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QUICK GUIDE SERIES: No. 8



USE VALUE SEARCHING TO FIND HIGH-POTENCY COMPOUNDS AND COMPARE STRUCTURES USING A SAR TABLE

In the Experimental Pharmacology and Pharmacokinetics/Metabolism knowledge areas of Thomson Reuters IntegritySM you can limit searches by numeric value to retrieve more targeted results. Additionally, filtering options allow you to drill down from a broader search into Integrity's comprehensive database of scientific information.

This tool adds versatility to the searches you can perform using Integrity as chemists, pharmacologists and information professionals. For example, you can create SAR tables based on a specific value range and export that dataset.

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

- Limit searches by numeric value ranges
- Easily create SAR tables based on a specific value range

EXAMPLE SCENARIO: EXPERIMENTAL PHARMACOLOGY STRUCTURE SEARCH LIMITED BY VALUE

A researcher working with a structure has found a new patent with compounds containing the same substructure that are reported to act with high potency on the histamine H4 target. He wants to find out if there are other known similar, high-potency molecules and to compare their structures.

1. SETTING UP A SEARCH

- Click on **Experimental Pharmacology** from the Home Page or select it from the pull-down menu of Knowledge Areas on other pages of Integrity.
- Click the **Structure Search** button (in the Product section of search fields) to open the structure drawing window within the Integrity Search Form.

Structures can either be drawn using the structure editor tools or they can be imported from an existing file.

To import the substructure you wish to query, right-click in the structure drawing window and click on File and then Open (ISIS/Draw, Symyx® Draw, CambridgeSoft CS ChemDraw™ users) or click on File and then Open (ChemAxon Marvin Applet users).

Tip:

- Refer to the *How to search by substructure Quick Guide* for further information.
- You can add further search criteria to your query by using the text fields displayed underneath the structure searching window.
- Open the first **Select Value** dropdown menu under the Experimental Pharmacology section and select **Value**. Click **Index** to open the **Value Browse Index**. Type **50** in the **Lookup box** and click **Lookup**. Click once to select the term **IC-50** and click **OK**.
- In the second box in this row select **M** from the dropdown list. In the third box select **Less than** from the dropdown list. Specify the range of interest in the fourth box. For this example we will search for values less than 10 nM. To do this type **10e-9**.

Tip:

- Type "e" in lower-case letters when entering value ranges in scientific notation format.



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2. WORKING WITH YOUR DATA

- You can refine the data you've retrieved with your search using the **Filter by Statistics** tool. For example, to filter your results to an experimental activity of interest, click **Experimental Activity** in the **Filter by Statistics** list to the right.

Tip:

- Hover over a bar in the chart to see the exact number of results. Hover over a category name to see the full name.

- In this case, scroll down to find the category for **Histamine H4 Receptor affinity, IN VITRO**. Click to enter a check in the checkbox and then click **View Subset(s)**. This will filter the original results list to a new list with about 32 results.

Tip:

- The list of values can be sorted in ascending numerical order by clicking on the underlined **Value** column header.
- The list of values can be further filtered by range by using the **Filter by Value Range** tool underneath the **Filter by Statistics** list.

- Display a SAR table for these values by opening the **Options** pull-down menu and selecting **Structure Activity**.

Tip:

- When there is a mixture of units of measurement on screen, such as M and g/L, you can convert for easy comparison using the unit conversion tool. Open the Options pull-down menu and click on **Convert Molar Units to Grams**.

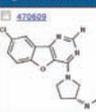
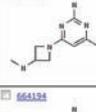
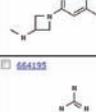
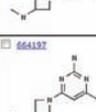
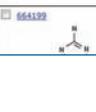


Records Retrieved: 32 in Experimental Pharmacology

Experimental Pharmacology Search Results

Experimental Activity: Histamine H4 Receptor affinity, IN VITRO

Pharmacological Activity: Histamine H4 receptor affinity

Drug Name & Structure	Mechanism of Action	Material	Method	Value	Details
 423693	Signal Transduction Inhibitors Histamine H4 Receptor Antagonists	Cells transfected with human receptor	Displacement of [3H]-Histamine	1.00 nM	Det. 2
 664132	Signal Transduction Inhibitors Histamine H4 Receptor Antagonists	CHO Chinese hamster ovary cells transfected with human receptor	Displacement of [3H]-Histamine	>> 1.00 µM	Det. 2
 664134	Signal Transduction Inhibitors Histamine H4 Receptor Antagonists	CHO Chinese hamster ovary cells transfected with human receptor	Displacement of [3H]-Histamine	>> 1.00 µM	Det. 2
 664135	Signal Transduction Inhibitors Histamine H4 Receptor Antagonists	CHO Chinese hamster ovary cells transfected with human receptor	Displacement of [3H]-Histamine	>> 1.00 µM	Det. 2
 664137	Signal Transduction Inhibitors Histamine H4 Receptor Antagonists	CHO Chinese hamster ovary cells transfected with human receptor	Displacement of [3H]-Histamine	>> 1.00 µM	Det. 2
 664139	Signal Transduction Inhibitors Histamine H4 Receptor Antagonists	CHO Chinese hamster ovary cells transfected with human receptor	Displacement of [3H]-Histamine	>> 1.00 µM	Det. 2

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