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Shaping Lives...
Empowering Communities...

Study of Various Ligand databases and structure importing from chemical databases



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Chemical databases

- A **chemical database** is a database specifically designed to store chemical information.
- This information is about chemical and crystal structures, spectra, reactions and syntheses, and thermophysical data.
- Chemical databases/resources are the backbone of computer-aided drug discovery, whether it is chemoinformatics or bioinformatics.
- These databases gives information which can be used to build knowledge-based models for discovering and designing drug molecules.



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List of major databases that are freely available and widely used:-

PubChem

The screenshot shows the PubChem website homepage. The browser's address bar displays 'pubchem.ncbi.nlm.nih.gov'. The website header includes the PubChem logo and navigation links: 'About', 'Blog', 'Submit', and 'Contact'. A notification banner states 'PubChemRDF 1.7β has been released >'. The main heading is 'Explore Chemistry' with the subtitle 'Quickly find chemical information from authoritative sources'. A yellow banner offers to 'Browse COVID-19 data available in PubChem'. Below this is a large search bar. Under the search bar, there are suggestions: 'Try aspirin EGFR C9H8O4 57-27-2 C1=CC=C(C=C1)C=O InChI=1S/C3H6O/c1-3(2)4/h1-2H3'. Below the suggestions are radio buttons for 'Use Entrez', 'Compounds' (selected), 'Substances', and 'BioAssays'. At the bottom, there are four icons with labels: 'Draw Structure' (pencil and structure), 'Upload ID List' (upload arrow), 'Browse Data' (data table), and 'Periodic Table' (periodic table grid).



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- **PubChem** is a database of chemical molecules and their activities against biological assays. The system is maintained by the National Center for Biotechnology Information (NCBI), a component of the National Library of Medicine, which is part of the United States National Institutes of Health (NIH).
- PubChem is the world's largest collection of freely accessible chemical information.
- Also search chemicals by name, molecular formula, structure, and other identifiers. Find chemical and physical properties, biological activities, safety and toxicity information, patents, literature citations and more.



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ChemSpider

Acetaminophen | C₈H₉ | eMolecules | ChemSpider | Search ar | ZINC | Chemical databases/re | ChemSpider | Search ar

Not secure | chemspider.com

ChemSpider

Search and share chemistry

Search ChemSpider

For medical information relating to Covid-19, please consult the [World Health Organisation](#) or local healthcare provision.

Simple Structure Advanced History

Search ChemSpider

Matches any text strings used to describe a molecule.

Search

Systematic Name, Synonym, Trade Name, Registry Number, SMILES, InChI or CSID ?

What is ChemSpider?	Search by chemical names	Search by chemical structure	Find important data
<p>ChemSpider is a free chemical structure database providing fast text and structure search access to over 67 million structures from hundreds of data sources.</p>	<ul style="list-style-type: none">• Systematic names• Synonyms• Trade names• Database identifiers	<ul style="list-style-type: none">• Create structure-based queries• Draw structures in the web page• Use structure files from your computer	<ul style="list-style-type: none">• Literature references• Physical properties• Interactive spectra• Chemical suppliers

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- ChemSpider is a web-based database of chemical data and links to related articles and patents.
- The range of data stored in ChemSpider includes chemical structures, identifiers (IUPAC/common/trade names, synonyms, SMILES, InChIs), properties (experimental and predicted), spectral, crystallographic, images and also draw a molecule.

What can I do with ChemSpider?

Search by chemical names

- Systematic names
 - Synonyms
 - Trade names
- Identifiers (molecular formulas, SMILES, InChIs, registry numbers)

Search by chemical structure

- Create structure-based queries
- Draw structures in the web page
- Use structure files from your computer
- Substructure searching
 - Similarity searching

Find important data

- Literature references
- Physical properties
- Interactive spectra
- Chemical suppliers

Predict Chemical Properties

- Log P
- Log D
- Polar Surface Area
- Surface Tension
- Refractive Index

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Deposit Data

- Chemical structures
- Chemical properties
- Spectra (NMR, IR, Raman, Mass Spectra, UV-Vis)
- Crystallographic Information Files

Curate Data

- Add names/identifiers
- Correct Name-Structure associations
- Add literature references



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eMolecules

The screenshot shows the eMolecules website in a web browser. The browser's address bar displays "emolecules.com". The website has a blue header with navigation links: "About Us", "Products", "Suppliers", and "Support". A search bar in the header contains the text "CAS/MFCD/Catalog#/SMILES" and a "Search" button. The user is logged in as "Hi Guest User".

The main content area features the eMolecules logo and the tagline "empowering drug discovery". Below this, a section titled "Search and order from over 7.3 million Building Blocks" is visible. It includes two tabs: "Structure Search" (selected) and "List Search".

On the left side, there is a blue sidebar with the following menu items: "Building Blocks" (with a right-pointing arrow), "Screening Compounds", and "Antibodies".

The central workspace is a large white area with a toolbar on the left containing various chemical building block icons (atoms, rings, functional groups). Below the toolbar is a large empty box for drawing or viewing chemical structures. At the bottom of this workspace are buttons for "Substructure Search", "Exact Structure Search", and "Similarity Search" (which includes a similarity score input field set to "0.8").

The footer of the website contains the copyright notice: "Copyright © 2020 eMolecules, Inc." and links to "Terms of Service", "Privacy Policy", "Feedback", and "Contact Us".



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ZINC15

The screenshot shows the ZINC15 website in a web browser. The browser tabs include 'eMolecules', 'ZINC', and 'Chemical databases/resources'. The address bar shows 'zinc15.docking.org'. The website has a dark navigation bar with links: ZINC, Substances, Catalogs, Tranches, Biological, More, and About. The main content area has a large 'ZINC15' heading. To the right, a paragraph states: 'ZINC is provided by the Irwin and Shoichet Laboratories in the Department of Pharmaceutical Chemistry at the University of California, San Francisco (UCSF). We thank NIGMS for financial support (GM71896).' Below this, a 'Welcome to ZINC' section describes the database. To the right, a citation is provided. At the bottom, there are three columns: 'Getting Started' with a list of links, 'Ask Questions' with a list of common queries, and 'ZINC15 News' with a list of recent updates. A 'Caveat Emptor' box is also present.

ZINC15

Welcome to ZINC, a free database of commercially-available compounds for virtual screening. ZINC contains over 230 million purchasable compounds in ready-to-dock, 3D formats. ZINC also contains over 750 million purchasable compounds you can search for analogs in under a minute.

ZINC is provided by the Irwin and Shoichet Laboratories in the Department of Pharmaceutical Chemistry at the University of California, San Francisco (UCSF). We thank NIGMS for financial support (GM71896).

To cite ZINC, please reference: Sterling and Irwin, *J. Chem. Inf. Model.*, 2015 <http://pubs.acs.org/doi/abs/10.1021/acs.jcim.5b00559>. You may also wish to cite our previous papers: Irwin, Sterling, Mysinger, Bolstad and Coleman, *J. Chem. Inf. Model.*, 2012 DOI: [10.1021/ci3001277](https://doi.org/10.1021/ci3001277) or Irwin and Shoichet, *J. Chem. Inf. Model.* 2005;45(1):177-82 PDF, DOI.

Getting Started

- [Getting Started](#)
- [What's New](#)
- [About ZINC 15 Resources](#)
- [Current Status / In Progress](#)
- [Why are ZINC results "estimates"?](#)

Explore Resources

Chemistry
[Tranches](#), [Substances](#), [3D Representations](#), [Rings](#), [Patterns](#)
[And More](#)

Ask Questions

You can use ZINC for **general** questions such as

- [How many substances in current clinical trials have PAINS patterns? \(150\)](#)
- [How many natural products have names in ZINC and are not for sale? \(9296\) get them as SMILES, names and calculated logP](#)
- [How many endogenous human metabolites are there? \(47319\) and how many of these can I buy? \(8271\) How many are FDA approved drugs? \(94\)](#)
- [How many compounds known to aggregate are in current clinical trials? \(60\)](#)
- [How many epigenetic targets have compounds known? \(53\) and Which of these substances can I buy? \(278\)](#)

ZINC15 News

- 2018-02-14 - ZINC reaches 213,235,528 purchasable leadlike 3D!
- 2018-02-13 - ZINC reaches 736,001,654 purchasable molecules 2D!
- 2018-01-14 - Klara Anu is born! Welcome Klara Anu, sister to Lisa!
- 2018-01-01 - Chinzo Dandar joins our team. Welcome Chinzo! Follow us on twitter @chem4biology Known limitations What's new

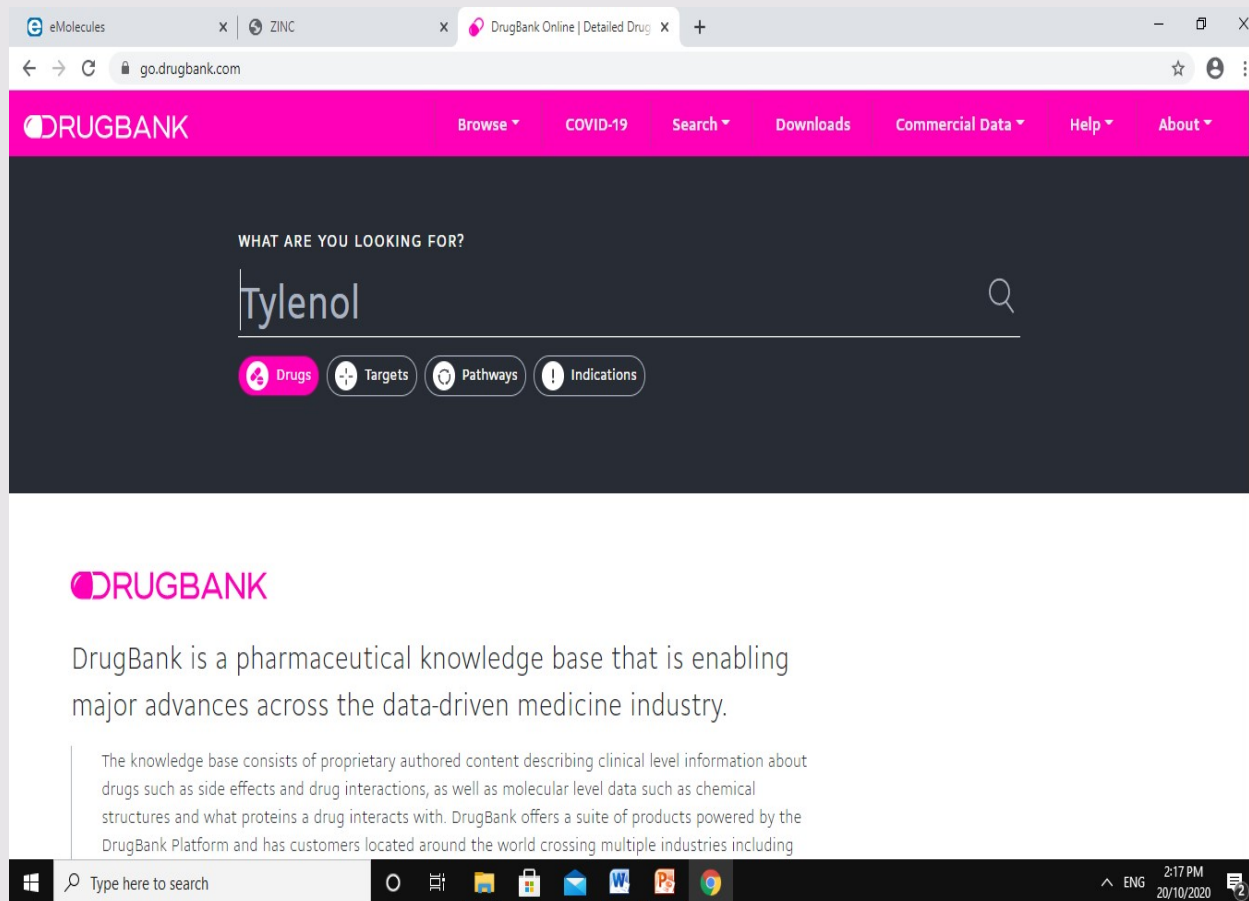
Caveat Emptor: We do not guarantee the quality of any molecule for any purpose and take no responsibility for errors arising from the use of this



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ZINC database contains 21 million compounds available for virtual screening. In this database various molecule features like molecular weight, logP etc are included.

DrugBank





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- The database that combines detailed drug (i.e. chemical, pharmacological and pharmaceutical) data with comprehensive drug target (i.e. sequence, structure, and pathway) information.
- The database contains 6712 drug entries including 1448 FDA-approved small molecule drugs, 131 FDA-approved biotech (protein/peptide) drugs, 85 nutraceuticals and 5080 experimental drugs.