Tutorials and worked examples for simulation, curve fitting, statistical analysis, and plotting.
https://simfit.org.uk

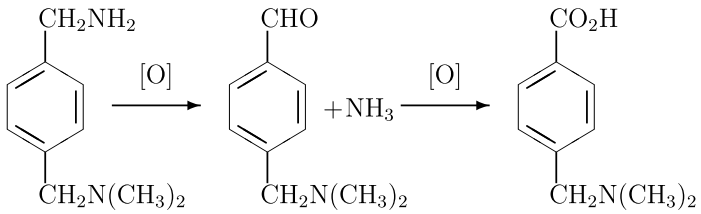
Sometimes it is required use LaTeX to display chemical structures inside a scientific plot, and this document describes how to do this using a condensed scheme for the oxidation of p-dimethylaminomethylbenzylamine. Note that all the files mentioned in this document are distributed as SimFIT test files so that users simply wishing to create the final composed document can proceed directly to the last section describing how to use **EditSVG**

The TEX source

This is the code contained in the file `latex_chemical_formula.tex`

```
\documentclass[12pt]{article}
\usepackage{carom}
\pagestyle{empty}
\begin{document}
{\begin{picture}(3000,600)(0,0)
\thicklines
\put(0,0){\bzdrv{1==CH$_{2}$NH$_{2}$;4==CH$_{2}$N(CH$_{3}$)$_{2}$}}
\put(700,450){\vector(1,0){400}}
\put(820,550){[O]}
\put(1000,0){\bzdrv{1==CHO;4==CH$_{2}$N(CH$_{3}$)$_{2}$}}
\put(1650,400){+}
\put(1750,400){NH$_{3}$}
\put(2000,450){\vector(1,0){400}}
\put(2120,550){[O]}
\put(2300,0){\bzdrv{1==CO$_{2}$H;4==CH$_{2}$N(CH$_{3}$)$_{2}$}}
\end{picture}}
\end{document}
```

which displays like this.



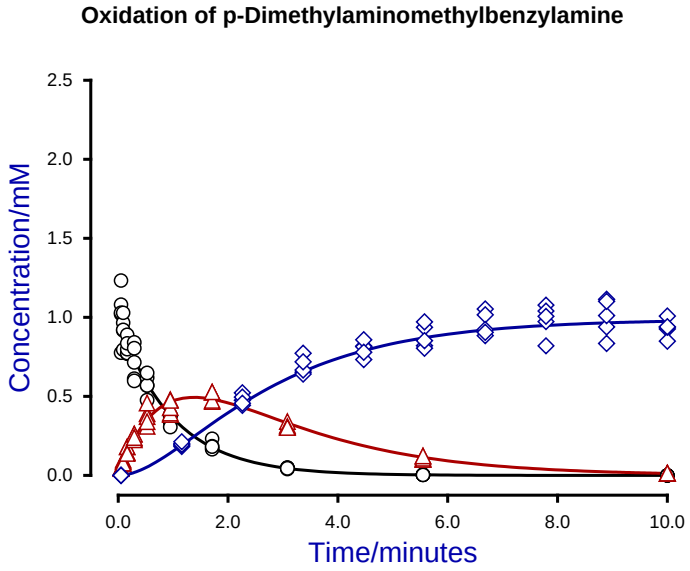
To import this formula into a graph using **EditSVG**, `latex_maths_equation.svg` can be made using the following commands, or `latex_maths_equation.tex` can be input directly into **EditSVG**.

- `latex latex_chemical_formula.tex`
- `dvips latex_chemical_formula.dvi`
- `dvisvgm -E latex_chemical_formula.ps`

The file `latex_chemical_formula.svg` created is then ready to be imported into **EditSVG** but, alternatively, the source file `latex_chemical_formula.tex` can be opened in or dragged and dropped directly onto **EditSVG** if there is a local installation of LaTeX. It should be realized that, when using LaTeX in this way to create a SVG file, the command line must be used from a folder containing the *.TEX file required as a local file and not as a fully qualified path–filename to a remote source file. The program **EditSVG** circumvents this issue when importing LaTeX source by creating local copies of all files.

Creating the plot file

The file `latex_chemical_plot.svg` with the time course data to be used looks like this before the equation is added.



This figure was created using **qnfit** fit three data sets for the consecutive reaction scheme

$$A \rightarrow B \rightarrow C$$

in the SimFIT test library file `consec3.tfl`, then fitted using the model in the model file `consec3.mod`.

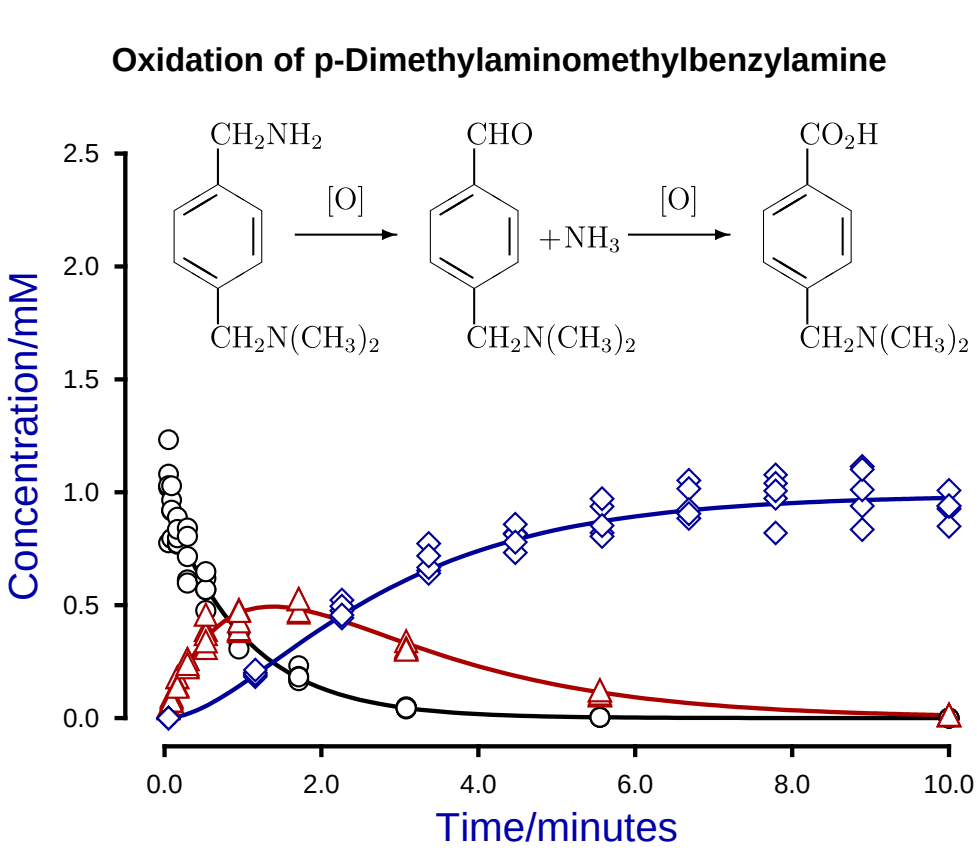
After manipulating the line thicknesses, title, legend, and colors, the files `latex_chemical_plot.svg`, and `latex_chemical_plot.eps` were created to archive the graph. In addition the SimFIT metafile `latex_chemical_plot.metafile` was saved so that users wishing generate this plot can easily do so using the SimFIT program **simplot**or the SimDEM program **simdem70**. Users wishing to avoid this process can simply read the SimFIT metafile `latex_maths_plot.metafile` directly into the SimFIT program **simplot**, or the SimDEM program `simdem70`.

Joining the SVG files using EditSVG

Open program **EditSVG** then input the test file `latex_chemical_plot.svg`. Then there are two options.

1. Input the test file `latex_chemical_formula.svg` directly; or
2. read in the test file `latex_chemical_formula.tex` which will then be used by LaTeX to generate an internal copy of `latex_chemical_formula.svg`.

Finally, just use the mouse to move the equation into position and alter the scaling as required to obtain the final plot saved as `latex_chemistry.svg` and shown next.



Summary

The programs referred to in this document are as follows.

1. **InkScape** is an OpenSource program that takes in SVG files and can write out EPS and other files.
2. **EditSVG** is a SimFIT and SimDEM program that takes in SVG or TEX files and writes out SVG and other files.
3. **editPS** is a SimFIT and SimDEM program that takes in EPS files and writes out only EPS files.
4. The SimFIT program **simplot** and the SimDEM program **simdem70** take in SimFIT metafiles and write out either SVG or EPS files.

Further, the SimFIT test files (*.TEX and *.SVG) described in this document that can be used by program **EditSVG**, and those (*.EPS) that can be used by program **editPS** are now listed.

File name	Data included
`latex_chemical_plot.metafile`	SimFIT or SimDEM metafile to create the plot without any equation
`latex_chemical_formula.tex`	LaTeX source file for the maths equation with no plot
`latex_chemical_formula.svg`	SVG file containing the formula only
`latex_chemical_plot.svg`	SVG file containing the plot only
`latex_chemistry.svg`	SVG file containing both the formula and plot
`latex_chemical_formula.eps`	EPS file containing the formula only
`latex_chemical_plot.eps`	EPS file containing the plot only
`latex_chemistry.eps`	EPS file containing both the formula and plot