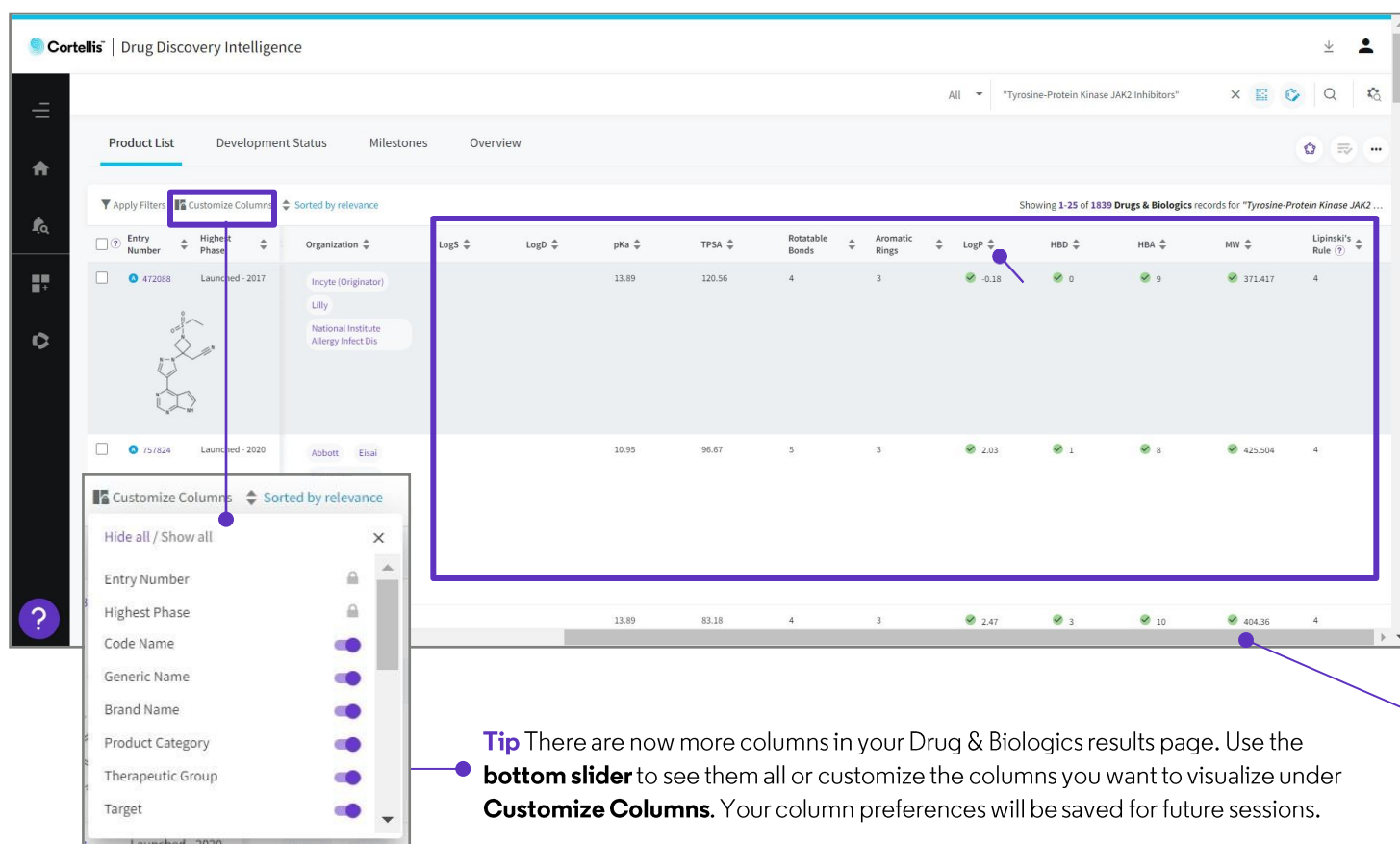


Find the physicochemical properties of your compound

Cortellis Drug Discovery Intelligence

You may need to identify structures with good solubility or that comply with Lipinski's rule of five. With Cortellis Drug Discovery Intelligence you can sort through physicochemical structure properties calculated by ChemAxon technology.

1. Run a compound/structure search in **Drugs & Biologics**.
2. In the results page, find up to 10 physiochemical properties of the compounds on the right of the table. Use the sorting options at the top of each column to arrange your results as needed.



The screenshot shows the Cortellis Drug Discovery Intelligence interface. The main table displays search results for "Tyrosine-Protein Kinase JAK2 Inhibitors". The table has columns for various physicochemical properties: LogS, LogD, pKa, TPSA, Rotatable Bonds, Aromatic Rings, LogP, HBD, HBA, MW, and Lipinski's Rule. A "Customize Columns" dialog is open, showing a list of columns that can be hidden or shown. A tip box points to the bottom slider of the table, indicating that it can be used to see all columns or customize the columns to visualize.











Tip There are now more columns in your Drug & Biologics results page. Use the **bottom slider** to see them all or customize the columns you want to visualize under **Customize Columns**. Your column preferences will be saved for future sessions.

3. Lipinski's rule of five

The **Lipinski's rule** states that the absorption or permeation of a molecule is more likely when the below 4 properties have the following value ranges:

$$\text{LogP} \leq 5 + \text{HBD} \leq 5 + \text{HBA} \leq 10 + \text{MW} \leq 500 \text{ g/mol}$$

Easily identify those structures which pass the Lipinski's rule indicated by **4 green check marks**.

LogP 	HBD 	HBA 	MW 	Lipinski's Rule  
 -0.18	 0	 9	 371.417	4

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