17-12-2021

EXPERIMENT NO : 01

AIM OF THE EXPERIMENT : Accessing biological databases.

THEORY : A biological database is a computerized biological data which are use to store and organize data in such way that information can be retrived easily via a variety of search criteria.

Types of databases based on datatypes –

ⓐ Nucleotide sequence database : GenBank.
ⓑ Protein sequence database : Uni-Port.
ⓒ Protein structure database : RCSB-PDB.
ⓓ Metabolic pathway database : KEGG pathway.
ⓔ Small molecules database : PubChem.
ⓕ Literature database : PubMed.
ⓖ Database of Drug : Drug Bank.

MATERIALS : Computer, Internet and Copy.

@ GenBank :

It is a nucleotide sequence database. GenBank is the NIH genetic sequence database an annotated collection of all publically available DNA sequences. GenBank is part of the International Nucleotide Sequence Database Collaboration (INSDC), which comprises the DNA DataBank of Japan (DDBJ), the European Nucleotide Archive (ENA) and GenBank at NCBI.

Procedure :

① The URL of database is -

https://www.ncbi.nlm.nih.gov/nucleotid

② The sequence for the gene of human hemoglobin was search with the search term "Human hemoglobin."

③ The results return were examined and one out of 23223 results was selected having accession number DQ659148.1.

(b) Uni-Prot:

It is a protein sequence database, it is the control hub for the collection of functional information on proteins, with accurate, consistent and rich annotation. It is maintained by European Bioinformatics Institute (EBI).

Procedure:

(1) The URL of the database is —

https://www.uniprot.org/uniprot/.

(2) The sequence for the protein human hemoglobin was search with the search term "Human hemoglobin."

(3) The result return were examined and one out of 864 results, was selected having entry P69892.

(c) RCSB- PDB:

It is protein structure database. This is powered by the protein Data Bank archive - information about 3D shape of proteins nucleic acids and complex assemblies. It is maintained by - ~~RCB~~ RCSB (Research Collaboratory for structural Bioinformatics).

Procedure:

(1) The URL of this database is -
https://www.rcsb.org

(2) The structure for protein - Hexokinase was search with search term "Hexokinase."

(3) The results return were examined and one out of 2 structure result was selected having ID: 1BDG.

Results:

Experimental data snapshot:

(a) Method: x-ray diffraction.
(b) Resolution: 2.60 Å
(c) DOI: 10.2210/pdb1BDG/pdb
(d) Classification: Hexokinase.

④ KEGG pathway:

It is a metabolic pathway database. It is a database of pathway of collection of manually drawn pathway maps representing our knowledge of molecular interaction, reaction and relation networks for:

(i) Metabolism (ii) Genetic information processing (iii) Cellular processes (iv) Human disease (v) Drug development, etc.

Procedure:

(1) The URL of this database is –
https://www.genome.jp/kegg/pathway.html.

(2) The pathway for Gluconeogenesis was search with search term "Gluconeogenesis."

(3) The result return were examined and one out of 50 results was selected having ID: map00010.

(e) PubChem:

It is small molecules database. PubChem is the world's largest collection of freely accessible chemical information, search chemicals by name, molecular formula, structure and other identifiers. Find chemical and physical properties, biological activities, safty, and toxicity information, patents, literature, citations and more.

It is maintained by NCBI of NLM of NIH of USA.

Procedure:

① The URL of this database is —

https://www.pubchem.ncbi.nlm.nih/gov/database

② The structure and information bore the compound "Citric acid" was search with the term "CITRIC ACID".

③ The results returned were examined and one out of 388 results was selected having compound CID: 311.

⑤ PubMed :

PubMed is a free search engine primarily the MEDLINE database of refferences and abstracts on life sciences and biomedical topics. The United States National Library of Medicine at the National Institute of Health maintain the database as a part of Entrez system of information retrival.

PubMed comprises more than 33 million citation for biomedical literature from MEDLINE life science journals and online books.

Procedure :

① URL of this database is -

https:// pubmed.ncbi.nlm.nih.gov.

② The literature for "Cell death pathway in Ischemic Strock and Targeted Pharmacotherapy" search with search term "Borah A".

③ The results return were examined and one out of 158 results was selected having PMID: 32219729

(9) Database of Drug: Drug Bank

The Drug Bank is a comprehensive, freely accessible, online database containing information on drug targets created and maintained by the University of Alberta and The Metabolomics innovation Centre located in Alberta, Canada.

Procedure:

(1) The URL of this database is —
https://go.drugbank.com.

(2) The drug "Paracetamol" was searched with the search term "Paracetamol".

(3) The results returned were examine having accession number - DB00316.
Generic name: Acetaminophen,

Results: The key features of this drug are -

(i) Drug name: Acetaminophen.
(ii) Types of drug: Small molecule.
(iii) Chemical formula: $C_8H_9NO_2$
(iv) Disease against the drug: Arthritis, Chills, Cold, Common cold, Cough, Fever, Sevear pain, Pollen Allergy etc.

(v) Mechanism of action of the drug:

According to its FDA labeling, acetaminophen's exact mechanism of action has not been fully established - despite this, it is often categorized alongside NSAIDs (nosteroidal antiinflammatory drugs) due to its ability to inhibit the cyclooxygenase (cox) pathways. It is thought to exert central actions which ultimately lead to the alleviation of pain symptoms.

One theory is that acetaminophen increses the pain threshold by inhibiting two isoforms of cyclooxygenase, cox-1 and cox-2, which are involved in prostaglandin synthesis. Prostaglandins are responsible for eliciting pain sensations. Acetaminophen does not inhibit cyclooxygenase in peripheral tissues and, therefore, has no peripheral anti-inflammatory effects. Though acetylsalicylic acid (aspirin) is an irreversible inhibitor of cox and directly blocks the active site of this enzyme, studies have shown that acetaminophen (paracetamol) blocks cox indirectly.