

So far, we've talked about

- DNA, RNA and protein sequences
- How to compare sequences to decide if they are related
- Having databases full of sequences and comparing them rapidly (BLAST)

In fact, <u>many</u> such databases exist, so today we'll start with a brief tour of <u>some</u> of the biological data on the web.

Edward Marcotte/Univ. of Texas/BCH391L/Spring 2015

Just some of

Database dbEST

Pride

SGD

Reactome

Yeast GFP database

	DIP	75,019 protein interactions	http://dip.doe-mbi.ucla.edu/
the resources	EcoCyc/MetaCyc	>1,900 pathways	http://www.ecocyc.org, http://www.metacyc.org
available for	Entrez Genome	1000's of genomes (including ~4,500 viruses)	http://www.ncbi.nlm.nih.gov/genome?db=genome
bioinformatics	Genbank	135,440,924 sequence records spanning 126 billion bases in traditional Genbank (as of 2013); 191 billion bases in WGS division	http://www.ncbi.nlm.nih.gov/Genbank/GenbankO verview.html
Think of these	Gene Expression Omnibus (GEO)	877,498 mRNA or protein expression data sets	http://www.ncbi.nlm.nih.gov/geo/
as the raw	Genomes Online Database (GOLD)	20,581 genome sequences (many in progress)	http://www.genomesonline.org/cgi- bin/GOLD/index.cgi
data for new	Human Protein Atlas	millions of images of ~14K human proteins' expression in 46 tissues, 20 cancers, 47 cell lines	http://www.proteinatlas.org/
discoveries	KEGG	Most known pathways, in 435 graphical diagrams and 2,455 organisms (via homology)	http://www.genome.ad.jp/kegg/
	Medline	>22 million references	http://www.ncbi.nlm.nih.gov/PubMed/
	Mouse Genome Informatics	~20,000 mouse genes, diverse associated data & annotations	http://www.informatics.jax.org/
	Online Mendelian Inheritance in Man (OMIM)	Compendium of human genes and genetic phenotypes, data for >12,000 genes	http://www.ncbi.nlm.nih.gov/omim/

> 342 million peptide mass spectra from 27K experiments

1,371 pathways involving 6,571 proteins, for human, similar for extra organisms

~6,000 yeast genes, diverse associated data &

protein subcellular localization for \sim 4,500 yeast proteins

~11,000 transcription factor/downstream gene pairs

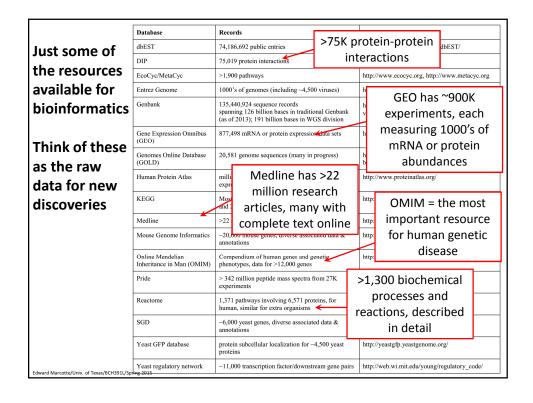
74,186,692 public entries

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

http://www.reactome.org/

http://www.yeastgenome.org/

http://yeastgfp.yeastgenome.org/



Live demo OMIM, Reactome, Human Protein Atlas

dward Marcotte/Univ. of Texas/BCH391L/Spring 2015

It's nice to know that all of this exists, but ideally, you'd like to be able to so something constructive with the data.

That means getting the data inside your own programs.

All of these databases let you download data in big batches, but this isn't always the case, so....

We saw one way to do this in AppSoma. Here's another.

Edward Marcotte/Univ. of Texas/BCH391L/Spring 2015

Let's empower your Python scripts to grab data from the web.

We'll use Python <u>library/module</u> = an optional, specialized set of Python methods

This particular Python module is called *urllib2*.

urllib2 is:

- A collection of programs/tools to let you to surf the web from inside your programs.
- Much more powerful than the simple tasks we'll do with it.
- More details: http://docs.python.org/2/library/urllib2.html

Edward Marcotte/Univ. of Texas/BCH391L/Spring 2015

The basic idea:

We first set up a "request" by opening a connection to the URL.

We then save the response in a variable and print it.

If it can't connect to the site, it'll print out a helpful error message instead of the page.

You can more or less use the commands in a cookbook fashion....

Edward Marcotte/Univ. of Texas/BCH391L/Spring 2015

For example:

```
import urllib2  # include the urllib2 module

url = "http://www.utexas.edu/"

try:  # this 'try' statement tells Python that we might expect an error.
  request = urllib2.urlopen(url)  # setup a request
  page = request.read()  # save the response
  print page  # show the result to the user

except urllib2.HTTPError:  # handle a page not found error
  print "Could not find page."
```

→ Run this...

Edward Marcotte/Univ. of Texas/BCH391L/Spring 2015

→ We just captured the UT web page and printed it out (minus the images)...

That was a static web page.

Let's try one that requires some sort of action, for example by entering a document id or an id code for a sequence.

Many web pages pass this information along in the web URL itself...

Edward Marcotte/Univ. of Texas/BCH391L/Spring 201

ward Marcotte/Univ. of Texas/BCH391L/Spring 2015

Here's a complete Python program to retrieve a single entry from Medline:

```
If you run that program, you should get back...
<?xml version="1.0" encoding="utf-8"?>
<!DOCTYPE html PUBLIC "-//W3C//DTD XHTML 1.0 Transitional//EN" "http://www.w3.org/TR/xhtml1/DTD/xhtml1-
transitional.dtd">
<
PMID-11237011
OWN - NLM
STAT- MEDLINE
                                                 the Medline entry for the human
DA - 20010309
DCOM- 20010322
                                                       genome sequence paper
LR - 20061115
IS - 0028-0836 (Print)
IS - 0028-0836 (Linking)
VI - 409
IP - 6822
DP - 2001 Feb 15
TI - Initial sequencing and analysis of the human genome.
AB - The human genome holds an extraordinary trove of information about human
   development, physiology, medicine and evolution. Here we report the results of an
   international collaboration to produce and make freely available a draft sequence
   of the human genome. We also present an initial analysis of the data, describing
   some of the insights that can be gleaned from the sequence.
FAU - Lander, ES
AU - Lander ES
AD - Whitehead Institute for Biomedical Research, Center for Genome Research,
   Cambridge, Massachusetts 02142, USA. lander@genome.wi.mit.edu
                                                                                  [and so on]
```

```
If you run that program, you should get back...
>>>
<?xml version="1.0" encoding="utf-8"?>
<!DOCTYPE html PUBLIC "-//W3C//DTD XHTML 1.0 Transitional//EN" "http://www.w3.org/TR/xhtml1/DTD/xhtml1-
PMID-11237011
OWN - NLM
STAT- MEDLINE
                                                 We just printed it. We could have
DA - 20010309
DCOM- 20010322
                                                 saved it or extracted data from it.
LR - 20061115
IS - 0028-0836 (Print)
                                                                 For example...
IS - 0028-0836 (Linking)
VI - 409
IP - 6822
DP - 2001 Feb 15
TI - Initial sequencing and analysis of the human genome.
PG - 860-921
AB - The human genome holds an extraordinary trove of information about human
   development, physiology, medicine and evolution. Here we report the results of an \,
   international collaboration to produce and make freely available a draft sequence
   of the human genome. We also present an initial analysis of the data, describing
   some of the insights that can be gleaned from the sequence.
FAU - Lander, ES
AU - Lander ES
AD - Whitehead Institute for Biomedical Research, Center for Genome Research,
   Cambridge, Massachusetts 02142, USA. lander@genome.wi.mit.edu
                                                                                   [and so on]
ward Marcotte/Univ. of Texas/BCH391L/Spring 2015
```

Here's our Python program again to retrieve a single entry from Medline. How would we modify this to count the authors?

dward Marcotte/Univ. of Texas/BCH391L/Spring 2015

Here's our Python program again to retrieve a single entry from Medline. How would we modify this to count the authors? import urllib2 pmid = 11237011 # Insert the pmid where the {} are in the following URL: url = "http://www.ncbi.nlm.nih.gov/pubmed/{0}?report=medline&format=text".format(pmid) # there might be an error! Medline begins request = urllib2.urlopen(url) author lines with page = request.read() "AU - ", so... print page.count("AU - ") except urllib2.HTTPError: # handle page not found error print "Could not connect to Medline!" So, there were 255 authors on one (of → Run this, & get ... >>> 255 the two) human genome papers ard Marcotte/Univ. of Texas/BCH391L/Spring 2015

- Queries to Medline or any other NCBI database, including GenBank, are described at: http://www.ncbi.nlm.nih.gov/books/NBK3862/
- You can often figure out the form of the URL just by looking something up in a database, then noting the address of the web page with the data.
- This very simple approach could easily be the basis for:
 - a home-made web browser
 - a program to consult biological databases in real time
 - a program to map the internet, etc.
- Of course, with this kind of power available to you, the imagination reels...

Edward Marcotte/Univ. of Texas/BCH391L/Spring 201