

生物資訊簡介

Introduction to Bioinformatics

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Outline

1. **What is bioinformatics?** 何謂生物資訊
2. **Molecular genetics** 分子生物學
3. **Human genome project** 人類基因體計畫
4. **Databases & information retrieval** 資料庫與資訊擷取
5. **Global research issues** 全球研究議題
6. **Applications** 相關應用
7. **Challenge and future work** 挑戰與未來

What is *Bioinformatics*?

- 生物與電腦兩種科學之結合
- 利用電腦發展資料庫與分析工具，以協助分子生物學家之研究

.....The staggering volume of molecular data and its cryptic and subtle patterns have led to an absolute requirement for **computerized databases and analysis tools**..... new approaches to deal with the volume and complexity of data, and in providing researchers with **better access** to analysis and computing tools **advance understanding of our genetic legacy and its role in health and disease**.....

(abstracted from 'general introduction of NCBI')

Definition

by National Human Genome Research Institute

- Bioinformatics, as related to **genetics** and **genomics**, is a scientific subdiscipline that involves using **computer technology** to **collect, store, analyze and disseminate** biological data and information, such as DNA and amino acid sequences or annotations about those sequences.
- Scientists and clinicians use databases that organize and index such biological information to increase our understanding of health and disease and, in certain cases, as part of medical care.

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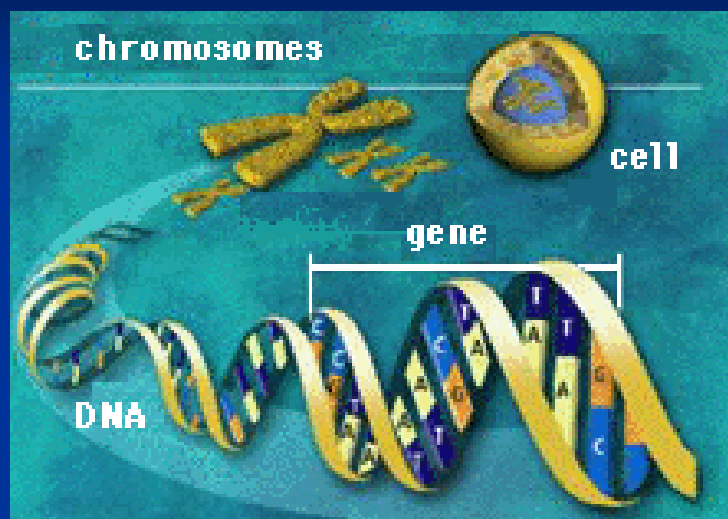
deoxyribonucleic acid
(DNA) in chromosome
can be represented as 4
characters: A, T, C, G

TTAGCTAGCCGCGC	TGCGACGTTAACGT
GATCTTAGCTAGCG	AGCAAGATCCTGAT
GGCATTATCTTCCG	TCGGATTCTAGAGG
GAGGCGCGATACGG	CGGAGGCGACGATG
AGGCGCGATATCTC	CGCGTATATGCGAC
TCTTATCTTCTTTC	GTTAACGTAGCAAG
GGAGGCGCGATATC	ATCCTGAGATTCTA
TCTCTTATCTTCCG	GAGGCGGAGGCGCT
GAGGCGCGATATCT	ATCTTCCGGAGGCG
CTCTTATCTTCTGA	CGATACGGAGGCGC
CGTTAACGTACGGA	GATATCTCTCTTAG
GGCGCGATATCTCT	CTAGCCGCGCGATC
CTTATCTTCTTAGC	TTAGCTAGCGGGCA
TAGCCGCGCGATCT	TCATGCTATTGAG
TAGCTAGCGGGCAT	GCGCTTAGCTAGCG
CATGCTCGGAGGCG	GGCATDOGCTATTTC
CGATATCTCTCTTA	GGATTCTAGAGGCG

Multi-disciplinary Research Group 跨多重領域研究

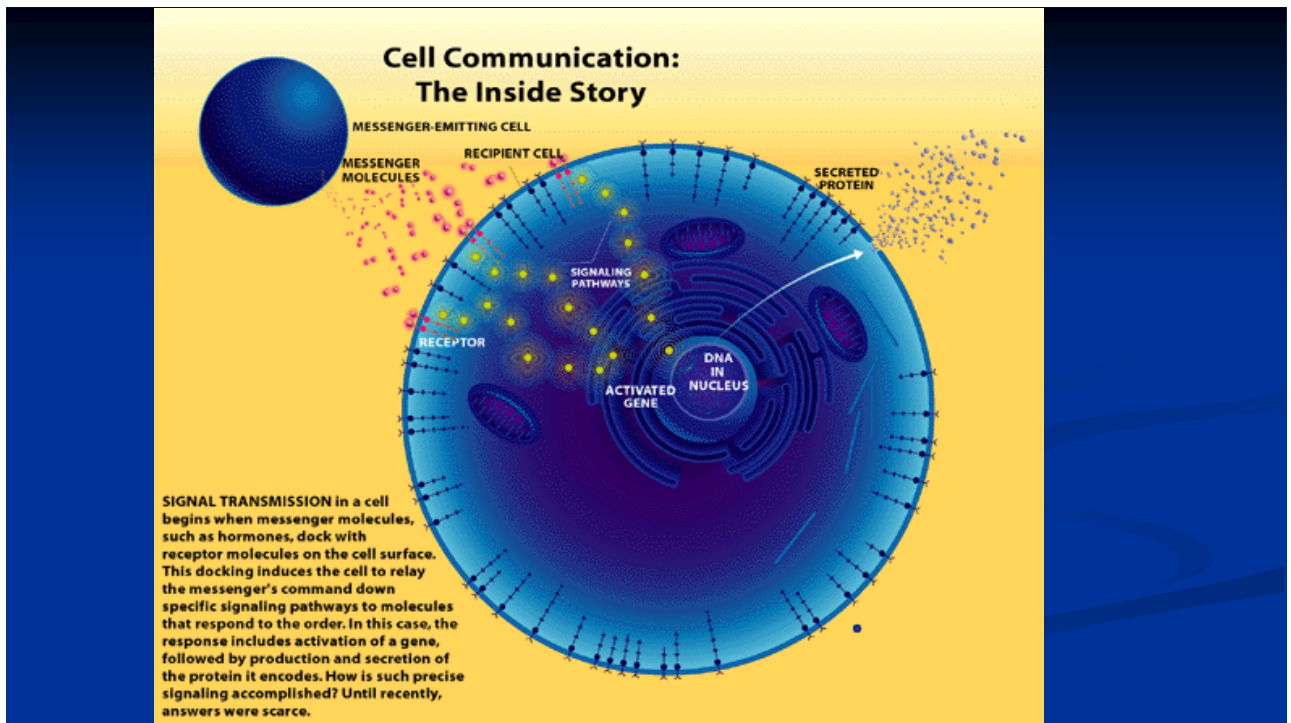
- Computer scientists
- Molecular biologists
- Mathematicians
- Biochemists
- Research physicians

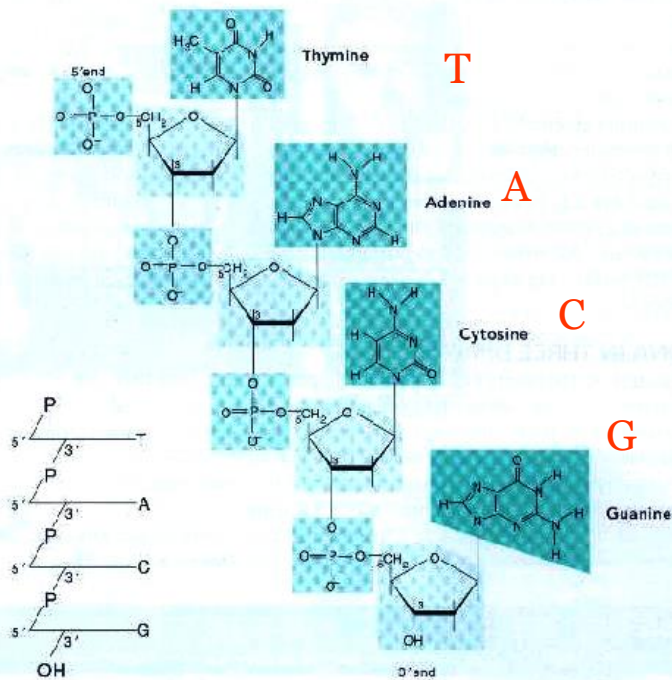
Molecular Genetics



Genes, DNA and Chromosomes explained

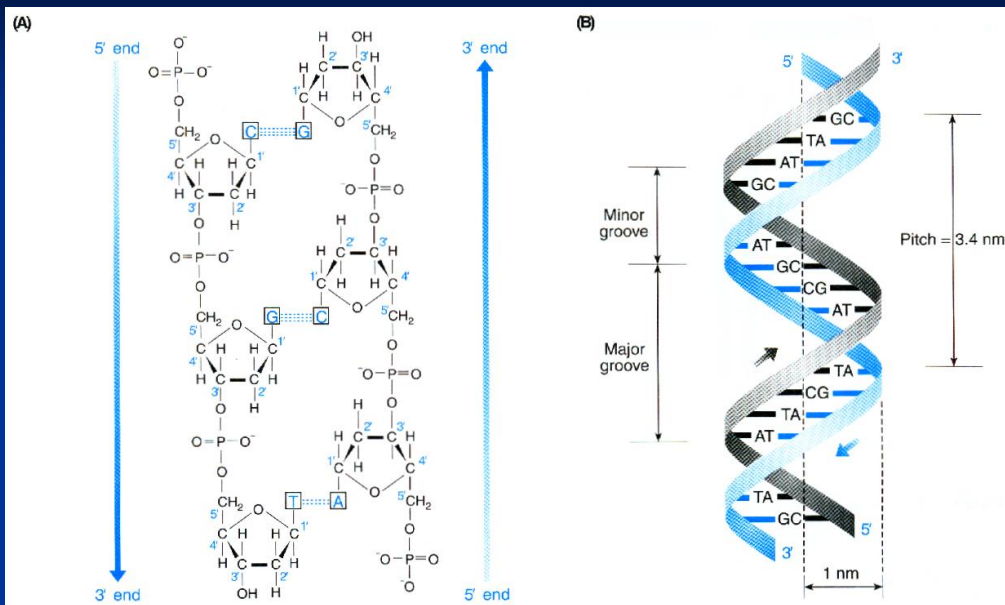
- https://www.youtube.com/watch?v=hywRdDVR76A&ab_channel=ScienceExplained





4 types of
DNA molecules

Double Strand



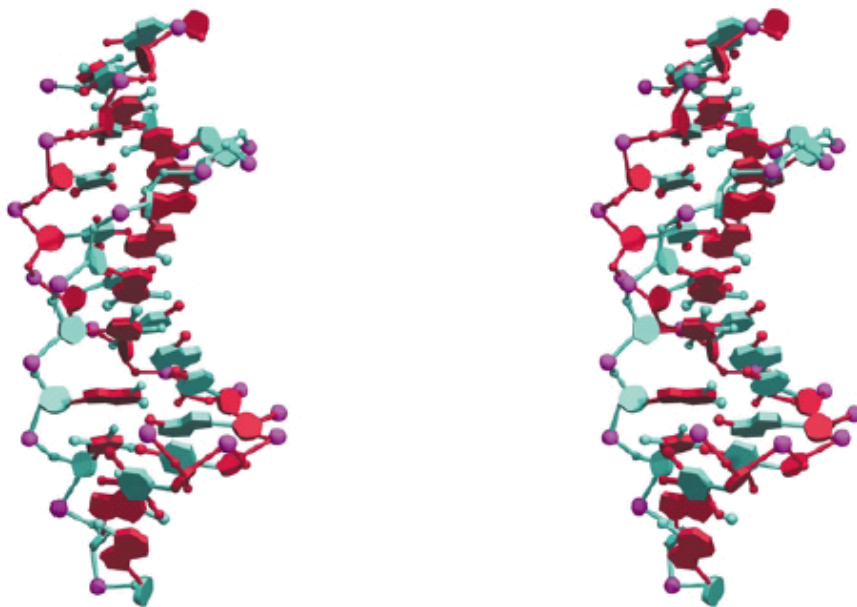
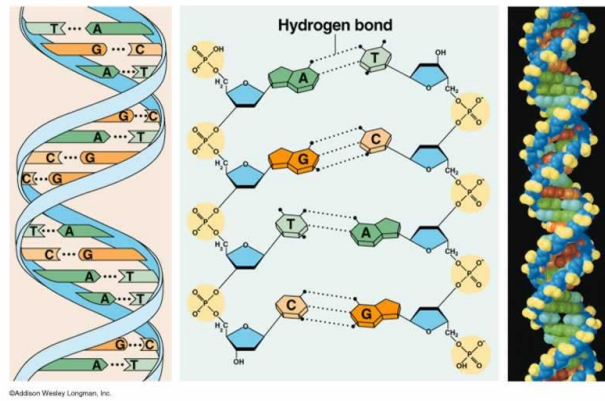
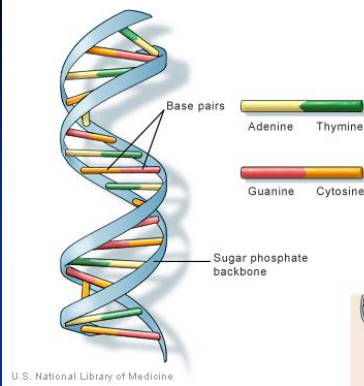
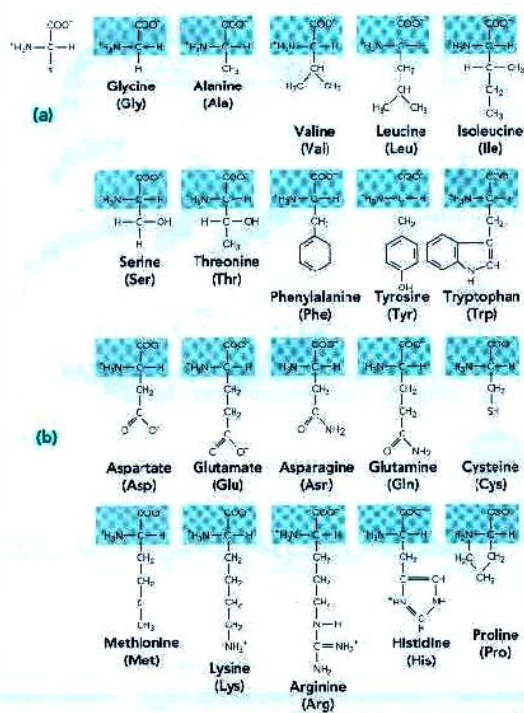
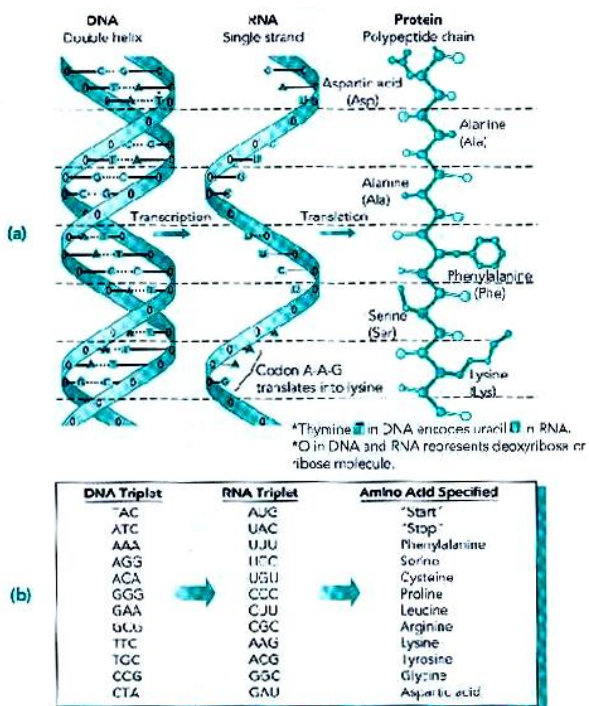


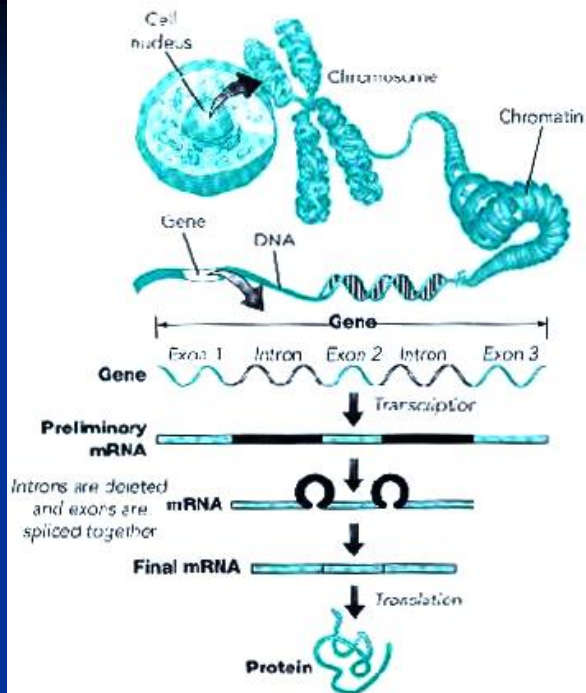
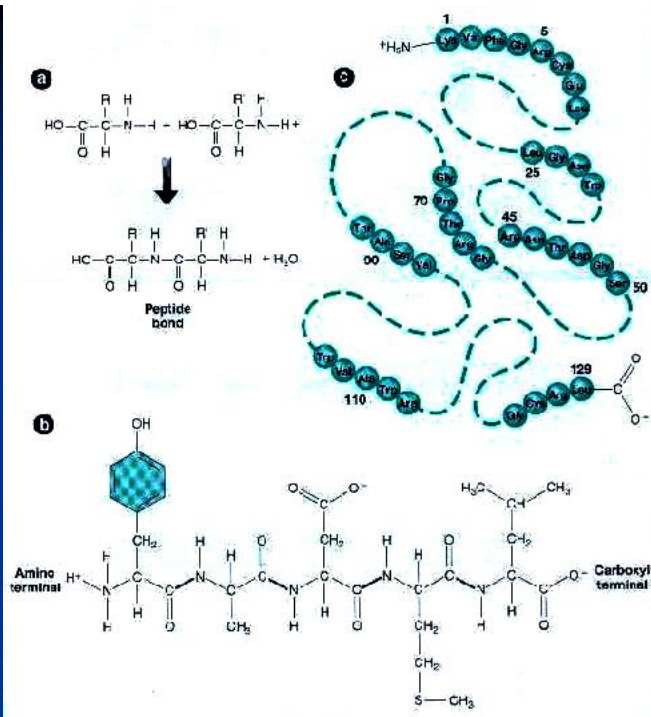
Plate I Double-helix of DNA. (See page 5.)



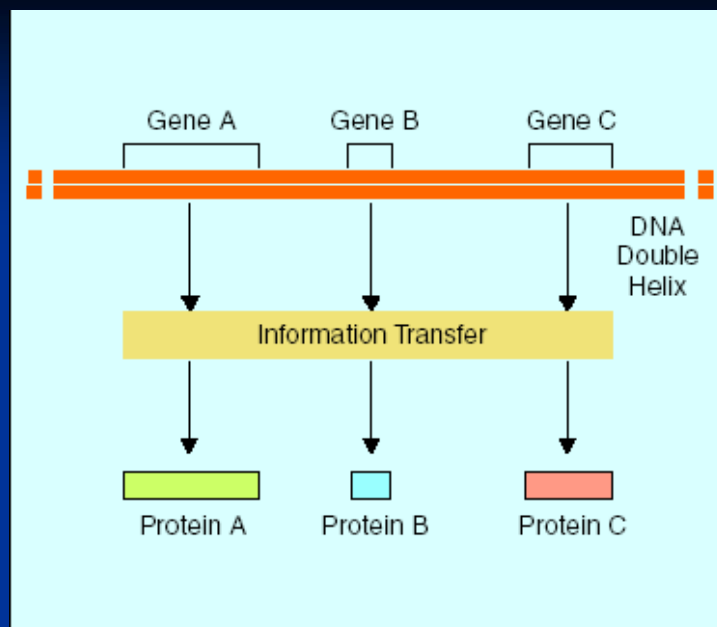
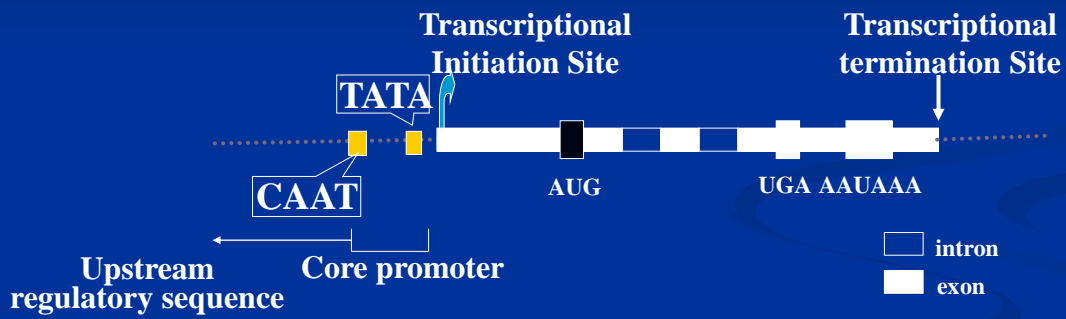
20 kinds of
amino acids
(氨基酸)



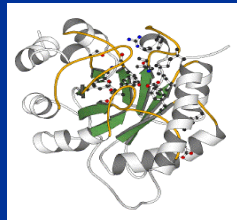
From DNA to Protein:
Transcription &
Translation



Gene Structure



Gene: protein-coding DNA



DNA

transcription

mRNA

translation

Protein

CCTGAGCCAAC TATTGATGAA



CCUGAGCCAACUAUUGAUGAA



PEPTIDE

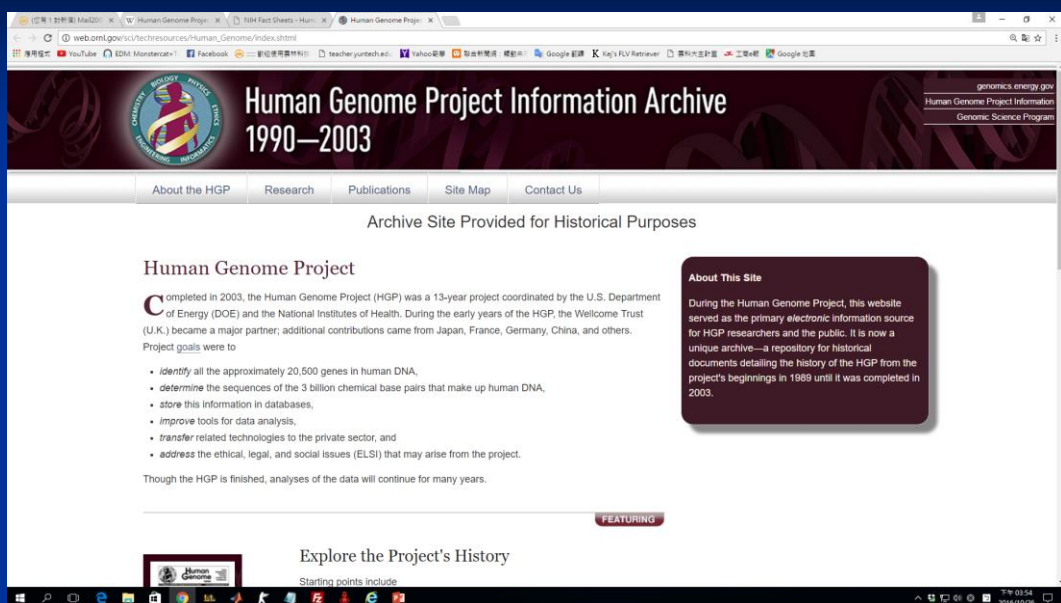
From DNA to protein - 3D film

<https://www.youtube.com/watch?v=gG7uCskUOrA>

人類基因體計畫 Human Genome Project

- 15-year-project; began in 1990, end in 2005
- Sponsored by the US Dept. of Energy and National Institute of Health; \$3 billion budget
- 18 countries worldwide participated, with significant contributions from the Sanger Center in the United Kingdom and research centers in Germany, France, and Japan. China recently joined the effort.

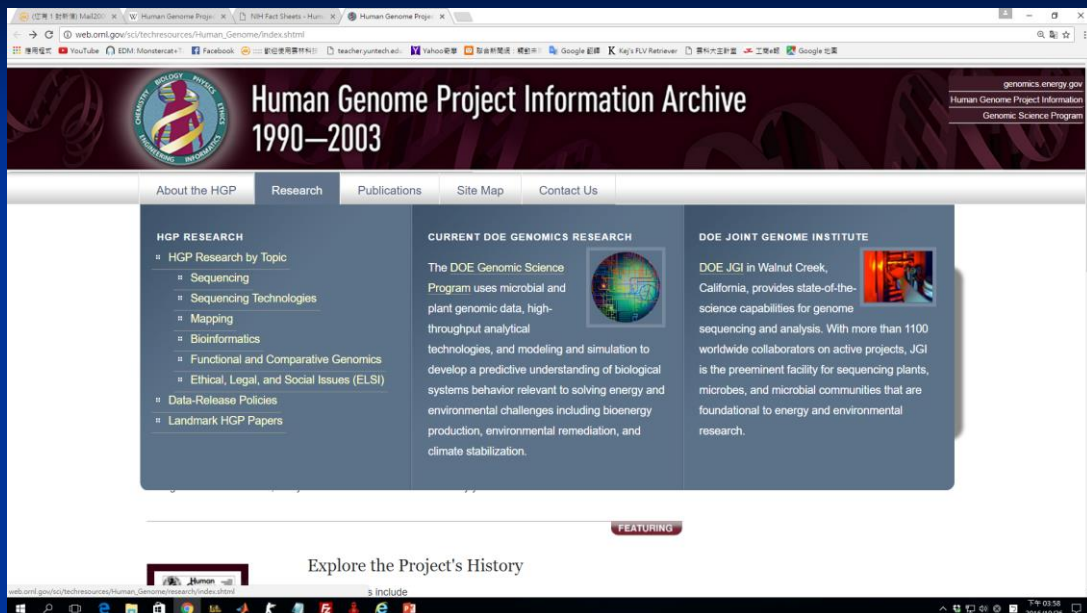
Human Genome Project



Project Goals

- **Identify** all the approximate 20,500 genes in human DNA
- **Determine** the sequences of the 3 billion chemical base pairs that make up human DNA
- **Store** this information in databases
- **Develop** tools for data analysis
- **Transfer** related technologies to the private sector
- **Address** the ethical, legal, and social issues

Human Genome Project



Highlights of the New 5-Year Plan for the U.S. Human Genome Project

■ Human DNA Sequencing

- Generate a working draft of 90% of the genome (2001).
- Obtain a complete, high-quality genomic sequence (2003).
- Make all data publicly available.

■ Sequencing Technology

- Create a long-term, sustainable sequencing capacity by improving current technology and developing highly efficient novel technologies.

■ Sequence Variation

- Develop technologies for rapid identification of DNA sequence variants.

■ Functional Genomics

- Expand support for current approaches and innovative technologies.

■ Comparative Genomics

- Obtain complete genomic sequences for *C. elegans* (1998), *Drosophila* (2002), and mouse (2008).

■ **Ethical, Legal, and Social Implications (ELSI)**

- Analyze and address implications of identifying DNA sequence information for individuals, families, and communities.
- Facilitate safe and effective integration of genetic technologies.
- Facilitate education about genomics in nonclinical and research settings.

■ **Bioinformatics and Computational Biology**

- Improve current databases and develop new databases and better tools for data generation and capture and comprehensive functional studies.

■ **Training**

- Nurture the training of genomic scientists and establish career paths.
- Increase the number of scholars knowledgeable in genomics and ethics, law, or the social sciences.

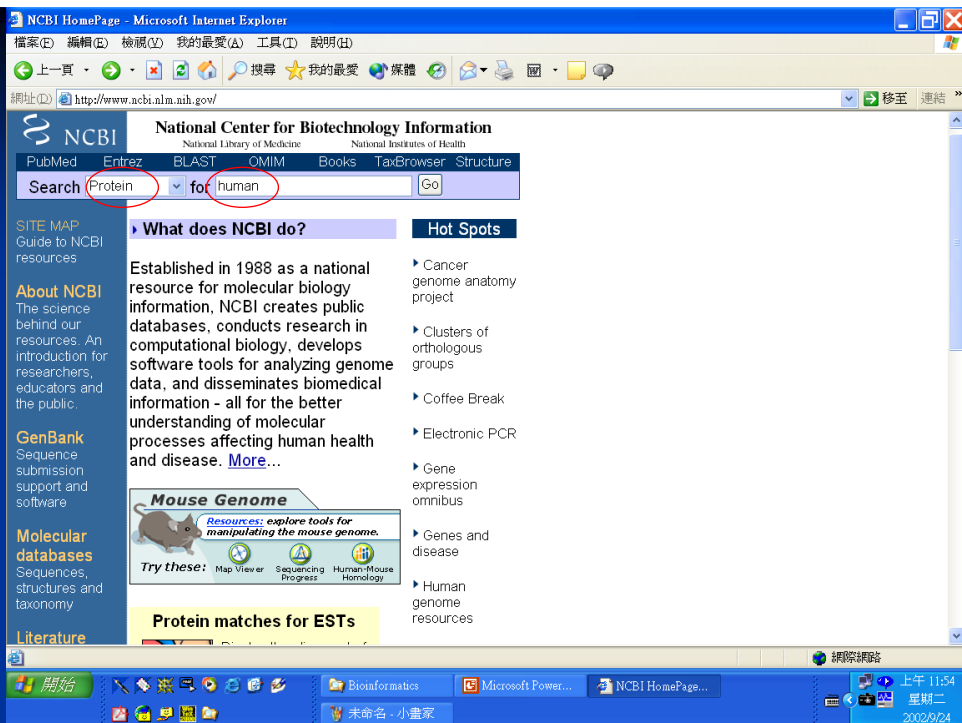
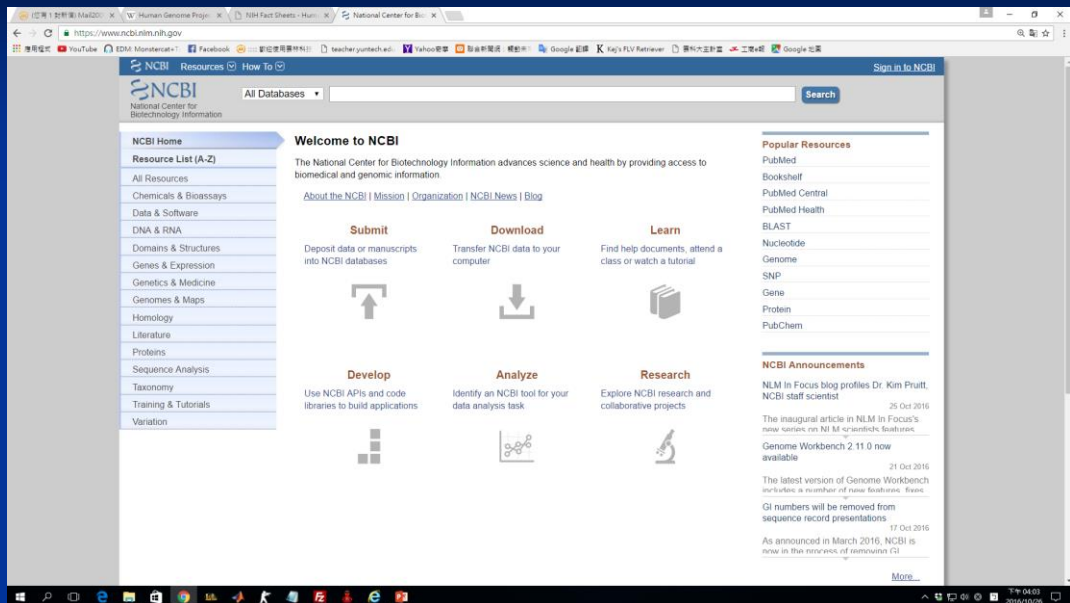
Genome Scientists' To-Do List

- Correct errors and proofread
- Fill tens of thousands of gaps
- Sequence the 7 percent
- Finish finding all the genes that make proteins
- Find the non-protein-making genes
- Discover the regulatory sequences
- Untangle the genes' intricate interactions with other molecules
- Identify gene functions

Databases & information retrieval

- **GeneBank** – Maintained by National Center for Biotechnology Information (NCBI), USA.
 - It is divided into several sections with sequences grouped according to species.
 - Searches can be made by keywords or by sequence.
 - <http://www.ncbi.nlm.nih.gov/>

NCBI website



Entrez-Protein - Microsoft Internet Explorer

檔案(F) 編輯(E) 檢視(V) 我的最愛(A) 工具(T) 說明(H)

網址(AD) http://www.ncbi.nlm.nih.gov/entrez/query.fcgi?db=protein&cmd=search&term=human

NCBI Protein

PubMed Nucleotide Protein Genome Structure PopSet Taxonomy OMIM Books

Search Protein for human Go Clear

Limits Preview/Index History Clipboard Details

About Entrez

Entrez Protein Help | FAQ

Batch Entrez: Upload a file of GI or accession numbers to retrieve sequences

Check sequence revision history

How to create WWW links to Entrez

LinkOut

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Display Summary Save Text Clip Add

Show: 20 Items 1-20 of 361255 Page 1 of 18063 Select page: 1 2 3 4 5 6 7 8 9 10

1: NP_003811 tumor necrosis factor receptor superfamily, member 14 precursor; herpesvirus entry mediator; CD40-like protein precursor; tumor necrosis factor receptor-like gene2; herpesvirus entry mediator A [Homo sapiens] gi23200041refINP_003811.2[23200041]

2: NP_683875 tumor necrosis factor receptor superfamily, member 12 isoform 11 precursor; translocating chain-association membrane protein; death domain receptor 3; death domain receptor 3 soluble form; apoptosis-mediating receptor; lymphocyte associated receptor of death; death receptor beta; apoptosis inducing receptor; WSL-1 protein [Homo sapiens] gi23200039refINP_683875.1[23200039]

3: NP_683874 tumor necrosis factor receptor superfamily, member 12 isoform 10 precursor; translocating chain-association membrane protein; death domain receptor 3; death domain receptor 3 soluble form; apoptosis-mediating receptor; lymphocyte associated receptor of death; death receptor beta; apoptosis inducing receptor; WSL-1 protein [Homo sapiens] gi23200037refINP_683874.1[23200037]

開始 生物informatics Microsoft Power... Entrez-Protein - ... 下午 01:00 星期二 2002/9/24

Limits Preview/Index History Clipboard Details

Display default Save Text Add to Clipboard Get Subsequence

1: NP_003811. tumor necrosis fa...[gi:23200041]

LOCUS TNFRSF14 283 aa linear PRI 19-SEP-2002

DEFINITION tumor necrosis factor receptor superfamily, member 14 precursor; herpesvirus entry mediator; CD40-like protein precursor; tumor necrosis factor receptor-like gene2; herpesvirus entry mediator A [Homo sapiens].

ACCESSION NP_003811

VERSION NP_003811.2 GI:23200041

DBSOURCE REFSEQ: accession NM_003820.2

KEYWORDS

SOURCE human.

ORGANISM Homo sapiens

REFERENCE 1 (residues 1 to 283)

AUTHORS Montgomery,R.I., Warner,M.S., Lum,B.J. and Spear,P.G.

TITLE Herpes simplex virus-1 entry into cells mediated by a novel member of the TNF/NGF receptor family

JOURNAL Cell 87 (3), 427-436 (1996)

MEDLINE 97053782

PUBMED 8898196

REFERENCE 2 (residues 1 to 283)

AUTHORS Hsu,H., Solovye,I., Colombero,A., Elliott,R., Kelley,M. and Boyle,W.J.

TITLE ATAR, a novel tumor necrosis factor receptor family member, signals through TRAF2 and TRAF5

JOURNAL J. Biol. Chem. 272 (21), 13471-13474 (1997)

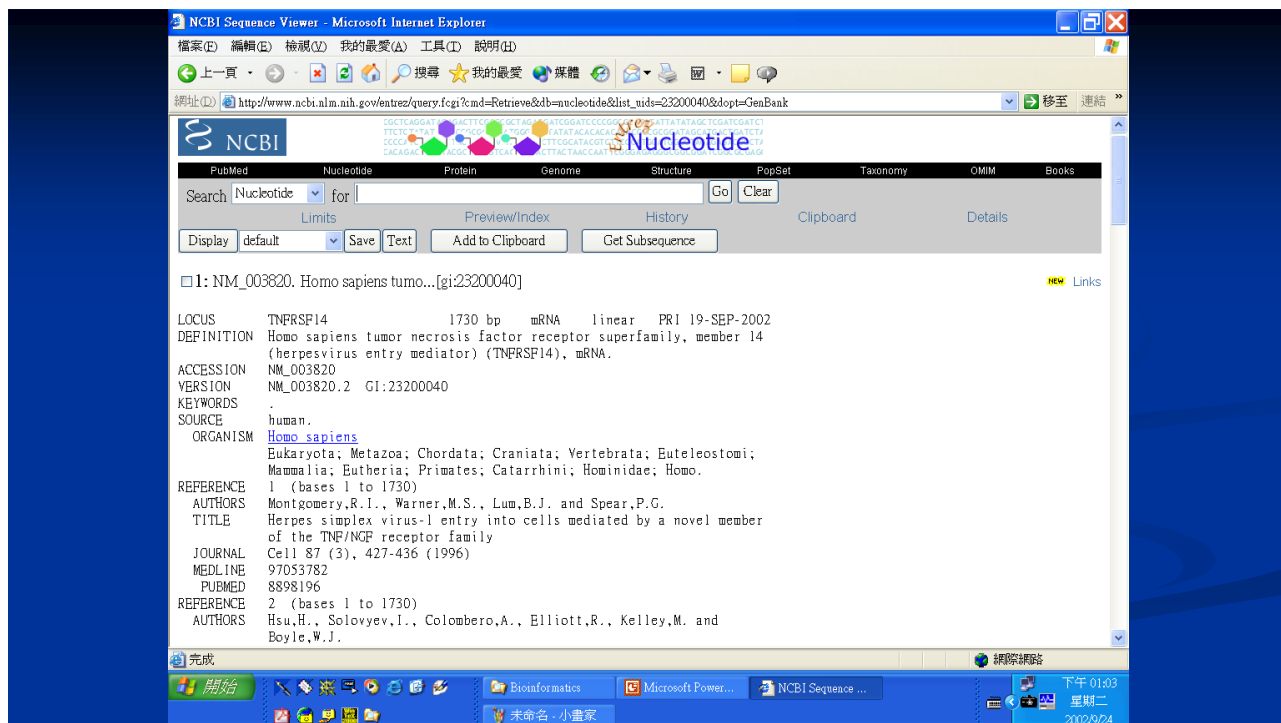
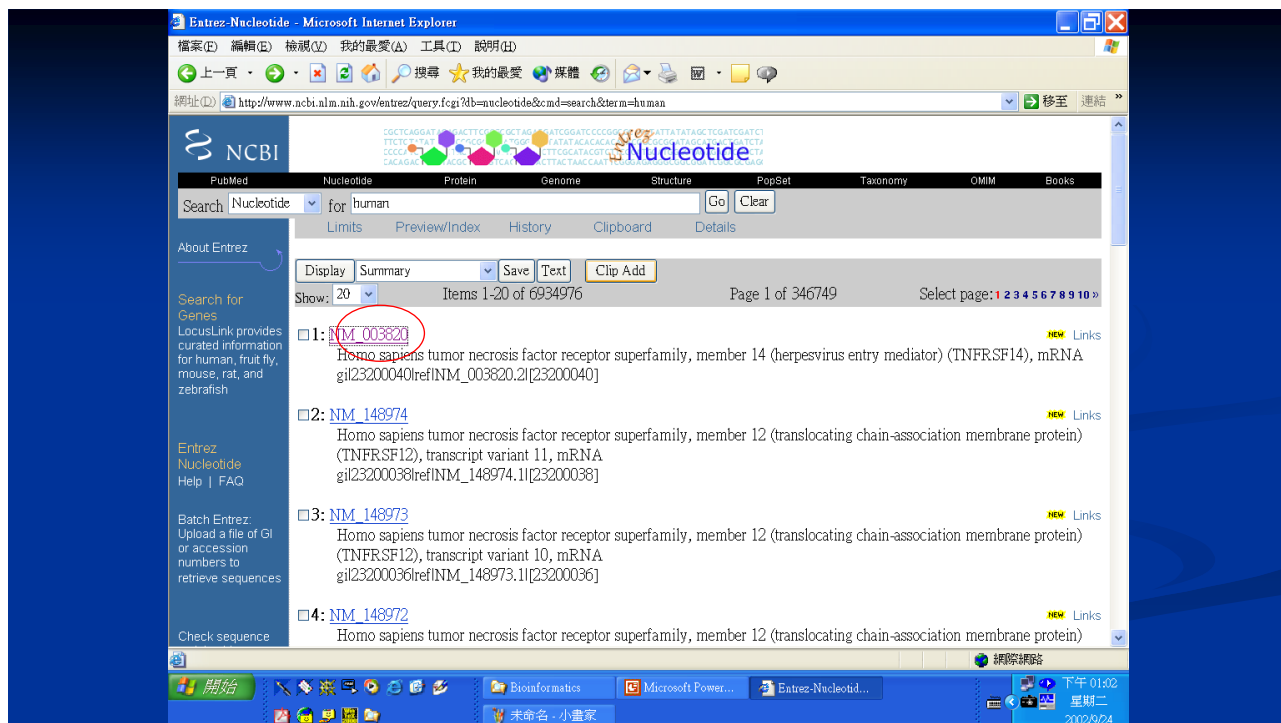
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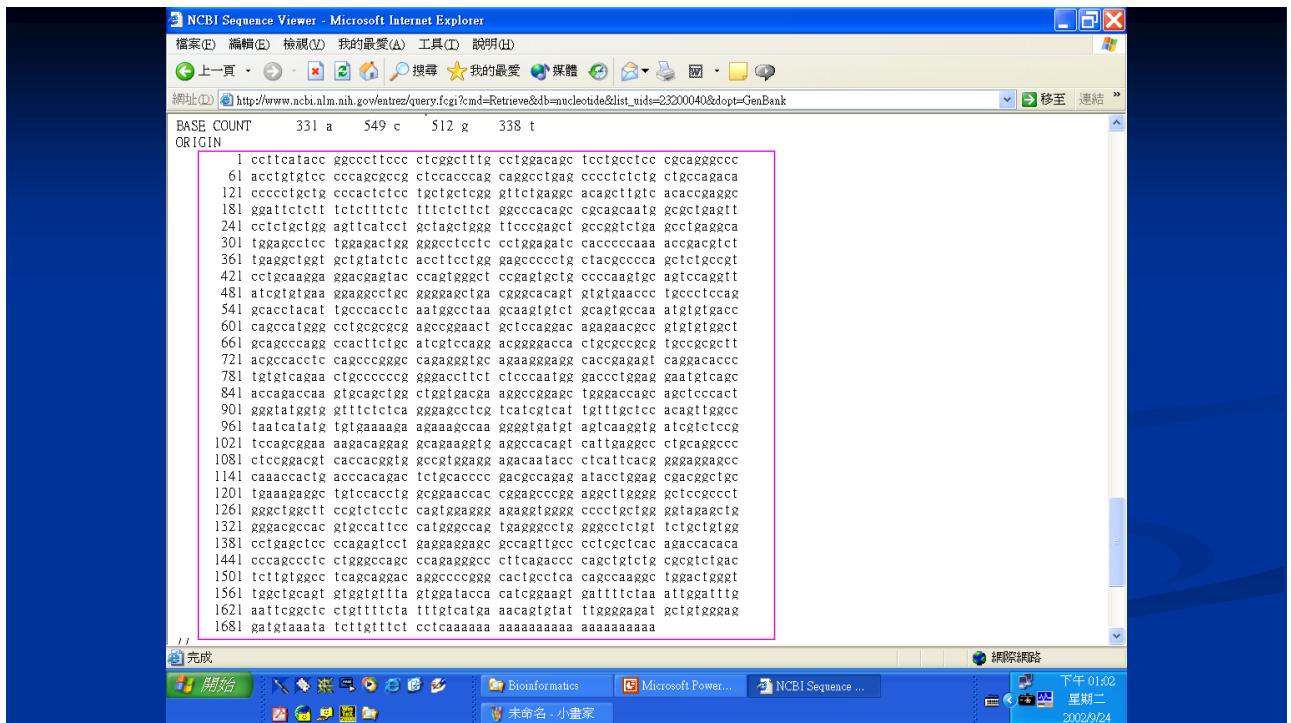
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REFERENCE 3 (residues 1 to 283)

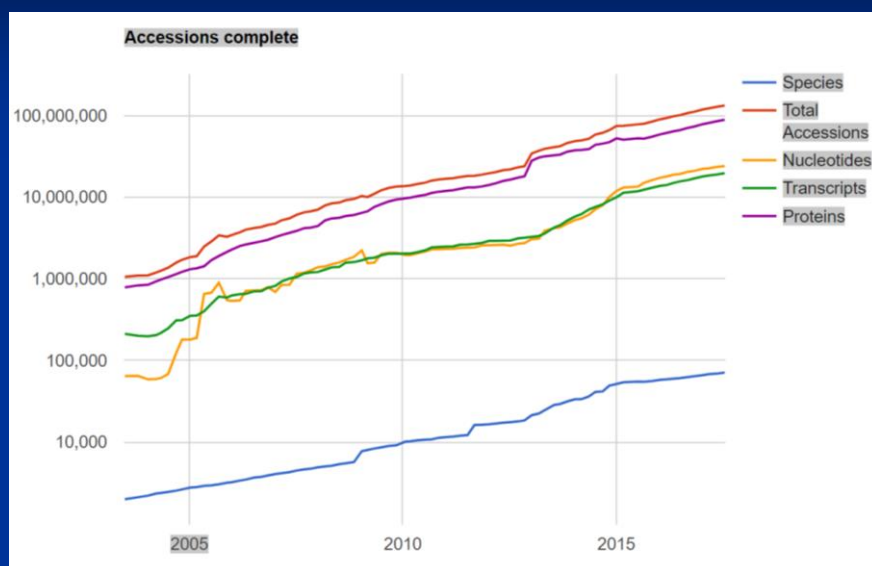
AUTHORS Marsters,S.A., Ayres,T.M., Skubatch,M., Gray,C.L., Rothe,M. and Ashkenazi,A.

TITLE Herpesvirus entry mediator, a member of the tumor necrosis factor receptor (TNFR) family, interacts with members of the TNFR-associated factor family and activates the transcription factors NF-kappaB and AP-1





RefSeq Growth Statistics



- **EMBL**: The European Molecular Biology Laboratory.

- <https://www.embl.org/>

- **GDB**: Genome Database

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

- **PDB**: The Protein Data Bank, a repository of 3-D structure of proteins.

- <https://www.wwpdb.org/>

RCSB PDB

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RCSB PDB PROTEIN DATA BANK

209,611 Structures from the PDB

1,068,577 Computed Structure Models (CSM)

3D Structures Enter search term(s), Entry ID(s), or sequence Include CSM

Advanced Search Browse Annotations Help

PDB-101 PDB EMDatResource NAKB wwPDB Foundation PDB-Dev

New: More Computed Structure Models (CSM) available Learn more

Welcome

Deposit Search Visualize Analyze Download Learn

RCSB Protein Data Bank (RCSB PDB) enables breakthroughs in science and education by providing access and tools for exploration, visualization, and analysis of:

- Experimentally-determined 3D structures from the Protein Data Bank (PDB) archive
- Computed Structure Models (CSM) from AlphaFold DB and ModelArchive

These data can be explored in context of external annotations providing a structural view of biology.

Explore NEW Features

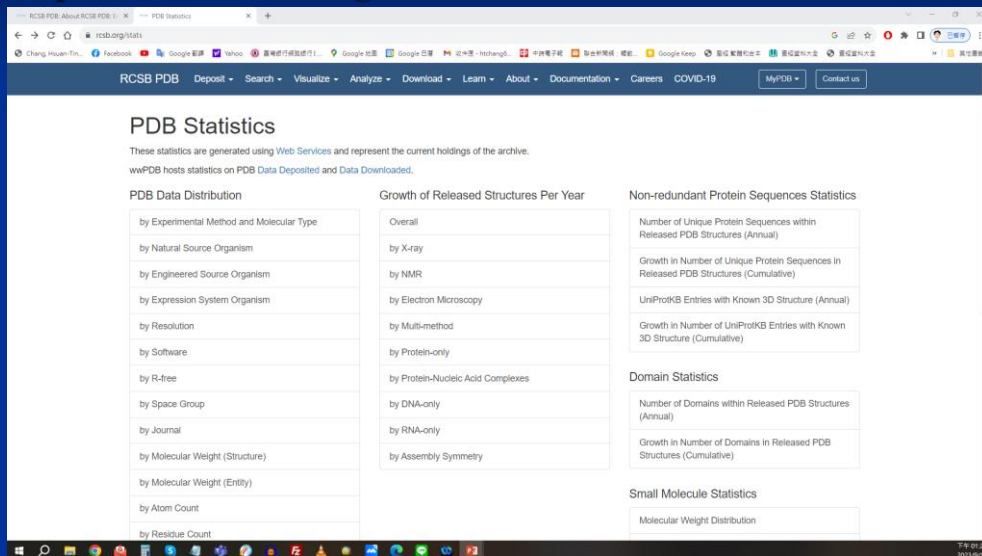
PDB-101 Training Resources

September Molecule of the Month

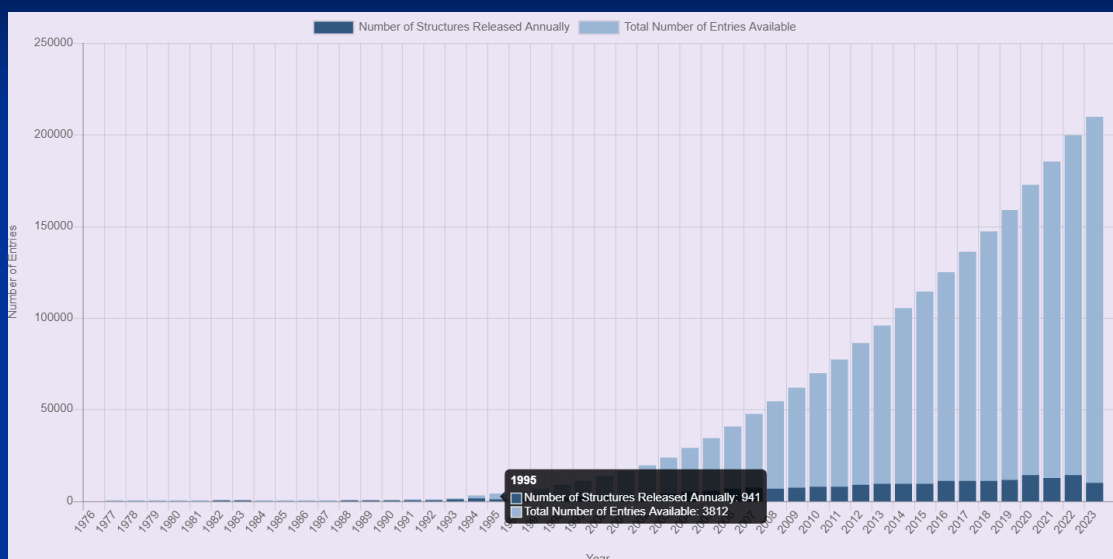
Histone Deacetylases

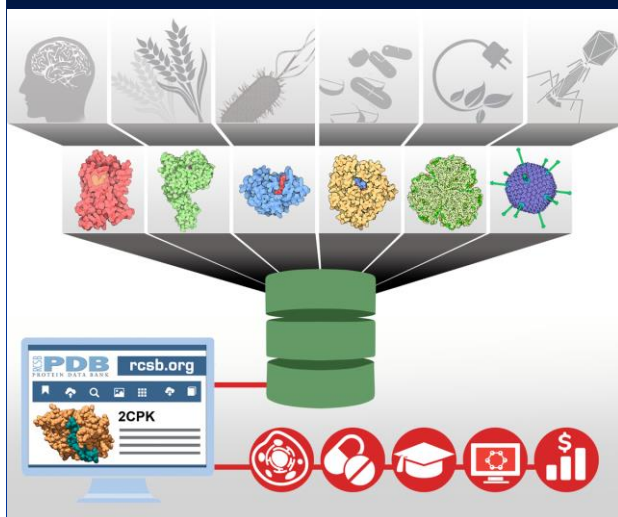
RCSB PDB Statistics

■ <https://www.rcsb.org/stats>



Protein Data Bank Overall Growth of Released Structures Per Year



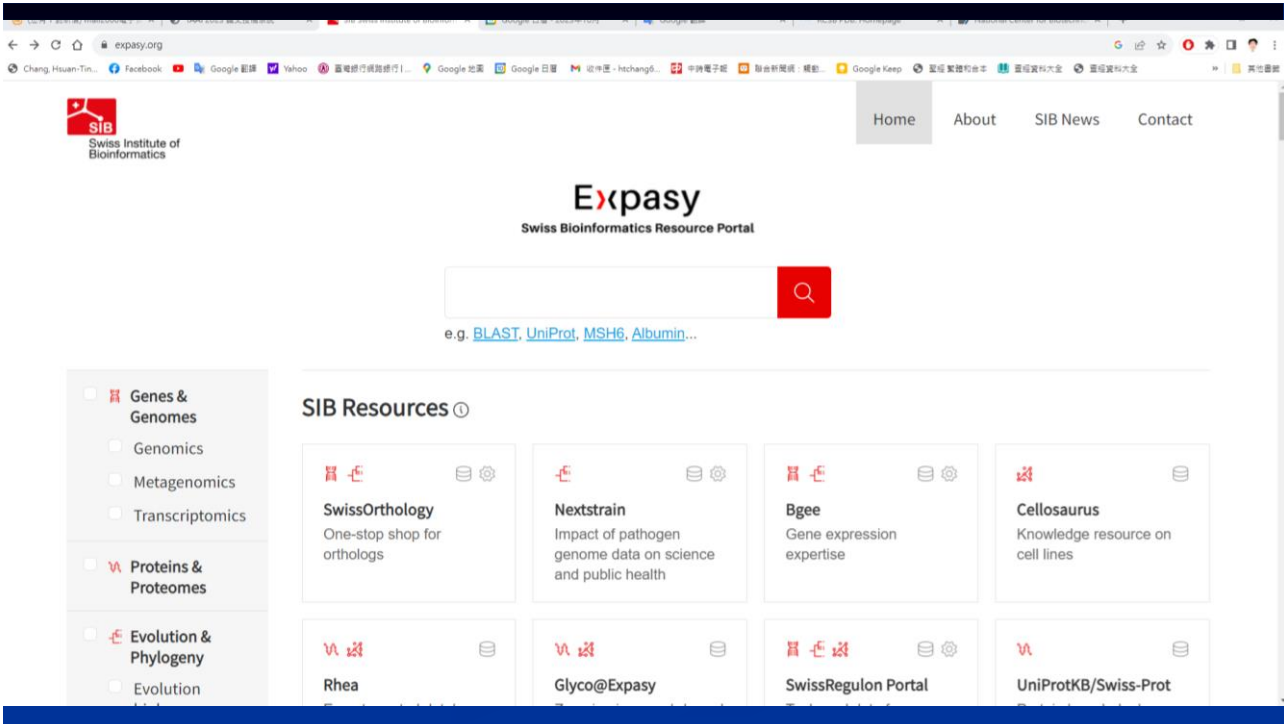
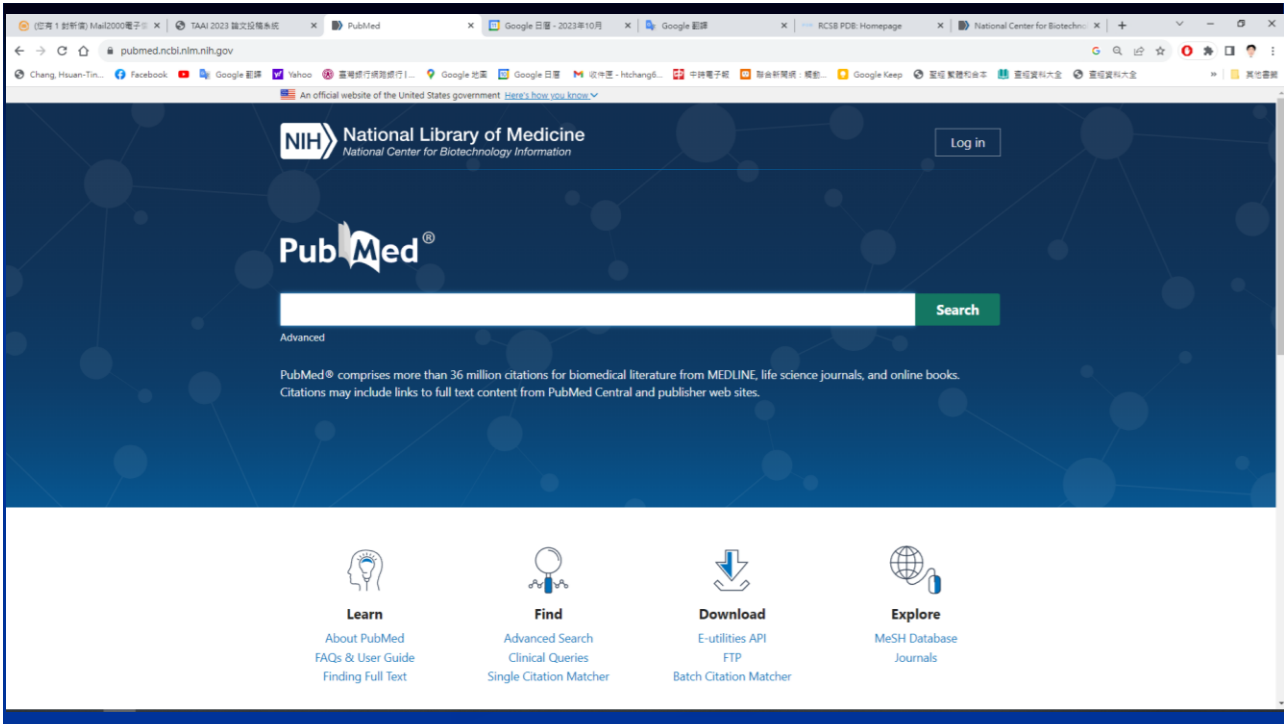


RCSB PDB (RCSB.org) is the US data center for the global Protein Data Bank (PDB) archive of 3D structure data for large biological molecules (proteins, DNA, and RNA) essential for research and education in fundamental biology, health, energy, and biotechnology.

PubMed Central® (PMC)



- A free full-text archive of biomedical and life sciences journal literature at the U.S. National Institutes of Health's National Library of Medicine (NIH/NLM).
- In keeping with NLM's legislative mandate to collect and preserve the biomedical literature, PMC is part of the NLM collection, which also includes NLM's extensive print and licensed electronic journal holdings and supports contemporary biomedical and health care research and practice as well as future scholarship.



ExPASy

- The ExPASy (the **Expert Protein Analysis System**) World Wide Web server (<http://www.expasy.org>), is provided as a service to the life science community by a multidisciplinary team at the Swiss Institute of Bioinformatics (SIB).
- It provides access to a variety of databases and analytical tools dedicated to proteins and proteomics.
- ExPASy databases include SWISS-PROT and TrEMBL, SWISS-2DPAGE, PROSITE, ENZYME and the SWISS-MODEL repository.

Research Issues

- Sequence comparison & database search
- Fragment assembly of DNA
- Physical mapping of DNA
- Phylogenetic trees
- Genome rearrangement
- Molecular structure prediction

Global Research on Bioinformatics

Major Cartels in the World

- In Europe
 - EMBL @ <https://www.embl.org/>
 - EBI @ <https://www.ebi.ac.uk/>
- In North America
 - NCBI @ <https://www.ncbi.nlm.nih.gov/>
- In Asia
 - GenomeNet @ https://www.genome.ad.jp/about_genomenet/about.html

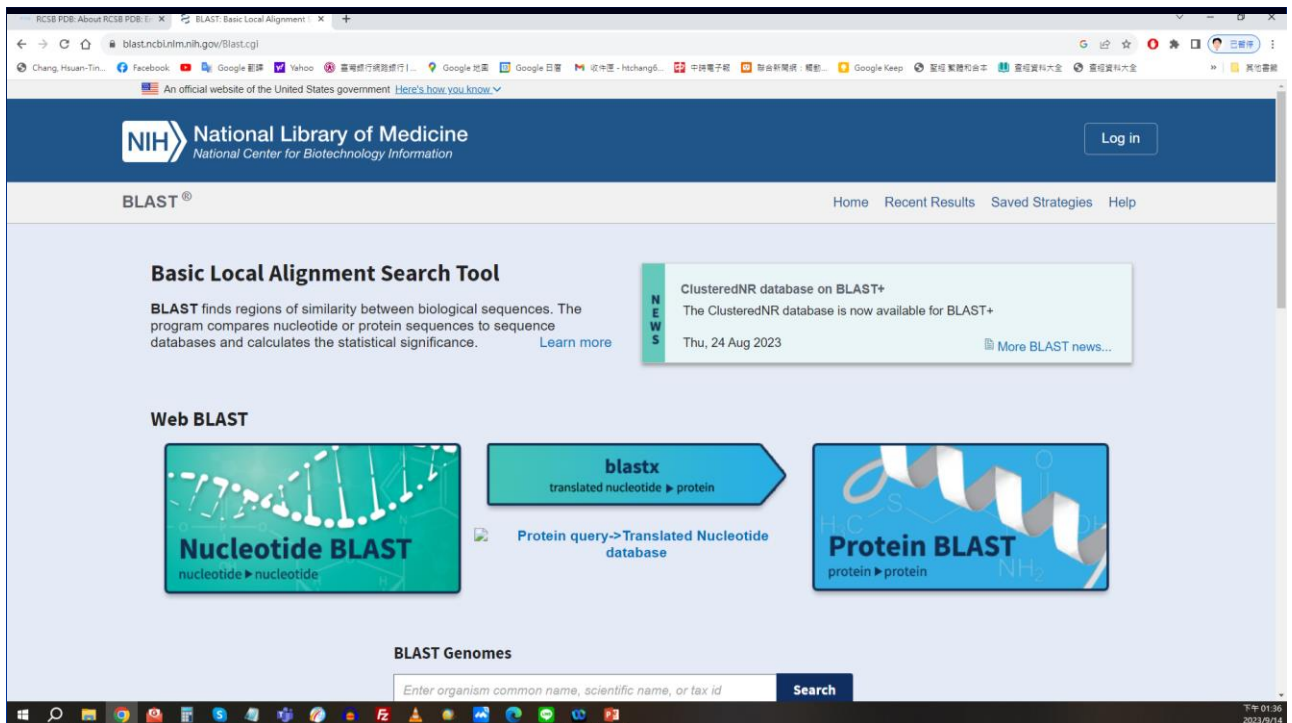
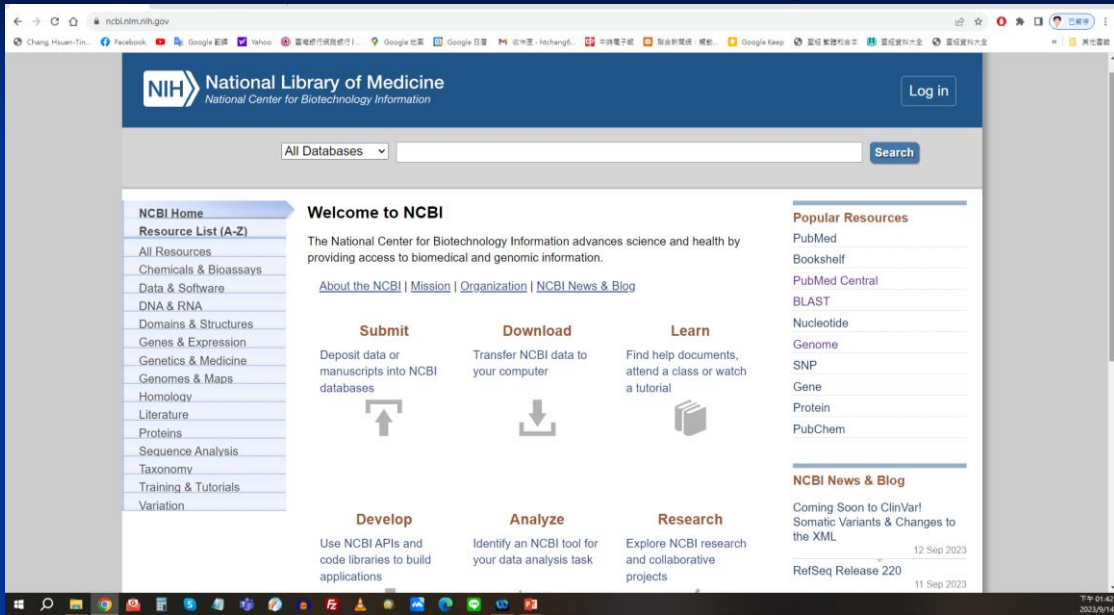
Global Research Projects on Bioinformatics

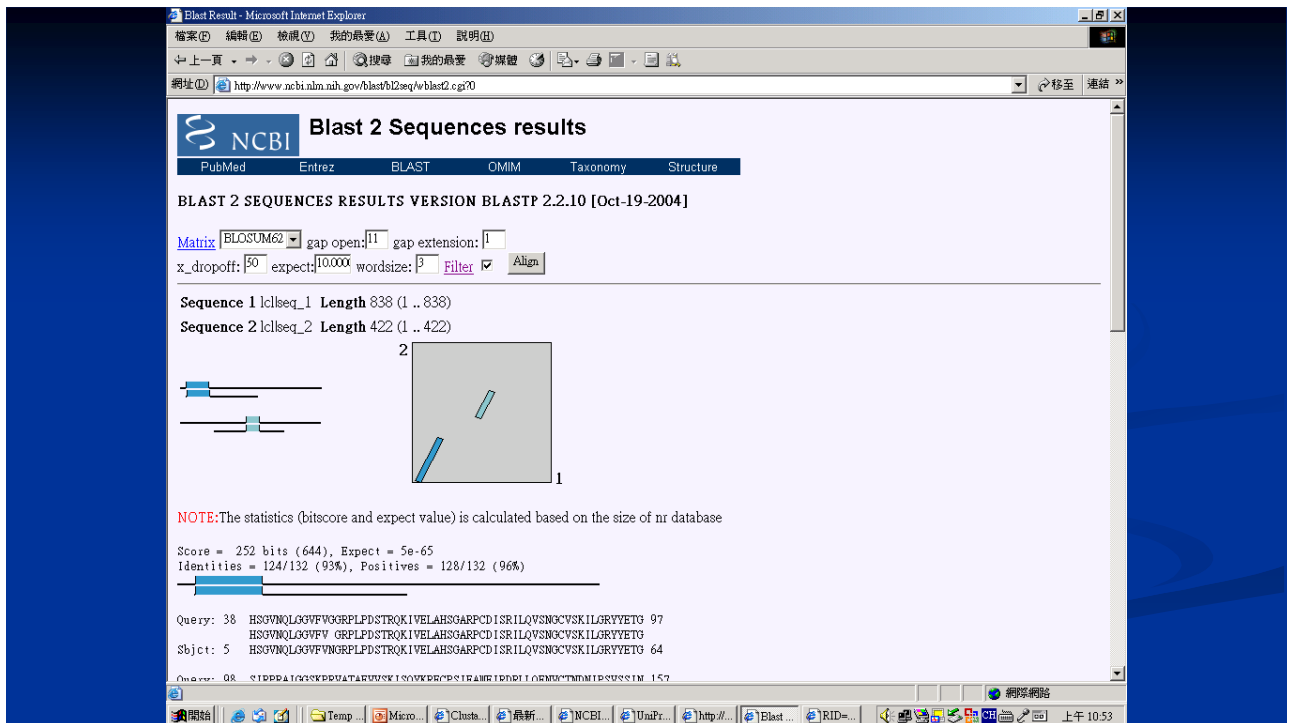
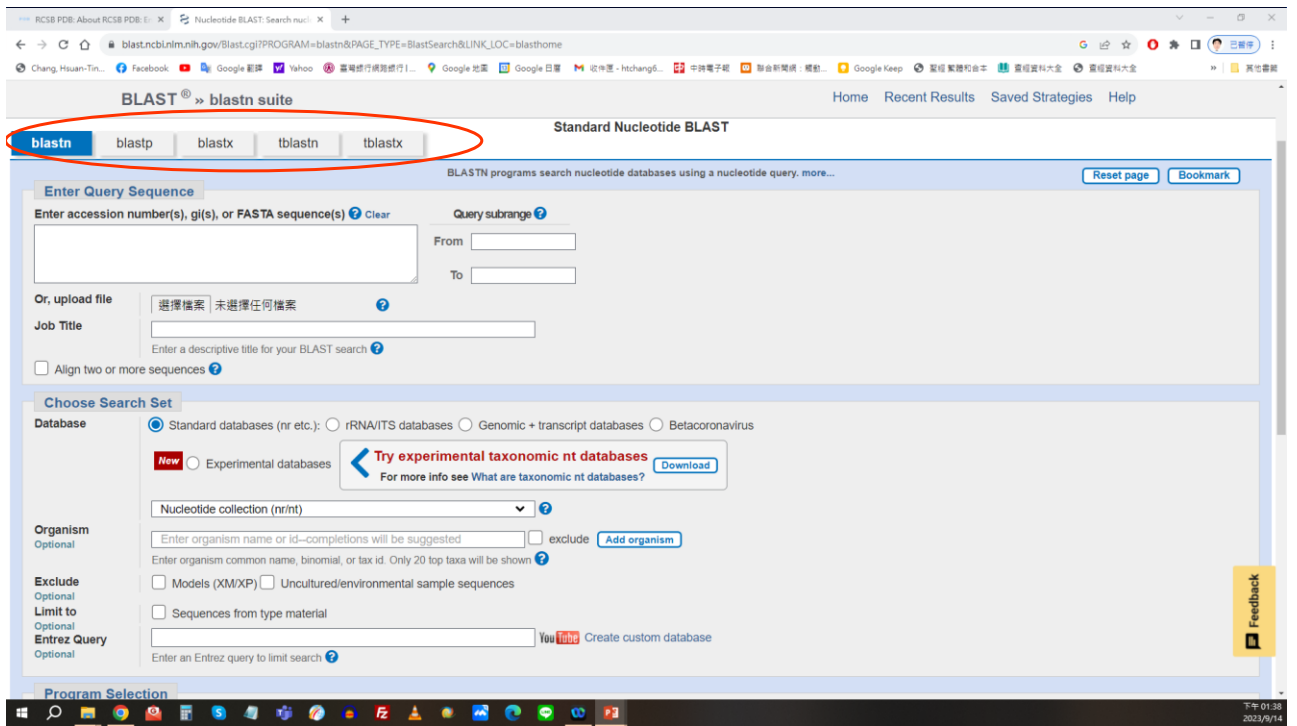
- Detection and analysis of gene organization
- Repeating sequence patterns
- Protein domains and structural elements
- Creation of a gene map of the human genome
- Analysis of effects of sequencing errors for database searching

Global Research Projects (cont.)

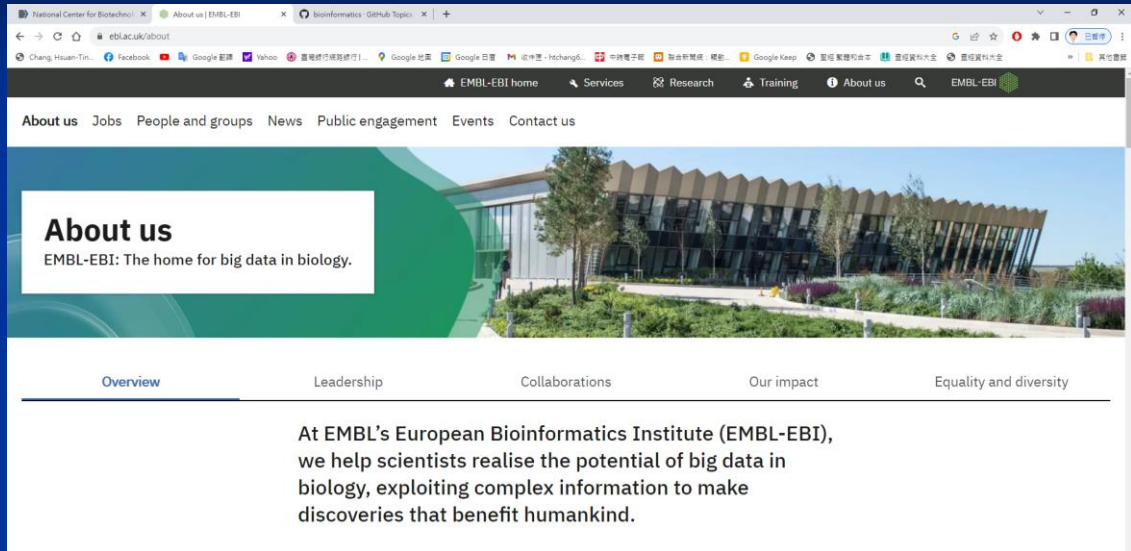
- Development of new algorithms for database searching and multiple sequence alignment
- Construction of non-redundant sequence databases
- Mathematical models for estimation of statistical significance of sequence similarity
- Establishment of microarray systems for screening disease genes

The National Center for Biotechnology Information





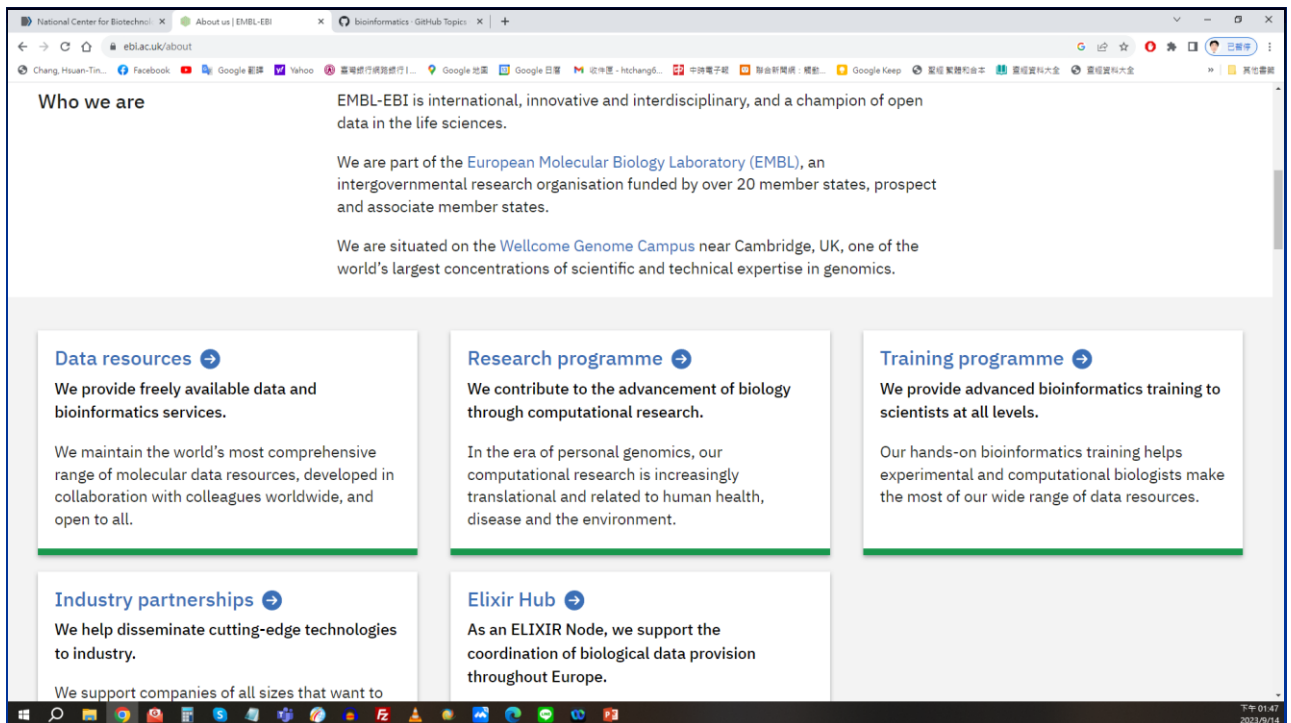
European Bioinformatics Institute



The screenshot shows the EMBL-EBI website with the following content:

- About us**
EMBL-EBI: The home for big data in biology.
- Navigation links:** Overview, Leadership, Collaborations, Our impact, Equality and diversity.
- Main text:**

At EMBL's European Bioinformatics Institute (EMBL-EBI), we help scientists realise the potential of big data in biology, exploiting complex information to make discoveries that benefit humankind.



The screenshot shows the EMBL-EBI website with the following content:

- Who we are**

EMBL-EBI is international, innovative and interdisciplinary, and a champion of open data in the life sciences.

We are part of the [European Molecular Biology Laboratory \(EMBL\)](#), an intergovernmental research organisation funded by over 20 member states, prospect and associate member states.

We are situated on the [Wellcome Genome Campus](#) near Cambridge, UK, one of the world's largest concentrations of scientific and technical expertise in genomics.
- Data resources**

We provide freely available data and bioinformatics services.

We maintain the world's most comprehensive range of molecular data resources, developed in collaboration with colleagues worldwide, and open to all.
- Research programme**

We contribute to the advancement of biology through computational research.

In the era of personal genomics, our computational research is increasingly translational and related to human health, disease and the environment.
- Training programme**

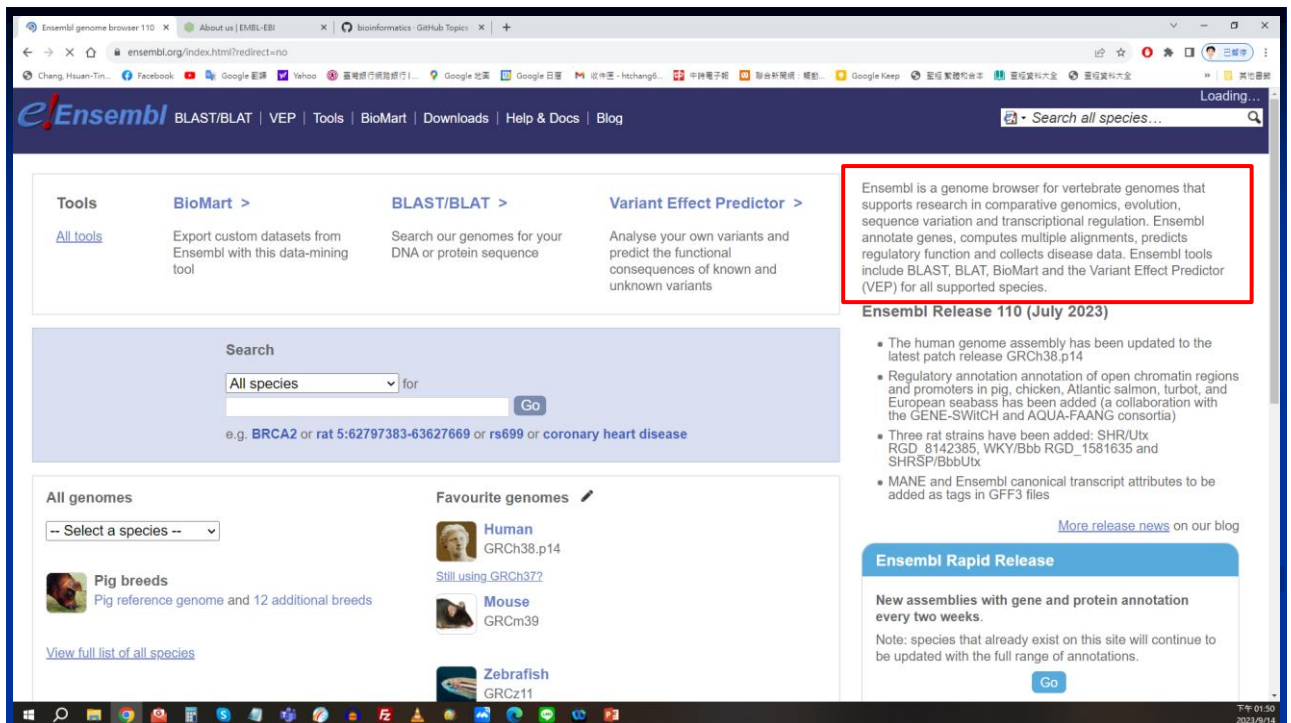
We provide advanced bioinformatics training to scientists at all levels.

Our hands-on bioinformatics training helps experimental and computational biologists make the most of our wide range of data resources.
- Industry partnerships**

We help disseminate cutting-edge technologies to industry.

We support companies of all sizes that want to
- Elixir Hub**

As an ELIXIR Node, we support the coordination of biological data provision throughout Europe.

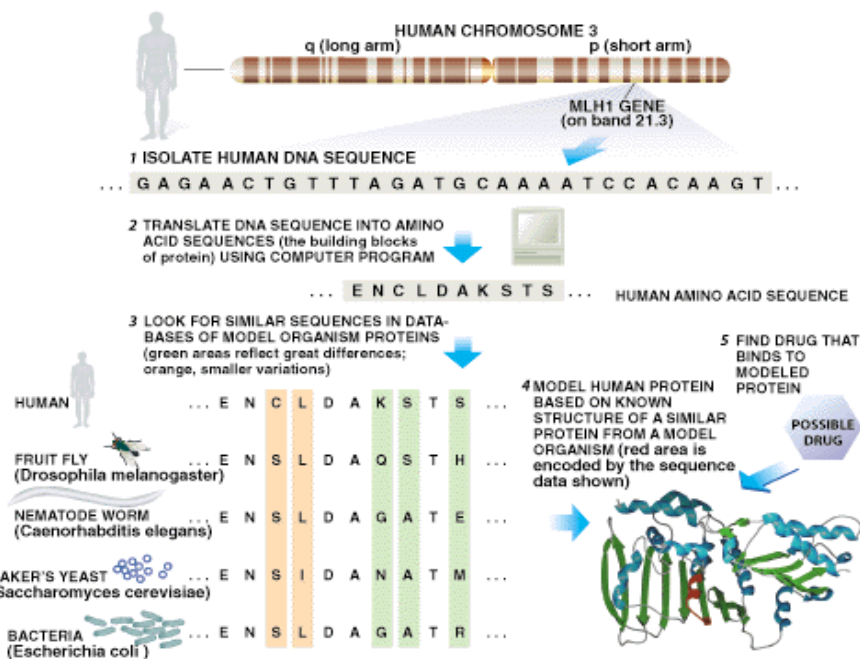


- Ensembl is a genome browser for vertebrate genomes that supports research in comparative genomics, evolution, sequence variation and transcriptional regulation. Ensembl annotate genes, computes multiple alignments, predicts regulatory function and collects disease data. Ensembl tools include BLAST, BLAT, BioMart and the Variant Effect Predictor (VEP) for all supported species.

- Ensembl 是一款脊椎動物基因組瀏覽器，支持比較基因組學、進化、序列變異和轉錄調控方面的研究。Ensembl 註釋基因、計算多重比對、預測調控功能並收集疾病數據。Ensembl 工具包括適用於所有受支持物種的 BLAST、BLAT、BioMart 和變異效應預測器 (VEP)。

Applications

- 遺傳學（動植物品種改良）Genetics (animal and plant breed improvement)
- 分子生物學（研究生命現象）Molecular biology (study of life phenomena)
- 臨床醫學（疾病治療）Clinical Medicine (Disease Treatment)
- 生物技術（環境保護與物種複製）Biotechnology (environmental protection and species replication)
- 食品藥物科學（食物改良與藥品設計）Food and Drug Science (Food Improvement and Drug Design)
- 法醫鑑識科學（DNA比對）Food and Drug Science (Food Improvement and Drug Design)
- 考古學（物種演化）Archeology (Evolution of Species)



Genomic Signal Processing

IEEE Signal Processing Magazine, July 2001

Dimitris Anastassiou

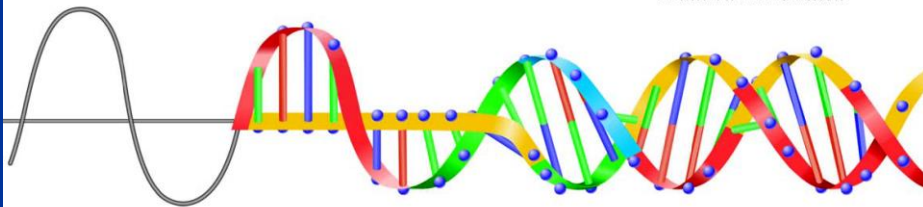


ILLUSTRATION: JIM HANKARD

Genomics is a highly cross-disciplinary field that creates paradigm shifts in such diverse areas as medicine and agriculture. It is believed that many significant scientific and technological endeavors in the 21st century will be related to the processing and interpretation of the vast information that is currently revealed from sequencing the genomes of many living organisms, including humans.

both the magnitude and the phase of properly defined Fourier transforms can be used to predict important features like the location and certain properties of protein coding regions in DNA. Even the process of mapping DNA into proteins and the interdependence of the two kinds of sequences can be analyzed using simulations based on digital filtering. These and other DSP-based approaches result in alternative mathematical formulations

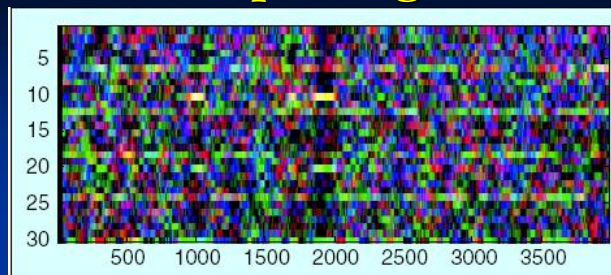
The Problem

- Genomic information is digital letters A, T, C and G
- Signal processing deals with numerical sequences, character strings have to be mapped into one or more numerical sequences
- Identification of protein coding regions
- Prediction of whether or not a given DNA segment is a part of a protein coding region
- Prediction of the proper reading frame
- Comparing to traditional methods, signal processing methods are much quicker, and can be even more accurate in some cases.

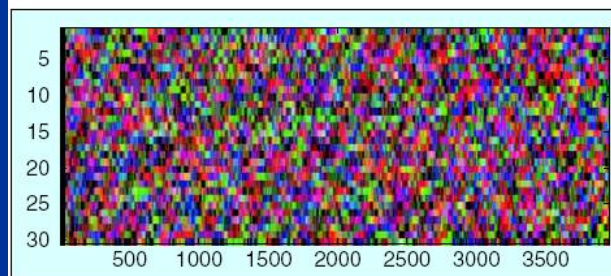
Genomic Signal Processing

- Digital Signal Processing Techniques
 - Fourier transform - spectrogram
 - Wavelet transform
- Visualization & Feature Selection
 - Genomic & protein sequences
 - Sequence representation
 - Database retrieval

DNA Spectrograms



▲ 7. Color spectrogram of a DNA stretch.



▲ 8. Color spectrogram of "totally random" DNA.

Z curve

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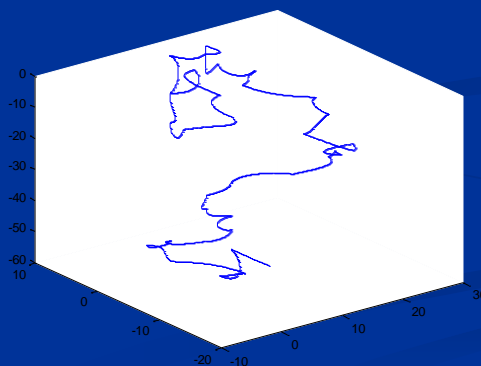
The Z curve database: a graphic representation of genome sequences Chun-Ting Zhang 1,*, Ren Zhang 2 and Hong-Yu Ou 1

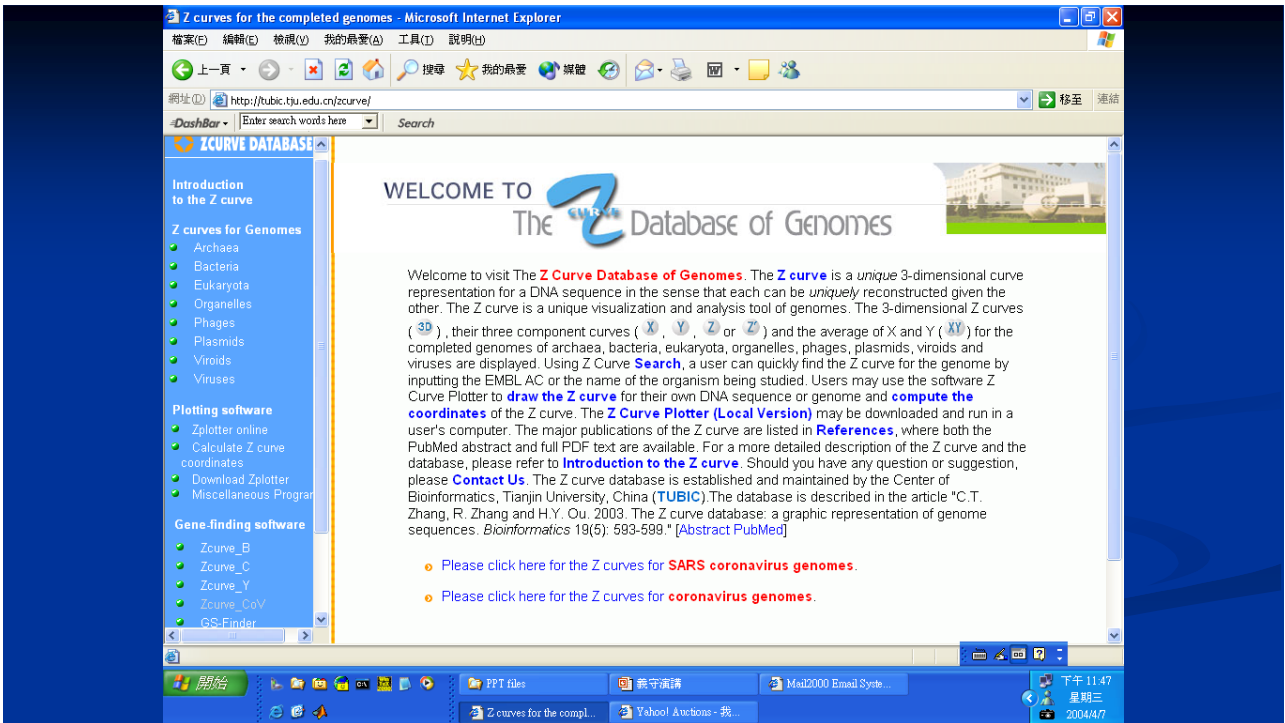
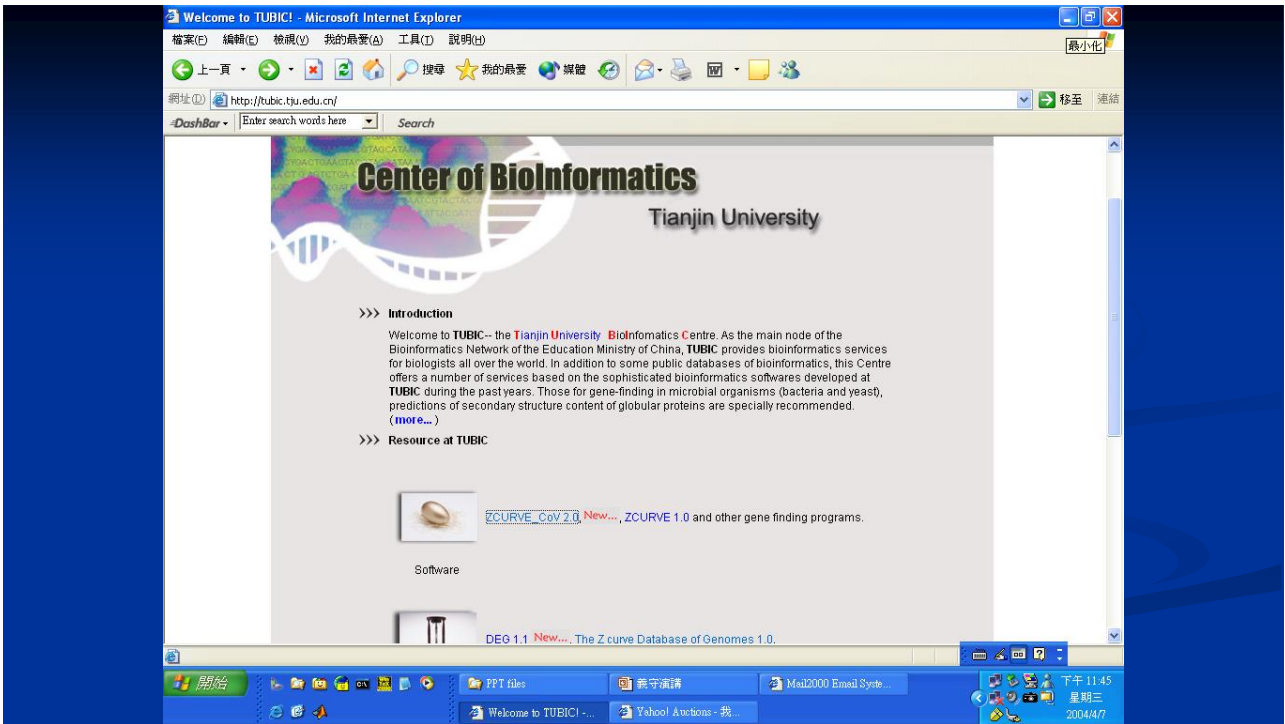
1 Department of Physics, Tianjin University, Tianjin 300072, People's Republic of China

2 Department of Epidemiology and Biostatistics, Tianjin Cancer Institute and Hospital, Tianjin 300060, People's Republic of China

$$\begin{cases} x_n = (A_n + G_n) - (C_n + T_n), \\ y_n = (A_n + C_n) - (G_n + T_n), \\ z_n = (A_n + T_n) - (C_n + G_n), \end{cases} \quad x_n, y_n, z_n \in [-N, N], \quad n = 0, 1, 2, \dots, N,$$

Z-curve flowchart





利用三維軌跡作為DNA序列的視覺化與比對

Visualization and Comparison of DNA Sequences by Use of
Three-Dimensional Trajectories

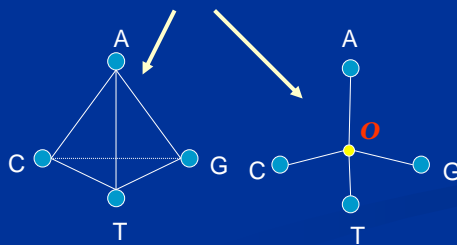
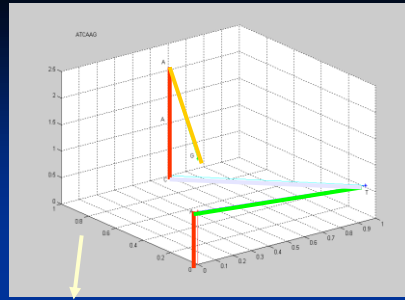
Presented in 2003 Asia Pacific Bioinformatics Conference
(APBC2003)
Adelaide Australia, Feb 2003

Three-dimensional trajectory (TDT)

- A global view visualization tool
- Presentation of *pseudo shape* of DNA sequences
- Low computational overhead
- Easy to find major similarity/difference among DNA sequences
- Use DSP algorithms for further processing

Algorithm

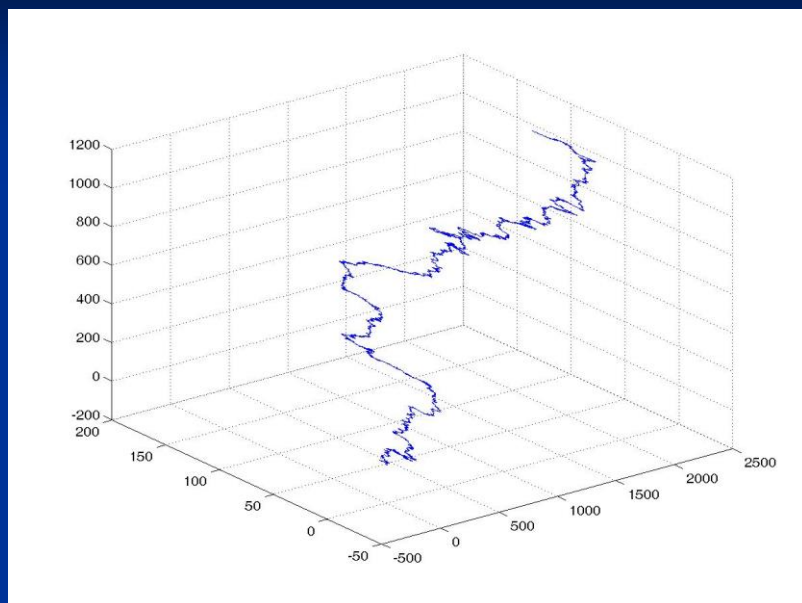
TTGCAAAGGTGACACTTGTAT
TTGCAACTGTGATGTTTG
GG....



Human DNA sequence

Homo sapiens chromosome 1 clone RP11-20L9, complete sequence.

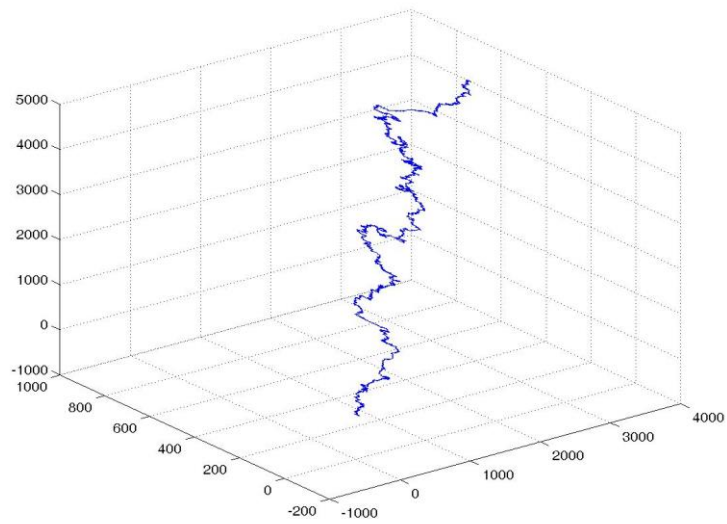
ACCESSION: AC095037, 15000 bp



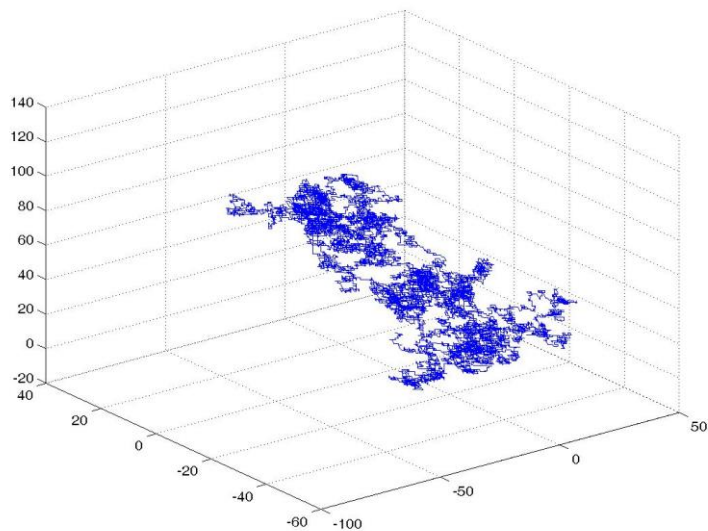
Human DNA sequence

From clone RP4-594L9 on chromosome 11p12-13, complete sequence

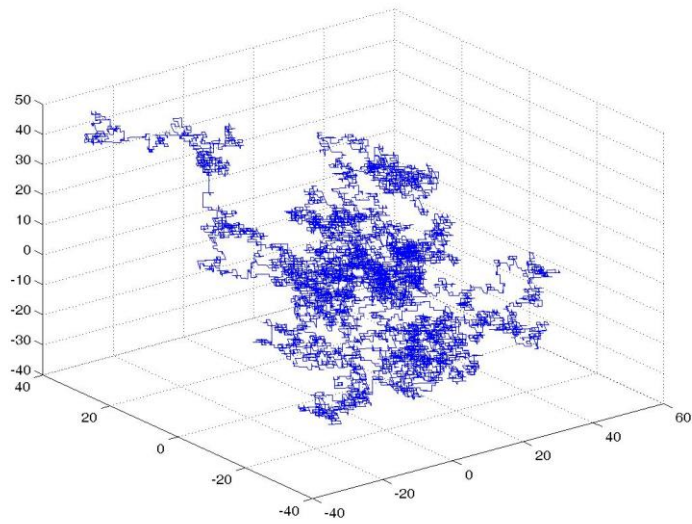
ACCESSION: AL137224 85138 bp



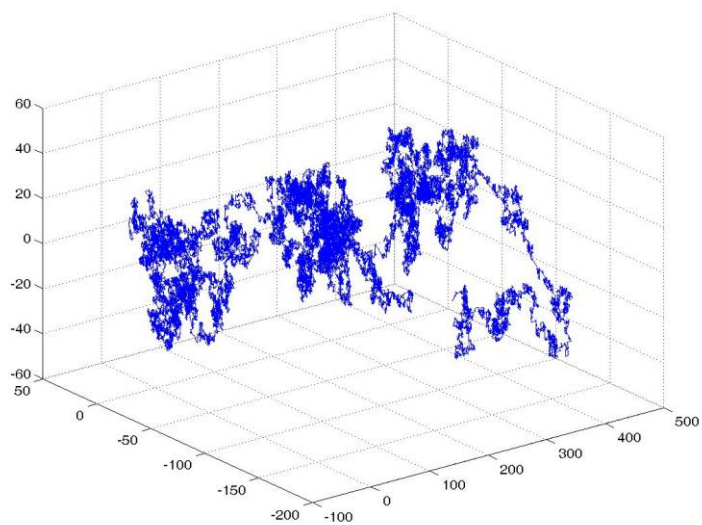
Computer-generated Random Sequence (1), 15000 bp

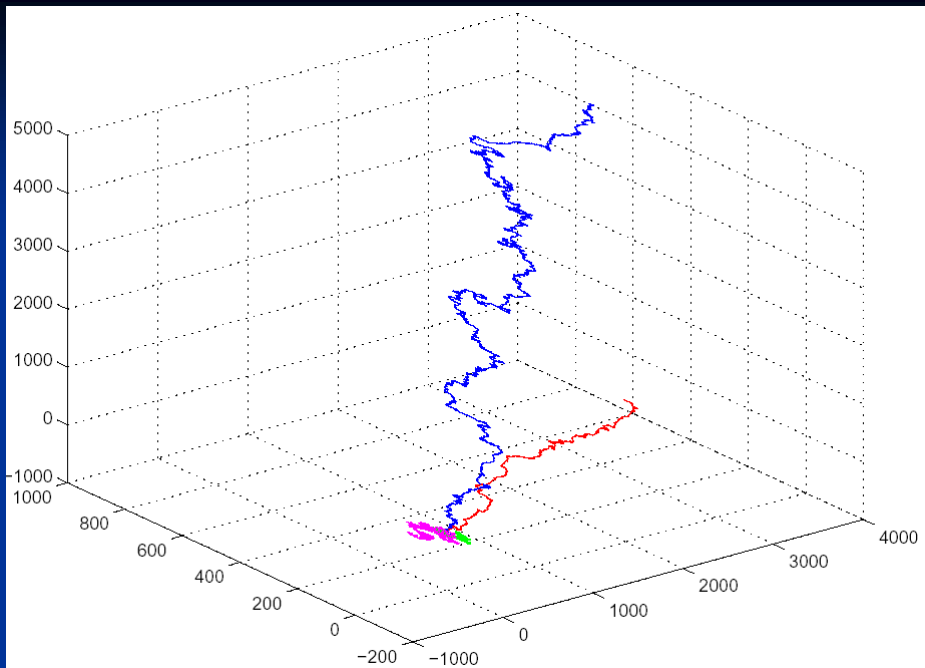
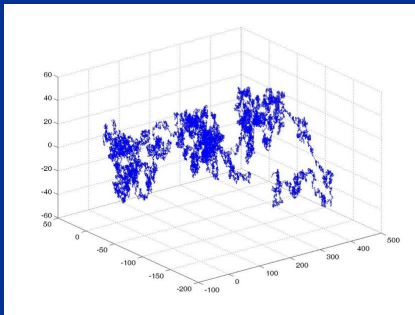
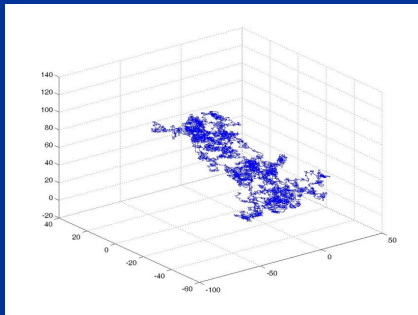
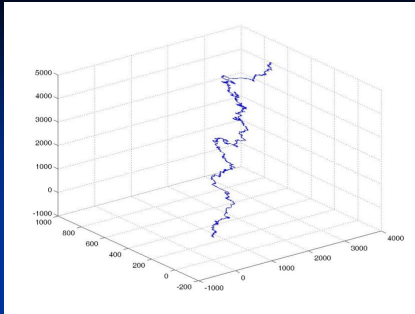
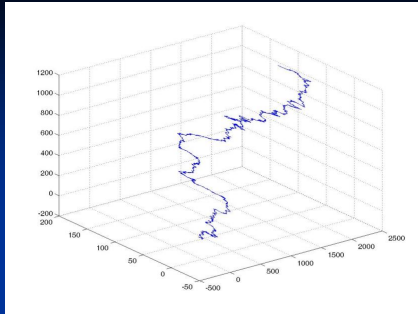


Random Sequence (2), 15000 bp



Random Sequence (3), 60000 bp

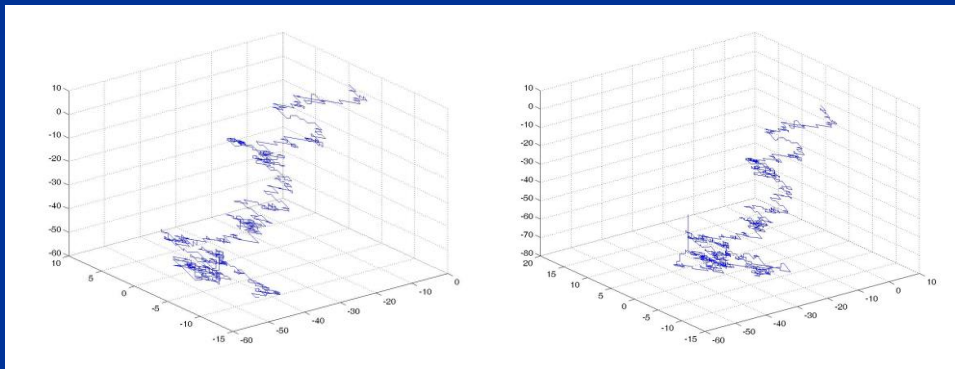




Same Gene From 2 Different Species

Human TGFA genes:
K03222, 867 bp

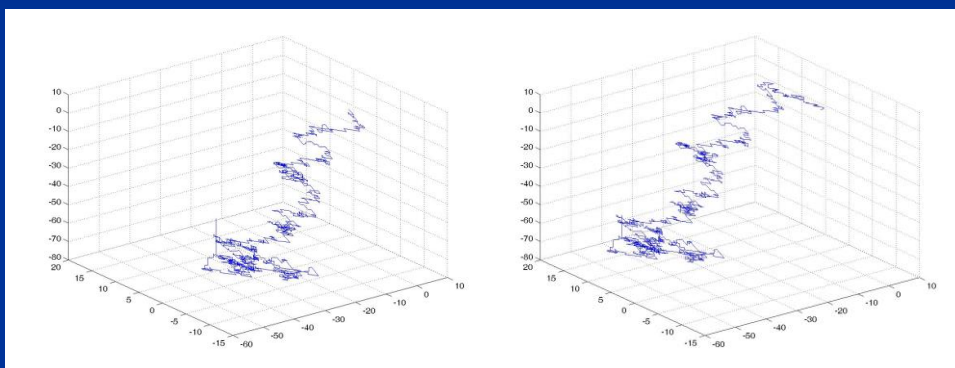
Mouse TGFA genes :
BC003895, 1042 bp



Two Different Sequences From Same Gene & Specie

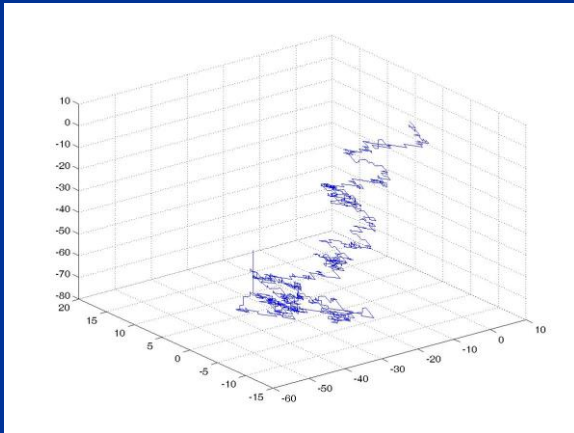
Mouse TGFA genes :
BC003895, 1042 bp

Mouse TGFA genes :
BC024928, 1097 bp

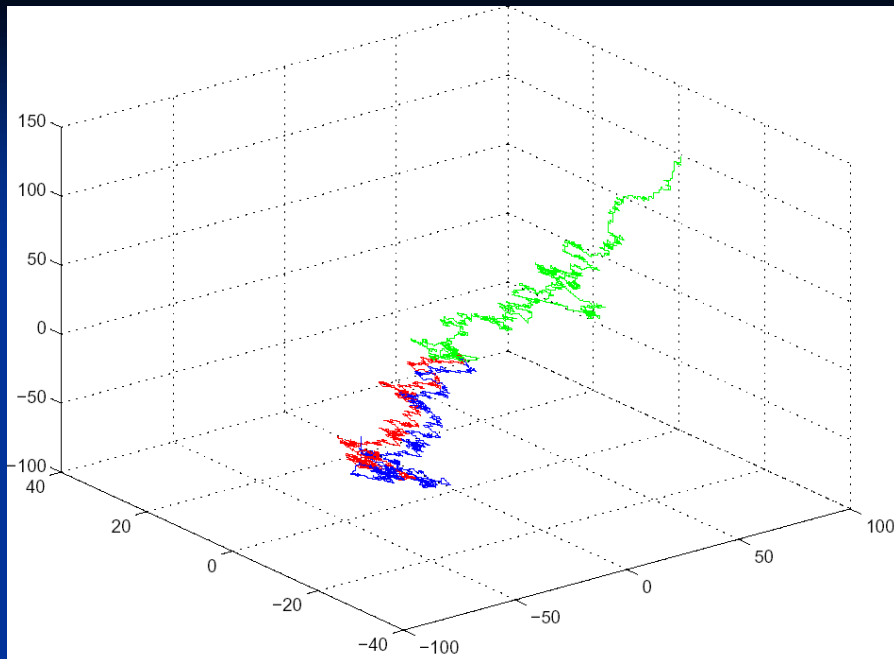
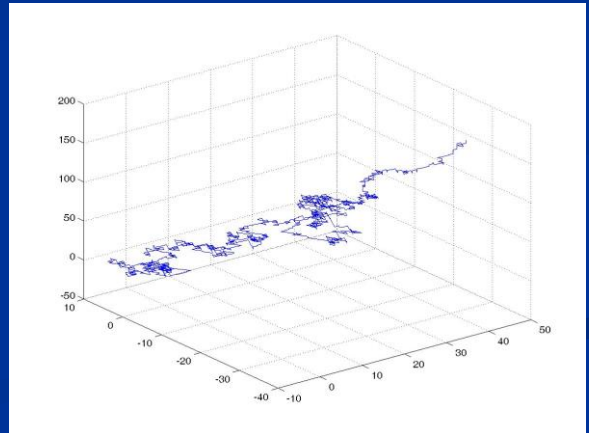


Different Sequences From One Specie

Mouse TGFA genes:
BC003895, 1042 bp



Mouse DHFR genes:
L26316, 1499 bp



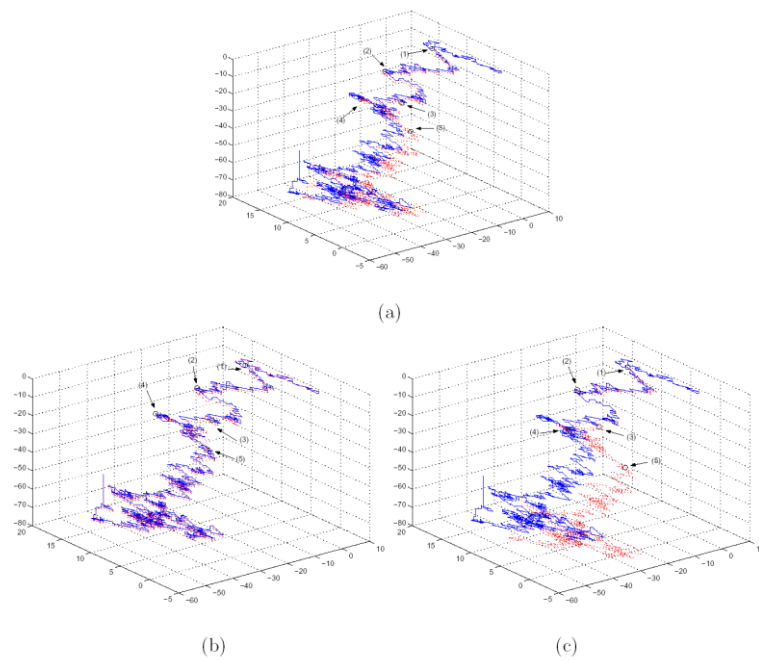
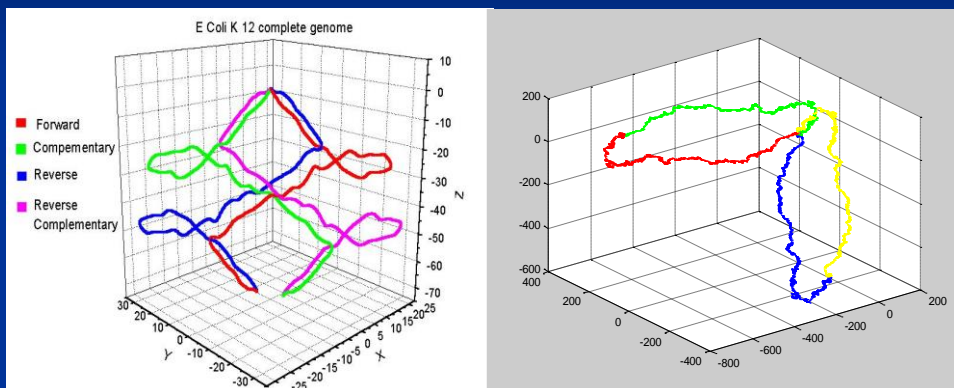
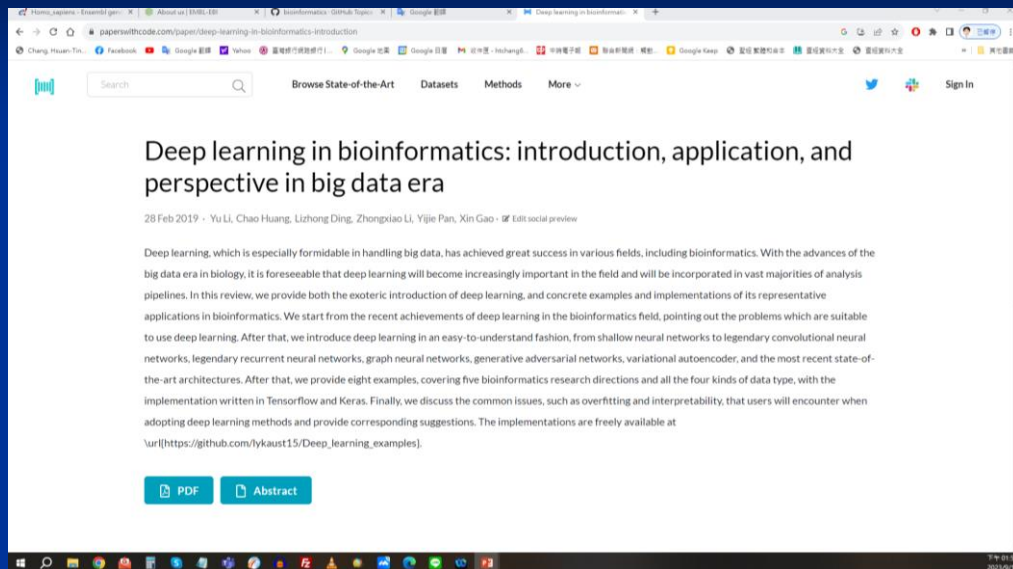


Figure 7: The TDTs for the mouse TGFA gene BC031432, 1109 bp, with (a) 5 bps deletion, (b) 5 bps insertion, and (c) 5 bps substitution.

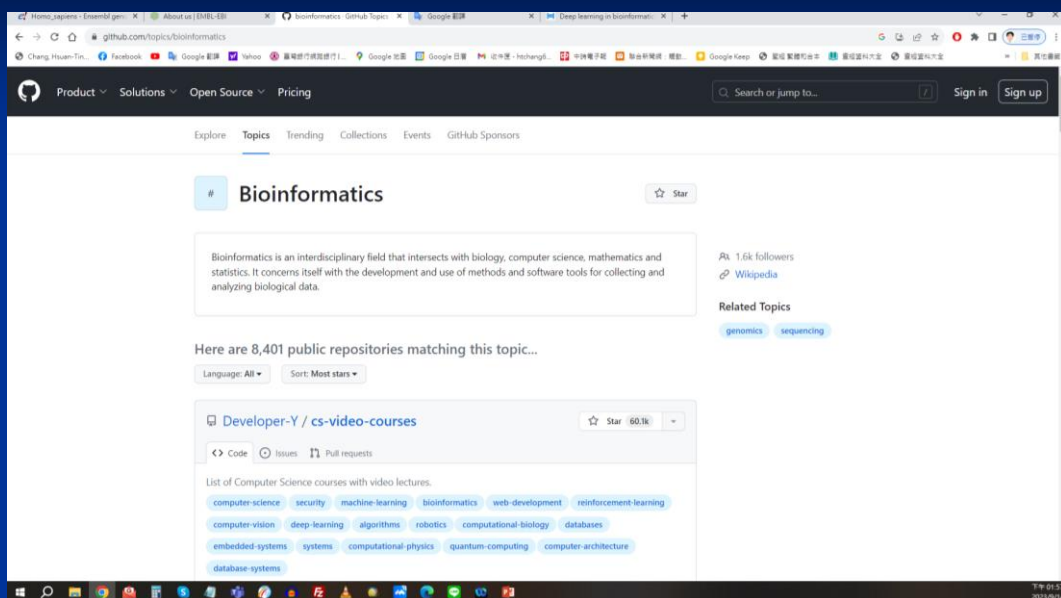
Z curve v.s. TDT



Deep Learning Techniques on Bioinformatics



GitHub topics related



Challenges & Future Work

- Genomic signal processing opens a new signal processing frontier
- Sequence analysis: symbolic or categorical signal, classical signal processing methods are not directly applicable
- Increasingly high dimensionality of genetic data sets and the complexity involved call for fast and high throughput implementations of genomic signal processing algorithms
- Future work: spectral analysis of DNA sequence and data clustering of microarray data. Modify classical signal processing methods, and develop new ones.

What are the major Challenges & Future Work of bioinformatics research?

Bioinformatics research faces several challenges and opportunities for future work, including:

1. **Data management:** As the amount of biological data continues to grow exponentially, managing and storing this data is becoming increasingly challenging. Future work in bioinformatics will focus on developing new tools and techniques for data management.
2. **Integration of data:** Integrating data from multiple sources is another major challenge in bioinformatics. Future work will focus on developing new methods for integrating and analyzing data from different sources.

- 3. Algorithm development: Developing new algorithms for analyzing biological data is a major focus of bioinformatics research. Future work in this area will focus on developing new algorithms that can handle increasingly complex datasets.
- 4. Interdisciplinary collaboration: Bioinformatics research requires collaboration between researchers from different disciplines, including biology, computer science, and statistics. Future work will focus on fostering interdisciplinary collaboration to advance the field.

- 5. Ethical considerations: As bioinformatics research becomes more advanced, ethical considerations are becoming increasingly important. Future work will focus on developing ethical guidelines for bioinformatics research.
- Overall, the future of bioinformatics research looks promising, with opportunities for new discoveries and advancements in the field.

- In molecular medicine
- In waste control
- In environmental cleanup
- In biotechnology
- In energy sources
- In risk assessment

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- [民視新聞台 科學再發現 解讀生命密碼按圖索驥DNA
1208080001](#)
- [揭開基因的奧秘-基因醫藥生物科技\(上\)](#)
- [揭開基因的奧秘-基因醫藥生物科技\(下\)](#)

TED Talks about bioinformatics

- 台灣的生物科技夢：林政和 (Jimmy Lin) at TEDxTaipei 2013
- The Human Genome: Collaboration is the New Competition | Dr. David Haussler | TEDxSantaCruz
- How to interpret the human genome | Alisha Holloway | TEDxClaremontColleges
- Bioinformatics: A way to decipher DNA and cure life's deadliest diseases | Spencer Hall | TEDxUGA

相關延伸演講

- 當深度學習與生物資訊在個人全基因體註解相遇
- 主講人：陳倩瑜 臺大生物產業機電工程學系教授
- <https://www.youtube.com/watch?v=JwTYvtUTiRM>

Thank you very much for your attention!

