Chemical Databases

Shatakshi Kulkarni

Introduction

- A chemical database is a database specifically designed to store chemical information
- Chemical Information:

- **Structural Information:**

  Molecular structures including 2D and 3D models.

  Stereochemistry, isomerism and molecular conformation

- **Chemical Properties:**

  Molecular weight, melting point, boiling point, solubility, density

- **Biological Activity:**

  Interaction of compounds with biological targets (e.g., enzymes, receptors, DNA)

- **Computational & Analytical tools:**

  Virtual screening, QSAR/Quantitative structure-activity relationship

PubChem

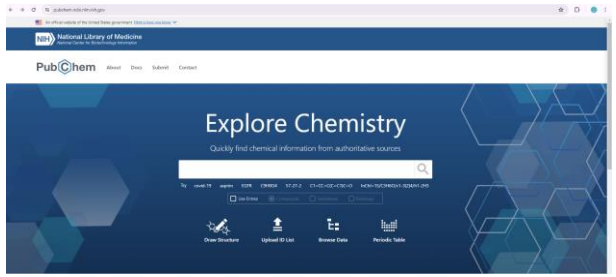
- Maintained by the National Center for Biotechnology Information (NCBI).
- Contains information on small molecules and their biological activities.

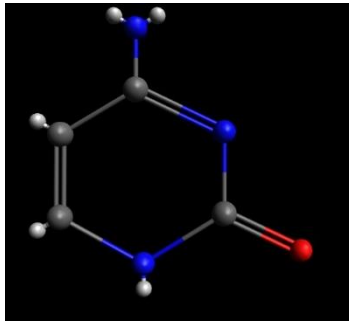
PubChem

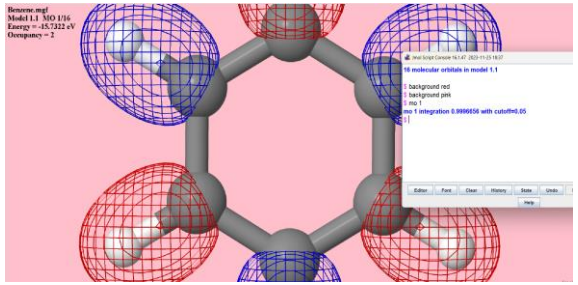
- PubChem:

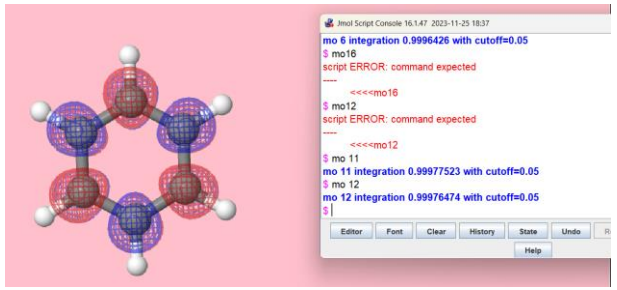
  https://pubchem.ncbi.nlm.nih.gov/

  Draw Structures: Structure of chemical compound drawn which can be further used to observe conformations and optimize energy



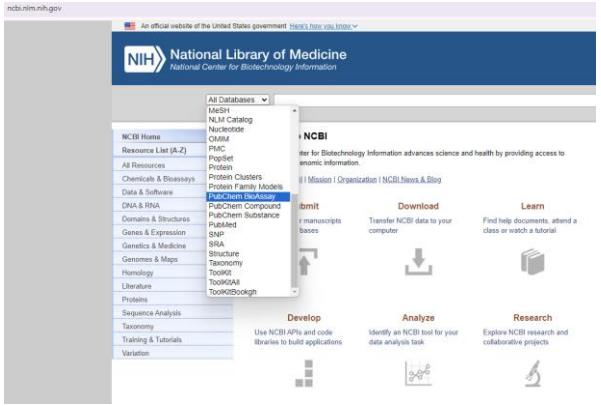






- NIH:

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



PubChem

- PubChem BioAssay (Drug candidate identification)

  Focuses on biological assay data and outcomes, linking tested substances to bioactivity results. Helps in assessing its effect on biological system. E.g., anti-inflammatory, anti-cancerous.

- PubChem Compound (Chemical, Physical properties)

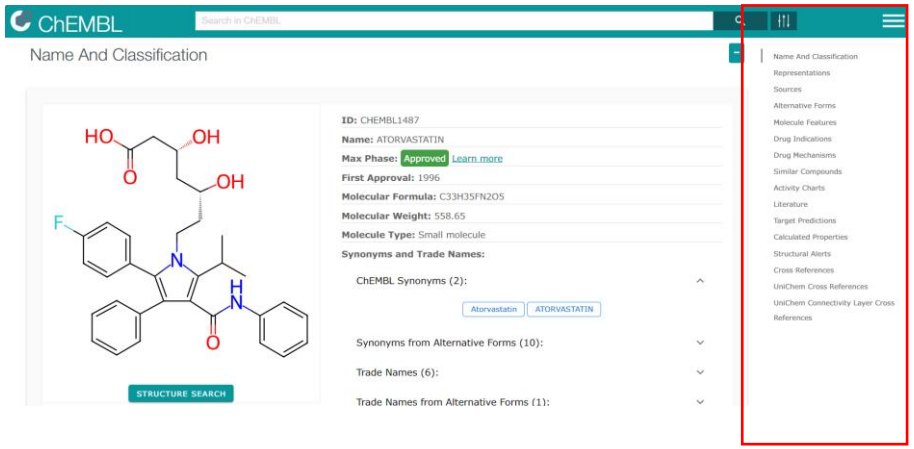
  Provides information on chemical structures (2D, 3D), physical properties(molecular weight, color, odor, boiling point, melting point), and synonyms of individual compounds.

- PubChem Substance (Trace origin)

  Catalogs chemical samples and their sources, facilitating the exploration and utilization of chemical data in diverse research fields.

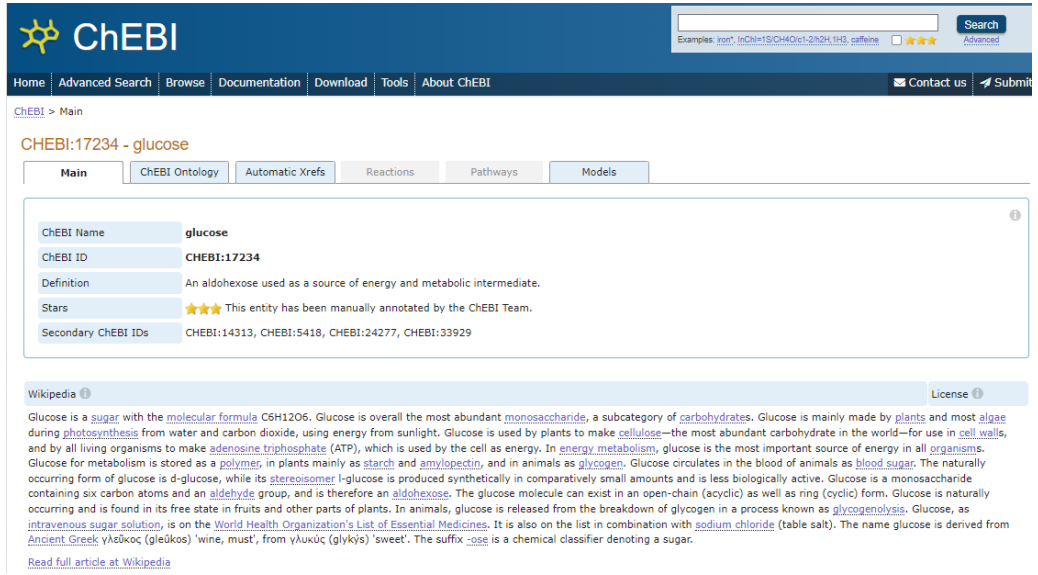
ChEMBL

- A manually curated chemical database of bioactive molecules with drug inducing properties.
- It is maintained by the European Bioinformatics Institute (EBI), of the European Molecular Biology Laboratory (EMBL).
- Provides data on compound bioactivity(Ki), drug targets (proteins, enzymes, receptors), and pharmacology.
- Mechanism of drug, target prediction, structure details provided.
- E.g., after searching for a drug such as atorvastatin (HMG CoA reductase inhibitor) a detailed description about target prediction, drug mechanism can be studied.
- https://www.ebi.ac.uk/chembl/



ChEBI

- Biological roles and physiological functions of chemical compounds.
- Ontology i.e., metabolic pathways, biochemical processes, disease mechanisms, reactions in which they are involved
- https://www.ebi.ac.uk/chebi/



Search result &
Ontology of glucose