

# 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

#### 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. 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:

- 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

Records Retrieved 193 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: 700939 Drug Name: Highest Phase: Biological Testing

Product Category: Steroids Therapeutic Group: Oncolytic Drugs Mechanism of Action: Organization: Jiciness Foundation for Cancer Research Tokyo University Pharmacy Life Sciences

Standard InChI: 1S/C30H50O4/c1-17(2)19(31)9-8-18(3)25-20(32)14-27(6)22-11-10-21-26(4,5)23(33)12-13-29(21)16-30(22,29)15-24(34)28(25,27)7/17-18,20-25,32-34H,8-16H2,1-7H3/t18-,20+,21+,22+,23+,24+,25+,27+,28-,29-,30+/m1/s1

Standard InChIKey: DOWYNWQMLPHSD-PCGSKIRXSA-N

Structure Feature Options

Entry Number: 700573 Drug Name: Highest Phase: Biological Testing

Product Category: Steroids Therapeutic Group: Oncolytic Drugs Mechanism of Action: Organization: Seoul National University

Standard InChI: 1S/C15H24O2/c1-13(2,17)10-5-12-14(3,8-11(10)16)6-9-7-15(9,12)4/h9-10,12,17H,5-8H2,1-4H3/t9-,10-,12+,14+,15+/m1/s1

Standard InChIKey: ZUTBZSJTAUXPB-SLFYDOTPSA-N

Structure Feature Options

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.

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
- Launch Year
- Target

Condition

Structure Search =

Diabetes

Obesity

Cancer

Hypertension

Hyperlipidemia

Gallstones

Anesthesia

Diabetes type 2

Non-alcoholic steatohepatitis

Dementia, Alzheimer's type

Atherosclerosis

Lipoprotein disorders

Records Retrieved 13 in Drugs & Biologics Search Results Options

Drugs & Biologics Search Results

Entry Number	Highest Phase	Code Name	Generic Name	Brand Name	Product Category	Therapeutic Group	Mec Act
070287	Launched-1975	CDCA	Chenic acid (formerly Chenodeoxycholic acid (Prop INN; BAN; JAN) Chenodiol (USAN)	Chenix Chenodal Chenofalk Chenorm Xenbilox	Steroids	Metabolic and Nutritional Genetic Disorders, Treatment of Agents for Gallstone Disease Therapy of Inborn Errors of Metabolism Metabolic Disorders (Not Specified) Lipoprotein Disorders, Treatment of	Farr Rec Ago 11-4 Hyd Deh Typ (11 Inhi) Sig Tar Mod
105245	Biological Testing						

Options: Keep Me Posted, Export Center, Integrity Reports, Full Records, Product List with Structures, Display Milestones, Gateways to Product Development Status, References, Patents, All Related Information via Quick Search

Drugs & Biologics 13 RECORDS RELATED INFO

Biomarkers 335 RECORDS RELATED INFO

Literature 1083 RECORDS RELATED INFO

Organic Synthesis 18 RECORDS RELATED INFO

Pharmacokinetics/ Metabolism 312 RECORDS RELATED INFO

Companies & Research Institutions 19 RECORDS RELATED INFO

Experimental Models 68 RECORDS RELATED INFO

Targets & Pathways 89 RECORDS RELATED INFO

Genomics 226 RECORDS RELATED INFO

Patents 226 RECORDS RELATED INFO

Experimental Pharmacology 342 RECORDS RELATED INFO

Clinical Studies 1 RECORDS RELATED INFO

Disease Briefings

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