

THOMSON REUTERS INTEGRITY

QUICK GUIDE SERIES: No. 3



HOW TO SEARCH BY SUBSTRUCTURE WITH ISIS/DRAW, ACCELRY'S DRAW, CS CHEMDRAW AND MARVIN

Use *Thomson Reuters Integrity*SM to search for all molecules that contain your query structure as the portion of the molecule to gain competitive intelligence, and identify potential new targets, or conditions.

This step-by-step guide will show you how to:

- Set up a structure search using *Accelrys Draw*, *ISIS/Draw*, *CambridgeSoft CS ChemDraw™ Plugin* or *ChemAxon Marvin Applet*.
- Filter and view subsets of your results and link to related information, such as experimental pharmacology values or pharmacokinetics data.

EXAMPLE SCENARIO: COMPOUND SUBSTRUCTURE SEARCH

A researcher wants 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.

1. SETTING UP A STRUCTURE 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 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. 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.



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Tip:

For more specific structure searching, for example stereochemistry, the following options can be applied:

- Under **Structure Representation: Normal** allows you to search for structures as they are displayed in *Integrity*, considering how salts, tautomers, or other structures are drawn; **Standardization** not only allows you to search for the structure displayed, but also other chemically equivalent structures irrespective of their structure representation in *Integrity*.
- **Match Stereochemistry** allows the results to consider, or ignore stereochemistry.
- To draw the substructure you wish to query, simply double-click in the structure drawing window to open the drawing package (*ISIS/Draw*, and *Accelrys Draw* users) or use the structure drawing tools that appear on screen (*ChemDraw* and *Marvin* users).
- When you have drawn your structure in the *ISIS/Draw* or *Accelrys Draw* application, click in the top left corner to transfer your structure back to *Integrity*. For this scenario the structure is part of an in-house COPD compound.
- 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.

2. 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** and **Phase I** 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** pulldown menu, and select **All Related Information via Quick Search**.
- Click the corresponding bar to go to **Experimental Pharmacology**, or **Pharmacokinetics** for related information.

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If you have any questions about using Integrity please contact us at: ts.support.emea@thomsonreuters.com