

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							
ААВ	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. <u>http://support.owlstonenanotech.com/entries/23207721-Request-Software</u>



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					
Export Lonestar [®] DF matrix file							
Exportir text file	ng DF matrix files using containing data collec	the Owlstone [®] Advanced Matrix Viewer Software results of the creation of a ted on the Lonestar [®] analyser.					
1	Exporting a Lonestar® DF matrix file can be realised using the Lonestar® Advanced Matrix Viewer software.	Advanced matrix viewer					
	be requested from	Link to Owlstone [®] website:					
	Owlstone [®] if not	http://support.owlstonenanotech.com/entries/23207721-Request-					
	already installed.	<u>Software</u>					
2	On the user's computer, open the Advanced Matrix Viewer (may also be called "Offline Viewer") In the Review DF Matrix File Offline window, load data of interest by selecting File / Load data.	Revolvery DF. Matrix File Offline Vsn 4.7 rie Cod Data Dist Based Station Based Based </td					

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Once the data file has been loaded, export it by selecting File / Export file .	Review DF Matrix File Offline Von 4.7 Image: Comparison Voltage Regative Mode Image: Comparison Voltage Regative Mode Image: Comparison Voltage Image: Comparison Voltage <td< th=""></td<>
4 A window called Export to Spreadsheet File opens with the corresponding tex file automatically named export_matrix_xxx Pressing the OK button will add th export_matrix_xxx text file into the D matrix file loaded previously.	Index DF Matrix File Offline Vin 4.7 Image: Contrast of Contr
	Open exported DF matrix file in Excel

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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.	Text Import Wizard - Step 3 of 3 Ø S2 This screen lets you select each column and set the Data Format. Column data format @ General General converts numeric values to numbers, date values to dates, and all remaining values to text. Data greview General Data greview Data greview Eneral File = C:\Lonestar Results\Owleston samples\220915 EM006\matrix_0001.dfm Start of File = 11:08:08 Start of Export = 11:08:08 Start of Export = 11:08:08 Start of Export = 11:08:08 Cancel (multicate)
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).	Inter Page Layout Formulat Data Review View Pitt C orgy Diff I
10	The actual values for the CV measurements can be found under the header //CV measurements.	Insert Page Layout Formulas Data Review ViewImage: Copy PasteCutCalibri11A* A*Image: Copy PasteImage: Copy PasteImag

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11	The actual values for the percentage DF measurements are found under the header DF% .	Home Insert Page Layout Formulas Data Review View Add-Ins Format Image Strape Fill Image Strape Fill Image Strape Fill Image Strape Fill Image Strape St
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"	Ref Inst Page Layout Formulas Data Review View Add-Inst Pate Copy + Pate Copy + Pate Copy + Pate Dial I II + Correction I II + Correctio
13	The Excel macro is titled ReversePivotTable . This can be verified by opening the Excel spreadsheet and clicking: View / Macros / View Macros .	Macro Macro § 53 Macro name: ReversePivotTable ReversePivotTable §tep Into Edit Create Delete Qptions Macros in: All Open Workbooks Description Cancel

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CV) to produce	10 12 11 14
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		1	A	В	С	D	E	F	G	Н	- I	J	K	L	М	N	0
	Make sure to paste	2		-6	-5.97653	-5.95306	-5.92959	-5.90613	-5.88266	-5.85919	-5.83572	-5.81225	-5.78878	-5.76531	-5.74184	-5.71838	-5.69
	selected raw data	4 5	0 2 4	-2.23E-03 1.59E-02	1.64E-02 -1.53E-03	-3.14E-03 -1.04E-02	-4.36E-03 -6.10E-04	-1.44E-02 9.46E-03	-1.87E-02 -9.16E-04	5.40E-03 -1.31E-02	4.49E-03 5.80E-03	-1.92E-03 -2.14E-03	9.37E-03 4.27E-03	-9.16E-05 -1.10E-02	-7.11E-03 -4.27E-03	-8.03E-03 6.10E-04	-8.85i
	into the Prep-Sheet	7	6	-1.97E-03 4.20E-03	1.82E-02 -1.63E-02	-1.97E-03 -7.63E-05	9.93E-03 -2.52E-03	9.32E-03 1.34E-02	-3.49E-03 -8.62E-03	2.91E-03 -9.84E-03	-2.58E-03 5.42E-03	-1.39E-02 5.11E-03	1.24E-02 2.98E-03	-9.29E-03 -1.56E-02	-8.07E-03 4.50E-03	-8.68E-03 6.33E-03	1.68
	tab.	9 10	10 12	1.40E-02	2.14E-03 -4.44E-03	8.55E-03 -2.91E-03	-1.89E-02 8.68E-03	6.10E-04 -2.61E-03	-1.83E-03 7.46E-03	-7.63E-03 -5.36E-03	6.10E-04 5.02E-03	-1.53E-03 8.07E-03	-2.44E-03 1.54E-02	9.46E-03	-1.80E-02	9.16E-03 2.03E-02	-6.71
	To convert the 2D	12	16 18	1.05E-02 -1.11E-02	-7.78E-04 3.27E-03	8.99E-03 6.93E-03	-1.02E-02 -8.03E-03	4.10E-03 8.24E-04	-1.08E-02 2.96E-03	-7.19E-03 9.98E-03	1.63E-02 5.40E-03	5.63E-03 8.76E-03	-5.97E-03 -5.28E-03	-4.14E-03 9.67E-03	2.33E-02 -1.62E-03	-7.80E-03 -8.03E-03	-1.39!
	To convert the 3D	14 15	20 22	-7.63E-04 2.85E-02	1.30E-02 -1.54E-02	-1.07E-03 -1.05E-02	-3.20E-03 1.97E-03	7.63E-04 -6.58E-03	1.17E-02 -1.45E-02	1.17E-02 5.63E-03	-1.60E-02 8.68E-03	-6.87E-03 1.36E-03	4.12E-03 6.55E-03	-9.31E-03 1.75E-02	2.46E-02 9.60E-03	-6.87E-03 4.43E-04	-1.078
	data into a data	17	24 26 28	6.27E-02 3.22E-02	-1.08E-02 -1.54E-02	1.69E-03 -7.48E-03	1.45E-02 -6.26E-03	-1.41E-02 -4.10E-03 2.29E-03	1.30E-02 9.31E-03	-1.59E-02 -8.07E-03 -1.68E-03	1.68E-04 1.33E-02	-7.42E-03 -4.10E-03 -1.42E-02	4.49E-03 6.58E-03 8.09E-03	3.83E-03 -3.51E-03	2.24E-02 -7.48E-03	-1.88E-02 -7.63E-04	1.121
	string, select the	19 20	30 32	3.46E-03 6.52E-03	3.77E-03 -2.64E-03	2.85E-03 1.05E-02	1.17E-02 -6.91E-03	-4.17E-03 3.16E-03	7.43E-03 1.14E-02	1.07E-04 1.02E-03	4.99E-03 7.43E-03	1.02E-03 -8.44E-03	-1.30E-02 -1.55E-02	7.17E-04 -5.39E-03	4.68E-03 2.76E-02	-2.52E-02 -2.06E-02	8.65i -5.69i
	pasted data along	21	34 36	4.88E-03 4.41E-03	1.86E-02 2.27E-03	3.36E-03 2.58E-03	3.66E-03 -1.12E-02	-7.93E-03 8.07E-03	1.31E-02 -6.58E-03	-1.74E-02 -1.08E-03	5.19E-03 1.51E-02	3.36E-03 3.49E-03	7.93E-03 2.61E-02	-6.10E-03 2.88E-03	2.44E-03 -7.78E-04	-1.07E-02 3.19E-03	6.108
	with the headers	23 24 25	38 40 42	1.45E-03 5.29E-03 2.46E-02	-5.57E-03 -7.52E-03 -1.75E-02	-1.20E-02 4.38E-03 2.07E-02	7.86E-03 -5.08E-03	-3.43E-03 5.91E-03 7 54E-03	9.99E-03 6.82E-03 6.32E-03	1.03E-02 7.17E-04 1.09E-02	-3.43E-03 6.52E-03 -1.75E-02	-9.92E-04 -3.25E-03 -1.14E-02	-4.65E-03 -1.15E-02	-5.87E-03 -2.95E-03 1.30E-02	1.75E-03 1.07E-04 2.35E-03	-1.60E-03 5.60E-03 -1.26E-02	4.501 3.461
	(CV and DF).	26 27	44 46	-6.44E-03 -4.52E-03	7.29E-03 1.89E-03	-4.30E-03 1.59E-03	-5.22E-03 -8.79E-03	-1.80E-02 2.20E-03	1.92E-02 -1.61E-02	1.03E-02 -1.09E-02	-1.62E-02 1.56E-02	3.94E-03 2.50E-03	6.99E-03 6.10E-05	-9.46E-04 3.66E-04	-2.17E-03 1.59E-03	1.31E-02 -7.26E-03	-6.13i 1.28i
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21 The resultant data strings (column 3, Intensities) can be copied in a structure suitable for multivariate analysis.	Inset Page Layout Formulas Data Review View Add-ins Fourt PDF Image: Solution of the

About Owlstone[®]

Owlstone[®] develops and commercializes innovative new technologies to address the critical need for compact, dependable and cost-effective chemical and biological detection solutions for a wide range of markets.

Owlstone[®] was formed through the recognition of the opportunities created by the application of microand 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.

Owlstone[®] is headquartered in the United States and has laboratory facilities in the United Kingdom. Owlstone[®] Ltd was founded in 2003 with a seed investment of two million dollars from Advance Nanotech, Inc., a New York based company specializing in the investment in and commercialization of nanotechnologies.