$\mathcal{O} \models R(X, Y)$ , i.e., if the statement defined by the relational pattern  $R$  is made true for classes  $X$  and  $Y$ .

# Beer ontology



# *Examples of bioontologies*

- GO
  - An ontology for describing the function of genes and gene products
- HPO
  - A structured and controlled vocabulary for the phenotypic features encountered in human hereditary and other disease.
- MA
  - A structured controlled vocabulary of the adult anatomy of the mouse (*Mus*)
- ENVO
  - Ontology of environmental features and habitats
- DO
  - An ontology for describing the classification of human diseases organized by etiology
- SO
  - A structured controlled vocabulary for sequence annotation, for the exchange of annotation data and for the description of sequence objects in databases.
- RO
  - Relationship types shared across multiple ontologies

## Gene Ontology

An ontology for describing the function of genes and gene products

[OntoBee](#) [AberOWL](#) [OLS](#) [AmiGO](#)

The goal of the GeneOntology (GO) project is to provide a uniform way to describe the functions of gene products from organisms across all kingdoms of life and thereby enable analysis of genomic data

### Products

[go.owl](#)

[go/extensions/go-plus.owl](#) GO-Plus The core ontology plus axioms connecting to select external ontologies

[go/extensions/go-taxon-groupings.owl](#) GO Taxon Groupings Classes added to ncbitaxon for groupings such as prokaryotes

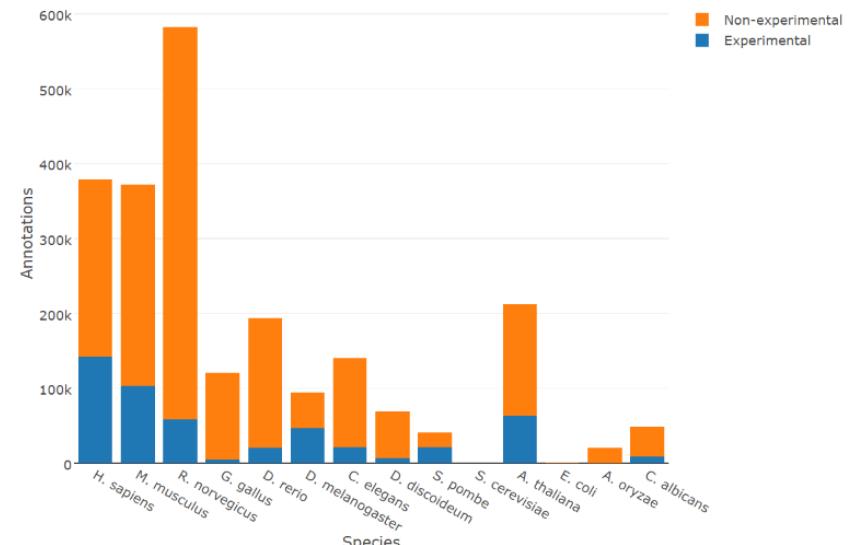
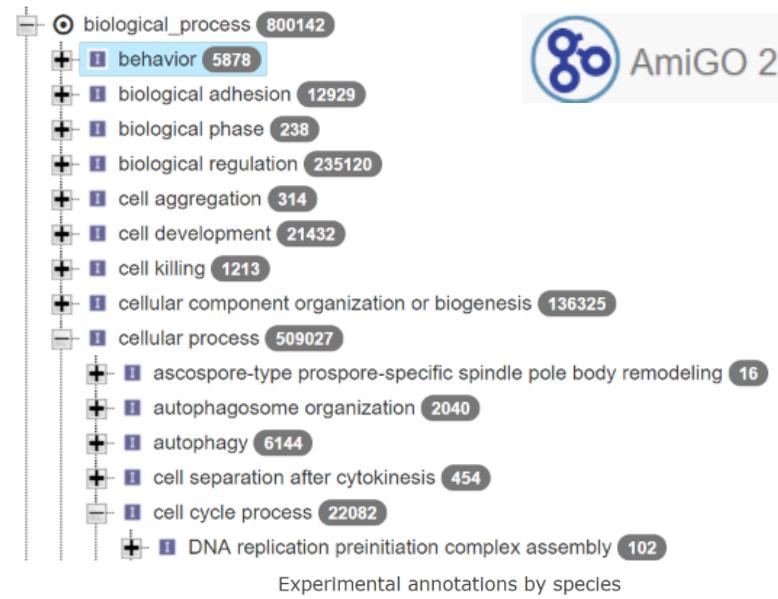
# Gene Ontology

Arguably one of the most successful ontology projects in the life sciences.

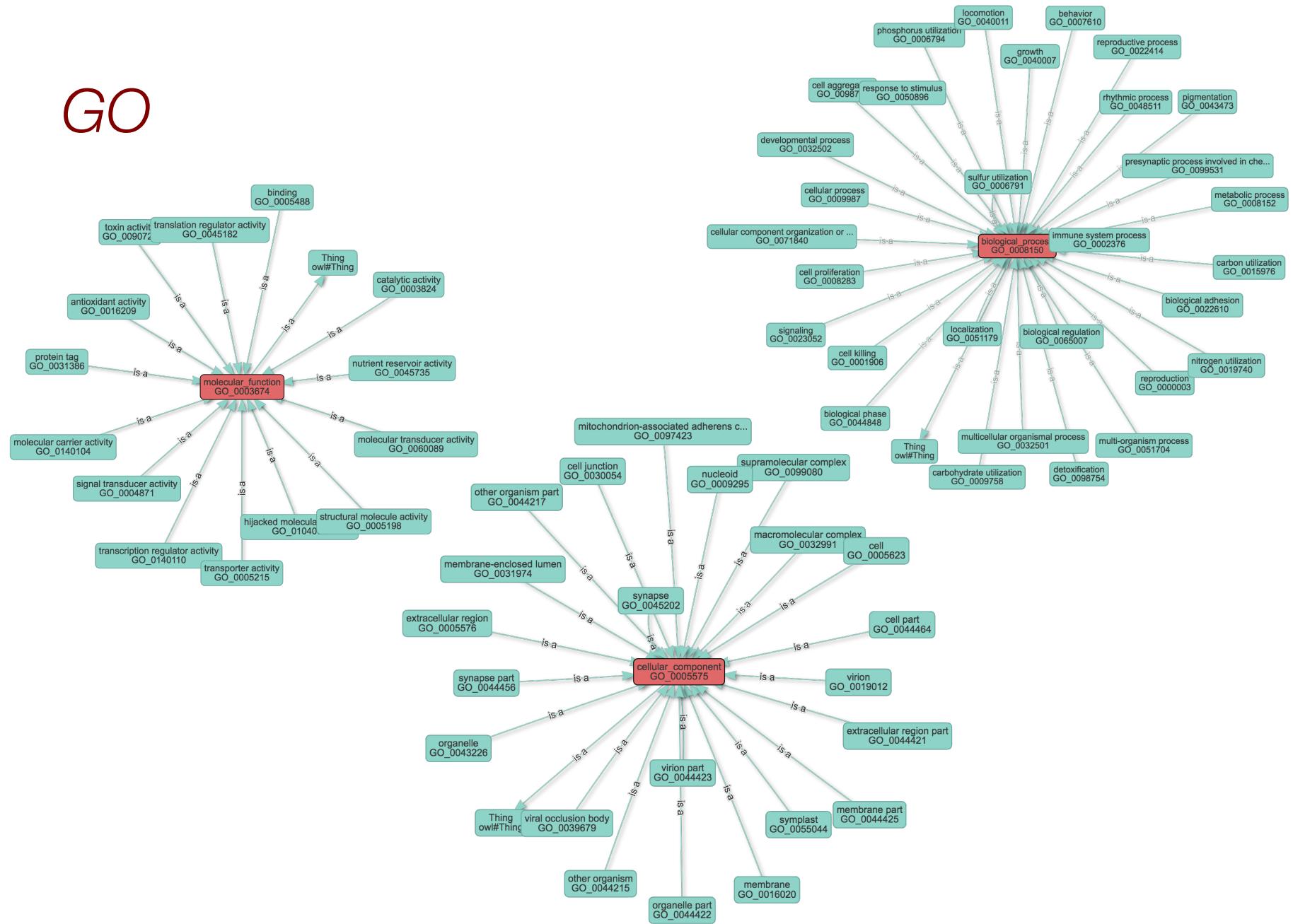
Millions of annotations on hundreds of thousands of genes using GO terms.

The GO defines types used to describe gene function. It classifies functions along three aspects:

- cellular component
  - where gene products operate
- molecular function
  - what gene products do
- biological process
  - The pathways and processes that gene products participate in



# GO



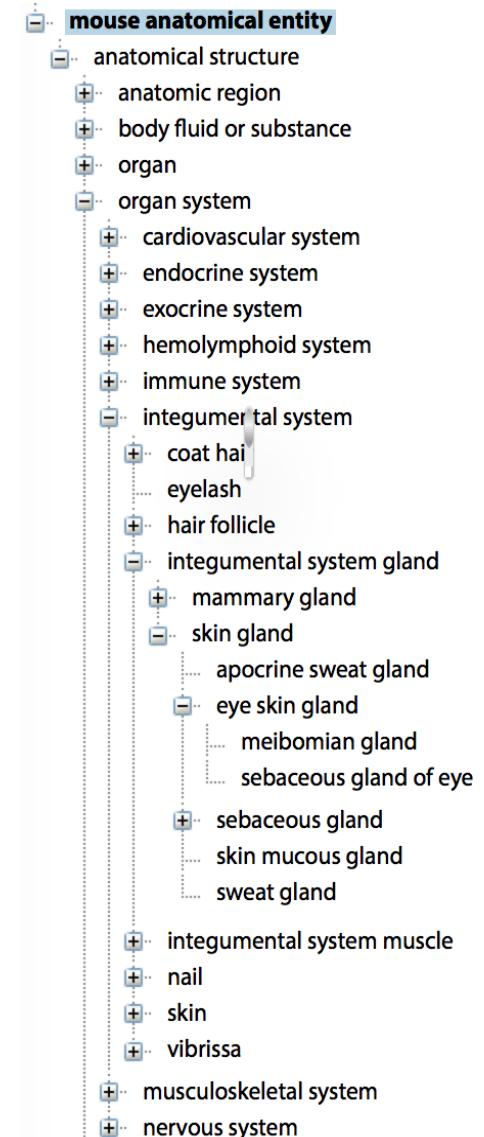
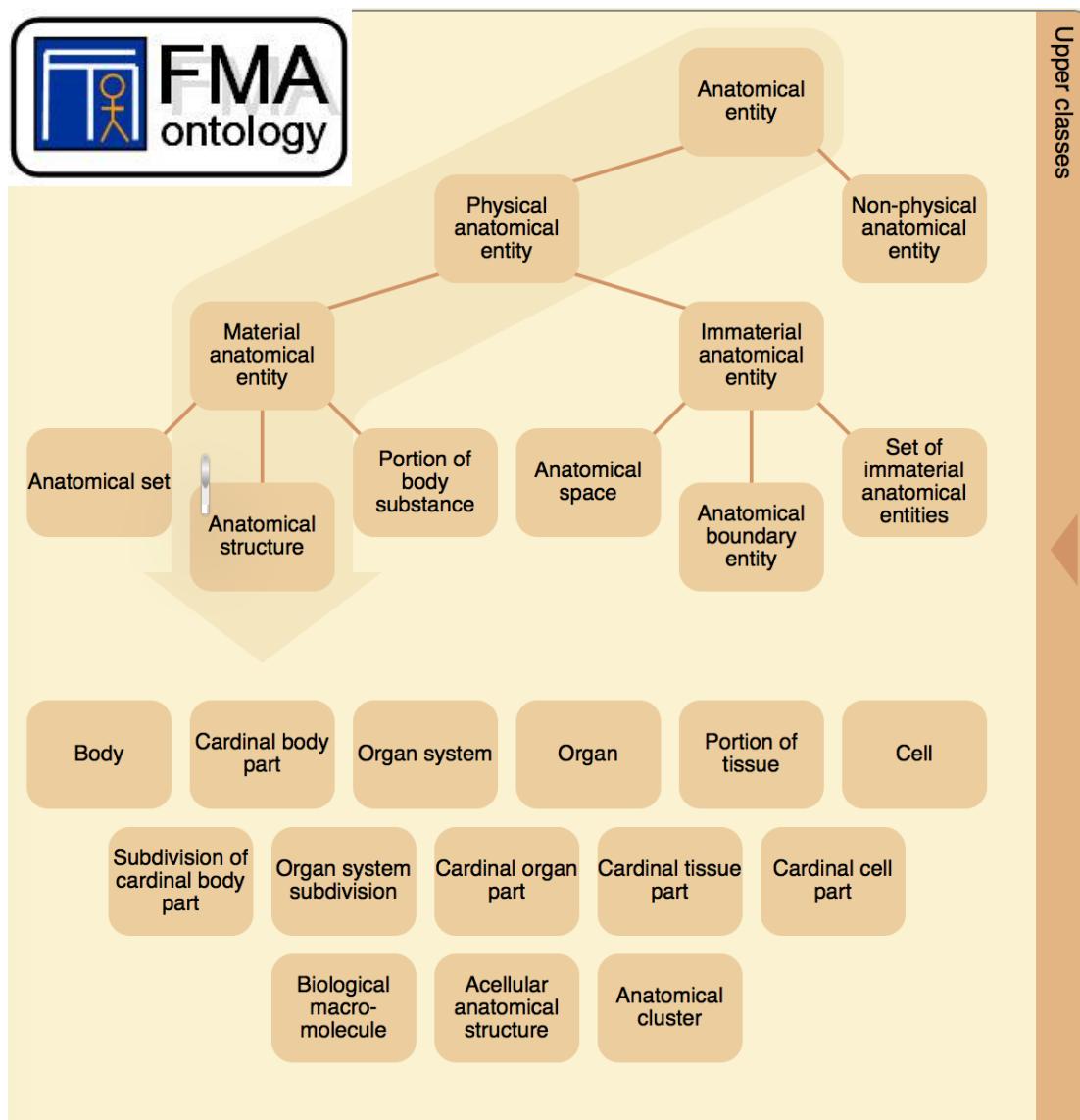
# *Main ontologies for diseases and phenotypes*

- Mammalian Pathology (MPATH)
  - 900 terms
  - mapped to other terminologies
  - describes pathological lesions and processes
- Disease Ontology (DO)
  - About 9000 terms
  - Semantically mapped to major terminologies, UMLS, MeSH, ICD10 etc.
- Experimental Factor ontology (EFO)
  - “application ontology” 18596 terms
  - Imports classes from other phenotype and related ontologies (MIREOT)
- Orphanet Ontology (ORDO)
  - 13105 terms
  - structured vocabulary for rare diseases capturing relationships between diseases, genes and other relevant features
- Human Phenotype Ontology ( HPO )
  - 15, 319 terms
  - derived from OMIM clinical synopses
- Mammalian Phenotype Ontology (MP)
  - 11, 720 classes
  - Used by MGI for annotating mutant strains from literature
  - Used by IMPC for annotating phenotyping pipeline
- Unified Medical Language System (UMLS)
  - US National Library of Medicine
  - terminology, classification and coding standards
  - 8M normalised concepts
- SNOMED-CT
  - 321,000 classes
  - clinical terminology
  - diseases diagnostics and procedures
  - proprietary
- NCI thesaurus
  - 119,000 classes
  - vocabulary for clinical care, translational and basic research, and public information and administrative activities.
- LOINC
  - medical diagnostics and observations
  - 180, 000 classes
- ICD-10
  - 12,450 classes
  - disease, epidemiology, billing
  - soon to be replaced with ICD-11

# Current anatomy ontologies

Ontology	Domain and applicability	Class count	Object Properties Count	Axioms count	Text definitions Count	Computable definitions Count	Text definitions %	Computable definitions %
Uberon	Animalia	14773	150	226887	11229	5190	76.01%	35.13%
FMA	Homo sapiens (A)	78977	7	484774	1118	0	1.42%	None
EHDAA2	Homo sapiens (AE)	2734	9	24773	234	0	8.56%	None
MA	Mus (A)	3257	1	19591	0	0	None	None
EMAPA	Mus (E)	6239	9	54307	77	0	1.23%	None
ZFA	Danio rerio (zebrafish) (AE)	3147	8	35497	2528	0	80.33%	*None
TAO	Teleosti (bony fishes) (AE)	3372	19	24109	1988	20	58.96%	0.59%
XAO	Xenopus (frog) (AE)	1521	6	16840	1492	0	98.09%	None
AAO	Amphibia (A)	1603	34	7846	0	0	None	None
FBbt	Drosophila (fruitfly) (AE)	9951	46	115964	9072	2767	91.17%	27.81%
WBbt	C. elegans (nematode) (AE)	7601	6	56114	6551	11	86.19%	0.14%

# Anatomy ontologies



# Where to find ontologies

- BioPortal: <https://bioportal.bioontology.org/>
- Ontology Lookup Service: <https://www.ebi.ac.uk/ols/>
- OntoBee: <http://www.ontobee.org/>
- AberOWL: <http://aber-owl.net>
- OBO Foundry: <http://www.obofoundry.org/>
- AgroPortal: <http://agroportal.lirmm.fr/>



Browse Ontologies

Add New Ontology

About

## AberOWL ontology repository and semantic search engine

Type any term or phrase to search the AberOWL ontology repository for a class that is described using the phrase (try [pancreas](#), [PATO:0001234](#), [sugar binding GO](#)), for ontologies that use the phrase in their description (try [integrated upper ontology](#), [infectious disease](#), [GFO](#) or [pathology](#)), or perform a Description Logic query across all ontologies in AberOWL (try [part of](#) some 'apoptotic process' and regulates some 'apoptotic process'):

Search

Query

Welcome to the EMBL-EBI Ontology Lookup Service.

Search OLS... Examples: diabetes, GO:0098743 Looking for a particular ontology?

About OLS Related Tools

### About OLS

The Ontology Lookup Service (OLS) is a repository for biomedical ontologies that aims to provide a single point of access.

Login Register

### Related Tools

In addition to OLS the SPOT team also provides [Zooma](#), a service to assist in mapping data to ontologies in OLS and [Webulous](#), a tool for building ontologies from spreadsheets. Also, look out in the new year for our new Ontology mapping service that will assist you in mapping between different but related ontologies.

### Contact Us

For feedback, enquiries or suggestion about OLS or to request a new ontology please contact [ols-support @ ebi.ac.uk](mailto:ols-support@ebi.ac.uk). For bugs or problems with the code or API please report on [GitHub](#) issue For announcements relating to OLS, such as new releases and new features sign up to the [OLS announce mailing list](#).

## *Exercise*

Find the Gene Ontology in BioPortal, OLS, or AberOWL

Find the GO-PLUS ontology in AberOWL

Find the Mammalian Phenotype (MP) ontology

Find the class “B cell apoptotic process” in GO (or GO-PLUS); what are its identifiers?

Find all the axioms pertaining to “B cell apoptotic process”

Find the class “decreased B cell apoptosis” in the MP; what are its identifiers and all the axioms?

# *Main applications of ontologies in biomedical data*

- Annotation of genes, genetic variants
  - OMIM, Orphanet, GWAS Catalog, Mouse Genome Informatics, Zfin, CLINVAR,
- Annotation of disease entities
  - OMIM, ORPHANET, Human Phenotype database (HPO), Aber-OWL-disease
- Ontology-based classification
  - Multi-modal learning
  - Neuro-symbolic systems
- Data recovery, integration and analysis
  - Literature, Electronic medical records and databases
  - Natural language processing and text mining
- Patient/animal data capture
  - *Phenotips/Phenome central*
  - International Mouse Phenotyping Consortium (IMPC)
  - Mouse Genome Informatics (MGI)
- Genome-Phenome relationships
  - Overrepresentation analysis of phenotypes on patient or animal cohorts
  - Correlation between variants and phenomes, eg in CNV analysis
  - Establishment of disease similarity, phenotype modularity, network identity, through constituent phenotypes.



# *What is an annotation?*

- Attribution of a property defined by an ontology class, to an entity
- Can be manually asserted, inferred electronically from annotations to similar or related entities etc.
- Can be inferred from the structure of an ontology
- Is usually maintained within a database, ie a dataset of annotations to specific entities

# *GO annotations*

A GO annotation is a statement about the function of a particular gene. Each GO annotation consists of an association between a gene and a GO term. ... Evidence is presented in the form of a GO 'evidence code' and either a published reference or description of the methodology used to create the annotation. <http://amigo.geneontology.org/amigo>

## Evidence codes

- Experimental Evidence codes
- High Throughput (HTP) evidence codes
- Computational Analysis evidence codes
- Author statement evidence codes
- Curator statement evidence codes
- Electronic Annotation evidence code

## Experimental evidence codes

- Inferred from Experiment (EXP)
- Inferred from Direct Assay (IDA)
- Inferred from Physical Interaction (IPI)
- Inferred from Mutant Phenotype (IMP)
- Inferred from Genetic Interaction (IGI)
- Inferred from Expression Pattern (IEP)

# GO annotation to *Mus musculus* IGF2

	Gene/product name	Annotation qualifier	GO class (direct)	Annotation extension	Contributor	Organism	Evidence	Evidence with	PANTHER family	Type	Isoform	Reference	Date
<input type="checkbox"/>	<a href="#">Igf2</a>	insulin-like growth factor 2	positive regulation of protein phosphorylation		BHF-UCL	Mus musculus	IMP		family not named pthr46886	protein		MGIdMGI:4438697 PMID:20032056	20110420
<input type="checkbox"/>	<a href="#">Igf2</a>	insulin-like growth factor 2	insulin receptor binding		MGI	Mus musculus	ISO	UniProtKB:P01344	family not named pthr46886	protein		GO_REF:0000096 MGI:MGI:4834177	20080606
<input type="checkbox"/>	<a href="#">Igf2</a>	insulin-like growth factor 2	insulin-like growth factor receptor binding		MGI	Mus musculus	ISO	UniProtKB:P01344	family not named pthr46886	protein		GO_REF:0000096 MGI:MGI:4834177	20150522
<input type="checkbox"/>	<a href="#">Igf2</a>	insulin-like growth factor 2	insulin-like growth factor receptor binding		MGI	Mus musculus	IPI	UniProtKB:Q07113	family not named pthr46886	protein		MGIdMGI:2679358 PMID:14566968	20041029

# GAF – GO annotation file format

## Annotation File Fields

The annotation flat file format is comprised of 17 tab-delimited fields.

Column	Content	Required?	Cardinality	Example
1	DB required	1	UniProtKB	
2	DB Object ID required	1	P12345	
3	DB Object Symbol required	1	PHO3	
4	Qualifier optional	0 or greater	NOT	
5	GO ID required	1	GO:0003993	
6	DB:Reference ( DB:Reference) required	1 or greater	PMID:2676709	
7	Evidence Code required	1	IMP	
8	With (or) From optional	0 or greater	GO:0000346	
9	Aspect required	1	F	
10	DB Object Name optional	0 or 1	Toll-like receptor 4	
11	DB Object Synonym ( Synonym)	optional	0 or greater	hToll Tollbooth
12	DB Object Type required	1	protein	
13	Taxon( taxon) required	1 or 2	taxon:9606	
14	Date required	1	20090118	
15	Assigned By required	1	SGD	
16	Annotation Extension	optional	0 or greater	part_of(CL:0000576)
17	Gene Product Form ID	optional	0 or 1	UniProtKB:P12345-2

# Annotation of mouse mutants

## Mammalian Phenotype Browser

**MGI**  
About | Help | FAQ  
Home | Contact  
Search | Download | More Resources | Submit  
  
Export: Excel File  
  
Allelic Composition  
Genetic Background  
  
[Igf2<sup>tm1.1Sson</sup>/Igf2<sup>+</sup>](#)  
involves: BALB/c \* C57BL/6  
  
[Igf2<sup>tm1Rob</sup>/Igf2<sup>+</sup>](#)  
involves: 129/Sv \* 129P2/OlaHsd \* 129S/S  
  
[Igf2<sup>tm1Rob</sup>/Igf2<sup>+</sup>](#)  
involves: 129S/SvEv  
  
[Igf2<sup>tm1Rob</sup>/Igf2<sup>+</sup>](#)  
involves: 129S/SvEv \* BALB/c  
  
[Igf2<sup>tm1Rob</sup>/Igf2<sup>+</sup>](#)  
involves: 129S/SvEv \* C57BL/6 \* DBA/2J  
  
  

Carbohydrate derivative binding  
Cytoskeletal protein binding  
DNA binding  
Enzyme regulator  
Hydrolyse  
Lipid binding  
Oxidoreductase  
Signaling

Click cells to view annotations.

### Phenotype Term Detail

Term: **delayed bone ossification**  
Definition: late onset of the formation of bone  
Parent Terms: [is-a abnormal bone ossification](#)  
ID: MP:0000060

### Phenotype Tree View

- ▶ I skeleton phenotype
  - ▶ I abnormal skeleton morphology
  - ▶ I abnormal skeleton physiology
    - ... I abnormal bone healing
    - ▶ I abnormal bone ossification
      - ▶ I abnormal bone mineralization
      - ▶ I abnormal endochondral bone ossification
      - ▶ I abnormal intramembranous bone ossification
      - ▶ I abnormal ossification involved in bone maturation
      - ... I abnormal ossification involved in bone remodeling
      - ... I decreased bone ossification
    - ▶ I **delayed bone ossification** (237 genotypes, 286 annotations)
      - ... I delayed endochondral bone ossification
      - ... I delayed intramembranous bone ossification
      - ... I failure of bone ossification
      - ... I increased bone ossification
      - ... I premature bone ossification
      - ... I abnormal bone remodeling
      - ... I abnormal bone stiffness
      - ... I abnormal bone strength
      - ... I abnormal chondrocyte physiology

Reference

[J:15108](#), [J:25091](#), [J:75054](#)

# Phenotype reports

Rb1<tm1Tyj>/Rb1<tm1Tyj>	Rb1<tm1Tyj>	MGI:1857242	involves:	129S2/SvPas	MP:0000600	12529408	MGI:97874	MGI:2166359
Rb1<tm1Tyj>/Rb1<tm1Tyj>	Rb1<tm1Tyj>	MGI:1857242	involves:	129S2/SvPas	MP:0001716	16449662	MGI:97874	MGI:2166359
Rb1<tm1Tyj>/Rb1<tm1Tyj>	Rb1<tm1Tyj>	MGI:1857242	involves:	129S2/SvPas	MP:0001698	16449662	MGI:97874	MGI:2166359
Rb1<tm1Tyj>/Rb1<tm1Tyj>	Rb1<tm1Tyj>	MGI:1857242	involves:	129S2/SvPas	MP:0001092	16449662	MGI:97874	MGI:2166359
Rb1<tm1Tyj>/Rb1<tm1Tyj>	Rb1<tm1Tyj>	MGI:1857242	involves:	129S2/SvPas	MP:0000961	16449662	MGI:97874	MGI:2166359
Rb1<tm1Tyj>/Rb1<tm1Tyj>	Rb1<tm1Tyj>	MGI:1857242	involves:	129S2/SvPas	MP:0000245	16449662	MGI:97874	MGI:2166359
Rb1<tm1Tyj>/Rb1<tm1Tyj>	Rb1<tm1Tyj>	MGI:1857242	involves:	129S2/SvPas	MP:0000828	16449662	MGI:97874	MGI:2166359
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Rb1<tm1Tyj>/Rb1<tm1Tyj>	Rb1<tm1Tyj>	MGI:1857242	involves:	129S2/SvPas	MP:0005039	12529408	MGI:97874	MGI:2166359
Rb1<tm1Tyj>/Rb1<tm1Tyj>	Rb1<tm1Tyj>	MGI:1857242	involves:	129S2/SvPas	MP:0002840	16449662	MGI:97874	MGI:2166359
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Rb1<tm1Tyj>/Rb1<tm1Tyj>	Rb1<tm1Tyj>	MGI:1857242	involves:	129S2/SvPas	MP:0009937	12529408	MGI:97874	MGI:2166359
Rb1<tm1Tyj>/Rb1<tm1Tyj>	Rb1<tm1Tyj>	MGI:1857242	involves:	129S2/SvPas	MP:0011098	16449662	MGI:97874	MGI:2166359
Rb1<tm1Tyj>/Rb1<tm1Tyj>	Rb1<tm1Tyj>	MGI:1857242	involves:	129S2/SvPas	MP:0011703	16449662	MGI:97874	MGI:2166359

[http://www.informatics.jax.org/downloads/reports/MGI\\_GenePheno.rpt](http://www.informatics.jax.org/downloads/reports/MGI_GenePheno.rpt)



## *Exercise*

Use AmiGO and find all gene products in humans associated with “B cell apoptotic process”; notice the difference between “direct” and “indirect” annotations!

<http://amigo.geneontology.org/amigo>

Download GO annotations in mouse (<http://www.informatics.jax.org/downloads/reports/index.html>, gene association.mgi.gz) and find all gene products associated with “B cell apoptotic process”

- Notice the identifiers
- How can you get “indirect” annotations?