

## Heatmap

The Heatmap view, which is available with a Reaxys Medicinal Chemistry (RMC) license, is available for all queries in substance, target and document result pages. It initially provides an overview on structure activity relationship by displaying by default chemical substances (Y-axis) vs. biological targets (X-axis) and activity potency as pX (Cells). These settings can be changed by accessing the heatmap settings button in the menu bar. A Navigator view (Navigator button) provides an overview and a quick navigation method in the heatmap.

The colors in the heatmap (Legend Button) and in the navigator panel refer to the potency of a substance with blue showing low potency and red showing high potency based on pX values. A gray color refers to a qualitative results or parameters and values for which the pX calculation is not designed for (AUC, Vd, Clearance, etc.). See below for more details.

The screenshot displays the Reaxys Heatmap interface with the following elements and callouts:

- 1**: Limit To button
- 2**: Exclude button
- 3**: Export button
- 4**: Settings button
- 5**: Navigator button
- 6**: Legend button
- 7**: Substances button
- 8**: Exit fullscreen button
- 9**: Ellipsis menu button in the heatmap grid
- 10**: A cell in the heatmap grid (Substance: EP128265, Target: Tubulin, pX: 6.4)
- 11**: Substances list on the left sidebar
- 12**: Heatmap settings dialog box
- 13**: Value of X-axis dropdown in the settings dialog
- 14**: Show substances radio buttons (Names selected, Structure drawing unselected)
- 15**: Display mode radio buttons (Normal unselected, Full Screen selected)
- 16**: Always show settings checkbox in the settings dialog
- 17**: Targets panel on the right sidebar

Substances	Caspase	Caspase [human]	Caspase-3	Tubulin
EP128265	8.7	8.7	8.7	6.4
(2-chloro-6...yl-amine		8.3	8.3	
(2-chloro-7...yl-amine		8.2		
2-chloro-... -4-amine		8.3		
2-chloro-... -4-amine		8.2		
(2-chloro-5...yl-amine		9		
2,7-dichlor...-4-amine		7.9		

## Legend:

1. **Limit to** – Click column or row headers to select columns or rows. Then click *Limit to*.
2. **Exclude** – Click column or row headers to select columns or rows. Then click *Exclude*.
3. **Export** – Yes, you can export the raw data like substances (Names, Smiles etc...), targets (Names, Species, mutations etc...), cell lines, Bioassays and bioactivities (pX, IC50, Ki etc.) that are used to construct and display the heatmap to excel, SD file or XML but not the heatmap itself as a picture or in excel.
4. **Settings** – Click on settings to define Heatmap settings and click *Apply*.
5. **Navigator** – Click to display a Navigator. Click within the map to jump to different data within the hit set.
6. **Legend** – View color coding legend.
7. **List view** – Click on *Substances*, *Targets* or *Documents* to switch to list view instead of the Heatmap view.
8. **Fullscreen display** – Click on *Exit fullscreen* to move to the normal display of the heatmap (filters and menu bar will be visible).
9. **3 dots** – Click on the *3 dots* button to display columns or rows actions.
10. **Data Density** – The circle size is related to the amount of cells filled in the row or the column.
11. **Filters** – Click to display filters.
12. **Cell** – Click to display Bioactivity details. Displayed numbers are pX, a value calculated from experimental data points. This allows you to compare data from different sources, different assays, or with different parameters. The pX value is hyperlinked to the real data. If multiple data points are available for an assay/target, select Max, Min, Median, or Average. Use the filters to limit results to a particular pX range.
13. **X and Y Axis Display** – Substances are displayed on the **Y** axis and Targets are displayed on the **X** axis by default. You can change this by selecting different options in the dropdown menu.
14. **Show Substances** – Select options to display *Names* or *Structure drawing*.
15. **Display Mode** – Select the default display mode *Normal* or *Full screen*.
16. **Always show settings** – Select this option if you want to see settings each time that heatmap is used otherwise unselect it.

## Heatmap Columns and Rows Management

Click the 3 dots to display options (columns or rows)

Drag to increase header size (columns or rows)

Displays Legend.

Hover over the column or row header to display more details such as chemical structure, target full name and synonyms.

Click header to select the column or row.

Drag and drop the rectangle to display other areas of the heatmap.

The interface displays a heatmap with a list of substances on the left and a list of targets on the top. A legend indicates that color represents bioactivity potency based on pX values, ranging from High (red) to Low (blue). A detailed view for the substance 'imatinib' is shown, including its chemical structure and associated identifiers: Reaxys ID: 7671333, CAS Registry Number: 152459-95-5, Molecular Formula: C<sub>29</sub>H<sub>31</sub>N<sub>7</sub>O, and Molecular Weight: 493.611.

## Heatmap Cell Click

Click cell to display Bioactivity details.

Click header to select the column or row.

The screenshot displays the Reaxys Medicinal Chemistry interface. On the left, a heatmap shows bioactivities for various substances across multiple targets. The 'imatinib' row is highlighted. A callout box titled 'Bioactivity detail' is open, showing the chemical structure and properties of imatinib. Below it, another callout box titled 'imatinib' shows a table of quantitative results.

**Bioactivity detail**

Targets: 1-phosphatidylinositol-3-phosphate 5-kinase >

Substances: imatinib >

Active substances

imatinib 5.3

C29H31N7O 493.611 7671333 152459-95-5 Maximum pX Value

Identification

Druglikeness

In vitro: Efficacy - 1

**imatinib**

Identification

Druglikeness

In vitro: Efficacy - 1

Quantitative Results Show/Hide columns

pX	Parameter	Value (qual)	Value (quant)	Unit	2..	Reference
5.38	IC50	=	4.2	µM		Patricelli, Matthew P.; Nomanbhoy, Tyzoon K.; Wu, Jiangyue; Brown, Heidi; Zhou, David; Zhang, Jianming; Jagannathan, Subadhra; (...) Gray, Nathanael S.; Kozarich, John W. - Chemistry and Biology, 2011, vol. 18, # 6, p. 699 - 710 Full Text <a href="#">↗</a> Cited 124 times <a href="#">↗</a> Show details <a href="#">&gt;</a>

- Targets and Substances.
- Name, Identification and Druglikeness.
- Bioactivities of the substance on the target. By default the cell displays the maximum of the pX so clicking on the cell will display all the bioactivities.