

## 3.5: Database Query Introduction

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### Basic Searches

After visiting a website that provides chemical information such as [PubChem](#), there was most likely a text field available that allows the user to input an alphanumeric name, number or combination of both to retrieve a chemical. Simple text input searches may seem like the most basic way to look for something in a database and often they are, but many allow for inputting characters to refine how the search is performed. Using a simple google search as an example, you can change how the search is performed by simply putting your terms into parenthesis. This tells the search engine that everything in parenthesis must be found before being included in the results. There are some common practices for these alterations that are used among many different search engines, but this should not be interpreted to think that they will all work the same.

Before performing a series of searches, look for documentation provided by the host of the search engine to see what alterations can be made so that the results found have more relevancy to what the user seeks. The reason for this is simply due to the fact that chemical databases can contain a lot of data and this will save on trying to sort through thousands of results. Review section 1.3 of this course to see some other alterations that are often allowed in text searches. Take note of using boolean characters along with some of the different ways chemicals can be represented in chapter 2 of this course.

### Custom Search Parameters

Advanced chemical searches may need to have several custom parameters used to narrow down a large list of chemicals into a smaller more relevant pool of results. The user interface for a custom search usually works similar to filling out an electronic form. After navigating to the advanced search on a website, the user will be presented with many options for defining a very specific search. Many of these advanced searches will contain checkboxes for selecting things like functional groups, experimental properties and other details for the compound. The user may also be able to specify ranges for things like density, number of atoms or other properties. Keywords can be valuable in searching the context of a chemical page to find a structure meeting certain categories.

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