EasySpec Manual

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1 Introduction

1.1 The aim of EasySpec

EasySpec refers to a suite of programs used to determine, from DF matrices taken with a Lonestar, whether or not a chemical of interest is present. EasySpec can also be used to create calibrations between a certain peak height and the concentration of an analyte.

EasySpec may be used for offline analysis of data that have been previously collected or to set up a Lonestar for online monitoring of samples.

1.2 The principles of EasySpec

EasySpec allows a Lonestar configuration file to be created, including not just Lonestar settings but also a set of rules for analysis of the input to the Lonestar. These rules are created from DF matrices taken under known conditions. This allows identification and quantification of the relevant chemicals.

A configuration file with a set of rules can be used either for online monitoring of sample input to a Lonestar, or for offline analysis of data already collected.

These are the modules of EasySpec software described in this introduction:

1. **Rule Builder**

   Based on Lonestar spectra taken under known conditions (e.g. a known concentration of a chemical or a clean system), the user sets **rules** to identify the relevant peaks. Rules are made up of a series of **waypoints** on the DF matrix: each waypoint has associated CV, DF and ion current (AU) values. If the ion current value at this waypoint is higher in a later DF matrix, the waypoint is triggered. This suggests a change in the input to the Lonestar, for instance an increase in chemical concentration.

   See Sections 2 and 4.

2. **Application Builder**

   Collects a set of rules and adds them to the **configuration file**. The user can adjust tolerances and set logic so that, when the Lonestar is running with this configuration file loaded, it gives an alarm under the right conditions. For example, an alarm is shown in the presence of a certain chemical, or if the degree of noise in the DF matrix is too high.

   See Section 3.

3. **Configuration Editor**

   The Lonestar configuration file contains all the information about the set-up of the Lonestar (for example, flow rates and heater settings). It also contains **rules** that allow online monitoring of signals from relevant chemicals. These are created in **Rule Builder** and added to the configuration file using **Application Builder**.

   See Section 4.

4. **EasyCheck**

   Efficiently checks a large number of DF matrices against rules or configuration files. EasyCheck exports the data in an easily-manipulated form (.csv).

1.3 List of terms

1.3.1 DF – dispersion field

The dispersion field (DF) is the field created by the dispersion voltage (DV). Dispersion voltage is the peak voltage of the asymmetric waveform applied to the electrodes in the FAIMS process. See Figure 1.

When taking a DF matrix with the Lonestar, the DF can be scanned from 0% to 100% of its set range.

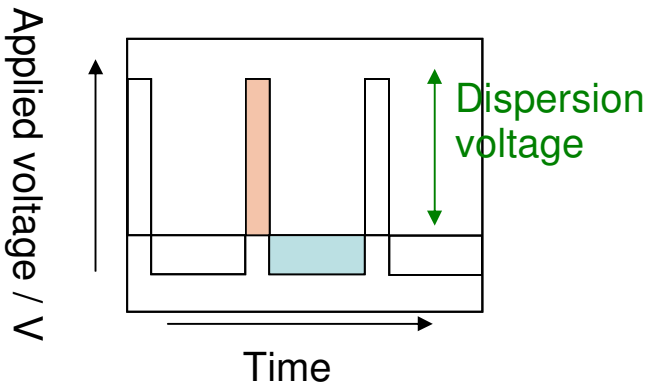


Figure 1 Asymmetric waveform applied to electrodes during FAIMS, showing dispersion voltage

1.3.2 CV – compensation voltage

A constant voltage is applied to the separator electrodes in the FAIMS process, in addition to the asymmetric waveform voltage (seen in Figure 1). This is called the compensation voltage (CV). Compensation voltage is scanned from -6.0 V to 6.0 V when collecting Lonestar data. The detector will pick up different analyte molecules at different combinations of CV and DF.

1.3.3 Ion current

The current generated by the ions that pass through the separator electrodes and are picked up by the ion detector plate. Ion current is measured in arbitrary units, A.U.

1.3.4 DF matrix / Lonestar spectrum

A DF matrix is the chart produced by scanning DF and CV and plotting the ion current produced. An illustration is shown in Figure 2.

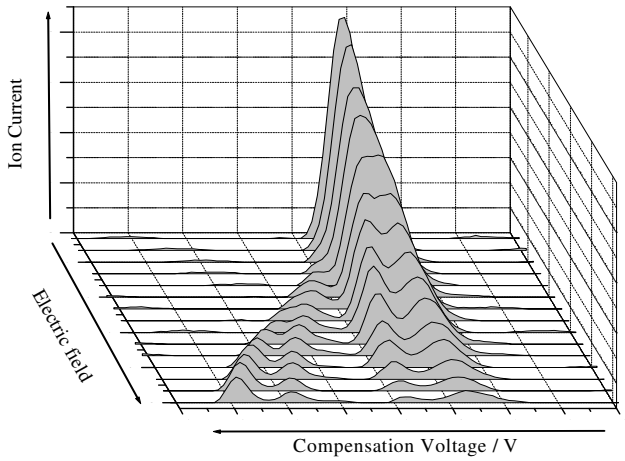


Figure 2 Illustration of a graph of ion current, produced by scanning dispersion field and compensation voltage.

DF matrices come in pairs: one for positive ions (positive mode) and one for negative ions (negative mode). These are shown in Figure 3.

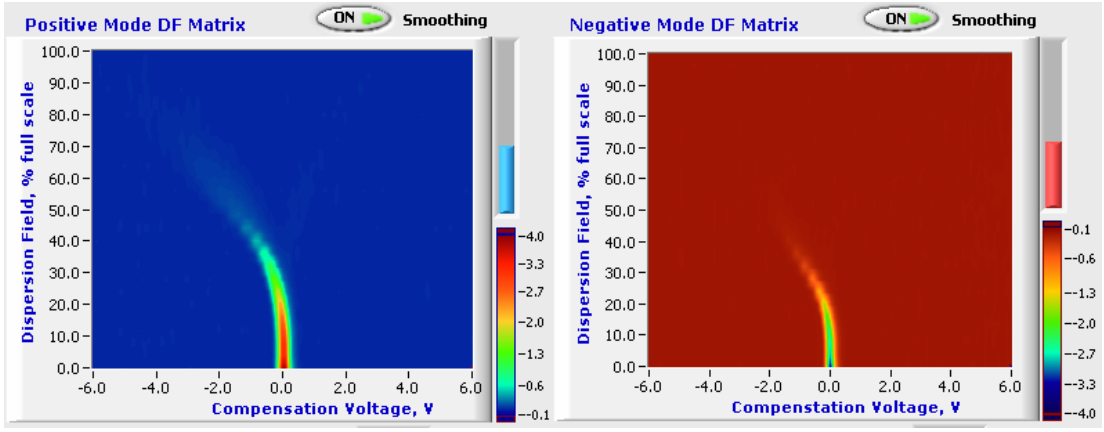


Figure 3 Positive mode and negative mode DF matrices. These matrices show a clean system blank. The RIP (Reactant Ion Peak) can be seen in each one.

1.3.5 RIP – reactant ion peak

Reactant ions are ion clusters formed from the ionisation of clean air in the reaction region of the detector.

The positive reactant ions are hydrated clusters of protons: $H^+(H_2O)_n$. The negative reactant ions are hydrated clusters of molecular dioxygen ions: $O_2^-(H_2O)_n$.

When an analyte is present, these ion clusters react with analyte molecules to give product ion clusters. These then pass into the detector to give the characteristic peaks for each chemical. When no analyte is present, a single peak is seen on the DF matrix in both the negative and the positive mode, due to the reactant ions. This is the RIP and can be seen in Figure 3 above.

2 EasySpec Rule Builder

2.1 Overview of EasySpec Rule Builder window

The EasySpec Rule Builder window is shown below, in Figure 4.

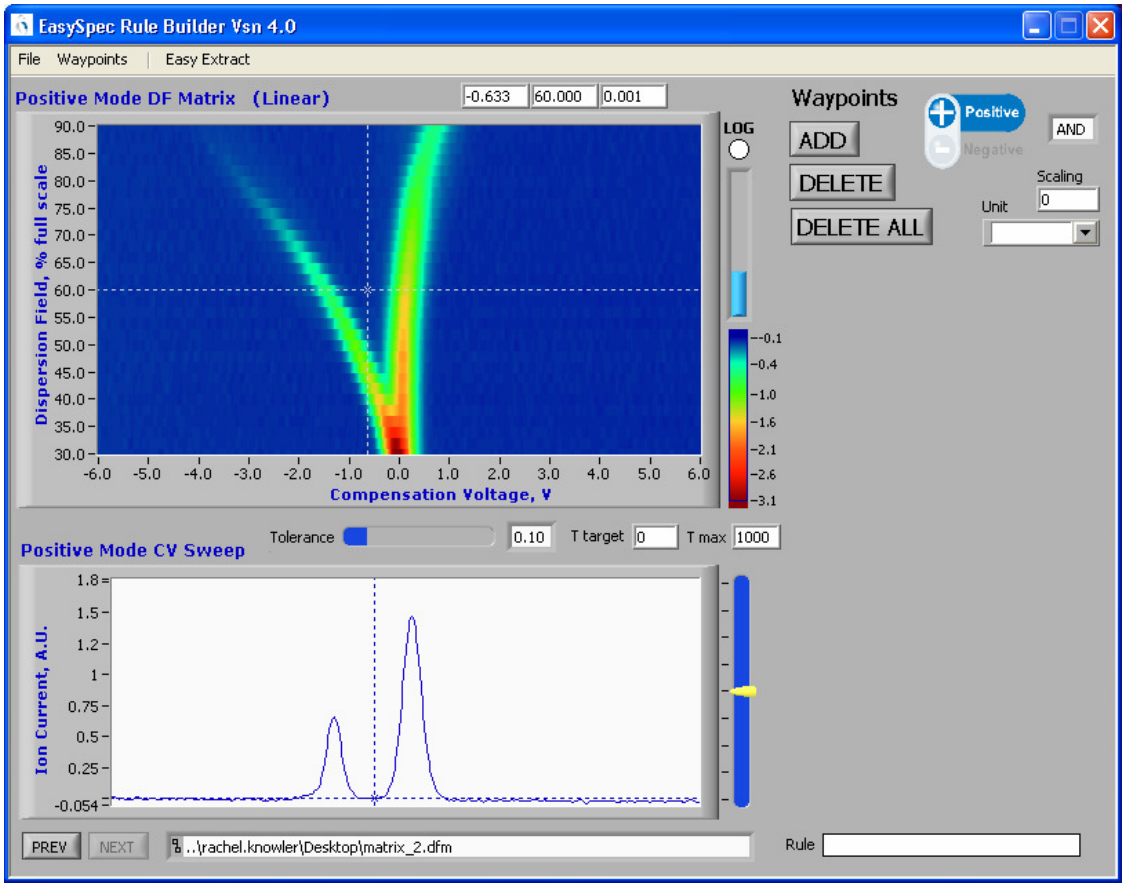


Figure 4 EasySpec Rule Builder window.

- The main feature of the window is the DF matrix. A horizontal and a vertical dashed line can be dragged across the matrix to select points.
- Beneath the DF matrix is shown a CV sweep corresponding to the position of the horizontal dashed line on the DF matrix.
- The PREV and NEXT buttons at the bottom of the Rule Builder window allow scrolling through matrices in the same folder.
- Toggle between positive and negative mode using the buttons in the top right corner.
- The position of the selected point is shown above the DF matrix, in the format:

Compensation Voltage (V)	Dispersion Field (%)	Ion Current (AU)

- To alter the contrast of the DF matrix, click and drag the pale blue slider to the right of the matrix, above the scale. The display can also be set to a log scale.
- In the top-right corner are controls for setting waypoints: ADD, DELETE and DELETE ALL.
- Beneath the DF matrix is a slider for setting the CV tolerance. See Section 2.4.
- Values for T target and T max can be set here. T max **must** be set higher than 0 if the rule is to be used in Analyser mode. See Section 2.7.
- There is a control to set the combination of positive and negative modes required to produce an alarm. Either both modes must be triggered (AND) or either one alone may produce an alarm (OR). See Section 3.3.
- Controls for setting scale and unit for concentration mode (see Section 4) are in the top right corner of the window.

2.2 Building a rule to check for the presence of a chemical

To begin, take Lonestar spectra of a chosen concentration of the chemical you are interested in detecting. The rule will trace the height and position of the relevant peaks on the spectrum.

Make sure to save the Lonestar configuration file used to take this data.

Open the program EasySpec Rule Builder. Go to *File > Load DF Matrix* and select an appropriate spectrum.

Rules are created by adding waypoints at particular points on the DF matrix, as shown by the white circles. Select a point on the spectrum by clicking and dragging the dotted lines. The bottom window shows a cross-section of the matrix for the selected DF value. Make sure your point is at the peak value of ion current. Then press ADD to add a waypoint.

Figure 5 shows a complete set of waypoints on an acetone spectrum.

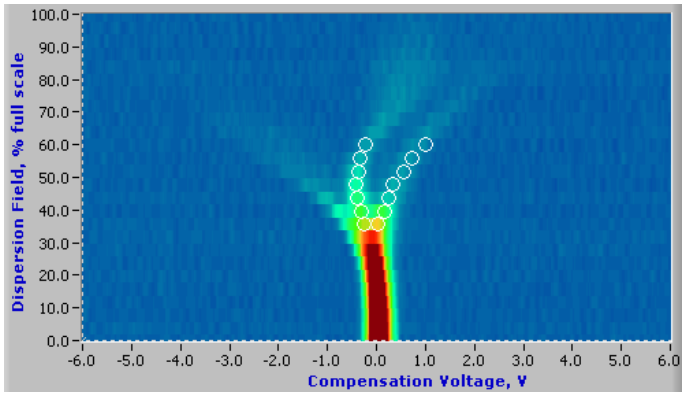


Figure 5 A completed set of waypoints on an acetone spectrum.

Positive Ion Mode Waypoints

-0.253	36.000	0.620
-0.002	36.000	0.736
0.137	40.000	0.365
-0.309	40.000	0.388
-0.393	44.000	0.261
0.221	44.000	0.108
-0.421	48.000	0.194
0.305	48.000	0.075
-0.365	52.000	0.132

Figure 6 Coordinates and values of a set of waypoints

Waypoints appear on the matrix as hollow white circles. A list of their coordinates and values appears beneath the ADD and DELETE buttons as they are added: see Figure 6. The columns have the same format as above.

2.3 Comparing the new rule with other DF matrices

By using the PREV and NEXT buttons at the bottom of the Rule Builder window, you can scroll through matrices in the same folder.

You should see that the hollow circles marking the waypoints become solid and either black or white. Black circles show waypoints that have been triggered – that is, the ion current at that point is greater than that set for the waypoint. White circles are un-triggered. See Figure 7.

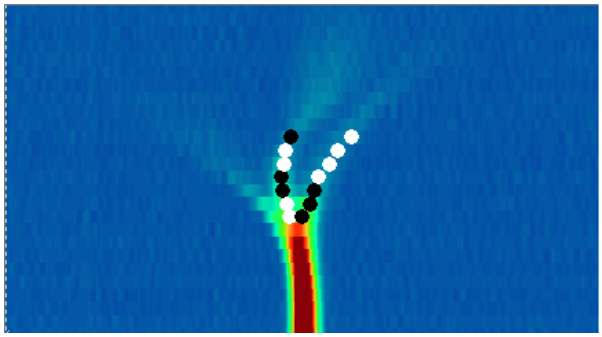


Figure 7 Comparing a rule with another DF matrix from the same set.

2.4 Adjusting waypoint tolerance

The blue bar marked Tolerance, beneath the DF matrix, allows you to take account of some uncertainty in the CV value of the peak.

This is useful because varying levels of humidity, for example, might shift the peak to a slightly lower or higher CV value.

When the tolerance is increased, a line appears on either side of the waypoints, as shown in Figure 8. The EasySpec programs will now look at the values of ion current at all the points along that line, and use the highest ion current value they find as the peak value.

The width of the line increases with tolerance. It also increases with increasing DF. This is because the peak usually shifts further at higher values of DF and very little or not at all with low values of DF.

It is not recommended to set the tolerance any lower than 0.05.

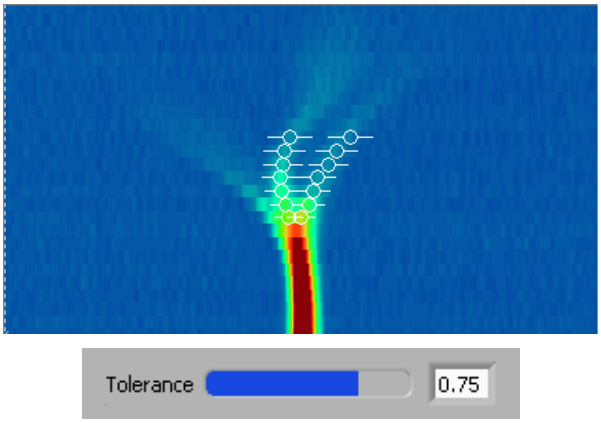


Figure 8 Changed appearance of rule with tolerance set to 0.75.

2.5 Setting the combination rule for positive and negative modes

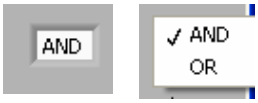


Figure 9 Setting AND or OR.

By clicking on the box beneath the positive/negative toggle, you can set the combination of positive and negative modes in this rule.

If AND is selected, waypoints will have to be triggered in both the positive and negative modes of a DF matrix for the alarm to be given.

If OR is selected, waypoints being triggered in either the positive mode or the negative mode alone will be sufficient to set off the alarm.

See Section 3.3 for more detail about the logic of combining rules.

2.6 Setting waypoints higher or lower than actual values

The slider to the right of the CV sweep graph allows you to set the value of the waypoint up to 20% above or below the actual value on the spectrum. This shows automatically on the CV sweep graph. See Figure 10.

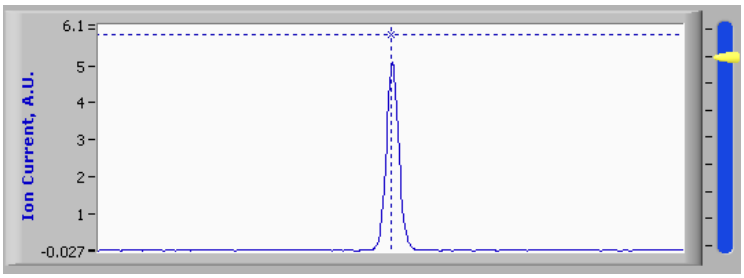


Figure 10 Offset of 20% above spectrum value.

Figure 11 and Figure 12 compare other spectra from the same set with the example acetone rule, where the waypoints have been set at 10% lower and 10% higher than the original values.

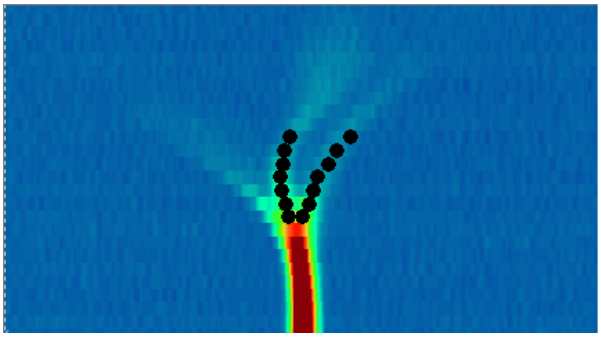


Figure 11 Waypoints set 10% lower than values. All waypoints have been triggered (black).

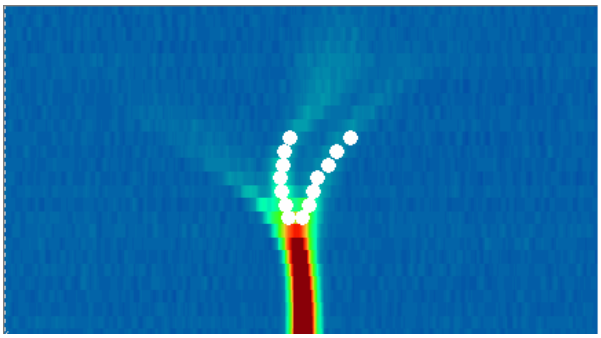


Figure 12 Waypoints set 10% higher than values. All waypoints are un-triggered (white).

These rules can be useful for setting an upper or lower acceptable value for the concentration of the chemical. They can also be used together in an application to set an acceptable range of variation for the concentration.

2.7 T target and T max

Figure 13 Setting T target and T max

Beneath the DF matrix in Rule Builder are boxes to change the settings of T target and T max (see Figure 13). The values are in seconds. These settings are important when creating a rule that will be used for online concentration monitoring using the Analyser tab in the Lonestar software.

Figure 14 Lonestar Analyser.

Figure 14 shows the Lonestar Analyser tab requesting a test sample for concentration measurement. When the sample is inserted and OK button pressed, it will take one DF matrix of the sample and compare it to the concentration rule for the required analyte.

T target specifies the time that should elapse between pressing OK and the Lonestar starting to collect the DF matrix. It is usually set to 0.

T max is the timeout value. If, after this time, the Lonestar has not been able to take the DF matrix, it will return a timeout and stop trying. If T max is set to 0, the rule will not work because it will always time out. T max should be set to a high value, for example 1000.

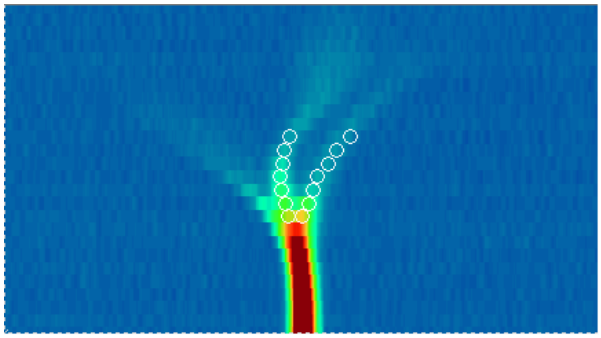
2.8 Migrating rules

A rule that has been created on one DF matrix can be migrated to another one. When this is done, the ion currents of the waypoints will change to match those at the same points of the new DF matrix.

To do this, first open a rule by selecting *File > Load Rule*.

Next, load a different DF matrix. Then select *File > Migrate Rule*. The ion current values of the waypoints will be changed to those of the new matrix. See Figure 15 and Figure 16.

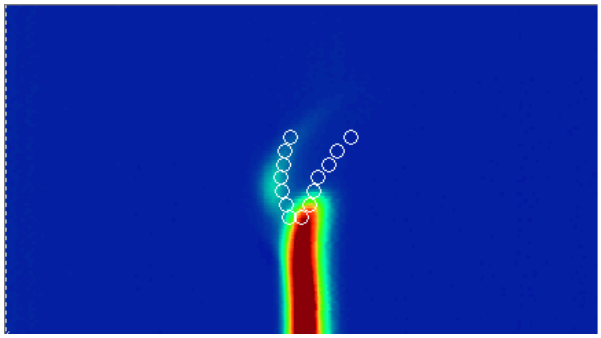
NOTE that if the peak position shifts then the migrated function will NOT attempt to follow the peak!



Positive Ion Mode Waypoints

-0.253	36.000	0.620
-0.002	36.000	0.736
0.137	40.000	0.365
-0.309	40.000	0.388
-0.393	44.000	0.261
0.221	44.000	0.108
-0.421	48.000	0.194
0.305	48.000	0.075
-0.365	52.000	0.132

Figure 15 Waypoints as set on the original DF matrix used to create this rule.



Positive Ion Mode Waypoints

-0.253	36.000	0.724
-0.002	36.000	3.621
0.137	40.000	1.944
-0.309	40.000	0.294
-0.393	44.000	0.362
0.221	44.000	0.298
-0.421	48.000	0.393
0.305	48.000	0.039
-0.365	52.000	0.294

Figure 16 The rule has been migrated to a different DF matrix. The waypoints are in the same positions but the ion current values have been increased to match the new matrix.

2.9 Exporting and importing waypoints

Once a rule has been created and saved, the waypoints may be exported as a comma-separated values (.csv) file that can be edited in a spreadsheet program.

To do this, go to Waypoints > Export and save the waypoints as a .csv file.

This method will export only the positive or negative waypoints, whichever mode is currently selected. If your rule has waypoints in both the positive and negative modes, you will have to save them separately. For example, save them as “acetone-rule-positive.csv” and “acetone-rule-negative.csv”.

The waypoints in Figure 17 have the positions and ion currents shown in Figure 18.

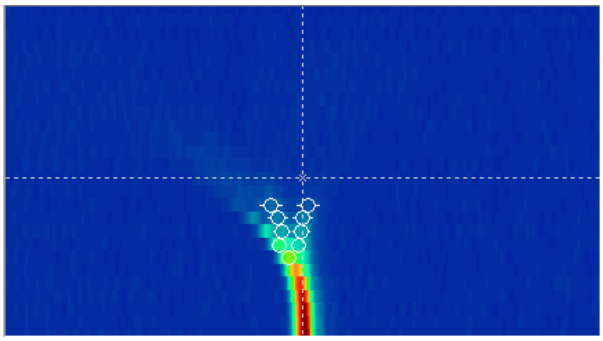


Figure 17 Waypoints in a rule based on an HCl spectrum.

Positive Ion Mode Waypoints

-0.281	24.000	1.336
-0.476	28.000	0.742
-0.030	32.000	0.259
-0.421	32.000	0.277
-0.002	36.000	0.187
-0.504	36.000	0.178
-0.086	28.000	0.365
0.081	40.000	0.077
-0.644	40.000	0.132

Figure 18 Positive ion mode waypoints for the rule in the previous figure.

These waypoints were exported as “HCl demo positive.csv”. Opened in a spreadsheet program, the data looks as shown in Figure 19.

HCl demo positive

	A	B	C	D
1	-0.2812	24	1.336054	1
2	-0.47647	28	0.741676	1
3	-0.03013	32	0.259453	1
4	-0.42068	32	0.277154	1
5	-0.00223	36	0.186682	1
6	-0.50437	36	0.177526	1
7	-0.08592	28	0.365078	1
8	0.081461	40	0.076937	1
9	-0.64385	40	0.132176	1

Figure 19 Waypoints from Figure 18 exported as a .csv file and opened in a spreadsheet program.

The columns are the same as before, except with a new fourth column. This is the weighting factor, which is used to set concentration output. For an explanation of concentration mode, see Section 4.

To import waypoints into a rule, go to Waypoints > Import and select the relevant .csv file. Note that the waypoints will be added to whichever of the negative and positive modes is currently selected. Make sure that, say, the negative mode is selected when importing a set of negative waypoints.

2.10 Setting multiple waypoints

It is possible to set several waypoints at the same coordinates on the Lonestar spectrum, but with different ion current values. An illustration of this on a CV sweep is shown in Figure 20.

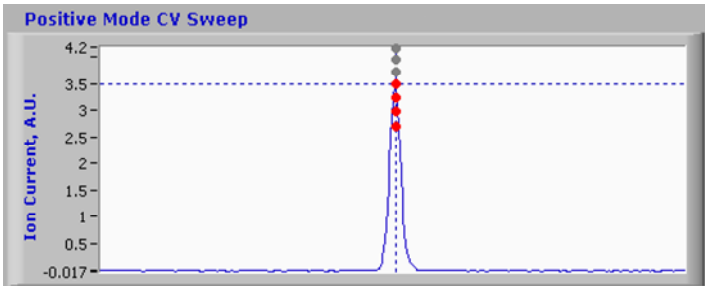


Figure 20 Illustration of multiple waypoints at the same point on the spectrum.

In this example, a waypoint has been set at the actual value and at 5% higher and lower, 10% higher and lower and 20% higher and lower. For illustration, the waypoints that have been triggered are shown in red and the un-triggered ones are shown in grey.

An easy way to do this is to first set an initial series of waypoints and save the rule. Then export the waypoints to a .csv file and open using a spreadsheet program. The values can be copied and adjusted as shown in Figure 21 and then imported back into the rule. (See Section 2.9.)

	A	B	C	D	E	F
1	0.025668	0	5.17488			
2	0.025668	12	4.376991	Original waypoints		
3	-0.03013	24	2.740887			
4	-0.00223	36	0.741873			
5	-0.39278	44	0.260114			
6	0.332531	48	0.074186			
7	0.695187	56	0.056336			
8	-0.2254	60	0.060155			
9	0.025668	0	5.433624			
10	0.025668	12	4.595841	Ion currents set 5%		
11	-0.03013	24	2.877931	higher than original		
12	-0.00223	36	0.778967			
13	-0.39278	44	0.27312			
14	0.332531	48	0.077895			
15	0.695187	56	0.059153			
16	-0.2254	60	0.063163			
17	0.025668	0	5.698034			
18	0.025668	12	4.819483	Ion currents set 10%		
19	-0.03013	24	3.017976	higher than original		
20	-0.00223	36	0.816873			
21	-0.39278	44	0.28641			
22	-0.42068	48	0.213388			
23	0.695187	56	0.062031			
24	-0.2254	60	0.066237			
25	0.040109	0	6.226854			
26	0.053565	12	5.211833	Ion currents set 20%		
27	-0.03013	24	3.298067	higher than original		
28	-0.00223	36	0.892685			
29	-0.39278	44	0.312991			
30	-0.42068	48	0.233192			
31	-0.36488	52	0.15808			
32	0.695187	56	0.067788			
33	-0.2254	60	0.072384			
34						
35						

Figure 21 Setting multiple waypoints using a spreadsheet program.

2.11 EasyExtract

EasyExtract compares large numbers of DF matrices, in one or more sets, to individual rules.

2.11.1 Loading EasySpec data into EasyExtract

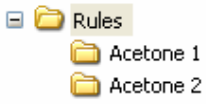


Figure 22 Correct file structure for using EasyExtract.

To use EasyExtract, a specific file structure must be used. Save rules in a folder called Rules, and save one or more folders containing DF matrices into the same folder. See Figure 22.

Click on EasyExtract in the main menu bar. It will ask you to select a rule within an EasyExtract structure, as shown in Figure 23.

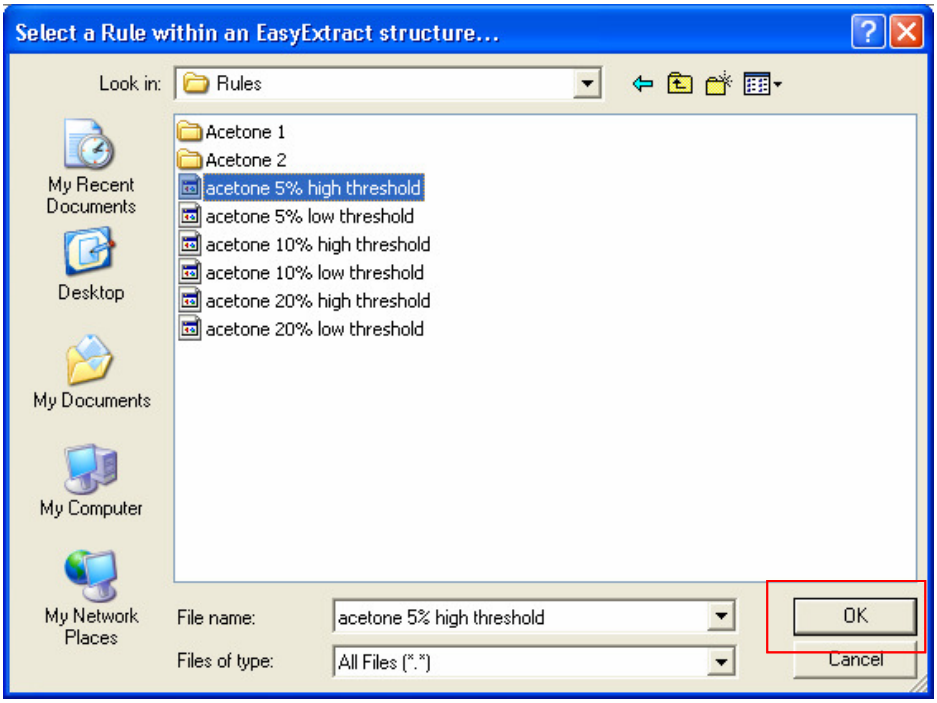


Figure 23 Selecting a rule for EasyExtract.

For each DF matrix in the Rules folder, EasyExtract finds the ion current at every waypoint in the rule. The results of the EasyExtract are then saved as a comma-separated values (.csv) file named results.csv in the Rules folder.

1.1.1 Interpreting EasyExtract results

An example results.csv file is shown in Figure 24.

UTC Date	UTC Time	Folder	Filename	DF%	CV	AU	W	AUmax	CV@AUmax	FW@HM	IonMode
22/07/2009	13:29:30	water 000 ppm	matrix_23.asc	60	-1.295326	0.064109	1	0.075604	-1.375495	2.770008	Pos
22/07/2009	13:34:47	water 000 ppm	matrix_24.asc	60	-1.295326	0.065538	1	0.078763	-1.586767	2.770008	Pos
22/07/2009	13:40:04	water 000 ppm	matrix_25.asc	60	-1.295326	0.065121	1	0.07031	-1.352021	2.863906	Pos
22/07/2009	13:59:01	water 020ppm	matrix_2.asc	60	-1.295326	0.070655	1	0.071774	-1.352021	2.98128	Pos
22/07/2009	14:04:17	water 020ppm	matrix_3.asc	60	-1.295326	0.079053	1	0.089328	-1.211173	0.492968	Pos
22/07/2009	14:09:36	water 020ppm	matrix_4.asc	60	-1.295326	0.049501	1	0.067405	-1.117274	0.446018	Pos
22/07/2009	14:40:45	water 040ppm	matrix_2.asc	60	-1.295326	0.131311	1	0.175054	-1.187698	0.422544	Pos
22/07/2009	14:46:04	water 040ppm	matrix_3.asc	60	-1.295326	0.13537	1	0.200883	-1.164224	0.446018	Pos
22/07/2009	14:51:23	water 040ppm	matrix_4.asc	60	-1.295326	0.088905	1	0.17629	-1.117274	0.446018	Pos
22/07/2009	15:27:47	water 060ppm	matrix_2.asc	60	-1.295326	0.238853	1	0.262047	-1.234647	0.399069	Pos
22/07/2009	15:33:04	water 060ppm	matrix_3.asc	60	-1.295326	0.288552	1	0.315714	-1.234647	0.399069	Pos
22/07/2009	15:38:23	water 060ppm	matrix_4.asc	60	-1.295326	0.290053	1	0.319147	-1.234647	0.399069	Pos
22/07/2009	16:49:23	water 100ppm	matrix_2.asc	60	-1.295326	0.601245	1	0.609078	-1.281597	0.399069	Pos
22/07/2009	16:54:40	water 100ppm	matrix_3.asc	60	-1.295326	0.669713	1	0.702266	-1.258122	0.399069	Pos
22/07/2009	16:59:59	water 100ppm	matrix_4.asc	60	-1.295326	0.676636	1	0.738283	-1.234647	0.399069	Pos

Figure 24 EasyExtract results.csv file.

Here, a calibration rule with one waypoint was compared with each matrix in a set. This included matrices taken from the headspace of an analyte in water, at several different concentrations.

The columns in the .csv file are as follows:

- **UTC Date:** The date the matrix was saved
- **UTC Time:** The time the matrix was saved
- **Folder:** The folder name
- **Filename:** The filename, including matrix number
- **DF%:** The DF of the waypoint
- **CV:** The CV of the waypoint
- **AU:** The ion current (in arbitrary units, AU) at that point, in this matrix
- **W:** Weighting – see Section 7.4
- **AUmax:** The maximum ion current along the tolerance bar for the current waypoint and matrix – see Section 2.4
- **CV@AUmax:** The CV at that maximum ion current
- **FW@HM:** The full width at half maximum for the peak at this DF
- **IonMode:** The ionisation mode (positive or negative)

For each matrix, the EasyExtract results give the ion current at each waypoint in the rule.

This is useful because it allows tracking over time of the ion current at one particular point. This can give a quick reflection of the change in the amount of the chemical over time.

See Figure 26 for an example graph. This shows the change with time in the height of an isoamyl acetate peak at 70% DF (Figure 25). The peak height increases over the first few matrices and then decreases, suggesting that the isoamyl acetate was drying up.

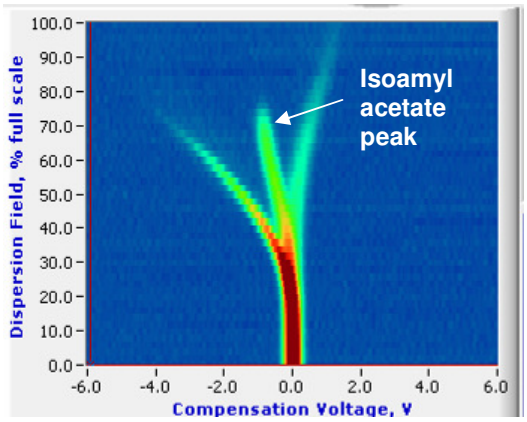


Figure 25 DF matrix showing isoamyl acetate peak.

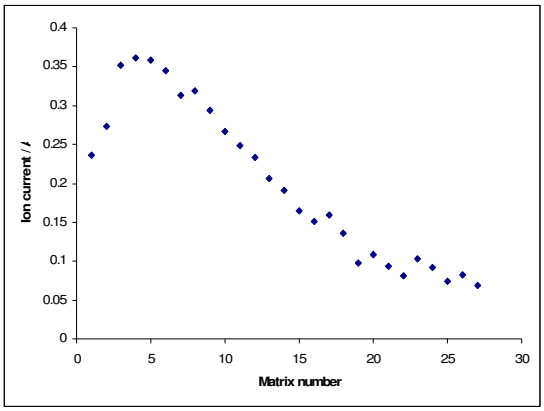


Figure 26 Variation of ion current at a waypoint over time. A graph produced from EasyExtract results.

3 EasySpec Application Builder

3.1 Overview of Application Builder window

The program Application Builder allows several rules to be brought together and added to a configuration file. DF matrices can be quickly compared against the rules inside Application Builder itself and an alarm given if any problems are seen. An example screen of Application Builder in use is shown in Figure 27.

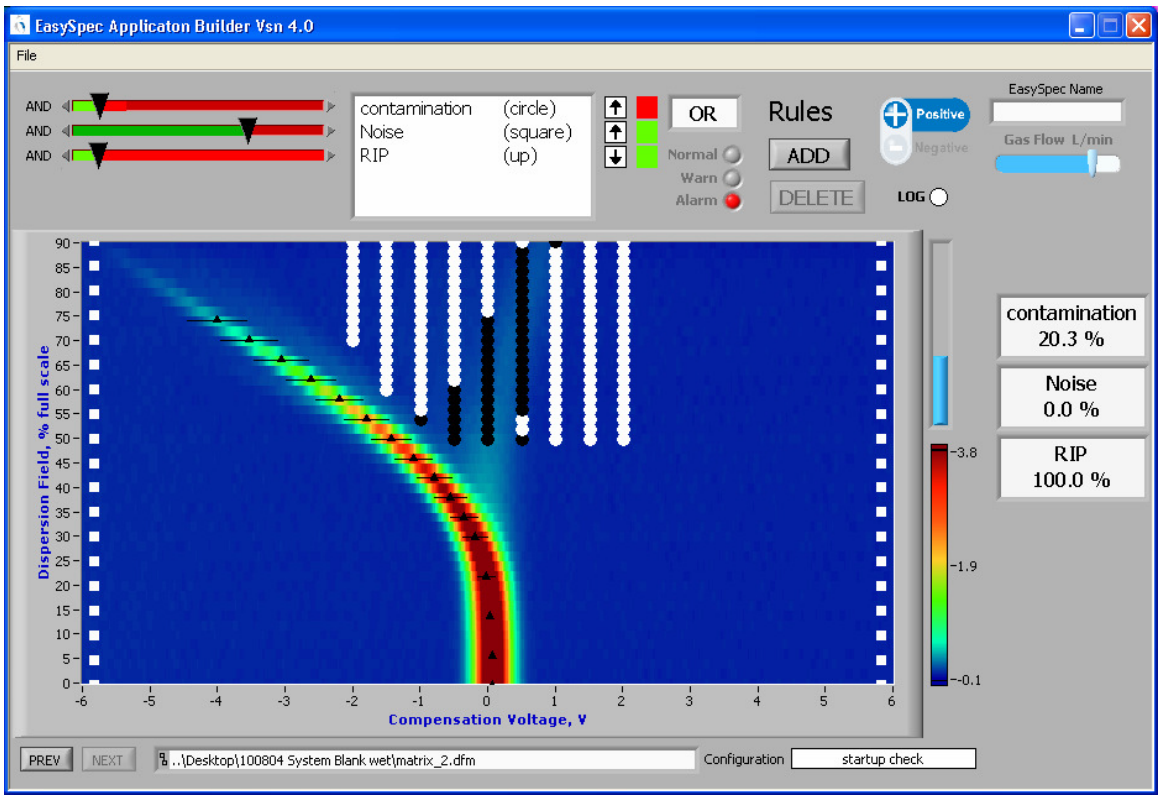


Figure 27 An application in Application Builder.

- The main feature of the Application Builder window is the DF matrix. This can be toggled between positive and negative mode with the buttons in the top right corner.
- Several rules have been added to this configuration file and they can be seen on the DF matrix, each represented by a different symbol.
- There is a list of the current rules in the white box above the DF matrix.

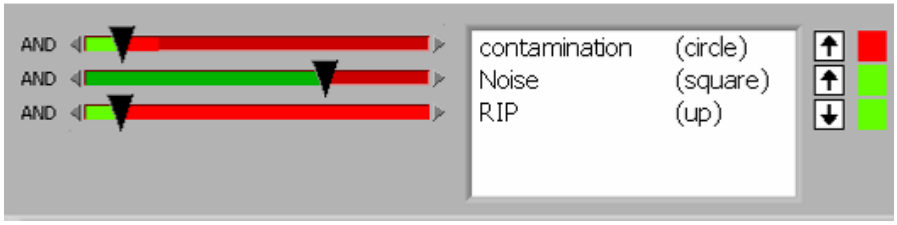


Figure 29 Sliders, list of rules and arrows.

- At the right of the window is a set of panels gives the result of each rule for the current DF matrix (see Figure 28). The scaling and units of the data in these panels can be set in Rule Builder when using EasySpec in concentration mode: see Section 7.5. If the scaling and units are not set, the panels will only show the names of the rules.

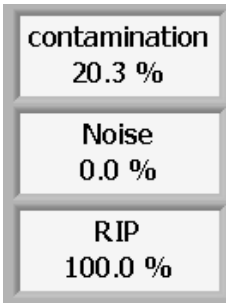


Figure 28 Outcome of each of the rules on the current DF matrix.

- The PREV and NEXT buttons at the bottom of the window allow the user to navigate through the DF matrices in a given folder.
- To the left of the list of rules, a set of red and green sliders allow the user to set tolerances for the proportion of waypoints that should be triggered before the alarm is given.
- To the right of the list, up or down arrows are used to set whether the alarm is given on the presence or absence of the condition in the rule. See Figure 30.
- Next to the list of rules is a small panel marked OR in the example (Figure 30). Clicking this allows you to select when the alarm is given. With OR, only one of the conditions must fail to be met for the alarm to show. With AND, all conditions must fail to be met.
- Beneath this panel is the alarm indicator. If the situation is Normal, a green circle shows. If there is an Alarm, a red circle shows.

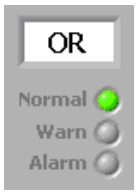


Figure 30 AND/OR selector and alarm indicator.

- At the top of the screen are buttons controlling the rules added to the application, labelled ADD and DELETE.

3.2 Creating a new application

To create a new application, begin with the configuration file that was used to take the relevant data. This can be saved using the software on the Lonestar, by selecting *File > Save Configuration*. Transfer the file to the computer that is to be used to create the application. Open Application Builder and select *File > Load Configuration*.

Next load a spectrum. Select *File > Load DF matrix*.

Add the rules created in Rule Builder one at a time by pressing ADD and selecting them from the menu.

As rules are added they will appear on the DF matrix, with waypoints black if triggered or white if not. Panels appear at the right hand side showing the name of each rule. If the rules include scaling and unit data (see Section 7.5) then the proportion of waypoints triggered in each rule, or concentration results, will appear in the panels.

Up to five rules may be combined into one application. This might include, for example, a check for cleanliness and four concentration rules. It might include checks for contamination, background noise and RIP to make sure the instrument is fit for use.

If the configuration file is to be used to take data with the **Analyser** tab on a Lonestar, the first rule added **must** be a check on the cleanliness of the instrument. The waypoints should cover the area of the DF matrix where the peak of interest emerges and the ion current should be set to a low value, <0.1 AU.

3.3 Overview of the logic of combining rules

Whether used online or offline, applications can give two types of output. One is a binary alarm/no-alarm (red light/green light) response when a peak height passes a threshold value. The other is a concentration value for a particular analyte.

Concentration analysis is described in greater detail in Section 6 (offline) and Section 7 (online).

Sections 3.4 to 3.6 below describe how to set the logic for each rule in an application to correctly give an alarm response. This can be applied to all rules, including those that give a concentration response.

Upper and/or lower boundaries on the ion current values of each waypoint are set in a rule. An alarm is triggered if the values go outside of these boundaries.

Several rules can be combined to give a system of logic to determine when the alarm should be given. This is summarised in Figure 31 below.

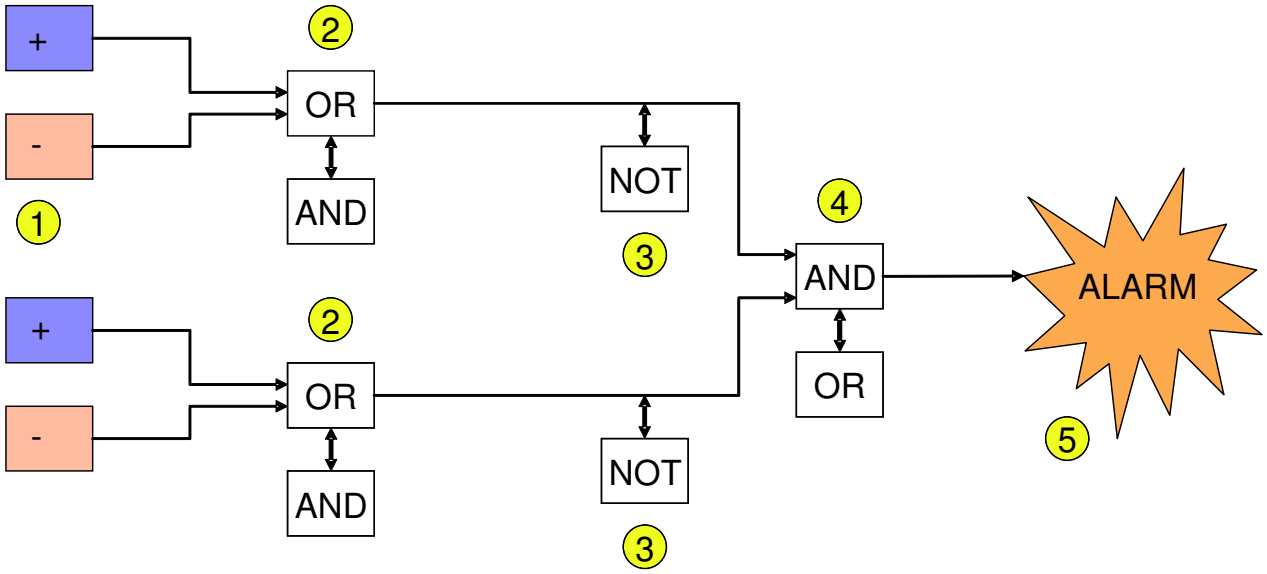


Figure 31 The logic determining whether the alarm should go off.

1. Rules are created in Rule Builder. They may have waypoints set in the positive mode (blue), the negative mode (red) or in both.

   See Section 2.2.

2. In Rule Builder, the logic for each rule can be set to AND (waypoints must be triggered in both positive and negative modes to trigger the rule) or OR (waypoints in only one mode need be triggered to trigger the rule).

   See Section 2.5.

3. Rules are added to the configuration file in Application Builder. Each rule can be set to produce an alarm on the presence or absence of a signal – giving an optional NOT gate. This can also be changed in Configuration Editor.

   See Section 3.4.

4. The master logic for the configuration file can also be set to AND (all rules must be triggered to give an alarm) or OR (only one rule need be triggered). This can be changed in Application Builder or in Configuration Editor.

   See Section 3.4.

3.4 Setting logic

Besides each rule in the application is a set of controls and indicators as shown in Figure 32.

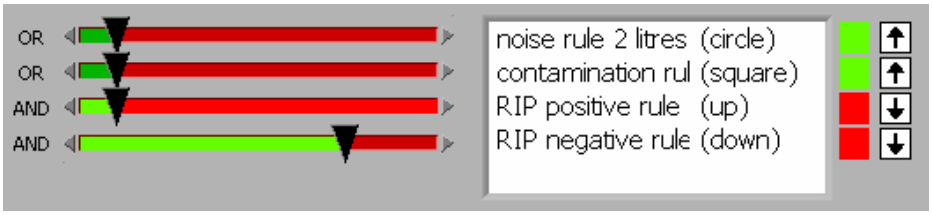


Figure 32 Rules and controls in an application.

The word at the far left of each line, either AND or OR, shows which was used to combine the positive and negative modes in each rule. See Section 2.5 for details of this.

The up or down arrow at the end of each line shows when the rule should set off an alarm.

If an **up arrow** is shown, then an alarm is set off in the **presence** of the condition. That is, if the waypoints in the rule are triggered, the alarm is set off.

If a **down arrow** is shown, then an alarm is set off in the **absence** of the condition. That is, if the waypoints in the rule are not triggered, the alarm is set off.

The green and red indicators show whether or not the waypoints in each rule are triggered. They should be read together with the arrows to see whether the situation is normal or alarmed.

Table 1 Outcome of each of the rules on the current DF matrix.

Appearance	Indicator meaning	Arrow meaning	Overall Result
	Green: Rule has not been triggered.	Up: Alarm set off when rule is triggered	Alarm is not set off. Situation is Normal. 
	Green: Rule has not been triggered.	Down: Alarm set off when rule is not triggered	Alarm is set off. 
	Red: Rule has been triggered.	Up: Alarm set off when rule is triggered	Alarm is set off. 
	Red: Rule has been triggered.	Down: Alarm set off when rule is not triggered	Alarm is not set off. Situation is Normal. 

Table 1 summarises the possibilities, assuming there is only one rule in the application.

The logic used to combine rules into applications is set by the box above the alarm buttons, which shows either AND or OR. If AND is selected, then all the rules must be alarmed for the alarm to show. If OR is selected, only one rule need be alarmed for the alarm to show.

3.5 Adjusting the threshold on each rule

The slider next to each rule adjusts the threshold number of waypoints that must be triggered before a rule is considered to be triggered.

The proportion of waypoints that have been triggered for this rule in the current DF matrix is shown by the bright part of the slider. The dull part shows the proportion that has not.

The pointer shows the proportion of waypoints that must have been triggered for the rule to be considered triggered. The slider bar is always green to the left of the pointer and red to the right of it.

Figure 33 Two threshold slider bars.

In Figure 33 above, the top rule has not been triggered and the bottom one has.

There is a set of sliders for each rule in the positive mode and a set in the negative mode. If your rules have waypoints set in both modes, you must be sure to adjust the thresholds for each.

3.6 Low thresholds vs. high thresholds

When trying to detect a chemical of interest, there are advantages and disadvantages to setting thresholds both low and high.

A low threshold gives a sensitive response, picking up peaks that only just exceed the ion current values set in the waypoints. On the other hand, false positives are common.

A high threshold will all but eliminate false positives. It may miss some borderline cases, though.

4 EasyCheck

4.1 Overview of EasyCheck window

The EasyCheck software has two functions designed to assist with the development and verification of applications that use EasySpec.

EasyCheck itself is designed to allow a large number of DF matrices to be checked against applications, without having to scroll through a folder full of files in Application Builder. Matrices can be checked against one application or several at a time. Data can be easily extracted in the form of comma-separated value (.csv) files that can be opened in a spreadsheet program. See Section 4.2.

EasyExtract compares a number of DF matrices against one individual rule at a time. The resulting data is exported as .csv files for analysis in a spreadsheet program. This function works exactly as in Rule Builder: see Section 2.11.

Figure 34 shows the appearance of EasyCheck in use.

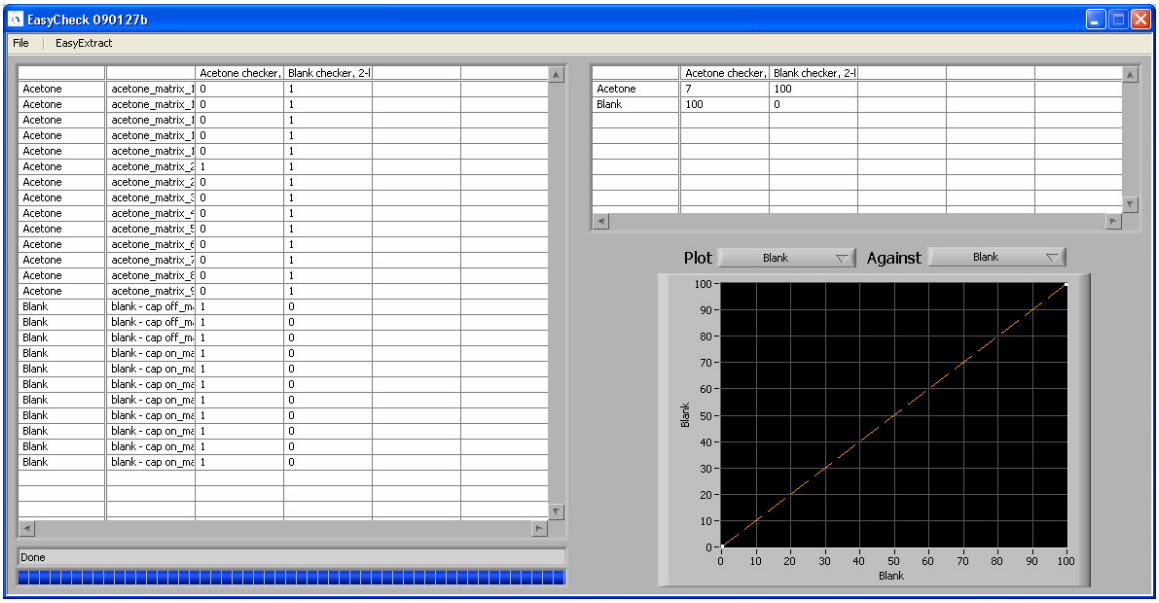


Figure 34 EasyCheck window in use.

- The EasyCheck window contains a large chart at the left, which shows a list of DF matrix files and the result of checking them against each of the applications used.
- A smaller chart summarises the percentage of each group of matrices that has set off an alarm in each of the applications.
- It is possible to plot the results of different groups of matrices against one another in the black graph on the right of the EasyCheck window.

- A status and progress bar at the bottom of the window updates as the program checks each of the requested DF matrices against the applications. See Figure 35.

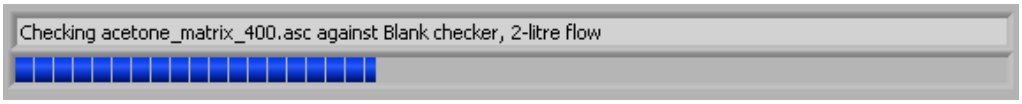


Figure 35 Status and progress bars.

4.2 Using EasyCheck

4.2.1 Loading EasySpec data into EasyCheck

EasySpec data must be saved with the correct folder structure to be opened by EasyCheck.

Save configuration files in a folder named Configurations. Save each set of Lonestar data in another folder. All of these must be saved in another folder, as seen in Figure 36.

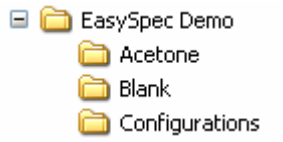


Figure 36 Correct folder structure for using EasyCheck.

To begin with EasyCheck, select *File > Open EasySpec*. Select the top-level EasySpec folder and click Current Folder, as shown by the red box in Figure 37.

In this example there are two sets of Lonestar data. One set has been taken with an airflow containing a known concentration of acetone. The other contains system blanks.

The Configurations folder also contains two configuration files. One is an acetone checker, to determine if acetone is present. The other is a blank checker, to check that the system is clean.

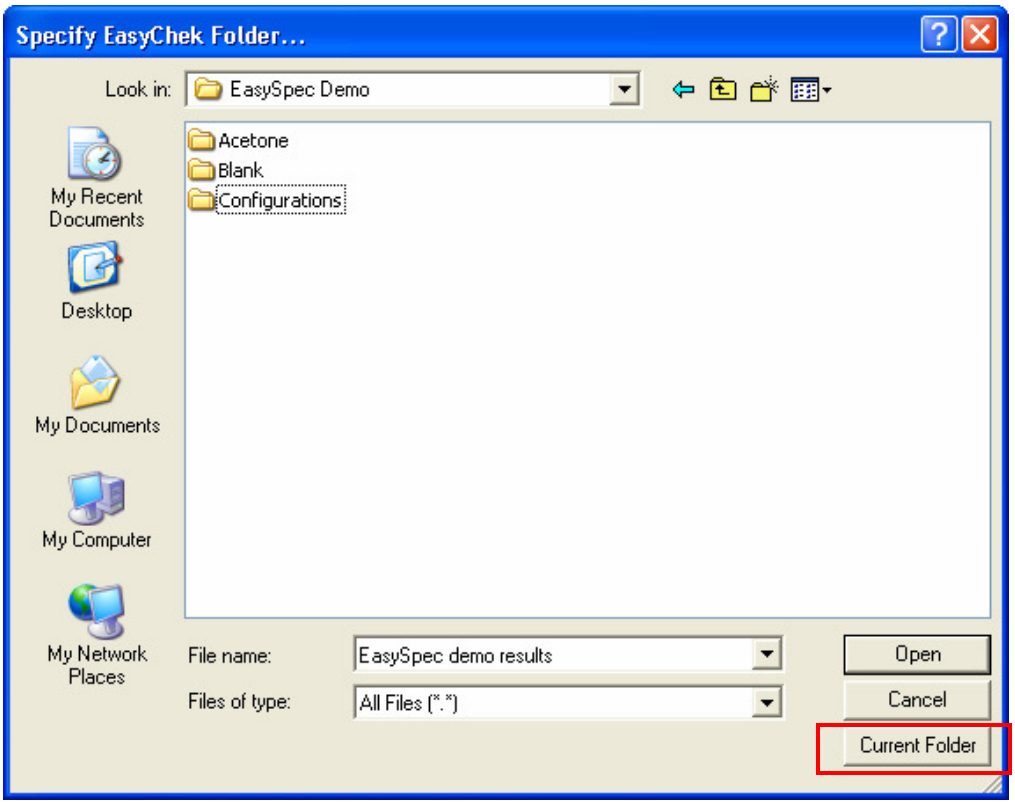


Figure 37 Opening EasySpec files.

EasyCheck checks the compatibilities of the files and then checks them against configuration files, with progress shown on the bar at the bottom of the window.

Sometimes an incompatibility report will appear, like that in Figure 38. If this happens, click to ACCEPT Incompatibility.

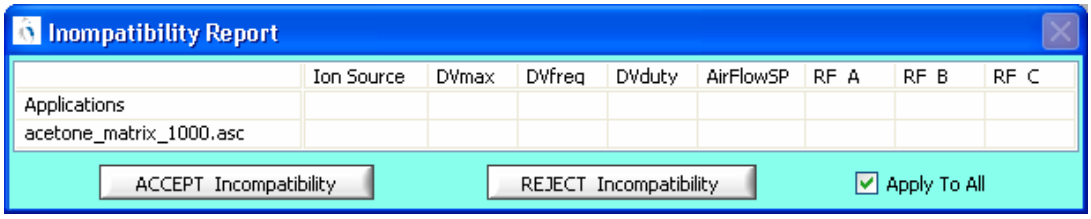
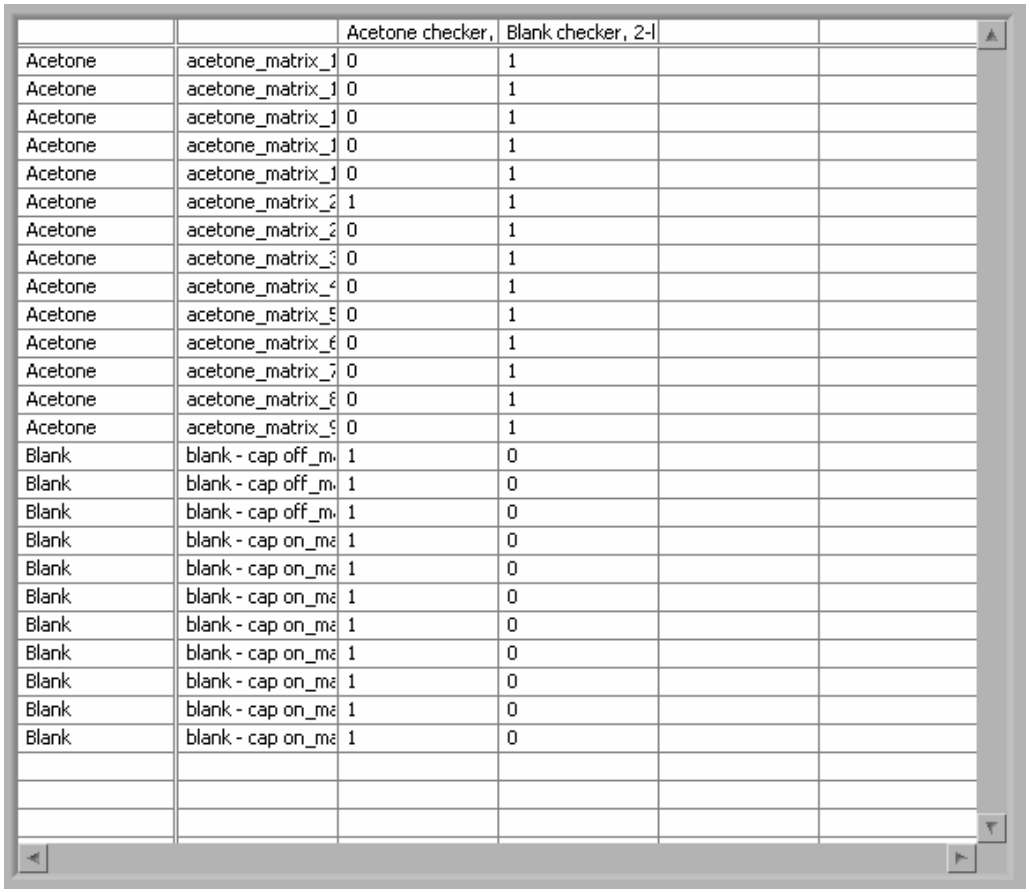


Figure 38 Incompatibility report.

Once this step is completed, a filled-out chart will appear, as shown in Figure 39.



		Acetone checker,	Blank checker, 2-I		
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		
Blank	blank - cap on_ma	1	0		

Figure 39 Appearance after successfully loading EasySpec data.

4.2.2 Interpreting EasyCheck Results

The EasyCheck results in Figure 39 give the following information:

- The first column here shows the name of the DF matrix folder.

  In this example, the names are “Acetone” and “Blank”.

- The next column shows the names of the individual files.

- The third and fourth columns are for each of the two configurations used.

  The values in the columns show whether or not the alarm has gone off. 1 means that there is an alarm. 0 means no alarm.

In this example, we would expect the acetone checker to alarm if acetone is not present. The blank checker should alarm if the system does not show a clean response with no contamination.

As expected, the acetone checker (third column) shows an alarm for the blank DF matrices, and no alarm for the acetone matrices (except one).

The blank checker (fourth column) shows an alarm for the acetone DF matrices but not for the blank matrices. This is summarised in the other chart: see Figure 40.

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

Figure 40 Summary of results.

Here, the percentage of each set of DF matrices which set off an alarm in each application is shown.

These results can be plotted against one another for indication. See Figure 41. This is not very useful in this example but may be in other cases.

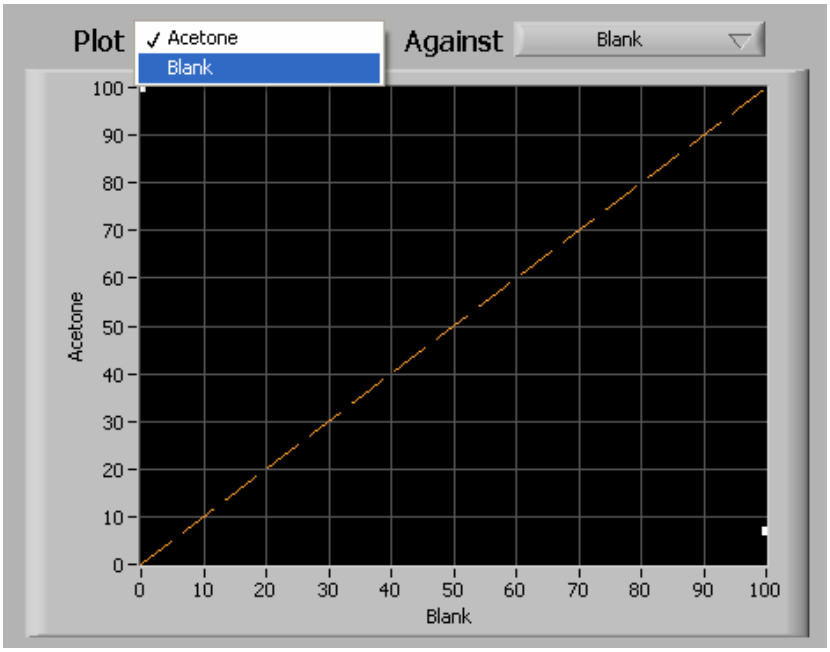


Figure 41 Plotting results for indication.

4.2.3 Exporting results

To quickly export the results, select *File > Export results*.

A comma-separated values (.csv) file is created, with exactly the same information as was shown in EasySpec. This file can be opened in a spreadsheet program, as seen in Figure 42, so the data can be more easily manipulated.

	A	B	C	D	E
1	Matrix Group	Matrix File	Acetone	Blank checker	
2					
3	Acetone	acetone_matr	0	1	
4	Acetone	acetone_matr	0	1	
5	Acetone	acetone_matr	0	1	
6	Acetone	acetone_matr	0	1	
7	Acetone	acetone_matr	0	1	
8	Acetone	acetone_matr	1	1	
9	Acetone	acetone_matr	0	1	
10	Acetone	acetone_matr	0	1	
11	Acetone	acetone_matr	0	1	
12	Acetone	acetone_matr	0	1	
13	Acetone	acetone_matr	0	1	
14	Acetone	acetone_matr	0	1	
15	Acetone	acetone_matr	0	1	
16	Acetone	acetone_matr	0	1	
17	Blank	blank - cap of	1	0	
18	Blank	blank - cap of	1	0	
19	Blank	blank - cap of	1	0	
20	Blank	blank - cap or	1	0	
21	Blank	blank - cap or	1	0	
22	Blank	blank - cap or	1	0	
23	Blank	blank - cap or	1	0	
24	Blank	blank - cap or	1	0	
25	Blank	blank - cap or	1	0	
26	Blank	blank - cap or	1	0	
27	Blank	blank - cap or	1	0	
28					
29					
30					
31					
32	Matrix Group		Acetone	Blank checker	
33					
34	Acetone		7	100	
35	Blank		100	0	

Figure 42 Exported data.

5 Configuration Editor

5.1 Overview of Configuration Editor window

Configuration Editor allows configuration files to be edited and created. It is possible to use Configuration Editor to change data-collection settings (e.g. DF range and number of lines sampled per DF matrix) and to directly edit rules that have been added to a configuration file.

Operational limits may be set so that, when running the Analyser tab in the Lonestar software, the Lonestar will not start taking data until gas flow rate, humidity measurements etc. are not within the correct ranges.

The program also allows changes to Lonestar system settings that are outside the scope of this manual.

The Configuration Editor window contains several panels, each containing a group of settings. These are shown in Figure 43.

Go to *File > Open* to open a configuration file or set up a new one by altering settings in the Configuration Editor window. Save your file by going to *File > Save*.

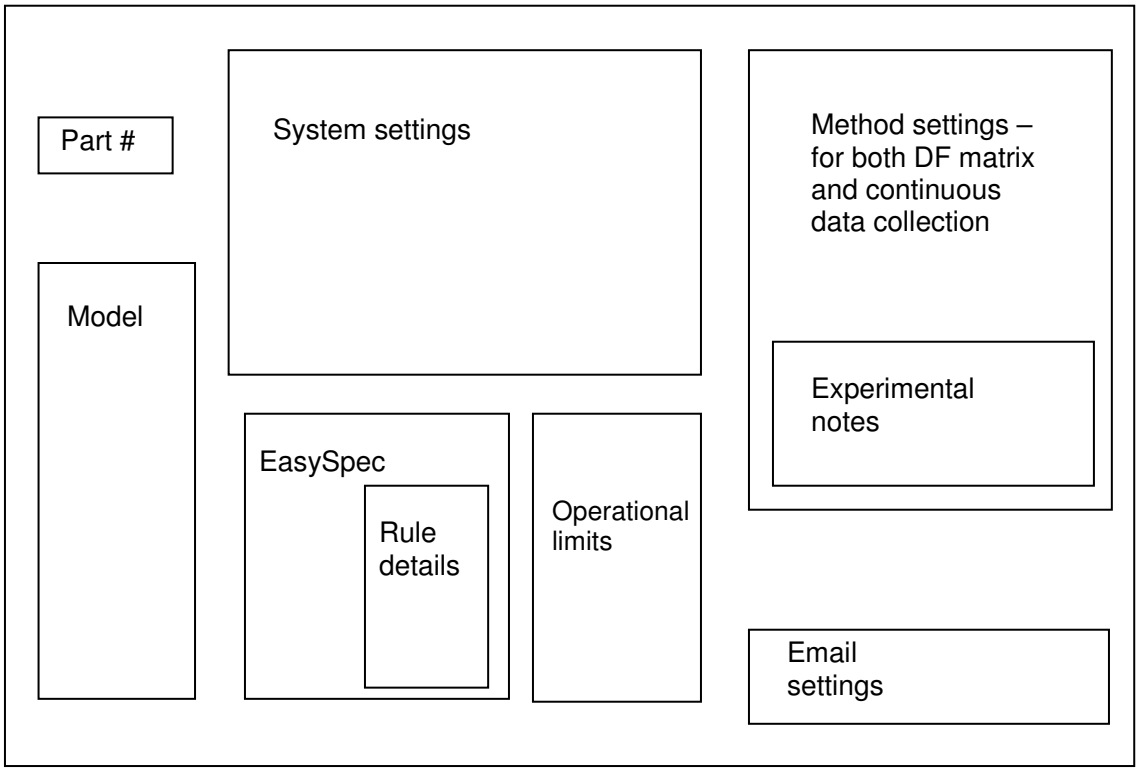


Figure 43 Configuration Editor screen.

5.2 Part

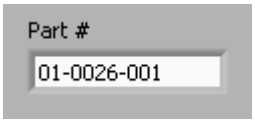


Figure 44 Part #.

The part # (Figure 44) may be filled in with the number of the Lonestar used to take the data.

For example, Lonestar 43 would have part # 01-0026-043.

This can be helpful but is not absolutely necessary.

5.3 Method settings

The method settings panel (Figure 45) contains the same controls as are found in the Settings tab in the Lonestar software. This panel can be set up in advance and the configuration file saved. When the file is loaded onto the Lonestar, monitoring can immediately begin.

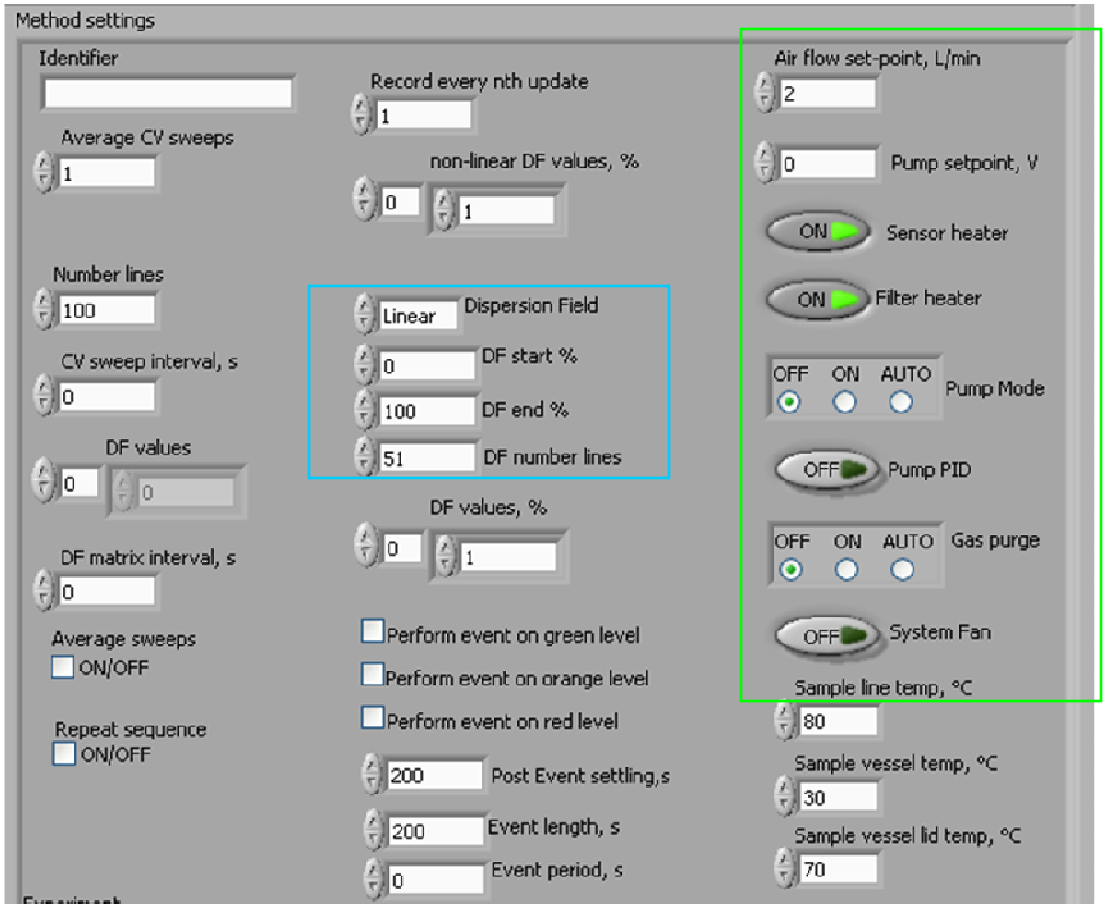


Figure 45 Method settings.

Some useful settings to check before saving the configuration file have been highlighted above.

In the blue box, the dispersion field range and number of lines to sample over in each DF matrix can be changed.

In the green box are heating and pump settings. For positive-pressure sampling under normal conditions, they should be as shown:

- Air-flow set point: the flow value used for sampling
- Pump set point: 0 V
- Sensor heater and filter heater ON
- Pump, pump PID, gas purge and system fan OFF

5.4 Operational limits

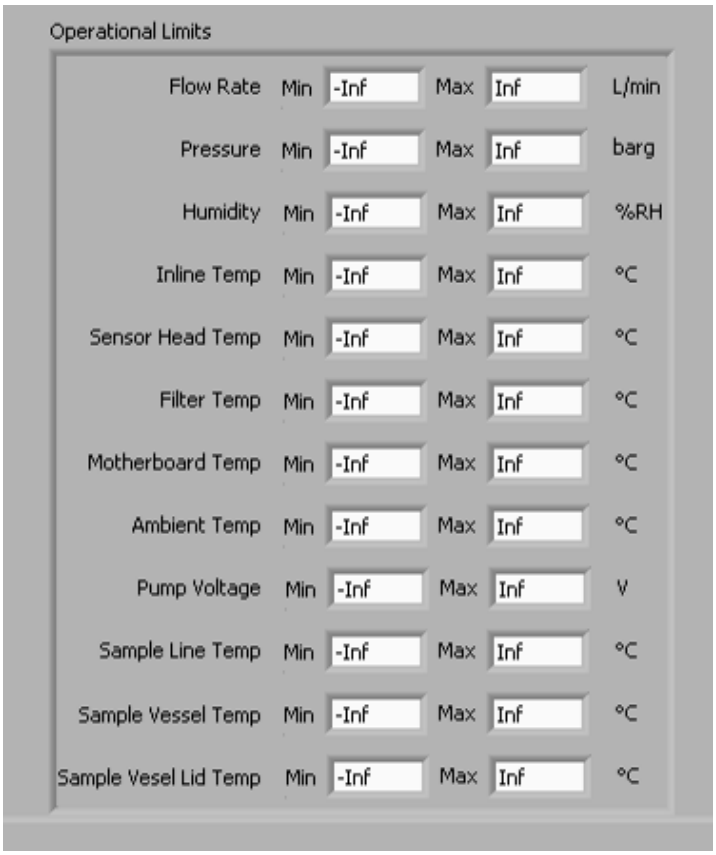


Figure 46 Operational limits panel.

The operational limits panel allows “good” ranges of system parameters to be set. When the Lonestar is run using the Analyser tab, it will check the value of the system parameters against the set limits. If they agree (Figure 47) then data may be taken. If they do not agree (Figure 48) the software will ask the operator to wait until the system parameters are within the set limits.

For example, the Lonestar could be set to only take data if the humidity is between 10% and 12% and the flow rate is between 1.95 l/min and 2.05 l/min.

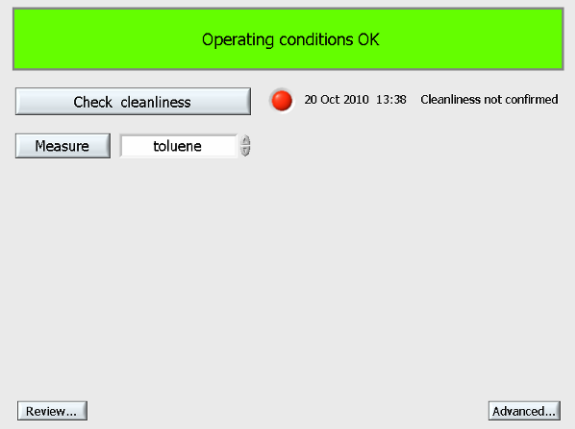


Figure 47 Operating conditions OK in Lonestar Analyser.

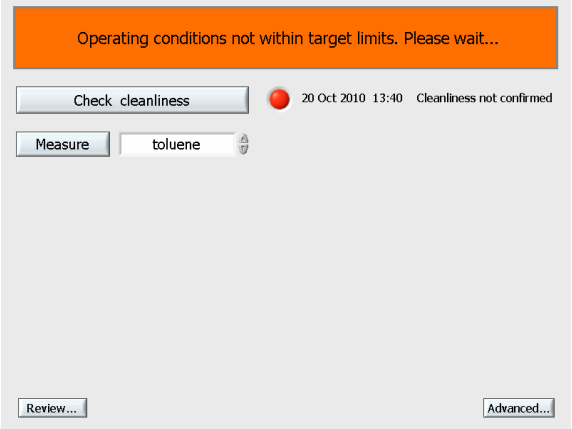


Figure 48 Operating conditions not within target limits.

The parameters that may be specified are:

- Flow rate
- Pressure
- Humidity
- Inline temperature
- Sensor head temperature
- Filter temperature
- Motherboard temperature
- Ambient temperature
- Pump voltage
- Sample line temperature
- Sample vessel temperature
- Sample vessel lid temperature

The last three parameters on the list refer to external heated apparatus (sample vessel, lid and inlet line) controlled by an Owlstone heater controller unit and corresponding software.

The values in the list default to ± infinity if they are not changed, as in Figure 46. If all the limits are at these default values, operating conditions will always be shown as OK in Analyser.

5.5 EasySpec panel settings

The EasySpec panel shows details of all the rules that have been loaded into the application. The DF values, CV values and ion currents of waypoints can all be adjusted in Configuration Editor, as well as scaling, units, weighting factors and tolerances. See Section 2 for more detail on creating rules.

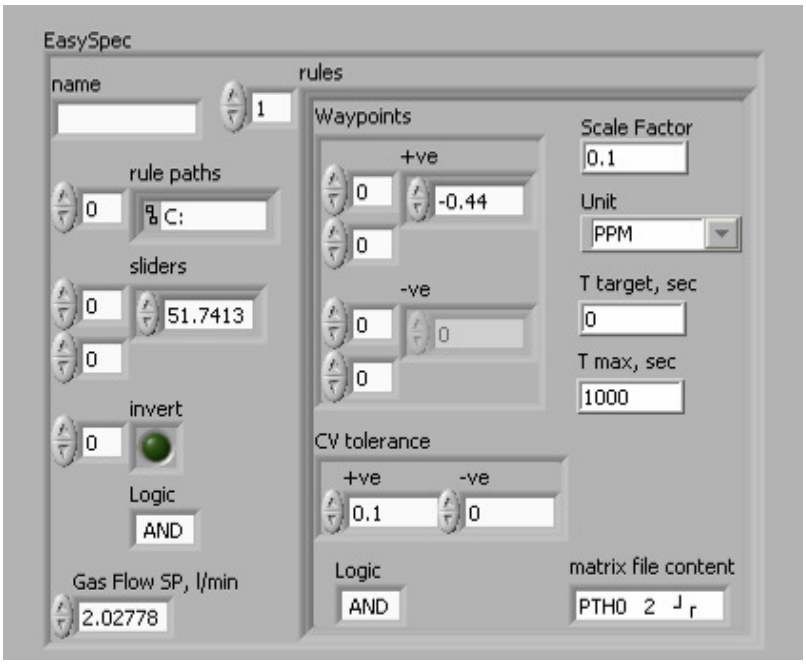


Figure 49 EasySpec panel.

5.5.1 Selecting a rule

The EasySpec panel allows you to scroll through the rules added to the current configuration file. To select a rule, click up and down on the counter next to the white box marked “name” at the top of the panel.

All counters begin at 0, not 1. If there are three rules in a configuration file, they will be numbered 0, 1 and 2.

When you have selected a rule with this counter, you can add a name for it into the “name” box. The details in the large panel to the right will be those for the selected rule.

This includes scaling and unit, CV tolerance, T target and T max.

It is also possible to change the Logic: whether both positive- and negative-mode waypoints must be triggered for the rule to be triggered (AND) or only one mode (OR). For more details on this, see Section 3.3.

5.5.2 Waypoints

The location of each of the waypoints in the rule may be seen and altered using the counters. The two counters to the left select the cell in the table of waypoints, and the larger box to the right displays the value.

Again, they count from 0 instead of from 1.

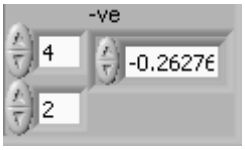
The upper counter selects the row and the lower counter selects the column.

This is illustrated in Figure 50 and Figure 51 below, using the .csv files created by exporting the rule from Rule Builder (see Section 2.9).

	A	B	C	D
1	-0.00223	20.40816	-0.36116	5
2	0.053564	24.4898	-0.35571	5
3	0.109358	28.57143	-0.32169	5
4	0.165151	32.65306	-0.3016	5
5	0.276737	36.7347	-0.26276	5
6	0.41622	40.81633	-0.20914	5
7	0.527807	44.89796	-0.17561	5
8	0.695187	48.97959	-0.13935	5

Figure 50 Displaying the waypoints in a rule in Configuration Editor.

In Figure 50, the first row and first column are selected. This displays the CV of the first waypoint in the rule, in the negative mode.



	A	B	C	D
1	-0.00223	20.40816	-0.36116	5
2	0.053564	24.4898	-0.35571	5
3	0.109358	28.57143	-0.32169	5
4	0.165151	32.65306	-0.3016	5
5	0.276737	36.7347	-0.26276	5
6	0.41622	40.81633	-0.20914	5
7	0.527807	44.89796	-0.17561	5
8	0.695187	48.97959	-0.13935	5

Figure 51 Displaying the waypoints in a rule in Configuration Editor.

In Figure 51, the 5th row and 3rd column are selected. This displays the ion current of the 5th waypoint in the rule, in the negative mode.

In general, for each waypoint:

- The first column (0) is the CV.
- The second column (1) is the DF.
- The third column (2) is the ion current.
- The fourth column (3) is the weighting.

5.5.3 Logic

Figure 52 shows the logic controls in the EasySpec panel.

As before, the counter is used to select a rule.

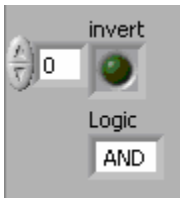


Figure 52 Logic controls.

When the “invert” button is selected, the logic for this rule is inverted. This means that the configuration file will give an alarm in the absence of this condition, when the rule is not triggered.

Inverting the logic of a rule is the same as giving it a **down arrow** in Application Builder. **Non-inverted logic** is the same as an **up arrow**. This is point (3) in Section 3.3.

The “Logic” box controls the master trigger logic: point (4) in Section 3.3**Figure 31**. If it is set to AND, all rules must be triggered for the alarm to go off. If it is set to OR, one rule being triggered is enough to produce the alarm.

6 Calibration for Offline Concentration Analysis

6.1 Overview of calibration for offline analysis

For online concentration monitoring, a concentration rule is created and added to the Lonestar configuration file, or application. This is loaded onto the Lonestar and data is taken in the Analyser tab. See Section 7.

A simpler, offline method of calculating concentrations from DF matrices is described here. This method uses EasyExtract to extract the height of a single point on the analyte peak at different concentrations. The data can then be plotted as a graph in Excel and an equation relating concentration and peak height can be calculated. The steps to create and use a calibration rule are as follows:

1 Take DF matrices from multiple concentrations of the analyte, with the same experimental procedure as will be used to take data later on.

2 Create the rule in EasySpec Rule Builder, with a single waypoint at a position along the peak. This might require some experimentation to identify a position on the analyte peak where the ion current is directly proportional to the concentration, and where the peak has good resolution.

3 Use EasyExtract to process a set of DF matrices taken at different, known concentrations of the analyte. This will extract the ion current at the waypoint in each matrix and save the data as a .csv file.

4 In a spreadsheet program, plot this ion current against concentration to give the calibration graph. Add a line of best fit to the graph.

5 Use EasyExtract to extract the ion current at the waypoint of the calibration rule from DF matrices taken from unknown samples. Use the equation of the line of best fit to calculate the concentration of 4-MeI in the sample.

6.2 Multiple concentrations

First, take multiple DF matrices of the analyte at three or more known concentrations.

At least three matrices should be taken at each concentration. To standardise the results, allow the system to stabilise before taking data.

Figure 53 shows spectra taken of 4-methylimidazole (4-MeI) in water at 20 ppm, 60 ppm and 100 ppm concentrations. The monomer peak (labelled M) can be seen to increase as the amount of 4-MeI in the system goes up. In the third DF matrix, the dimer peak D can also be seen. At the same time the RIP decreases. This makes 4-MeI a suitable chemical for EasySpec concentration monitoring.

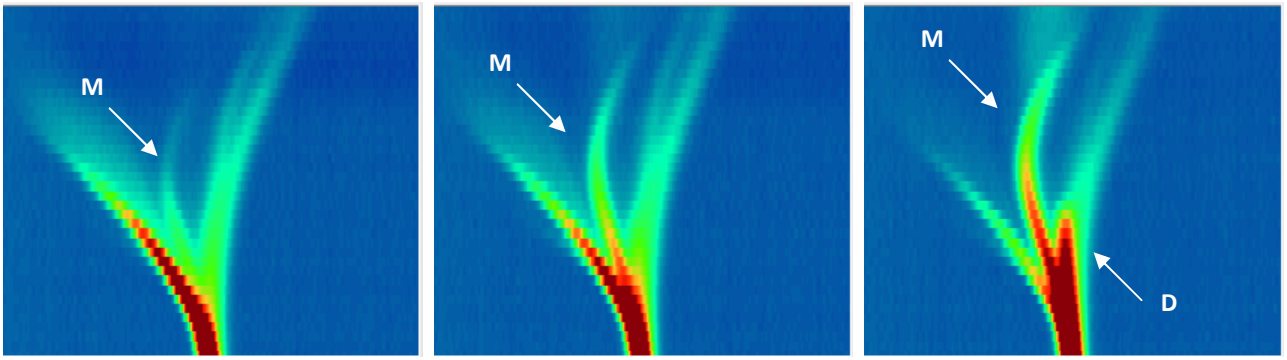


Figure 53 Positive-mode spectra of 20 ppm, 60 ppm and 100 ppm concentrations of 4-Mel.

6.3 Building the rule

The single waypoint on the rule should be positioned on the analyte peak, as in Figure 54. For advice on where to put it, see Section 6.5.

Remember to set a tolerance value of at least 0.05. Here it has been set to 0.25. See Section 2.4 for more information.

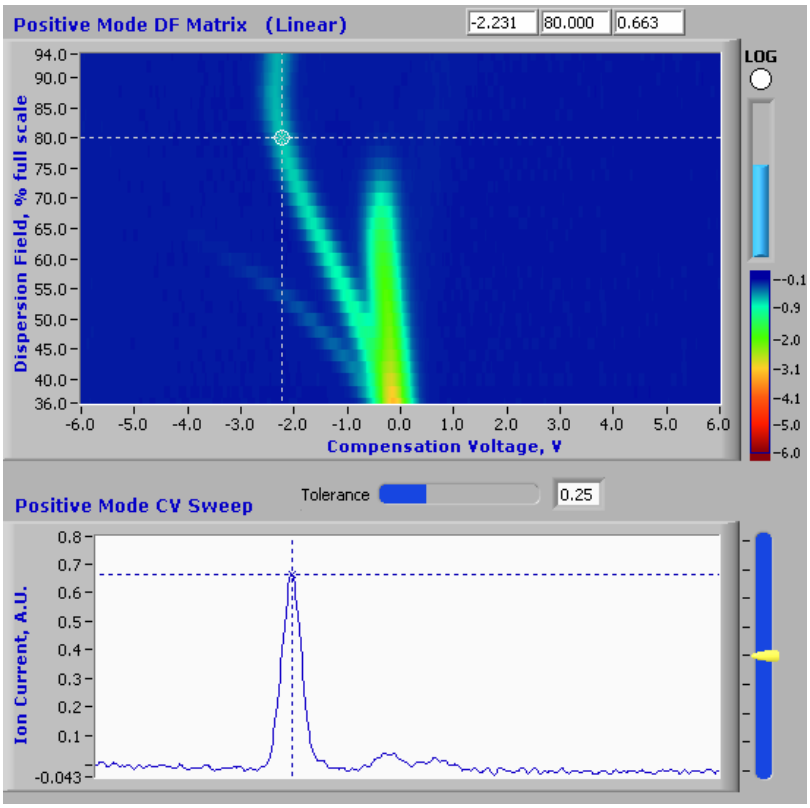


Figure 54 Placing a waypoint on a 50 ppm 4-Mel spectrum.

Save the rule in a folder that also contains the folders of DF matrices taken from known concentrations of the analyte (see 2.11.1).

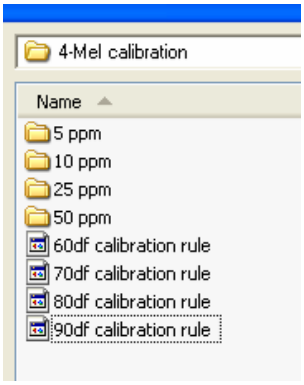


Figure 55 Correct file structure for saving the calibration rule.

6.4 Extracting and handling results

Use the EasyExtract function in EasySpec Rule Builder to create a results.csv file as described in Section 2.11. For each of the DF matrices, this gives the ion current at the waypoint.

Open results.csv in Excel or another spreadsheet program. The peak height is given in the column headed AUmax. Use Excel to plot peak height vs. concentration, as shown in Figure 56.

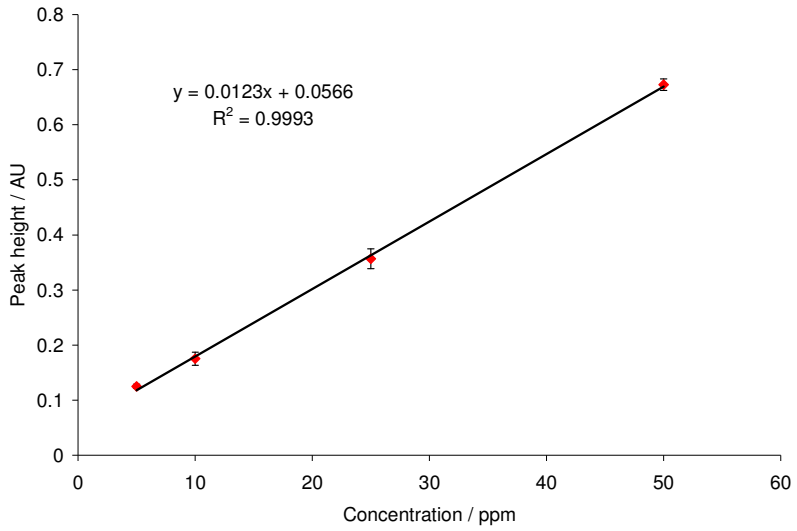


Figure 56 Calibration curve for 4-MeI between 5 ppm and 50 ppm.

6.5 Selecting a position to place the waypoint

Different positions along the analyte peak might give slightly different relationships between concentration and peak height. In Figure 57, four calibration curves are plotted together, derived from the same set of 4-MeI data. The waypoint for the different calibration rules was placed at 60% DF, 70% DF, 80% DF or 90% DF.

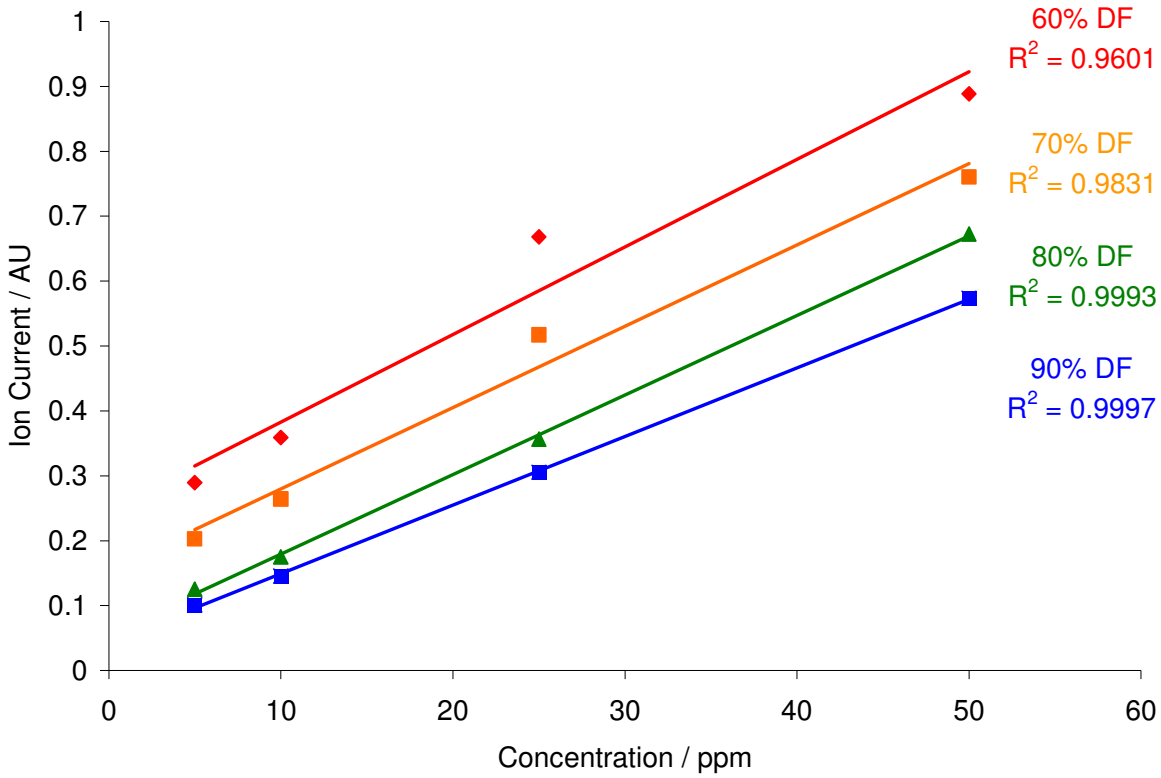


Figure 57 Comparison of the linearity of the calibration curve for 4-Mel, for calibration rule waypoints at different values of DF.

As can be seen, the relationship between peak height and concentration, for this concentration range, was more linear for higher DF values of the waypoint. A waypoint placed at 80% or 90% DF would be suitable in this situation.

It is also useful to put the waypoint in a position that gives the greatest resolution between the analyte peak and any nearby background peaks.

6.6 Calculating concentrations from unknown samples

To calculate the concentration of an unknown sample, first take data from it with a Lonestar using the same experimental setup as used for the calibration.

Extract the peak height at the waypoint from the DF matrices using EasyExtract, as above.

Average the peak height values from the set of matrices and use the trend line equation to calculate the concentration of the analyte in this sample.

7 Calibration for Online Concentration Monitoring

To use the Analyser tab in the Lonestar software, a calibrated concentration rule is added to the configuration file (application). When data is taken using the Analyser tab, the concentration of the analyte in question will be returned.

An overview of this method is given in Section 7.1. Explanations of terms used are given in sections 7.3, 7.4 and7.5. A description of setting up the calibrated concentration is given in Section 7.7.

7.1 Overview of concentration monitoring setup

An overview of the method used to set up concentration monitoring is shown in Figure 58.

Sets of DF matrices are taken from sample inputs at three or more concentrations of the relevant analyte. As in the offline method in Section 6, a rule is created with a single waypoint on the analyte peak. Peak height vs. concentration is extracted and graphed in Excel (or a similar program) to give a linear equation.

A .csv file can then be created with waypoints spanning the concentration range. The peak height of each waypoint is calculated from the linear equation.

Each waypoint is given a weighting factor (see Section 7.4) determined by the concentration.

The waypoints are now imported into a new rule (see Section 2.9). The scaling factor for the rule (see Section 0) is determined and the unit of concentration is set.

When the concentration-monitoring rule is completed, it can be added to the configuration file (using Application Builder, see Section 3).

New samples are analysed using Lonestar Analyser, which immediately gives the concentration of the analyte.

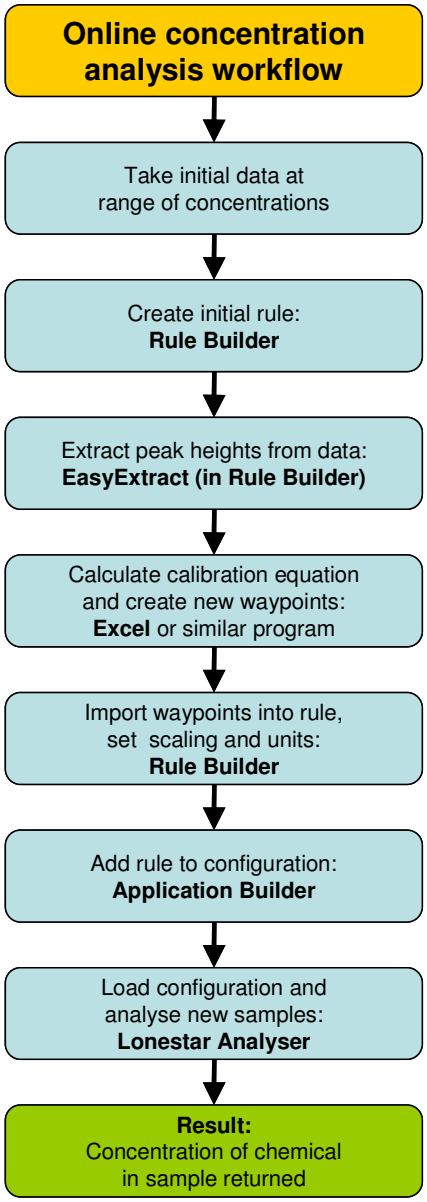


Figure 58 Creating and using an online concentration rule in EasySpec

7.2 Using the Lonestar Analyser tab

Figure 59 and Figure 60 illustrate the use of the Lonestar Analyser tab to measure the concentration of an analyte. For a more detailed guide, see the Lonestar manual.

The green bar at the top of the screen shows that the operating conditions are OK. (For information on how to set the operational limits, see Section 5.4.)

Next, the cleanliness of the system is confirmed by pressing the “Check clean” button. A DF matrix will be taken, checking the ion current in the relevant areas for contamination peaks, and a red or green light is returned.

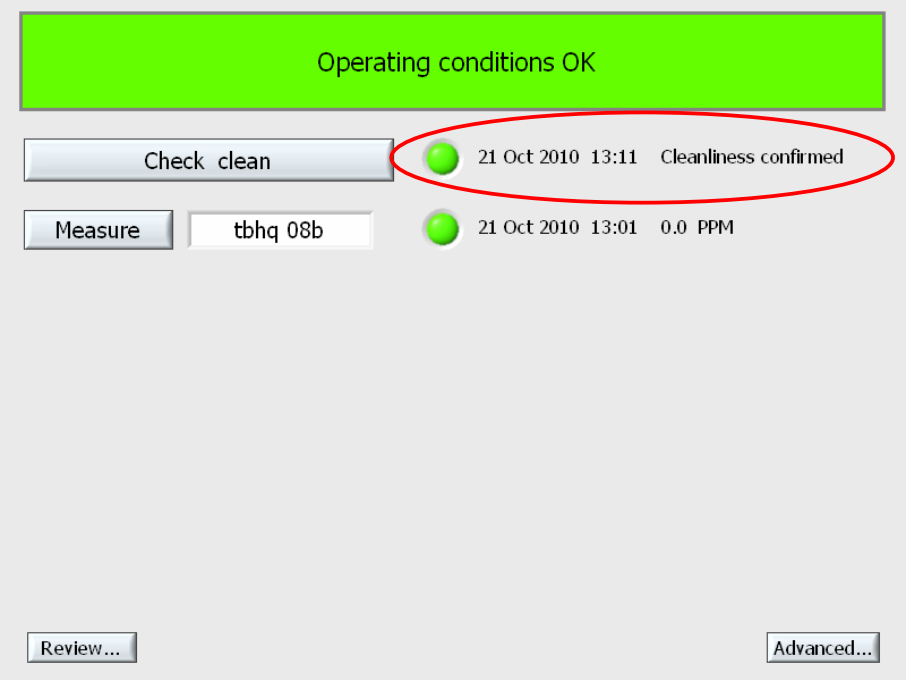


Figure 59 The Lonestar Analyser tab: cleanliness is confirmed.

In this example there is only one analyte to measure. The name of the analyte is shown in the panel by the “Measure” button. The sample is put into the sample conditioning manifold and “Measure” is pushed. Again, the Lonestar takes one DF matrix and at the same time compares it to the concentration rule. The concentration is returned immediately. There is also a red or green light response, which can be adjusted as described in Section 3.5, for a visual sign of contamination.

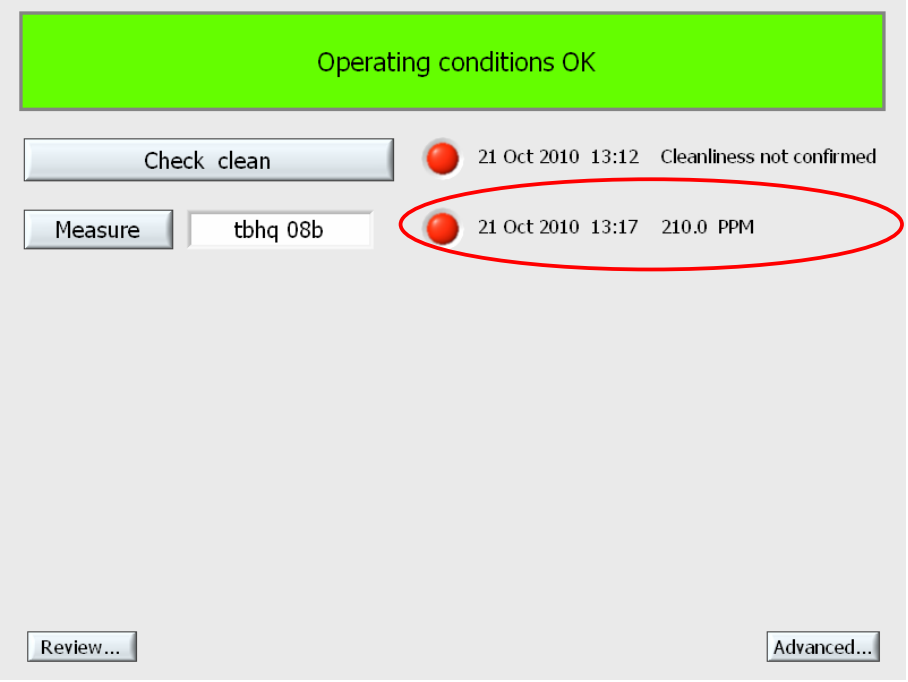


Figure 60 The Lonestar Analyser tab: returning the concentration of the analyte TBHQ.

7.3 Multiple concentrations

As with any calibration, at least three concentrations of the relevant analyte should be used to set up the concentration monitoring. It is important that the peak that is monitored is one that increases with increased concentration. If not, EasySpec concentration monitoring will not be suitable for this analyte.

Generally speaking, the monomer peak of a chemical is a better choice for calibration than the dimer peak. At low levels, the monomer peak height will increase linearly with concentration, before becoming saturated at higher levels.

7.4 Weighting factor

HCl demo positive

	A	B	C	D
1	-0.2812	24	1.336054	1
2	-0.47647	28	0.741676	1
3	-0.03013	32	0.259453	1
4	-0.42068	32	0.277154	1
5	-0.00223	36	0.186682	1
6	-0.50437	36	0.177526	1
7	-0.08592	28	0.365078	1
8	0.081461	40	0.076937	1
9	-0.64385	40	0.132176	1

Figure 61 Exported waypoints, showing columns for CV, DF, ion current and weighting factor.

When a set of waypoints is exported from a rule and saved as a .csv file, the result looks like Figure 61. Each line represents one waypoint, showing the following information:

Compensation Voltage (V)	Dispersion Field (%)	Ion Current (AU)	Weighting factor

The weighting factor determines how much weight to give each waypoint when analysing results. A waypoint with a weighting of 2 counts twice as much as one with a weighting of 1.

Weighting factors for exported waypoints can be edited in the .csv file. This can then be saved and the waypoints re-imported into a rule.

7.5 Scaling and units

The scaling and unit inputs in Rule Builder (see Figure 62) allow you to set the correlation between the number of waypoints triggered by a DF matrix and the figure calculated for concentration.

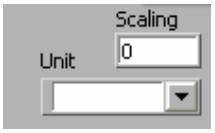


Figure 62 Scaling and unit inputs.

The unit can be set using the drop-down menu to PPM, PPB or %. Alternatively, a suitable unit can be typed in.

7.6 Weighting and scaling combined

When analysing the results, the weighting factor determines how much each waypoint counts for. This can be set differently for different waypoints.

The scaling relates the number of waypoints in the rule that are triggered to the concentration given. This is the same for the whole rule.

The concentration is calculated as follows:

Concentration = (scaling)(weighting factor 1)(number of these waypoints triggered)
+ (scaling)(weighting factor 2)(number of these waypoints triggered)
+ (scaling)(weighting factor 3)(number of these waypoints triggered)
+ …

It is usually easiest to set the scaling to 1 and adjust the weighting accordingly.

If scaling is set to 0, no concentration data will be given.

Individual waypoints in a rule can be weighted to give correct concentration data. For example, a waypoint with a weighting factor of 5 is treated as 5 waypoints when setting the scaling.

In a case where 5 waypoints were set with a weighting of 1, and another waypoint was set with a weighting of 5, the total number of waypoints would be treated as (5 × 1) + (1 × 5) = 10.

If the output required was simply a percentage, out of 100%, then:

- **either** scaling could be set to 10 (= 100 / 10) and units set to be %;
- **or** the weightings of the waypoints could be set to 10, 10, 10, 10, 10 and 50, giving a total of 100. The scaling would be 1 and units would be %.

7.7 Calculating the calibration curve and setting the waypoints

As described in Sections 6.2 to 6.4 for offline concentration monitoring, the online method begins by taking data at three concentrations of the analyte. A single-waypoint rule is created with the waypoint on the peak at a suitable position (see Section 6.5). The peak height and concentration are plotted against one another and an equation of the relationship is derived. This is illustrated in Figure 63.

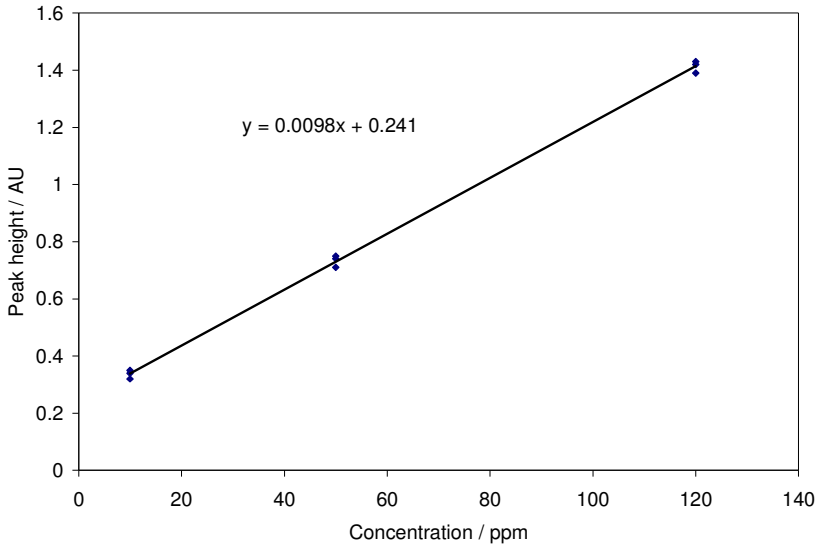


Figure 63 A graph of peak height vs. concentration giving the equation: y = 0.0098x + 0.241.

A set of waypoints that spans the range can be created in Excel, by listing the concentration values and calculating the theoretical peak height that would be produced. See Figure 64.

	A	B	C
1	Concentration	Peak height	
2			
3	10	= 0.0098 * A3 + 0.241	
4	15	0.388	
5	20	0.437	
6	25	0.486	
7	30	0.535	
8	35	0.584	
9	40	0.633	
10	45	0.682	

Figure 64 Calculating peak heights for intermediate concentrations.

Finally, the waypoints are listed and saved in a new .csv file as shown in Figure 65.

As before, the columns represent:

Compensation Voltage (V)	Dispersion Field (%)	Ion Current (AU)	Weighting factor

	A	B	C	D
1	-0.5	82	0.339	10
2	-0.5	82	0.388	5
3	-0.5	82	0.437	5
4	-0.5	82	0.486	5
5	-0.5	82	0.535	5
6	-0.5	82	0.584	5
7	-0.5	82	0.633	5
8	-0.5	82	0.682	5
9	-0.5	82	0.731	5
10	-0.5	82	0.78	5
11	-0.5	82	0.829	5
12	-0.5	82	0.878	5
13	-0.5	82	0.927	5
14	-0.5	82	0.976	5
15	-0.5	82	1.025	5
16	-0.5	82	1.074	5
17	-0.5	82	1.123	5
18	-0.5	82	1.172	5
19	-0.5	82	1.221	5
20	-0.5	82	1.27	5
21	-0.5	82	1.319	5
22	-0.5	82	1.368	5
23	-0.5	82	1.417	5
24				

Figure 65 Waypoints for online concentration rule.

Note that the CV and DF for each waypoint are the same, because they are layered on top of one another.

The first waypoint has the weighting 10, because if only this waypoint has been triggered then the concentration of the analyte in the sample is 10 ppm.

Subsequent waypoints are weighted at 5, because the concentration has a precision of 5 ppm.

The scaling should be set to 1 and the units to ppm.

As an example, say a sample is analysed with this rule. At a CV of -0.5 V and DF of 82%, it is found to give an ion current of 0.71 AU.

This would trigger the first 8 waypoints in the rule. The concentration would be calculated as so:

(1 ppm x 1 waypoint x 10 weighting/waypoint)

+ (1 ppm x 7 waypoints x 5 weighting / waypoints)

= **45 ppm**.

If the concentration falls below the lower limit of the calibration, it will be shown as 0 ppm.

If the concentration falls higher than the upper limit, it will be shown as whatever value the upper limit is (here, 120 ppm).