ChemSpider is a freely available database, based on chemical structures, that provides information on over 26 million de-duplicated compounds derived from over 400 sources. These sources include a wide variety of government databases, chemical supplier catalogs, academic and commercial websites, that are listed at: [http://www.chemspider.com/DataSources.aspx](http://www.chemspider.com/DataSources.aspx)

“Before you do anything with ChemSpider it is important to remember that it isn’t yet either perfect or exhaustive” [http://www.chemspider.com/GettingStarted.aspx](http://www.chemspider.com/GettingStarted.aspx)

Each of the listed sources has a brief popup description, with the full record providing a web link to the source. ChemSpider augments the default information from these sources with additional of property data. For example, the record display for Pyridine provides a 2d or 3d chemical structure with MF and MW, systematic name, SMILES and InChI.

If available, each chemical compound record also includes:

- Names and Identifiers: Names, Synonyms and Database Identifier Numbers.
- ChemSpider/Google Searches: MF, Skeleton, Structure, Synonym or INChI Key.
- Properties/Predicted: ACD Labs, EPISuite, & ChemAxon’s chemicalize.org
- Spectra: HNMR & CNMR.
- CIFs: Crystallographic Information Files.
- Articles/Links & References & RSC journals: Articles recommended by users.
- Articles/PubMed & Google Books: Articles/Books recommended by users.
- Chemical Vendors: List of suppliers with product numbers.
- Data Sources: All, Biological, Syntheses, Publishers, Metabolism, Screening, Phys. Properties, Theor., Personal, Publication, Web Article, Compound Aggreg., Xtal Structures, Natural Products, Spectral Data, Data Aggregators, Safety Data.
- Wikipedia Article(s): Introduction with link to full article and option to edit article.
- RSC Databases: Mass Spectrometry Bulletin, Laboratory Hazards Bulletin, Methods in Organic Synthesis/ Catalysts & Catalysed Reactions, Natural Product Updates, Analytical Abstracts (only article titles, authors for non-subscribers)
- MESH Headings: PubMed Terms that include the compound name.
- Pharmacological Links: DailyMed, PillBox
- Curation: Feedback with response

Search options include:

- Simple:
Systematic Name, Synonym, Trade Name, Registry Number, SMILES, InChI or CSID with additional options for: Single/Multi-component, Isotopically Labeled, and additional filters.

Structure:

Upload a structure or image file or Convert Name, SMILES, InChI or ChemSpider ID to structure, or Draw a structure (Accelrys JDraw, Elemental, ACD/Labs SDA, Ketcher, JME, or JChempaint). Searches can be Exact or Substructure or Similarity with additional options for: Exact Match, All Tautomers, Same Skeleton (including or excluding H) and All isomers.

Display options are: Grid, Tile, Table, Names/Structures.

Advanced:

Search by Structure, Identifier, Elements, Properties, Calculated Properties, Data Source, etc., and by LASSO (Ligand Activity in Surface Similarity Order) Similarity.

Search History:

Each search is assigned an internal ID number, date/time started & Updated, Status, Progress, Predicate (search string) and system Message.

Web API:

Web services for both query and access are available.

Help:

ChemSpider FAQs, Help (for links to various Help Topics), Getting Started, Forum, and Site Map.

ChemSpider
http://www.chemspider.com