

Bioinformatics

CS300/BIO300

The Great Review

Fall 2019

Oliver BONHAM-CARTER



Thursday, 5th Dec

- Dr. Thu of the Dept of Biology will present on Thursday at 11:45am – 12:15pm
- **Main ideas**
 - *How do we make sense of a large amount of data in gene expression analysis or proteomics?*
 - *Looking for patterns, instead of focusing on one gene/protein at a time*
 - *Computational tools to look for pattern (hierarchical clustering, pathway enrichment analysis)*
 - *Examples of how we use these data (cancer subtyping, proteins involved in regeneration in planarian worm)*



Course Summary

\subsection*{\textbf{Academic Bulletin Description}}

An introduction to the development and application of methods, from the computational and information sciences, for the investigation of biological phenomena. In this interdisciplinary course, students integrate computational techniques with biological knowledge to develop and use analytical tools for extracting, organizing, and interpreting information from genetic sequence data. Often participating in team-based and hands-on activities, students implement and apply useful bioinformatics algorithms. During a weekly laboratory session students employ cutting-edge software tools and programming environments to complete projects, reporting on their results through both written assignments and oral presentations. Prerequisites: BIO 221 and FSBIO 201, or CMPSC 111. Distribution Requirements: QR, SP.



Course Objectives

- **Students successfully completing this class will have developed:**
 - A “big-picture” view of bioinformatics.
 - An ethical foundation
 - An understanding of the objectives and limitations of bioinformatics.
 - An understanding of the biological foundations (genes and genomes, gene expression, etc.).
 - An understanding of the computational foundations (programming, databases, etc.).
 - An understanding of how genetic information is obtained and processed.
 - The ability to use basic bioinformatics software tools to study genetic information.



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An Ethically Conscious Course

- We had lab assignments in which ethical considerations were explored
- We met **speakers** who came to talk about
 - The ethical use of data in the health sciences
 - The responsible use of robotics technology in automation

Responsible Computer Science Challenge

With Great Code Comes Great Responsibility

a partnership of

ON OMIDYAR NETWORK **moz://a** SCHMIDT FUTURES Craig Newmark Philanthropies

moz://a



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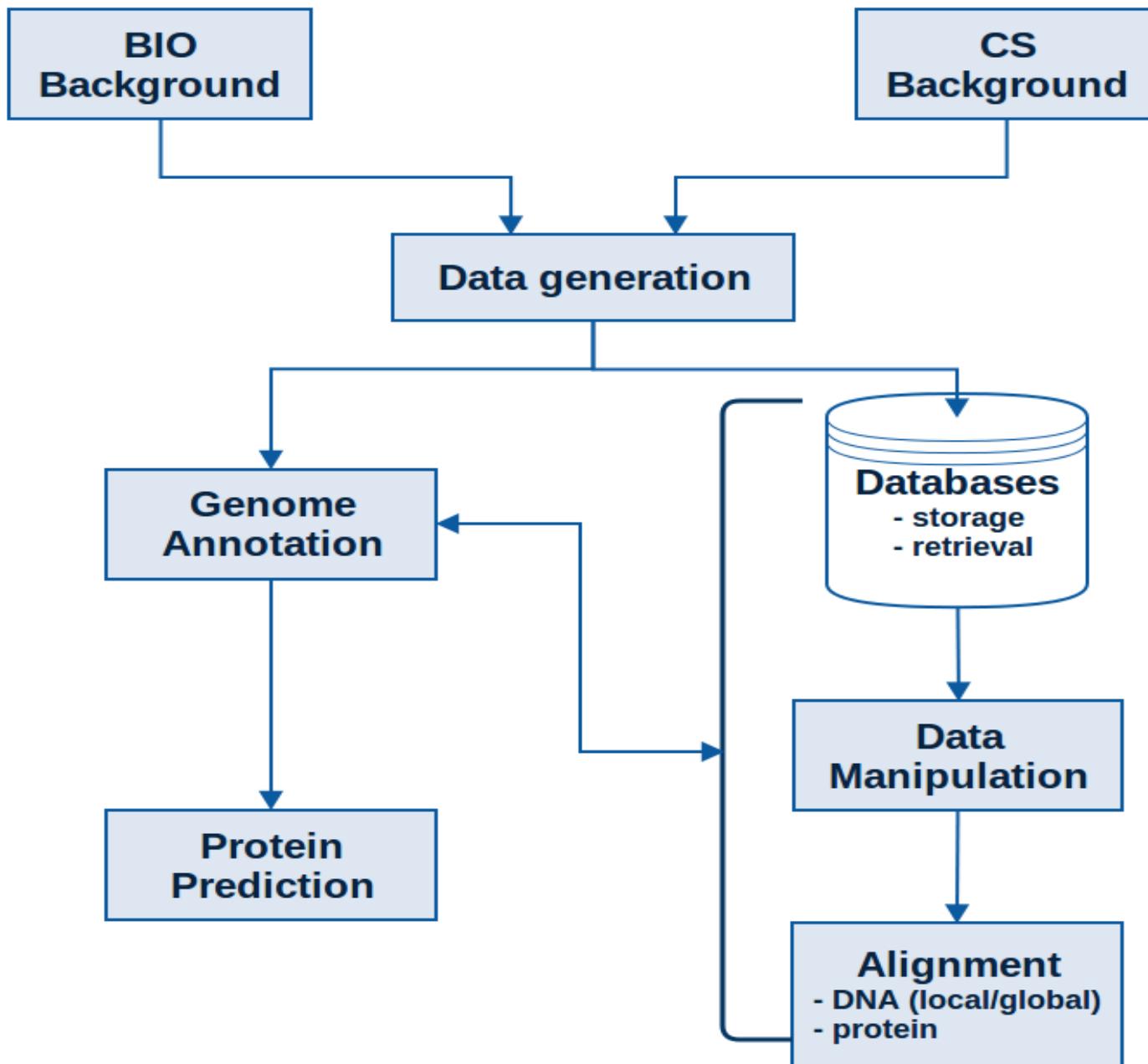
How Did We Meet These Objectives?



Let's go back and
revisit some of our
discussions and slides.



Course Outline





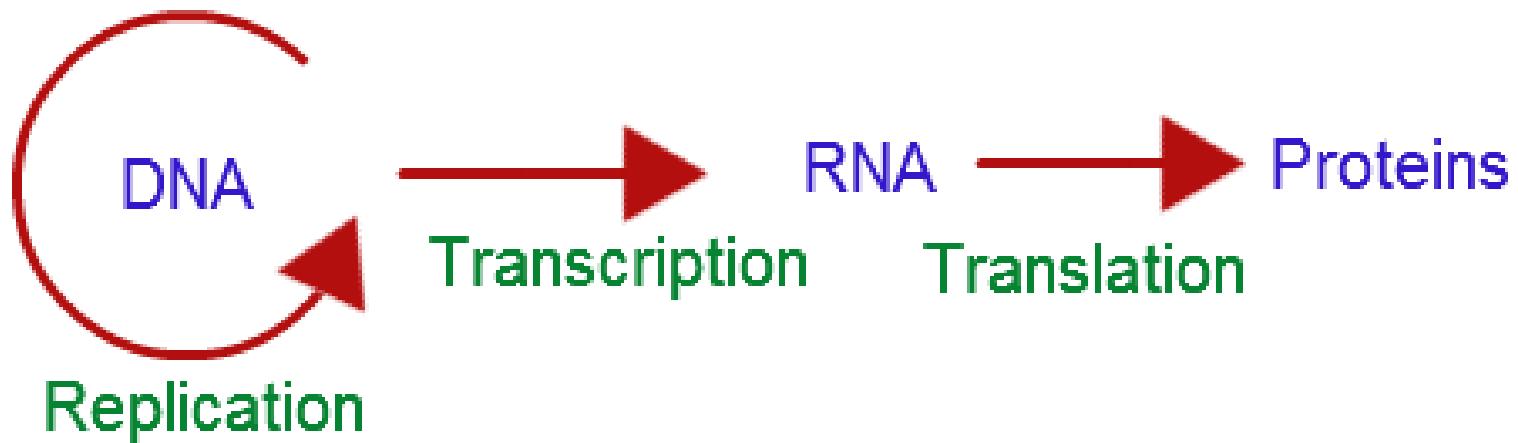
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We Started With ...

The Central Dogma Of Biology



The Central Dogma Of Biology

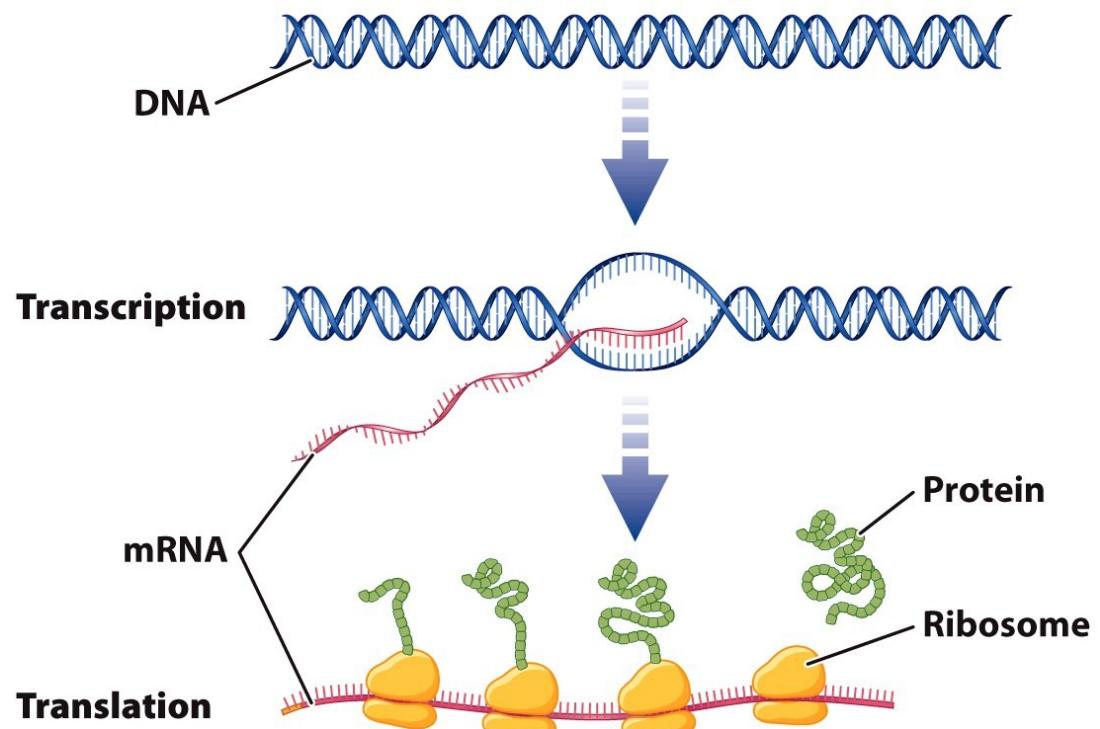
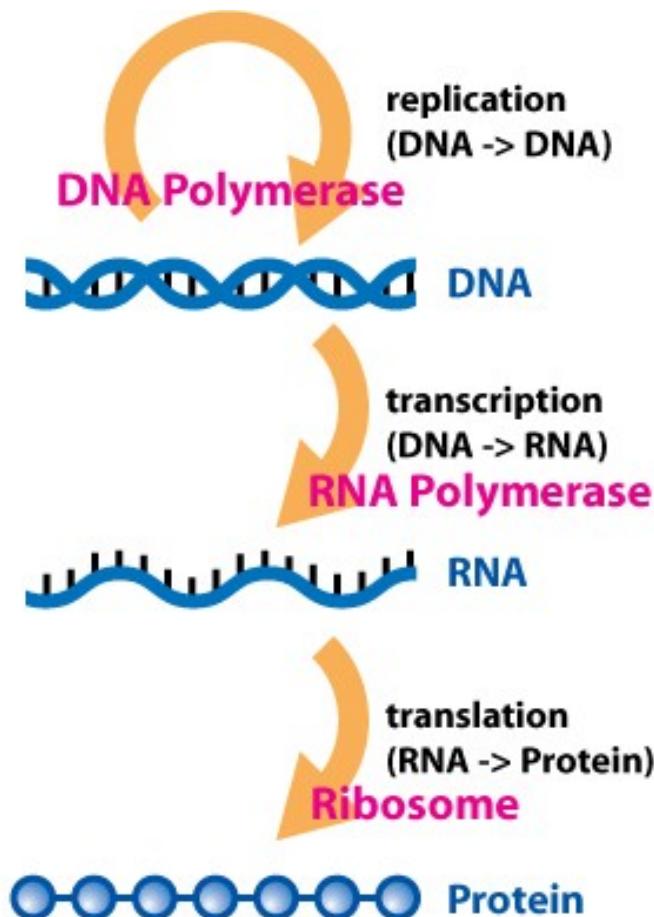


"the coded genetic information hard-wired into DNA is transcribed into individual transportable cassettes, composed of messenger RNA (mRNA); each mRNA cassette contains the program for synthesis of a particular protein (or small number of proteins)" - NCBI



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The Central Dogma of Molecular Biology



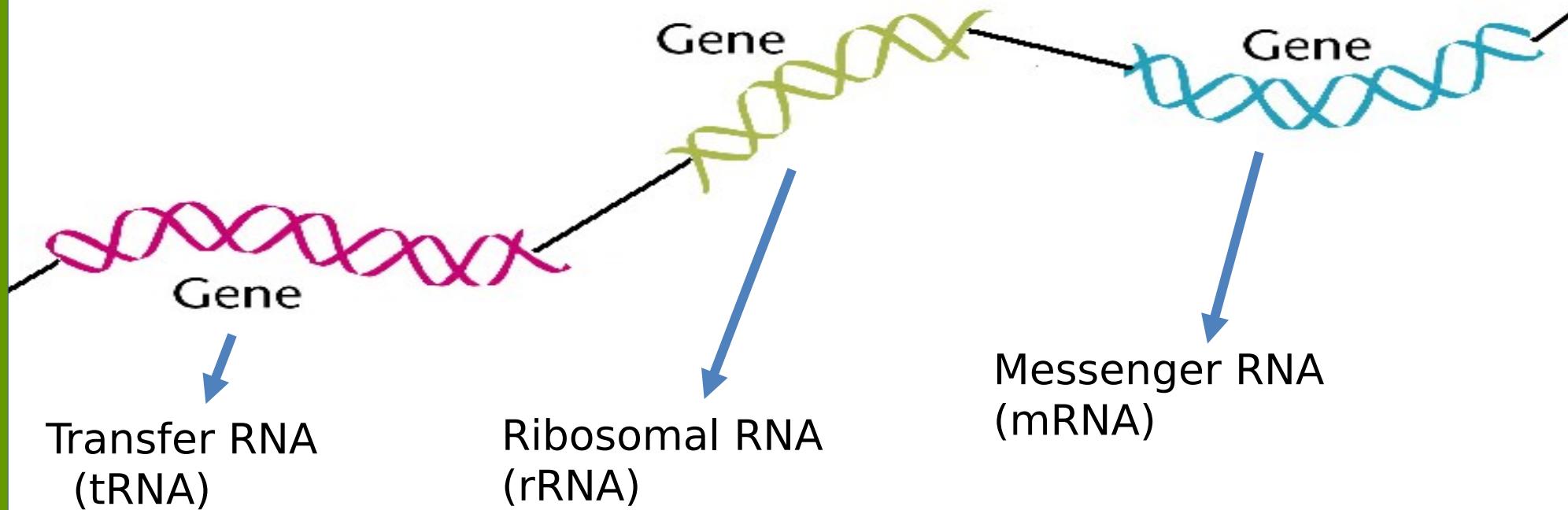
Proteins provide structure
and carry out many
essential activities in a cell.

Figure 3.3
How Life Works
© 2014 W. H. Freeman and Company



Transcription

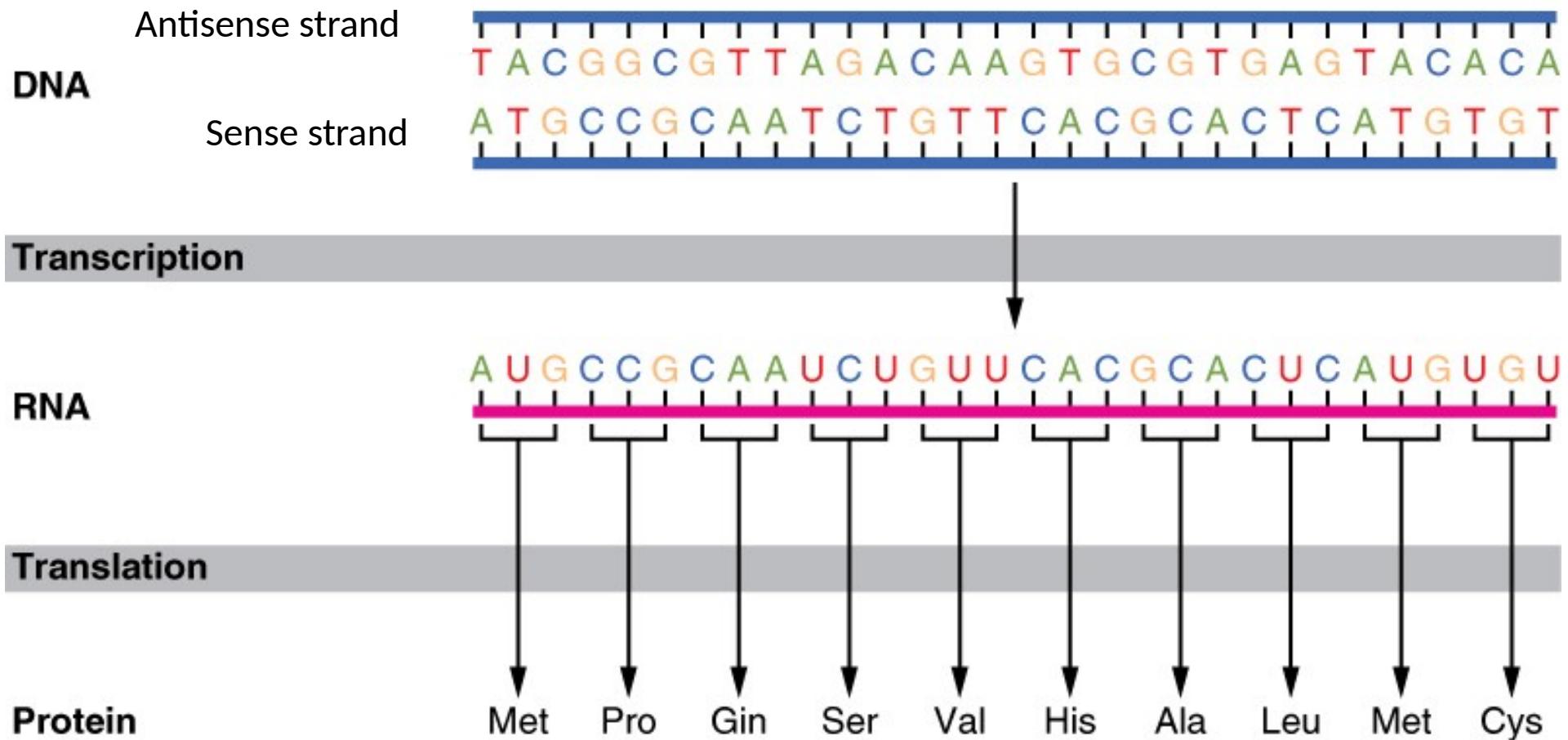
- **Transcribe** specific regions of DNA – **genes**
 - Human genome ~25,000 genes (just 1.5% of genome)
- **RNA** is the direct **product** of transcribing a gene (DNA)
 - DNA -> RNA
 - same language (nucleotides)





Translation

- The information from DNA is rewritten in a new language: RNA





Translation

- Triplet code
 - Combinations of three nucleotides code for one amino acid
 - Three nucleotides = codon
- Redundancy
 - Sometimes >1 codon codes for same amino acid
 - 20 amino acids, 64 possible codons

- Start and Stop codons
 - First codon of many transcripts is “AUG”, which codes for methionine
 - Codons UAA, UAG, and UGA indicate the end of the transcript

		Standard genetic code											
1st base	2nd base	A				G				C			
		T	C	T	A	T	G	T	C	A	G	T	
T	TTT	(Phe/F) Phenylalanine		TCT	(Ser/S) Serine	TAT	(Tyr/Y) Tyrosine		TGT	(Cys/C) Cysteine		T	
	TTC			TCC		TAC			TGC			C	
	TTA			TCA		TAA ^[B]	Stop (Ochre)		TGA ^[B]	Stop (Opal)		A	
	TTG			TCG		TAG ^[B]	Stop (Amber)		TGG	(Trp/W) Tryptophan		G	
C	CTT	(Leu/L) Leucine		CCT	(Pro/P) Proline	CAT	(His/H) Histidine		CGT			T	
	CTC			CCC		CAC			CGC			C	
	CTA			CCA		CAA	(Gln/Q) Glutamine		CGA	(Arg/R) Arginine		A	
	CTG			CCG		CAG			CGG			G	
A	ATT			ACT	(Thr/T) Threonine	AAT	(Asn/N) Asparagine		AGT	(Ser/S) Serine		T	
	ATC	(Ile/I) Isoleucine		ACC		AAC			AGC			C	
	ATA			ACA		AAA	(Lys/K) Lysine		AGA	(Arg/R) Arginine		A	
	ATG ^[A]	(Met/M) Methionine		ACG		AAG			AGG			G	
G	GTT			GCT	(Ala/A) Alanine	GAT	(Asp/D) Aspartic acid		GGT			T	
	GTC	(Val/V) Valine		GCC		GAC			GGC			C	
	GTA			GCA		GAA	(Glu/E) Glutamic acid		GGA	(Gly/G) Glycine		A	
	GTG			GCG		GAG			GGG			G	



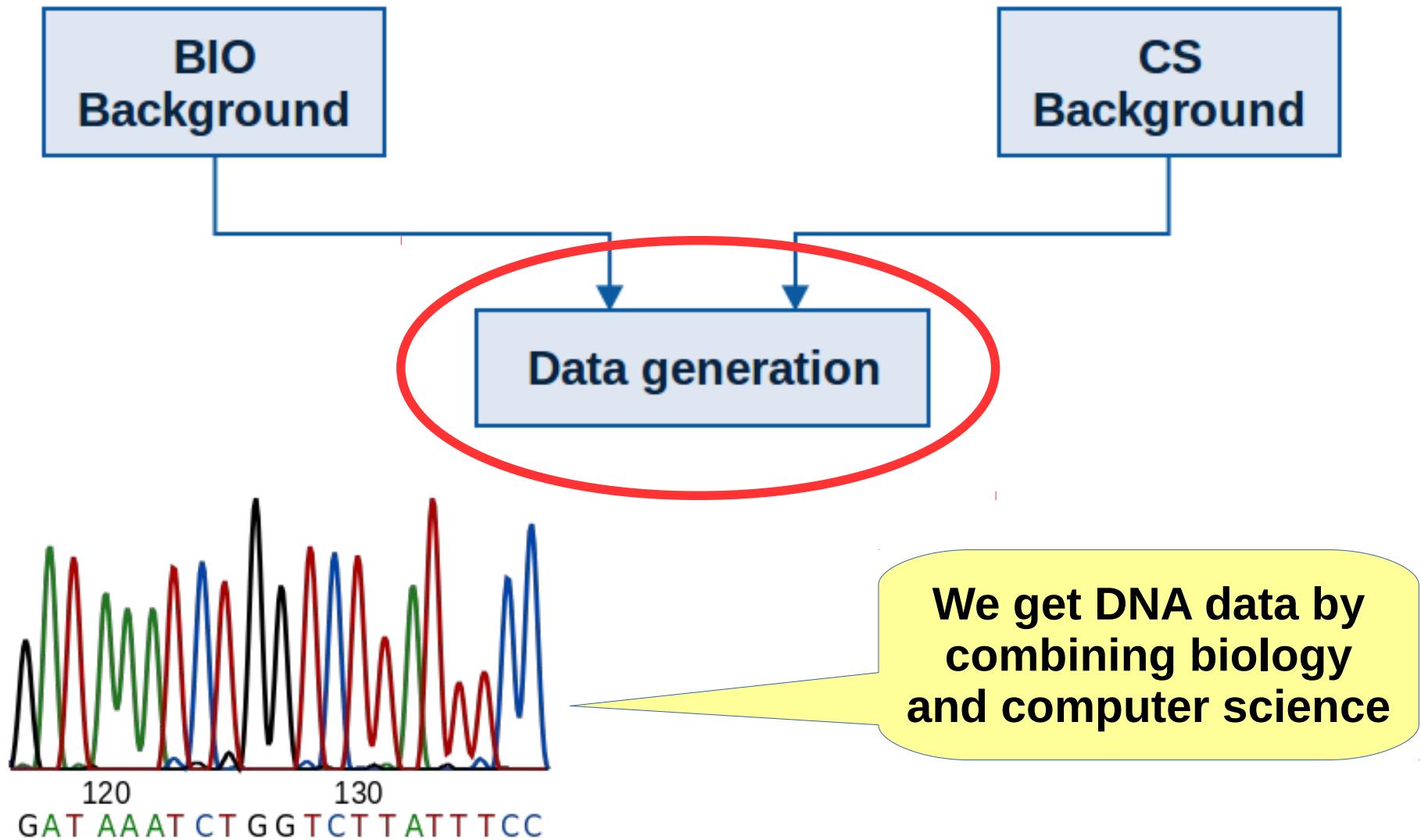
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We Talked About...

Data Generation:
Or where the data
comes from for research
in Bioinformatics

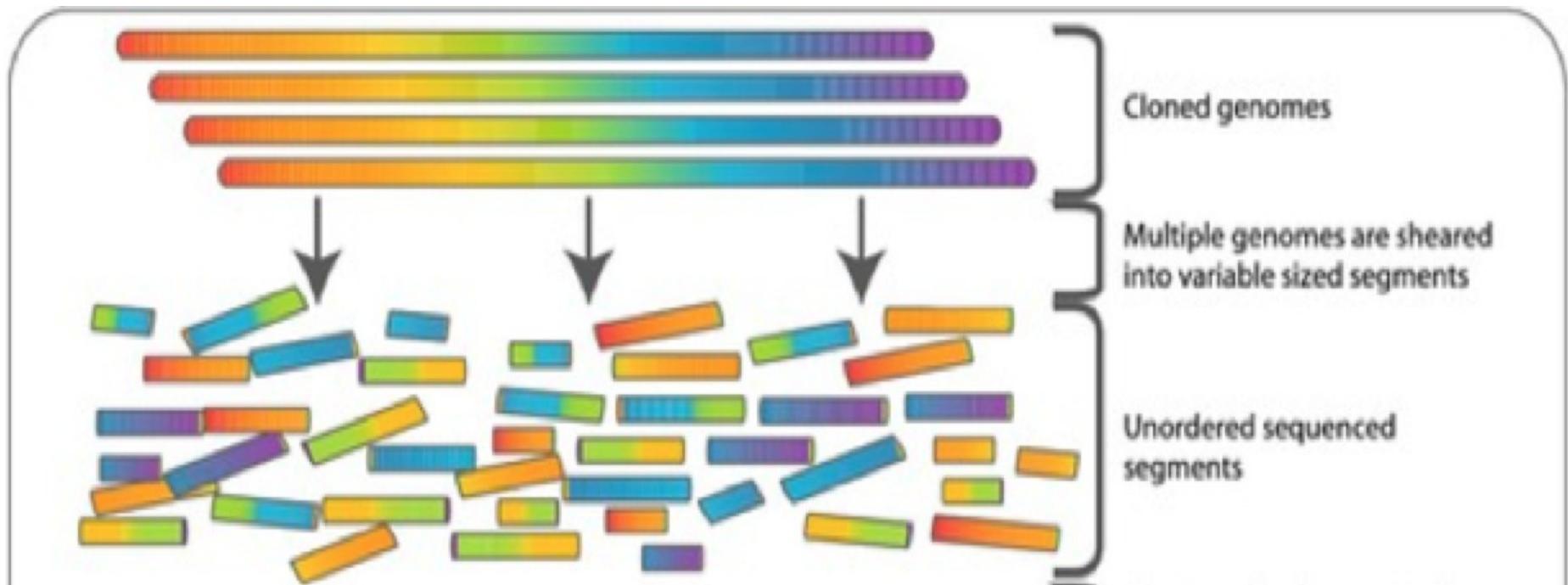


From The Course Outline



Genome Sequencing

- The technology works by “exploding” DNA into smaller, manageable pieces
- Then it recombines pieces (*Reads*) into bigger pieces (*Contigs*)
- And then it combines contigs bigger chunks like a jigsaw puzzle



times, it was the age

It was the best of

age of wisdom, it was

best of times, it was

it was the age of

it was the age of

it was the worst of

of times, it was the

of times, it was the

of wisdom, it was the

the age of wisdom, it

the best of times, it

the worst of times, it

worst of times, it was

wisdom, it was the age

was the worst of times,

was the best of times,

was the age of foolishness,

was the age of wisdom

times, it was the worst

Repeats pile up – actual placement of each individual fragment unknown

Repeats can cause ambiguity and prevent proper assembly

It was the best of

was the best of times,

the best of times, it

best of times, it was

of times, it was the

of times, it was the

times, it was the age

times, it was the worst

It was the best of times, it was the [age/worst]

Assembly Parameter:
100% identify across 4 words

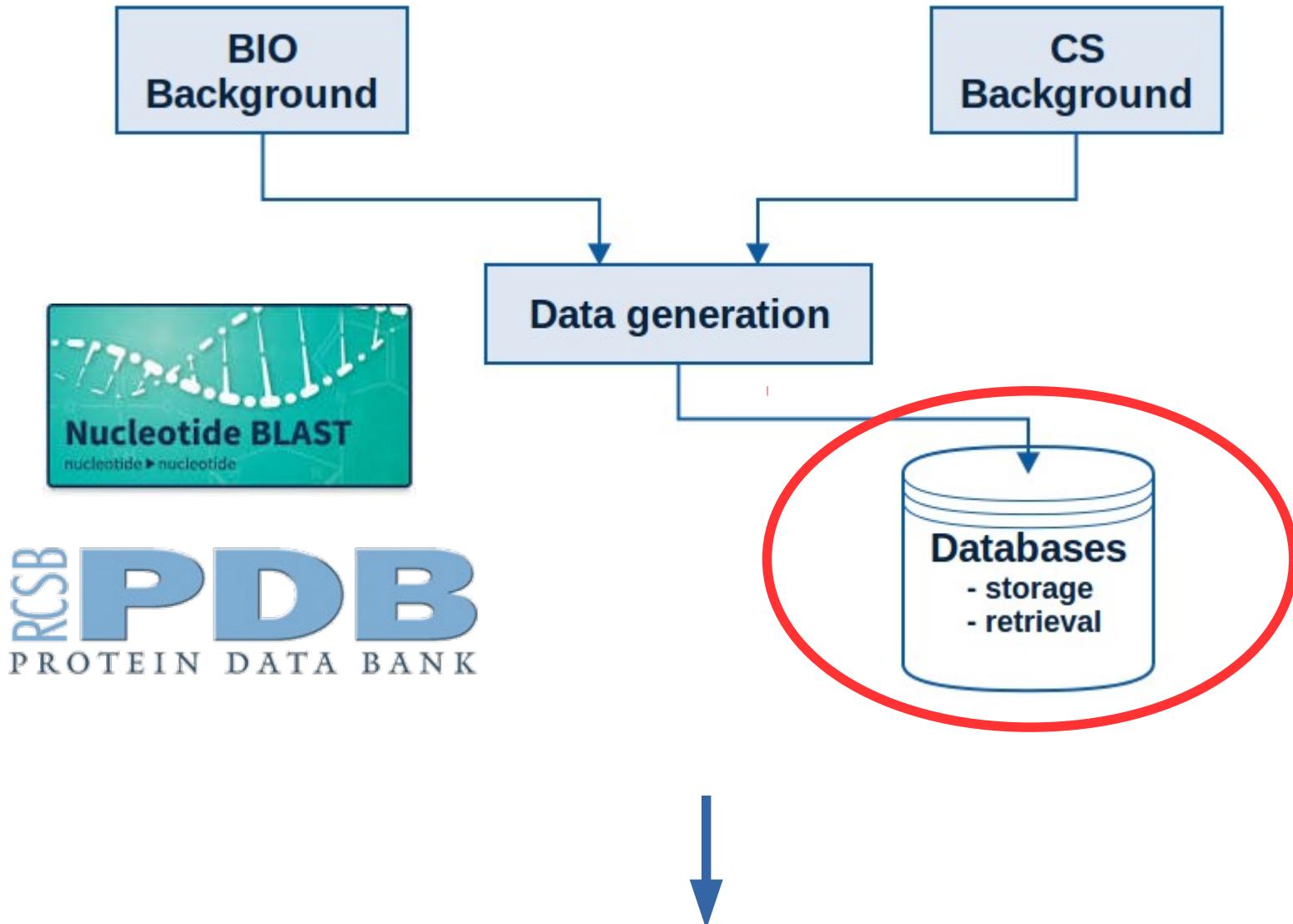


We Talked About...

Databases:
Places where data
is stored for further
research



From The Course Outline



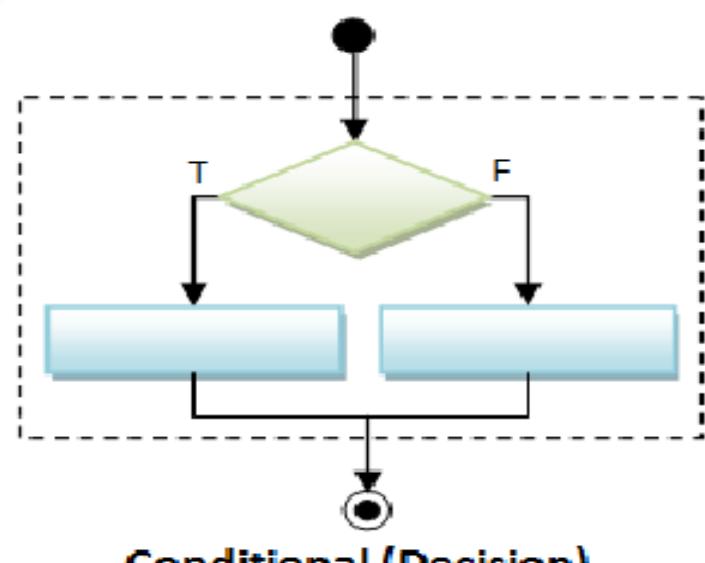
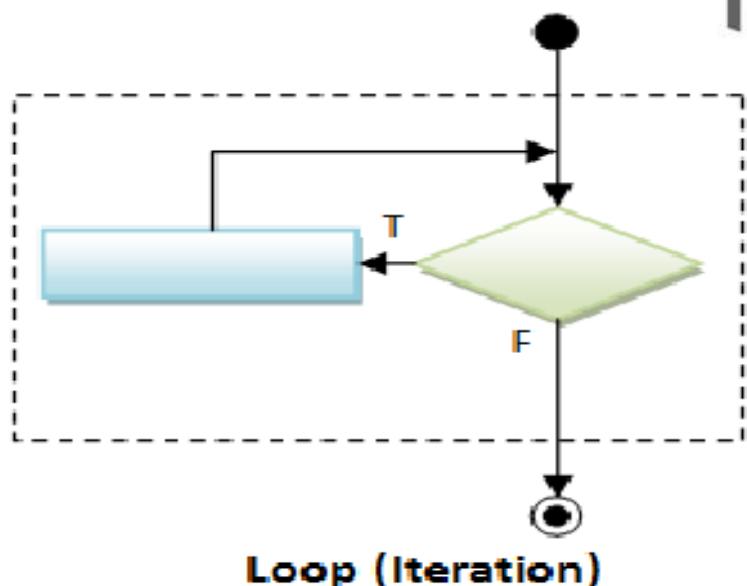


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Databases (and Tools)



GitHub





Biological Data and Databases

- To learn how to use a Web-based genomic databases and tools.
- To understand the types of information stored in genomic databases.
- To learn how to use different interfaces to find and retrieve genomic information.
- Write Python program to find patterns (start and stop codons) in DNA sequences



NCBI Resources How To Sign in to NCBI

All Databases Search

NCBI Home

Resource List (A-Z)

All Resources

Chemicals & Bioassays

Data & Software

DNA & RNA

Domains & Structures

Genes & Expression

Genetics & Medicine

Genomes & Maps

Homology

Literature

Proteins

Sequence Analysis

Taxonomy

Training & Tutorials

Variation

Welcome to NCBI

The National Center for Biotechnology Information advances science and health by providing access to biomedical and genomic information.

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Download
Transfer NCBI data to your computer


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Find help documents, attend a class or watch a tutorial


Develop
Use NCBI APIs and code libraries to build applications


Analyze
Identify an NCBI tool for your data analysis task


Research
Explore NCBI research and collaborative projects


Popular Resources

PubMed

Bookshelf

PubMed Central

PubMed Health

BLAST

Nucleotide

Genome

SNP

Gene

Protein

PubChem

NCBI News & Blog

NCBI to assist in Southern California genomics hackathon in January
30 Nov 2017

From January 10-12, 2018, the NCBI will help with a bioinformatics hackathon in

December 6th NCBI Minute: Keeping Current and Getting Help with NCBI Resources
30 Nov 2017

NCBI Browser



DB Interfaces: UniProt

The mission of [UniProt](#) is to provide the scientific community with a comprehensive, high-quality and freely accessible resource of protein sequence and functional information.

UniProtKB
UniProt Knowledgebase
Swiss-Prot (556,196)
Manually annotated and reviewed.
TrEMBL (98,705,220)
Automatically annotated and not reviewed.

UniRef
Sequence clusters

UniParc
Sequence archive

Proteomes

Supporting data

Literature citations
Cross-ref. databases

Taxonomy
Diseases

Subcellular locations
Keywords

News [BLOG](#) [TWITTER](#) [FACEBOOK](#) [RSS](#)

Forthcoming changes
There are currently no changes planned

UniProt release 2017_11
Sex determination in insects: 50 ways to achieve sex-specific splicing

UniProt release 2017_10
Of smell and social life

UniProt release 2017_09
News archive

[Getting started](#)



[UniProt data](#)

[Text search](#)

Our basic text search allows you to search all the resources available

[Download latest release](#)

Get the UniProt data

UniProt Browser



DB Interfaces: UniProt

- Domains give the protein special qualities:
 - Domain Names: *Alpha1, Alpha2, Alpha3, Ig-like C1-type*

Family & Domainsⁱ

Domains and Repeats

Feature key	Position(s)	Description	Actions	Graphical view	Length
Domain ⁱ	209 – 297	Ig-like C1-type	Add BLAST		89

Region

Feature key	Position(s)	Description	Actions	Graphical view	Length
Region ⁱ	25 – 114	Alpha-1	Add BLAST		90
Region ⁱ	115 – 206	Alpha-2	Add BLAST		92
Region ⁱ	207 – 298	Alpha-3	Add BLAST		92
Region ⁱ	299 – 309	Connecting peptide	Add BLAST		11

UniProt ID: P01899
A Protein Knowledge Base

http://www.uniprot.org/uniprot/P01899#family_and_domains

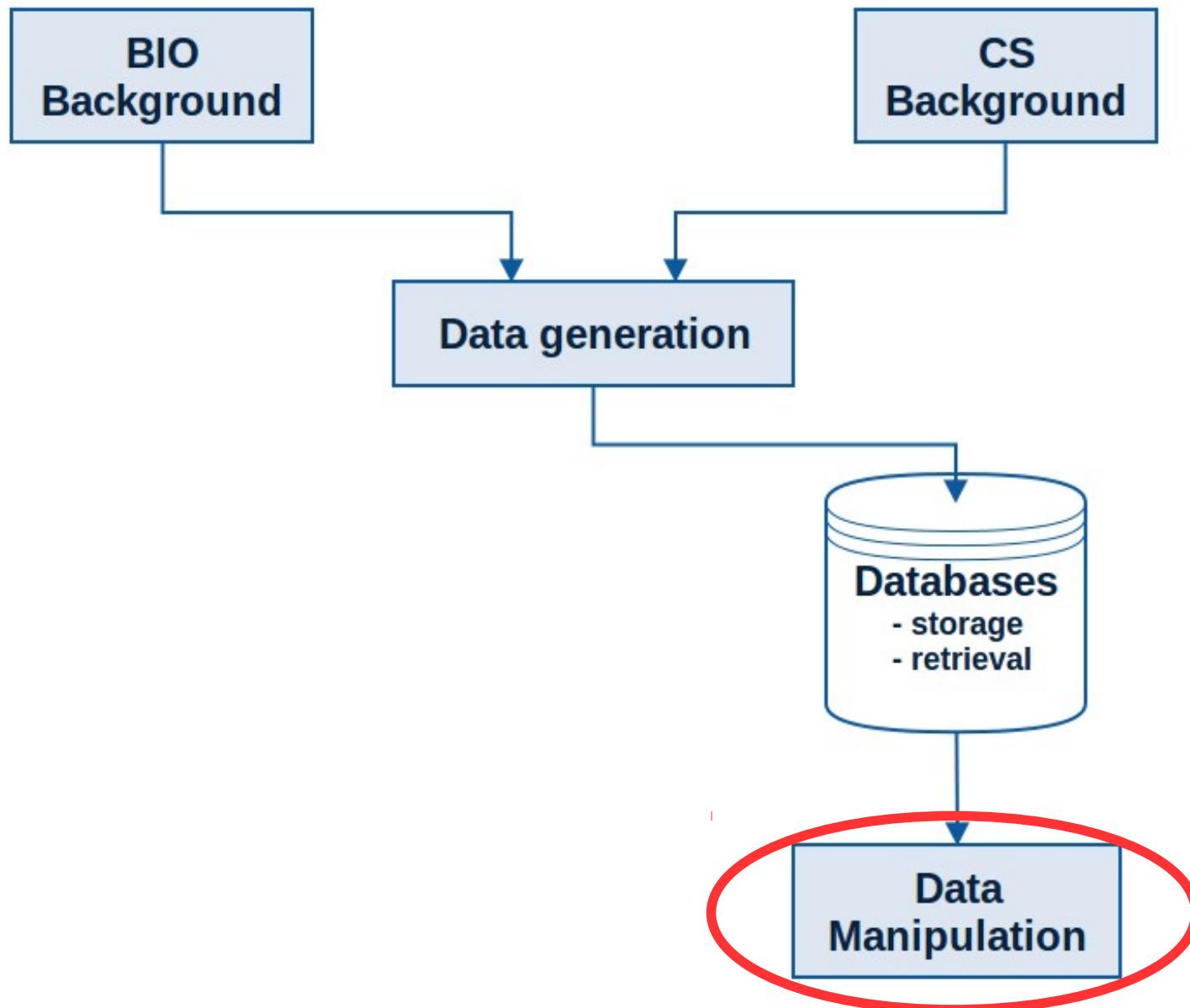


We Talked About...

Data Manipulation:
How we begin to find
meaning in the data



From The Course Outline





Databases...

Filter byⁱ

	Entry	Entry name	Protein names	Gene names	Organism	Length
Reviewed (556,196) Swiss-Prot	<input type="checkbox"/> Q91G88	006L_IIV6	Putative KilA-N domain-containing ...	IIV6-006L	Invertebrate iridescent virus 6 (IIV-6) (Chilo iridescent virus)	352
Unreviewed (98,705,220) TrEMBL	<input type="checkbox"/> Q6GZW6	009L_FRG3G	Putative helicase 009L	FV3-009L	Frog virus 3 (isolate Goorha) (FV-3)	948
Popular organisms	<input type="checkbox"/> Q91G70	026R_IIV6	Uncharacterized protein 026R	IIV6-026R	Invertebrate iridescent virus 6 (IIV-6) (Chilo iridescent virus)	59
Human (161,042)	<input type="checkbox"/> Q6GZU9	027R_FRG3G	Uncharacterized protein 027R	FV3-027R	Frog virus 3 (isolate Goorha) (FV-3)	970
Rice (122,677)	<input type="checkbox"/> Q197D7	023R_IIV3	Uncharacterized protein 023R	IIV3-023R	Invertebrate iridescent virus 3 (IIV-3) (Mosquito iridescent virus)	106
A. thaliana (89,135)	<input type="checkbox"/> Q91G65	032R_IIV6	Uncharacterized protein 032R	IIV6-032R	Invertebrate iridescent virus 6 (IIV-6) (Chilo iridescent virus)	100
Mouse (83,100)	<input type="checkbox"/> Q6GZU3	033R_FRG3G	Transmembrane protein 033R			

UniProt Browser



Pulling Data From Databases...

Homo sapiens genomic DNA, chromosome 21q

GenBank: BA000005.3

[FASTA](#) [Graphics](#)

[Go to:](#)

LOCUS BA000005 33543332 bp DNA linear CON 12-JUL-2008
DEFINITION Homo sapiens genomic DNA, chromosome 21q.
ACCESSION BA000005
VERSION BA000005.3
KEYWORDS .
SOURCE Homo sapiens (human)
ORGANISM [Homo sapiens](#)
Eukaryota; Metazoa; Chordata; Craniata; Vertebrata; Euteleostomi;
Mammalia; Eutheria; Euarchontoglires; Primates; Haplorrhini;
Catarrhini; Hominidae; Homo.
REFERENCE 1

Homo sapiens genomic DNA, chromosome 21q

GenBank: BA000005.3

[GenBank](#) [Graphics](#)

>BA000005.3 Homo sapiens genomic DNA, chromosome 21q
CATGTTCCACTTACAGATCTTCAAAAAGAGTGTTCAAAAGCTCTATGAAAAGGAATGTTAAC' TGTGAGTTAAATAAAAGCATCAAAAAAAAGTTCTGAGAATGCTCTGTCTAGTTTTATGTGAAGAT' TTCCATTTCCTCTATAAGCCTCAAAGCTGTCCAATGTCCACTTGAGATACTACAAAAGAGTGTTC' AAAGTGCTCAATGAAAAGGAATGTTCAGCTCTGTGAGTTAAATGCAAACATCACAAATAAGTTCTGA' ATGCTTCTGTCTAGTTTATGGGAAGATAATTCCGTGCCAGCGAAGGCTCAAGCTTCAAAGATA' CACTGCAAATTCTACAAAAGAGTGTTCAGTGTCTTATCAAAGAAAGTTCAACTCTGTGAG' GAATGTGCACATCACAAAGAAGTTCTGAGAATGCCTTCAGTGTGGTTTATGTGAAGATATTCCCT'

Mitochondrial processing				
Feature key	Position(s)	Description	Actions	Graphical view
Transit peptide ⁱ	1 - 77	Mitochondrion Sequence analysis	Add BLAST	
Chain ⁱ PRO_0000024369	78 - 581	Serine/threonine-protein kinase PINK1, mitochondrial	Add BLAST	

Amino acid modifications

Feature key	Position(s)	Description	Actions	Graphical view
Modified residue ⁱ	228	Phosphoserine; by autocatalysis 1 Publication		
Modified residue ⁱ	402	Phosphoserine; by autocatalysis 1 Publication		



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Using Tools With Databases

NIH > U.S. National Library of Medicine > NCBI

BLAST® » blastn suite

Home Recent Results Saved

I Nucleotide BLAST

blastn blastp blastx tblastn tblastx

Enter Query Sequence

BLASTN programs search nucleotide databases using a nucleotide query. [more...](#)

Enter accession number(s), gi(s), or FASTA sequence(s) [?](#) [Clear](#)

BA000005.3

Query subrange [?](#)

From To

Or, upload file [Choose File](#) No file chosen [?](#)

Job Title

Enter a descriptive title for your BLAST search [?](#)

Align two or more sequences [?](#)

Choose Search Set

Database Human genomic + transcript Mouse genomic + transcript Others (nr etc.):
Nucleotide collection (nr/nt) [?](#)

Organism Optional Enter organism name or id--completions will be suggested Exclude [+](#)
Enter organism common name, binomial, or tax id. Only 20 top taxa will be shown [?](#)

Exclude Optional Models (XM/XP) Uncultured/environmental sample sequences

Limit to Optional Sequences from type material

Entrez Query Optional [YouTube](#) [Create custom database](#)
Enter an Entrez query to limit search [?](#)

BLAST

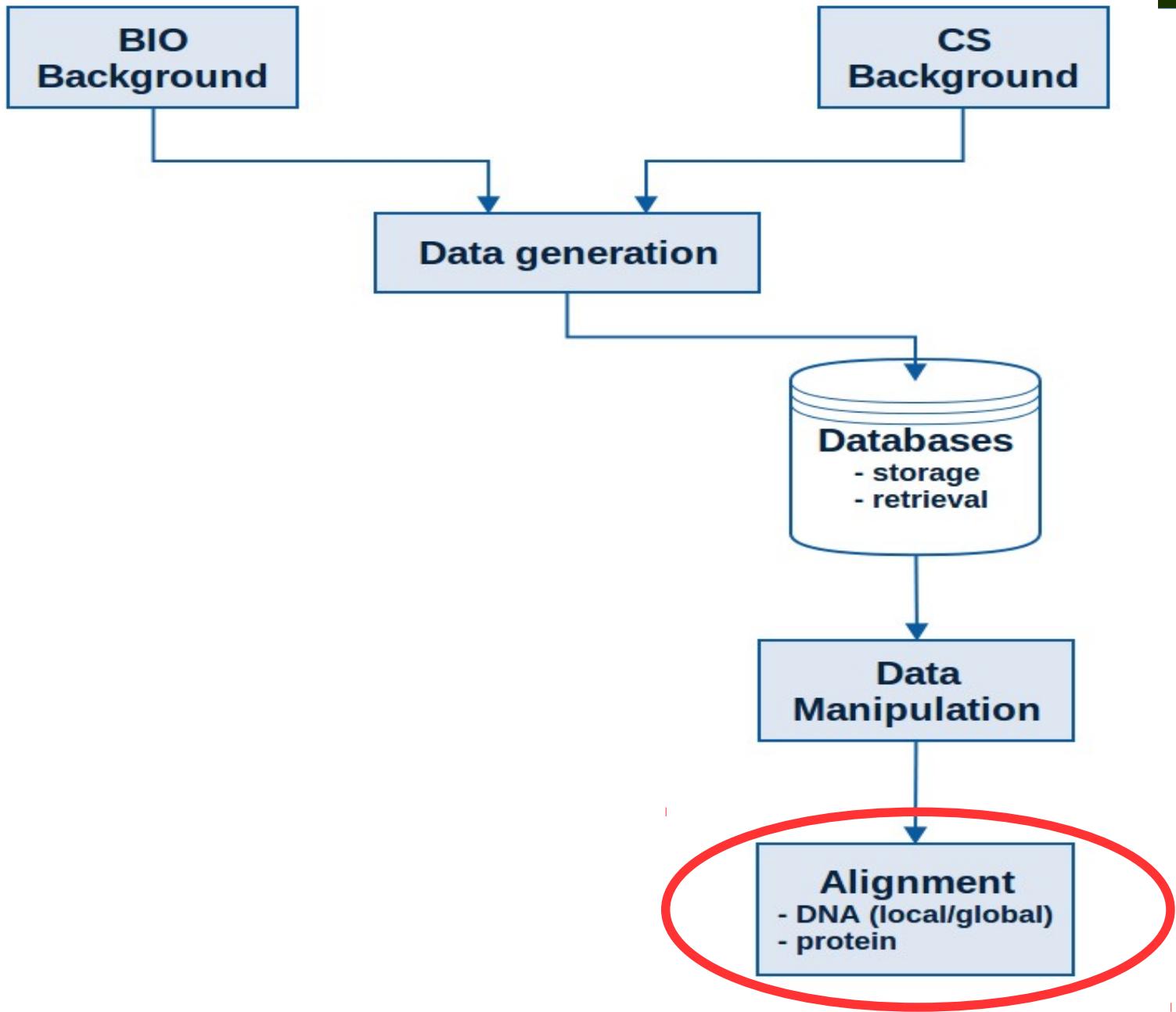


We Talked About...

Sequence Alignment:
Comparing sequences
to discover similarities
and differences



From The Course Outline





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Comparing Things!

- DNA sequences
- Genes
- Proteins
- Organisms



- **How to compare these things?**
- **What do we learn by comparison?**



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Sequence Alignment

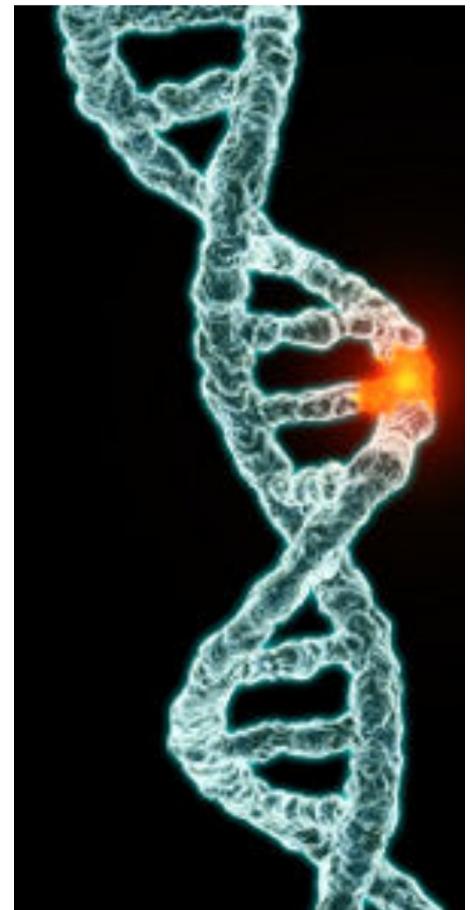
DNA - Nucleotides

- To understand the value of aligning genes and recognize the practical applications of this technique.
- To gain familiarity with the use of Web-based alignment tools to explore sequence similarity and understand how to modify their parameters.
- To know how the Needleman-Wunsch algorithm optimally aligns any two sequences.
- Understand how the Needleman-Wunsch algorithm can be modified to yield other alignments.



Aligning Sequences To Locate Mutations

- A natural process that changes the DNA sequence
- A common process
 - during replication of the human genome a “typo” occurs every 100,000 or so nucleotides
 - that’s about 120,000 typos each time one of our cells divides
 - most are repaired





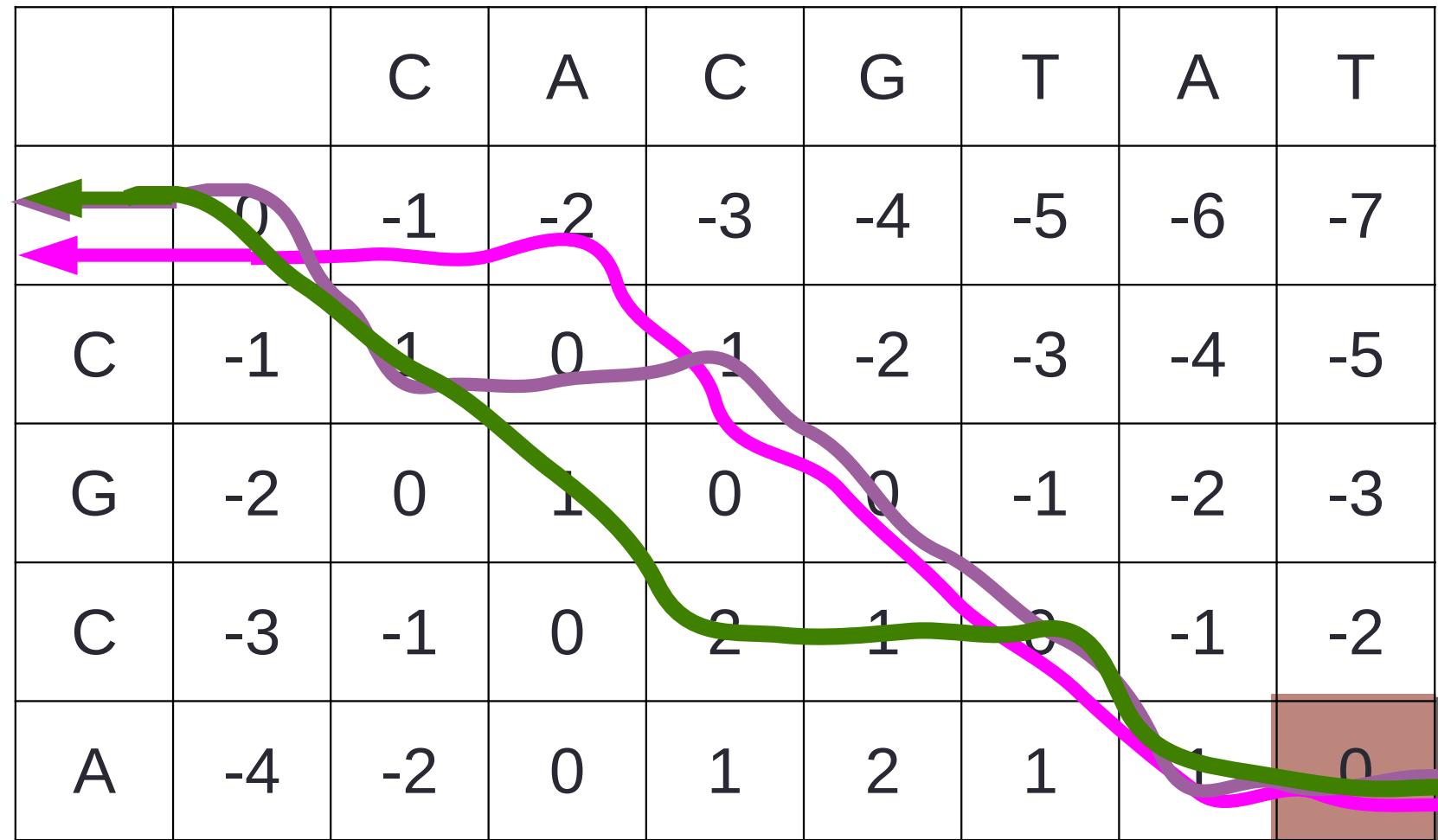
Sequence Alignment: Needleman-Wunsch

Let:

Match = +1

Mismatch = 0

Gap = -1



CACGTAT
--CGCA--

CACGTAT
C--GCA-

CACGTAT
CGC--A-



Global Pairwise Alignment

- Steps to begin
 - Initialization of the matrix
 - Calculation of the scores given for a character by character comparison.
 - Filling in a system of arrows in a trace-back matrix to uncover a path back to the start in the score matrix.
 - Deducing the alignment by following the arrows in the trace-back matrix.

	C	A	C	G	T	A	T	
0	-1	-2	-3	-4	-5	-6	-7	
C	-1	1	0	-1	-2	-3	-4	-5
G	-2	0	1	0	0	-1	-2	-3
C	-3	-1	0	2	1	0	-1	-2
A	-4	-2	0	1	2	1	1	0

op alignm



Pairwise Alignment Similarity and Relatedness

Alignment of a gene from two closely related viruses

Hemagglutinin gene from virus A: ATGAACGCAATACTCGTAGTT...

||||| ||||||||| |||||

Hemagglutinin gene from virus B: ATGAAGGCAATACTAGTAGTT...

Few Mismatches



Alignment of a gene from two distantly related viruses

Hemagglutinin gene from virus A: ATGAACGCAATACTCGTAGTT...

||| ||| ||| ||| | |

Hemagglutinin gene from virus C: ATGCACGAAATGCTCGGACCT...

Lots of Mismatches





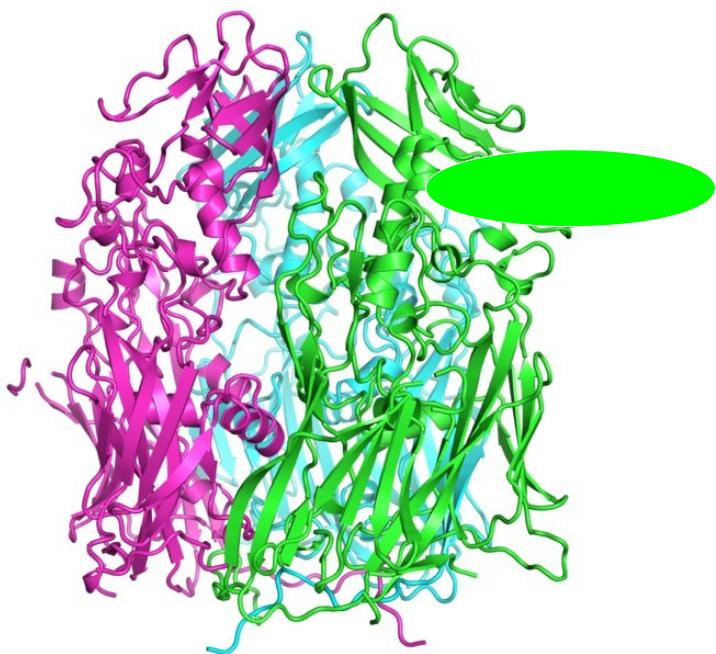
Sequence Alignment

Protein – Amino Acids

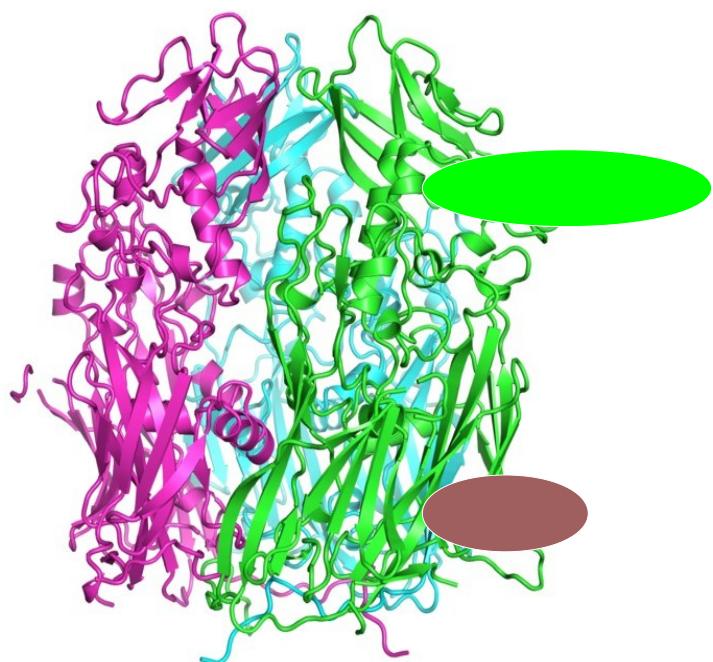
- Understand the use of a substitution matrix to score amino acid similarity in a protein sequence alignment.
- Gain experience using protein alignment to develop hypotheses about protein function based on sequence similarity.
- Know how protein alignment differs algorithmically from DNA alignment.
- Know how substitution matrix is developed and how different matrices might be used to produce better alignments in particular situations.

Comparing Protein

- Two proteins (wildtype, non-wildtype) are compared to find causes of disorder.



Healthy



Unhealthy



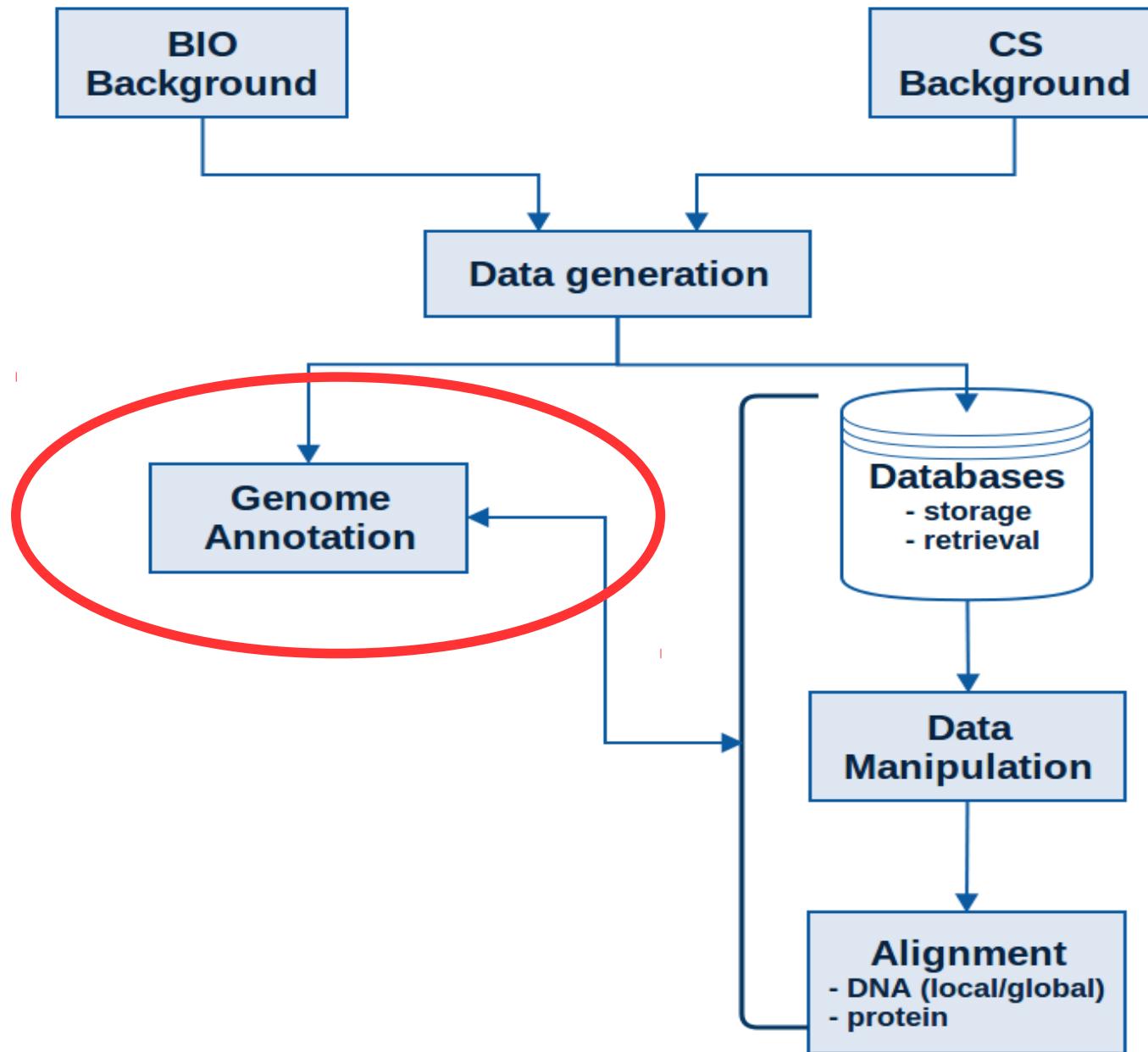
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We Talked About...

Genome annotation:
Finding relevant
regions in sequences



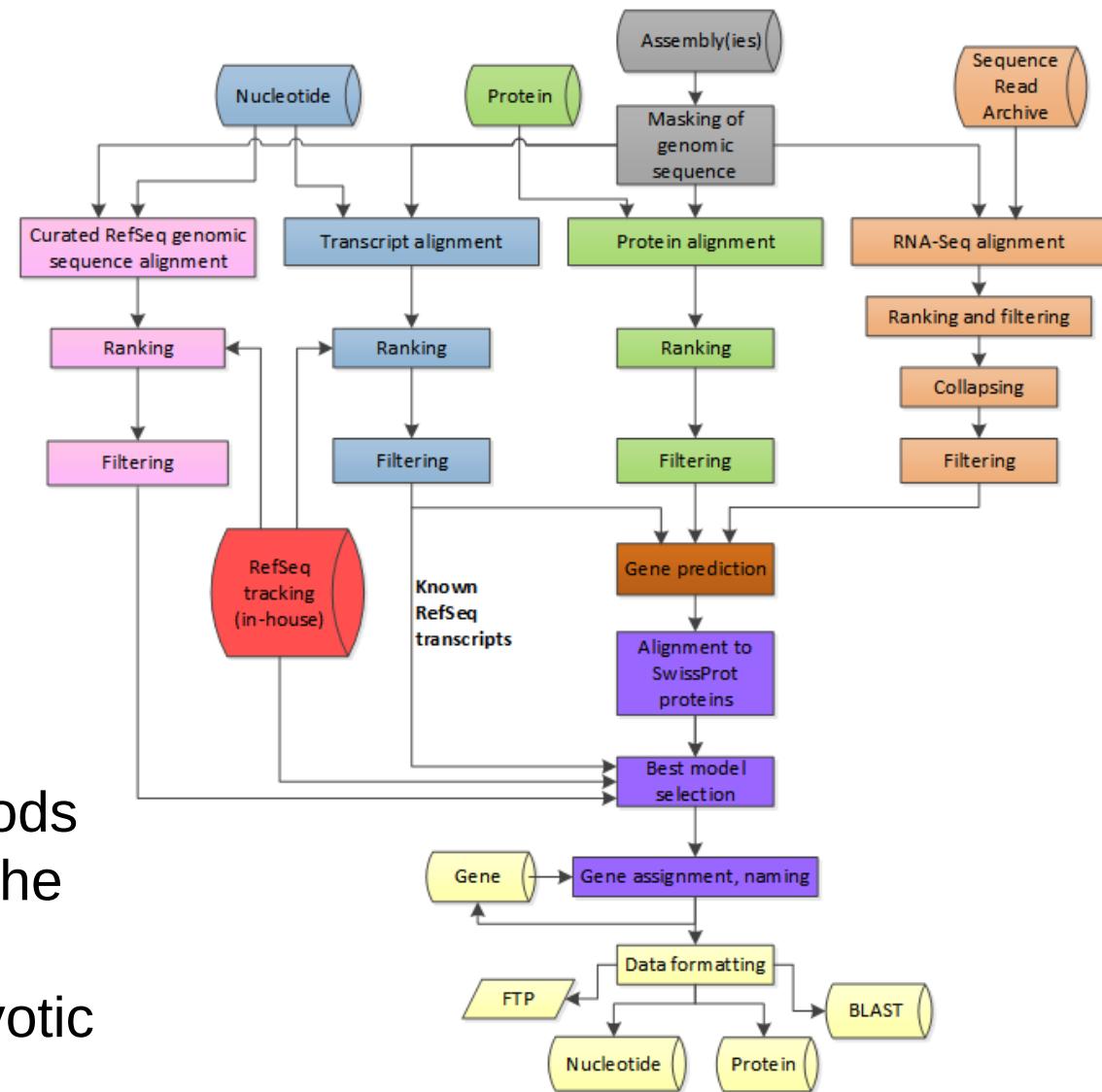
Course Outline





Genome Annotation: Algorithms

- Alignment-based
- Sequence-based
- Content-based
- Probabilistic
- Be able to combine content-based and probabilistic methods of **gene discovery** to identify the most probable locations of introns and exons in a eukaryotic DNA sequence





Genome Annotation

- Locate genes for proteins in sequences.

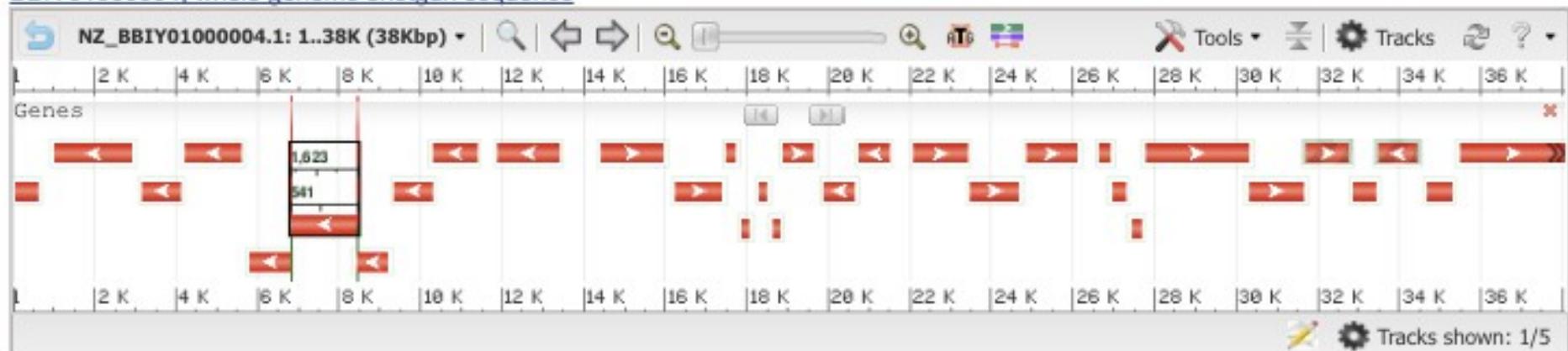
Genome Assembly Annotation

Type	Name	RefSeq	INSDC	Size (Mb)	GC%	Protein	tRNA	Other RNA	Gene	Pseudogene
master WGS	NZ_BBIY00000000.1	BBIY00000000.1		0.74	27.6	901	27	-	928	-

Genome Region

'Chrysanthemum coronarium' phytoplasma strain OY-V
BBIY01000004, whole genome shotgun sequence

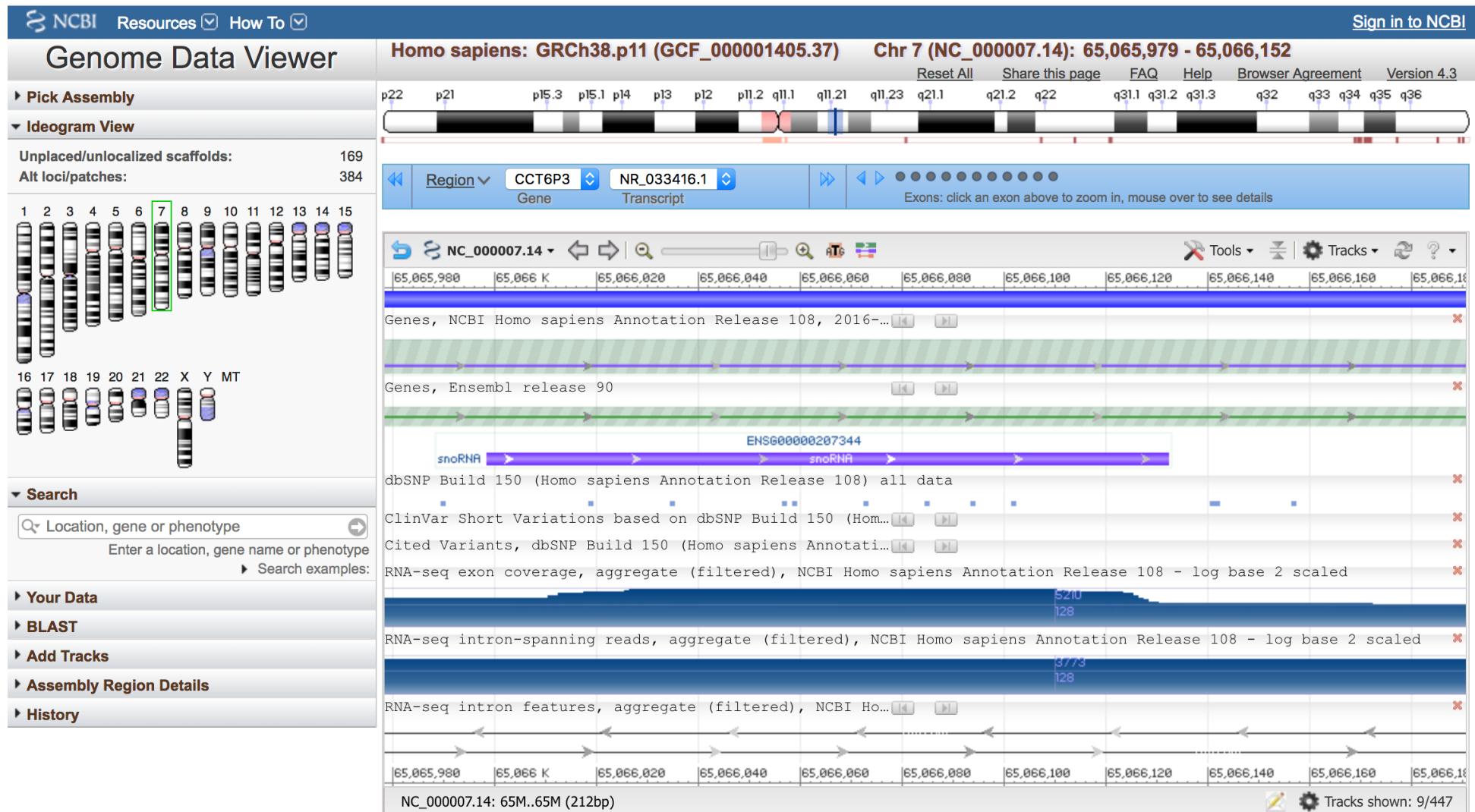
Go to nucleotide: [Graphics](#) [FASTA](#) [GenBank](#)



<https://www.ncbi.nlm.nih.gov/genome/browse/>



Genome Annotation



https://www.ncbi.nlm.nih.gov/genome/gdv/browser/?context=Nucleotide&acc=NR_145729.1

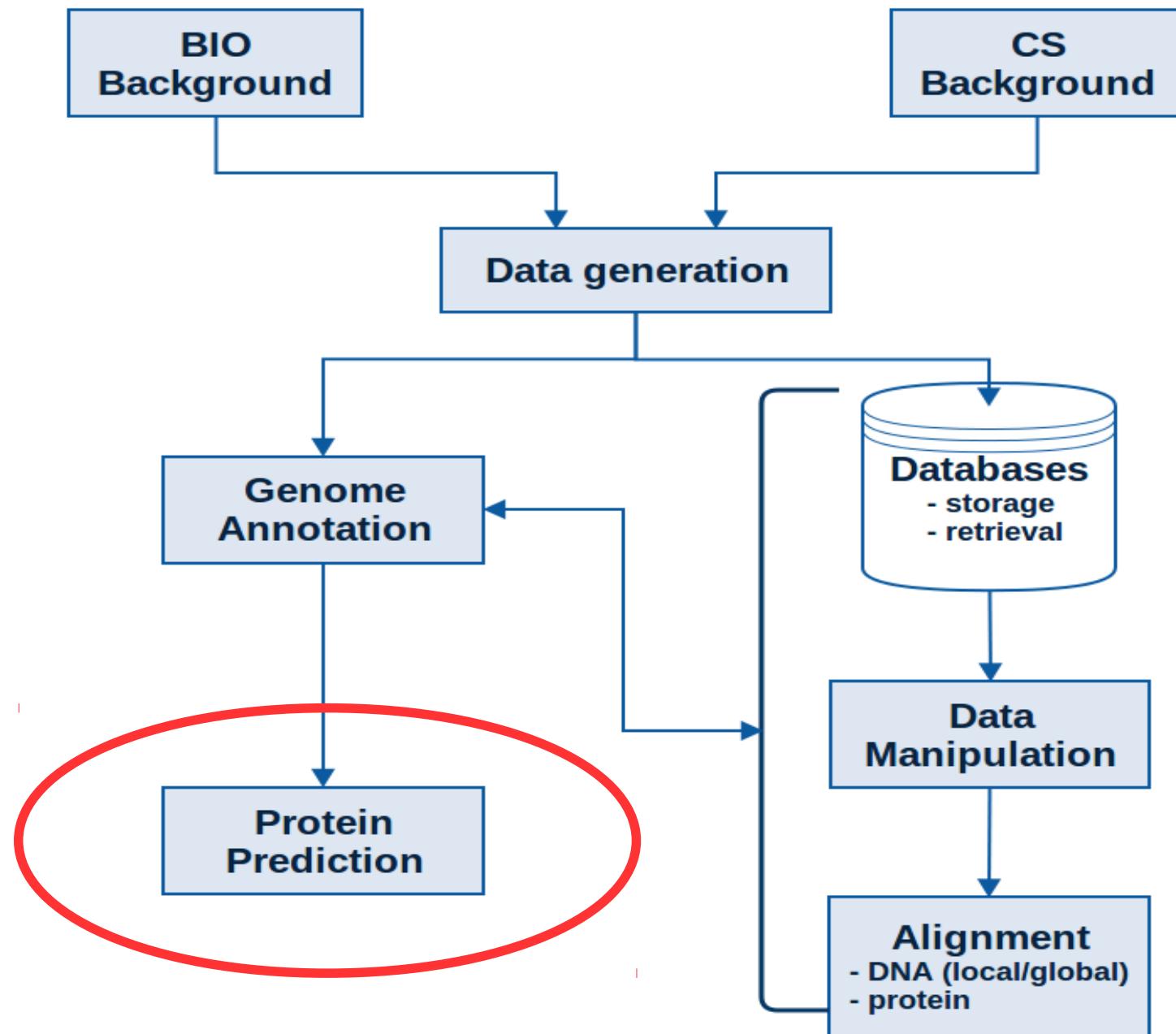


We Talked About...

Protein Prediction:
Determining what
protein exist in a
sequence and how they
might *behave*.



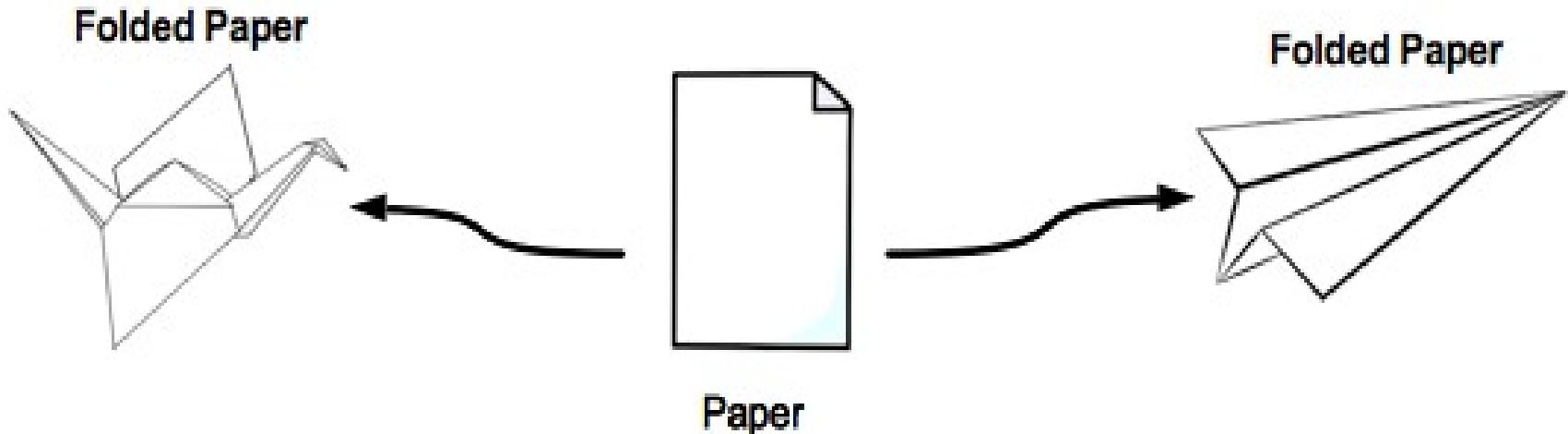
Course Outline





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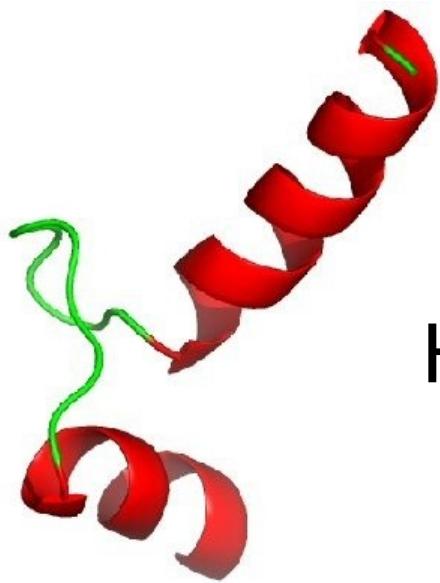
Properties From Folding



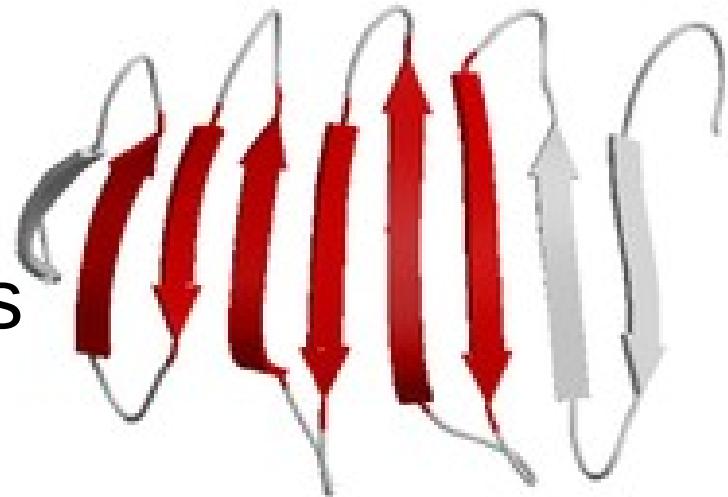


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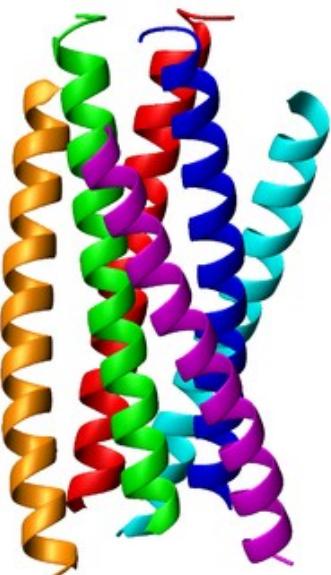
Parts of Protein (Structures)



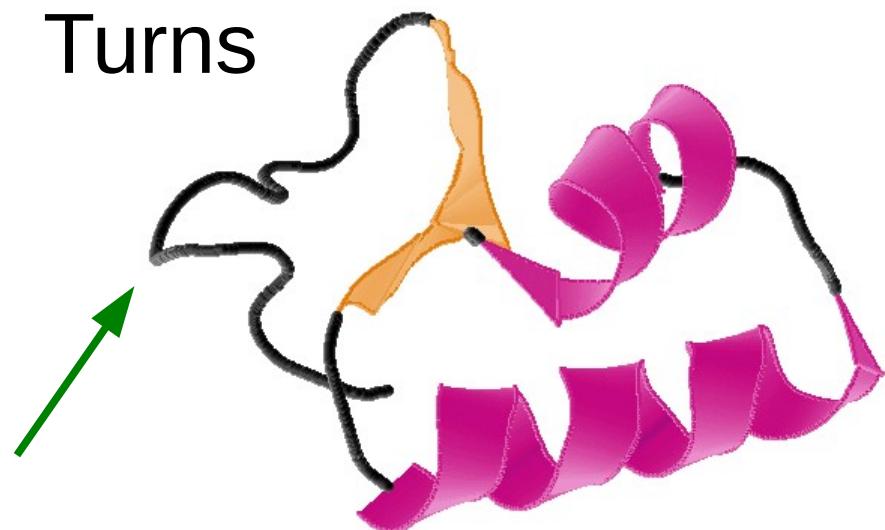
Helices



Sheets



Coils

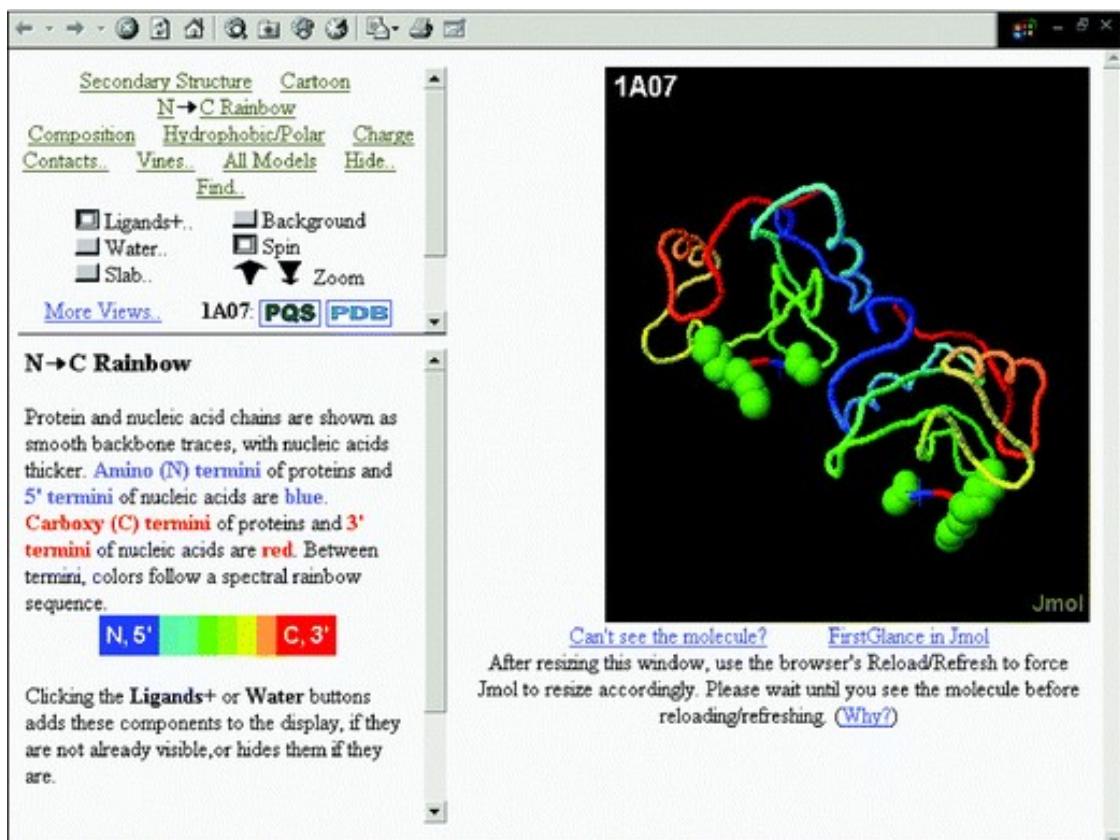


Turns



Protein Prediction

- Know how to use available tools to examine the experimentally determined structures of proteins and visualize structural and functional features
- Appreciate the value and limitations of predicting 3-D structure from sequence alone





Protein Folding - Applications

- **Protein must fold correctly to function**
- Misfolded proteins
 - Accumulation – Huntington's and Parkinson's disease
 - Tagged for degradation – emphysema, cystic fibrosis
 - Pharmaceutical chaperones – fold mutated proteins to render them functional
- Antiviral drug development
 - Antibiotics vs antivirals
 - Bacteria – cells
 - Viruses – invade host's cells



Bacteria



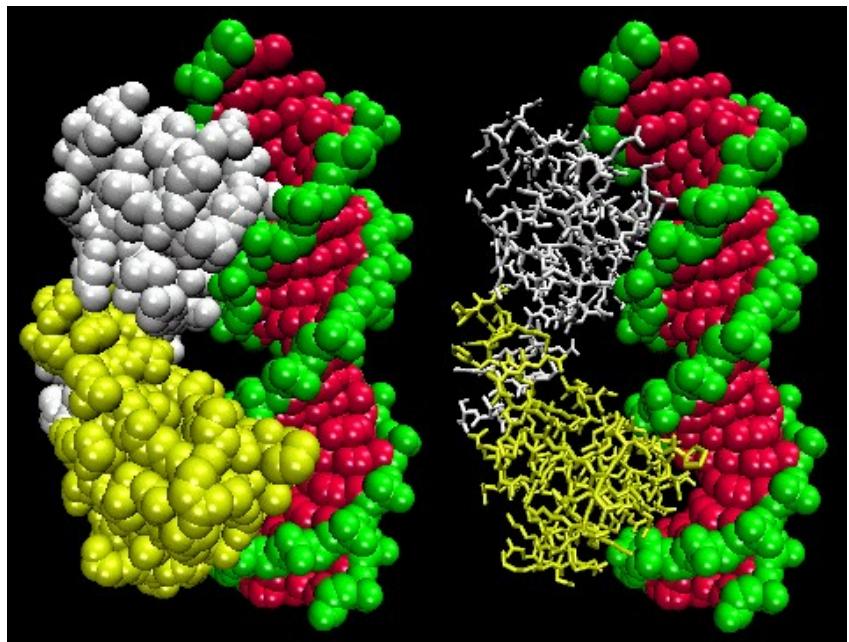
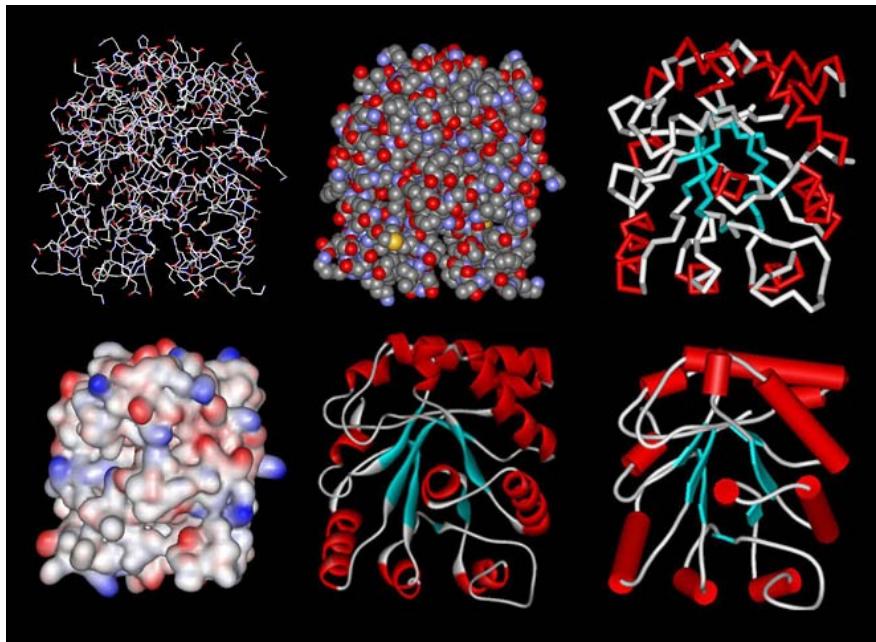
Virus

VS.



Protein DataBase (PDB)

- Database for 3-D structural data of large biological molecules
- <https://www.rcsb.org/>
- Data is viewable using jmol.





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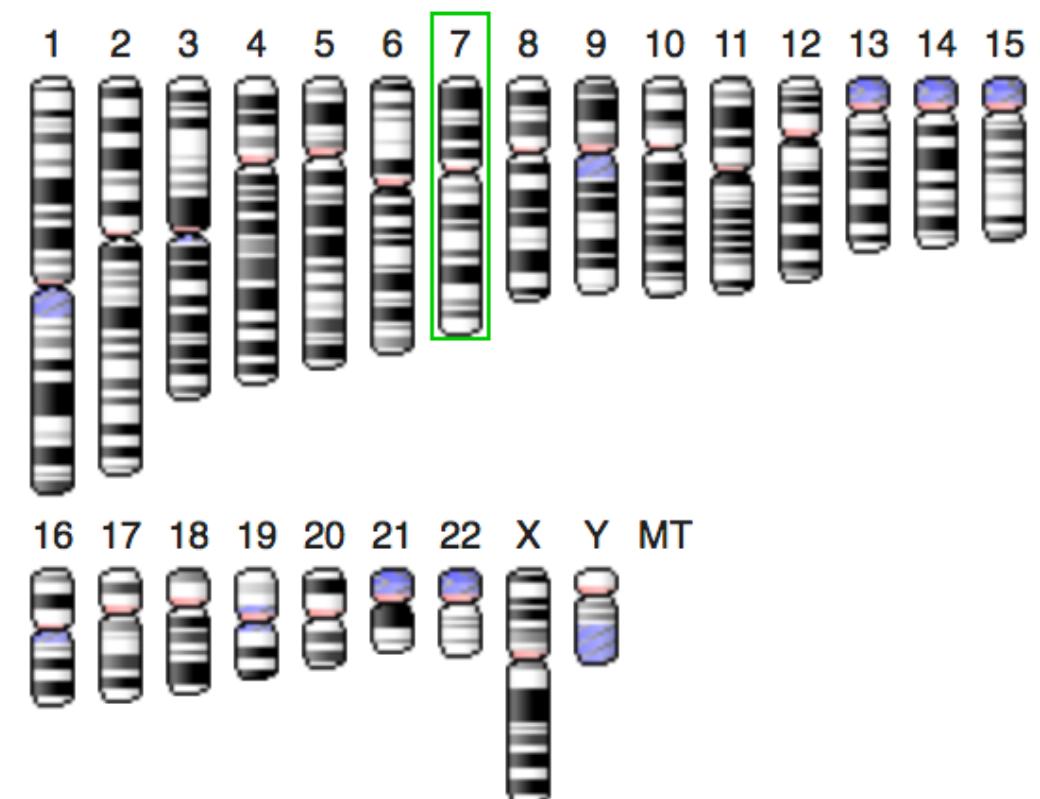
In Closing ...

Bioinformatics
is diverse
and exciting!



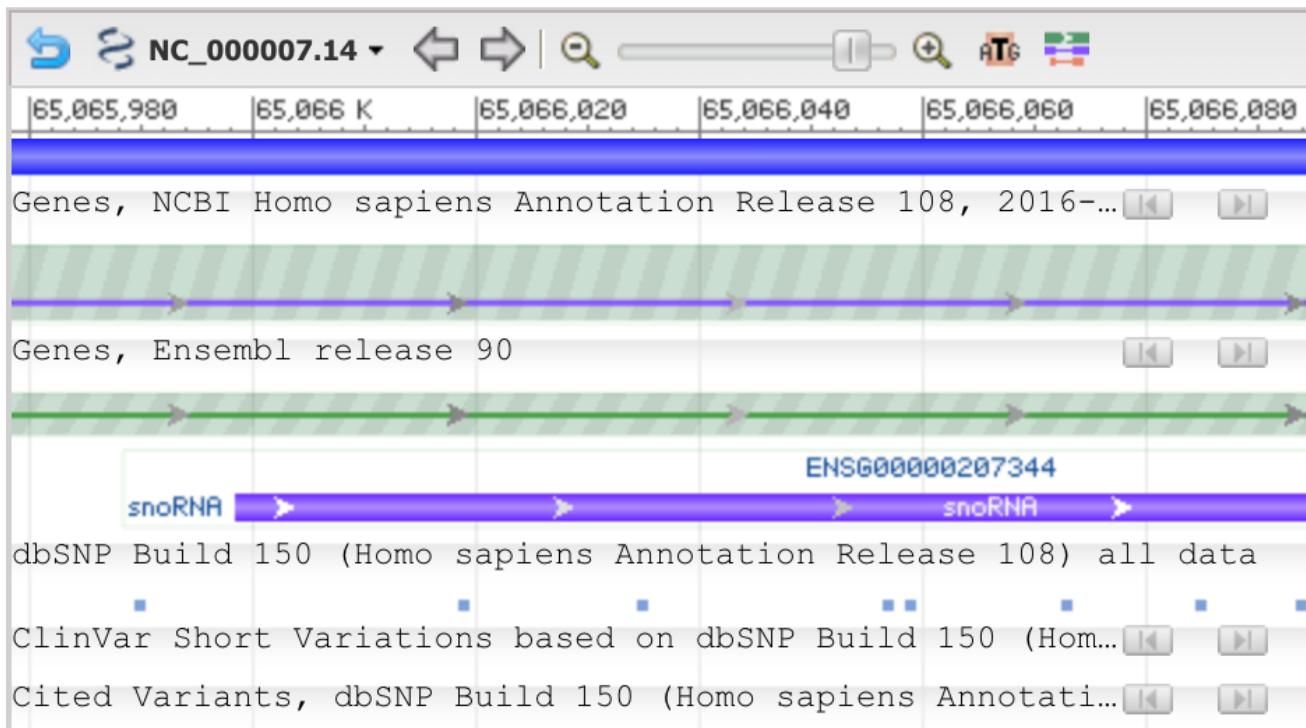
Bioinformatics Accomplishments

- ✓ A “big-picture” view of bioinformatics.
- ✓ An understanding of the objectives and limitations of bioinformatics.
- ✓ An understanding of the biological foundations of bioinformatics (genes and genomes, gene expression, etc.).





Bioinformatics Accomplishments



- An understanding of the computational foundations of bioinformatics (programming, databases, etc.).
- An understanding of how genetic information is obtained and processed.
- The ability to use basic bioinformatics software tools to study genetic information.



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What's Next?

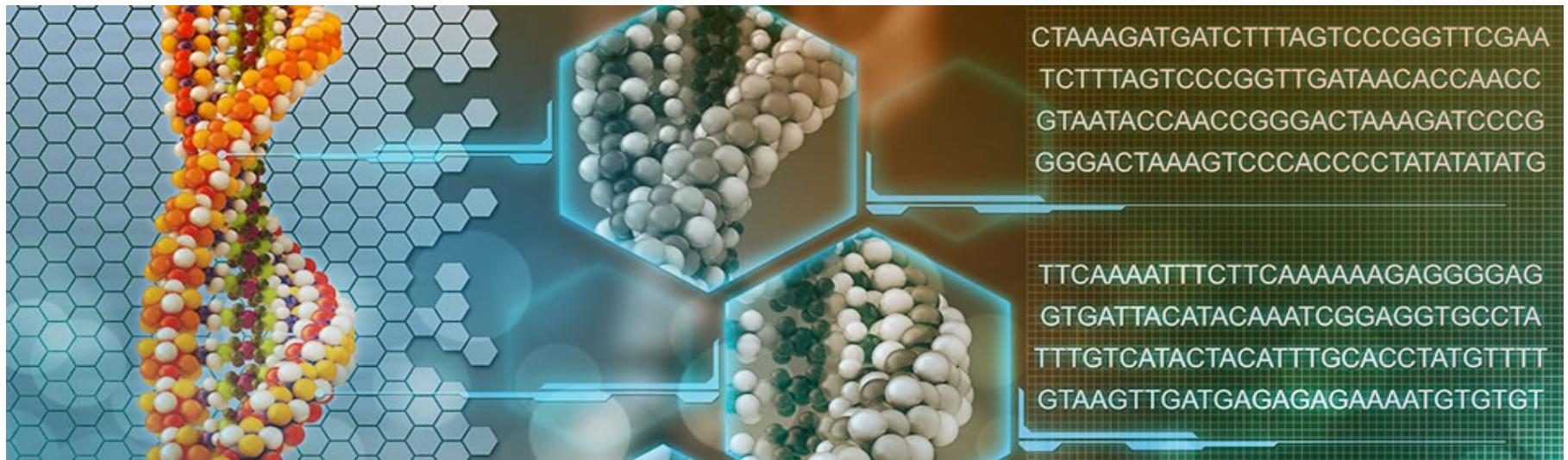
Bioinformatics could provide you with a satisfying career and plenty of room to advance



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The Value of the Bioinformatics Skills

There is a great need for Bioinformaticians!





Skills in Careers

- Biologists:
 - Computational skills
 - Mathematical /statistical
 - Programming for Automation
- Computer scientists
 - BioMedical skills
 - Understanding of biological systems and mechanisms
 - Early detection of disease by data
 - Modeling of therapeutic remedies
 - Others





Skills in Careers

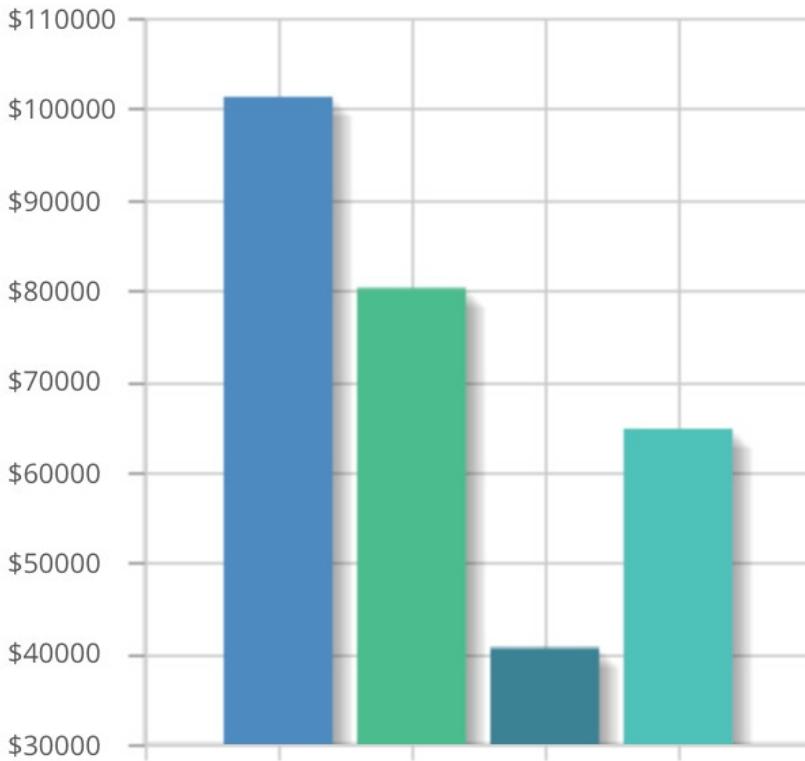
- Software (bioinformatics) engineer
- Research scientist in biotechnology
- Data scientist
- Project manager (pharmaceuticals, medical, etc)
- Computational immunologist
- Medical doctor (in clinical and research applications)





High Paying Careers

Avg. Wages For Related Jobs



- Biological science teachers, postsecondary
- Biomedical engineers
- Biological technicians
- Biological scientists, all other



High Paying Careers

Bioinformatics Research Scientist Salaries

36,327 Salaries Updated Aug 10, 2015

All Industries

All Company Sizes

All Years of Experience

Average Base Pay

\$90,214 /yr

Not enough reports to show salary distribution



Additional Cash Compensation [\(?\)](#)

Average \$xx,xxx

Range \$xx,xxx

How much does a Bioinformatics Research Scientist make?

The national average salary for a Bioinformatics Research Scientist is \$90,214 in United States. Filter by... [More](#)



High Paying Careers

Bioinformatics Scientist Salaries

287 Salaries Updated Nov 27, 2017

All Industries

All Company Sizes

All Years of Experience

Average Base Pay

\$113,545 /yr



Additional Cash Compensation [\(?\)](#)

Average **\$9,721**

Range **\$1,511 - \$17,411**

How much does a Bioinformatics Scientist make?

The national average salary for a Bioinformatics Scientist is \$113,545 in United States. Filter by location... [More](#)

Salaries for Related Job Titles

[Bioinformatics Analyst](#) \$76K

[Bioinformatics Research Scienti...](#) \$90K

[Senior Scientist, Computation...](#) \$129K

[Bioinformatics Engineer](#) \$101K



Careers in Bioinformatics

- Research scientist
 - Bioinformatician
 - Bioinformatics programmer
 - Software Developer
 - Analyst
 - Statistician
 - Physician
 - Project manager
 - Database developer and administrator
 - Technical assistant and technical sales representative
 - or any jobs where biologists are currently hired
- (some of these may require graduate education)



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Bioinformatics Internship and Career resources

Resources

<http://www.iscb.org/iscb-careers-job-database>

<http://www.bioinformatics.org/jobs/>

<http://www.bioplanet.com/>

<http://www.bio-itworld.com/BioIT/JobOpenings.aspx>

<http://www.biospace.com/>

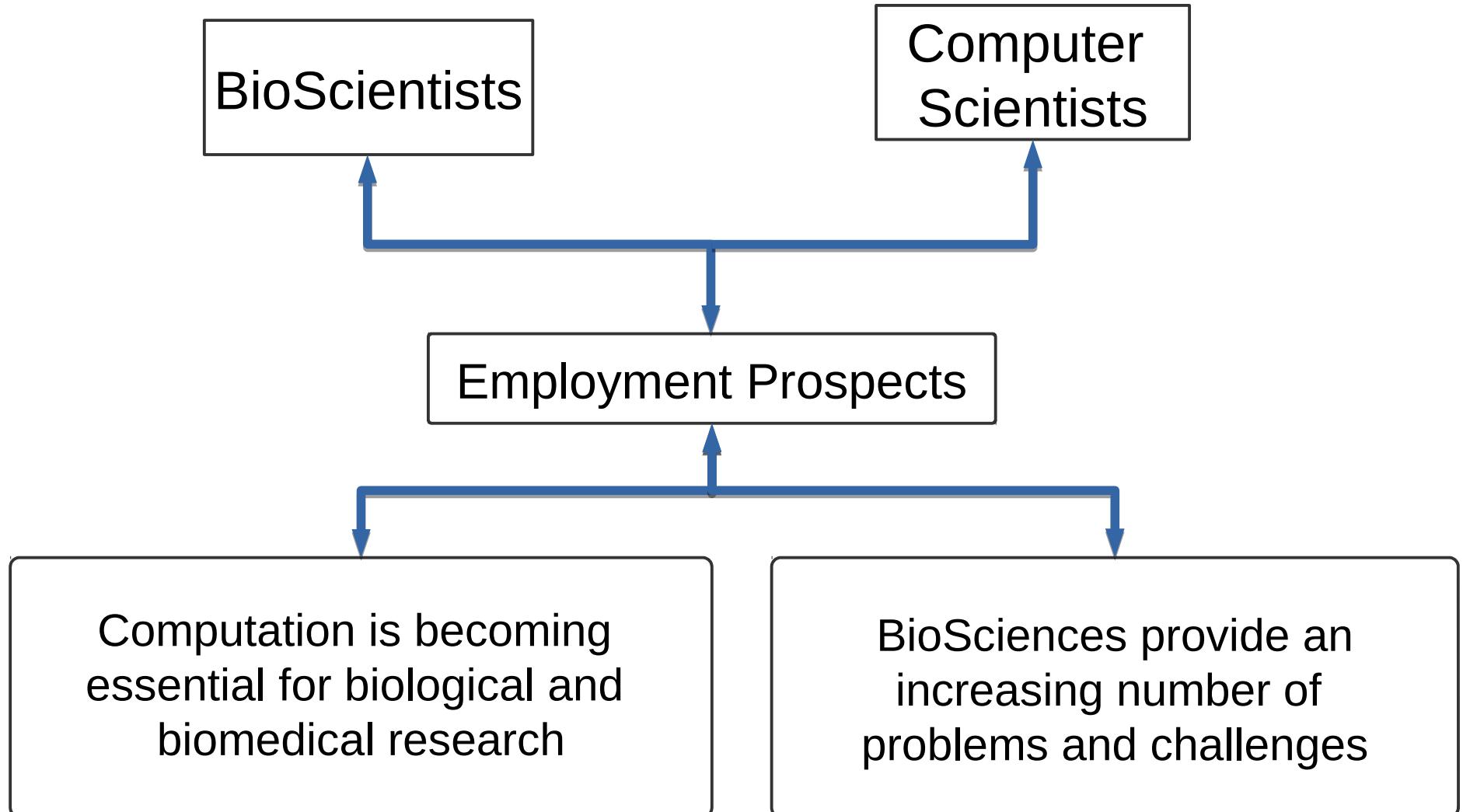
www.glassdoor.com

<http://www.jobs-salary.com/jobs.php?>

Campus Resources



The Value of the Bioinformatics Skills





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In Bioinformatics,
there is ...

S O M U C H

M O R E