

Chemical Databases

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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

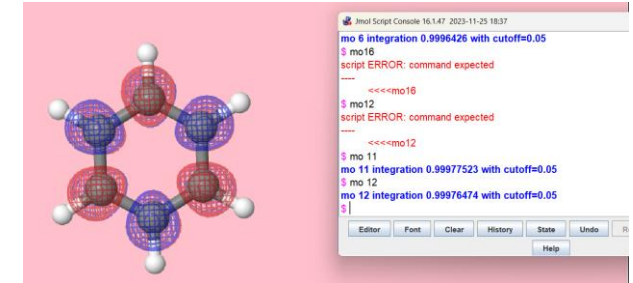
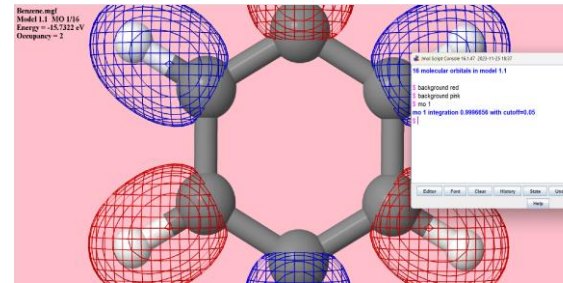
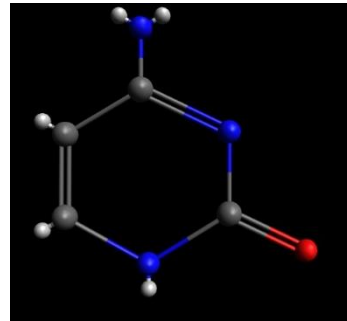
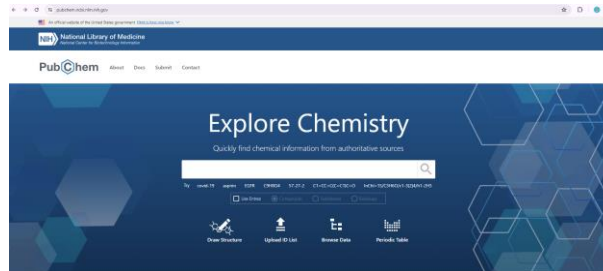
- ❑ Maintained by the National Center for Biotechnology Information (NCBI).
- ❑ Contains information on small molecules and their biological activities.

PubChem

❑ PubChem:

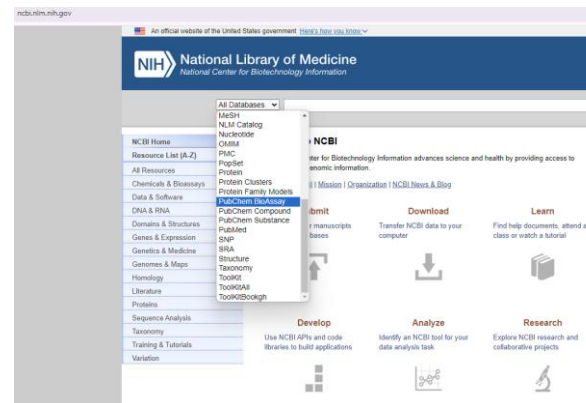
<https://pubchem.ncbi.nlm.nih.gov/>

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)

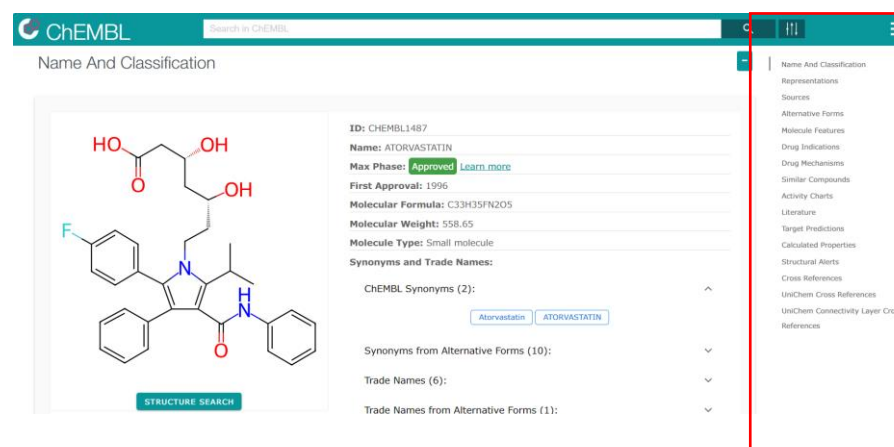
Provides information on chemical structures (2D, 3D), physical properties(molecular weight, color, odor, boiling point, melting point), and synonyms of individual compounds.

❑ 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/>

ChEBI

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ChEBI:17234 - glucose

Main | ChEBI Ontology | Automatic Xrefs | Reactions | Pathways | Models

ChEBI Name	glucose
ChEBI ID	ChEBI:17234
Definition	An aldohexose used as a source of energy and metabolic intermediate.
Stars	☆☆☆ This entity has been manually annotated by the ChEBI Team.
Secondary ChEBI IDs	ChEBI:14313, ChEBI:5418, ChEBI:24277, ChEBI:33929

Wikipedia

Glucose is a [sugar](#) with the [molecular formula](#) C₆H₁₂O₆. Glucose is overall the most abundant [monosaccharide](#), a subcategory of [carbohydrates](#). Glucose is mainly made by [plants](#) and most [algae](#) during [photosynthesis](#) from water and carbon dioxide, using energy from sunlight. Glucose is used by plants to make [cellulose](#)—the most abundant carbohydrate in the world—for use in [cell walls](#), and by all living organisms to make [adenosine triphosphate](#) (ATP), which is used by the cell as energy. In [energy metabolism](#), glucose is the most important source of energy in all [organisms](#). Glucose for metabolism is stored as a [polymer](#), in plants mainly as [starch](#) and [amylopectin](#), and in animals as [glycogen](#). Glucose circulates in the blood of animals as [blood sugar](#). The naturally occurring form of glucose is d-glucose, while its [stereoisomer](#) l-glucose is produced synthetically in comparatively small amounts and is less biologically active. Glucose is a monosaccharide containing six carbon atoms and an [aldehyde](#) group, and is therefore an [aldohexose](#). The glucose molecule can exist in an open-chain (acyclic) as well as ring (cyclic) form. Glucose is naturally occurring and is found in its free state in fruits and other parts of plants. In animals, glucose is released from the breakdown of glycogen in a process known as [glycogenolysis](#). Glucose, as [intravenous sugar solution](#), is on the [World Health Organization's List of Essential Medicines](#). It is also on the list in combination with [sodium chloride](#) (table salt). The name glucose is derived from [Ancient Greek](#) γλυκός (gleukós) 'wine, must', from γλυκύς (glykys) 'sweet'. The suffix [-ose](#) is a chemical classifier denoting a sugar.

[Read full article at Wikipedia](#)

Search result & Ontology of glucose

