

Intended Users:	Students (High School and Above)	Information Professionals	Researchers
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## PubChem

**Description:** PubChem is the world's largest collection of freely accessible chemical information. People can search by name, structure, and other identifiers. The site provides information on physical and biological properties, safety, toxicity, patents, and available literature. PubChem mostly contains small molecules, but includes certain larger molecules such as nucleotides, carbohydrates, lipids, peptides, and chemically modified macromolecules.

### Popular uses of this product:

Students (High School and Above)	Information Professionals	Researchers
<ul style="list-style-type: none"> <li>• Use the Draw Structure Tool to model chemicals.</li> <li>• Use the Periodic Table to find information about the characteristics of elements.</li> <li>• Play the Periodic Table matching game to study how the elements are organized.</li> <li>• Find Laboratory Chemical Safety Summaries.</li> </ul>	<ul style="list-style-type: none"> <li>• Direct researchers to tutorials and provide guidance on how to find and use information on PubChem.</li> <li>• Find relevant blog articles about updates and changes to the site.</li> <li>• Help researchers find programming language resources to aid in analyzing content.</li> <li>• Embed PubChem widgets onto any webpage.</li> </ul>	<ul style="list-style-type: none"> <li>• Use PubChemRDF to explore semantic relationships among compounds, substances, proteins, etc.</li> <li>• Perform a 3D similarity search to identify molecular similarity.</li> <li>• Use programmatic access to search and retrieve non-textual information about compounds and chemical structures.</li> <li>• Find Laboratory Chemical Safety Summaries.</li> </ul>

### Key Points:

1. The data on PubChem is gathered from over 800 different sources to provide information on hundreds of millions of compounds, substances, bioactivities, and patents.
2. People can use the Entrez search option to search all PubChem resources at once; bulk download of different record type; or use programmatic access to find URLs, annotations, and associations.

### Potential Predicaments:

1. The Entrez search function is primarily for text-based searches. Researchers may prefer programmatic access to retrieve information, but there are request volume limits.
2. Submissions on PubChem go through a standardization process to validate chemical contents and normalize chemical representations. Researchers may need to be more familiar with this process in case any submissions are modified during standardization.

### Teaching Examples:

1. On the PubChem homepage, select the "About" tab at the top. Have participants search for information in the "About" pages. Find the number of compound records on the website (under PubChem Statistics, about 111 million). Find the Request Volume limitations (under Programmatic Access). While exploring the "About" pages, find and access a PubMed article that discusses ways to use PubChem.
2. Type "57-27-2" in the search bar. The results should bring back the compound morphine. On the right-hand side of the page, select "Search in Entrez." A new window will open. Select "PubMed (MeSH Keyword)" to find PubMed articles related to that compound.

### Real Life Examples:

1. An information professional finds tutorial on using XML, C++, and C# so researchers can better access programmatic information from PubChem.
2. A researcher uses the PUG tools to find tabular bioactivity data on PubChem.

**More Information:**

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[PubChem Substance and Compound Databases PMID: 26400175](#)