95-0011 User Guide- TD-GC-Lonestar: Offline data processing using the FAIMS Viewer Lonestar GC software

Contents

1 Introduction

The purpose of this document is to provide a guide on how to process data offline which has been captured from a TD-GC-Lonestar system, using the **91-0259 FAIMS Viewer Lonestar GC** software.

This document will explain how to

- set up and launch the “FAIMS Viewer”,
- load matrix files generated by the Lonestar system
- generate plot overlays using the “Multi-ROI” function integrated in the software
- export the plot overlay data into MS Excel.

2 Definitions

Abbreviation/Term	Definition
FAIMS	Field Asymmetric Ion Mobility Spectrometry
DF	Dispersion Field
LNS	Lonestar
RIP	Reactant Ion Peak
SOP	Standard Operation Procedure
CV	Compensation Voltage
CF	Compensation Field

3 Procedure

3.1 How to install and launch the FAIMS Viewer.

3.1.1 The FAIMS Viewer software is packed in a compressed zip. file named **91-0259 FAIMS Viewer Lonestar GC**

FAIMS Viewer software download instructions are located within Owlstone Medical's Knowledge Base. Please click here to access our guidance, or visit www.owlstonemedical.com, click on Support, and search for FAIMS Viewer.

Unzip the file to extract the folder containing the software files (Figure 1)

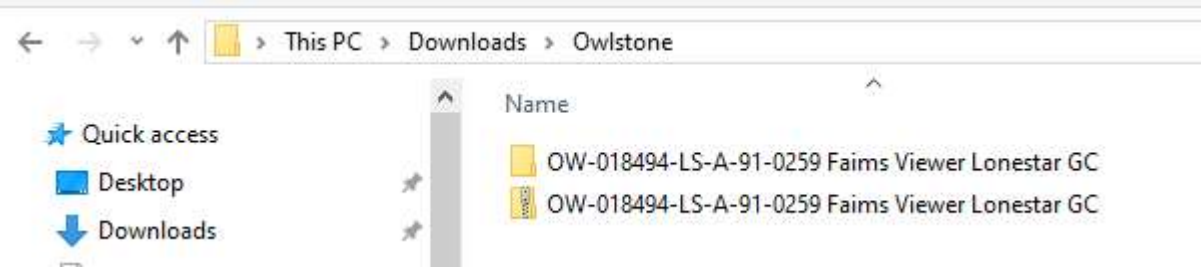


Figure 1. 91-0259 FAIMS Viewer Lonestar GC software pack. The file folder is generated by extracting the zip file.

3.1.2 The folder generated will contain several files. Find the “FaimsViewer” application file (Figure 2) by using the “Search” box and execute it to launch the software.

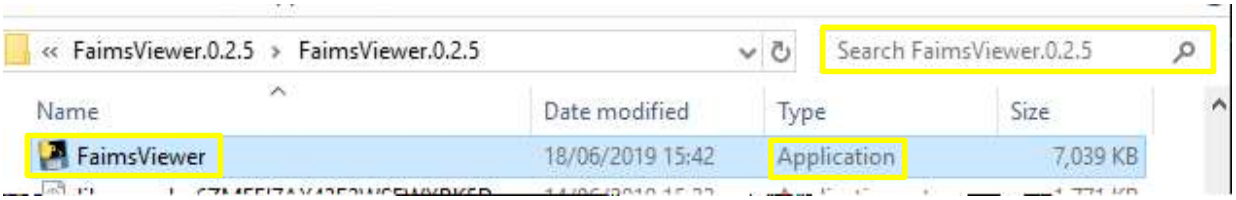


Figure 2. FaimsViewer launcher. Create a short cut and place it in the desktop for future data processing.

3.1.3 If using Windows 10, in the “Windows Defender” box you may need to select “more info” and then “Run Anyway”.

3.1.4 A black window will pop up and after a few seconds, the FAIMS Viewer interface will appear (Figure 4). Click on both “*ROI*” buttons to display the positive and negative mode 2D CV sweep.

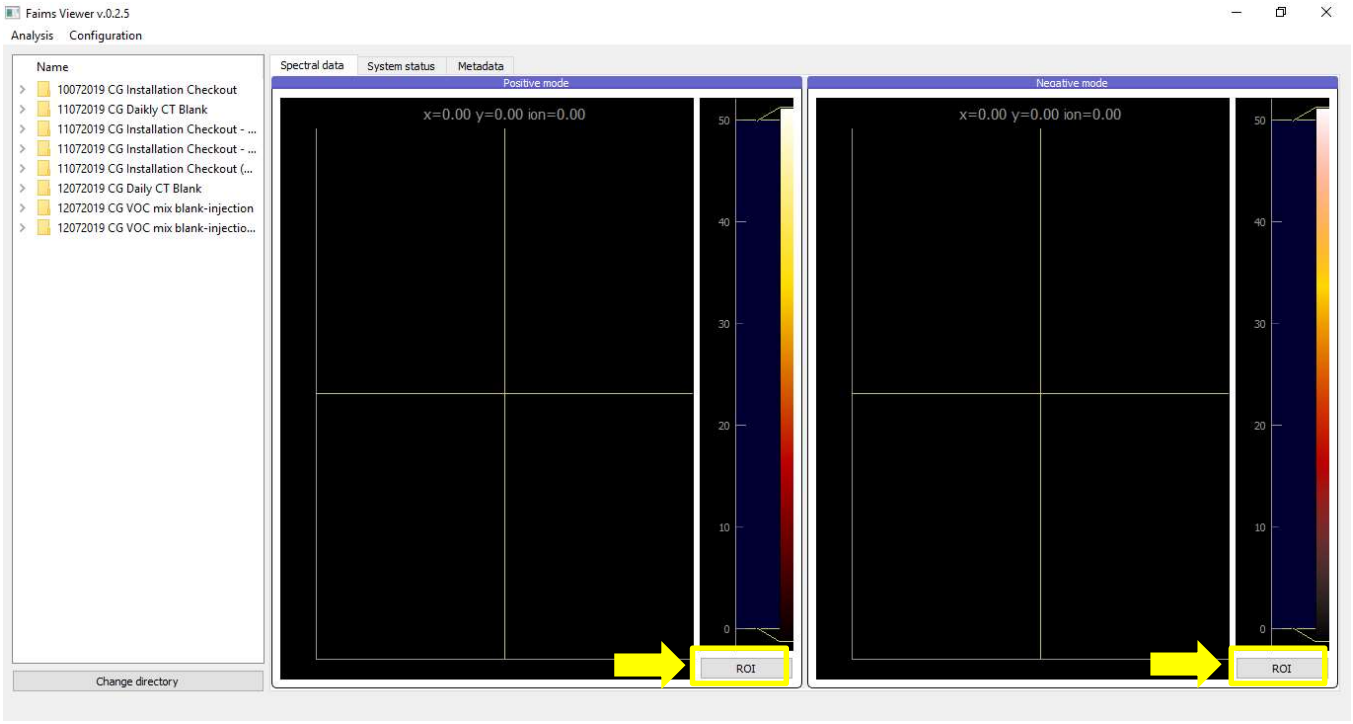


Figure 3. FAIMS Viewer launcher interface. Click on both “ROI” buttons.

3.1.5 The software is now ready to be used. The FAIMS Viewer main interface is shown in Figure 4.

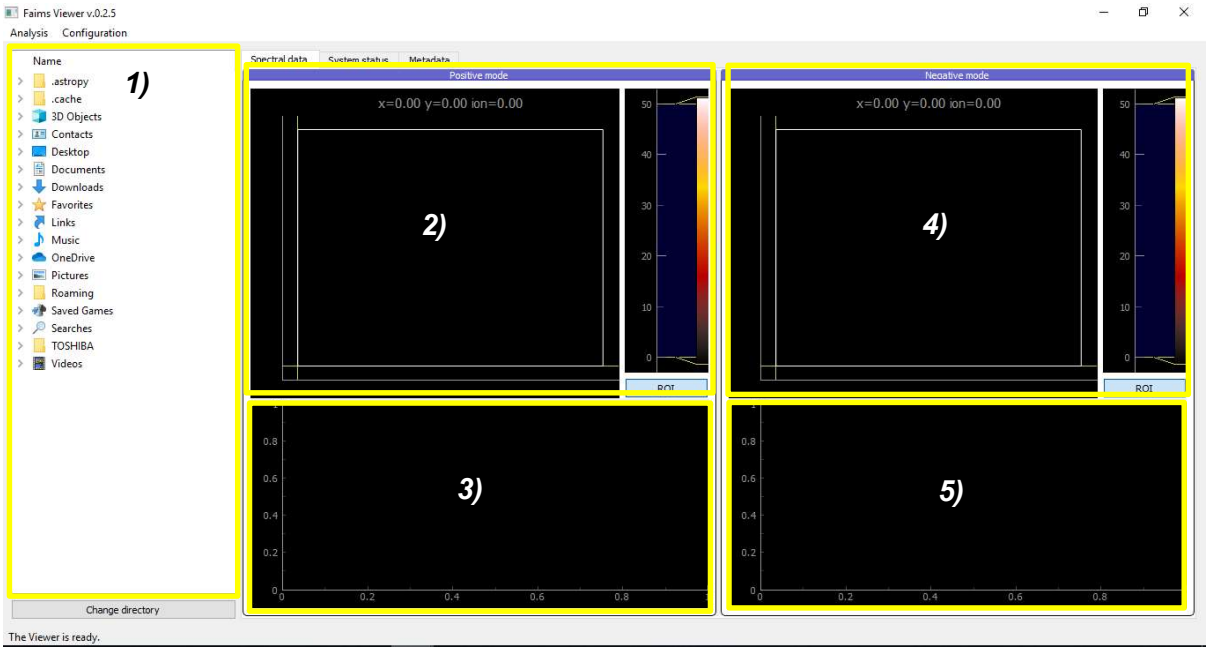


Figure 4. FAIMS Viewer interface. Press the ROI button to display the 2D CV sweep graphs. The interface is divided in 5 main sections: 1) File directory panel – used to select matrix files, 2) Positive mode DF matrix viewer with ion current adjuster column, 3) Positive mode 2D CV sweep, 4) Negative mode DF matrix viewer with ion current adjuster column, and 5) Negative 2D CV sweep.

3.2 How to load DF matrices onto the FAIMS Viewer.

3.2.1 Use the left panel to find the folder and select the matrix file to be loaded onto the viewer (Figure 5). Once found, click on the matrix file. The matrix will be loaded after a few seconds. The file path is displayed at the top of the interface. The message “Processing done”, located at the bottom of the interface, confirms the file loading has been completed.

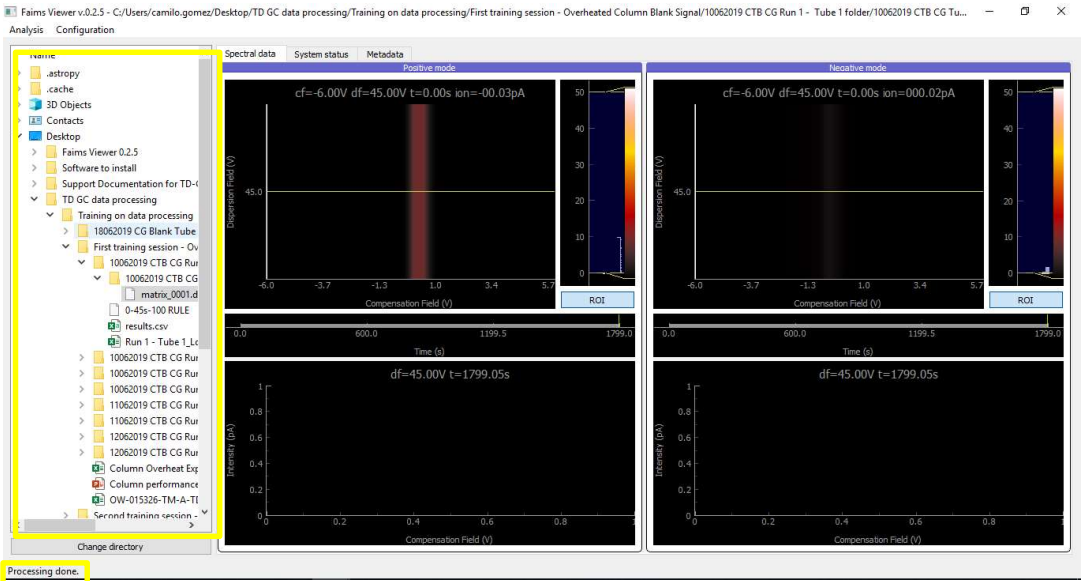


Figure 5.How to load a matrix file. The top banner shows the file path and document being displayed. The bottom bar message describes the current status of the software.

3.2.2 Right click on the positive mode DF matrix displayed and select 3D Visualization > Fixed axis > Dispersion Field. The Dispersion Filed (V) - Compensation Field (V) plot will be replaced with the Compensation Field (V) - Time (s) plot (Figure 6).

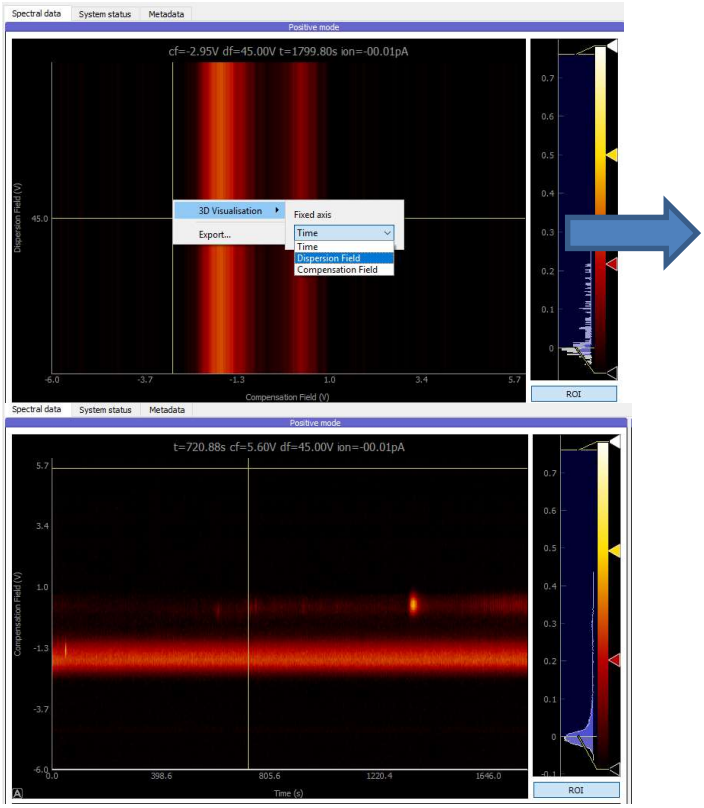


Figure 6. How to display the Compensation Field (V) – Time (s) plot. If the "3D Visualization" option does not appear, right click on the positive mode 2D CV sweep plot (box number 3 in Figure 3) and then right-click back gain on the 3D matrix. The 3D visualization option should now appear.

3.2.3 In order to visualize the matrix, adjust the bar panel located to the right of the positive DF matrix viewer (Figure 7).

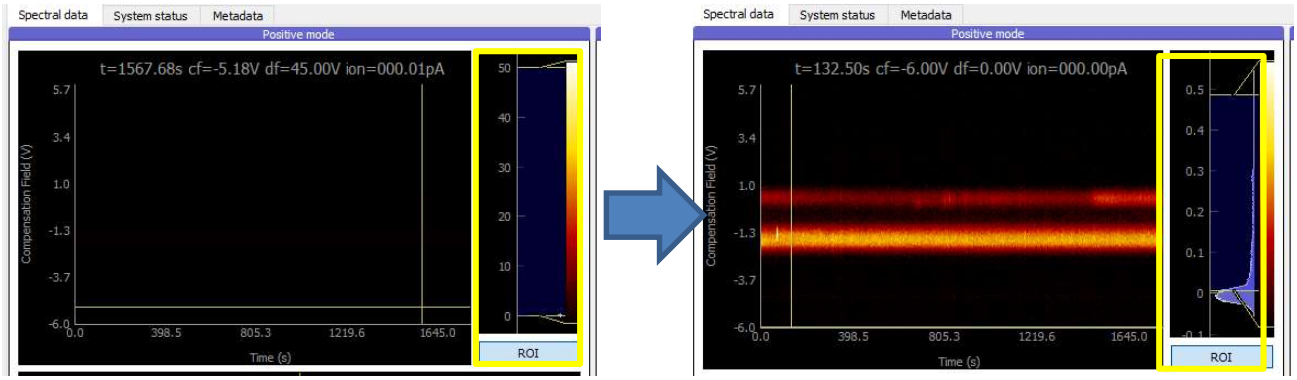


Figure 7.How to visualize the DF matrix. It is possible to change the colour scheme by right-clicking on the coloured bar.

3.2.4 Select a cf in the positive DF matrix viewer to display a chromatogram (Intensity over retention time) in the 2D CV sweep plot (Figure 8). Do not select the cf within the RIP's area.

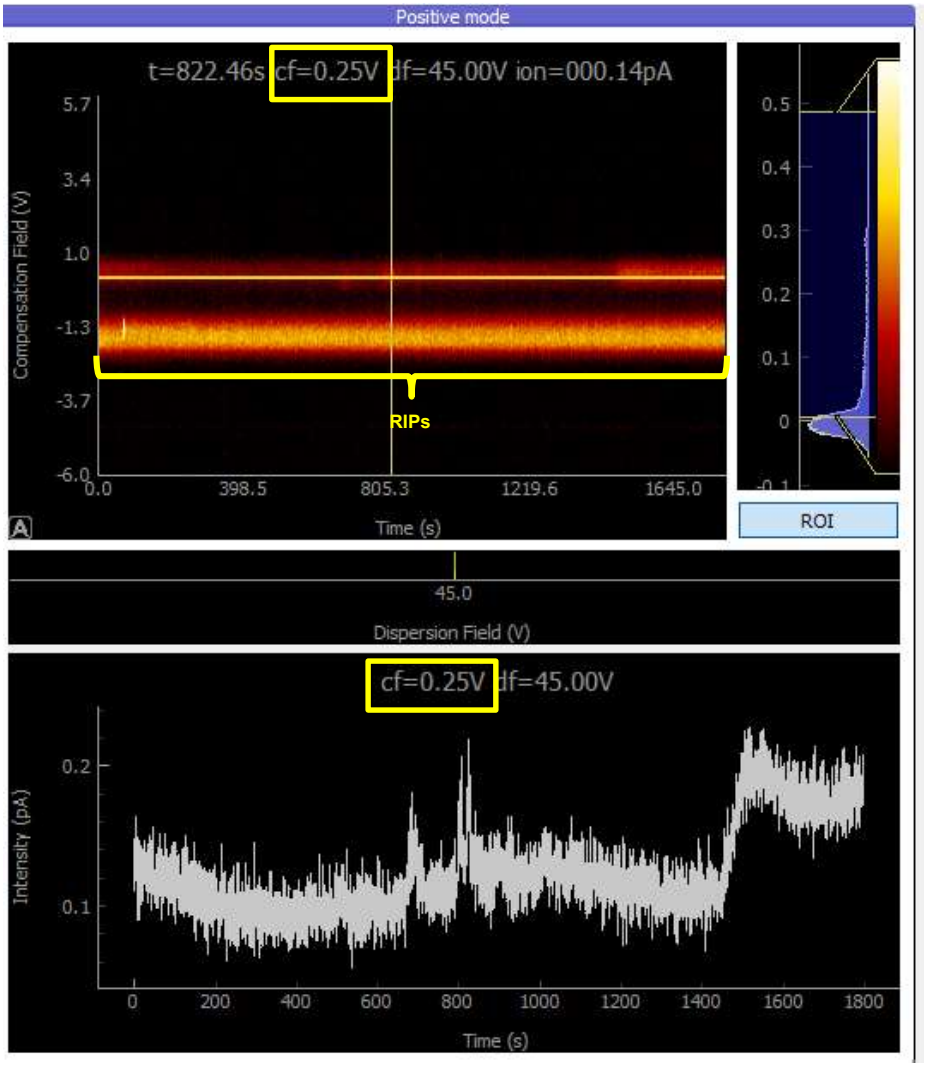


Figure 8. Chromatograph visualization. In this example, the chromatograph corresponds to a cold trap blank. Notice scaling on Intensity axis will be automatically adjusted.

3.3 How to generate plot overlays using the "Multi-ROI" option.

3.3.1 Follow steps described in sections from 3.2.1 to 3.2.4 3.2.4 to visualize a chromatograph. Right-click on the positive mode 2D CV sweep and select "Add to Multi-ROI". Enter the name of the series and press "OK" (Figure 9).

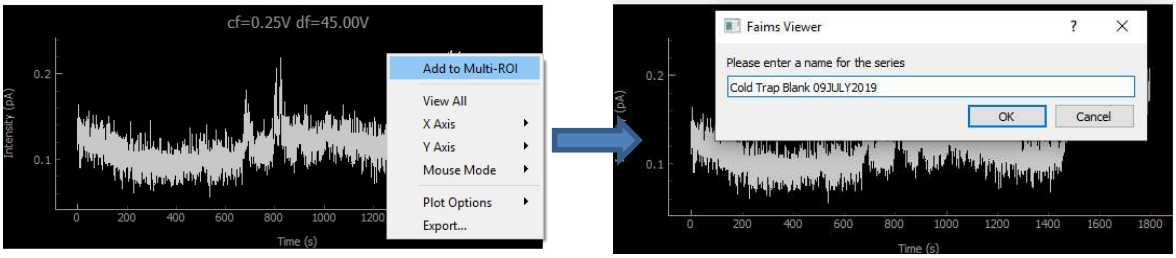


Figure 9. How to add a chromatograph plot in the overlay. In this example a cold trap blank will be used.

3.3.2 The negative mode side screen will be covered by the “Multi-ROI” plot, in where the CV sweep graph will be plotted and labelled with the name entered (Figure 10). Double-click on the “Multi-ROI” tab at the top to open a single window for the overlay.

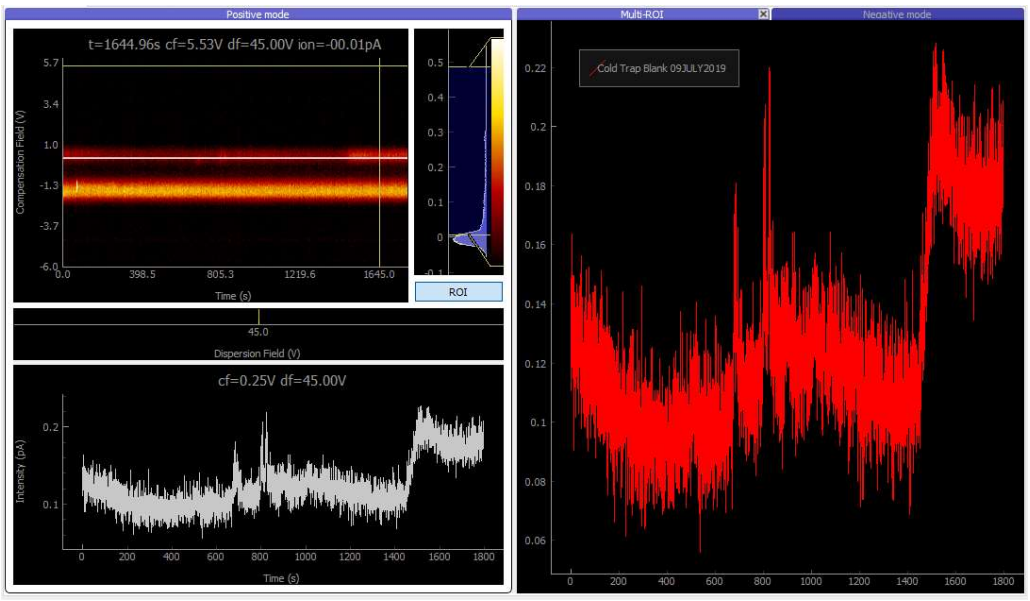


Figure 10. Generation of a chromatograph overlay. Notice scaling will be adjusted automatically. Series labels can be moved.

3.3.3 Repeat the process to add new series to the Multi-ROI plot (Figure 11). Maintain the same cf when adding more chromatograph series. This also applies for the negative mode. Note: when loading the second matrix, it is required to return the 3D Visualization back to “time” and then to “dispersion field” it is also required to right click down so that the menu.

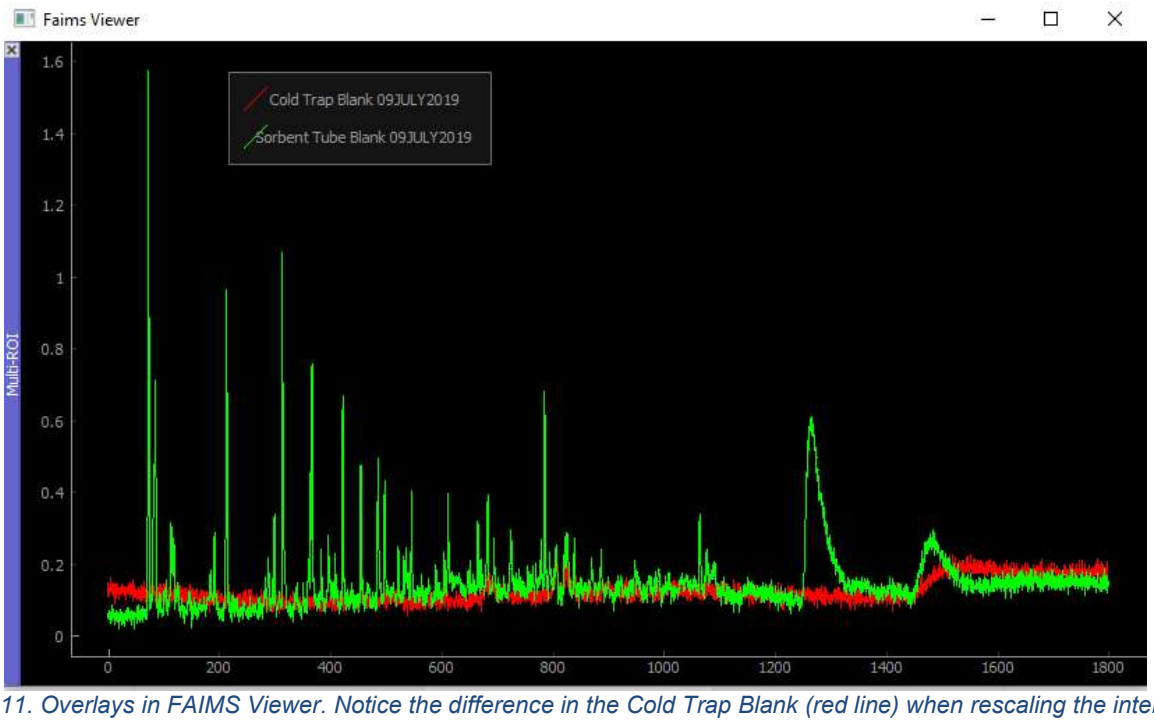


Figure 11. Overlays in FAIMS Viewer. Notice the difference in the Cold Trap Blank (red line) when rescaling the intensity axis (y).

3.4 How to export data to Excel.

3.4.1 To export to a excel (.csv) file, right click on the Multi-ROI plot, select “Export”. Select “CSV from plot data” and click on export (Figure 12) Select the file location and the excel file name. The Multi-ROI plot can be exported either by using the “Export” option or by coping using the computer screenshot command.

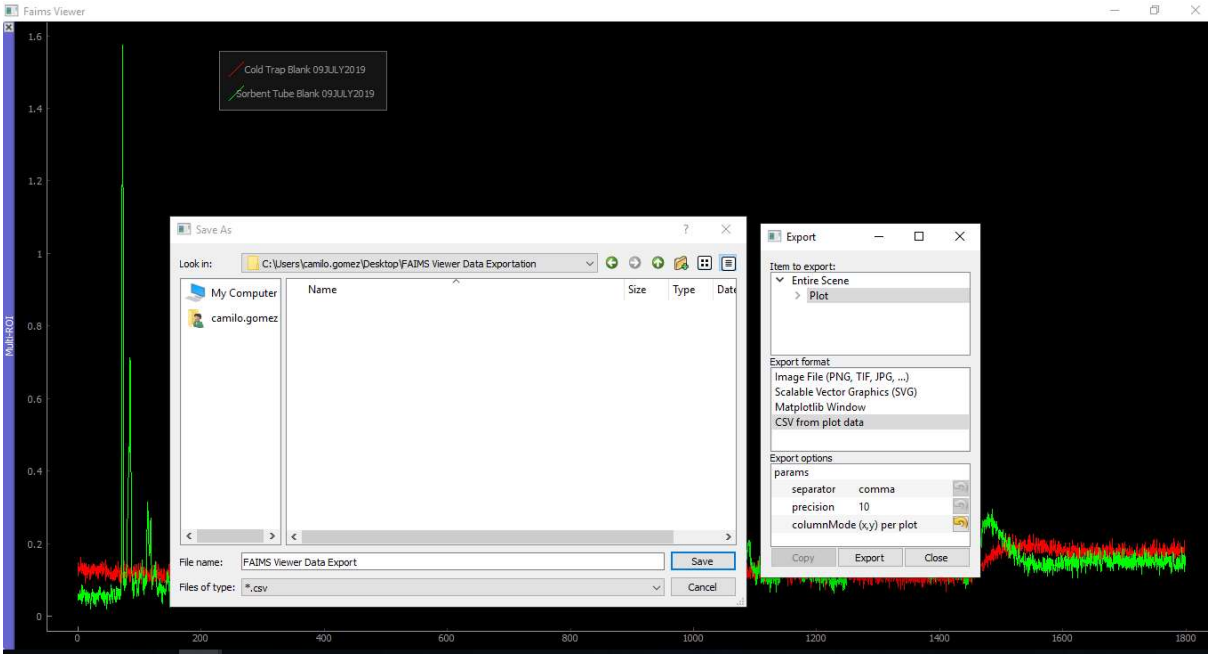
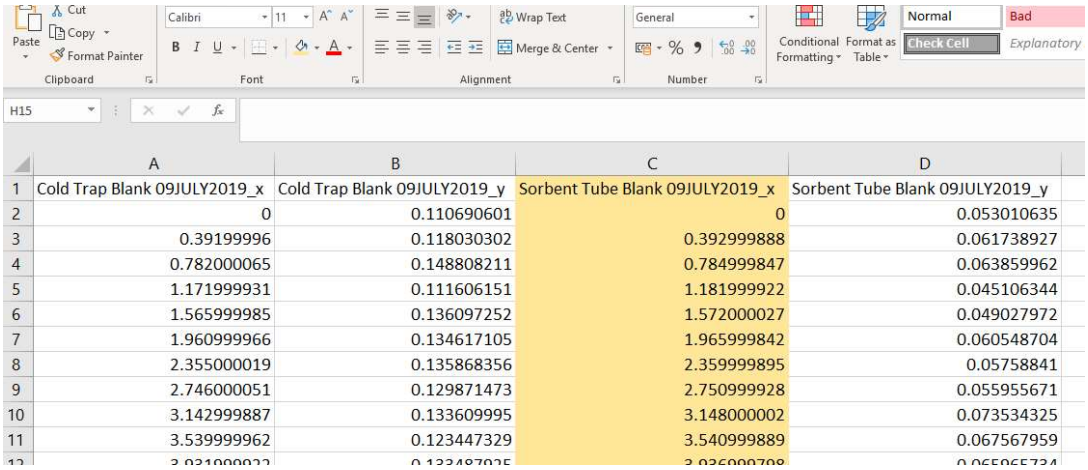


Figure 12. Data export function. Select “CSV from plot data” to export into Excel format.

3.4.2 Save the Excel CSV file as an Excel Workbook.

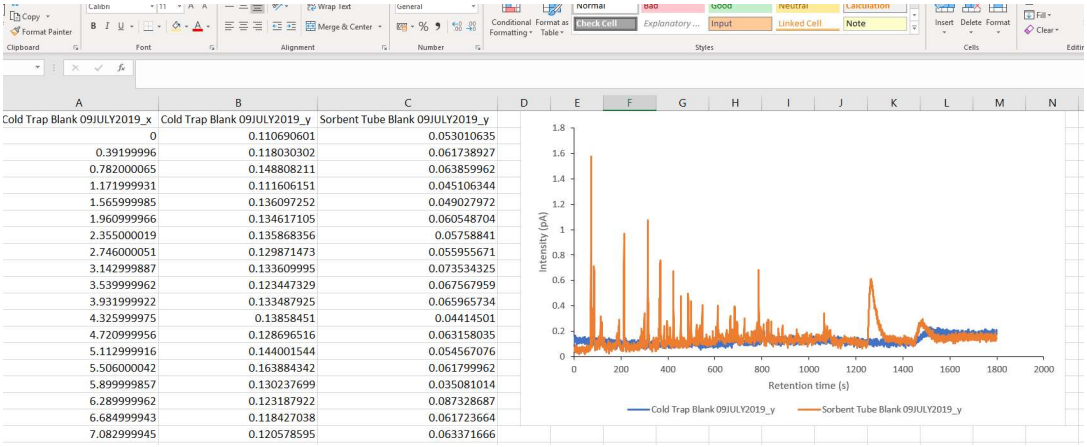
3.4.3 The same Multi-ROI plot can be obtained from the excel file exported. Open the Excel file generated. As the x-axis (retention time in seconds) for both matrices are the same, only one x-axis values column is required (Figure 13).



	A	B	C	D
1	Cold Trap Blank 09JULY2019_x	Cold Trap Blank 09JULY2019_y	Sorbent Tube Blank 09JULY2019_x	Sorbent Tube Blank 09JULY2019_y
2	0	0.110690601	0	0.053010635
3	0.39199996	0.118030302	0.392999888	0.061738927
4	0.782000065	0.148808211	0.784999847	0.063859962
5	1.171999931	0.111606151	1.181999922	0.045106344
6	1.565999985	0.136097252	1.572000027	0.049027972
7	1.960999966	0.134617105	1.965999842	0.060548704
8	2.355000019	0.135868356	2.359999895	0.05758841
9	2.746000051	0.129871473	2.750999928	0.055955671
10	3.142999887	0.133609995	3.148000002	0.073534325
11	3.539999962	0.123447329	3.540999889	0.067567959

Figure 13. Excel file generated. The x axis is the retention time in seconds, which is same for all the series overlaid. The column in yellow can be deleted/omitted when performing further statistical analysis.

3.4.4 In this example, select the three columns. On Excel, go to “insert”, and select “scatter plot with straight lines”. The plot generated will be the same as the one displayed on the FAIMS Viewer (Figure 14).

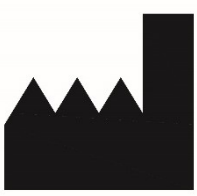


Cold Trap Blank 09JULY2019_x	Cold Trap Blank 09JULY2019_y	Sorbent Tube Blank 09JULY2019_y
0	0.110690601	0.053010635
0.39199996	0.118030302	0.061738927
0.782000065	0.148808211	0.063859962
1.171999931	0.111606151	0.045106344
1.565999985	0.136097252	0.049027972
1.960999966	0.134617105	0.060548704
2.355000019	0.135868356	0.05758841
2.746000051	0.129871473	0.055955671
3.142999887	0.133609995	0.073534325
3.539999962	0.123447329	0.067567959
3.931999922	0.133487925	0.065965734
4.325999975	0.13858451	0.04414501
4.720999956	0.128696516	0.063158035
5.112999916	0.144001544	0.054567076
5.506000042	0.163884342	0.061799962
5.899999857	0.130237699	0.035081014
6.289999962	0.123187922	0.087328687
6.684999943	0.118427038	0.061723664
7.082999945	0.120578595	0.063371666

Figure 14. Data analysis on Excel: chromatograms overlay.

4 Contacts and support

Owlstone Medical Ltd is dedicated to providing excellent support.
For all technical and safe use question relating to this manual, contact as at:



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