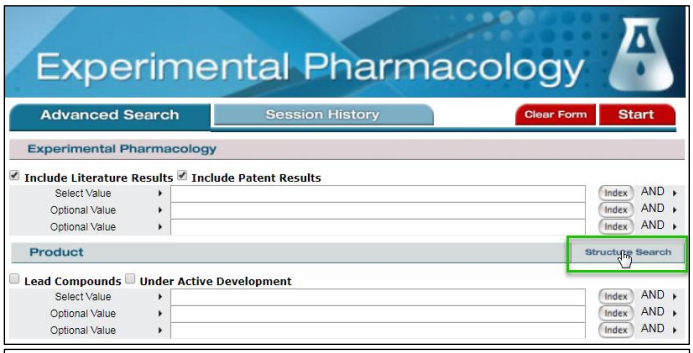
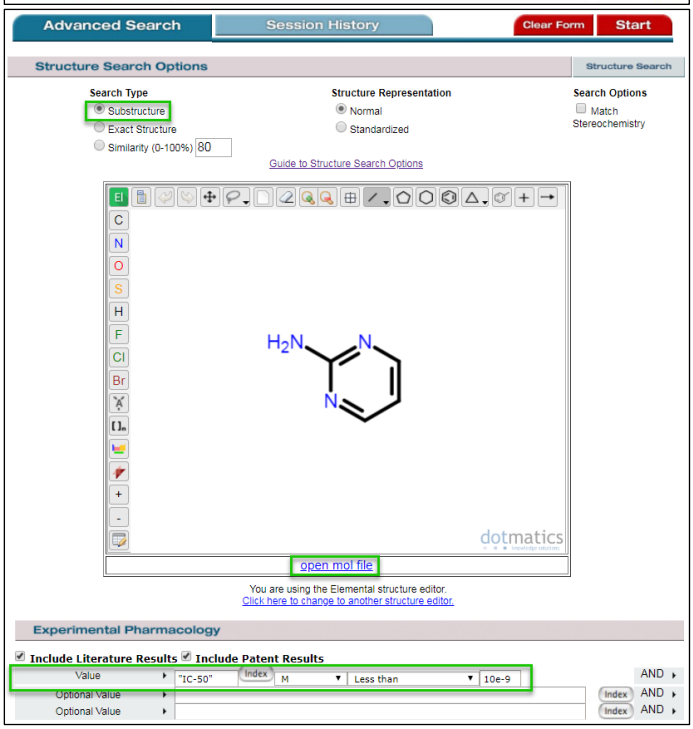
Find high-potency compounds and compare structures using value search and SAR table

Searching for compounds with very specific parameters of pharmacological activity?

In the Experimental Pharmacology and Pharmacokinetics/Metabolism Knowledge Areas of *Clarivate Analytics Integrity* 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. With help of *Integrity* you can easily create SAR tables based on a specific value range and export this table for further analysis outside of the system. **Example Scenario**: you are a researcher working with a structure and have found a new patent with compounds containing the same structure that are reported to act with high potency on the histamine H4 receptor. You want to find out if there are other known similar, high-potency molecules and to compare their structures.

Set up a search:





Select **Experimental Pharmacology** from 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 field) to open the structure drawing window within the *Integrity* Search From.

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, click on **open mol file**.

Tip:

- Find out more information about structure search in Guide to Structure Search Options.

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** drop-down 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**.

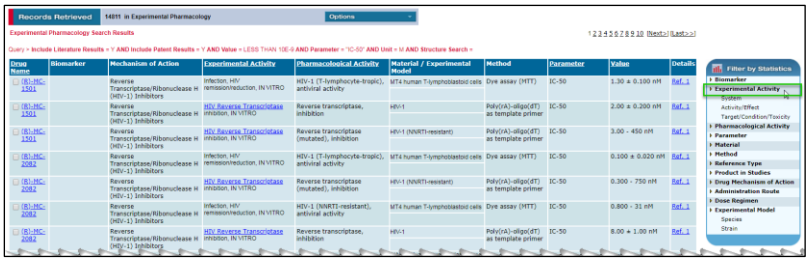
In the second box in this row select **M** from the drop-down list. In the third box select **Less than** from the drop-down list. Specify the range of interest in the fourth box. For this example, we will search for value less than 10nM. To do this type 10e-9.

Tip:

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

Clarivate Analytics

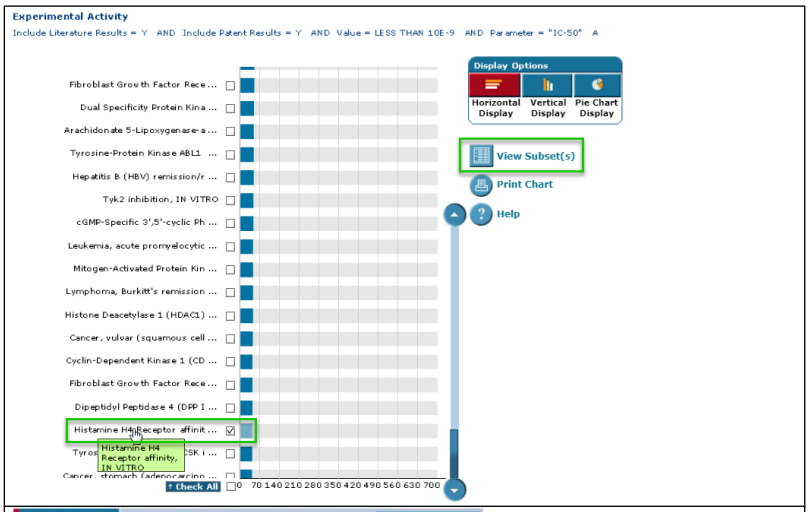
Working with your data:



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 the bar in the chat 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 42 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**.