

# 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 [link] or by downloading the shiny script from Zenodo [link] or GitHub [link] 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.

The code has been published under GNU General Public License Version 3 – for the full license statement see the “LICENSE” file on the repository.

## Parameters

## Panel

The screenshot shows the 'Parameters' panel of the EveRplot application. It is divided into several sections: 'Input Data', 'Aesthetics', 'Curve', 'Labels', and 'Axes'. Each section contains various controls for customizing the plot. Red circles with numbers 1 through 17 are placed over specific features to indicate where they are explained in the document. The features include: 1. 'Choose CSV File' button; 2. 'Shape of Datapoints' (Dots selected); 3. 'Size of Datapoints' slider; 4. 'Select Datapoint Colour' (purple); 5. 'Colour by Pathway' checkbox; 6. 'Type of Plot' (Gaussian selected); 7. 'Size of Curve' slider; 8. 'Opacity of Curve' slider; 9. 'Select Curve Colour' (black); 10. 'Labels' section (Energies selected); 11. 'Position of Labels' slider; 12. 'Size of Labels' slider; 13. 'Axes' section (Verdana font selected); 14. 'Axis Element Font Size' slider; 15. 'Axis Thickness' slider; 16. 'y-Axis Label' (ΔG (kcal/mol)); 17. 'Show y-Axis' checkbox.

**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

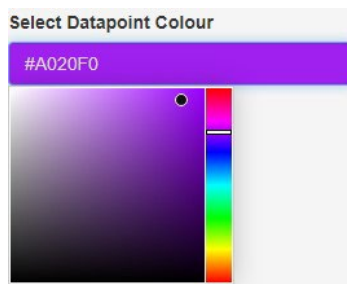
The user may upload .csv files to the application, whose data will be used to create the desired plot and will be displayed in the table (see section on Graph Panel for more information regarding the data table). An example .csv file is found on the repository accompanying this documentation (“EveRplot\_example\_data.csv”). Alternatively, the data table (see Graph Panel – 4) may be used as a template.

### 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 slider changes the size of the shape that represents the data.



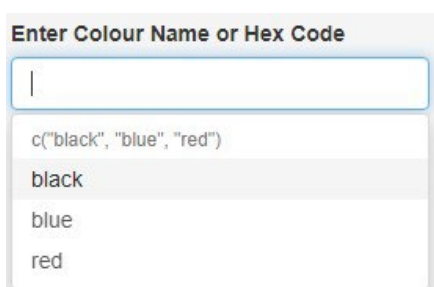
**Figure 2.** Colour selection tool.

### 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 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).

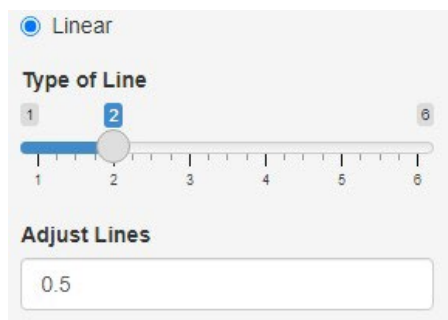


**Figure 3.** Conditional text input field when “Colour by pathway” is enabled.

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 `geom_segment`.

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 ( $\Delta$ rc) 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 – 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` 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 reserve issues for some users.

## 11 – Position of Labels

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

## 12 – Size of Labels

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

## 13 – Axis Font

Allows the selection of fonts for the axis elements by entering the name of the desired font. Most common fonts are supported. For a comprehensive list, the user should consult the documentation of the R package “extrafont”.

## 14 – Axis Element Font Size

Affects the size of the title and numbers on the axes.

## 15 – Axis Thickness

Changes the thickness of the axis itself.

## 16 – y-Axis Label

Allows the user to define the title of the y axis by text input. Does not support subscripts and superscripts but does support special characters such as Greek letters.

## 17 – Show Axis Buttons

Deselecting either option hides the corresponding axis. If the x-axis option is selected an additional options appears, identical in appearance and function to “y-Axis Label”.

## 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.

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.