

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:

Select a Structure Editor from the list below.

[Accelrys Draw](#)
[ISIS/Draw](#)
[ChemAxon Marvin Applet](#)
[CambridgeSoft CS ChemDraw™ Plugin](#)
[Elemental](#)

Loading the Marvin Applet and Accelrys Draw in the same browser session provokes Java conflicts. Please restart your browser after changing from one of these structure editors to the other in the same session. When you re-enter Integrity, the last editor chosen will be the default structure editor.

Please contact [Customer Care](#) for additional information

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.

Records Retrieved 118 Record(s) Retrieved Options

Drugs & Biologics Search Results 1 2 3 4 5 6 7 8 9 10 [Next>] [Last>>]

Query > Structure Search =

Entry Number: 122175 *	Drug Name: 4',5,7-Trihydroxyisoflavone	Highest Phase: Phase II	Under Active Development
Product Category	Therapeutic Group	Mechanism of Action	Organization
Isoflavones	Prostate Cancer Therapy	Cystic Fibrosis	National Cancer Institute
Phytoestrogens	Cystic Fibrosis, Treatment of	Transmembrane Conductance Regulator (CFTR)	Bausch & Lomb
	Anti-HIV Agents	Modulators	Astellas
	Melanoma Therapy	Signal Transduction	Pharma
	Treatment of Erectile Dysfunction	Modulators	Humantec
	Bladder Cancer Therapy	EGFR (HER1; erbB1)	National Institutes of Health
	Chemopreventive Agents	Inhibitors	US Army
	Treatment of Poisoning	NADPH Oxidase (NOX)	Med Res Inst of Chemical Defense
	Radioprotectants/Radiomitigators	Inhibitors	University of Mississippi
	Ophthalmic Drugs	Apoptosis Inducers	Uniformed Services University
	Endometriosis Therapy	DNA Topoisomerase II Inhibitors	SurModics
	Gynecological Disorders, Treatment of	Angiogenesis Inhibitors	
	Renal Failure, Agents for	Tyrosine Kinase Inhibitors	
	Bone Diseases, Treatment of		
Standard InChI 1S/C15H10O5/c16-9-3-1-8(2-4-9)11-7-20-13-6-10(17)5-12(18)14(13)15(11)19/h1-7,16-18H			
Standard InChIKey TZBJGXHYKVUXJN-UHFFFAOYSA-N			

Structure Feature Options

Entry Number: 134669	Drug Name:	Highest Phase: Biological Testing
Product Category	Therapeutic Group	Mechanism of Action
Isoflavones	Immunosuppressants	Apoptosis Inducers
	Oncolytic Drugs	Antioxidants
Standard InChI 1S/C22H18O10/c1-3-29-20(26)19-16(18)25(17-14(24)9-12(23)10-15(17)32-19)11-5-7-13(8-6-11)31-22(28)21(27)30-4-2/h5-10,23-24H,3-4H2,1-2H3		
Standard InChIKey ZFVANSRVZDYRK-UHFFFAOYSA-N		

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:

Filter by Statistics

- ▶ **Development Status**
- ▶ Organization
- ▶ Major Therapeutic Groups
- ▶ Therapeutic Group
- ▶ Major Condition Groups
- ▶ Condition
 - ▶ Mechanistic Scope
 - Molecular Mechanisms
 - Cellular Mechanisms
- ▶ Major Product Categories
- ▶ Product Category

Biological Testing 100

Preclinical 25

Phase I/II 5

Phase II 5

↑ Check All 0 10 20 30 40 50 60 70 80 90 100

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**.

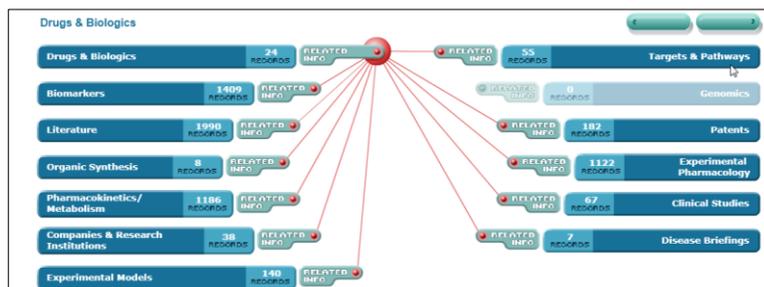
In this case, select the **Preclinical, Phase I/II and Phase II** checkboxes.

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.

If you have any questions please contact us at: DTStraining@clarivate.com