

# Project Design

Genome 559: Introduction to Statistical and  
Computational Genomics

**Elhanan Borenstein**

# Hypothesis:

The average degree in the metabolic networks of Prokaryotes is higher than the average degree in the metabolic networks of Eukaryotes

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## KEGG: Kyoto Encyclopedia of Genes and Genomes

KEGG is a database resource for understanding high-level functions and utilities of the biological system, such as the cell, the organism and the ecosystem, from molecular-level information, especially large-scale molecular datasets generated by genome sequencing and other high-throughput experimental technologies (See [Release notes](#) for new and updated features).

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**Entry point for wider society**

**KEGG MEDICUS**    [Health-related information resource](#)

**Organism-specific entry points**

**KEGG Organisms**    Enter org code(s)   [hsa](#) [hsa eco](#)



## KEGG Organisms: Complete Genomes

Eukaryotes: 180   Bacteria: 2149   Archaea: 149

[ [Genomes](#) | [Draft](#) | [ESTs](#) | [Meta](#) | [Pan](#) ]

### Eukaryotes

Category	Species	Source	
Vertebrates	hsa Homo sapiens (human)	RefSeq	
	ptr Pan troglodytes (chimpanzee)	RefSeq	
	pps Pan paniscus (bonobo)	RefSeq	
	ggo Gorilla gorilla gorilla (western lowland gorilla)	RefSeq	
	pon Pongo abelii (Sumatran orangutan)	RefSeq	
	mcc Macaca mulatta (rhesus monkey)	RefSeq	
	mmu Mus musculus (mouse)	RefSeq	
	rno Rattus norvegicus (rat)	RefSeq	
	cfa Canis familiaris (dog)	RefSeq	
	aml Ailuropoda melanoleuca (giant panda)	RefSeq	
	fca Felis catus (domestic cat)	RefSeq	
	bta Bos taurus (cow)	RefSeq	
	ssc Sus scrofa (pig)	RefSeq	
	ecb Equus caballus (horse)	RefSeq	
	mdo Monodelphis domestica (opossum)	RefSeq	
	shr Sarcophilus harrisii (Tasmanian devil)	RefSeq	
	oaa Ornithorhynchus anatinus (platypus)	RefSeq	
	Birds	gga Gallus gallus (chicken)	RefSeq
		mgp Meleagris gallopavo (turkey)	RefSeq
		tgu Taeniopygia guttata (zebra finch)	RefSeq
Reptiles	acs Anolis carolinensis (green anole)	RefSeq	

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KEGG: Kyoto Encyclopedia of Genes and Genomes

www.genome.jp/kegg/

KEGG Organisms: Complete

www.genome.jp/kegg/catalog/org\_list.html

KEGG GENOME: Rhodobacter

www.genome.jp/kegg-bin/show\_organism?org=rsp

# KEGG Rhodobacter sphaeroides 2.4.1

Genome info   Pathway map   Brite hierarchy   Module   Genome map   Blast   Taxonomy

Search genes:

### Genome information

<b>T number</b>	T00284
<b>Org code</b>	rsp
<b>Aliases</b>	RHOS4, 272943
<b>Full name</b>	Rhodobacter sphaeroides 2.4.1
<b>Definition</b>	Rhodobacter sphaeroides 2.4.1
<b>Annotation</b>	manual
<b>Taxonomy</b>	TAX: 272943
<b>Lineage</b>	Bacteria; Proteobacteria; Alphaproteobacteria; Rhodobacterales; Rhodobacteraceae; Rhodobacter
<b>Data source</b>	RefSeq (Project:57655)
<b>Original DB</b>	JGI, Texas
<b>Comment</b>	Photosynthetic alpha-proteobacterium
<b>Chromosome</b>	1; Circular
<b>Sequence</b>	RS: NC_007493
<b>Length</b>	3188609
<b>Chromosome</b>	2; Circular
<b>Sequence</b>	RS: NC_007494
<b>Length</b>	943016

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www.genome.jp/kegg/catalog/org\_list.html

KEGG GENOME: Rhodobacter

www.genome.jp/kegg-bin/show\_organism?org=rsp

KEGG T00007: b2799

www.genome.jp/dbget-bin/www\_bget?eco:b2799

Boreinstein Lab Notebook | MyF1000 Home - F1000 | Google Scholar | "elhanan boreinstein" | IMG Home | Other bookmarks

## KEGG Escherichia coli K-12 MG1655: b2799

Help

Entry	b2799	CDS	T00007
Gene name	fucO		
Definition	L-1,2-propanediol oxidoreductase (EC:1.1.1.77)		
Orthology	K00048 lactaldehyde reductase [EC:1.1.1.77]		
Organism	eco Escherichia coli K-12 MG1655		
Pathway	<a href="#">eco00620</a> Pyruvate metabolism <a href="#">eco00630</a> Glyoxylate and dicarboxylate metabolism <a href="#">eco01120</a> Microbial metabolism in diverse environments		
Class	Metabolism; Carbohydrate metabolism; Pyruvate metabolism [PATH:eco00620]		
Annotation	Metabolism; Carbohydrate metabolism; Glyoxylate and dicarboxylate metabolism [PATH:eco00630]		
Taxonomy	<a href="#">BRITE hierarchy</a>		
SSDB	<a href="#">Ortholog</a> <a href="#">Paralog</a> <a href="#">Gene cluster</a> <a href="#">GFIT</a>		
Motif	Pfam: <a href="#">Fe-ADH Fe-ADH_2</a> <a href="#">Motif</a>		
Other DBs	NCBI-GI: 345452723 NCBI-GeneID: 947273 Pasteur: fucO RegulonDB: ECK120000345 EcoGene: EG10351 ECOCYC: EG10351 ASAP: ABE-0009177 UniProt: P0A9S1		
Position	complement(2929887..2931035) <a href="#">Genome map</a>		
AA seq	382 aa		

**All links**

- Pathway (3)
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  - KEGG COMPOU
  - Chemical react
  - KEGG ENZYME
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- Gene (9)
  - KEGG ORTHOI
  - NCBI-Gene
  - NCBI-GI (1)
  - ASAP (1)
  - ECOCYC (1)
  - ECOGENE (1)
  - OC (1)
  - PASTEUR-ECC
  - REGULONDB-E
- Protein sequer
  - UniProt (1)
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- Protein domain
  - Pfam (2)
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Genome

Search gene

Genome

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Org code

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Full name

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Chromosome

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KEGG GENOME: Rhodobacter

www.genome.jp/kegg-bin/show\_organism?org=rsp

KEGG T00007: b2799

www.genome.jp/dbaet-bin/www\_baet?eco:b2799

KEGG ORTHOLOGY: K00048

www.genome.jp/dbget-bin/www\_bget?ko:K00048

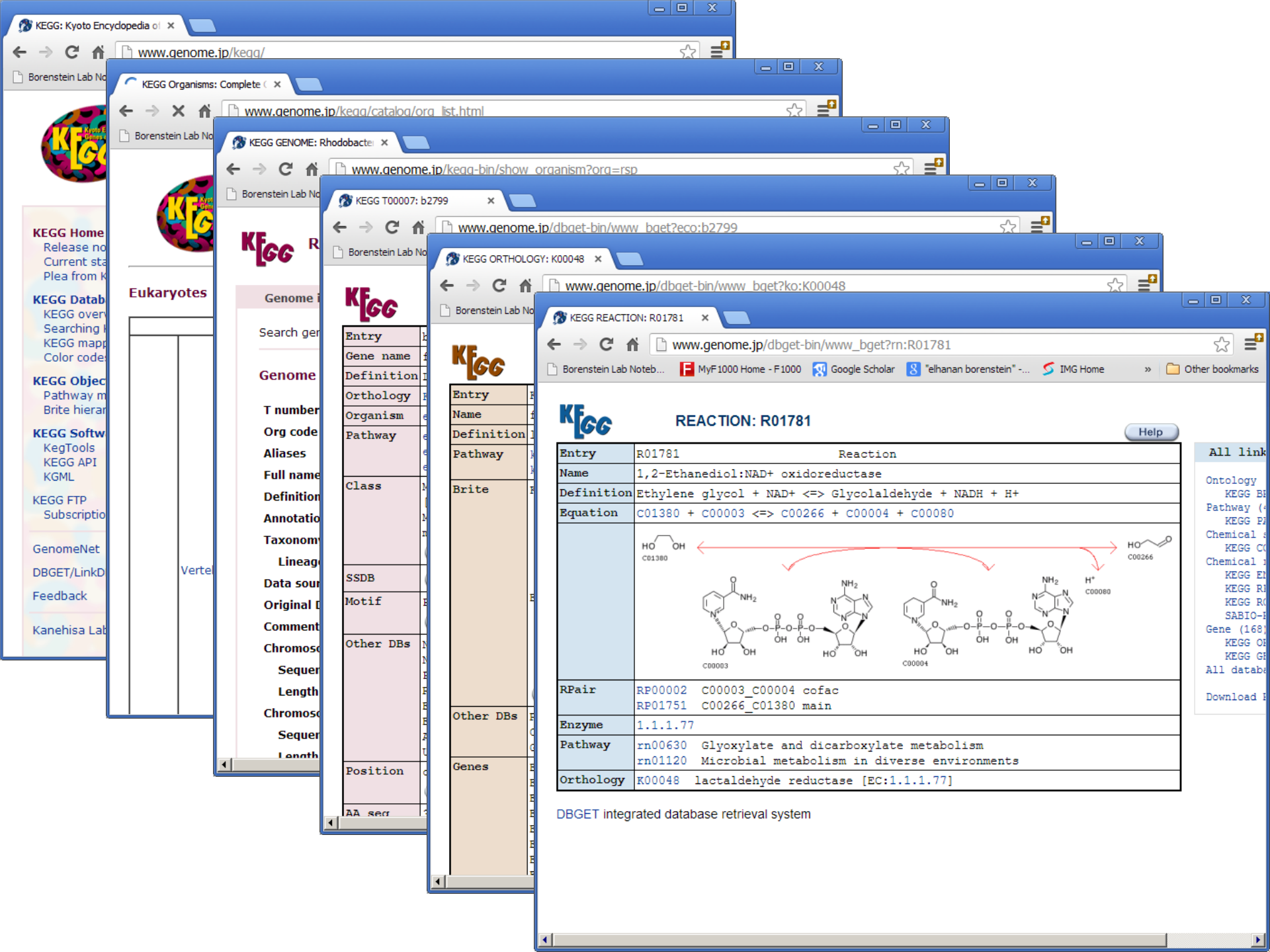
**KEGG ORTHOLOGY: K00048** Help

Entry	K00048	KO
Name	fucO	
Definition	lactaldehyde reductase [EC:1.1.1.77]	
Pathway	ko00620 Pyruvate metabolism ko00630 Glyoxylate and dicarboxylate metabolism	
Brite	KEGG Orthology (KO) [BR:ko00001] Metabolism Carbohydrate metabolism 00620 Pyruvate metabolism K00048 fucO; lactaldehyde reductase 00630 Glyoxylate and dicarboxylate metabolism K00048 fucO; lactaldehyde reductase Enzymes [BR:ko01000] 1. Oxidoreductases 1.1 Acting on the CH-OH group of donors 1.1.1 With NAD+ or NADP+ as acceptor 1.1.1.77 lactaldehyde reductase K00048 fucO; lactaldehyde reductase <a href="#">BRITE hierarchy</a>	
Other DBs	UniProt: R01781 R02257 COG: C03145 GO: 0008912	
Genes	ECO: b2799(fucO) ECJ: Y75_p2736(fucO) ECD: ECDH10B_2968(fucO) EBW: BWG_2537(fucO) ECE: Z4116(fucO) ECS: ECs3659 ECF: ECH74115_4063(fucO) EFW: EFW_2751(fucO)	

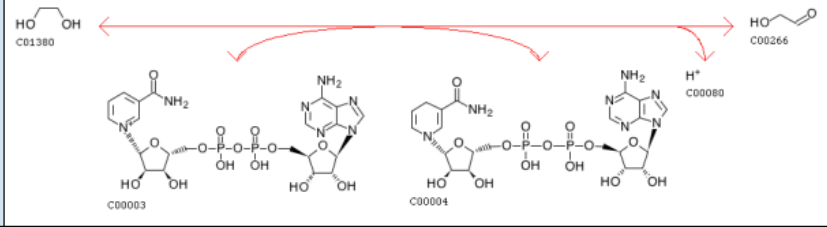
All links

- Ontology (4)
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  - GO (1)
  - COG (1)
- Pathway (6)
  - KEGG PATHWAY
  - Chemical reaction
  - KEGG ENZYME
  - KEGG REACTION
  - KEGG RCLASS
- Gene (11345)
  - KEGG GENES
  - KEGG MGENSE
- Protein sequence
  - UniProt (15)
- All databases
- Download RDF





## REACTION: R01781

Entry	R01781	Reaction
Name	1,2-Ethanediol:NAD <sup>+</sup> oxidoreductase	
Definition	Ethylene glycol + NAD <sup>+</sup> <=> Glycolaldehyde + NADH + H <sup>+</sup>	
Equation	C01380 + C00003 <=> C00266 + C00004 + C00080	
		
RPair	RP00002 C00003_C00004 cofac RP01751 C00266_C01380 main	
Enzyme	1.1.1.77	
Pathway	rn00630 Glyoxylate and dicarboxylate metabolism rn01120 Microbial metabolism in diverse environments	
Orthology	K00048 lactaldehyde reductase [EC:1.1.1.77]	

DBGET integrated database retrieval system

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## KEGG FTP

### KEGG FTP Site for Academic Users

The KEGG data may be downloaded by academic users from the KEGG FTP site:

<ftp://ftp.genome.jp/pub/kegg/>

Non-academic users are required to obtain a license agreement for downloading KEGG.

- [Terms of use](#)
- [Licensing from Pathway Solutions](#)

**Announcement:**

A new directory, "module", is created.

Posted on December 22, 2010 » [Past announcements](#)

## Directories and Files

<a href="#">pathway/</a>	KEGG PATHWAY (daily updated)
<a href="#">map/</a>	Reference pathway maps
<a href="#">ko/</a>	Reference pathway maps (KO)
<a href="#">ec/</a>	Reference pathway maps (EC)
<a href="#">rn/</a>	Reference pathway maps (reaction)
<a href="#">organisms/</a>	Organism-specific pathway maps
<a href="#">pathway</a>	Pathway entries (text data)
<a href="#">map_title.tab</a>	List of pathways available
<a href="#">module/</a>	KEGG MODULE (daily updated) <i>New!</i>
<a href="#">ko/</a>	Reference module maps (KO) - to be added
<a href="#">organisms/</a>	Organism-specific module maps - to be added
<a href="#">module</a>	Module entries (text data)

# genome.txt

```
ENTRY      T00001          Complete Genome
NAME       hin, H.influenzae, HAEIN, 71421
DEFINITION Haemophilus influenzae Rd KW20 (serotype d)
ANNOTATION manual
TAXONOMY   TAX:71421
  LINEAGE  Bacteria; Proteobacteria; Gammaproteobacteria; Pasteurellales;
           Pasteurellaceae; Haemophilus
DATA_SOURCE RefSeq
ORIGINAL_DB JCVI-CMR
DISEASE    Meningitis, septicemia, otitis media, sinusitis and chronic
           bronchitis
CHROMOSOME Circular
  SEQUENCE RS:NC_000907
  LENGTH   1830138
STATISTICS Number of nucleotides:      1830138
           Number of protein genes:    1657
           Number of RNA genes:        81
REFERENCE  PMID:7542800
  AUTHORS  Fleischmann RD, et al.
  TITLE    Whole-genome random sequencing and assembly of Haemophilus
           influenzae Rd.
  JOURNAL  Science 269:496-512 (1995)
///
ENTRY      T00002          Complete Genome
NAME       mge, M.genitalium, MYCGE, 243273
DEFINITION Mycoplasma genitalium G-37
ANNOTATION manual
TAXONOMY   TAX:243273
  LINEAGE  Bacteria; Tenericutes; Mollicutes; Mycoplasmataceae; Mycoplasma
  ...
```

# hin\_ko.txt

ace:Acel_0001	ko:K02313
ace:Acel_0002	ko:K02338
ace:Acel_0003	ko:K03629
ace:Acel_0005	ko:K02470
ace:Acel_0006	ko:K02469
ace:Acel_0012	ko:K03767
ace:Acel_0018	ko:K01664
ace:Acel_0019	ko:K08884
ace:Acel_0020	ko:K05364
ace:Acel_0026	ko:K01552
ace:Acel_0029	ko:K00111
ace:Acel_0031	ko:K00627
ace:Acel_0032	ko:K00162
ace:Acel_0033	ko:K00161
ace:Acel_0035	ko:K00817
ace:Acel_0036	ko:K07448
ace:Acel_0039	ko:K04750
ace:Acel_0041	ko:K03281
ace:Acel_0048	ko:K08323
ace:Acel_0051	ko:K03734
ace:Acel_0052	ko:K03147
ace:Acel_0057	ko:K03088
ace:Acel_0059	ko:K01010
ace:Acel_0061	ko:K03711
ace:Acel_0062	ko:K06980
ace:Acel_0063	ko:K07560
ace:Acel_0072	ko:K12373
ace:Acel_0075	ko:K01834
ace:Acel_0076	ko:K09796

...

# ko.txt

```
ENTRY          K00001                KO
NAME           E1.1.1.1, adh
DEFINITION    alcohol dehydrogenase [EC:1.1.1.1]
PATHWAY       ko00010  Glycolysis / Gluconeogenesis
              ko00071  Fatty acid metabolism
MODULE        M00236  Retinol biosynthesis, beta-cacrotene => retinol
CLASS         Metabolism; Carbohydrate Metabolism; Glycolysis / Gluconeogenesis
              [PATH:ko00010]
              Metabolism; Lipid Metabolism; Fatty acid metabolism [PATH:ko00071]
              Metabolism; Amino Acid Metabolism; Tyrosine metabolism
              [PATH:ko00350]
              Metabolism; Metabolism of Cofactors and Vitamins; Retinol metabolism
DBLINKS       RN: R00623 R00754 R02124 R04805 R04880 R05233 R05234 R06917 R06927
              R07105 R08281 R08306 R08310
              COG: COG1012 COG1062 COG1064 COG1454
              GO: 0004022 0004023 0004024 0004025
GENES         HSA: 124 (ADH1A) 125 (ADH1B) 126 (ADH1C) 127 (ADH4) 130 (ADH6) 131 (ADH7)
              PTR: 461394 (ADH4) 461395 (ADH6) 461396 (ADH1B) 471257 (ADH7)
              744064 (ADH1A) 744176 (ADH1C)
              MCC: 707367 707682 (ADH1A) 708520 711061 (ADH1C)
...
              PAS: Pars_0396 Pars_0534 Pars_0547 Pars_1545 Pars_2114
              TPE: Tpen_1006 Tpen_1516
///
ENTRY          K00002                KO
NAME           E1.1.1.2, adh
DEFINITION    alcohol dehydrogenase (NADP+) [EC:1.1.1.2]
PATHWAY       ko00010  Glycolysis / Gluconeogenesis
              ko00561  Glycerolipid metabolism
...

```

# reaction.txt

```
R00005: 00330: C01010 => C00011
R00005: 00791: C01010 => C00011
R00005: 01100: C01010 <=> C00011
R00006: 00770: C00022 => C00900
R00008: 00362: C06033 => C00022
R00008: 00660: C00022 => C06033
R00010: 00500: C01083 => C00031
R00013: 00630: C00048 => C01146
R00013: 01100: C00048 <=> C01146
R00014: 00010: C00022 + C00068 => C05125
R00014: 00020: C00068 + C00022 => C05125
R00014: 00290: C00022 => C05125
R00014: 00620: C00068 + C00022 => C05125
R00014: 00650: C00068 + C00022 => C05125
R00014: 01100: C00022 <=> C05125
R00018: 00960: C00134 => C06366
R00019: 00630: C00080 => C00282
R00019: 00680: C00080 => C00282
R00021: 00910: C00025 <= C00064
R00022: 00520: C01674 => C00140
...
```

# From Small Scripts to Full Projects

- *Use a top-down approach*
- *Divide and conquer*

# Designing with Pseudo-Code Comments

```
# Preprocessing  
# =====
```

```
# Build networks and calc degree  
# =====
```

```
# Print output  
# =====
```



# Add details

```
# Preprocessing
# =====

# Read and store mapping from KO to RN

# Read and store mapping from RN to edges

# Read and store species list and lineages
```

```
# Build networks and calc degree
# =====

# Loop over species

    # Read KO list of current species

    # Map KO to RN and RN to edges

    # Calculate degree

    # Store: species, degree, phyla

# Print output
# =====

# Calculated average degree per P and per E

# Print
```

# Add notes to self

```
# Preprocessing
# =====

# Read and store mapping from KO to RN

# Read and store mapping from RN to edges

# Read and store species list and lineages
```

```
# Build networks and calc degree
# =====

# Loop over species

    # Read KO list of current species

    # Map KO to RN and RN to edges

    # -> Here I should have a full network
    # -> TBD: What data structure should I use?

    # Calculate degree

    # Store: species, degree, phyla
    # -> TBD: How do I store results?

# Print output
# =====

# Calculated average degree per P and per E

# Print
```

# Add variables, loops, if-s, function calls

```
# Preprocessing
# =====

# Read and store mapping from KO to RN
KO_file = 'ko.txt'
KO_to_RN = {}

# Read and store mapping from RN to edges
RN_file = 'reaction.txt'
RN_to_EDGES = {}

# Read and store species list and lineages
Genomes_file = 'genome.txt'
species_list = []
species_lineage = {}
```

```
# Build networks and calc degree
# =====

# Loop over species
for species in species_list:

    # Read KO list of current species

    # Map KO to RN and RN to edges

    # -> Here I should have a full network
    # -> TBD: What data structure should I use?

    # Calculate degree
    degree = CalcDegree(network)

    # Store: species, degree, phyla
    # -> TBD: How do I store results?

# Print output
# =====

# Calculated average degree per P and per E

# Print
```

# Start coding small chunks

```
# Preprocessing
# =====

# Read and store mapping from KO to RN
KO_file = 'ko.txt'
KO_to_RN = {}

# Read and store mapping from RN to edges
RN_file = 'reaction.txt'
RN_to_EDGES = {}

# Read and store species list and lineages
Genomes_file = 'genome.txt'
species_list = []
species_lineage = {}
< LET'S WRITE THIS PART >
```

```
# Build networks and calc degree
# =====

# Loop over species
for species in species_list:

    # Read KO list of current species

    # Map KO to RN and RN to edges

    # -> Here I should have a full network
    # -> TBD: What data structure should I use?

    # Calculate degree
    degree = CalcDegree(network)

    # Store: species, degree, phyla
    # -> TBD: How do I store results?

# Print output
# =====

# Calculated average degree per P and per E

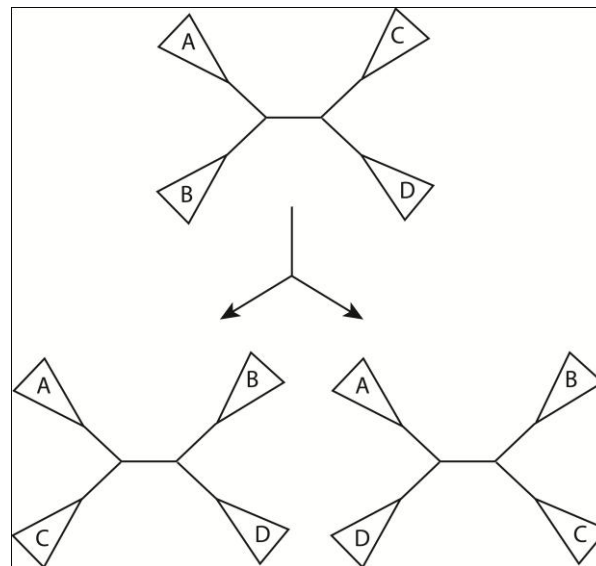
# Print
```

# Final Exam

- **Two parts:**
  - *The first will focus on the bioinformatics topics covered in class.*
  - *The second on programming.*
- Both parts will comprise very simple and brief questions to account for the short time allowed for the exam.
- Open books (basically, any static resource you want is ok).

# Common Mistakes: Parsimony

- Figure out how many possible Nearest-Neighbor Interchanges there are on a specific unrooted tree with 8 leaves (that is, the number of competing trees that would be considered in one step of the hill-climbing method using NNIs). Hint: a subtree can be any part of the tree, including a single leaf. Justify your answer.



# Common Mistakes: Programming

- Comments !!!
- continue, elif, if ...

```
for items in list:  
    if (...):  
        do_something  
    else:  
        continue
```

```
if (a > 10):  
    do_nothing  
else:  
    print ...
```

- Lists vs. Dictionaries

... it's a wrap ...  
Hope you enjoyed!



