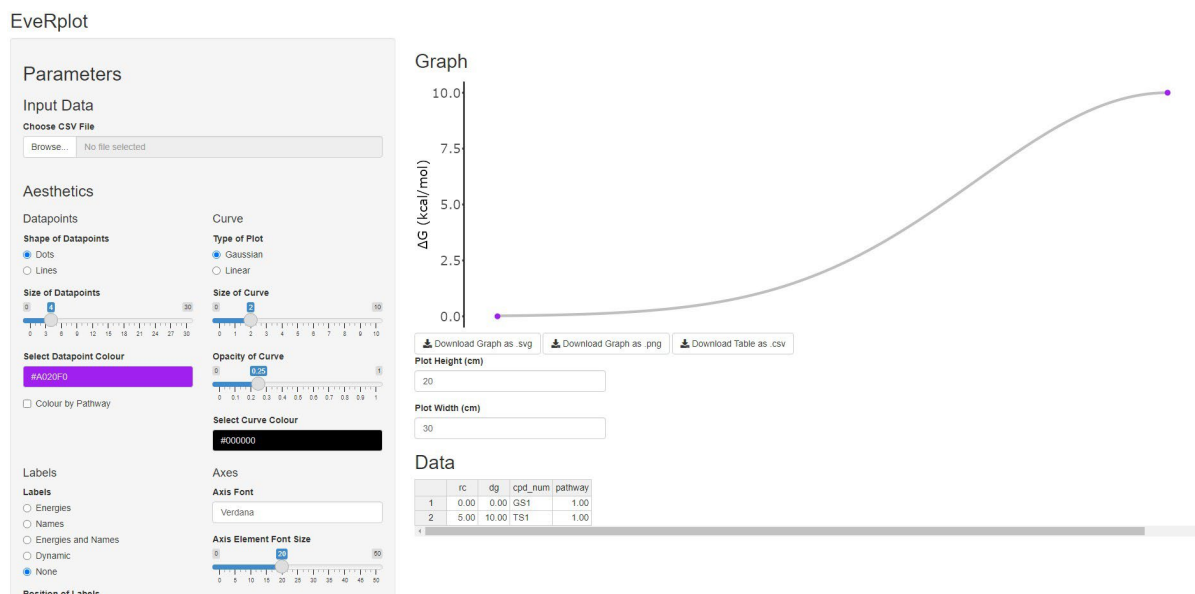# EveRplot Tutorial

This document is a step-by-step guide to creating an example energy vs. reaction coordinate diagram using EveRplot. The example diagram is that seen in Figure 1 of the publication associated with the app.
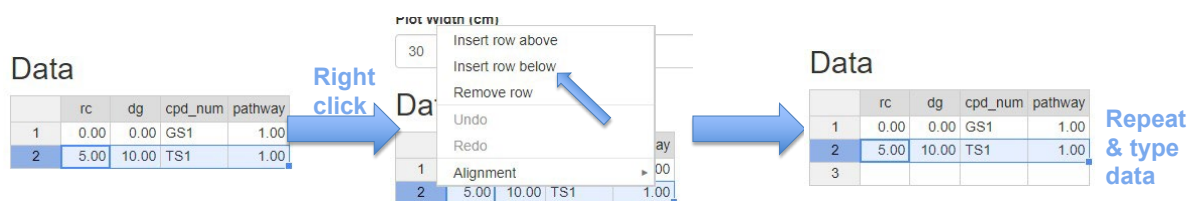
- Launch app (see documentation)

- Input the appropriate data – in this case we know from the source material that 7 points are required, with energies of 0, 43, 21, 25, 21, 43 and 0 kJ/mol (see publication for the reference to the source material) – these correspond to "dg".
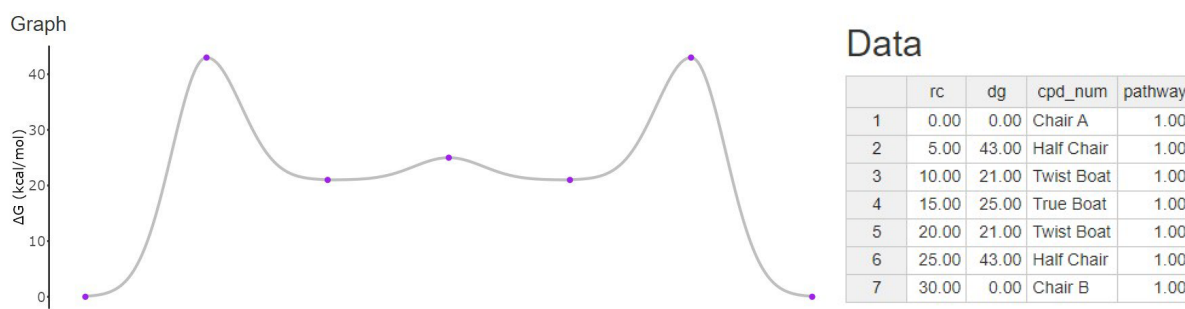
    The "rc" values may be anything, in this case we continue the pattern in the default data, which is spacing evenly by 5 units. It is not necessary to space points evenly, but it will generally give more aesthetically pleasing results.

    In "cpd_num" we will enter the names of the conformations. All pathways are numbered "1" as we do not wish to have multiple pathways represented.

   The data are added by modification of the table:

Which results in:

|	rc	dg	cpd_num	pathway
1	0.00	0.00	Chair A	1.00
2	5.00	43.00	Half Chair	1.00
3	10.00	21.00	Twist Boat	1.00
4	15.00	25.00	True Boat	1.00
5	20.00	21.00	Twist Boat	1.00
6	25.00	43.00	Half Chair	1.00
7	30.00	0.00	Chair B	1.00

- The aesthetics are modified next, beginning with labels. In this case, selecting "Energies and Names" under labels provides a satisfactory result.
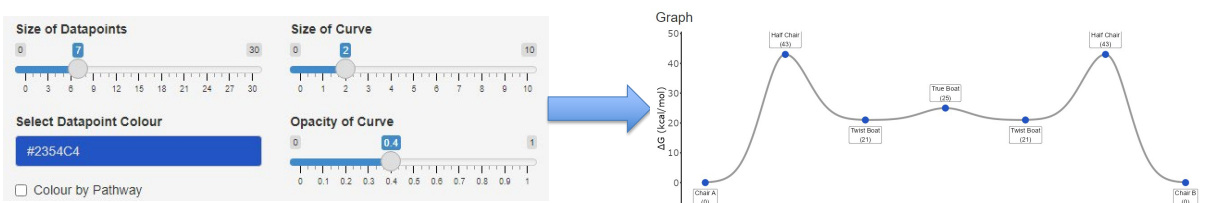
- To match the aesthetics of the figure in the paper, the appropriate colour for the datapoints is selected, as well as the appropriate size and curve opacity.
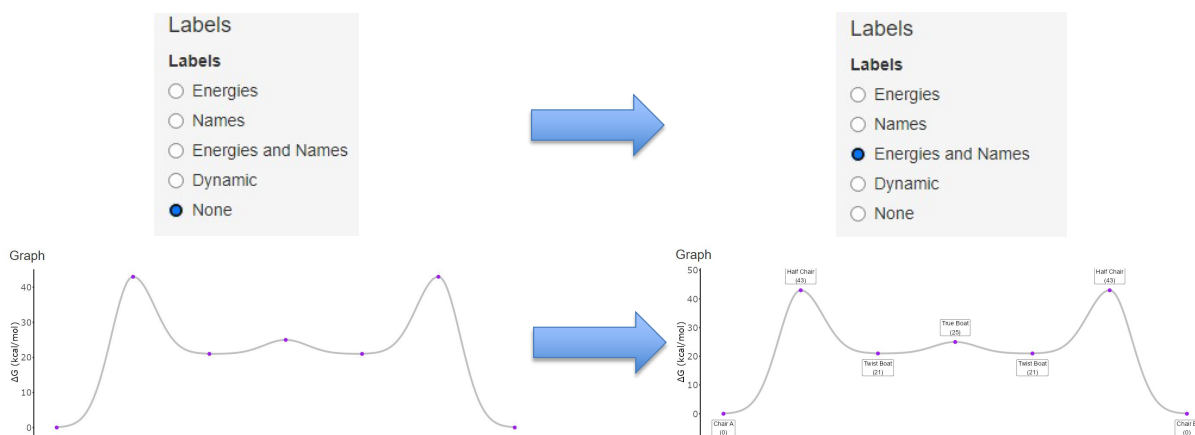
- The axis label is changed from "ΔG (kcal/mol)" to "Energy (kJ/mol)":
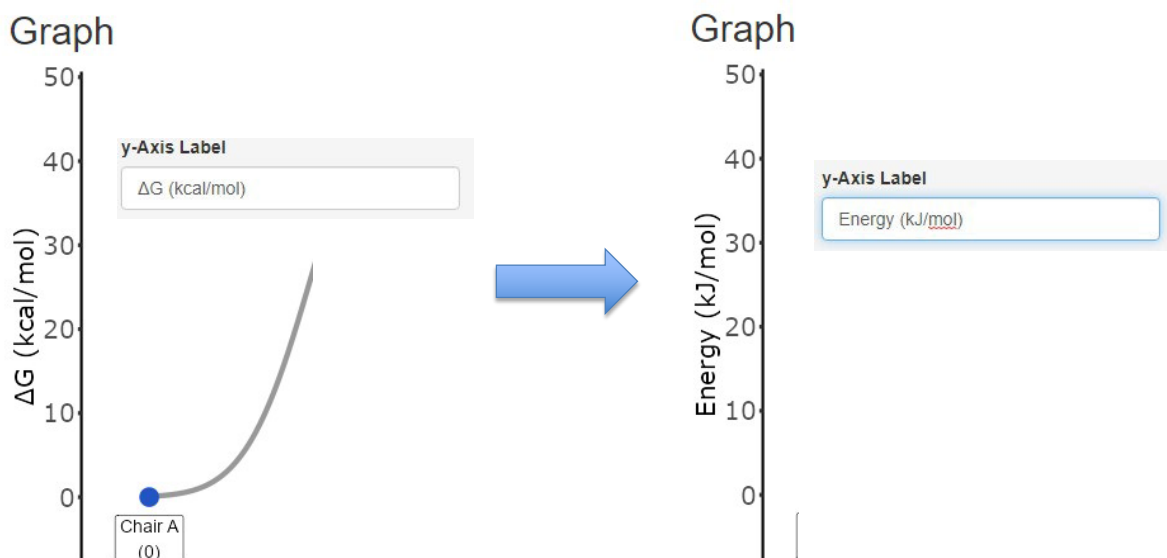

- The graph is now ready and may be saved. The graph in the manuscript has a ratio of 2:1 width:height – for .svg files the absolute values in cm are not relevant, so here the height and width are modified to 20 x 40 cm from 20 x 30 cm.

Once these parameters are set, we can download the plot using the desired download button:

- The graph is added to an appropriate image editor (it has a transparent background – Microsoft PowerPoint will also work) and ChemDraw objects may be added:
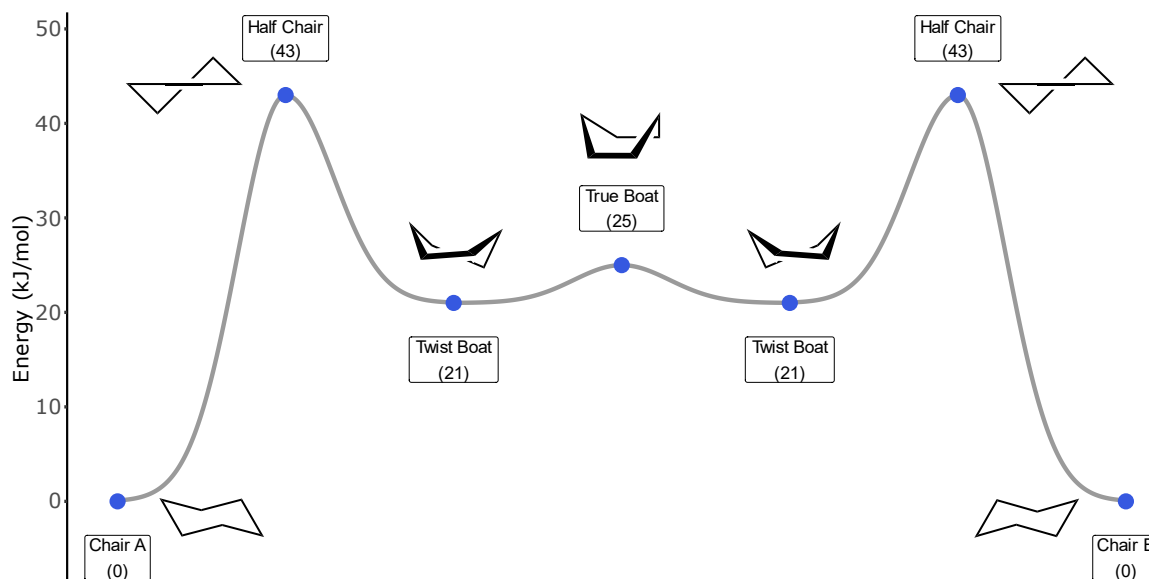
This concludes the tutorial. Different types of diagrams will have a slightly different workflow, however the core ideas are similar. For additional details please see the documentation. If you are experiencing problems making a particular diagram please contact the developer.