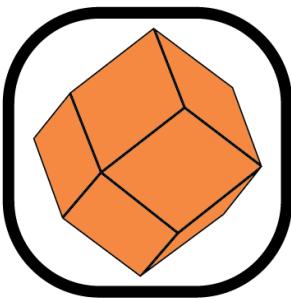


Quick Start Guide



MinPlotX

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1 General Information

MinPlotX is downloaded and installed as an application and compiled versions are available for Windows, Mac, and Linux users. **Download MinPlotX here!** <https://github.com/NilsGies/MinPlotX/releases/latest>

1.1 What is MinPlotX?

MinPlotX is an open-sourced MATLAB®-based mineral formula recalculation and compositional plotting program with an easy-to-use stand-alone graphical user interface (GUI) as well as an advanced programming interface (API). Compiled versions of MinPlotX do not require a MATLAB® license to run. The uncompiled version is also available for users who wish to modify the source code.

1.1.1 Highlights of MinPlotX

- The program can read as input various types of data files (*e.g.*, .txt, .csv, .xlsx) that contain columns of data as mass percents (wt %) of oxides (or elements for sulfides). Input data columns can be arranged in any order.
- Input data can include metadata such as mineral name, sample name, analysis location (*e.g.*, core, mantle, rim), rock type, metamorphic grade, transect/line distance, or any other kind of metadata.
- Metadata can be used to classify mineral analyses during plotting (*e.g.*, plotting cores vs rims with different colors, symbols, etc.).
- In addition to predefined classification plots provided automatically for various minerals, users can create and modify their own diagrams.
- Advanced users can modify or create new functions for mineral formula recalculation and plotting routines in the uncompiled version of MinPlotX.

MinPlotX currently offers recalculation and structural formula assignment for 21 different minerals/mineral groups: Allanite, amphibole, apatite, chlorite, chloritoid, cordierite, epidote, feldspar, garnet, ilmenite, lawsonite, mica, olivine, oxyspinel, pyroxene, scapolite, serpentine, staurolite, sulfides, talc, and titanite.

1.1.2 The MinPlotX download includes:

- A Quick Start Guide with examples and information for an easy start with MinPlotX
- A documentation file explaining the recalculation and plotting procedures for each mineral
- Example input files of natural and synthetic mineral data (in the installation directory of MinPlotX)
 - Synthetic mineral data are calculated from ideal endmember formulas in various ways (*e.g.*, including or excluding H₂O)

1.2 Report Issues

MinPlotX was developed by a small, dedicated team of two geoscientists without special training in software development as a side project within a relatively short time frame. Despite our best efforts to test all features and implement routines to prevent errors, as with any complex software, there may still be ways in which users could potentially cause the software to malfunction. If you encounter problems, please send us a description of the issue and an example dataset so that we can work on improving MinPlotX. Send us a message [here!](#)

1.3 Citation Guidelines

We recommend that you use the following citations in your publications or presentations when referring to data processed and visualization with MinPlotX, *e.g.*, data were processed and visualized with MinPlotX (Walters & Gies 2024).

Jesse B. Walters & Nils B. Gies, MinPlotX: A powerful tool for formula recalculation, visualization, and comparison of large mineral compositional datasets, <https://doi.org/10.31223/X5FX5N>

It is not recommended to cite MinPlotX only in the supplementary material, as these citations are not taken into account by citation statistics platforms.

textit{Note}: Please check for the latest citation information on the MinPlotX GitHub page, once the peer reviewed paper is published please cite the paper instead of the preprint. **Check for updates on the MinPlotX GitHub Page!** <https://github.com/NilsGies/MinPlotX>

1.4 License

This work is licensed under a GPL-3.0 license.

2 MinPlotX Getting Started

2.1 Installation

MinPlotX is available on Windows and MacOS as standalone and does not require a MATLAB licence, but you will have to install the MATLAB Runtime libraries during the installation. For Mac users: It is recommended to start the installation with right click - open (Some versions of MacOS block the installation when starting it with a double click). The installation files including all needed libraries which are needed for computers without access to the internet are available on request. To install MinPlotX execute the installation file and follow the instructions:



Note: On the first startup MinPlotX will try to create the default working directory in Documents>MinPlotX. If MinPlotX can not create this folder it will request the user to chose an existing folder with read and write permission as default working directory. After the first successful startup MinPlotX will create a file containing the path of the default working directory in the installation directory > Dev > "MinPlotXWorkingDir". The user can change this path to an existing directory with read and write permission to change the default working directory.

2.2 MinPlotX for advanced MATLAB users

Execution in this method is only suitable for advanced users, requires a MATLAB licence and is not recommended for standard use of MinPlotX. To run MinPlotX without installation in matlab, the directory with the files must be added to the MATLAB path with the following syntax:

```
addpath(genpath('Your MinPlotX directory'))
```

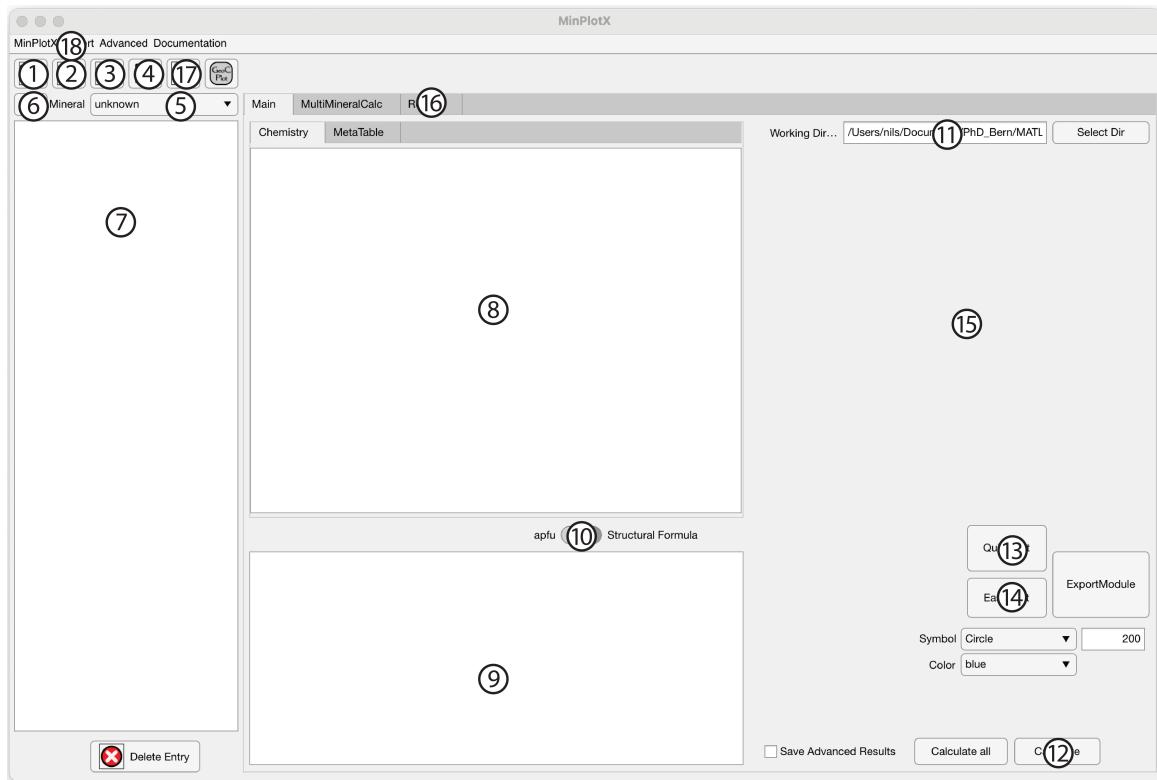
After that, modifications or extensions can be implemented using the MATLAB App Designer. Further information on execution, public properties and public functions is available in the MinPlotX API.

2.3 MinPlotX input data

MinPlotX reads tables of mass percent of the oxides of the elements (for silicate, oxide, and phosphate minerals) or atomic proportions of elements (for sulfides only). Some oxides are required for minerals (e.g., SiO₂ in silicates) whereas others are optional (e.g., SrO in feldspar, K₂O in pyroxene). All possible inputs (required and optional), calculated outputs, and mineral specific options are given in MinPlotX_InputsOutputs which can be accessed in the top Menu ? > InputOutput Documentation. This document should be checked in detail before loading any data into MinPlotX. If the Mineral name (or a specified alternative spelling from the MineralNames.csv file) is included in the file name MinPlotX automatically assigns the Mineral to the imported data.

2.4 MinPlotX GUI

The graphical user interface (GUI) of MinPlotX:



1. Load MinPlotX Project
2. Load Data From Folder
3. Load Data From File
4. Save MinPlotX Project
5. Mineral Selection
6. Input Data Files Filter
7. Input Data Files
8. Input Data Table
9. Output Data Table
10. Change Output Data Table
11. Current Working Directory
12. Calculate Button
13. Plot Diagrams (Single)
14. Plot Diagrams (Separated)
15. Calculation Options
16. Additional Modules
17. Table Calculator
18. Top Menu

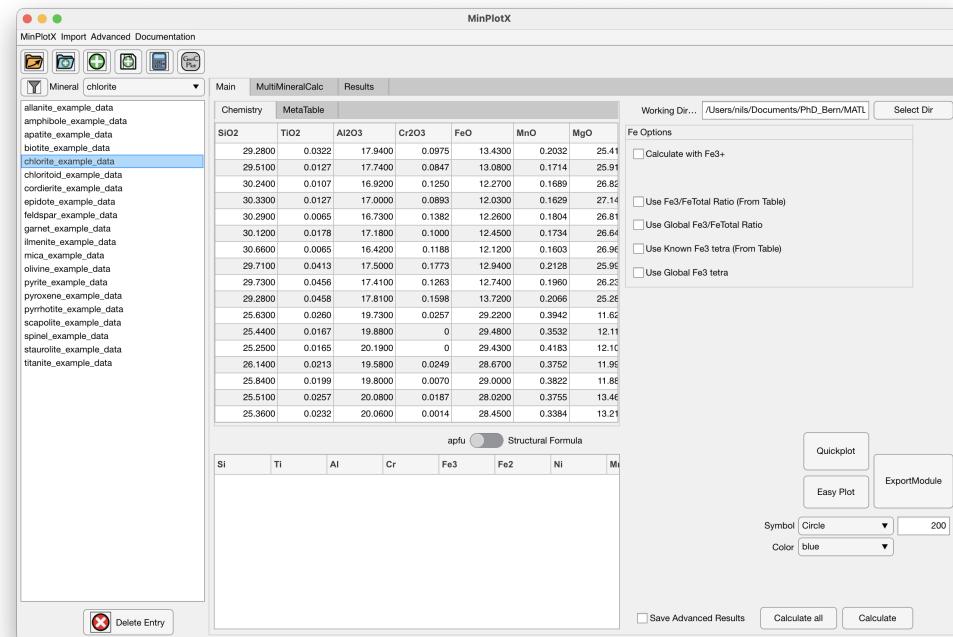
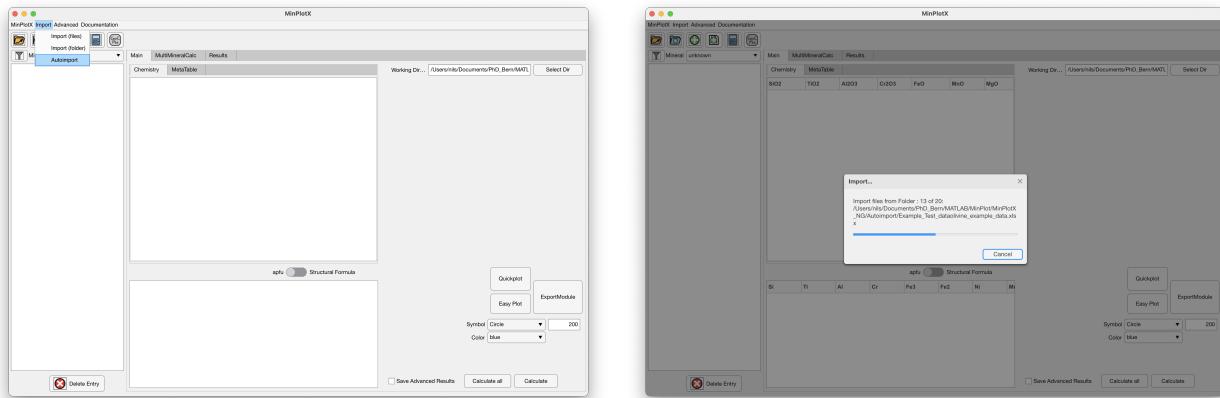
3 Quick Start Guide

This document is intended to introduce the most important features of MinPlotX. More advanced workflows to for example custom plotting will be explained in an additional document.

3.1 MinPlotX Autoimport

MinPlotX comes with a set of example datafiles, which are located in the Autoimport folder in the installation directory. To automatically import all files in the Autoimport folder use Import > Autoimport

Note: You can replace the files in the Autoimport folder in the installation directory of MinPlotX with any files you want to automatically import

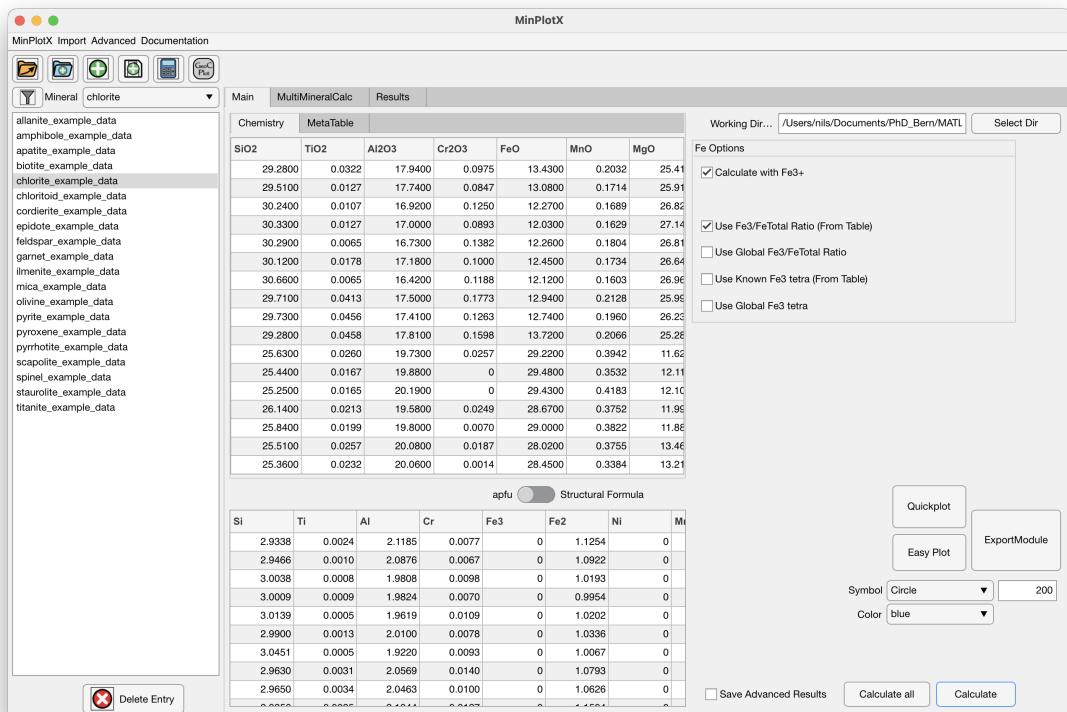
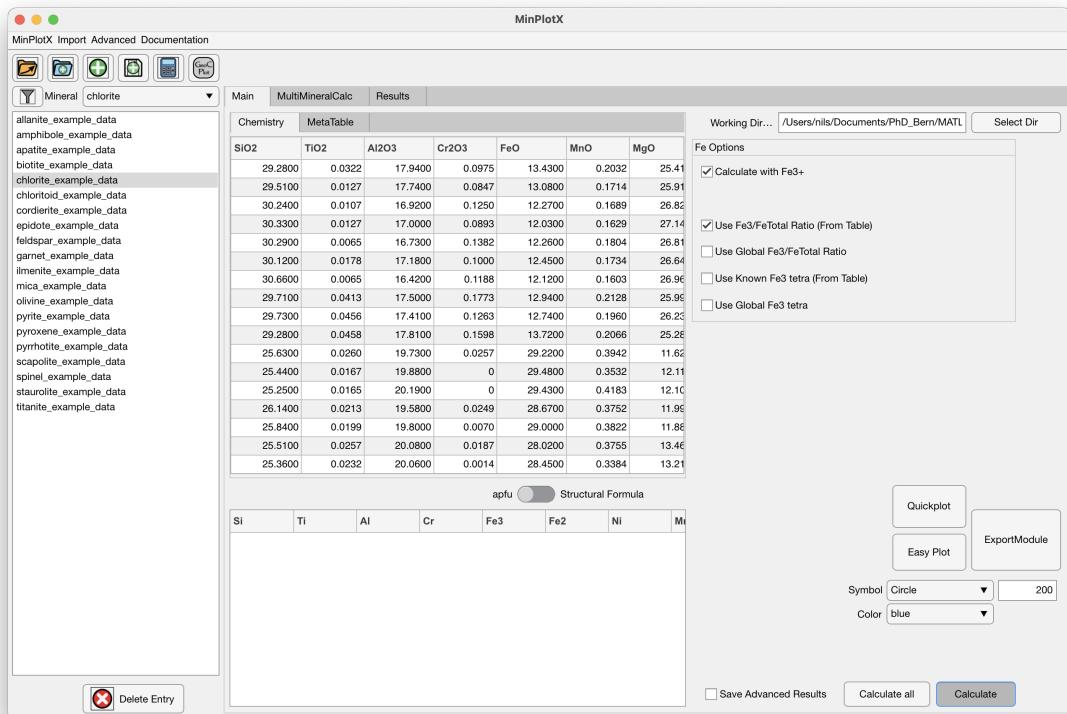


3.2 MinPlotX Manual Import

To Import data manually you can either chose to import all compatible files from a directory using either button (2) or import a single file using button (3).

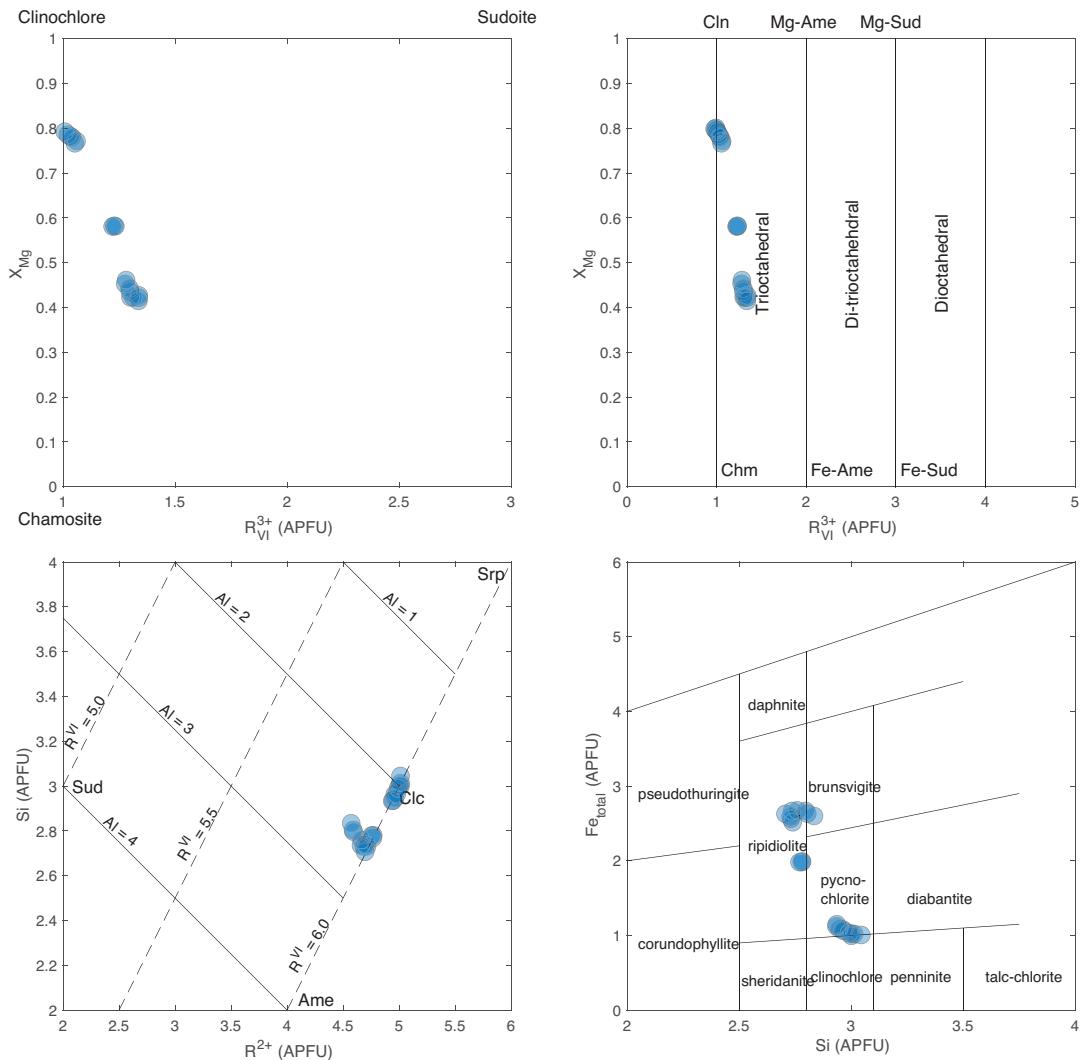
3.3 MinPlotX Calculation

To calculate make sure the correct mineral is chosen in the "Mineral" drop down menu (5) and if need for the mineral, calculation settings for Fe, Mn and MineralSpecific options are set as desired. After pressing the "Calculate" Button the results will appear in the Output Table (9). Use the switch (10) to change between atoms per formula unit and structural formula. When the "Calculate" Button is pressed again with different settings previous calculation results will be replaced with the latest calculation results.



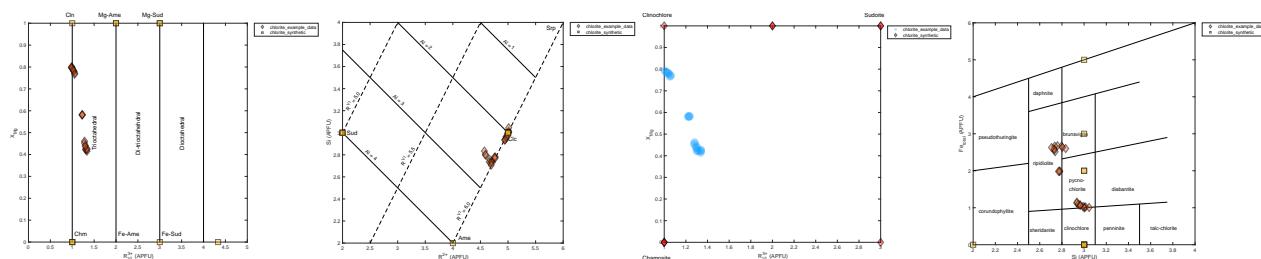
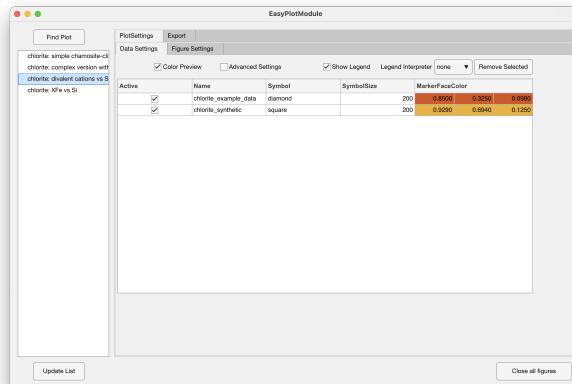
3.4 MinPlotX Quickplot

MinPlotX includes many mineral specific diagrams. The easiest way to generate these plots is to use the Quickplot Button (13). If the mineral is specified in the Mineral DropDown (5) and mineral specific diagrams are available for the selected mineral the diagrams will be generated as subplots in a single figure.



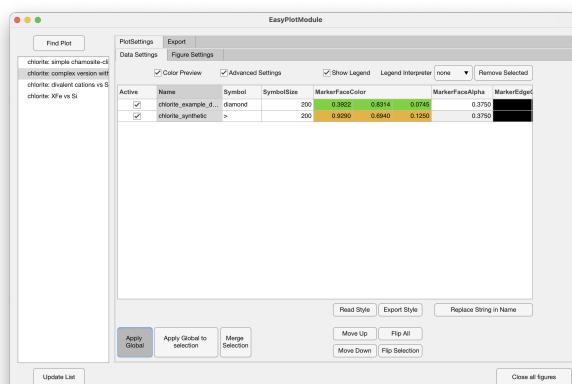
3.5 MinPlotX EasyPlot

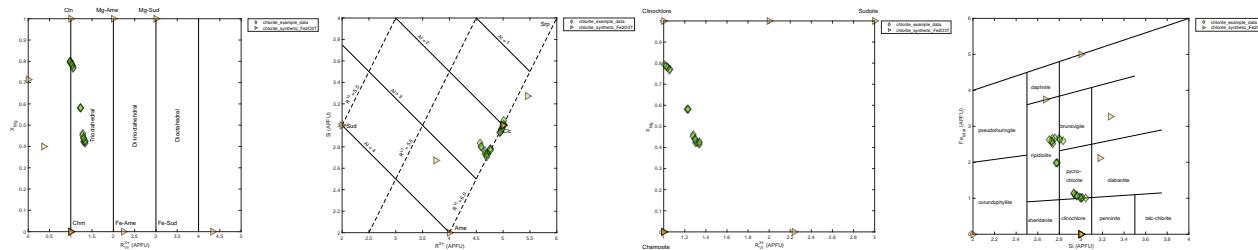
To further customise plots we developed the Easy Plot Module. With the Easy Plot Button (14). All mineral specific diagrams will be generated as individual figures. If the mineral specific figure already exists the data will be added onto the existing plot with a new legend entry. The EasyPlot Module which opens together with the plots allow to further customise these plots. Here the appearance of all symbols and legend entries can be changed by simply editing the table.



To apply the changes to all open figures, check the all settings box, select the entries you want to update in all figures and press the Apply Global button. The settings will be applied to all entries in all figures with the same names as the selected entries. If you want to change a name in all figures change the entry you want to edit, select the entry in the table, press the apply global to selection button, chose the entry with the old name you want to change and agree in the dialogue box to change the name.

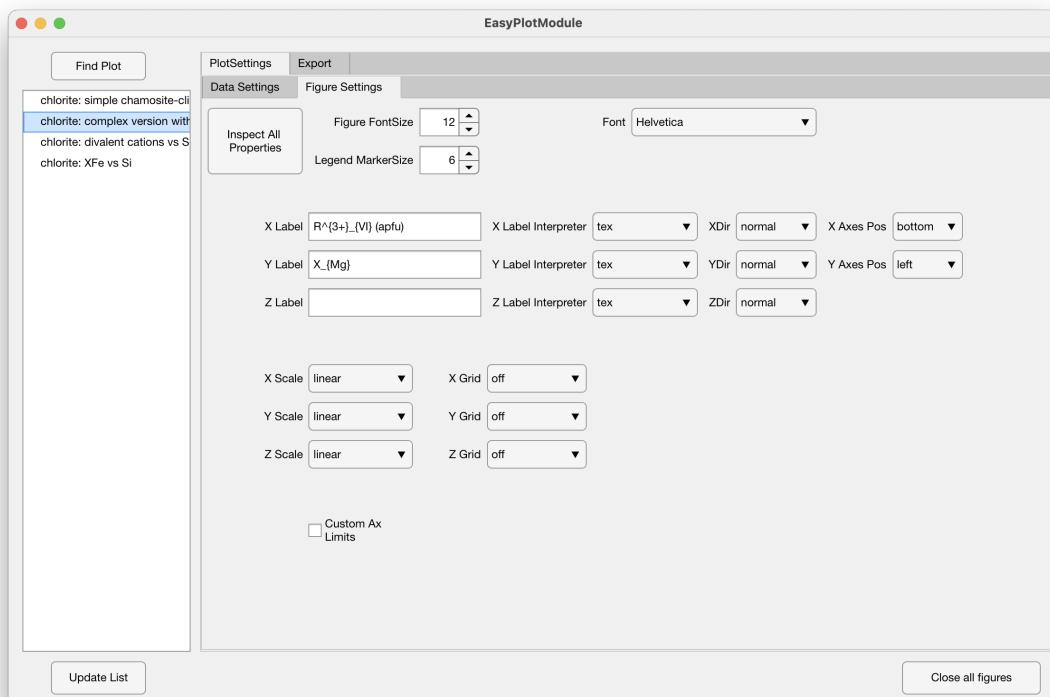
Note: to change the colors of the spots or the outlines double right click in the table.



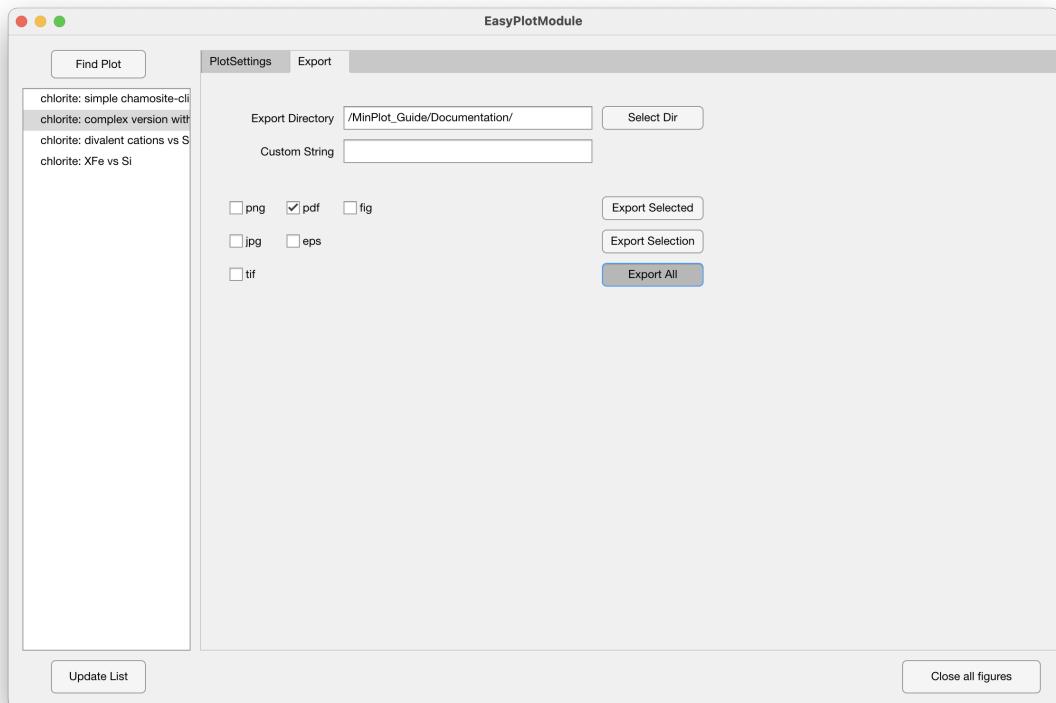


To merge entries, use the button labelled Merge Selection.ⁱⁱ If the selected objects have different appearances, a list box will open, allowing the user to select the target object to which all other selected data points will be merged. Please note that merging is an irreversible process. It does not affect any data stored in MinPlotX; only the data displayed in the plot is affected. Consequently, the original plot can be regenerated using the same method as the original figure.

Additional figure properties such as font, fontsize or axis properties can be changed in the Figure Settings tab.

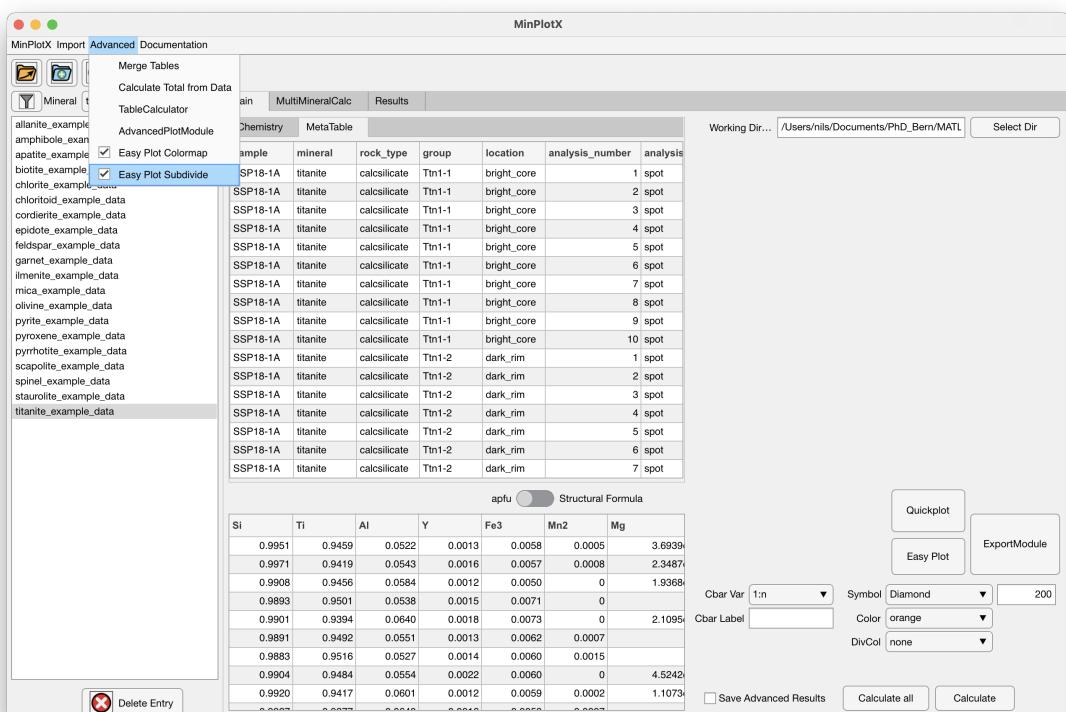


To export EasyPlot figures, navigate to the "Export" tab, select the desired files and export directory, and export the figures.



3.6 EasyPlot Data Subdivision and Colormap

The following options can be used either individually or in combination and provide the ability to visualise additional features in a dataset. To enable these additional features, the appropriate menu item must be activated. These features are available for both EasyPlot and Quickplot.

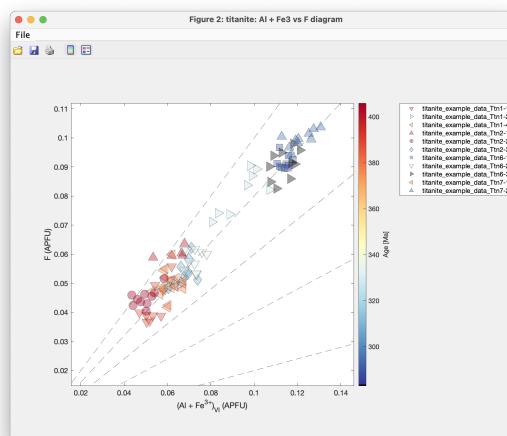
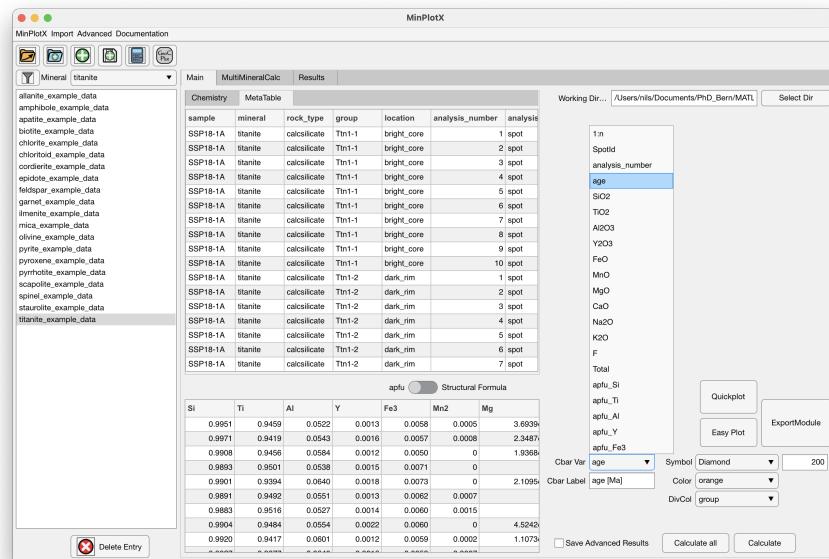


3.6.1 Subdivision

For subdivision, columns containing strings can be used to subdivide the dataset into individual subsets using the unique strings in the selected column. The column to be used for subdivision can be selected from the DivCol drop down menu.

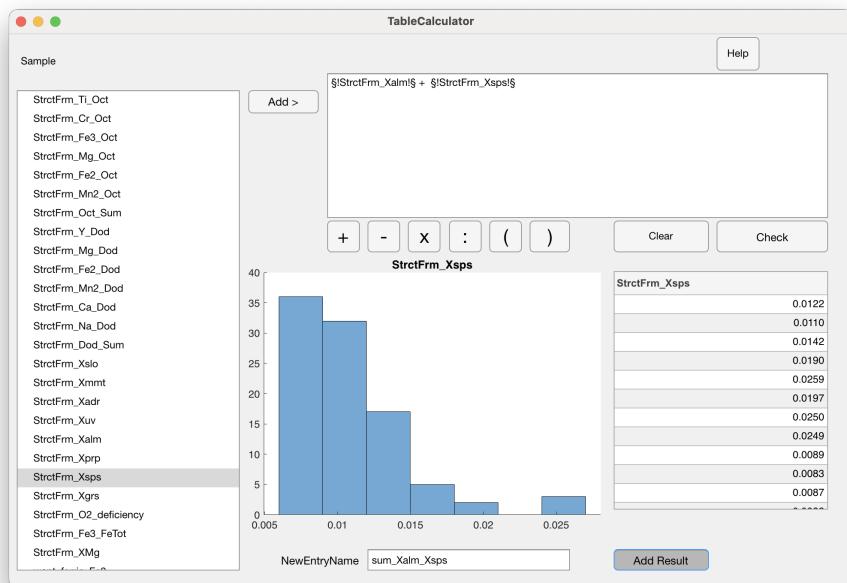
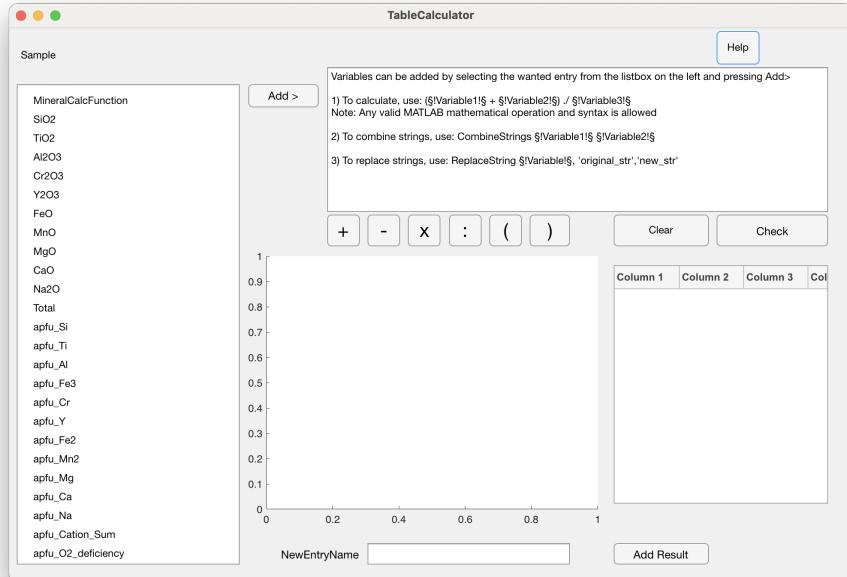
3.6.2 Colormap

Columns containing numeric variables can be used to apply a colormap to the data points. The column used for the colour map values can be selected from the CbarVar drop down menu. The colormap can be changed in the Results tab when the Advanced>Easy Plot Colour Map option is enabled.



3.7 TableCalculator

To perform mathematical calculations with the available numeric data columns in a single dataset, we have included the TableCalculator. The module can be accessed via the calculator symbol or "Advanced">>TableCalculator. Further the table calculator can be used to combine strings or remove strings from columns.



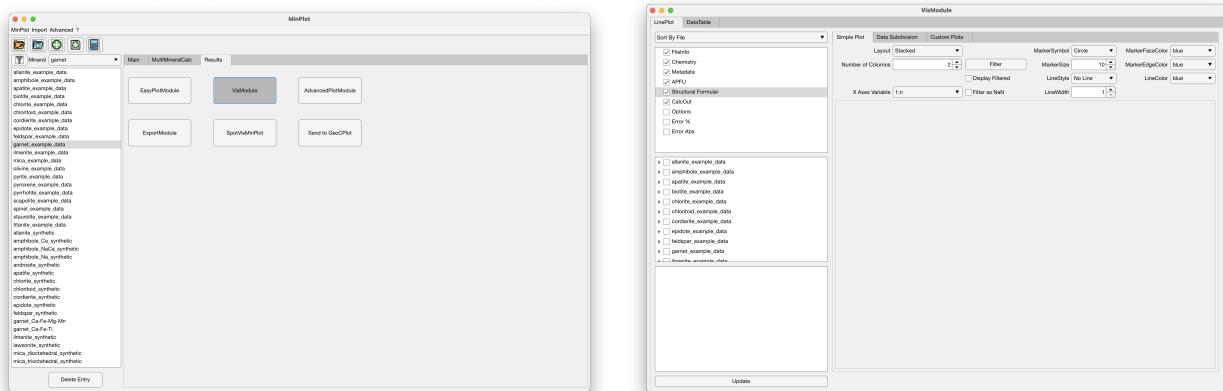
Select the column to be used for the calculation and use the "add >" button to generate the identifier. For simple calculations, the symbols of the mathematical operators can be used to generate the calculation to be performed. However, any mathematical operation can be performed using a valid MATLAB syntax. To check that the calculation syntax is correct, use the 'Check' button to generate a histogram of the resulting output values. A custom column name can be specified and the calculation result added to the data set.

Note: To perform multiplication and division of two columns “.” and “./“ respectively needs to be used.*

3.8 VisModule

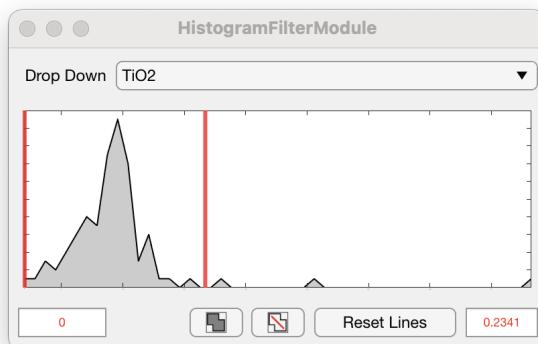
3.8.1 Data selection and filtering

For more customised data visualisation routines, we have created the VisModule. The user can build the data table used for plotting by selecting the samples, tables and variables to be used in the plots. The VisModule can be accessed via the button located in the Results tab. It should be used after the calculations have been completed for all datasets that are to be used for plotting.



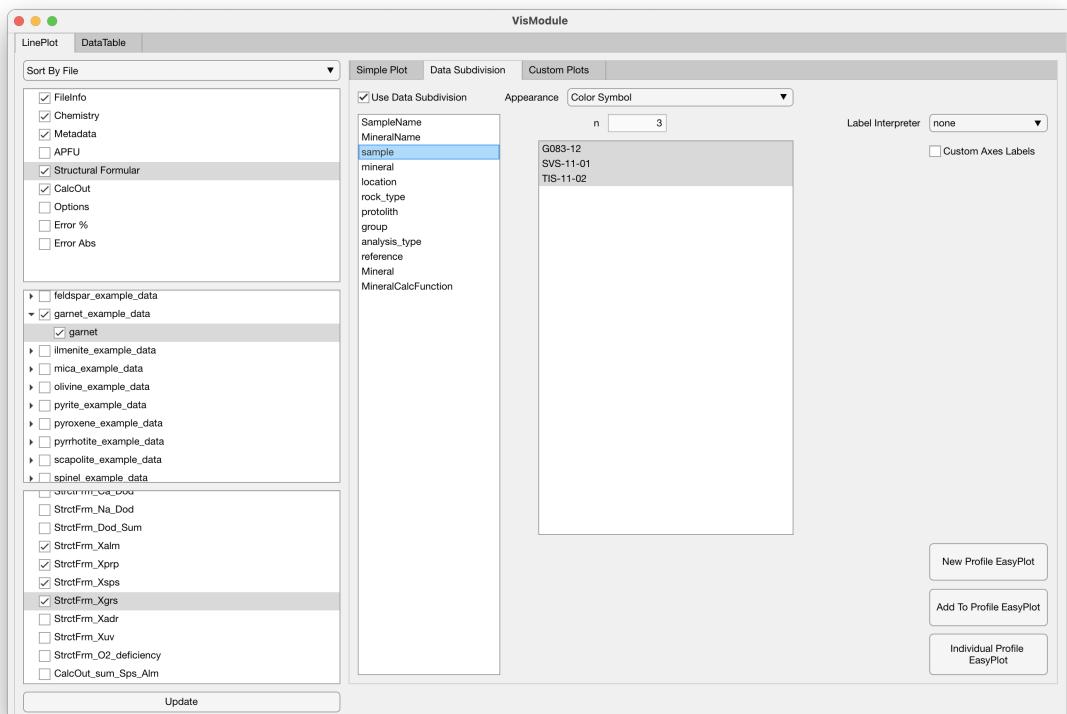
3.8.2 Data selection and filtering

The initial step is to choose the tables and datasets to be utilized for plotting in the tree menus on the left side. In an optional step, the HistogramFilterModule can be used to filter data points outside the selected threshold for any numeric data column. The HistogramFilterModule can be activated with the "Filter" button.



3.8.3 Data Subdivision

Another powerful routine we have implemented allows a data table to be further subdivided using unique strings present in the data table. Each selected unique string is used to create a subset of the data and can be visualised with different symbols and colours. Each individual subset can be further customised in the EasyPlot Module. To use the data subdivision, activate the "Use Data Subdivision" in the "Data Subdivision" tab and select the column you want to use for the data subdivision in the left list box. All unique strings will appear in the right list box. Only the selected unique strings will be included in any further plotting operations.

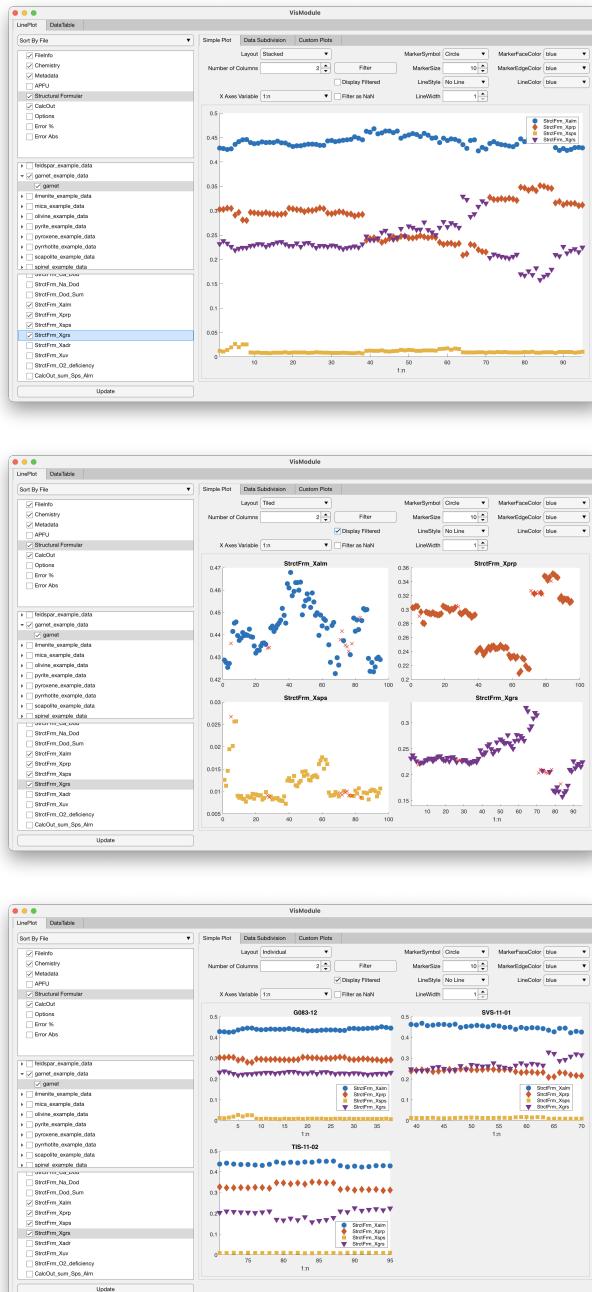


Note: Plotting a very large number of subdivisions might be slow

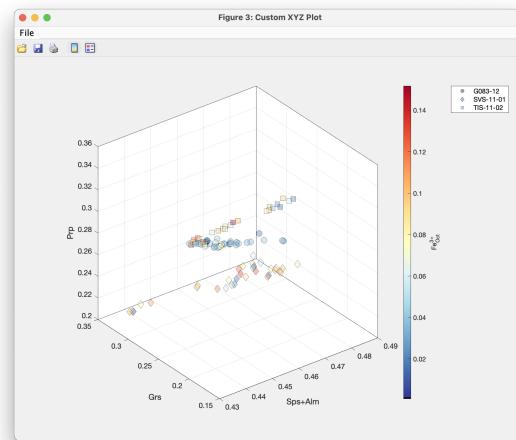
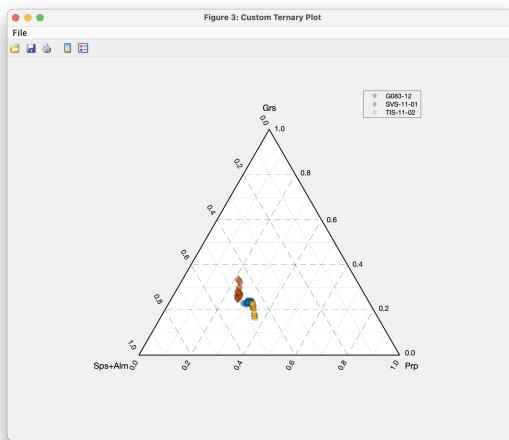
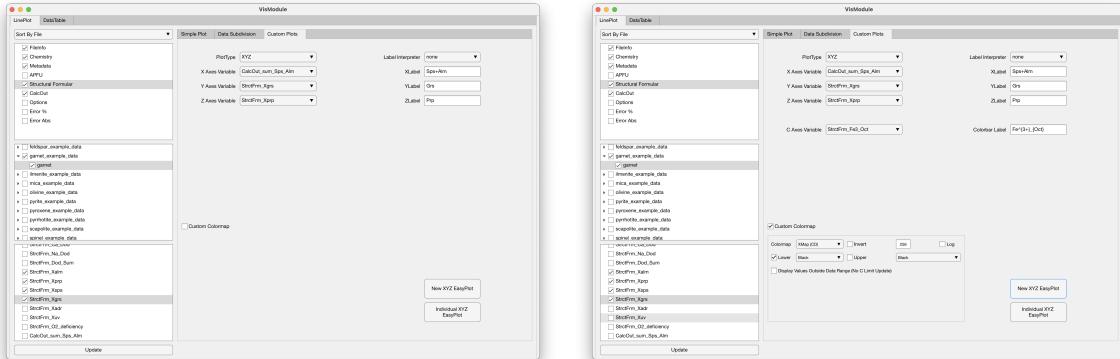
3.8.4 Data Visualization

There are several ways to generate plots in the VisModule. These are presented in the following with increasing complexity and customisation.

3.8.4.1 Simple XY Plots Simple XY Plots are intended to be used to visualise profiles or ratios of different columns of data. The default X-axis variable is 1:n (n=number of data points) and can be changed in the drop-down menu above the plot. The default visualisation offers two different types of plots which either plot all selected Y-variables (lower left tree menu) in a single plot or generate individual plots for each selected Y-variable. A more complex plot type is only enabled when the data is subdivided by a unique string (see Data Subdivision), where the data set is subdivided by another variable in the table and each subdivision is visualised in an individual plot. The plot types can be changed in the top left drop-down menu.



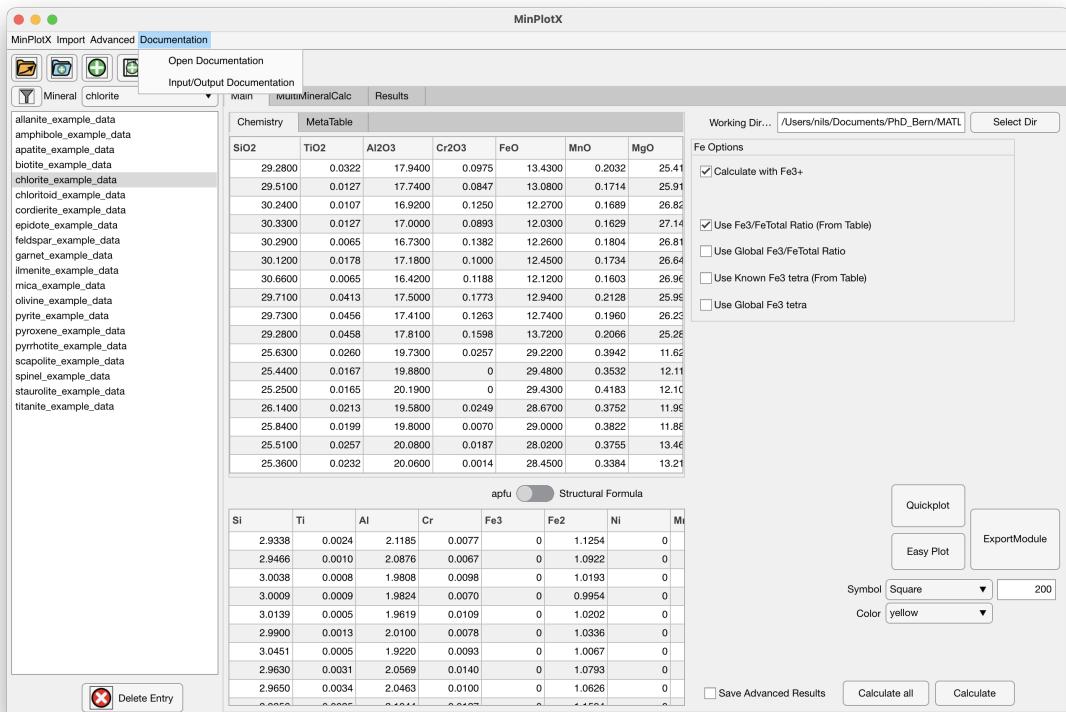
3.8.4.2 Custom Plots To provide full flexibility in plotting different variables, we have created the Custom Plots section. Here it is possible to select any numerical variables for different axes and create XY, XYZ, Ternary and Tetrahedron plots. These plots can be further extended by adding a colour map to the symbols using an additional variable. Custom plots can be used in combination with the EasyPlot module and allow further customisation of e.g. symbol appearance or legend entries.



Note: Custom ratios or other calculation results can be calculated with the CalculatorModule and also used in Custom Plots.

3.9 Additional Documentation and Information

You can find additional documentation about the required input and output for each mineral in the top menu (18) > Documentation > Input/Output Documentation. A detailed Documentation about all mineral calculation functions can be accessed in the top menu (18) > Documentation > Open Documentation.



3.10 AdvancedPlotModule

The AdvancedPlotModule is our most complex but most powerful data visualisation module. It is intended to be used to create customised mineral specific graphs as well as to explore a data set using scatterplot matrices. These allow any selected variables to be plotted against each other to explore the correlation of different variables. The workflow follows a specific/streamlined workflow and is structured to follow the tabs from left to right.

To use the AdvancedPlotModule, the user first creates a custom data table, which can be filtered by any variable present in the table, allowing a specific data table to be created to investigate a specific problem. The next step is to select the column that will be used to divide the data into sub-groups. These groups can be saved as a plot group and customised (icon, colour, transparency, etc.). It is possible to store multiple subgroups from different filtered datasets, allowing different filtering approaches to be combined in a single plot. Further customization of mineral specific diagrams is possible in the EasyPlotModule.

Note: The code to handle the complex multi-layer data structure of this module is a modification of the GeoCPlot module of the SpecXY software. The modified version has not been fully tested and bugs may occur. It is anticipated that the code and workflow will undergo modification to enhance the usability of the AdvancedPlotModule. Therefore, a comprehensive documentation guide of the AdvancedPlotModule will be compiled in the future as an additional document.

4 Problem Report

MinPlotX was developed by a small, dedicated team of two geoscientists without special training in software development as a side project within a relatively short time frame. Despite our best efforts to test all features and implement routines to prevent errors, as with any complex software, there may still be ways in which users could potentially cause the software to malfunction. To assist with troubleshooting, MinPlotX generates a log file, accessible in the MinPot working directory and titled "MinPlotX_log.txt". Should you encounter an error while using MinPlotX please send us a description of the problem, the "MinPlotX_log.txt" log file and an example dataset so that we can work to improve the software.