EveRplot Documentation

Michael K. Bogdos

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/EveRplot_app/ 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.

Parameters Panel

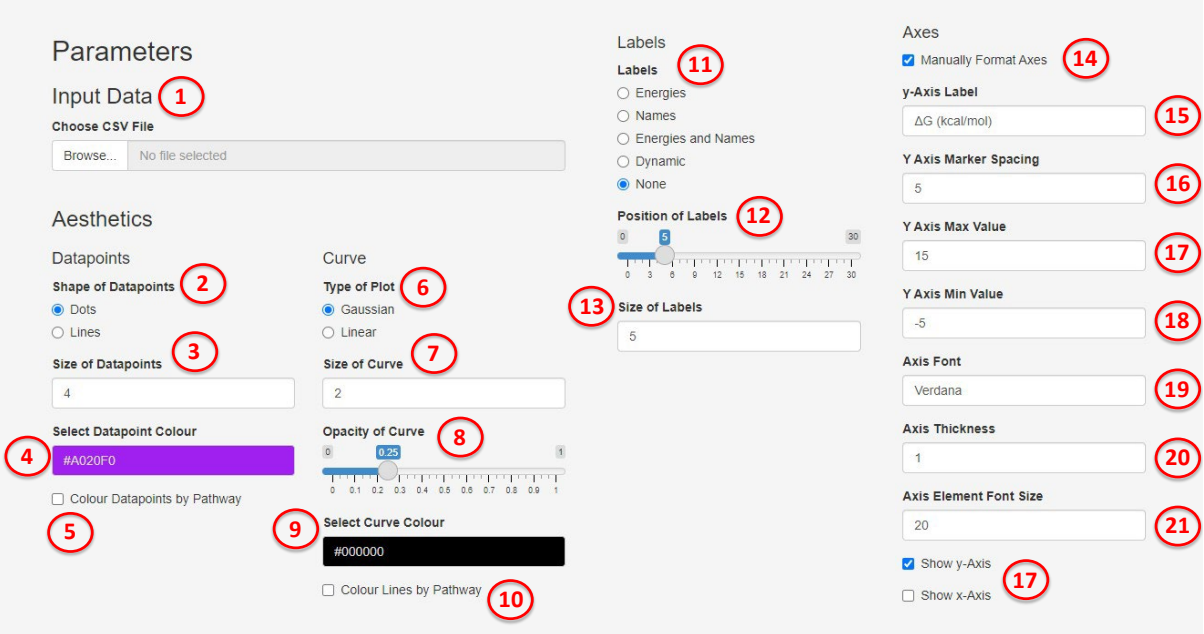

Figure 1. Screenshot of Parameters side of UI. The various features are annotated with numbers and are explained in this document in that order.

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 accompanying this documentation ("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 – 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.

3 – Size of Datapoints

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

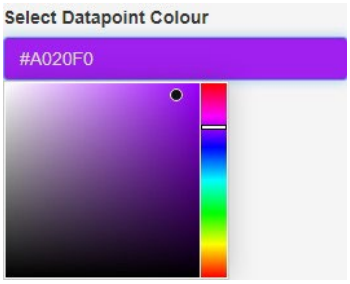

Figure 2. Colour selection tool.

4 – 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.

5 – 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.

6 - 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).

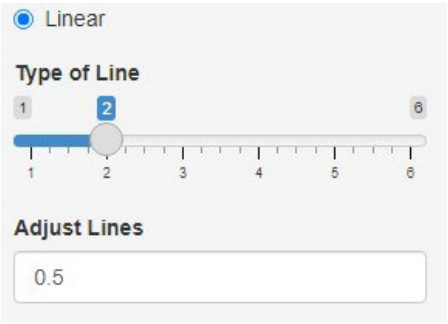

Figure 4. Additional options visible on selecting the linear option under Type of Plot.

Type of line allows the user to cycle through the various default linetype options offered by the geom_segment() offered by 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”, when “Lines” is selected in the “Shape of Datapoints” option.

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.

7 – Size of Curve

Adjusts the thickness of the curve.

8 – 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 cause what is technically a different colour appear in the plot, due to transparency being applied.

9 – Select Curve Colour

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

10 – Colour Lines by Pathway

Functions exactly like the “Colour Datapoints by Pathway”.

11 – 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.

12 – Position of Labels

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

13 – Size of Labels

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

14 – Manually Format Axes

Disabling this option (default) will result in the axes being automatically formatted.

15 – y-Axis Label

Here the user can type in desired label for the y axis

16 – 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.

17 – Y Axis Max Value

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

18 – Y Axis Min Value

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

19 – Axis Font

Sets the font for all elements of the axes.

20 – Axis Thickness

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

21 – Axis Element Font size

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

22 – 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. 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 changes 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.