EasySpec Quick-Start Guide

27th October 2010

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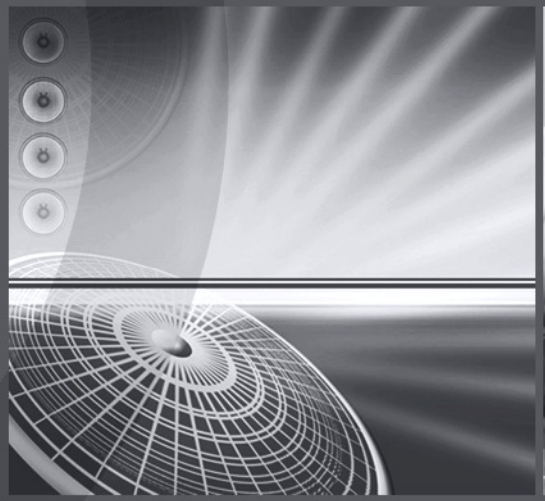


NEXT GENERATION DETECTION

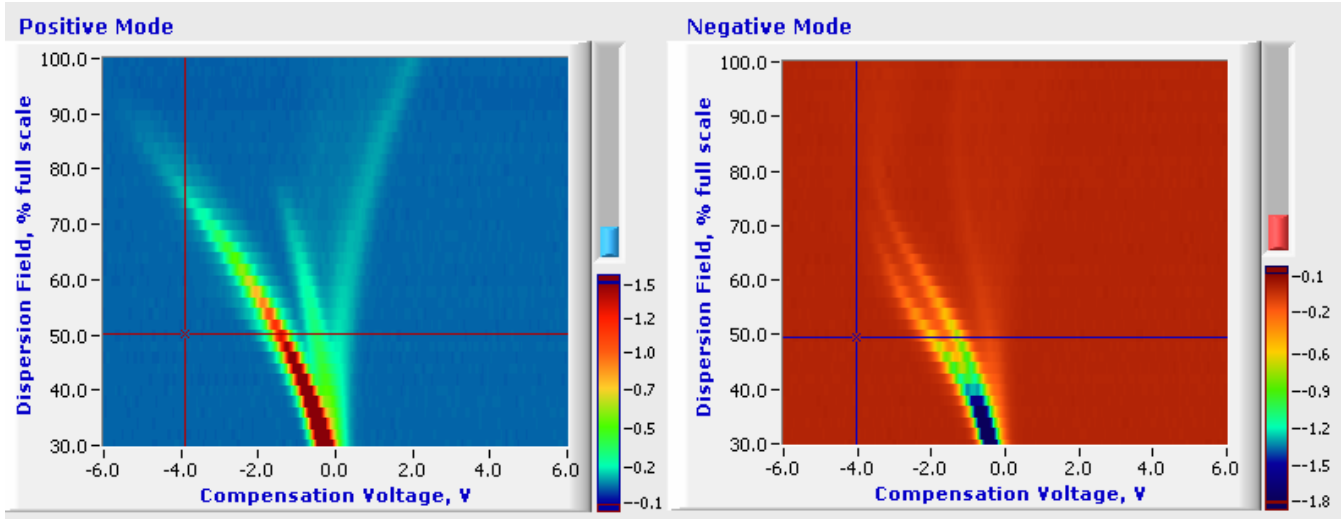
Topics covered in this guide

- **Introduction**
- **Basics of EasySpec**
- **DF Matrix Viewer**
- **Rule Builder** – making rules
- **EasyExtract** – exporting data from DF matrices
- **Application Builder** – combining rules
- **EasyCheck** – comparing data against your rules
- **Configuration Editor** – setting experimental parameters and operational limits
- **Calibration for Online Concentration Monitoring**
- **Calibration for Offline Concentration Monitoring**

Introduction

- This presentation is intended to be used as a quick-start guide to using the EasySpec suite of programs.
- The information here is correct as of EasySpec version 4.0.
- There is more detail on everything mentioned in the EasySpec Manual v3.0.

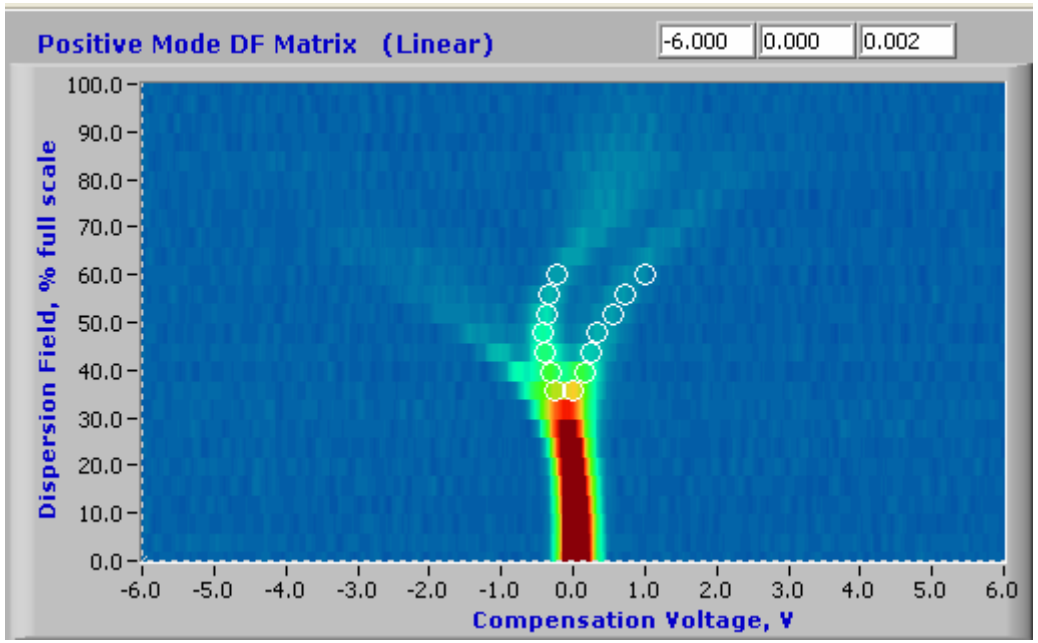
EasySpec Basics 1



- The images produced by Lonestar are called DF matrices.
- They are 3d graphs with **dispersion field (DF)** plotted against **compensation voltage (CV)** and the **ion current (AU)** at each point represented by colour.
- There are two plots in each matrix: **positive mode** looks at the positive ions present, and **negative mode** looks at the negative ions.
- DF matrices can be viewed in **DF Matrix Viewer**.

EasySpec Basics 2

- EasySpec works by creating **rules** made up of one or more **waypoints**. Each waypoint records the coordinates of a point on the 3d graph (DF, CV and AU).
- Rules can be created in **Rule Builder** to identify a peak or peaks.

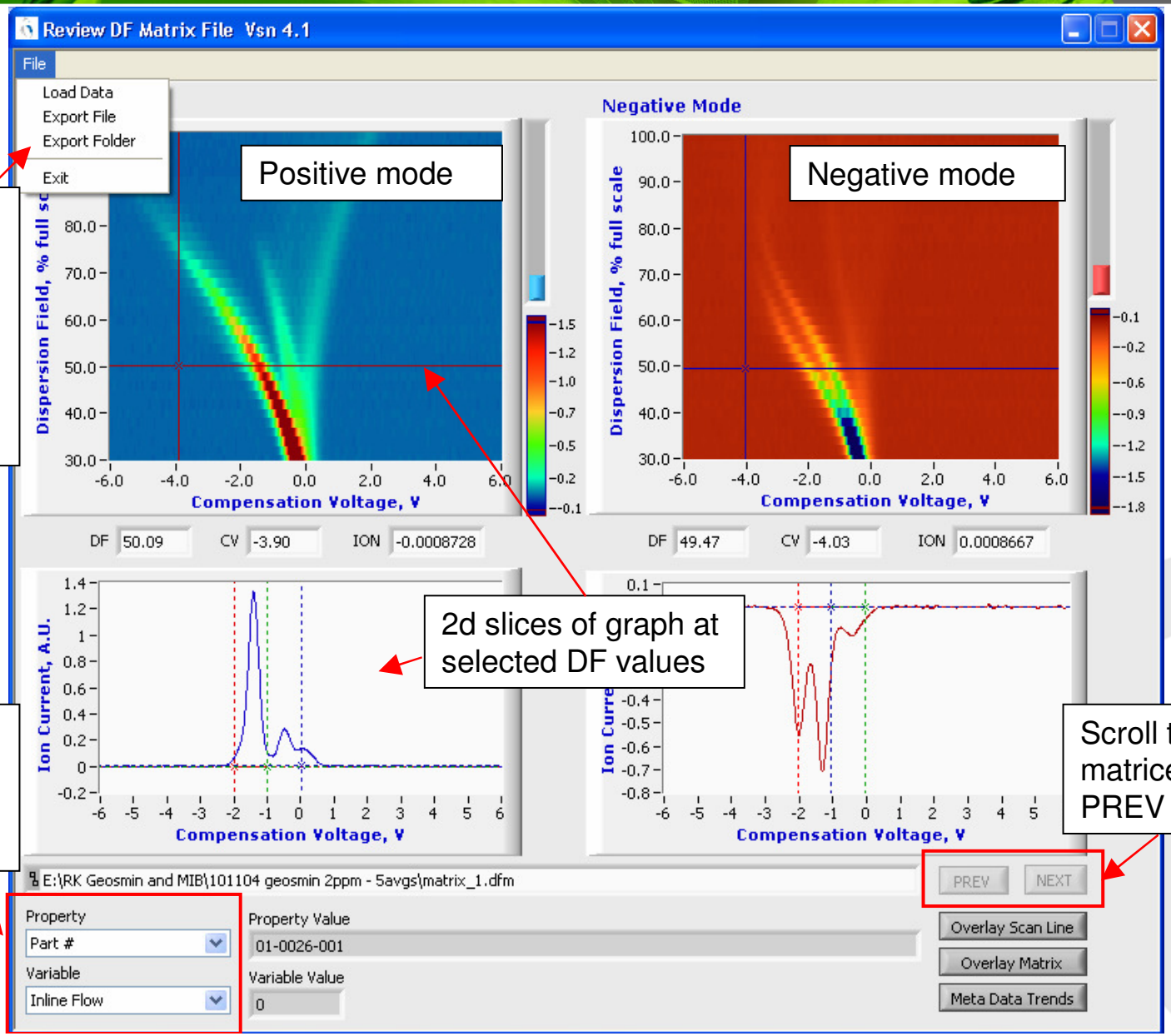


In the matrix shown here, the two peaks identify the chemical as acetone. They are traced out by waypoints.

EasySpec Basics 3

- Several rules can be brought together and added to a Lonestar configuration file, using **Application Builder**. The rule set can be adjusted to give an alarm or an OK signal for DF matrices.
- Multiple sets of data can be compared to the rule sets in configuration files, using **EasyCheck**.
- **EasyExtract**, a feature in both EasyCheck and Rule Builder, will compare a set of data to a rule and export the ion current value at each waypoint in each DF matrix.
- **Configuration Editor** allows other details of the Lonestar configuration files to be adjusted, for example which DF values to sample at when taking data. When the configuration file is loaded onto the Lonestar, these experimental parameters will automatically be set.
- If a calibration rule is added to a configuration file, **online concentration analysis** is possible.

DF Matrix Viewer

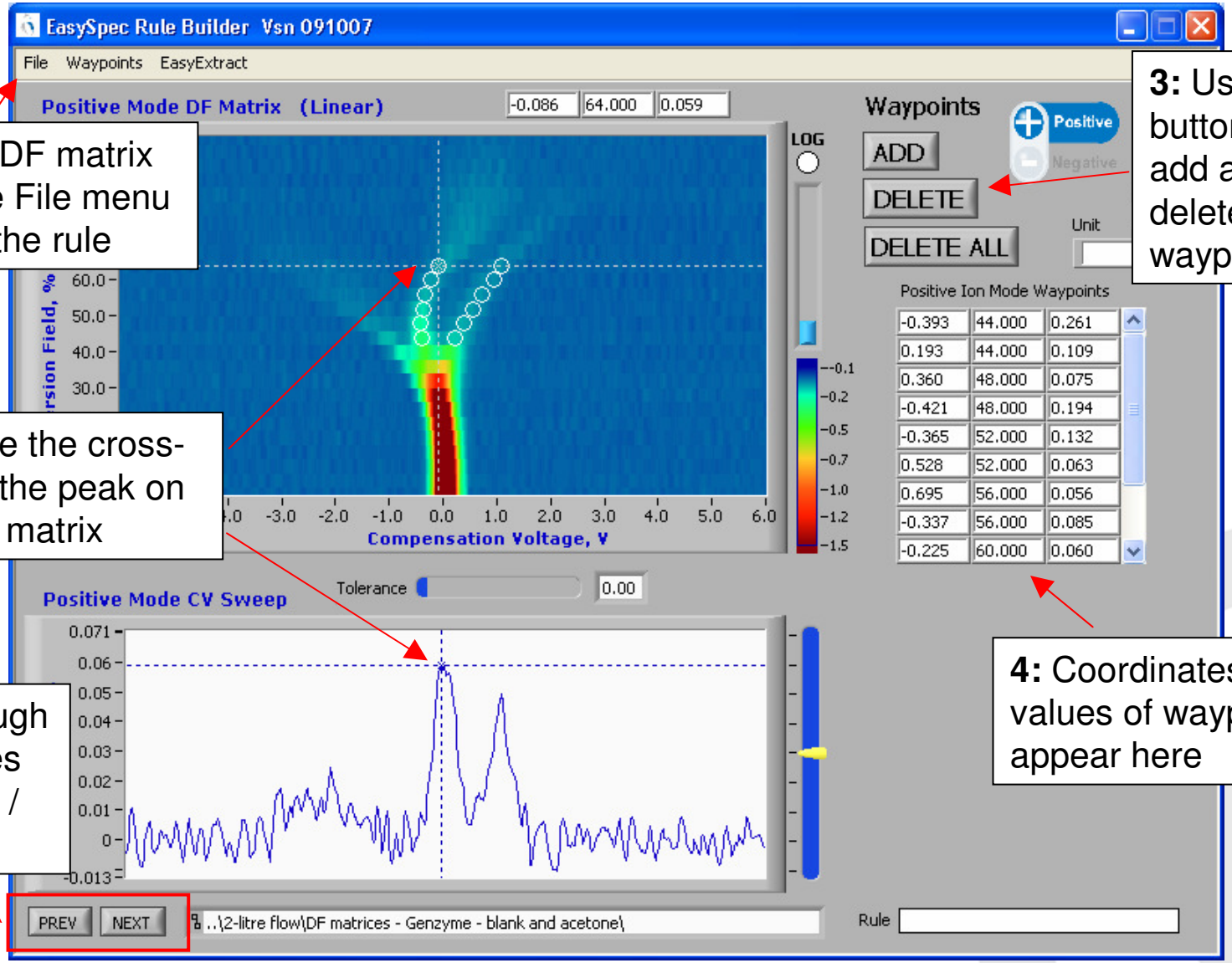


Load data from file. Export DF matrices as comma separated values (.csv) files.

View experimental variables and properties

Scroll through DF matrices with PREV / NEXT

Rule Builder 1: creating a rule



1: Open DF matrix using the File menu
5: Save the rule

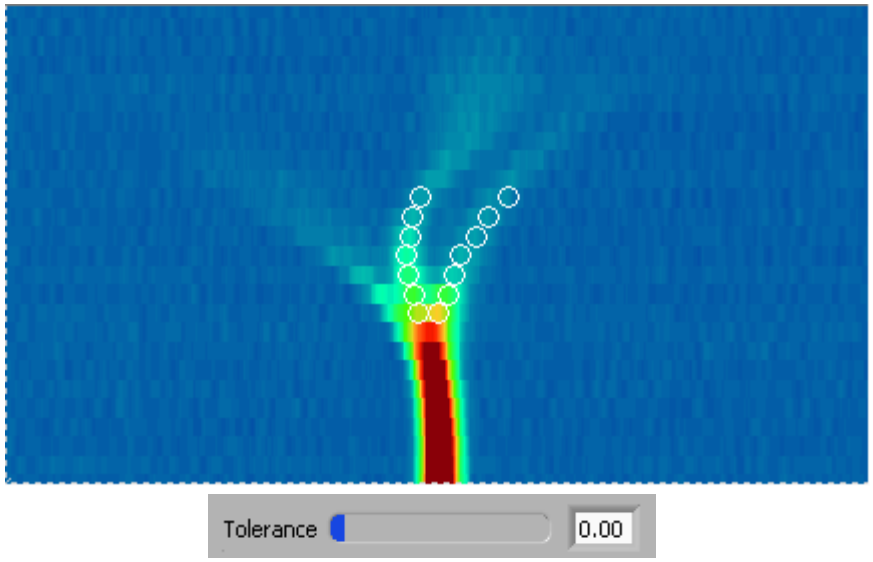
2: Move the cross-hair to the peak on the DF matrix

Scroll through DF matrices with PREV / NEXT

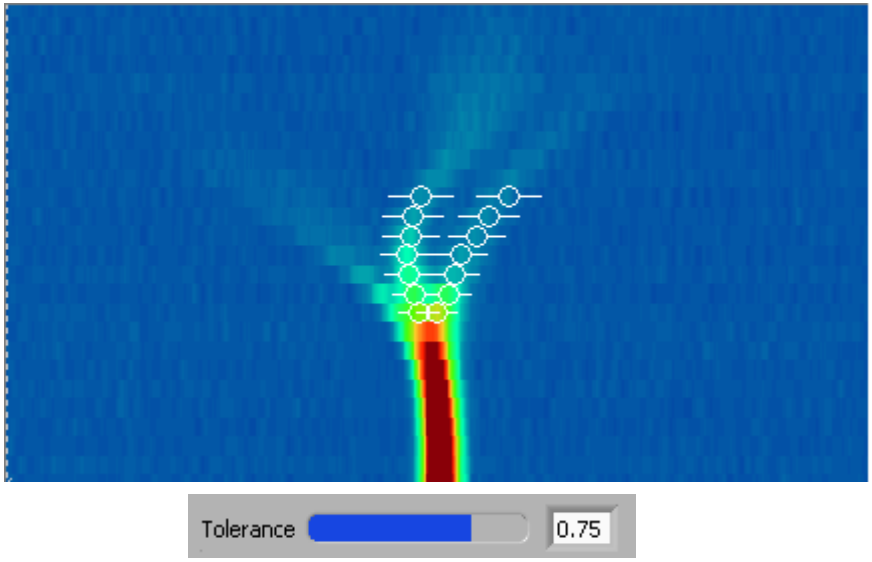
3: Use these buttons to add and delete waypoints

4: Coordinates and values of waypoints appear here

Rule Builder 2: setting tolerance



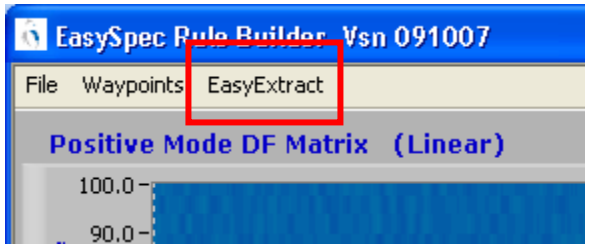
Low tolerance

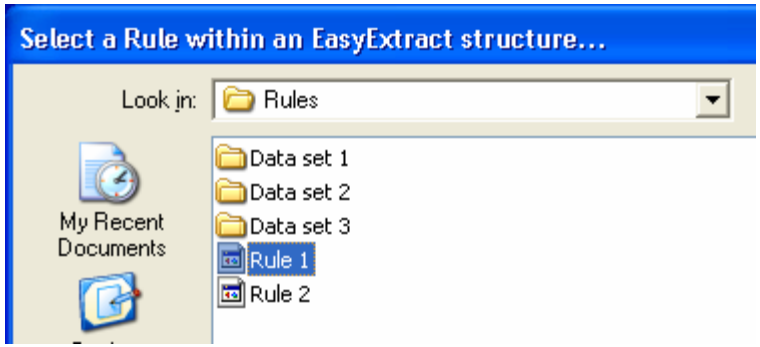


High tolerance

- Setting a tolerance in your waypoints is useful if the peaks move from side to side between scans – for example if humidity varies.
- The maximum ion current along the tolerance line is used as the peak value (**AUmax**).
- Tolerance should be set to at least 0.05.

EasyExtract

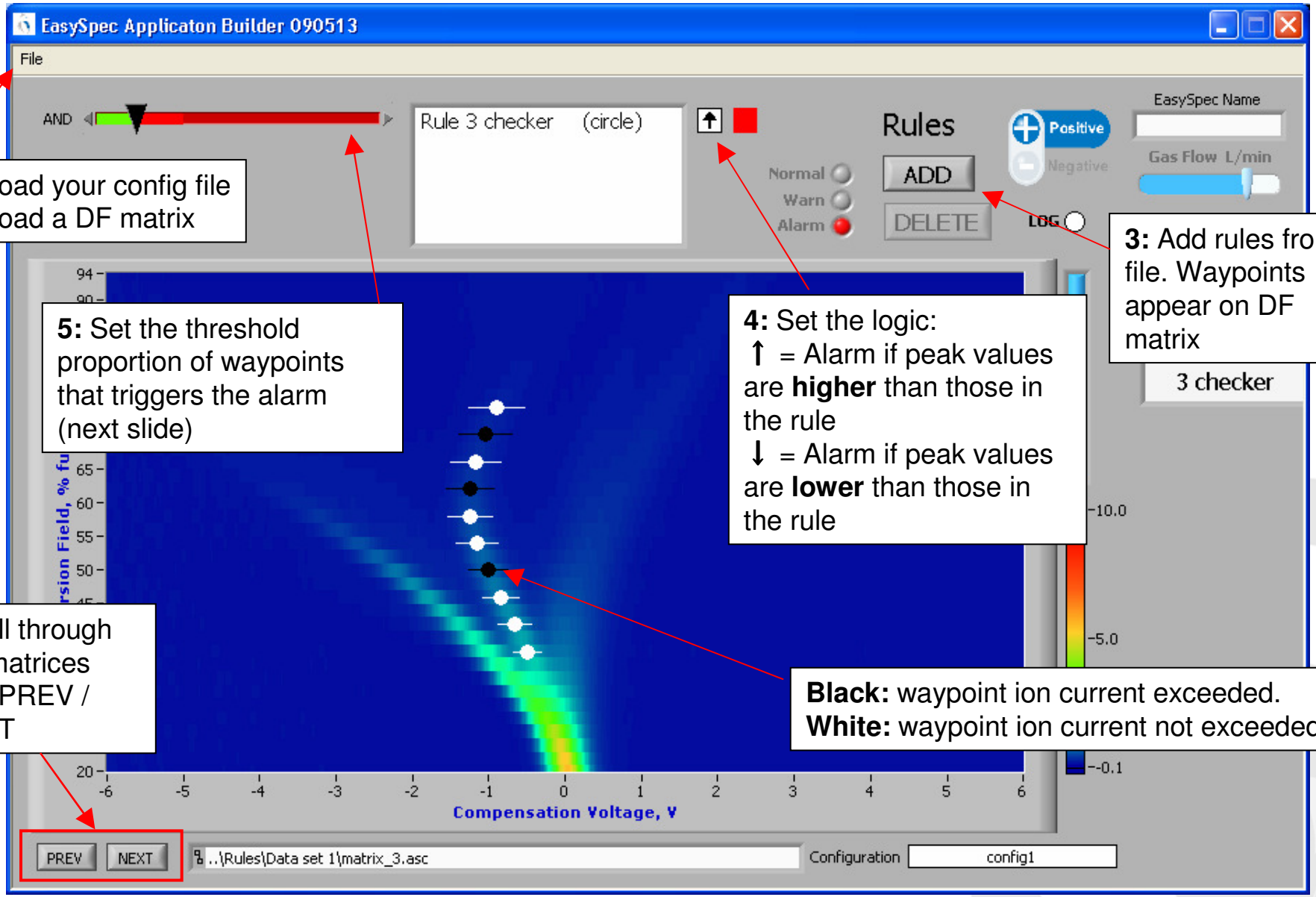




- The function EasyExtract in the programs Rule Builder and EasyCheck compares DF matrices with a rule.
- The rules and data must be saved in a specific structure, as shown.
- Results are given as a .csv file (can be opened in Excel).
- For every DF matrix, the ion current value at each waypoint in the rule is given.

	A	B	C	D	E	F	G	H	I	J	K	L
1	UTC Date	UTC Time	Folder	Filename	DF%	CV	AU	W	AUmax	CV@AUmax	FW@HM	IonMode
2												
3	22/07/2009	15:38:23	Data set 1	matrix_1.asc	72	-1.185275	0.078667	1	0.078667	-1.187698	0.65729	Pos
4	22/07/2009	15:38:23	Data set 1	matrix_1.asc	48	0.890463	0.010392	1	0.010392	0.901545	4.131537	Pos
5	22/07/2009	15:27:47	Data set 1	matrix_2.asc	72	-1.185275	0.061719	1	0.061719	-1.187698	0.65729	Pos
6	22/07/2009	15:27:47	Data set 1	matrix_2.asc	48	0.890463	0.013215	1	0.013215	0.901545	4.178486	Pos
7	22/07/2009	15:33:04	Data set 1	matrix_3.asc	72	-1.185275	0.081444	1	0.081444	-1.187698	0.610341	Pos
8	22/07/2009	15:33:04	Data set 1	matrix_3.asc	48	0.890463	0.01088	1	0.01088	0.901545	4.037639	Pos
9	22/07/2009	14:09:36	Data set 2	matrix_1.asc	72	-1.185275	-0.005076	1	-0.005076	-1.187698	0	Pos
10	22/07/2009	14:09:36	Data set 2	matrix_1.asc	48	0.890463	0.021475	1	0.021475	0.901545	3.544671	Pos
11	22/07/2009	13:59:01	Data set 2	matrix_2.asc	72	-1.185275	0.007909	1	0.007909	-1.187698	0.563391	Pos
12	22/07/2009	13:59:01	Data set 2	matrix_2.asc	48	0.890463	0.026317	1	0.026317	0.901545	3.63857	Pos

Application Builder 1: adding a rule to a configuration file



1: Load your config file
2: Load a DF matrix

3: Add rules from file. Waypoints appear on DF matrix

4: Set the logic:
↑ = Alarm if peak values are **higher** than those in the rule
↓ = Alarm if peak values are **lower** than those in the rule

5: Set the threshold proportion of waypoints that triggers the alarm (next slide)

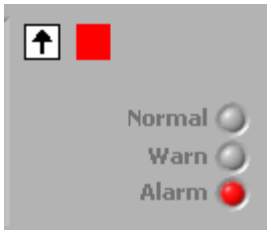
Scroll through DF matrices with PREV / NEXT

Black: waypoint ion current exceeded.
White: waypoint ion current not exceeded.

Application Builder 2: altering confidence levels

25% of waypoints must be triggered to initiate alarm

35% of waypoints have been triggered

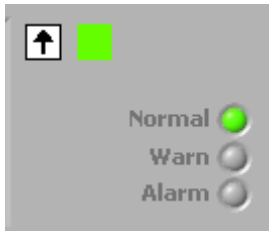


Alarm

- Low threshold: high sensitivity but can give false positives

50% of waypoints must be triggered to initiate alarm

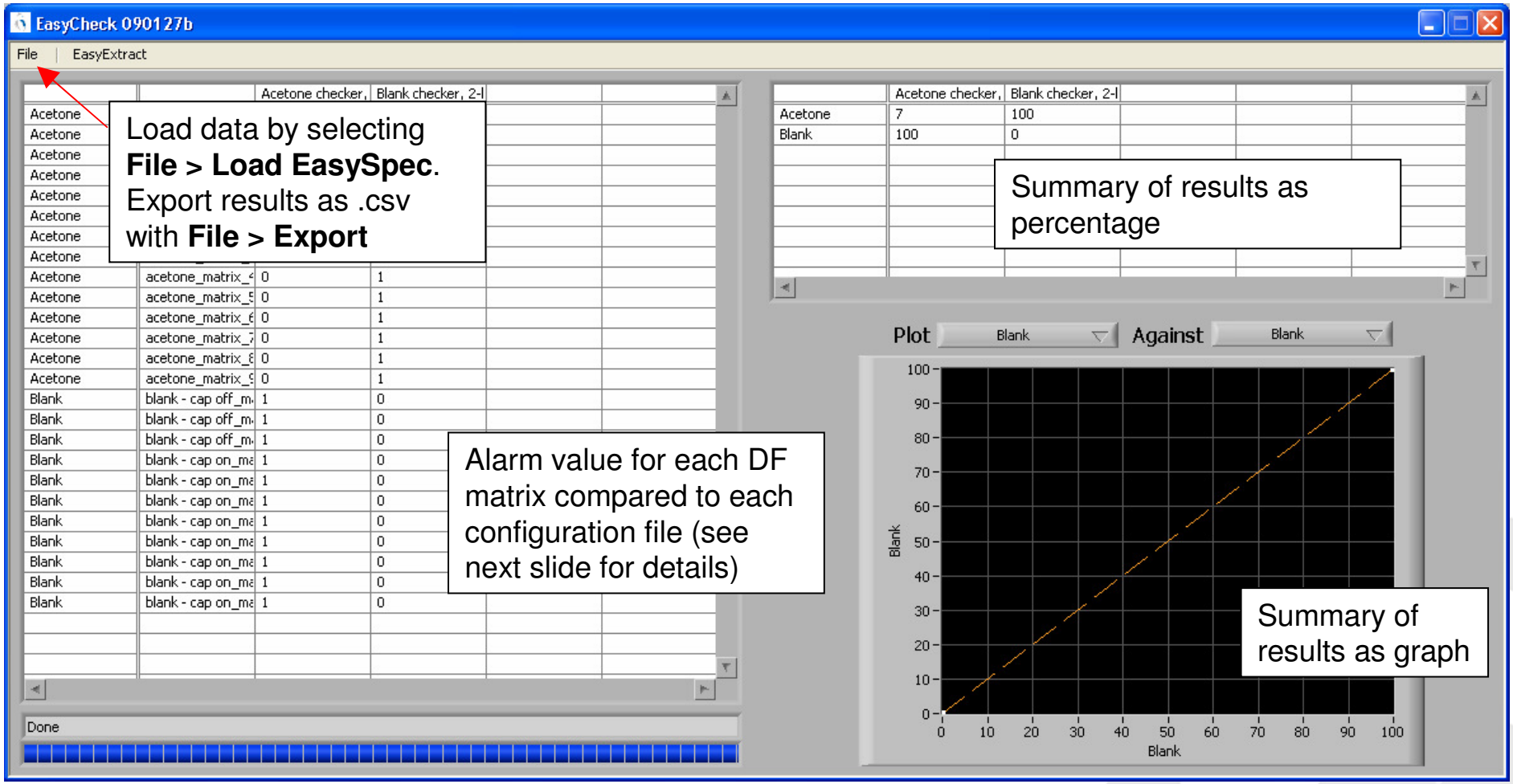
35% of waypoints have been triggered



No alarm

- High threshold: no false positives but may miss some borderline cases

Using EasyCheck 1: overview



		Acetone checker,	Blank checker, 2-I
Acetone			
Acetone			
Acetone			
Acetone			
Acetone			
Acetone			
Acetone			
Acetone			
Acetone	acetone_matrix_4	0	1
Acetone	acetone_matrix_5	0	1
Acetone	acetone_matrix_6	0	1
Acetone	acetone_matrix_7	0	1
Acetone	acetone_matrix_8	0	1
Acetone	acetone_matrix_9	0	1
Blank	blank - cap off_m	1	0
Blank	blank - cap off_m	1	0
Blank	blank - cap off_m	1	0
Blank	blank - cap on_ma	1	0
Blank	blank - cap on_ma	1	0
Blank	blank - cap on_ma	1	0
Blank	blank - cap on_ma	1	0
Blank	blank - cap on_ma	1	0
Blank	blank - cap on_ma	1	0
Blank	blank - cap on_ma	1	0
Blank	blank - cap on_ma	1	0

	Acetone checker,	Blank checker, 2-I
Acetone	7	100
Blank	100	0

Again, the configuration files and data must be saved in a specific structure, as shown. To load data, select the top-level folder (here it is EasySpec Demo).

Using EasyCheck 2: results

DF Matrices | First rule | Second rule

First data set

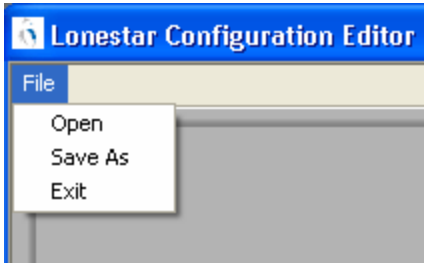
Second data set

		Acetone checker,	Blank checker, 2-l
Acetone	acetone_matrix_1	0	1
Acetone	acetone_matrix_1	0	1
Acetone	acetone_matrix_1	0	1
Acetone	acetone_matrix_1	0	1
Acetone	acetone_matrix_1	0	1
Acetone	acetone_matrix_2	1	1
Acetone	acetone_matrix_2	0	1
Acetone	acetone_matrix_3	0	1
Acetone	acetone_matrix_4	0	1
Acetone	acetone_matrix_5	0	1
Acetone	acetone_matrix_6	0	1
Acetone	acetone_matrix_7	0	1
Acetone	acetone_matrix_8	0	1
Acetone	acetone_matrix_9	0	1
Blank	blank - cap off_m	1	0
Blank	blank - cap off_m	1	0
Blank	blank - cap off_m	1	0
Blank	blank - cap on_ma	1	0
Blank	blank - cap on_ma	1	0
Blank	blank - cap on_ma	1	0
Blank	blank - cap on_ma	1	0
Blank	blank - cap on_ma	1	0
Blank	blank - cap on_ma	1	0
Blank	blank - cap on_ma	1	0

1 = Alarm.
0 = No alarm.

Configuration Editor: overview

- The Configuration Editor has controls to set most aspects of the Lonestar's running. Only the sections most relevant to the user are described here:
  - Method settings
  - Operational limits
- To open and save configuration files, use the File menu as shown.

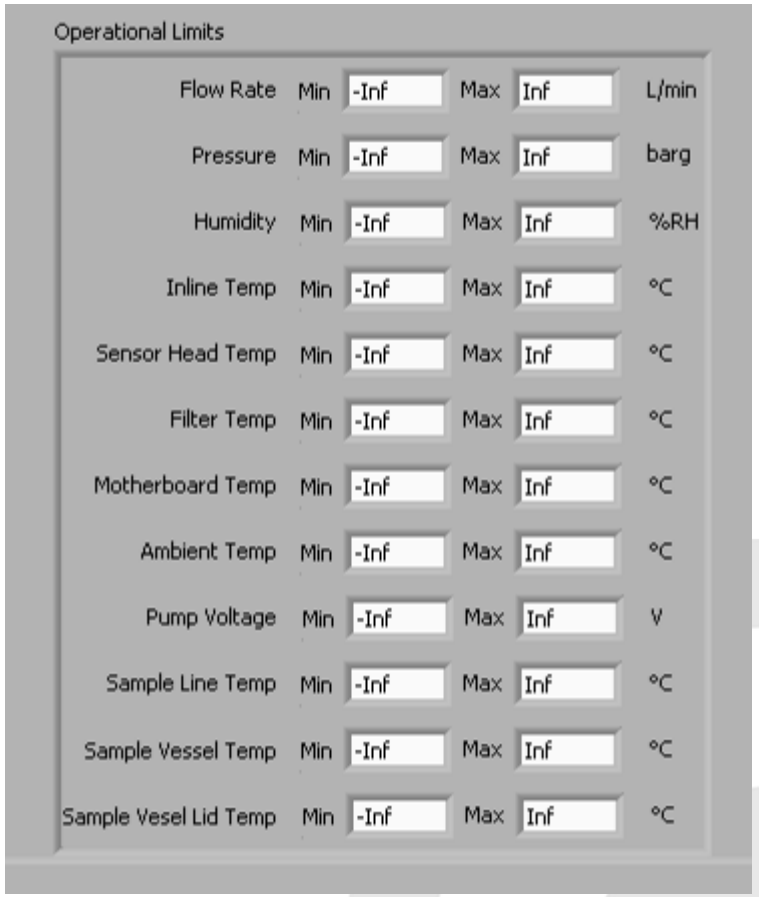


Configuration Editor: method settings

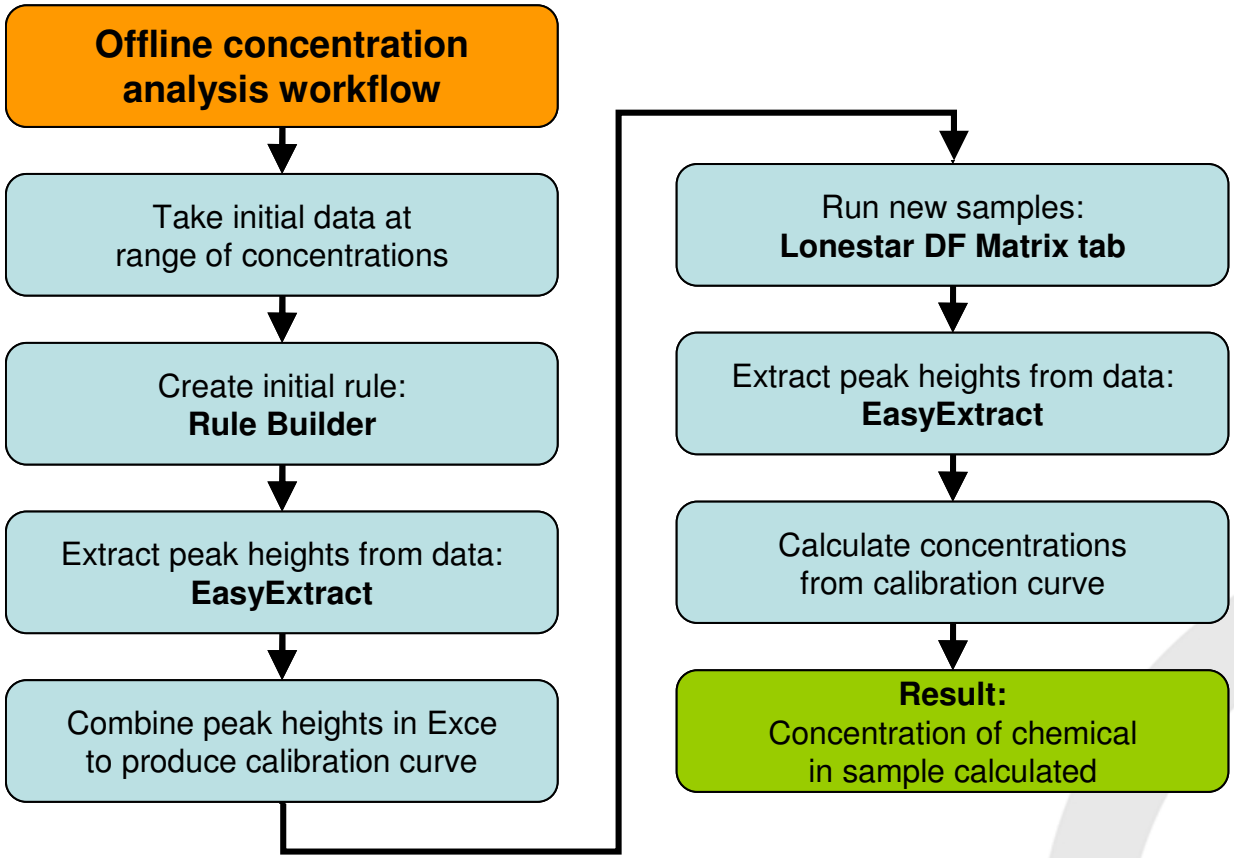
- The method settings correspond to the parameters found in the Lonestar Settings tab.
- The values in the green box should usually be set as shown.
- The values in the blue box control the dimensions of the DF matrix.
- The settings in the pink boxes control the averaging of data taken.

Configuration Editor: operational limits

- The operational limits allow good ranges of system parameters to be set.
- For example, if it is necessary that the filter temperature is between 95°C and 105°C, these values can be entered into the configuration file.
- When running the Lonestar in Analyser mode, it will report whether conditions are within the set limits. Data will not be recorded until all conditions are OK.

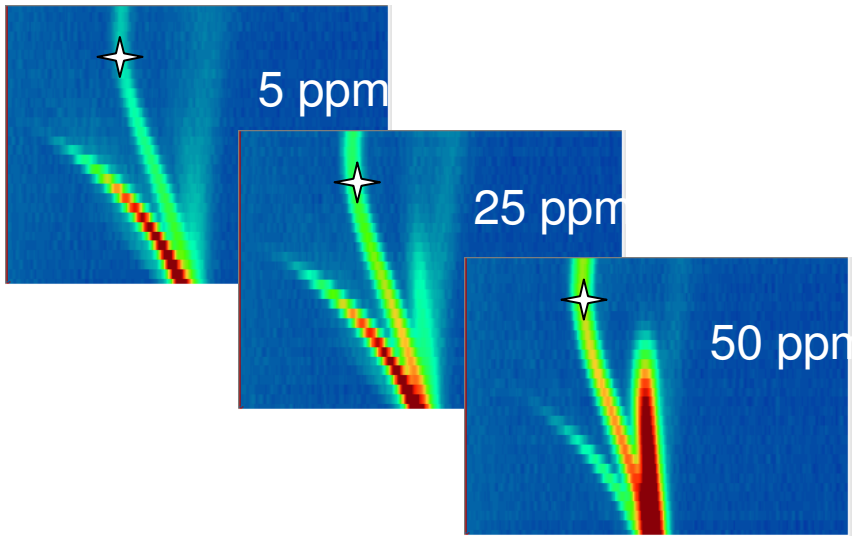


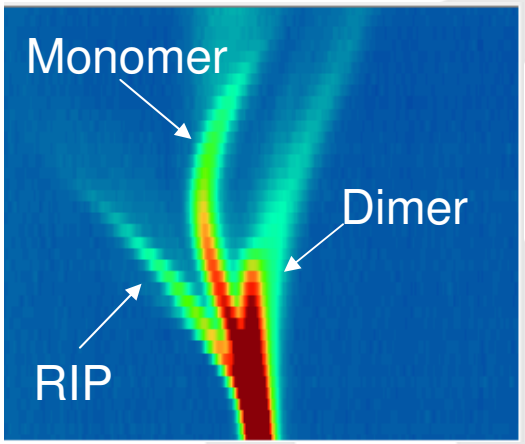
Calibration for Offline Concentration Analysis 1: workflow



Calibration for Offline Concentration Analysis 2: initial data

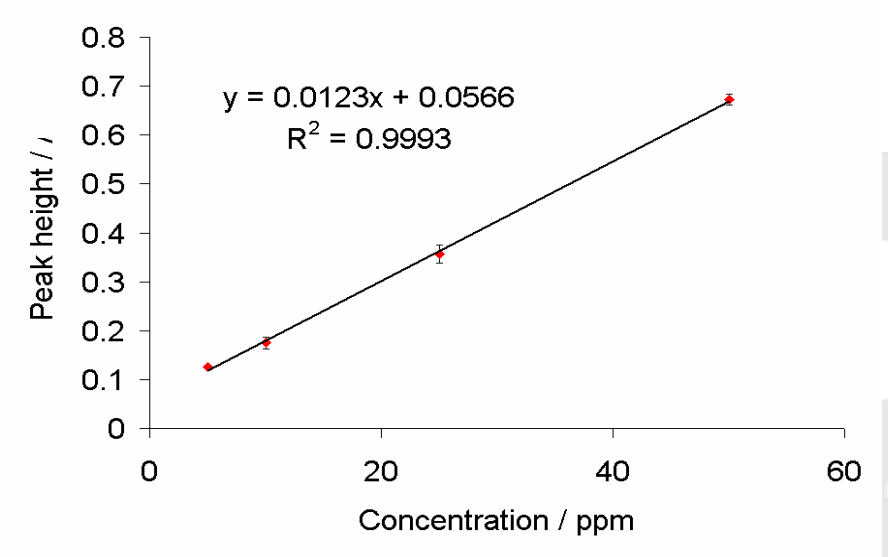
- Take data from at least 3 concentrations of the chemical in question, and at least 3 repetitions at each concentration.
- Use the monomer peak for calibration, not the dimer, and make sure the RIP is present in the DF matrices to avoid saturation.
- Create a rule with a single waypoint on the monomer peak, at a position where it is well separated from any background peaks.



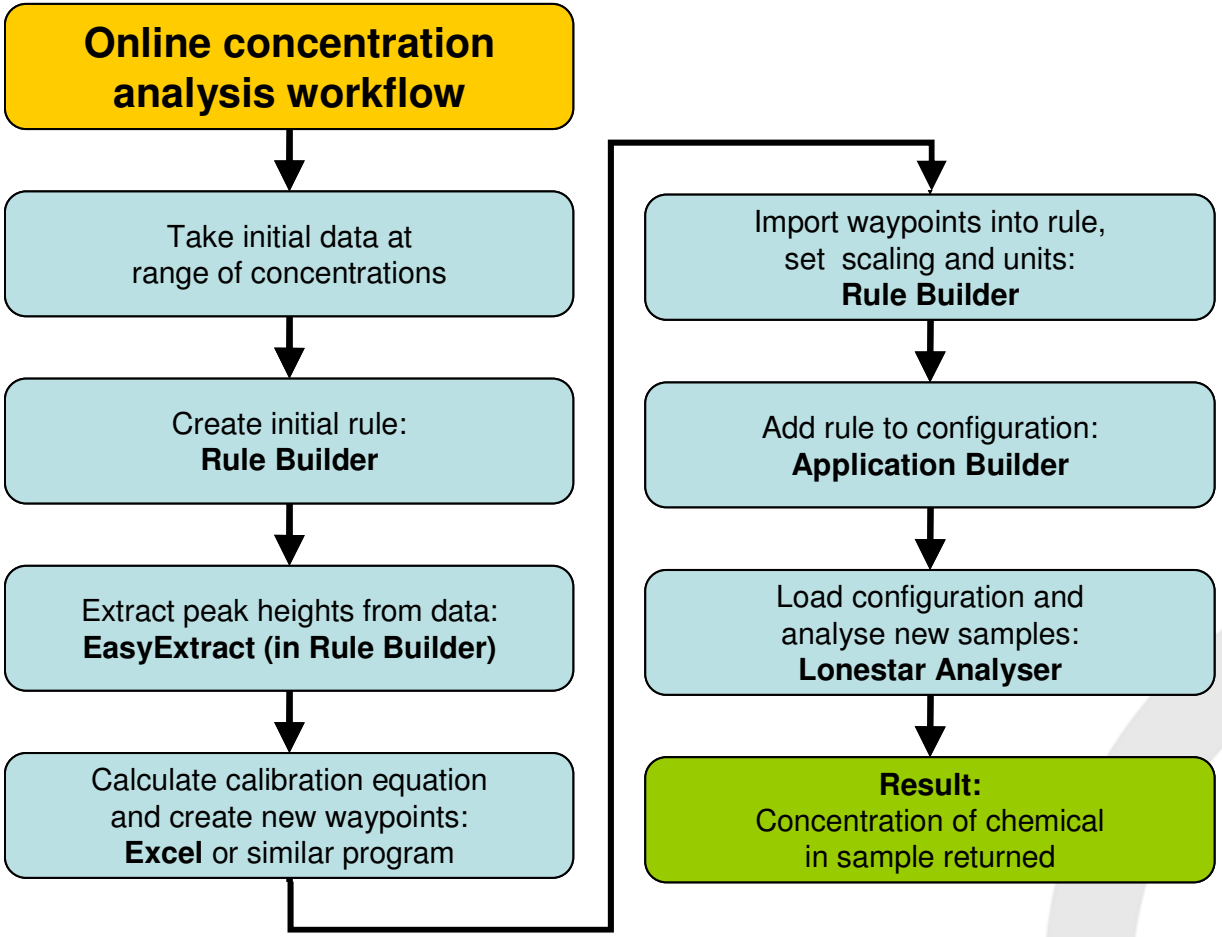


Calibration for Offline Concentration Analysis 3: data processing

- Extract the height of the peak at this point in all of your calibration DF matrices by using **EasyExtract**.
- Now use Excel to plot ion current vs. concentration and find the equation of the calibration curve.
- When you take new data, use EasyExtract and the same rule to give the height of the peak.
- Use the calibration equation to calculate the concentration of the chemical in the new samples.



Calibration for Online Concentration Analysis 1: workflow



Calibration for Online Concentration Analysis 2: overview

- The online concentration analysis requires two rules to be created and added to a configuration file: a rule to check instrument cleanliness and a calibration rule.
- This configuration file is then loaded onto the Lonestar and the Analyser mode is used to run samples and return a concentration value.

- As with the offline calibration, the process begins by taking initial data and calculating the equation of the calibration curve.
- A set of waypoints are then created in Excel. They will be imported into a rule using Rule Builder.
- Scaling, units and times must be set in the rule.
- The rule is added to the configuration file with Application Editor.

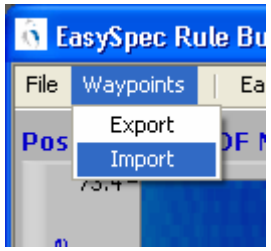
Calibration for Online Concentration Analysis 3: creating waypoints

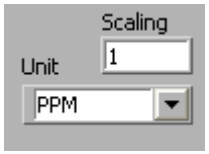
CV value | DF value | Ion current | Weighting

	A	B	C	D
1	-0.38519	73.15	0.1181	5
2	-0.38519	73.15	0.1796	5
3	-0.38519	73.15	0.2411	5
4	-0.38519	73.15	0.3026	5
5	-0.38519	73.15	0.3641	5
6	-0.38519	73.15	0.4256	5
7	-0.38519	73.15	0.4871	5
8	-0.38519	73.15	0.5486	5
9	-0.38519	73.15	0.6101	5
10	-0.38519	73.15	0.6716	5

- The rules are saved as a .csv file in Excel. Each row represents one waypoint. The columns are as shown on left.
- CV and DF values should be the same for each entry as the waypoints are at the same position.
- The ion current is calculated from the calibration curve: here the equation is y = 0.0123x + 0.0566.
- The weighting determines the concentration that is shown. Here it goes up in 5s. The concentration value is **cumulative**.
- For example, if the analyte peak in a new DF matrix had a height of 0.25 AU, it would have triggered 3 of the waypoints. The value given would be 3 x 5 = 15 ppm.

Calibration for Online Concentration Analysis 4: setting up the rule

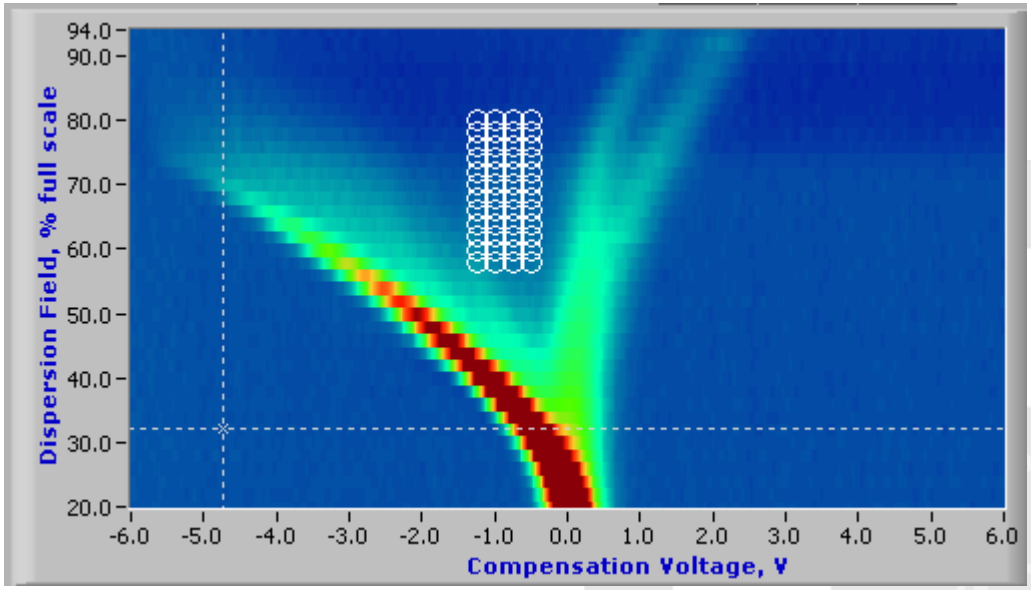




- Load a DF matrix into Rule Builder as usual.
- To import the waypoints into the rule, select Waypoints > Import and choose the file. The waypoints should appear on the DF matrix.
- Set the scaling to 1 and unit to the required unit.
- Set T target to 0 and T max to a large value, e.g. 1000.
- Otherwise set up the rule as usual and save it with the name of the chemical to be measured, e.g. toluene.

Calibration for Online Concentration Analysis 4: cleanliness rule

- The waypoints for the cleanliness checker rule are created in much the same way.
- Make sure they are distributed over the area of the DF matrix that must be clean before taking data in order to get a reliable concentration result.
- Set the ion current of the waypoints to a low value, e.g. 0.1 AU.
- Set the weighting to 1.
- Import the waypoints into Rule Builder as before.
- Set T target to 0.
- Set T max to 1000.
- Set scaling to 0.
- Otherwise set the rule up as usual.
- Save it with the name “cleanliness” or similar.



Calibration for Online Concentration Analysis 5: configuration

- Either save the configuration file that was used to take the data originally, or create a new one with the right parameters in Configuration Editor.
- Open the configuration file in Application Builder.
- First add the cleanliness rule and then add the calibration rule.
- Set the logic and sliders in Application Builder to show an alarm (red light) if the system is not clean.
- You can also set it to show a red light when the concentration is above or below a certain value.

Calibration for Online Concentration Analysis 6: Lonestar Analyser

- Load the configuration and open the Analyser tab in the Lonestar software.
- The bar at the top indicates whether operating conditions are OK.
- When they are, run a blank and check the cleanliness of the system.
- Once cleanliness has been confirmed, connect a sample to the Lonestar. Select the correct rule from the list of rules loaded and hit Measure.
- A scan will be made and the concentration appear on screen.