

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:

The screenshot shows the 'Experimental Pharmacology' search interface. The top section is titled 'Advanced Search' and includes 'Session History', 'Clear Form', and 'Start' buttons. Below this, there are sections for 'Include Literature Results' and 'Include Patent Results', each with 'Select Value', 'Optional Value', and 'Index AND' options. A 'Product' section is also visible, with a 'Structure Search' button highlighted in green. The main search area is titled 'Structure Search Options' and includes 'Search Type' (Substructure, Exact Structure, Similarity), 'Structure Representation' (Normal, Standardized), and 'Search Options' (Match Stereochemistry). A chemical structure editor is shown with a pyridine ring and an amino group, and an 'open mol file' button is highlighted in green. The bottom section shows the 'Value' search criteria set to 'IC-50', 'M', 'Less than', and '10e-9'.

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.

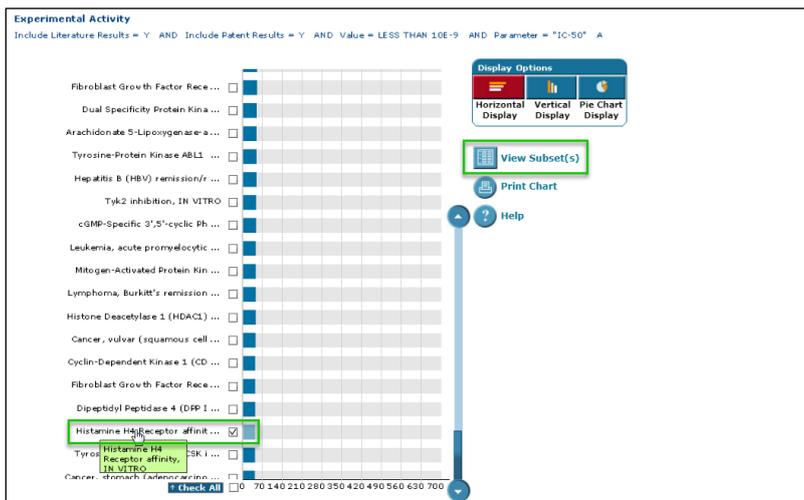
Working with your data:

Drug Name	Biomarker	Mechanism of Action	Experimental Activity	Pharmacological Activity	Material / Experimental Model	Method	Parameter	Value	Details
470609		Reverse Transcriptase/Ribonuclease H (RT/RNase H) Inhibitors	Infection, HIV recombination, IN VITRO	Reverse transcriptase (reversed), inhibition	HIV-1 (T-lymphocyte-98)PC, antihiviral activity	MT4 human T-lymphoblastoid cells	Dye assay (HTT)	IC-50	3.30 ± 0.100 nM Ref.1
664192		Reverse Transcriptase/Ribonuclease H (RT/RNase H) Inhibitors	Infection, HIV recombination, IN VITRO	Reverse transcriptase (reversed), inhibition	HIV-1 (T-lymphocyte-98)PC, antihiviral activity	MT4 human T-lymphoblastoid cells	Dye assay (HTT)	IC-50	2.00 ± 0.200 nM Ref.1
664192		Reverse Transcriptase/Ribonuclease H (RT/RNase H) Inhibitors	Infection, HIV recombination, IN VITRO	Reverse transcriptase (reversed), inhibition	HIV-1 (T-lymphocyte-98)PC, antihiviral activity	MT4 human T-lymphoblastoid cells	Dye assay (HTT)	IC-50	3.00 - 450 nM Ref.1
664192		Reverse Transcriptase/Ribonuclease H (RT/RNase H) Inhibitors	Infection, HIV recombination, IN VITRO	Reverse transcriptase (reversed), inhibition	HIV-1 (T-lymphocyte-98)PC, antihiviral activity	MT4 human T-lymphoblastoid cells	Dye assay (HTT)	IC-50	0.550 ± 0.020 nM Ref.1
664192		Reverse Transcriptase/Ribonuclease H (RT/RNase H) Inhibitors	Infection, HIV recombination, IN VITRO	Reverse transcriptase (reversed), inhibition	HIV-1 (T-lymphocyte-98)PC, antihiviral activity	MT4 human T-lymphoblastoid cells	Dye assay (HTT)	IC-50	0.300 - 750 nM Ref.1
664192		Reverse Transcriptase/Ribonuclease H (RT/RNase H) Inhibitors	Infection, HIV recombination, IN VITRO	Reverse transcriptase (reversed), inhibition	HIV-1 (T-lymphocyte-98)PC, antihiviral activity	MT4 human T-lymphoblastoid cells	Dye assay (HTT)	IC-50	0.800 - 31 nM Ref.1
664192		Reverse Transcriptase/Ribonuclease H (RT/RNase H) Inhibitors	Infection, HIV recombination, IN VITRO	Reverse transcriptase (reversed), inhibition	HIV-1 (T-lymphocyte-98)PC, antihiviral activity	MT4 human T-lymphoblastoid cells	Dye assay (HTT)	IC-50	8.00 ± 1.00 nM Ref.1

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.

Drug Name	Biomarker	Mechanism of Action	Experimental Activity	Pharmacological Activity	Material	Method	Parameter	Value	Details
470609		Histamine H4 Receptor Antagonists	Histamine H4 Receptor affinity, IN VITRO	Histamine H4 receptor affinity	an receptor	Displacement of [3H]-histamine	IC-50	1.00 nM	Ref.2
664192		Histamine H4 Receptor Antagonists	Histamine H4 Receptor affinity, IN VITRO	Histamine H4 receptor affinity	my cells transfected	Displacement of [3H]-histamine	IC-50	51.00 µM	Pat.2
664192		Histamine H4 Receptor Antagonists	Histamine H4 Receptor affinity, IN VITRO	Histamine H4 receptor affinity	my cells transfected	Displacement of [3H]-histamine	IC-50	51.00 µM	Pat.2
664192		Histamine H4 Receptor Antagonists	Histamine H4 Receptor affinity, IN VITRO	Histamine H4 receptor affinity	my cells transfected	Displacement of [3H]-histamine	IC-50	51.00 µM	Pat.2
664192		Histamine H4 Receptor Antagonists	Histamine H4 Receptor affinity, IN VITRO	Histamine H4 receptor affinity	my cells transfected	Displacement of [3H]-histamine	IC-50	51.00 µM	Pat.2
664192		Histamine H4 Receptor Antagonists	Histamine H4 Receptor affinity, IN VITRO	Histamine H4 receptor affinity	my cells transfected	Displacement of [3H]-histamine	IC-50	51.00 µM	Pat.2

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**.

Pharmacological Activity: Histamine H4 receptor affinity
Parameter: IC-50

Drug Name & Structure	Mechanism of Action	Material	Method	Value	Details
470609	Signal Transduction Modulators Histamine H4 Receptor Antagonists	Cells transfected with human receptor	Displacement of [3H]-histamine	1.00 nM	Ref.2
664192	Histamine H4 Receptor Antagonists	CHO Chinese hamster ovary cells transfected with human receptor	Displacement of [3H]-histamine	51.00 µM	Pat.2
664192	Histamine H4 Receptor Antagonists	CHO Chinese hamster ovary cells transfected with human receptor	Displacement of [3H]-histamine	51.00 µM	Pat.2