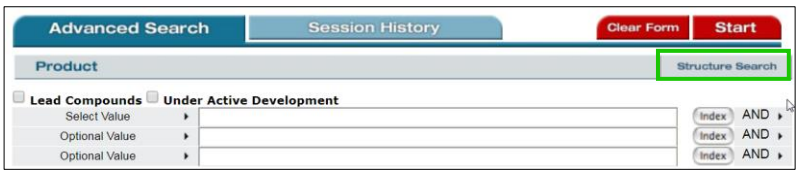
Clarivate Analytics Integrity

# Search by substructure

*Want to know which molecules contain your query structure as a portion? What are these compounds being developed for?*

*Integrity* helps you gain competitive intelligence, and identify potential new targets or conditions related to your candidate molecule. **Example Scenario:** You are a researcher and want to find compounds containing the same substructure core that an in-house molecule has, and review any activity those compounds demonstrate against other targets, or in other disease areas.

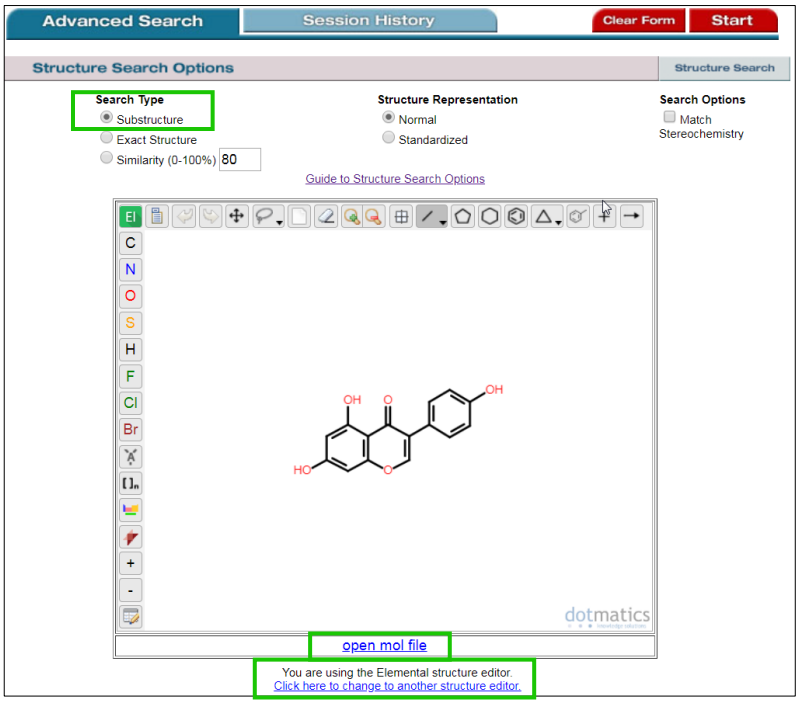
## Setup a substructure search:




Starting in the **Drugs & Biologics** knowledge area click the **Structure Search** button.

**Tip:**

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

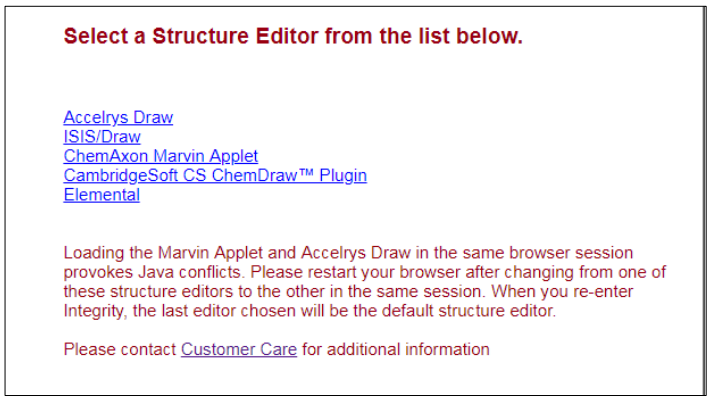



You are taken to an **Advanced Search** page containing a structure drawing window.

*Integrity* is compatible with four different drawing package (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.

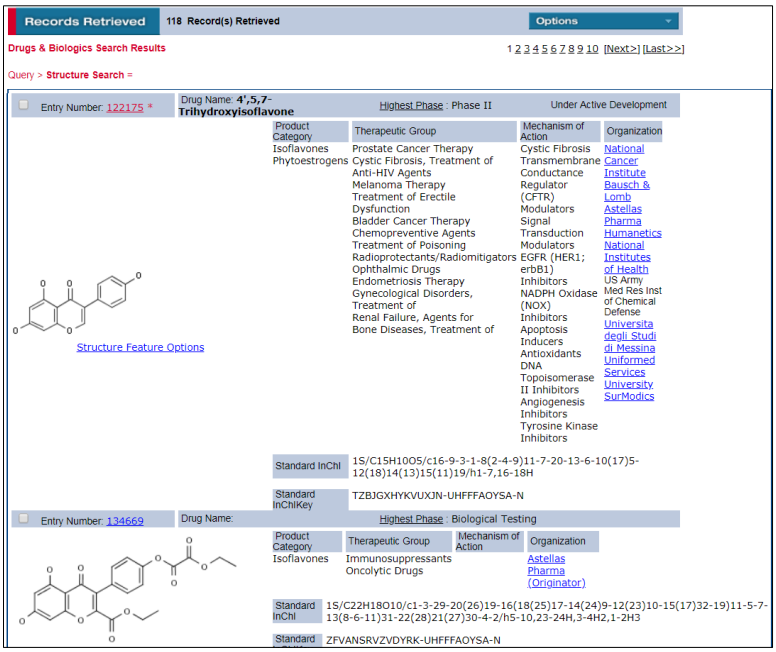



Simply click the link below the structure drawing window to install (or to change) a structure editor. A pop-up box with installation instructions appears.

**Tip:**

- For further details on how the available drawing packages work with *Integrity*, see **Guide to Structure Search Options** above the structure drawing window.

Ensure **Substructure** radio button is selected.




To draw the substructure you wish to query, use the structure drawing tools that appear on screen or click on **open mol file** to upload the structure.

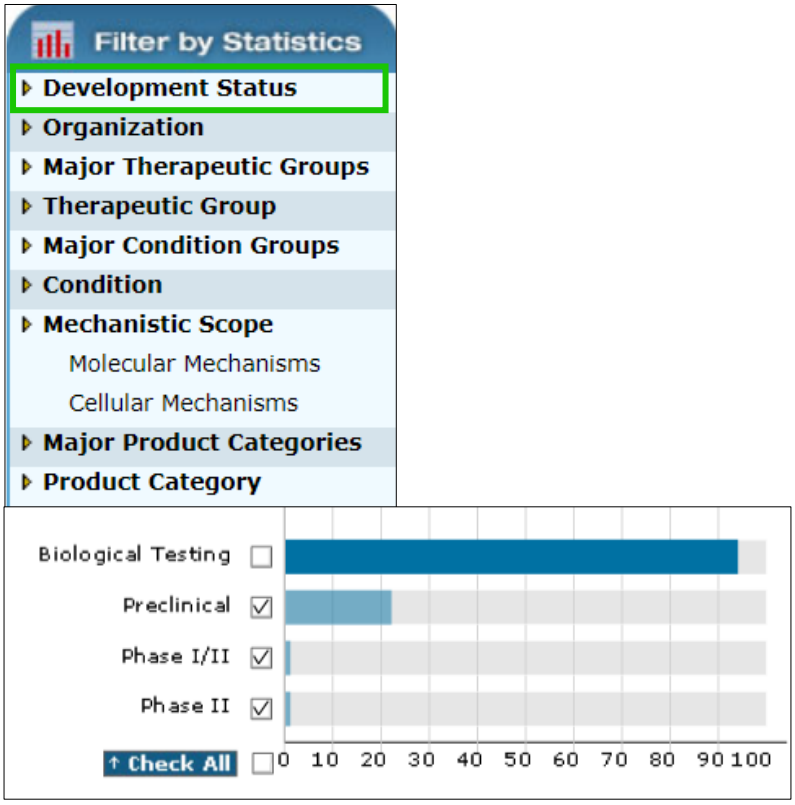
For this scenario, the structure belongs to isoflavone family for cancer chemotherapy.

When your substructure appears in the *Integrity* structure drawing box, click **Start** to launch your search.

**Tip:**

- For more specific results, combine substructure searches with text and data searches.

# Working with your data:




You can refine your data using the **Filter by Statistics** tool. For example, to remove all compounds in biological testing status, and find only those that have progressed further in the pipeline, click **Development Status**.

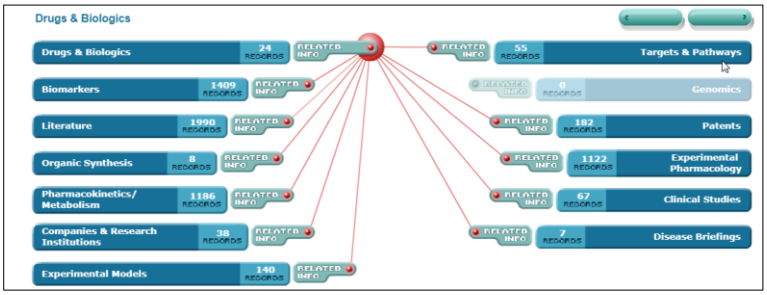
In this case, select the **Preclinical, Phase I/II and Phase II** checkboxes.

Click **View Subset(s)** for a list of results.

You can then use the **Filter by Statistics** tool to view, or further filter by other fields such as **Condition**, **Target**, or **Therapeutic Group**.

**Tip:**

- To see the structures at any time, select **Options**, and **Product List with Structures.**




To find other information around these compounds, for example experimental pharmacology or pharmacokinetic data, click the checkbox for each compound you want to include in your search, or leave unchecked to include all compounds.

Open the **Options** pull down menu, and select **All Related Information via Quick Search**.

Click the corresponding bar to go to **Experimental Pharmacology**, or **Pharmacokinetics** for related information.