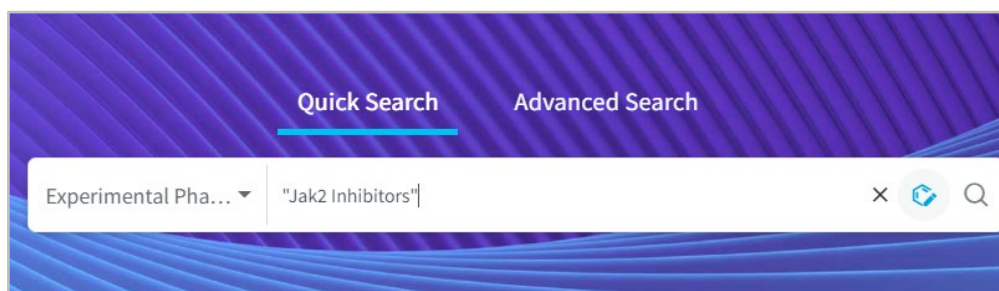


Cortellis Drug Discovery Intelligence

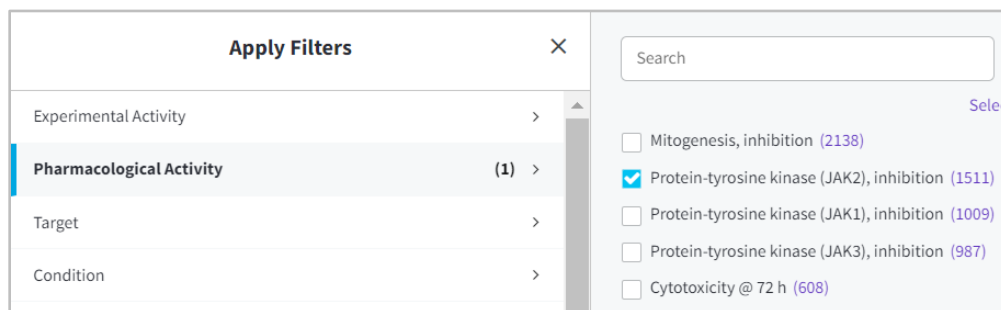
Experimental pharmacology analytics

Easily benchmark your drugs of interest using the analytical tools in the **Experimental Pharmacology Knowledge Area**.

1. Run a quick search in **Experimental Pharmacology**, for example to find experimental data on Jak2 inhibitors.



2. In the results page, use **Apply Filters** to select the **Pharmacological Activity** you'd like to benchmark, for instance Jak2 inhibition.



- Parameters and Values in the results page may appear in different form (**Log/Non-log**) and units (**Grams/Molar**) depending on the source of the data. Use the **Unify - Convert** functionality to solve that.

The screenshot shows the 'Unify - Convert' dialog box with options to toggle between Log and Non-log, and Molar and Grams. In the background, a table of experimental pharmacology records is visible, with a purple box highlighting the 'Parameter' and 'Value' columns.

Material/Experimental Model	Method	Parameter	Value	Source
	ATP assay	IC-50	39 ± 13 nM	Literature
recombinant human enzyme	Fluorescence resonance energy transfer (FRET) assay	IC-50	824 nM	Patent
F1 human erythro leukemia cells	Chemiluminescent assay	IC-50	2.3 µM	Literature
Human enzyme	ATP assay	IC-50	7.2 nM	Literature

- To see all results normalized into the same unit, click on **Show normalized units**. This will add an extra column to the results page where you can select your preferred normalized unit (**µmol** or **µg**).

The screenshot shows the 'Show normalized units' dialog box. In the background, a table of experimental pharmacology records is visible, with a purple box highlighting the 'Value (µg)' column.

Drug Name	System	Experimental Activity	Pharmacological Activity	Material/Experimental Model	Method	Parameter	Value	Value (µg)	Source
814804		Tyrosine-Protein Kinase JAK2 (JAK-2) inhibition, IN VITRO	Protein-tyrosine kinase (JAK2), inhibition			Ki	1000 mM	320.37x10 ⁶ µg/l	Literature
814802		Tyrosine-Protein Kinase JAK2 (JAK-2) inhibition, IN VITRO	Protein-tyrosine kinase (JAK2), inhibition			Ki	1000 mM	295.34x10 ⁶ µg/l	Literature
814801		Tyrosine-Protein Kinase JAK2 (JAK-2) inhibition, IN VITRO	Protein-tyrosine kinase (JAK2), inhibition			Ki	1000 mM	309.33x10 ⁶ µg/l	Literature
814805		Tyrosine-Protein Kinase JAK2 (JAK-2) inhibition, IN VITRO	Protein-tyrosine kinase (JAK2), inhibition			Ki	1000 mM	309.37x10 ⁶ µg/l	Literature

Tip: Sort your experiments by **Value** to get the most active drugs on the top of your list.

- Once your results are unified and converted, you may see many experiments measuring the same drug for the same activity with the same parameter. Use the **Mean / Median** tab on the top of the page to calculate the mean and median values for those similar experiments.

Mean / Median

* Select at least one of the sources of records you would like included.

Literature Patents

Would you want to consider only the same Material in the calculation?
 Yes No

Would you want to consider only the same Method in the calculation?
 Yes No

* Select at least one parameter:

Select all / Clear all

IC-50 (M) IC-90 (M) Kd (M)
 Ki (M)

Reset Calculate

Specify what terms to consider for your calculation under the Mean/Median tab. Then hit **Calculate**.

- You can now easily benchmark drugs with the most interesting pharmacological values in the Mean/Median results page.

Experimental Pharmacology **Mean / Median**

Showing 1-20 of 640 Mean/Median calculations

Drug Name	Pharmacological Activity	Parameter	Mean	Median
1009088	Protein-tyrosine kinase (JAK2), inhibition	IC-50	6.2 nM [6.2 - 6.2] (n=3)	6.2 nM [6.2 - 6.2] (n=3)
1009089	Protein-tyrosine kinase (JAK2), inhibition	IC-50	1 pM [1 - 1] (n=3)	1 pM [1 - 1] (n=3)
1009090	Protein-tyrosine kinase (JAK2), inhibition	IC-50	2.1 nM [2.1 - 2.1] (n=3)	2.1 nM [2.1 - 2.1] (n=3)
1009091	Protein-tyrosine kinase (JAK2), inhibition	IC-50	1.4 nM [1.4 - 1.4] (n=3)	1.4 nM [1.4 - 1.4] (n=3)
1009092	Protein-tyrosine kinase (JAK2), inhibition	IC-50	5.53 nM [5.4 - 5.6] (n=3)	5.6 nM [5.4 - 5.6] (n=3)

(n=x) reflects the number of data points used to calculate the mean/median

For more information contact Customer Service at [LS Product Support](#)