EveRplot Documentation

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This document serves as a guide to the features on EveRplot, an application for the creation of energy vs. reaction coordinate diagrams.

EveRplot may be launched either by using the in-browser web-app hosted at http://mor-vm-shiny.ethz.ch:3838/ or by downloading the shiny script from GitHub https://github.com/mbogdos96/EveRplot and running it in an appropriate R environment such as RStudio. Running the app locally allows for modifications of the code and may prove faster than using the web-app.

A backup web-based version of EveRplot may be found at https://mkb96.shinyapps.io/EveRplot/.

Parameters Panel

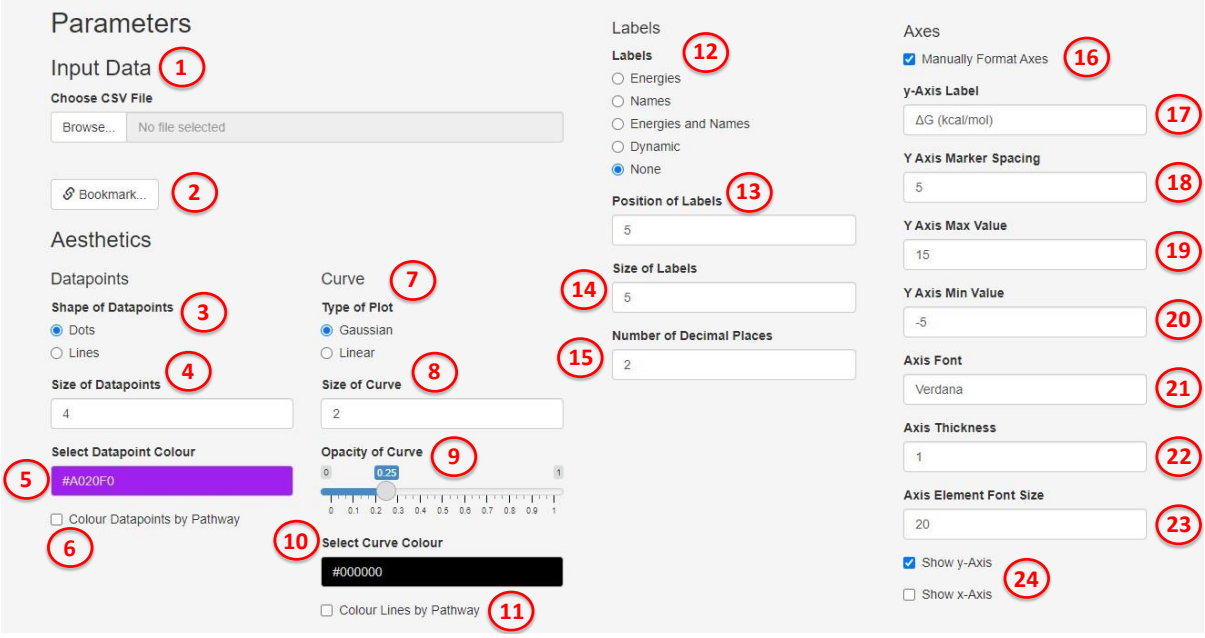

Figure 1. Screenshot of Parameters side of UI. The various features are annotated with numbers and are explained in this document in that order.

1 – Input Data

The user may upload .csv files to the application, whose data will be used to create the desired plot and will be displayed in the table (see section on Graph Panel for more information regarding the data table).

An example .csv file is found on the repository ("EveRplot_example_data.csv"). The column names shown in that example data and the data table (see Graph Panel – 4) must be followed for the app to function correctly.

2 – Bookmark

If you are part way through creating your graph and want to continue later, you can use this button. It will create a popup window with a URL.

Save this URL and use it in your browser to return to the settings you had. This will only save parameters on the "Parameters" side of EveRplot, this means that you should download your data table using the appropriate button (see Graph Panel Section).

3 – Shape of Datapoints

The user may select between dots and lines to represent the individual datapoints that are provided either by the Input Data tool or the Data table.

4 – Size of Datapoints

The text input changes the size of the shape that represents the data.

5 – Select Datapoint Colour

A colour may be selected using the selection tool that appears on clicking the ribbon (Fig. 2). Alternatively, a hex code may be provided and the appropriate colour will be automatically selected.

Figure 2. Colour selection tool.

6 – Colour Datapoints by Pathway

This option may be enabled if multiple pathways have been specified in the data. Enabling it will reveal a text input field (Fig. 3).

Figure 3. Conditional text input field when "Colour by pathway" is enabled.

The field accepts names of common colours and hex codes as input – it is not necessary to select an option from the dropdown list, these are there to give some examples and to prompt the user. After a name or hex code is typed, pressing the enter key will add it to the list. A list of colours at least as long as the number of pathways specified in the data must be entered, else the plot will not be rendered.

Keep in mind that colours are layer on top of each other, starting from the leftmost which is applied to pathway 1 and so on – this can have implications when it comes to overlaps.

7 - Type of plot

This input determines the shape of the lines that connect the various datapoints. Gaussian is the default option; by selecting linear, the user changes the generated plot and reveals additional options in the UI (Fig. 4).

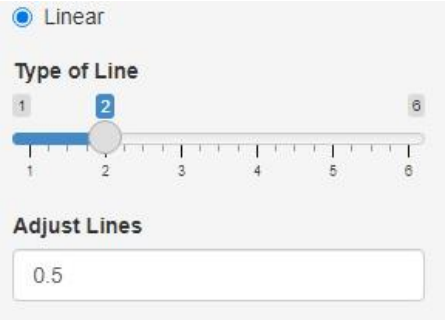

Figure 4. Additional options visible on selecting the linear option under Type of Plot.

Type of line allows the user to cycle through the various default linetype options offered by the geom_segment() function of the ggplot2 R package.

Adjust lines allows fine-tuning of the distance of the lines from the edges of the shapes that represent the datapoints. This parameter has a strong influence on the shape of the graph and will depend on both the selected size of the shapes in "Size of Datapoints" and the size of the graph (more or fewer datapoints). For this reason, it is necessary for the user to adjust it so that a satisfactory outcome is achieved. As a general guideline, a good starting point is approximately 1 % of the value selected for "Size of Datapoints".

If a satisfactory graph is not obtained, it is advisable to change the spacing between the reaction coordinate (Δrc) in the data and try adjusting this value again *e.g.* with spacing between points along the reaction coordinate of 5 no satisfactory result is obtained, but with spacing of 10 or 1 maybe a better result can be obtained.

Keep in mind that the dimensions of the graph seen in the preview may be different than the dimensions which you choose to save the graphs as (see Graph Panel Section), so it is advisable to decide on the dimensions you want beforehand if you plan on using the Linear option. Testing by saving a graph in the desired dimensions before setting the rest of the options is highly advisable.

8 – Size of Curve

Adjusts the thickness of the curve.

9 – Opacity of Curve

Adjusts the opacity of the curve. Low values create a more transparent curve. Caution should be used to coordinate this value with the colour of the curve, as values different than 1 in this field will result in a perceived different colour appear in the plot, due to transparency being applied.

10 – Select Curve Colour

Functions exactly like "Select Datapoint Colour" but changes the colour of the curve instead.

11 – Colour Lines by Pathway

Functions exactly like the “Colour Datapoints by Pathway”.

12 – Labels

This option allows for either the names (column “cpd_num” in the data table) or the energies (column “dg” in the data table) or both to be displayed near the datapoints.

The “Dynamic” option enables the function geom_label_repel() offered by the ggrepel R package and will cause the labels to try to avoid each other and the datapoints, but not the curve. It is reserved for cases where label overlap is an issue and is available only with both names of points and energies, not each individually.

It is generally not advisable to use this option, although it may automatically resolve issues for some users.

13 – Position of Labels

Increasing the value of this option will cause any labels to be moved further away from datapoints on the graph.

14 – Size of Labels

Alters the size of the text (and boxes) of the labels, if any are selected for display.

15 – Number of Decimal Places

This only applies if the data in the table has values that are not integers. It affects the number of decimal places shown on labels, if these are enabled.

For example, using the value 1 in this field when the energies have values of 0 and 25.58 will lead to labels which show 0.0 and 25.6.

16 – Manually Format Axes

Disabling this option (default) will result in the axes being automatically formatted. If it is enabled, additional options appear.

17 – Y Axis Label

Here the user can type in the desired label for the y axis. A similar field will appear for the x axis if the “Show x-Axis” option is enabled.

18 – Y Axis Marker Spacing

This value affects how many markers (ticks) appear on the y axis. For example, using a range of 0 to 10 with this options set to 5 will result in a y axis with ticks marks at 0, 5 and 10.

19 – Y Axis Max Value

Sets the maximum value displayed on the y axis; this does not affect the range displayed on the plot.

20 – Y Axis Min Value

Functions as Y Axis Max Value (17) but for the minimum value.

21 – Axis Font

Sets the font for all elements of the axes.

22 – Axis Thickness

Determines the thickness of all features of the axes (line thickness, marker thickness).

23 – Axis Element Font size

Determines the font size of all features of the axes (label, values displayed).

24 – Show Axes

Controls whether either the y or x axes are shown.

Graph Panel

Figure 5. Screenshot of Graph side of UI. The various features are annotated with numbers and are explained in this document in that order.

1 – Plot Area

This is where the output of the application is displayed. Right clicking on the plot allows copying of the plot to the clipboard for quick sharing.

2 – Download Buttons

These buttons allow the plot to be downloaded in both vector (.svg) and bitmap (.png) file formats. The app automatically downloads plots with transparent backgrounds. Vector format is recommended in order to achieve the smallest file size combined with the highest quality.

ChemDraw is able to open .png files which allows importing of the graphs into a .cdxml file

The third button allows one to save the Data table as a .csv, in case the user has manipulated the table and wishes to continue later.

3 – Plot Dimensions

These values determine the height and width of the plot in cm when downloaded. This does not apply to the displayed plot, but solely to the plot that is downloaded using the download buttons. These parameters apply to both .svg and .png downloads.

4 – Data Table

This table displays any data uploaded as .csv in the Input Data field. In addition, the cells are editable if changes are required.

Right clicking on the table reveals options for adding and removing rows, as well as undo and redo functions.

Note: there exists a known bug where the cpd_num column is not editable but is only a dropdown list. A .csv with any value in that column may still be uploaded.

This bug exists only in the primary web-based version of the app, not in the backup web hosting or the locally run app, despite using the same code.

We could not resolve the issue, which we believe is due to the versioning of some packages in the linux distribution we are using to host the web-based version.