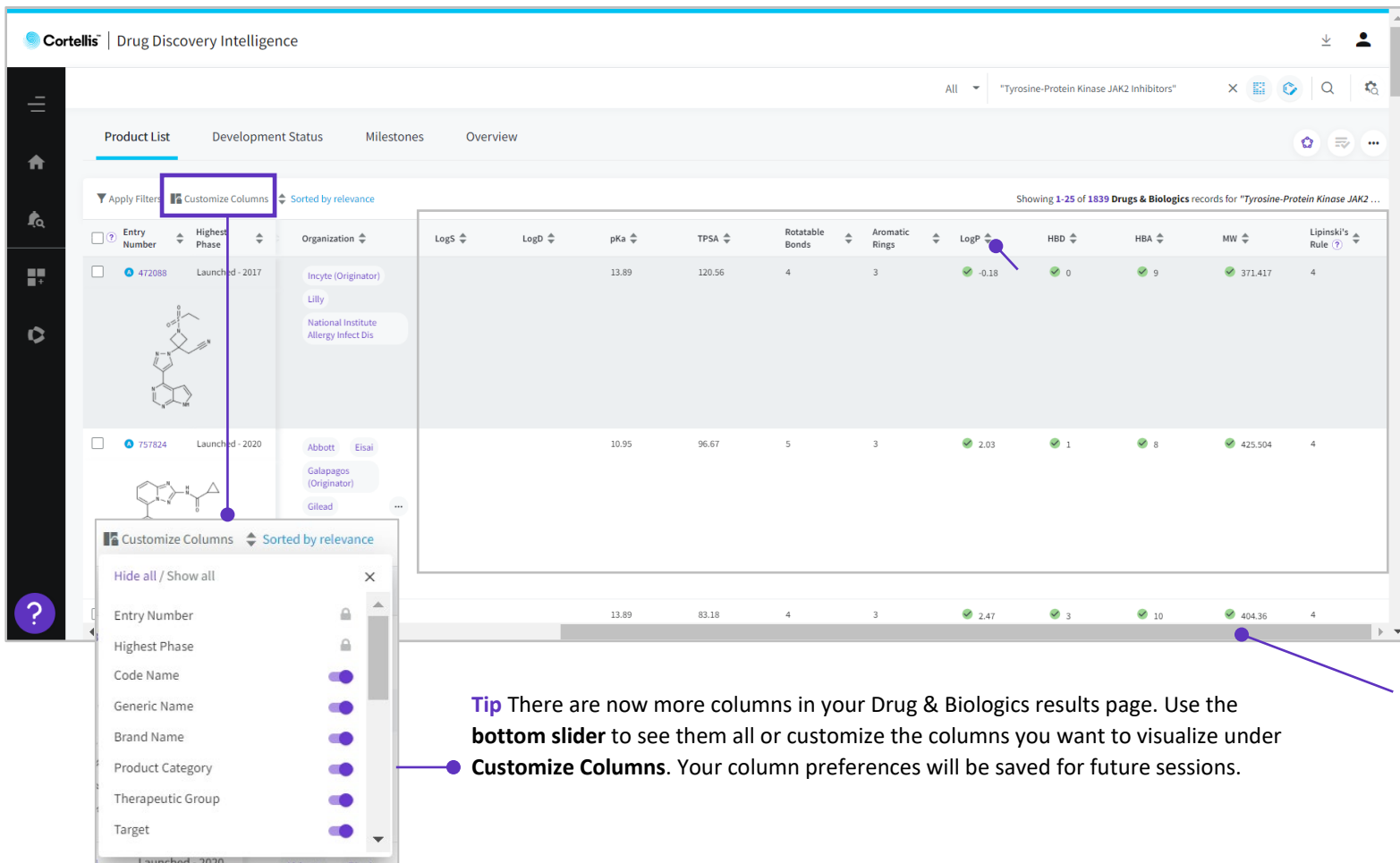


# Find the physicochemical properties of your compound

## 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 physicochemical 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 displays the Cortellis Drug Discovery Intelligence interface. The main table shows results for "Tyrosine-Protein Kinase JAK2 Inhibitors". The table columns include Entry Number, Highest Phase, Organization, LogS, LogD, pKa, TPSA, Rotatable Bonds, Aromatic Rings, LogP, HBD, HBA, MW, and Lipinski's Rule. A "Customize Columns" dialog box is open, showing a list of columns with toggle switches to enable or disable them. A blue arrow points to the "LogP" column in the table, and another blue arrow points to the "Customize Columns" dialog box. A tip box is also present, explaining the "Customize Columns" feature.

**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.

Entry Number	Highest Phase	Organization	LogS	LogD	pKa	TPSA	Rotatable Bonds	Aromatic Rings	LogP	HBD	HBA	MW	Lipinski's Rule
472088	Launched - 2017	Incyte (Originator) Lilly National Institute Allergy Infect Dis			13.89	120.56	4	3	-0.18	0	9	371.417	4
757824	Launched - 2020	Abbott Eisai Galapagos (Originator) Gilead			10.95	96.67	5	3	2.03	1	8	425.504	4
			13.89	83.18			4	3	2.47	3	10	404.36	4

### 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](#)