Charts view

Data displayed in both Connect grid and form view can be visualized using an integrated component called Charts view. For instance, displaying molecular weight distribution within a data set as a histogram.

The Charts view component was implemented in v18.17 of Plexus Connect. In v19.7 (LTS Deuterium) its new version has been integrated. This version brings a lot of significant improvements in data discovery workflow and offers a better usability than the previous version. As a result of design upgrades, the overall look of the component has been modernized. The new toolbars with added options make creating a chart more intuitive. Thanks to bright colors, the charts are easier to read and provide better user experience for scientific data visualization.

Adding a Charts view

Data can be visualized from any given result set (e.g. open a view or load a list). Click on the Charts icon within the blue control panel on the left and choose one of the available chart types:

- Histogram - displays frequency distributions
- Scatter plot - displays correlation between two data sets

After chart-type selection, choose fields you want to visualize on the x and y axes. Please note that only the parent table fields can be selected.

The Charts view component enables the user to display chemical structures on the axes in the chart. Displaying R-groups is also possible. This functionality offers enhanced support of research workflows and improved examination of relationships between your molecules.

How to create a histogram?

Please note that only the dependent variable along the horizontal axis can be chosen. The vertical axis contains the independent variable and its scaling can be changed from arithmetic to logarithmic by clicking on the axis title.

How to create a scatter plot?

Beyond to the field selection for horizontal and vertical axes, coloring of data points is also customizable by a selected field. Below the dropdown menus for field selection, the properties displayed in the Card can be selected by clicking on the corresponding fields.

There are two options available in the dropdown menus of axis titles. The first one is for changing of Dimension Mapping. By clicking on this option, a scrollable menu opens. It contains a list of all fields available for selection and enables the user to restore the chart with the newly selected field. The second option is Change Scaling. By clicking this option the axis scale switches from linear to logarithmic and back.

The legend panel of the data point coloring is also scrollable and contains a list of all available fields. Switching to a new field changes the color scheme accordingly. Below the legend panel, the colors of the current color scheme and the values they represent are listed. When the user hovers over a discrete value, an eye icon appears on the right. By clicking the eye icon, all data points corresponding to the selected value can be hidden/restored in the chart.
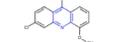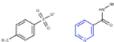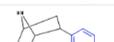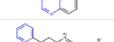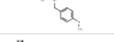
Data selection

Data displayed in a chart are automatically synchronized with a corresponding view. This means that only data selected in the chart are displayed in the view and vice versa. Selection can be done either within the view by filtering your result set (by a query), or within the chart by one of the available selection tools:

- Rectangular selection
- Rectangular deselection
- Freehand selection
- Freehand deselection
- Cherry picking (selection of individual data points)

The selection tools for rectangular selection and deselection, freehand selection and deselection are available in the dropdown menu on the legend panel.

The cherry picking selection option is available by simply clicking on individual data points in the chart.

By clicking on the Deselect All icon on the legend panel, the whole result set reappears both in the view and in the chart.

Curve fitting

Several curve fitting options can be used to highlight trends in your data set. Click on the Add Regression icon on the legend panel to open an option menu and choose one of the following regression options:

- Linear regression
- 4PL regression
- Exponential regression
- Power regression
- Logarithmic regression

The corresponding regression parameters can be found under the legend panel. You can exclude any point from the curve fitting by rectangular or freehand selection or by selection of individual data points. On that occasion the regression curve will be recalculated and the regression parameters will be adjusted and displayed.
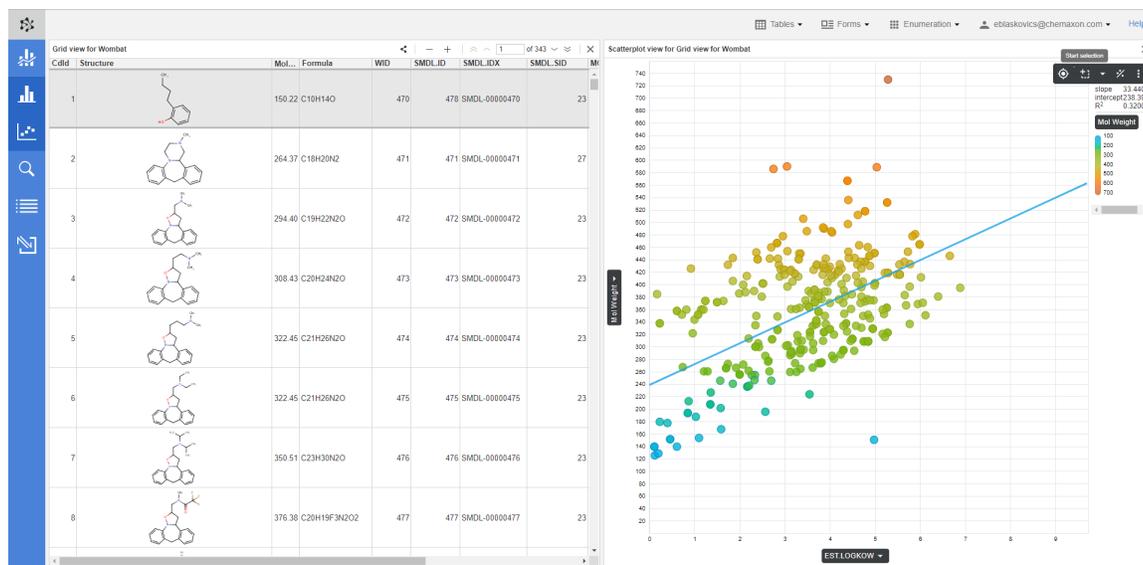
Saving a chart

The chart can be saved as PNG or SVG file. This functionality is available by clicking the menu option on the legend panel.
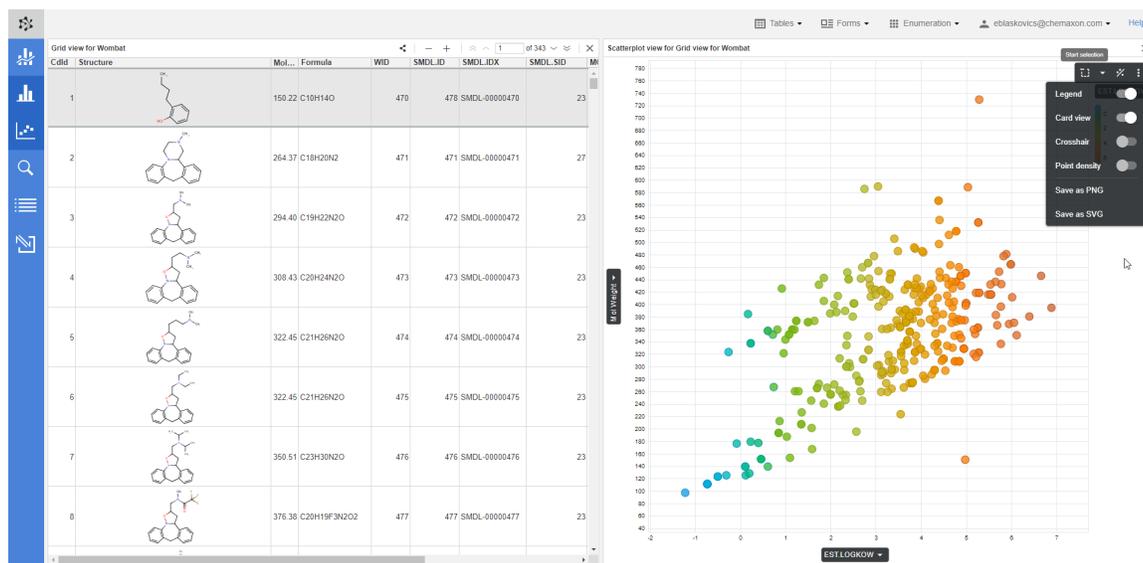
Scatter plot specific options

Hexbin view

To enhance usability and performance, large data sets are initially displayed as hexbins which represent clusters of data points. The lightness of the hexbins corresponds to point density - the lighter the hexbin, the fewer data points it represents. After zooming in (thus decreasing the number of displayed data points) the hexbin view switches to a view which displays separate data points.

The default hexbin view can be switched off in the menu on the legend panel so even big data sets can be displayed as individual data points. Please note that the big data sets displayed as data points lack some functionalities compared to the hexbin view. The panning, zooming and screen reader functionalities are disabled.
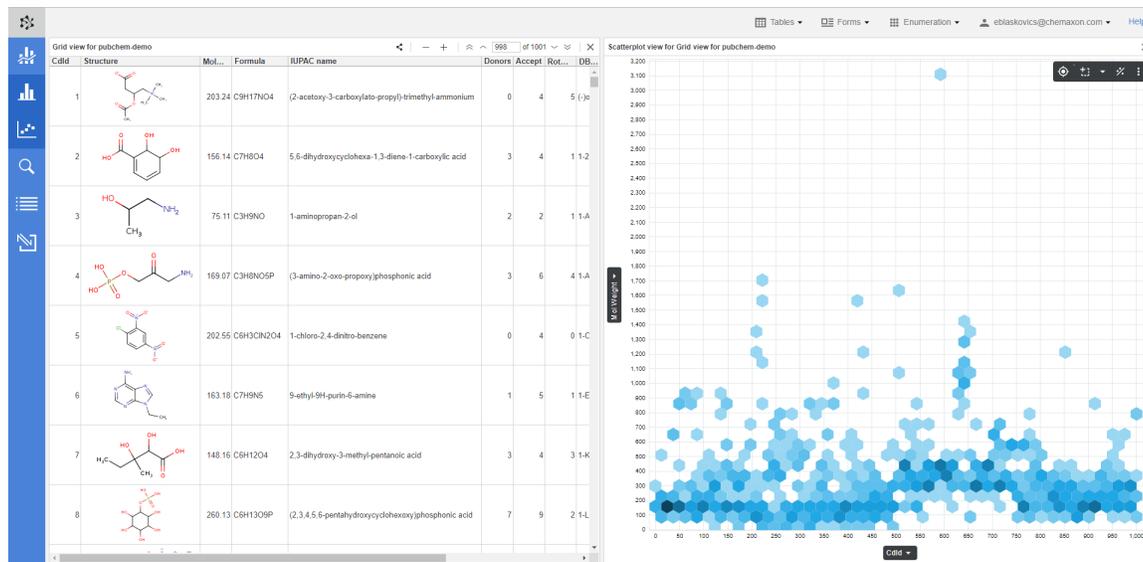
Screen Reader (Crosshair)

The Screen Reader (Crosshair) makes the position of a data point better readable. When the user hovers on a data point, the Screen Reader (Crosshair) displays the corresponding coordinate values on x and y axes. This functionality can be turned on and off in the menu on the legend panel.

Cards

This option offers an advanced way to visualize properties of a molecule in the chart. By hovering on a data point, properties of the related molecule appear on the Card. By default, these properties include the values displayed on the chart (x axis dimension and value, y axis dimension and value, dimension and value of the field selected for datapoint coloring). Additional fields can be selected in the first step of chart creation. Below the dropdown menus for x and y axes field selection, the properties displayed in the card can be selected by clicking on the corresponding fields. Worth noting, the molecule structure can be also displayed this way on the Card. Displaying of a structure and relevant properties on the Card can be helpful to discover your molecules and their characteristics in the context of other molecules visualized in the same chart.
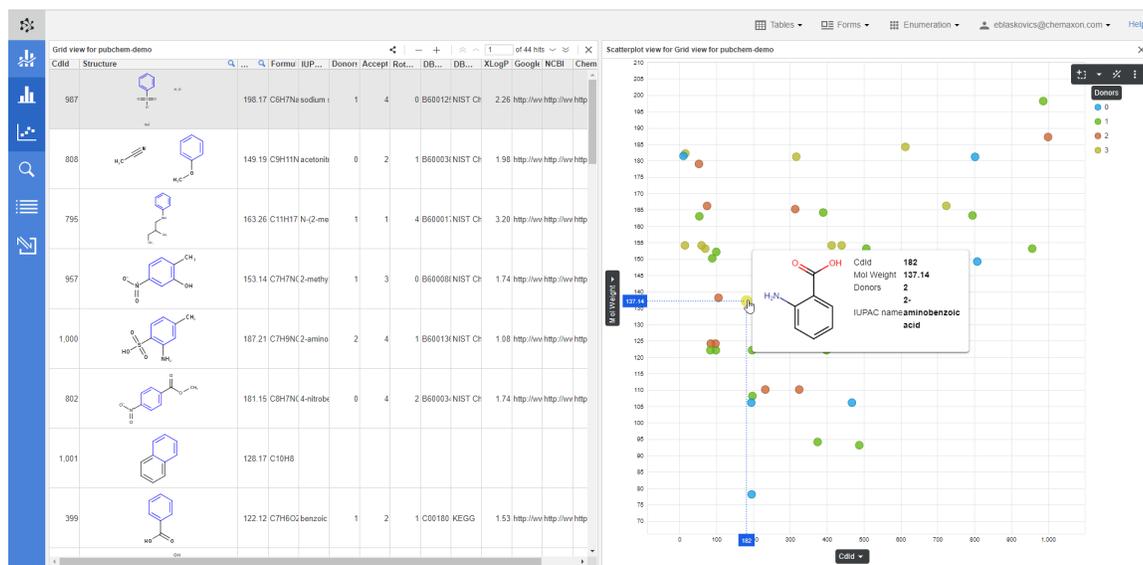
Histogram specific options

Cumulative curve

A cumulative curve of the percent distribution of the data points can be displayed by clicking the corresponding option in the menu on the legend panel. A separate vertical axis showing the percent distribution appears on the right side of the histogram.
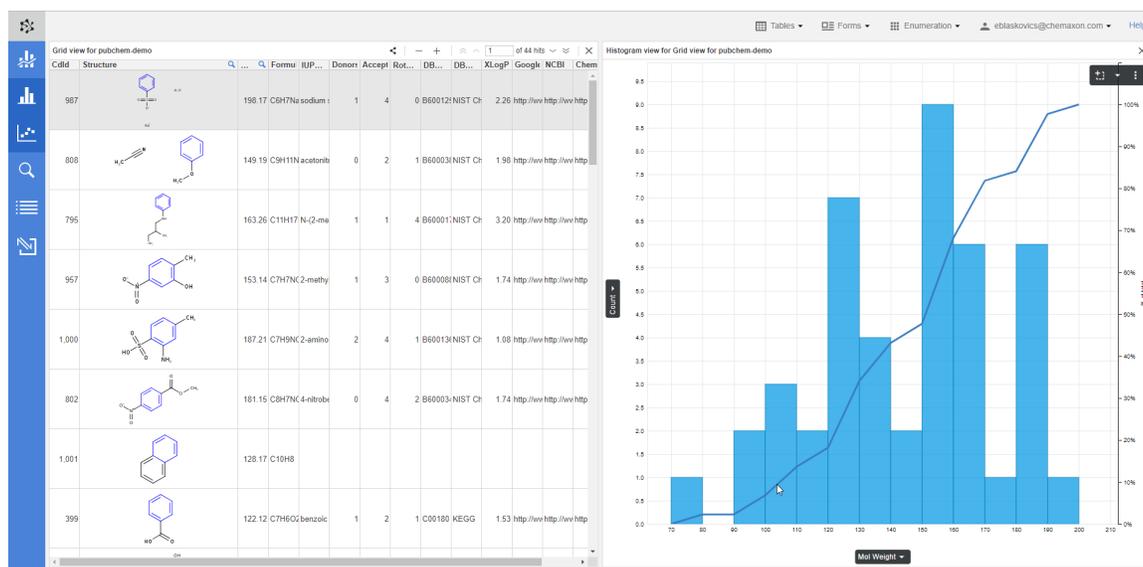
Administration

Charts integration and related functionalities can be enabled / disabled by Plexus Connect administrator using PLEXUS_CHARTS business flag available in the *featureFlags.properties* file by setting the property to *true* or *false*, respectively. The changes will take effect the next log-in to Plexus Suite.