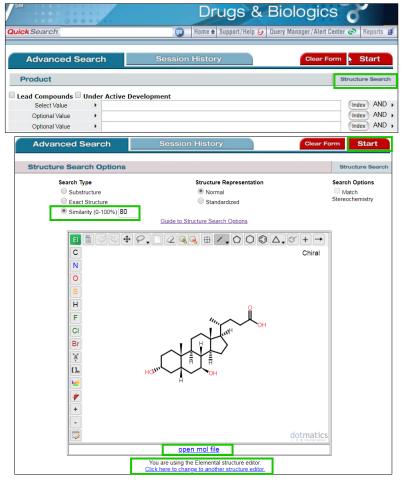# Structure Similarity Search

Interested in compounds structurally similar to your target molecule?

Use *Clarivate Analytics Integrity* to search for compounds similar to your target molecule. Similarity searching is different from substructure searching in that it relies on molecular descriptors, fingerprints and algorithms. It is complementary to substructure and exact structure searches because it returns answers not found with these chemical structure search strategies. **Example Scenario:** You are a researcher working on biliary tract disorders and want to review the landscape of compounds obtained by similarity searching on your candidate molecule. Additionally, you are also interested in the indications these compounds are being developed for.

Setting up a Structure Search and refining search results:

Structure search

Starting in the **Drugs & Biologics** Knowledge Area click the **Structure Search** button.

Tip:

o   The **structure search** feature is available in all knowledge areas except **Targets & Pathways**, **Genomics**, and **Biomarkers**.

You are taken to an **Advanced Search** page containing a structure drawing window.   Click to select the **Similarity** radio button. The default similarity value is 80%; this can be manually adjusted by the user (in this example, the value has been set to 80%).

Tip:

o   If you're using the structure search feature for the first time please see the end of this guide for further details about compatible drawing packages (structure editors).

To draw the structure you wish to query, use the structure drawing tools that appear on screen to draw directly in the structure drawing window. Alternately, you can upload a mol file by clicking the **open mol file** link.
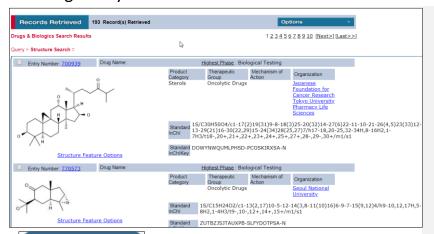
For this scenario, a structure mol file was uploaded into the structure editor and is a candidate for biliary disorders.

To use a different structure editor, use **Click here to change to another structure editor** option at the bottom.
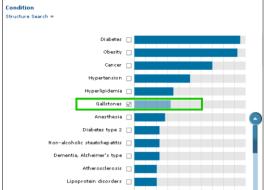
When your structure is complete in the *Integrity* structure drawing box, click **Start** to launch your search.
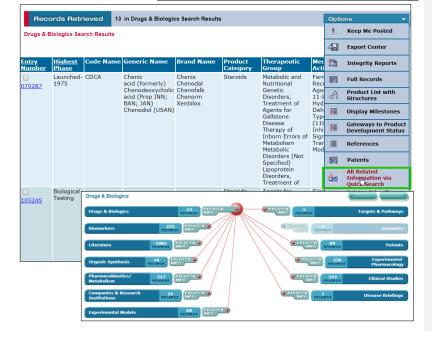
Working with your data

You can refine the data you've retrieved with your search using the **Filter by Statistics** tool.

For example, to see what conditions are associated with your results click **Condition** in the **Filter by Statistics** list.

For example, click on the **Gallstones** bar to view a refined list of drugs specific for this indication.

Using the **Options** pull down menu you can select **All Related Information via Quick Search** to view related information to **Experimental pharmacology** or **Pharmacokinetics**.

Compatible Drawing Packages (structure editors)

Integrity is compatible with four different drawing packages (structure editors):

- *Accelrys Draw* (existing license and prior installation required).

- *ISIS/Draw* (existing license, prior installation, and Chime plugin required).

- *ChemAxon Marvin Applet* (no-charge license, automatic installation).

- *CambridgeSoft CS ChemDraw™ Plugin* (installation required; no-charge download available).

If you are using the structure search feature for the first time, a plugin may need to be installed, depending on which structure editor has been chosen as the default value for your company's license.

Simply click the link below the structure drawing window to install (or to change) a structure editor.

Note: Compared to the other structure editors listed ChemDraw uses a unique algorithm and the number of hits returned may differ.