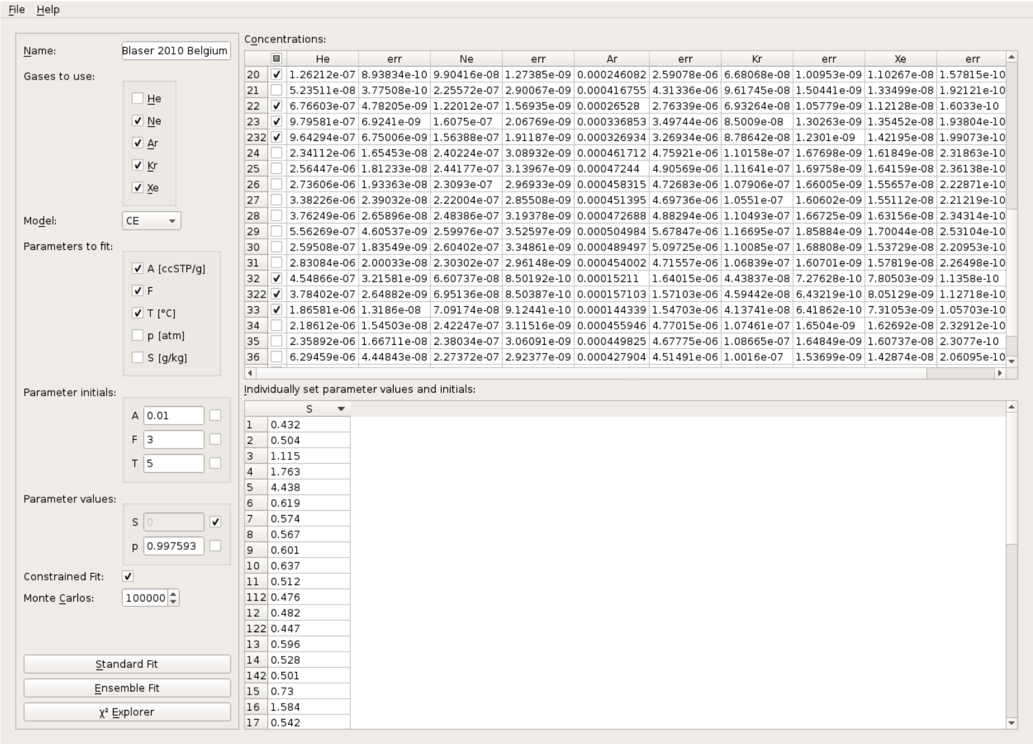
1 PANGA manual



Name: Blaser 2010 Belgium

Gases to use:

- ☐ He
- ☑ Ne
- ☑ Ar
- ☑ Kr
- ☑ Xe

Model: CE

Parameters to fit:

- ☑ A [ccSTP/g]
- ☑ F
- ☑ T [°C]
- ☐ p [atm]
- ☐ S [g/kg]

Parameter initials:

A 0.01 ☐
F 3 ☐
T 5 ☐

Parameter values:

S 0 ☑
p 0.997593 ☐

Constrained Fit: ☑
Monte Carlos: 100000

Concentrations:

	▣	He	err	Ne	err	Ar	err	Kr	err	Xe	err
20	☑	1.26212e-07	8.93834e-10	9.90416e-08	1.27385e-09	0.000246082	2.59078e-06	6.68068e-08	1.00953e-09	1.10267e-08	1.57815e-10
21	☐	5.23511e-08	3.77508e-10	2.25572e-07	2.90067e-09	0.000416755	4.31336e-06	9.61745e-08	1.50441e-09	1.33499e-08	1.92121e-10
22	☑	6.76603e-07	4.78205e-09	1.22012e-07	1.56935e-09	0.00026528	2.76339e-06	6.93264e-08	1.05779e-09	1.12128e-08	1.6033e-10
23	☑	9.79581e-07	6.9241e-09	1.6075e-07	2.06769e-09	0.000336853	3.49744e-06	8.5009e-08	1.30263e-09	1.35452e-08	1.93804e-10
232	☑	9.64294e-07	6.75006e-09	1.56388e-07	1.91187e-09	0.000326934	3.26934e-06	8.78642e-08	1.2301e-09	1.42195e-08	1.99073e-10
24	☐	2.34112e-06	1.65453e-08	2.40224e-07	3.08932e-09	0.000461712	4.75921e-06	1.10158e-07	1.67698e-09	1.61849e-08	2.31863e-10
25	☐	2.56447e-06	1.81233e-08	2.44177e-07	3.13967e-09	0.00047244	4.90569e-06	1.11641e-07	1.69758e-09	1.64159e-08	2.36138e-10
26	☐	2.73606e-06	1.93363e-08	2.3093e-07	2.96933e-09	0.000458315	4.72683e-06	1.07906e-07	1.66005e-09	1.55657e-08	2.22871e-10
27	☐	3.38226e-06	2.39032e-08	2.22004e-07	2.85508e-09	0.000451395	4.69736e-06	1.0551e-07	1.60602e-09	1.55112e-08	2.21219e-10
28	☐	3.76249e-06	2.65896e-08	2.48386e-07	3.19378e-09	0.000472688	4.88294e-06	1.10493e-07	1.66725e-09	1.63156e-08	2.34314e-10
29	☐	5.56269e-07	4.60537e-09	2.59976e-07	3.52597e-09	0.000504984	5.67847e-06	1.16695e-07	1.85884e-09	1.70044e-08	2.53104e-10
30	☐	2.59508e-07	1.83549e-09	2.60402e-07	3.34861e-09	0.000489497	5.09725e-06	1.10085e-07	1.68808e-09	1.53729e-08	2.20953e-10
31	☐	2.83084e-06	2.00033e-08	2.30302e-07	2.96148e-09	0.000454002	4.71557e-06	1.06839e-07	1.60701e-09	1.57819e-08	2.26498e-10
32	☑	4.54866e-07	3.21581e-09	6.60737e-08	8.50192e-10	0.00015211	1.64015e-06	4.43837e-08	7.27628e-10	7.80503e-09	1.1358e-10
322	☑	3.78402e-07	2.64882e-09	6.95136e-08	8.50387e-10	0.000157103	1.57103e-06	4.59442e-08	6.43219e-10	8.05129e-09	1.12718e-10
33	☑	1.86581e-06	1.3186e-08	7.09174e-08	9.12441e-10	0.000144339	1.54703e-06	4.13741e-08	6.41862e-10	7.31053e-09	1.05703e-10
34	☐	2.18612e-06	1.54503e-08	2.42247e-07	3.11516e-09	0.000455946	4.77015e-06	1.07461e-07	1.6504e-09	1.62692e-08	2.32912e-10
35	☐	2.35892e-06	1.66711e-08	2.38034e-07	3.06091e-09	0.000449825	4.67775e-06	1.08665e-07	1.64849e-09	1.60737e-08	2.3077e-10
36	☐	6.29459e-06	4.44843e-08	2.27372e-07	2.92377e-09	0.000427904	4.51491e-06	1.0016e-07	1.53699e-09	1.42874e-08	2.06095e-10

Individually set parameter values and initials:

	S
1	0.432
2	0.504
3	1.115
4	1.763
5	4.438
6	0.619
7	0.574
8	0.567
9	0.601
10	0.637
11	0.512
112	0.476
12	0.482
122	0.447
13	0.596
14	0.528
142	0.501
15	0.73
16	1.584
17	0.542

Figure 1.1: *PANGA* main window

1.1 Loading data

Noble gas concentrations can be loaded from a file or imported from the clipboard using the respective entries in the file menu or the shortcuts `Ctrl+L` / `Ctrl+V`. The file or clipboard contents must meet the following specifications:

- The data need to be arranged in eleven columns: sample name, He, He error, Ne, Ne error, Ar, Ar error, Kr, Kr error, Xe and Xe error.
- Noble gas concentrations and their errors need to be given in cm^3 STP/g.
- The columns need to be separated by either comma or tab.

- The decimal mark must be a dot. Other decimal mark system settings will be ignored.
- If no concentrations are available for some gases, their fields may also be left empty.

Lines not fulfilling the above conditions will be ignored. Just using copy and paste from a spreadsheet program should generally work.

1.2 Setting up the fit

On the left side of the main window, the fit can be configured:

Gases to use Here, the individual noble gases can be added to or removed from the fit. If a noble gas is selected here, but no concentrations are given, the gas will not be fitted for that sample.

Model The excess air model to fit to the data.

Parameters to fit The model parameters to be fitted need to be selected here.

Parameter initials Here, the initial parameter guess for the fitter can be configured. To set different initial values for each sample, check the checkbox on the right side of the parameter.

Parameter values Fixed values for the model parameters not to be fitted. To set different parameter values for each sample, check the checkbox on the right side of the parameter.

Constrained Fit If this checkbox is checked, the range of possible values for the fit parameters will be constrained. In the CE model the constraints are: $A \geqslant 0$ and $F \geqslant 0$. In the OD model the contraints restrict P_{OD} to $1 \leqslant P_{OD} \leqslant 1.26$.

Monte Carlos The number of Monte Carlo fits to be carried out for each sample.

The table on the bottom can be used to assign each sample individual values for certain model parameters or individual initial guesses for certain fit parameters. First, the parameters need to be selected under *parameter initials* or *parameter values*. A column will be added to the table for each selected parameter. By clicking on the head line cell of a column, it is possible to set the parameter this column is used for. The values may be filled in using copy and paste from, e.g., a spreadsheet software.

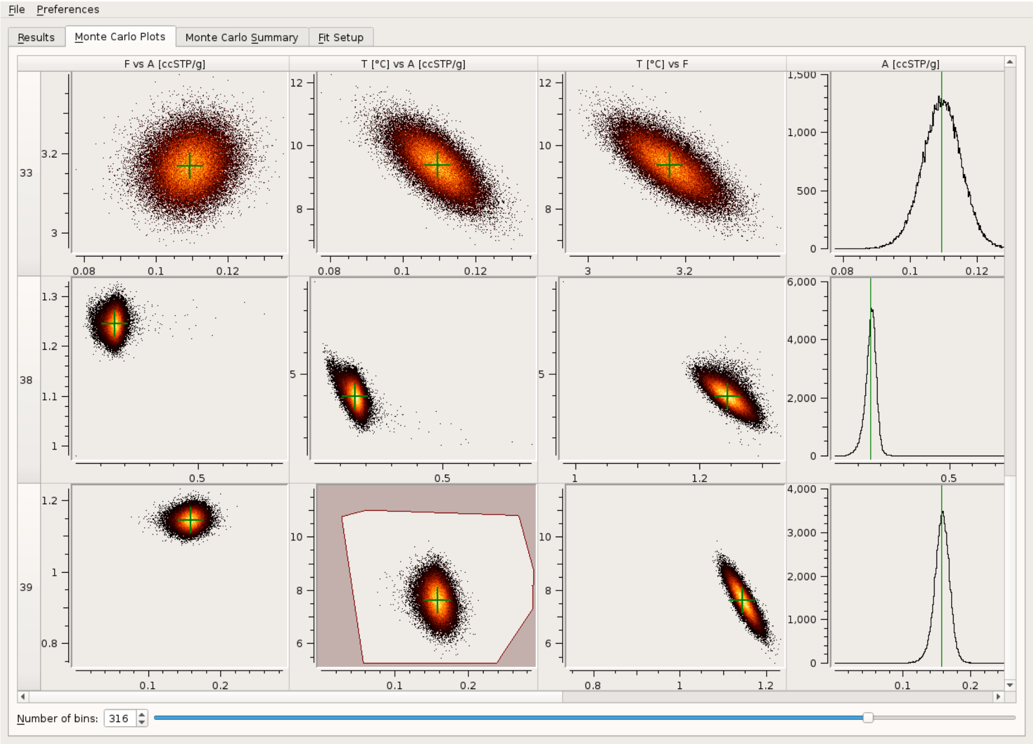
After the fit has been set up, one can choose between two different fitting modes and the χ^2 explorer:

Standard Fit Each sample is fitted separately.

Ensemble Fit All samples are combined in a single fit. In this mode each fit parameter can either be varied independently for each sample or it can be fitted to the ensemble of samples, i.e., it has the same value for every sample.

χ^2 Explorer In this mode the χ^2 surface of the fit can be analyzed interactively.

1.3 Evaluation of the fit results



Number of bins: 316

Figure 1.2: Overview of the Monte Carlo results

When the fit has finished, a new window will pop up containing the fit results. The *Results* tab contains the complete fit output for all samples.

For the CE model, *PANGA* gives hints as to when an additional Monte Carlo analysis is recommended: If any result is outside of the normal range, the respective value is shown in red and the whole sample is marked in yellow.

1.3.1 Monte Carlo analysis

The *Monte Carlo Plots* tab contains an overview of the Monte Carlo histograms of the different samples. By default, the following plots are shown: two-dimensional histograms of all possible pairs of fit parameters and one-dimensional plots of all fit parameters. The green crosses and vertical lines mark the position of the original fit results. The number of histogram bins can be set globally using the slider on the bottom of the window.

The plot window

A double click on a plot will open the plot window. Here, the plot may be zoomed, selections are made and masks are set.

The plot can be zoomed by drawing a rectangle around the desired area using the left mouse button. With a right click you can zoom out again. When the shift button is pressed, a selection is made instead. In a one-dimensional plot an interval of values is selected. In a two-dimensional plot a polygon can be selected using several clicks of the left mouse button. The polygon will be completed if the right mouse button is used. The selected area will then be highlighted. Note, that the red-shaded region indicates the areas that are not selected. With the buttons on the right side, the selection can be modified as well as applied to the sample's mask.

With the slider on the bottom, the bin number of the histogram can be changed individually for this plot.

Using masks

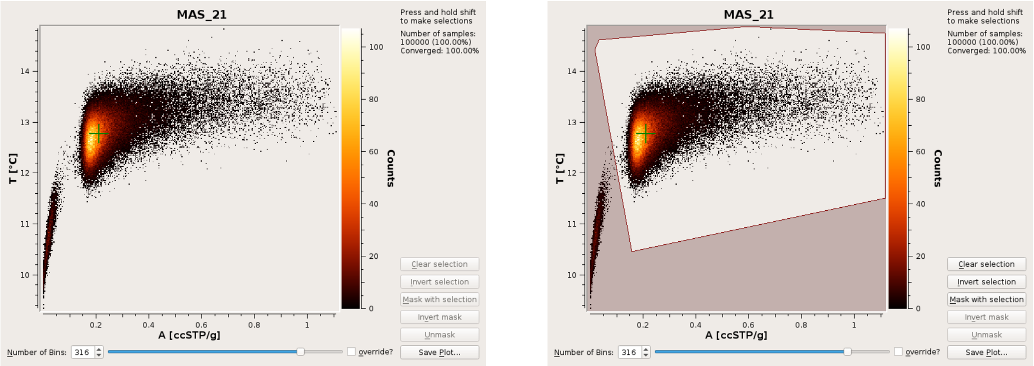
A mask is used to switch on or off specific Monte Carlo realizations for the statistical evaluation. Its use is illustrated in figure 1.3. Masks are modified using selections in the plot window: the selection needs to be done so that the Monte Carlo realizations to be removed are in the red-shaded area. After a click on *Mask with selection*, only the Monte Carlo realizations in the selected area (not shaded in red) will remain activated. This process may be repeated to combine several selections in one mask. Note that a mask always affects the whole sample, not only the plot in which it is created.

Monte Carlo results

On the right side of the plot window, the results of the statistical analysis are displayed. For 1D plots this analysis consists of mean value and standard deviation of the respective parameter. 2D plots show mean values and standard deviations of both parameters as well as their correlation coefficient. The statistical analysis is restricted to the Monte Carlo realizations not disabled via the mask. The Monte Carlo results of all samples are summarized in a table under the tab *Monte Carlo Summary.*

Add other plots or parameters

By default, *PANGA* shows plots and carries out a statistical analysis for all fit parameters. Two-dimensional plots are created for all possible pairs of fit parameters. If needed, additional plots can be created via *Preferences* ⟶ *Choose Monte Carlo Plots.* A window will show up, which contains a list of all available parameters and the list of the currently shown ones. Parameters can be added to right light list by dragging them from the left-side and dropping them at the end of the list or between two existing entries. If the parameter is dropped on an existing list entry, both entries will be combined for a two-dimensional plot. Entries can be removed by dragging them from the right list and dropping them on the left one.



Press and hold shift
to make selections

Number of samples:
100000 (100.00%)
Converged: 100.00%

Number of Bins: 316

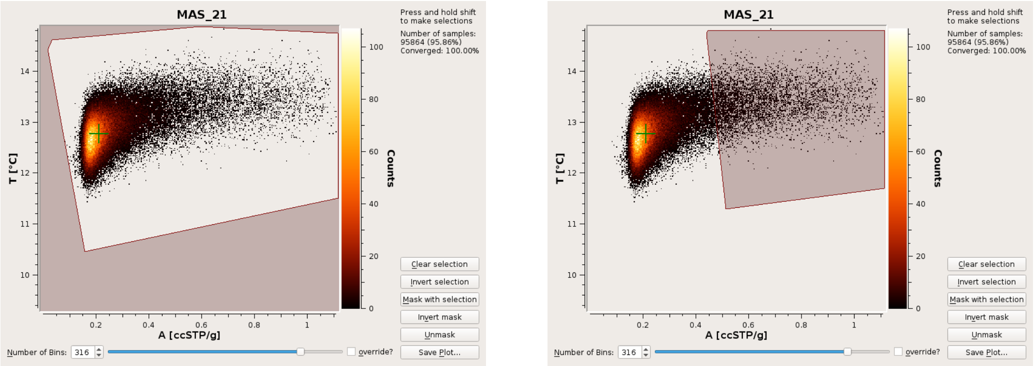
Press and hold shift
to make selections

Number of samples:
100000 (100.00%)
Converged: 100.00%

Number of Bins: 316

(a) No selection

(b) First selection, not yet applied to the mask



Press and hold shift
to make selections

Number of samples:
95864 (95.86%)
Converged: 100.00%

Number of Bins: 316

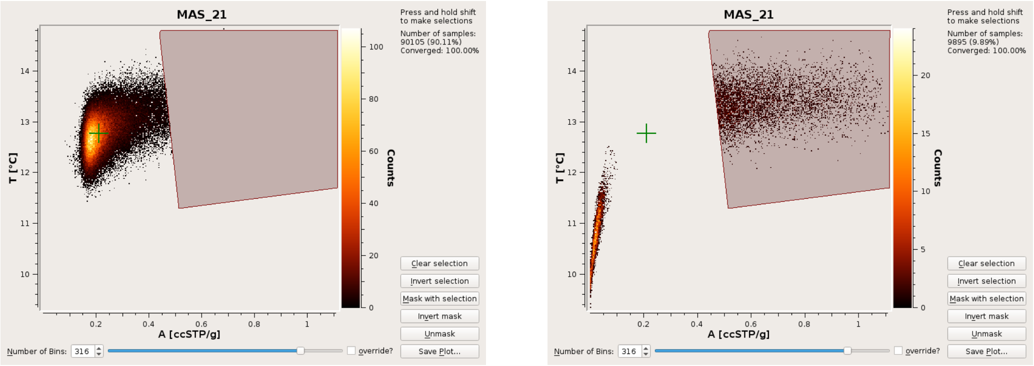
Press and hold shift
to make selections

Number of samples:
95864 (95.86%)
Converged: 100.00%

Number of Bins: 316

(c) First selection, applied to the mask

(d) Second (inverted) selection, not yet applied to the mask



Press and hold shift
to make selections

Number of samples:
90105 (90.11%)
Converged: 100.00%

Number of Bins: 316

Press and hold shift
to make selections

Number of samples:
9895 (9.89%)
Converged: 100.00%

Number of Bins: 316

(e) Second selection applied to the mask

(f) Mask inverted

Figure 1.3: Illustration of masks in *PANGA*. Note that this illustration does not represent a real evaluation. It is only meant to demonstrate the masking feature.

1.3.2 Saving and loading results

The results of a fit, including Monte Carlo results, selections, masks, etc., can be saved to a file using *File* ⟶ *Save*. There are two different file types available: binary files and portable files. The binary files can be saved and loaded much faster than the portable files. They are, however, not portable, which means that, e.g., a file saved in the 32-bit Windows version cannot be read with the 64-bit Windows version. Also, the files saved under another operating system cannot be opened. So if cross-architecture or cross-platform compatibility is required, the slower portable format should be used. Saved files can be opened with *File* ⟶ *Open results*.

The settings of fits from a saved file (and also of a new fit) can be seen under the *Fit Setup* tab in the results window. If needed, they can be loaded back into the main window by clicking *Load into Main Window*.

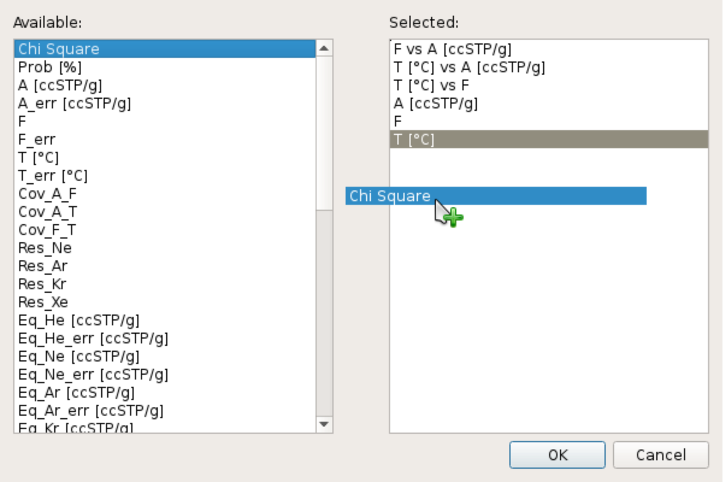
If the simple statistical evaluation carried out by *PANGA* is not sufficient, the Monte Carlo results can be exported to a text file, from where they may be processed with other software. The export can be done by choosing *Export Monte Carlo Data* from the *File* window. The file will be in the *csv* format and will contain, for every Monte Carlo realization, all of the columns shown under the *Results* tab. Only the Monte Carlo realizations which are enabled by the sample's mask will be exported.

1.4 The χ^2 explorer

The plot in the χ^2 explorer shows χ^2 as a function of two model parameters. The plot is configured in the table on the right side of the window. It contains options for all the parameters chosen to be fit parameters in the main window. The columns *X* and *Y* are used to set the parameters which are currently displayed on the plot's axes. Their *min* and *max* values determine the range of the axes. The remaining parameters may either be set to fixed values or included in the fit. This is determined by the *fit?* column. If a model parameter is not fitted, a slider will appear, which can be used to set its value. Alternatively, it can also be set in the table. The *min* and *max* values of these parameters only determine the range of the their sliders.

If *auto-update* is selected, the plot will be updated whenever any setting is changed. Otherwise, updates need to be triggered manually with the *Update plot* button.

By default, the scale of the χ^2 colorbar is set to range from the minimal to the maximal value visible in the plot. It may be readjusted with the *Minimum* and *Maximum* fields.



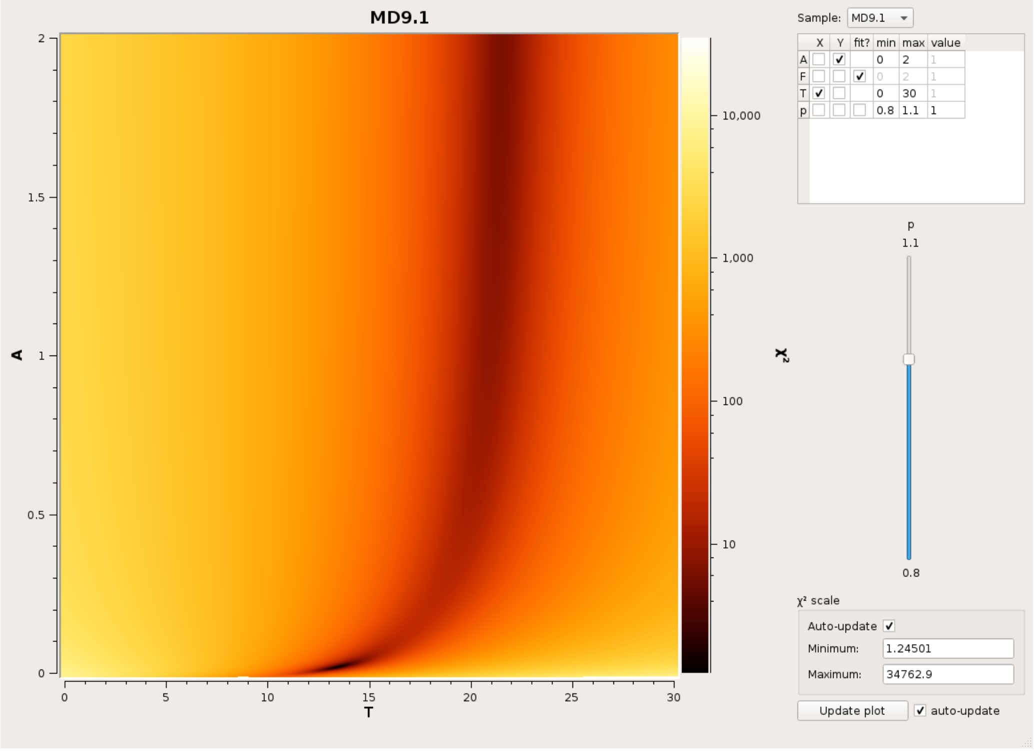
Available:

Chi Square
Prob [%]
A [ccSTP/g]
A_err [ccSTP/g]
F
F_err
T [°C]
T_err [°C]
Cov_A_F
Cov_A_T
Cov_F_T
Res_Ne
Res_Ar
Res_Kr
Res_Xe
Eq_He [ccSTP/g]
Eq_He_err [ccSTP/g]
Eq_Ne [ccSTP/g]
Eq_Ne_err [ccSTP/g]
Eq_Ar [ccSTP/g]
Eq_Ar_err [ccSTP/g]
Eq_Kr [ccSTP/g]

Selected:

F vs A [ccSTP/g]
T [°C] vs A [ccSTP/g]
T [°C] vs F
A [ccSTP/g]
F
T [°C]

Figure 1.4: Monte Carlo plots setup



Sample: MD9.1

	X	Y	fit?	min	max	value
A	☐	☑		0	2	1
F	☐	☐	☑	0	2	1
T	☑	☐		0	30	1
p	☐	☐	☐	0.8	1.1	1

Auto-update ☑
Minimum: 1.24501
Maximum: 34762.9
☑ auto-update

Figure 1.5: The χ^2 explorer