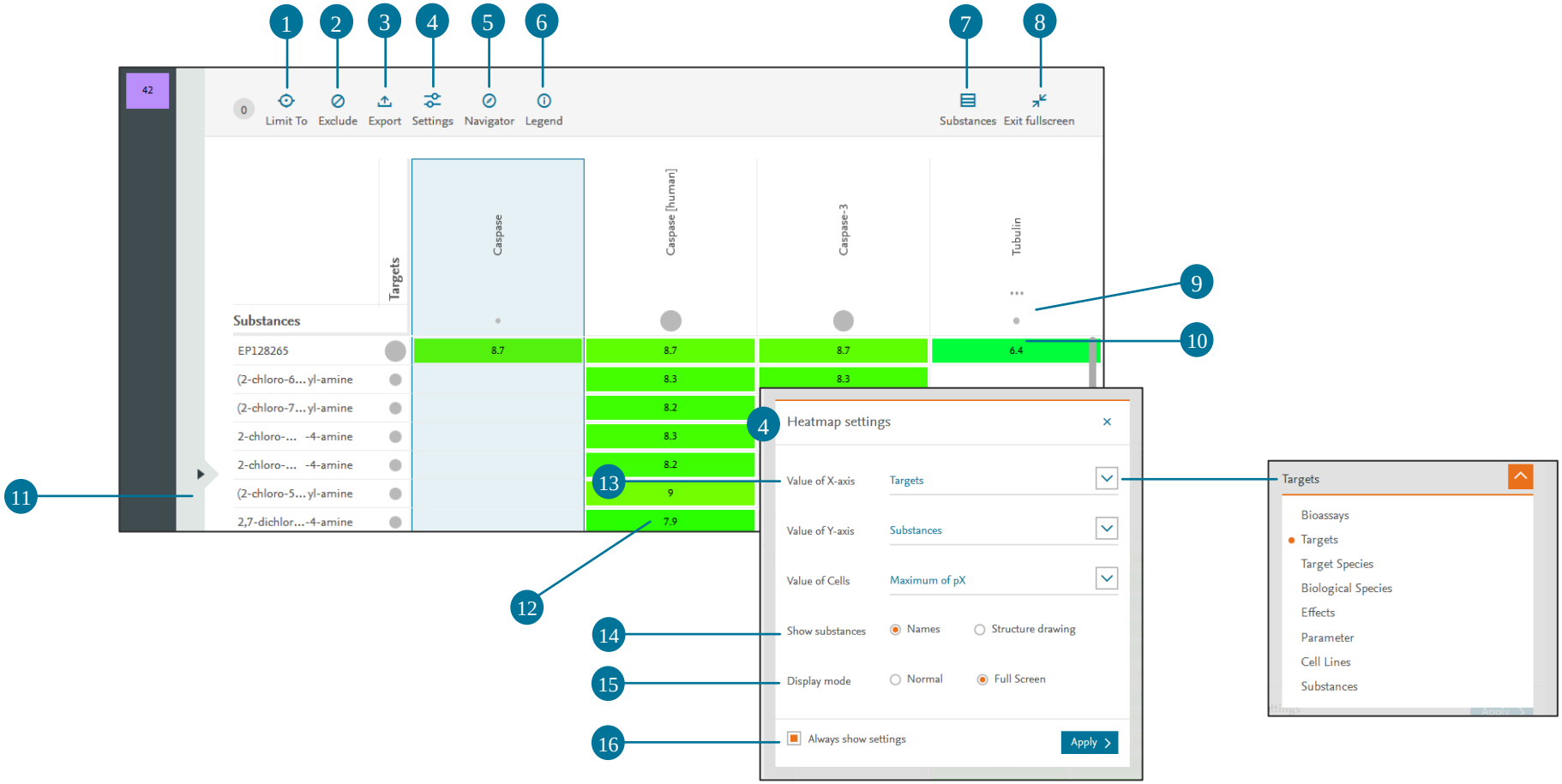
Heatmap

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.



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.

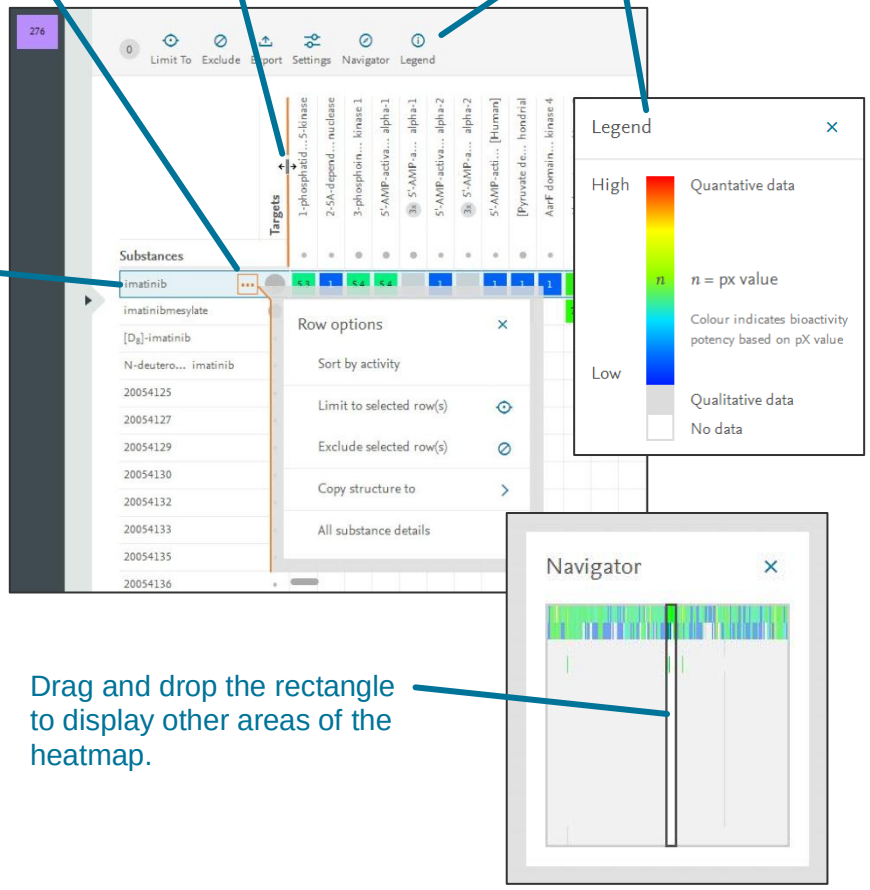
Heatmap Columns and Rows Management

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

Drag to increase header size (columns or rows).

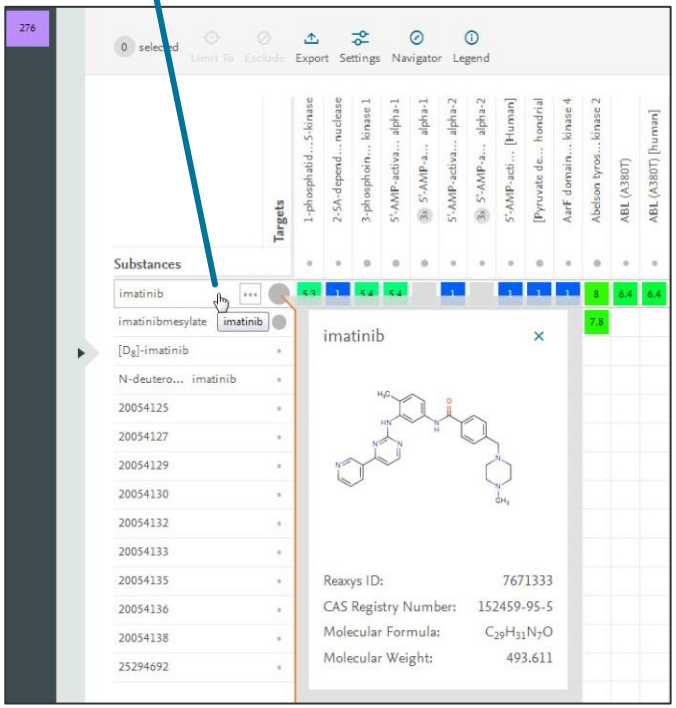
Displays Legend.

Click header to select the column or row.



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

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



Heatmap Cell Click