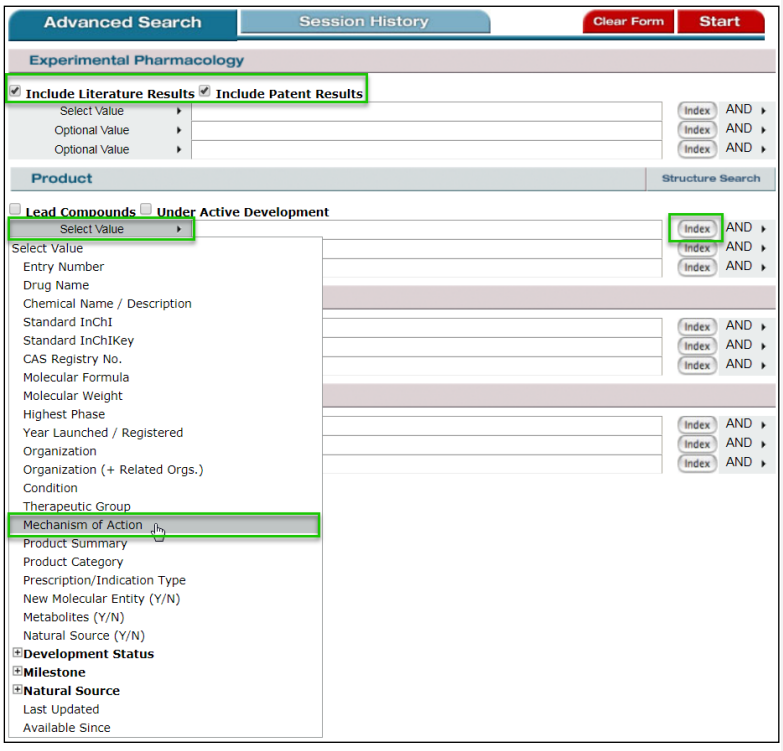
Generate a SAR table from the Experimental Pharmacology Knowledge Area

Do you need to predict or compare pharmacological activity of in-house compounds?

Clarivate Analytics Integrity enables you to compare the measured pharmacological activity values of a series of related compounds to identify those with the greatest activity and to predict biological activity of in-house compounds. With help of *Integrity* you can quickly create a Structure Activity Relationship (SAR) table for compounds based on the mechanism of action and easily work with the data and draw insight from your findings by using data management options in the Experimental Pharmacology knowledge area. **Example Scenario**: you are developing an inhibitor of type 4 phosphodiesterase B (PDE4B) and are searching for compounds that exhibit the same mechanism of action.

Retrieve data:

Run your search



Within Integrity go to the **Experimental Pharmacology** knowledge area.

Note that **Include Literature Results** and **Include Patent Results** are checked by default.

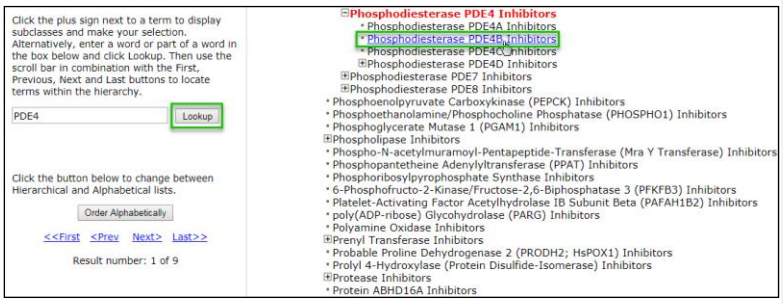
Under the **Product** section select **Mechanism of Action** as the search field.

Click the **Index** button on the right to open the **Browse Index** box for this field.

Type “Phosphodiesterase” or “PDE4” in the Lookup box and click **Lookup**.

Tip:

- Click **Order Alphabetically** to obtain a short list of all the search terms that contain your lookup term and make your selection from here.



Select the mechanism of action of your interest (Phosphodiesterase PDE4B Inhibitors in this example).

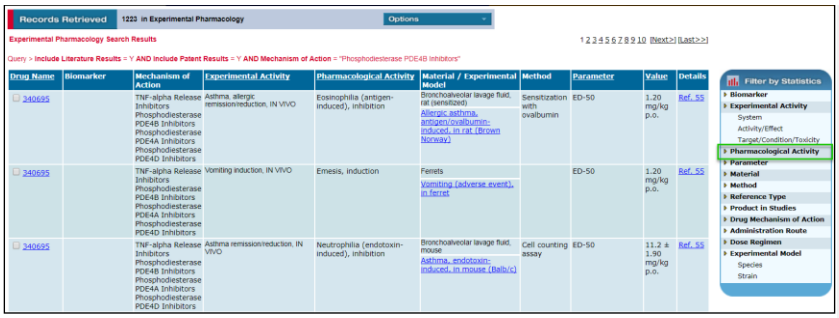
Click **Start** to run your search.

Results appear in the table format.

Clarivate Analytics

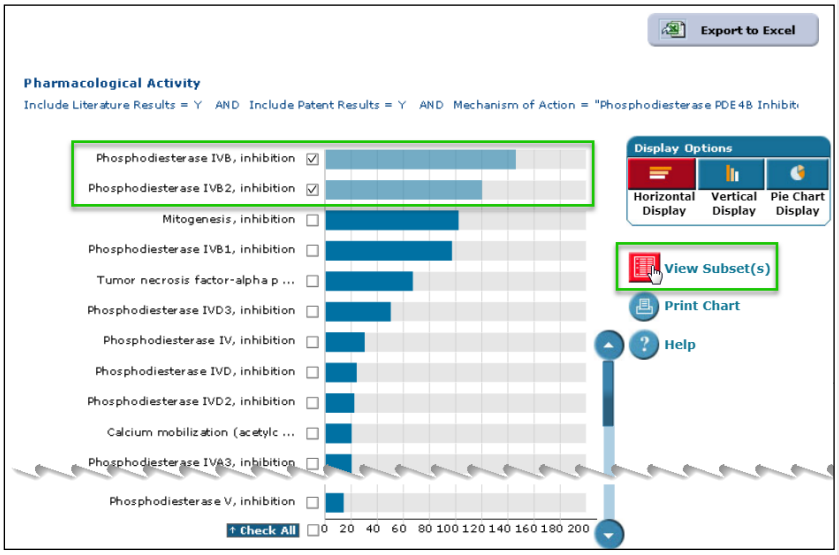
Working with your data:

Refine by pharmacological activity



You can view the data retrieved by categories and refine them using the **Filter by Statistics** tool (at the right of the table results).

Click **Pharmacological Activity** to open this chart, review the data categories and select subsets of data.



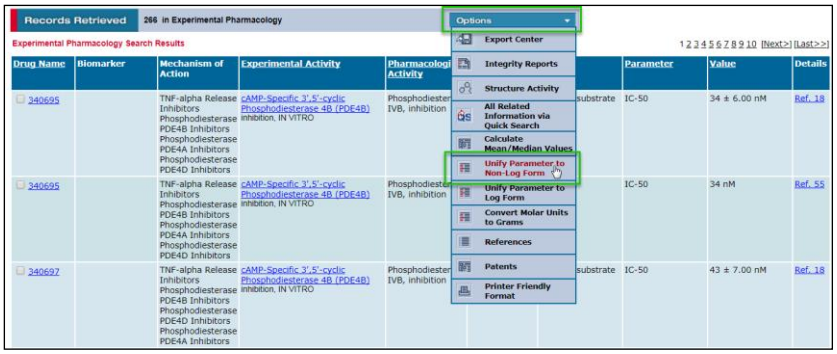
Tip:

- Use the chart scroll bar to view and select categories below the scroll line in the chart. Click the **Export to Excel** button at the top to export all categories and their corresponding numeric values to spreadsheet format for easy visualization and sorting.

Click the checkboxes to select the top two pharmacological activity categories – Phosphodiesterase IVB, inhibition and Phosphodiesterase IVB2, inhibition.

To return results for these two categories only click **View Subset(s).**

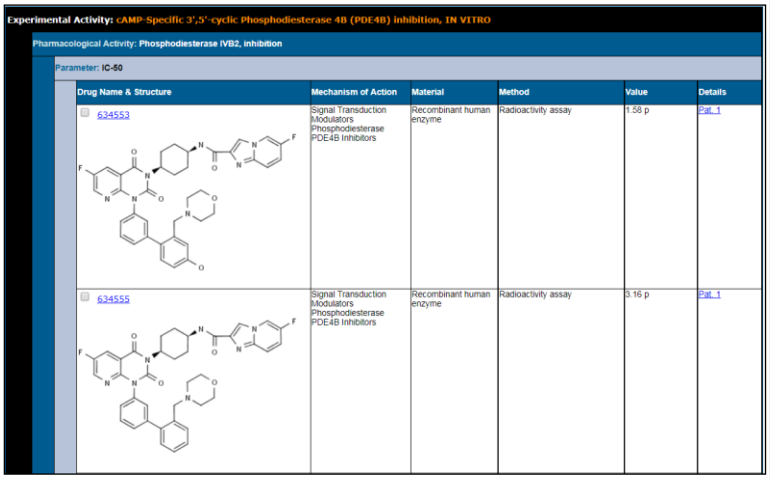
Unify parameters so values are directly comparable



To facilitate comparison of data represented by different parameters – in this case, IC50 and pIC50, open the **Options** pull-down menu. Select **Unify Parameters to Non-Log Form**. Results are displayed as IC50 values.

__Tip:__ You can click the underlined column header __Value__ to display data in ascending numeric order.

Display SAR table



Open the **Options** pull-down menu and select **Structure-Activity** to generate the SAR table as shown.

Tip:

- You can return to the Experimental Pharmacology data display format (via the **Options** menu or by using the **Back** button of your browser) and further refine data using **Filter by Statistics** feature should you wish to compare data for a specific material or method.