



90-0632 Lonestar® Data Export for Multivariate Analysis Using an Excel Macro

Issue/Version	Date	Author	Details
AAA	26/07/2016	Aditya Malkar	The Original
AAB	27/07/2016	Céline Lainé	Reformat. Complete introduction. Detail DF matrix data exporting procedure.
AAC	08/08/2016	Aditya Malkar	Complete missing screenshots and corresponding instructions.
AAD	08/08/2016	Céline Lainé	Complete instructions #8 and 18.
AAE	11/08/2016	Céline Lainé	Add Excel macro part number for reference.
001	11/08/2016	Andrew Pauza	Tidy formatting, change software request links, release as 001

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Introduction

This document outlines the process for exporting Lonestar® Dispersion Field (DF) matrix data for multivariate statistical analysis (MVA).

This procedure takes place in three steps:

1. Export Lonestar® DF matrix file using the Owlstone® Advanced Matrix Viewer Software.
2. Open the exported Lonestar® DF matrix file in an Excel spreadsheet.
3. Re-arrange the Owlstone® Excel spreadsheet, Part Number 90-0634, using the Excel macro to create a suitable format for multivariate statistical analysis.

The Excel macro converts the exported 3-dimensional DF matrix into a data string, as explained in Figure 1 Overview of the data re-arrangement.

The Excel spreadsheet, Part Number 90-0634, is available by submitting a request through our support site. <http://support.owlstonenanotech.com/entries/23207721-Request-Software>

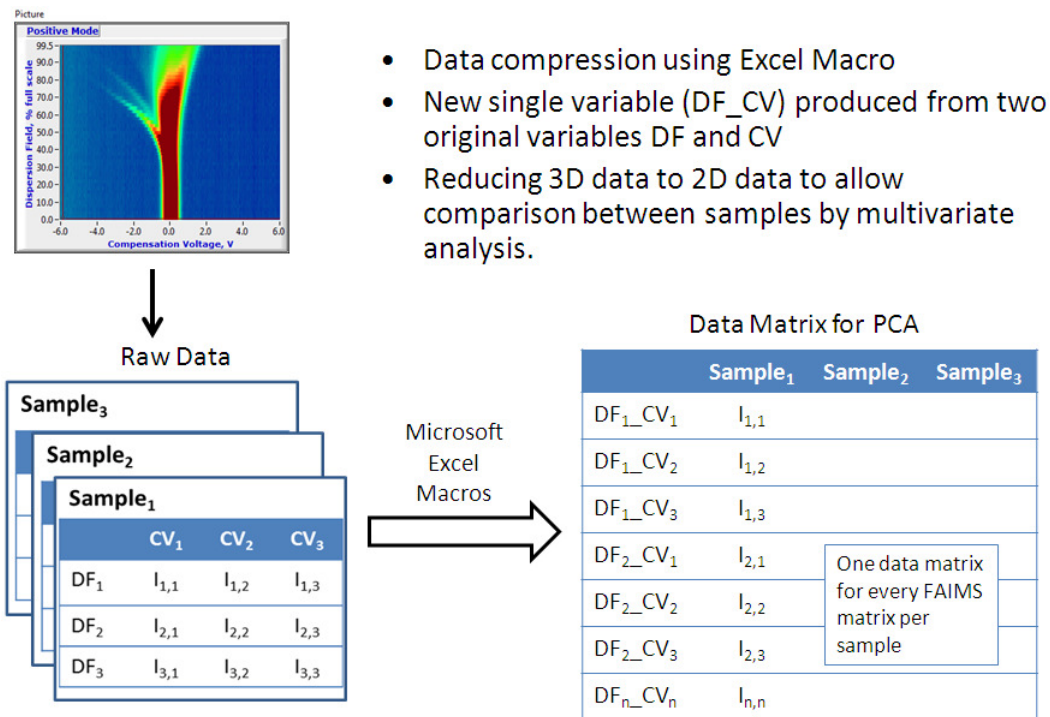



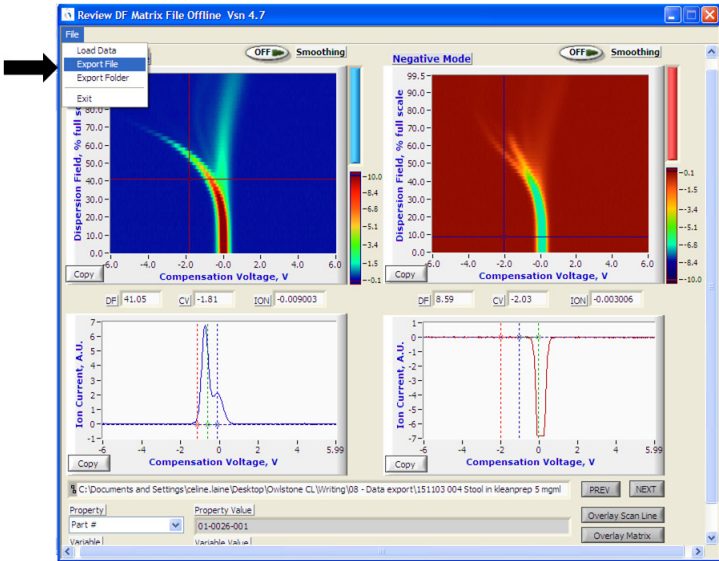
Figure 1 Overview of the data re-arrangement

Instructions

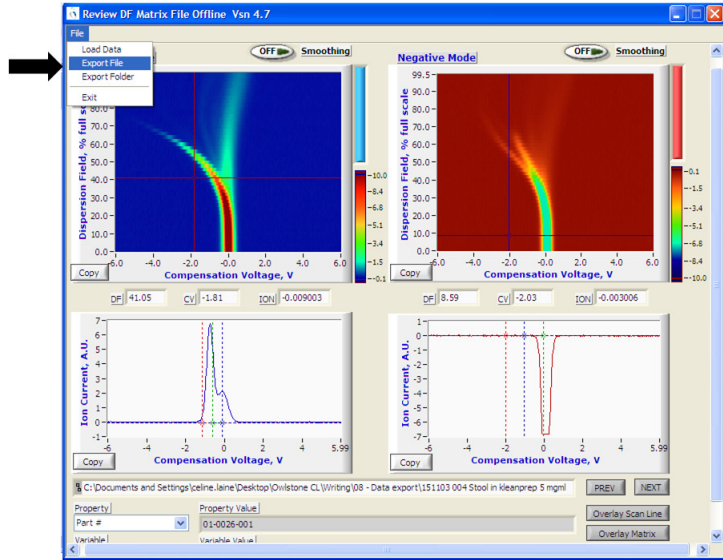
The instructions below detail the procedure to export Lonestar® DF matrix data for multivariate statistical analysis.

Instructions can be divided in three major steps:

1. Export Lonestar® DF matrix file.
2. Open exported Lonestar® DF matrix file in Excel.
3. Re-arrange the Excel spreadsheet.

Step #	Instructions	Pictures
<h2 style="margin: 0;">Export Lonestar® DF matrix file</h2> <p style="margin: 0;">Exporting DF matrix files using the Owlstone® Advanced Matrix Viewer Software results of the creation of a text file containing data collected on the Lonestar® analyser.</p>		
1	<p>Exporting a Lonestar® DF matrix file can be realised using the Lonestar® Advanced Matrix Viewer software.</p> <p>This software can be requested from Owlstone® if not already installed.</p>	 <p style="margin-top: 20px;">Link to Owlstone® website: http://support.owlstonenanotech.com/entries/23207721-Request-Software</p>
2	<p>On the user's computer, open the Advanced Matrix Viewer (may also be called "Offline Viewer")</p> <p>In the Review DF Matrix File Offline window, load data of interest by selecting File / Load data.</p>	

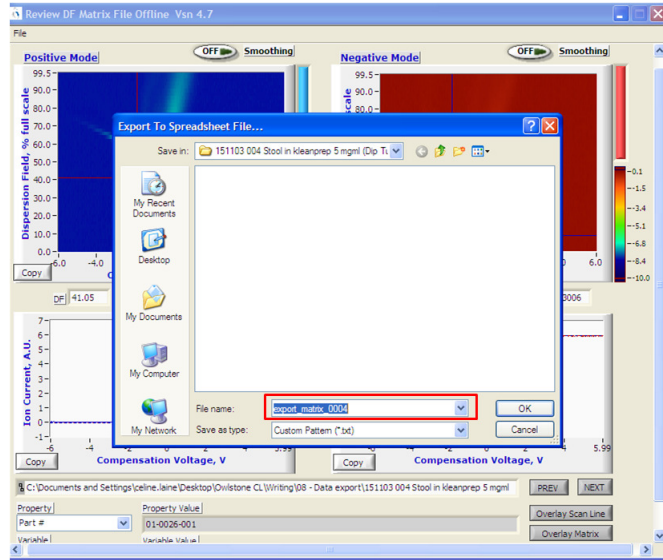
Once the data file has been loaded, export it by selecting **File / Export file.**



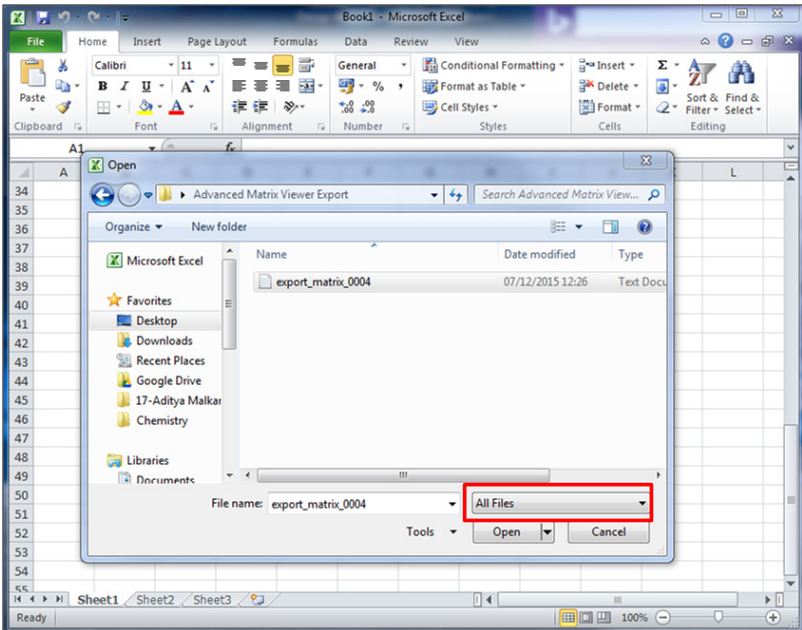
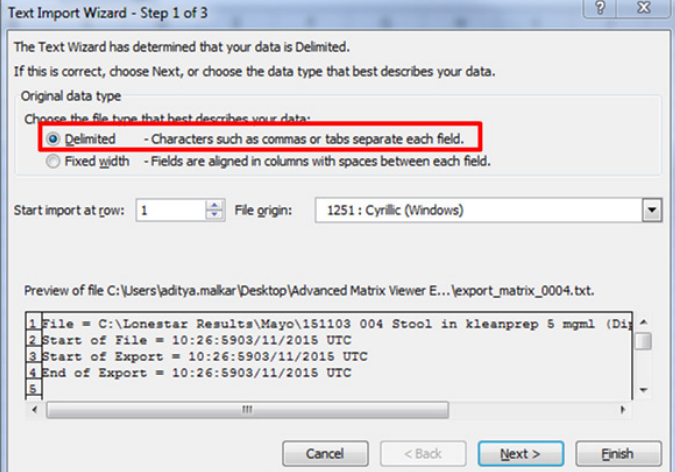
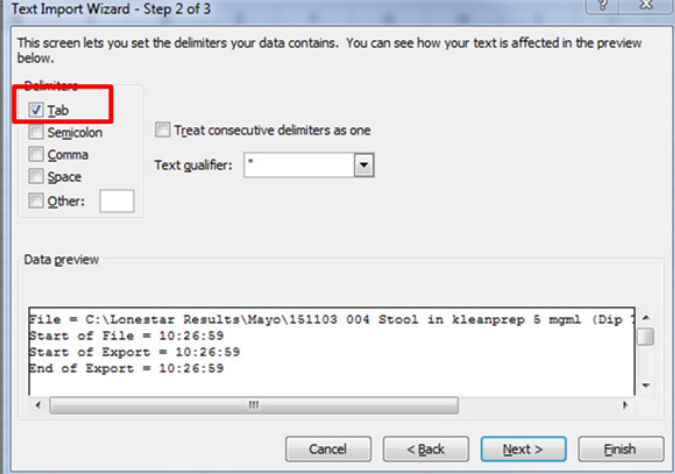
4

A window called **Export to Spreadsheet File** opens with the corresponding text file automatically named `export_matrix_xxx`.

Pressing the **OK** button will add the `export_matrix_xxx` text file into the DF matrix file loaded previously.

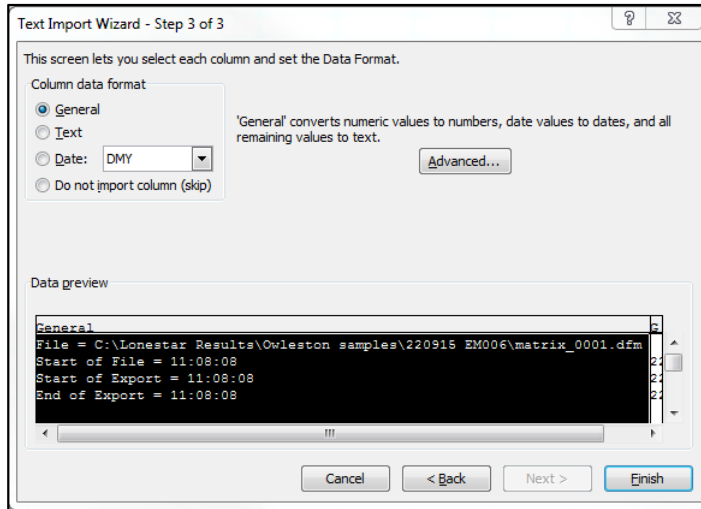


Open exported DF matrix file in Excel

<p>5</p> <p>The exported DF matrix file is a text document that can be opened in Excel.</p> <p>Open Excel and click File / Open.</p> <p>In the separated window named Open, navigate to the DF matrix file of interest.</p> <p>Make sure to select All Files in Files of types to see the export_matrix_xxx text file.</p> <p>Press the Open button.</p>	
<p>6</p> <p>In the Text Import Wizard window, Step 1 of 3 is to select the Delimited option to get characters such as commas or tabs separating each field.</p> <p>Press the Next button.</p>	
<p>7</p> <p>In the Text Import Wizard window, Step 2 of 3 is to select the Tab option as delimiter.</p> <p>This should open up the exported data matrix in the required format in Excel.</p> <p>Press the Next button.</p>	

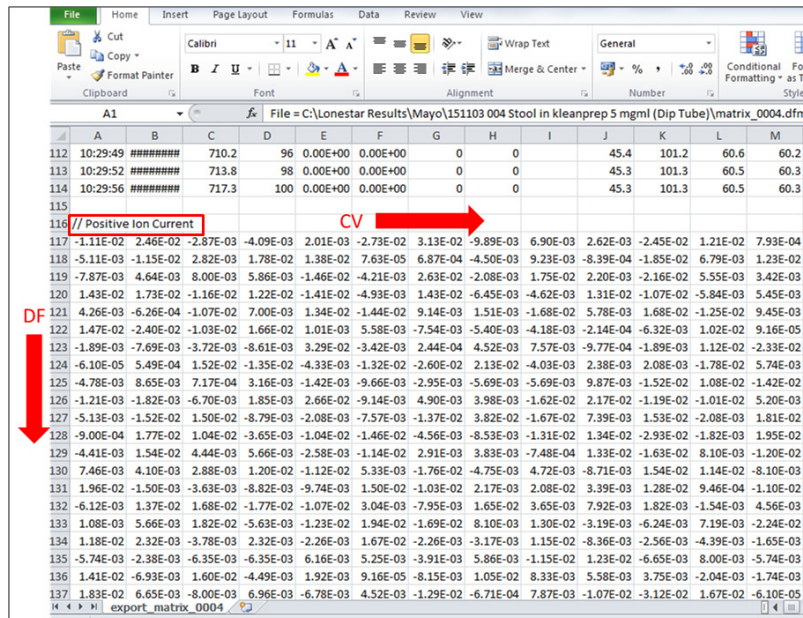
8 The **Text Import Wizard** window, Step 3 of 3 opens, select the **Finish** button.

The exported DF matrix file contains all the raw data as well as all the Lonestar® analyser metadata (i.e. temperature, pressure, flow...) associated with data collection.

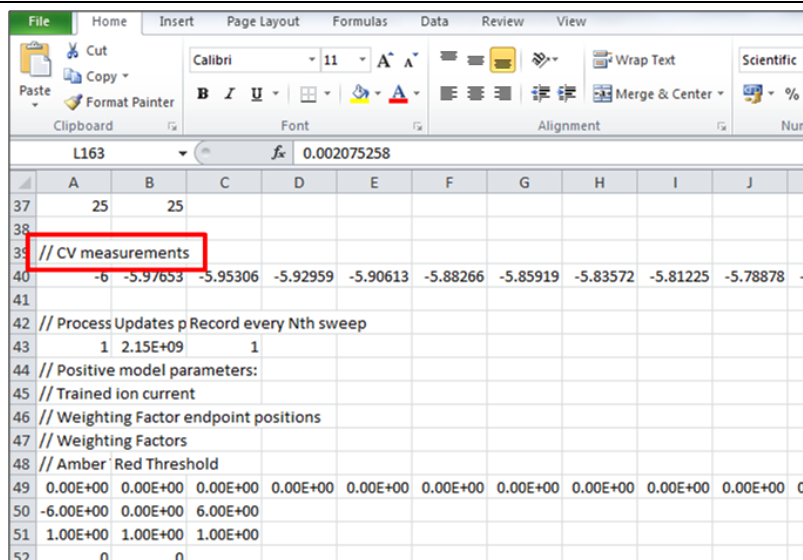


9 In the Excel spreadsheet export_matrix_xxx tab, scroll down to the raw data in the file. These are divided as **Positive Ion Current** and **Negative Ion Current**.

The Compensation Voltage (CV) values are on the X-axis whereas the DF values are on the Y-axis (both without the header row and column).



10 The actual values for the CV measurements can be found under the header **//CV measurements**.



11

The actual values for the percentage DF measurements are found under the header **DF%**.

	A	B	C	D	E	F	G	H	I	J	K	L	M
58	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
59	-6.00E+00	0.00E+00	6.00E+00										
60	1.00E+00	1.00E+00	1.00E+00										
61	0	0											
62													
63	// Process	UTdate	El	d	DF(%)	Positive	ic Negative	Positive A	Negative	Event	File	Motherbo	Filter Tem
64	09:20:11	#####			0	0.00E+00	0.00E+00	0	0			46.9	101.1 59.8 53.4
65	09:20:14	#####			3.3	2	0.00E+00	0.00E+00	0	0		47	101 59.8 54.7
66	09:20:18	#####			7.7	4	0.00E+00	0.00E+00	0	0		46.9	101 59.8 55.9
67	09:20:21	#####			10.4	6	0.00E+00	0.00E+00	0	0		46.9	101 59.8 56.7
68	09:20:25	#####			14.1	8	0.00E+00	0.00E+00	0	0		47	101.2 59.8 57.4
69	09:20:28	#####			17.7	10	0.00E+00	0.00E+00	0	0		47	101.3 59.9 57.9
70	09:20:32	#####			21.3	12	0.00E+00	0.00E+00	0	0		47	101.4 59.9 58.3
71	09:20:35	#####			24.9	14	0.00E+00	0.00E+00	0	0		47.1	101.4 59.9 58.5
72	09:20:39	#####			28.5	16	0.00E+00	0.00E+00	0	0		47.1	101.4 60 58.7
73	09:20:42	#####			32.1	18	0.00E+00	0.00E+00	0	0		47.1	101.4 60.1 58.9
74	09:20:46	#####			35.7	20	0.00E+00	0.00E+00	0	0		47.1	101.4 60.1 59.2
75	09:20:49	#####			39.3	22	0.00E+00	0.00E+00	0	0		47.1	101.3 60.2 59.1
76	09:20:53	#####			42.9	24	0.00E+00	0.00E+00	0	0		47.1	101.4 60.2 59.2
77	09:20:56	#####			46.5	26	0.00E+00	0.00E+00	0	0		47.1	101.3 60.3 59.2

12

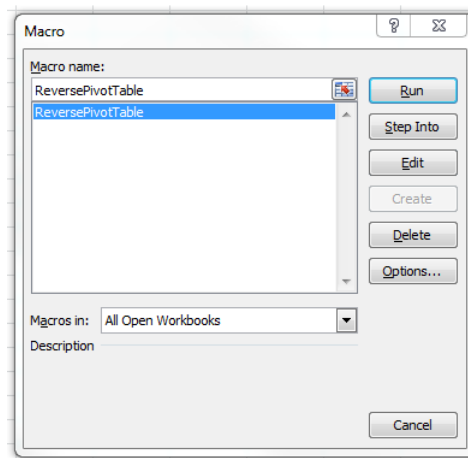
These CV and DF measurements should be copied out into the Excel spreadsheet provided by Owlstone®, Part Number 90-0634.

The Excel spreadsheet tab is named “Prep-Sheet”

	A	B	C	D	E	F	G	H	I	J	K	L	M
1													
2													
3													
4													
5													
6													
7													
8													
9													
10													
11													
12													
13													
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26													
27													

13

The Excel macro is titled **ReversePivotTable**. This can be verified by opening the Excel spreadsheet and clicking: **View / Macros / View Macros**.



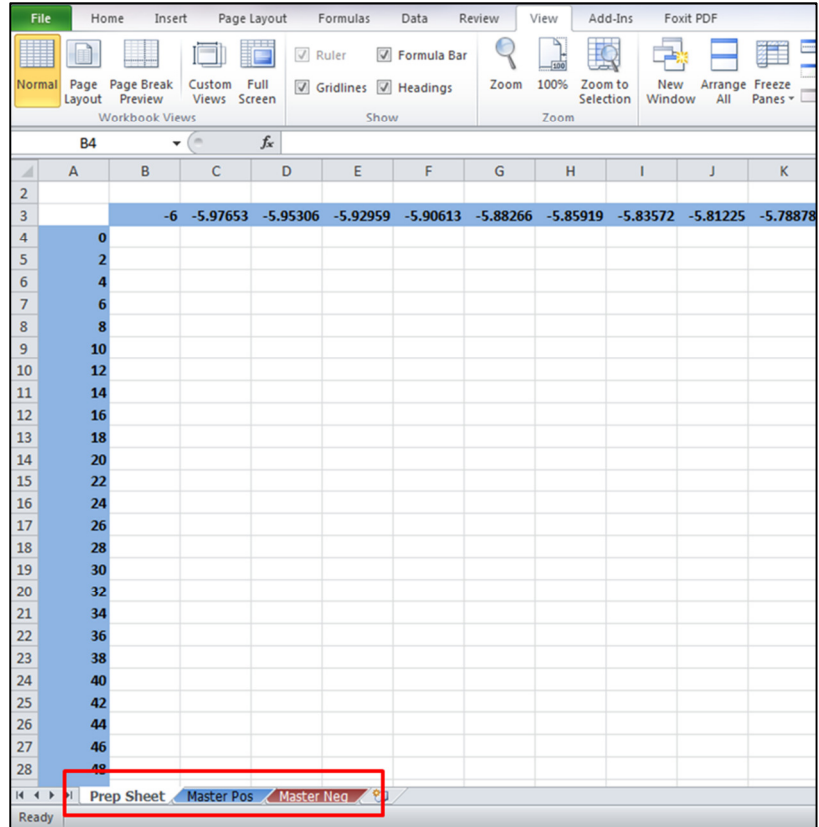
14

The worksheet will have three tabs: **Prep-Sheet, Master Pos and Master Neg.**

The Prep-Sheet contains the structure required to combine the two variables (DF and CV) to produce DF_CV variable.

The Master Pos and Master Neg sheets are available to store the resultant positive or negative mode data respectively.

N.B. These sheets can be renamed as per requirement.

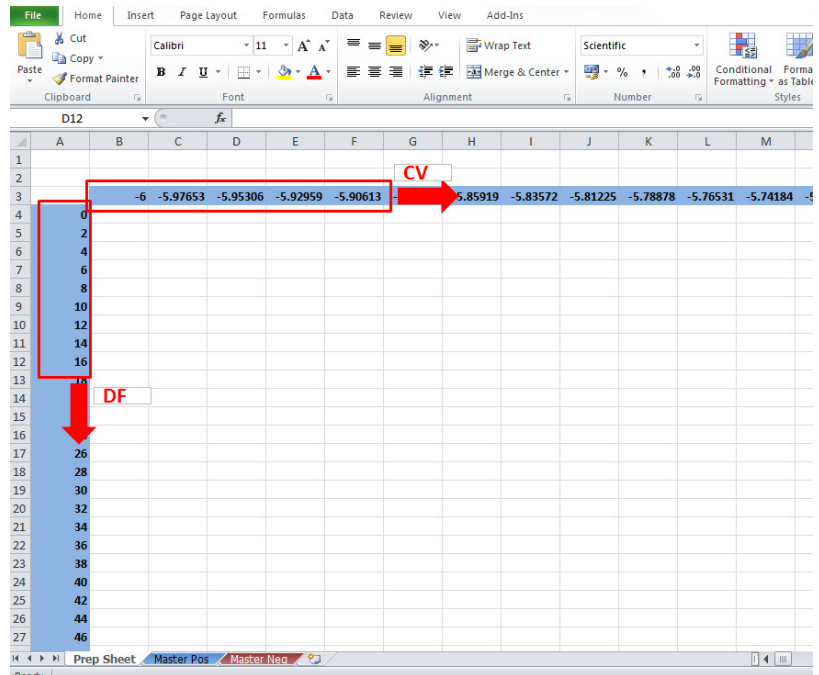


15

CV and DF values are dependent on the Lonestar® configuration parameters used for data collection.

Copying all CV and DF values in the Prep-Sheet tab needs to be performed only once for all the files acquired using the same Lonestar® configuration.

DF values should be copied in column A and CV values in row from

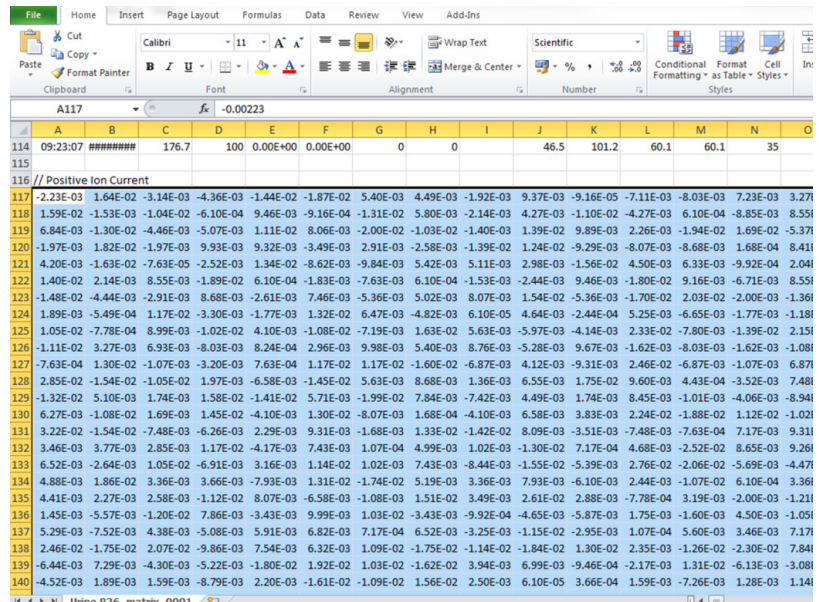


column B.

16 To start copying, select raw data in the Excel spreadsheet containing the export_matrix_xxx tab.

Scroll down to raw data and copy the entire positive or negative mode data (as per requirement).

Tip: Hold down Control + shift and use arrow keys to select the data to make the process of copying easier.

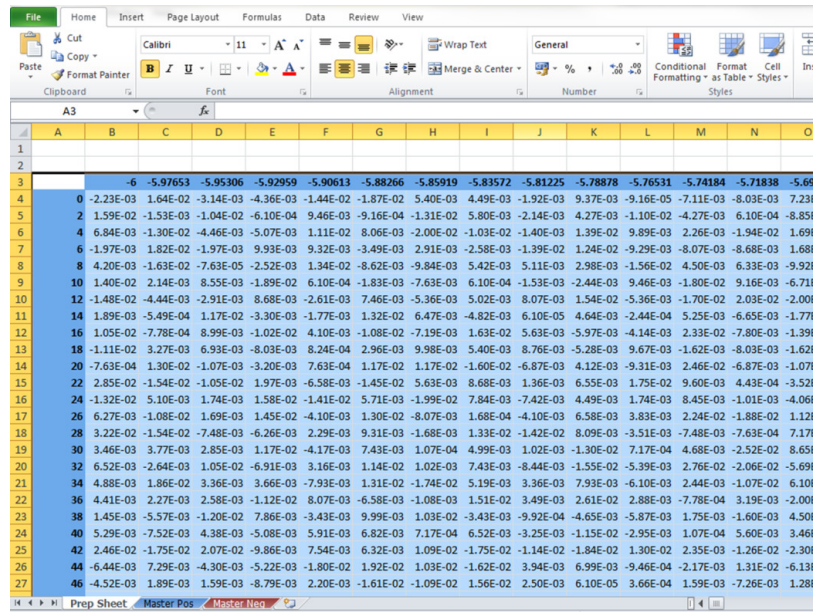


17 Paste the copied data in the Excel spreadsheet, Part Number 90-0634, containing the macro.

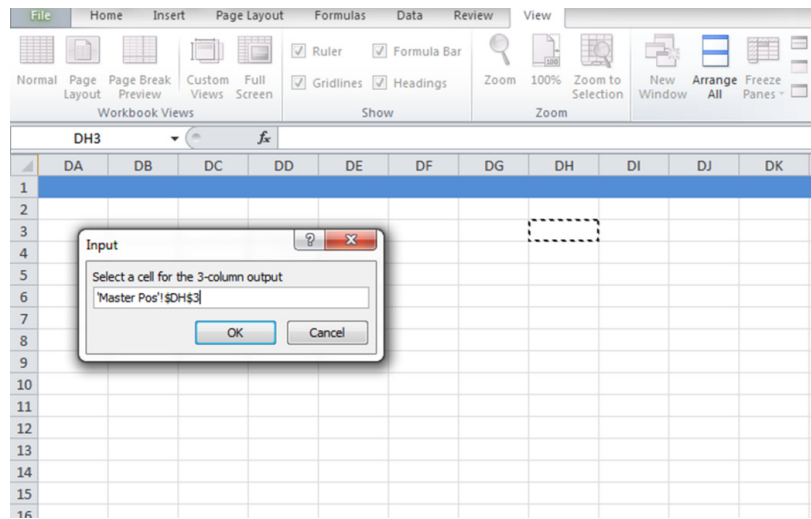
Make sure to paste selected raw data into the Prep-Sheet tab.

To convert the 3D data into a data string, select the pasted data along with the headers (CV and DF).

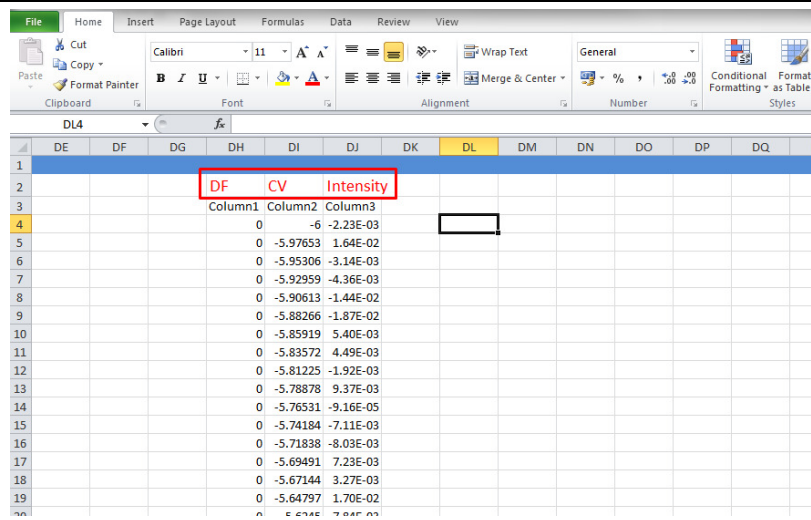
Select **View / Macros / Show Macros**



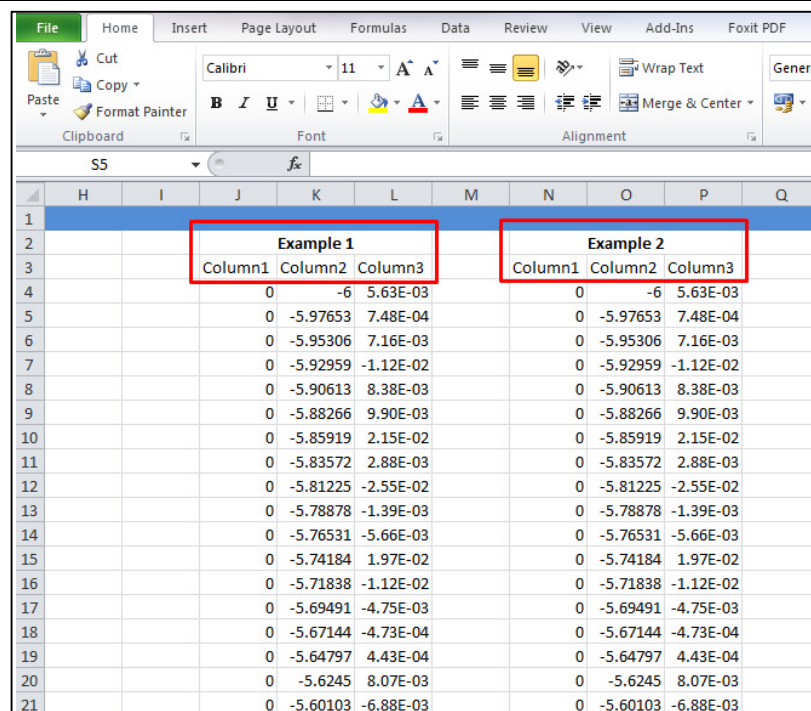
18 Select **Run Macro** in the dialogue box.
 This will produce a second dialogue box which will prompt to select a three-cell-output.
 Select an output cell in either the positive mode or the negative mode sheet in the Excel worksheet as applicable.



19 On clicking **OK** after selecting the appropriate output destination, the macro will run and produce an output.
 The intensity column can be renamed as required (e.g. sample name).

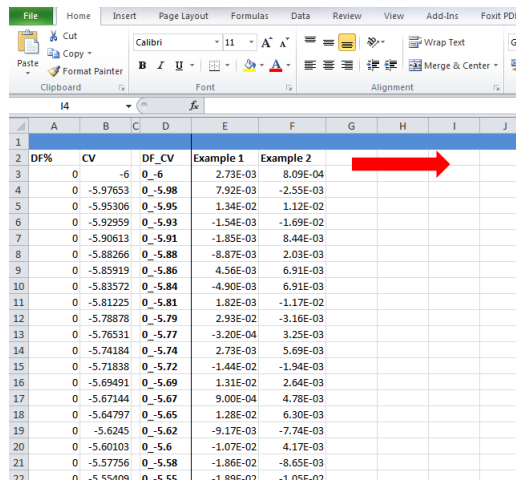


20 This data re-arrangement can be repeated for all samples for both positive and negative modes.



21

The resultant data strings (column 3, Intensities) can be copied in a structure suitable for multivariate analysis.



	A	B	C	D	E	F	G	H	I	J
1										
2	DF%	CV	DF_CV		Example 1	Example 2				
3	0	-6	0_-6		2.73E-03	8.09E-04				
4	0	-5.97653	0_-5.98		7.92E-03	-2.55E-03				
5	0	-5.95306	0_-5.95		1.34E-02	1.12E-02				
6	0	-5.92959	0_-5.93		-1.54E-03	-1.69E-02				
7	0	-5.90613	0_-5.91		-1.85E-03	8.44E-03				
8	0	-5.88266	0_-5.88		-8.87E-03	2.03E-03				
9	0	-5.85919	0_-5.86		4.56E-03	6.91E-03				
10	0	-5.83572	0_-5.84		-4.90E-03	6.91E-03				
11	0	-5.81225	0_-5.81		1.82E-03	-1.17E-02				
12	0	-5.78878	0_-5.79		2.93E-02	-3.16E-03				
13	0	-5.76531	0_-5.77		-3.20E-04	3.25E-03				
14	0	-5.74184	0_-5.74		2.73E-03	5.69E-03				
15	0	-5.71838	0_-5.72		-1.44E-02	-1.94E-03				
16	0	-5.69491	0_-5.69		1.31E-02	2.64E-03				
17	0	-5.67144	0_-5.67		9.00E-04	4.78E-03				
18	0	-5.64797	0_-5.65		1.28E-02	6.30E-03				
19	0	-5.6245	0_-5.62		-9.17E-03	-7.74E-03				
20	0	-5.60103	0_-5.6		-1.07E-02	4.17E-03				
21	0	-5.57756	0_-5.58		-1.86E-02	-8.65E-03				
22	0	-5.55409	0_-5.55		-1.88E-02	-1.05E-02				

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Owlstone® was formed through the recognition of the opportunities created by the application of micro- and nano- technology to develop improved sensing solutions.

Owlstone® is focused on the innovation of detection technologies to address unmet needs, developing solutions that are flexible enough to target a range of markets with the potential for growth by enabling new application opportunities.

From homeland security to home safety, Owlstone® is working with leading manufacturers and integrators across a range of markets to develop products incorporating our microchip chemical sensing solution.

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