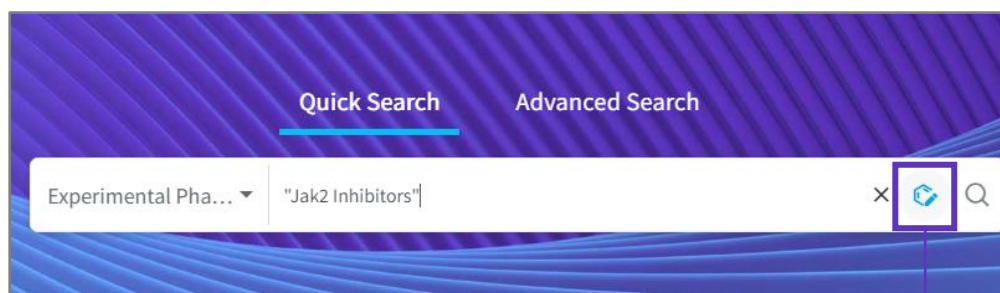


# Benchmarking the performance of your drug

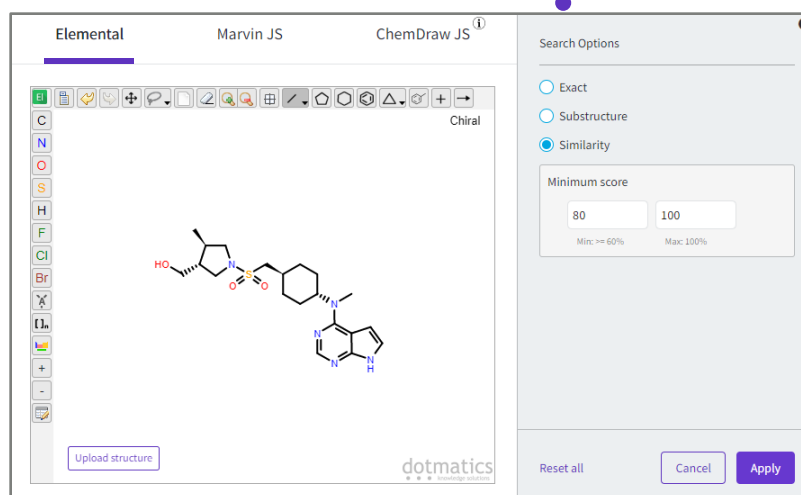
## Cortellis Drug Discovery Intelligence

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

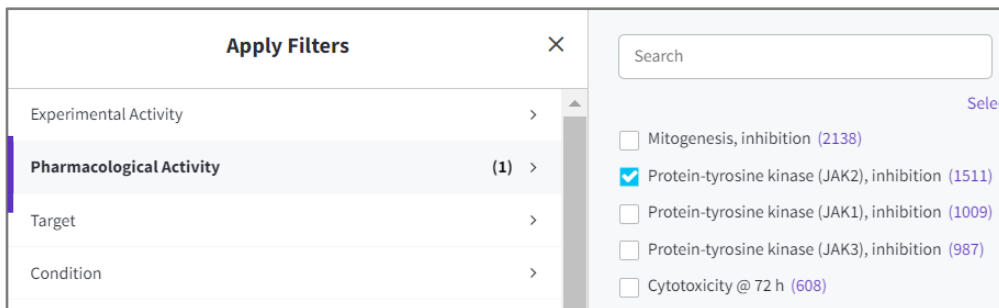
1. Run a quick search in **Experimental Pharmacology**, for example to find experimental data on Jak2 inhibitors.



**Tip** To benchmark the performance of a specific structure, start with a structure similarity search. This will retrieve experimental data for structures similar to yours so that you can then compare performances.



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



**Apply Filters** X

Search

Experimental Activity >

**Pharmacological Activity (1) >**

Target >

Condition >

☐ Mitogenesis, inhibition (2138)

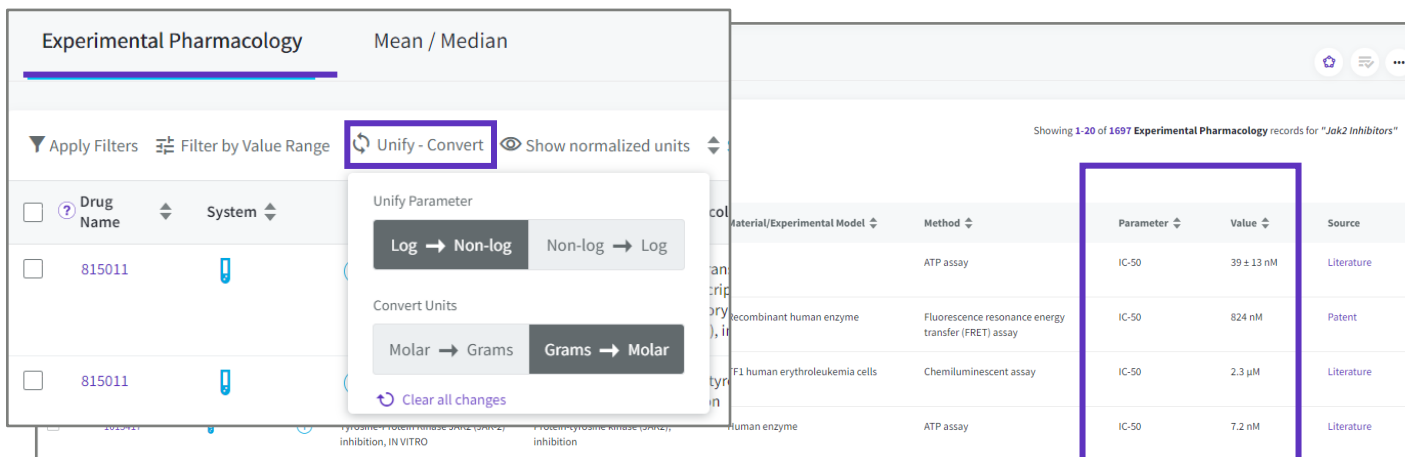
☒ Protein-tyrosine kinase (JAK2), inhibition (1511)

☐ Protein-tyrosine kinase (JAK1), inhibition (1009)

☐ Protein-tyrosine kinase (JAK3), inhibition (987)

☐ Cytotoxicity @ 72 h (608)

- 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.



**Experimental Pharmacology** Mean / Median

Apply Filters Filter by Value Range **Unify - Convert** Show normalized units

Drug Name System

815011

815011

Unify Parameter

Log → Non-log Non-log → Log

Convert Units

Molar → Grams Grams → Molar

Clear all changes

Showing 1-20 of 1697 Experimental Pharmacology records for "Jak2 Inhibitors"

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 erythroleukemia 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 ( $\mu\text{mol}$  or  $\mu\text{g}$ ).

Experimental Pharmacology

Mean / Median

Apply Filters

Filter by Value Range

Unify - Convert

Show normalized units

Sorted by relevance

Showing 1-20 of 1697 Experimental Pharmacology records for "Jak2 Inhibitors"

Drug Name	System	Experimental Activity	Pharmacological Activity	Material/Experimental Model	Method	Parameter	Value	Value ( $\mu\text{g}$ )	Source
814804		Tyrosine-Protein Kinase JAK2 (JAK-2) inhibition, IN VITRO	Protein-tyrosine kinase (JAK2), inhibition			Ki	1000 nM	320.37x10 <sup>6</sup> $\mu\text{g}/\text{l}$	Literature
814802		Tyrosine-Protein Kinase JAK2 (JAK-2) inhibition, IN VITRO	Protein-tyrosine kinase (JAK2), inhibition			Ki	1000 nM	295.34x10 <sup>6</sup> $\mu\text{g}/\text{l}$	Literature
814801		Tyrosine-Protein Kinase JAK2 (JAK-2) inhibition, IN VITRO	Protein-tyrosine kinase (JAK2), inhibition			Ki	1000 nM	309.33x10 <sup>6</sup> $\mu\text{g}/\text{l}$	Literature
814805		Tyrosine-Protein Kinase JAK2 (JAK-2) inhibition, IN VITRO	Protein-tyrosine kinase (JAK2), inhibition			Ki	1000 nM	309.37x10 <sup>6</sup> $\mu\text{g}/\text{l}$	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)
 ☐ Ki (M)

Reset

Calculate

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

6. 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](#).