

Unscrambler
ONLINE 

User Manual
for
Unscrambler Online 2.2

Table of Contents

Unscrambler-Online User Manual	1
1 Introduction	1
2 Getting started	2
2.1 Package contents	2
2.1.1 Setup.exe	2
2.1.2 Unscrambler-Online .msi	2
2.2 Installation	2
2.3 Application Startup.....	2
3 Configuration settings.....	4
3.1 Configuration file	4
3.1.1 Creating a New Configuration file	5
3.1.1.1 Model Tab	6
3.1.1.1.1 Add button.....	6
3.1.1.1.2 Set MSC Path	8
3.1.1.1.3 Remove button	8
3.1.1.1.4 Back button	8
3.1.1.1.5 Next button.....	8
3.1.1.1.6 Output tab.....	8
3.1.1.1.7 File Format.....	9
3.1.1.1.8 Limit.....	9
3.1.1.1.9 Output folder	9
3.1.1.1.10 File Prefix.....	10
3.1.1.1.11 Result Matrices.....	10
3.1.1.1.11.1 Level of Detail	10
3.1.1.1.11.2 Prediction	10
3.1.1.1.11.3 Classification.....	11
3.1.1.1.12 Numeric Format	11
3.1.1.1.13 PC Settings	11
3.1.1.1.13.1 Model.....	11
3.1.1.1.13.2 Number of PCs	11
3.1.1.1.13.3 PC to Plot	11
3.1.1.2 Input tab.....	11
3.1.1.2.1 File Information	12
3.1.1.2.1.1 Input Directory.....	12
3.1.1.2.1.2 Move to Directory	13
3.1.1.2.2 Spectral Information.....	13
3.1.1.2.3 Polling Settings	15
3.1.1.2.4 Save Configuration.....	15
3.1.2 Edit a configuration.....	15
3.1.3 Delete a configuration	16
4 Prediction / Classification	16
4.1 Plot View	17
4.2 Grid View	18

Table of Figures

Figure 1-1 : Unscrambler Online Schematic	1
Figure 2-1 : Startup screen	3
Figure 3-1 : Configuration management	4
Figure 3-2 : Creation of a new configuration file.....	5
Figure 3-3 : Location of Input, model and results	6
Figure 3-4 : Model file selection	7
Figure 3-5 : Model loading and Model information.....	7
Figure 3-6 : The prediction/classification results settings	9
Figure 3-7 : The default Output folder	10
Figure 3-8 : Input Data/Sample settings.....	12
Figure 3-9 : Default data/sample input folder	13
Figure 3-10 : Folder for moving the predicted samples	13
Figure 3-11 : Editing an existing configuration.....	15
Figure 3-12 : Deleting a configuration file.....	16
Figure 4-1 : Select a configuration for prediction/classification	17
Figure 4-2 : Unscrambler Online is waiting for input samples	17
Figure 4-3 : Plots screen with the predicted Y values	18
Figure 4-4 : Results shown as a data grid.....	19
Figure 4-5 : Sample files written by the instrument to the input folder	20
Figure 4-6 : Results of prediction/Classification in Output folder	20

Table of Tables

Table 3-2 : Result matrices in case of prediction	10
Table 3-3 : Result matrices in case of Classification.....	11
Table 3-4 : Supported OEM Formats	14

1 Introduction

Unscrambler Online is a powerful tool that can be used in prediction and classification applications. This application facilitates the user with tools for defining the parameters that are required for classification or prediction viz., source of samples, source of model, location for storing the results of prediction and classification and location for storage of samples that have already predicted. Refer Figure 1 below.

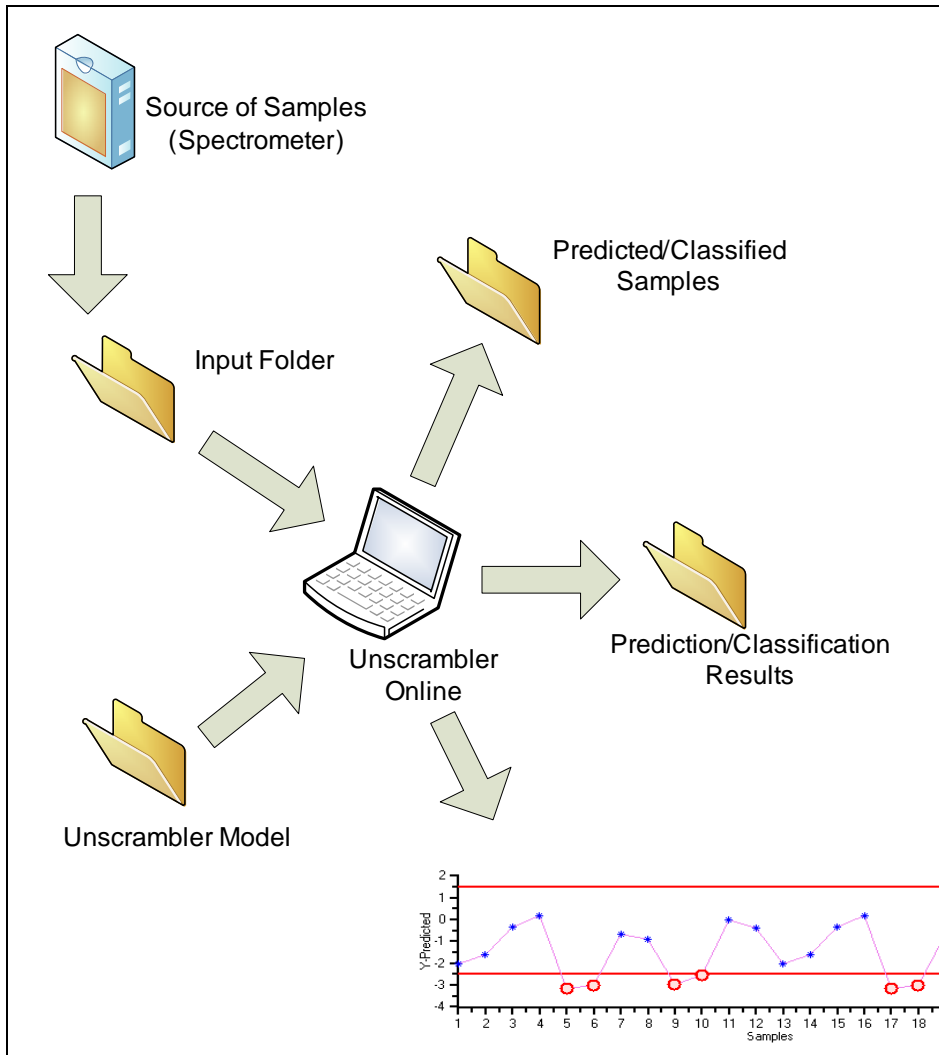


Figure 1-1 : Unscrambler Online Schematic

2 Getting started

2.1 Package contents

2.1.1 Setup.exe

Setup.exe is the main binary executable that is used when installing Unscrambler-Online software. You should not terminate this process part-way through installing a new program as this may cause the installation to fail, or only be part-completed

2.1.2 Unscrambler-Online .msi

Unscrambler-Online .msi is a binary file that contains other binary components, which will be installed in a target machine when executing setup.exe.

2.2 Installation

Installation manual can be downloaded from the following link ()

2.3 Application Startup

Launching the application by double clicking on the application icon, Unscrambler Online displays a splash screen as in Figure 2-1 : Startup screen, below

The splash screen captures the User name, for tagging the configurations, results etc with the user name. The user name should be in plain text alpha numeric (no special characters are allowed). The password field is disabled in this version

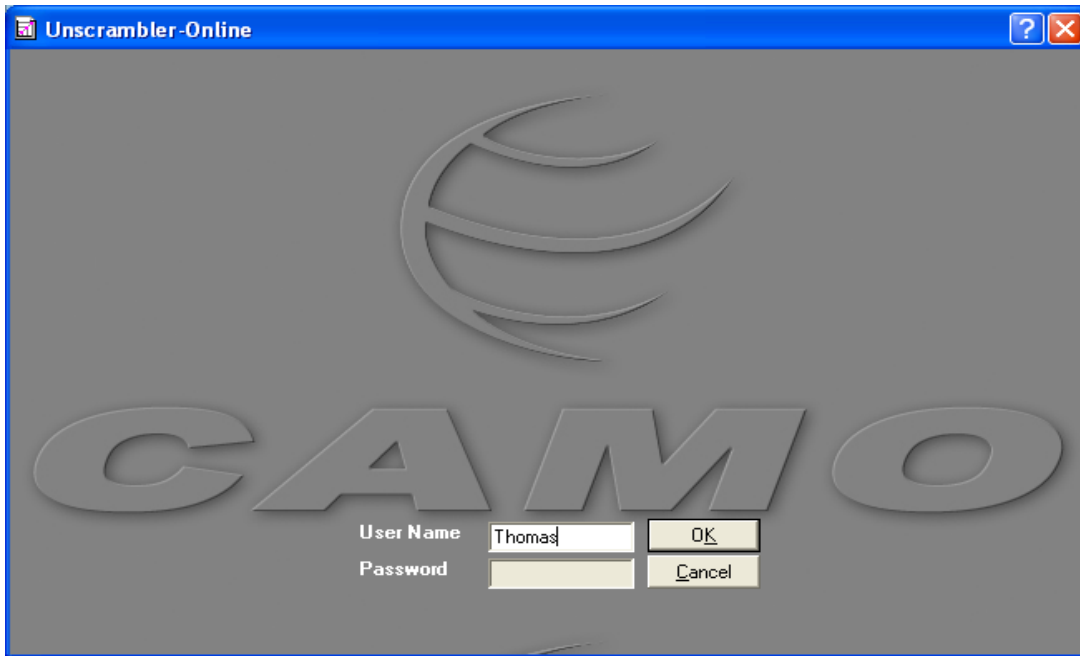


Figure 2-1 : Startup screen

3 Configuration settings

In order to use the application for prediction and/or classifications, the following are essential.

- An Unscrambler model file
- A location for storing the samples from a data source (spectrometer or other)
- A location for storing the samples that have already been predicted
- A location for storing the results of prediction or classification
- A sampling/polling frequency (measured in milliseconds)
- Selection of prediction or classification

A file that stores these parameters is referred to as a configuration file.

3.1 Configuration file

After entering the user information in the splash screen, the application displays the configuration management screen as in Figure 3-1 : Configuration management below.

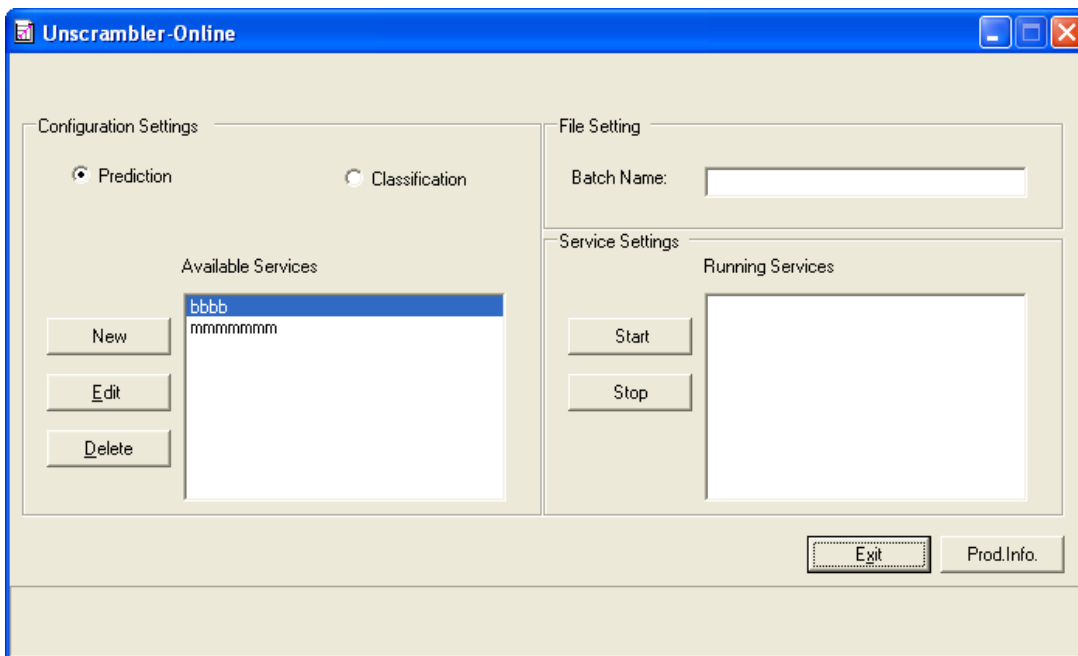


Figure 3-1 : Configuration management

The configuration management screen facilitates in creation of a new configuration, modify the existing configuration and delete a configuration when no longer needed.

3.1.1 Creating a New Configuration file

Click on the button labeled New to start building a configuration as in Figure 3-2 : Creation of a new configuration file

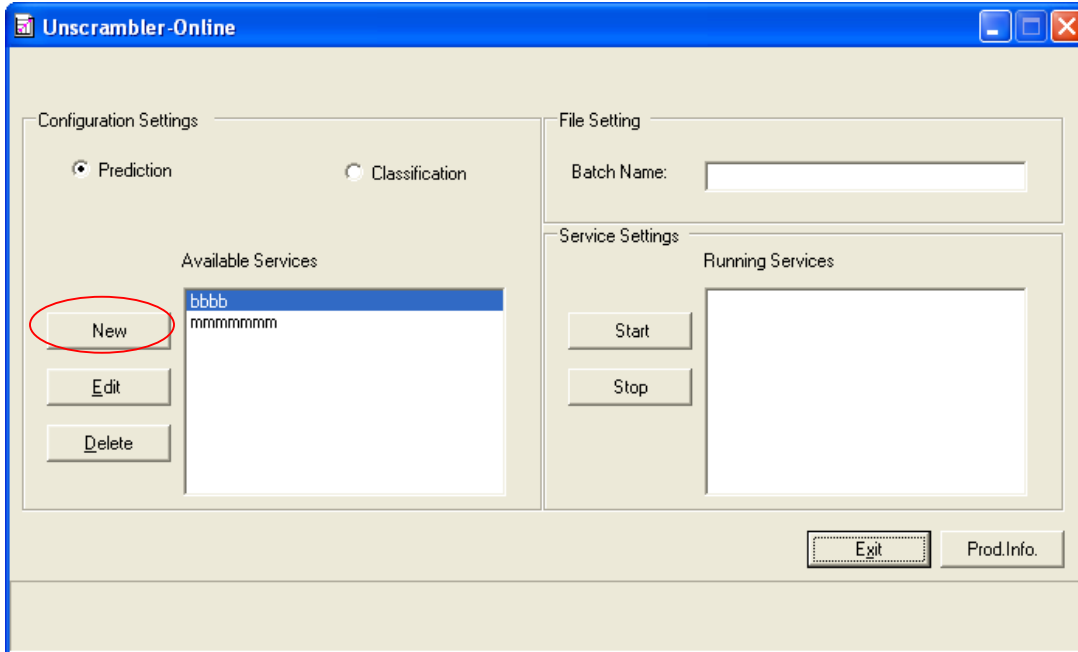


Figure 3-2 : Creation of a new configuration file

The user is presented with a screen (Figure 3-3 : Location of Input, model and results) where some of the configuration parameters are entered.

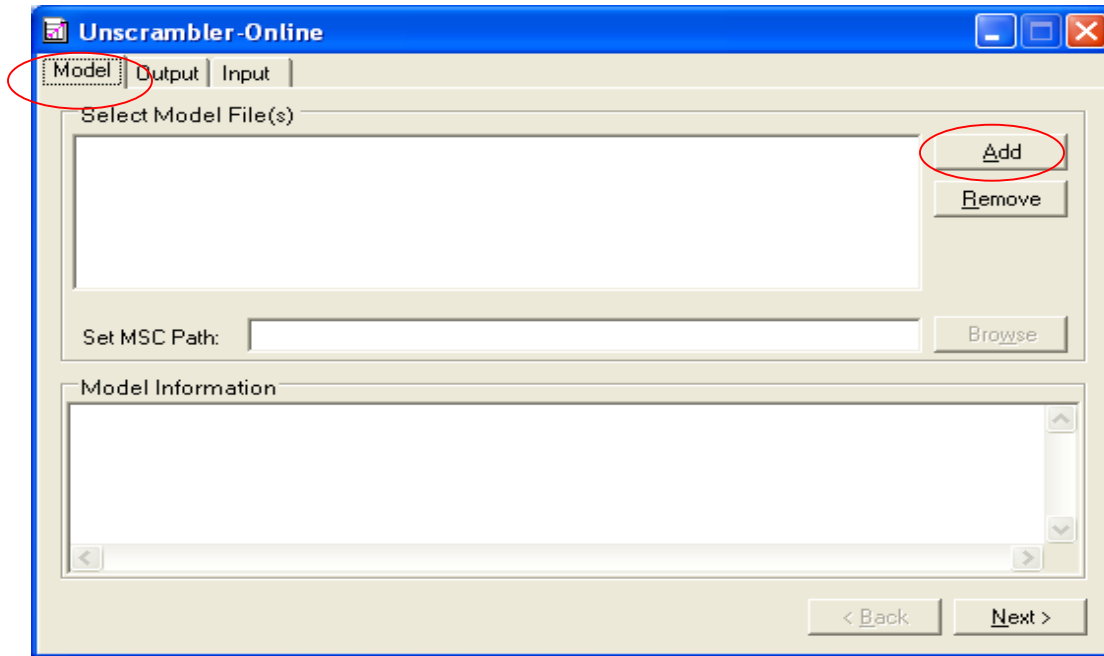


Figure 3-3 : Location of Input, model and results

3.1.1.1 Model Tab

Model tab in the dialog is for loading Unscrambler model files that are to be used for prediction or classification. More than one model can be loaded and used for prediction or classification purposes. Each sample that is read in during the prediction or classification process are predicted using each of the models that are selected.

3.1.1.1.1 Add button

Click on the Add button for loading the Unscrambler model files for prediction and classification, A standard windows file selection dialog pops up listing the files, as shown in Figure 3-4 : Model file selection, below

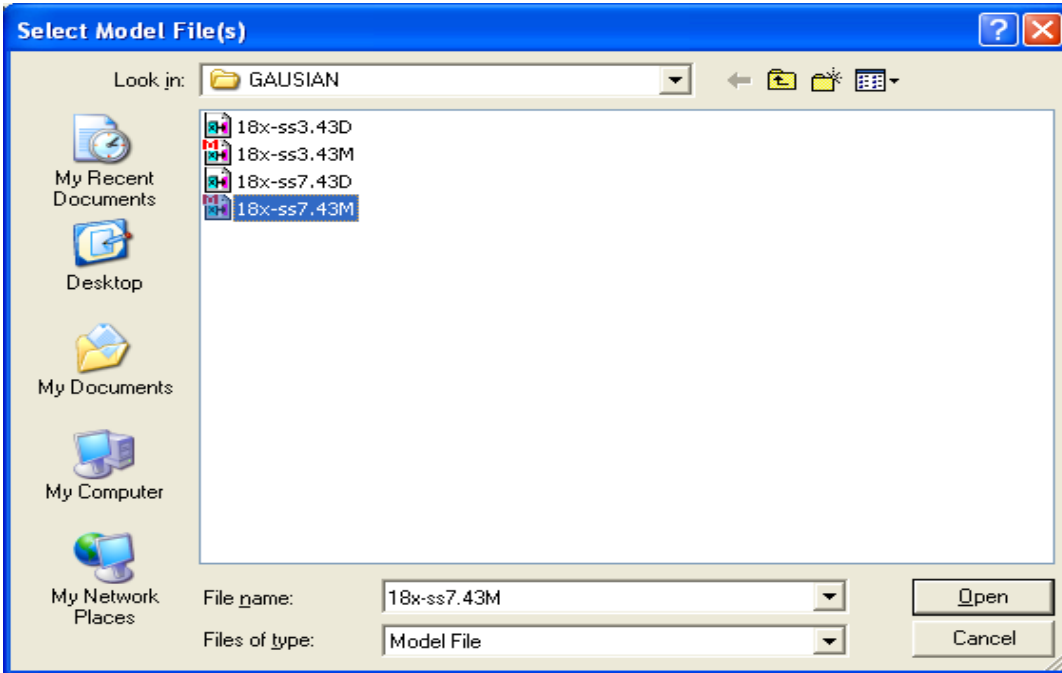


Figure 3-4 : Model file selection

Select the model file that is to be loaded and click the Open button. The path of the file now appears in the selected model files area, along with the information regarding the model is shown in the model information text area such as Model File Name, Calibration Method, Variables and Components are displayed as shown in Figure 3-5 : Model loading and Model information.

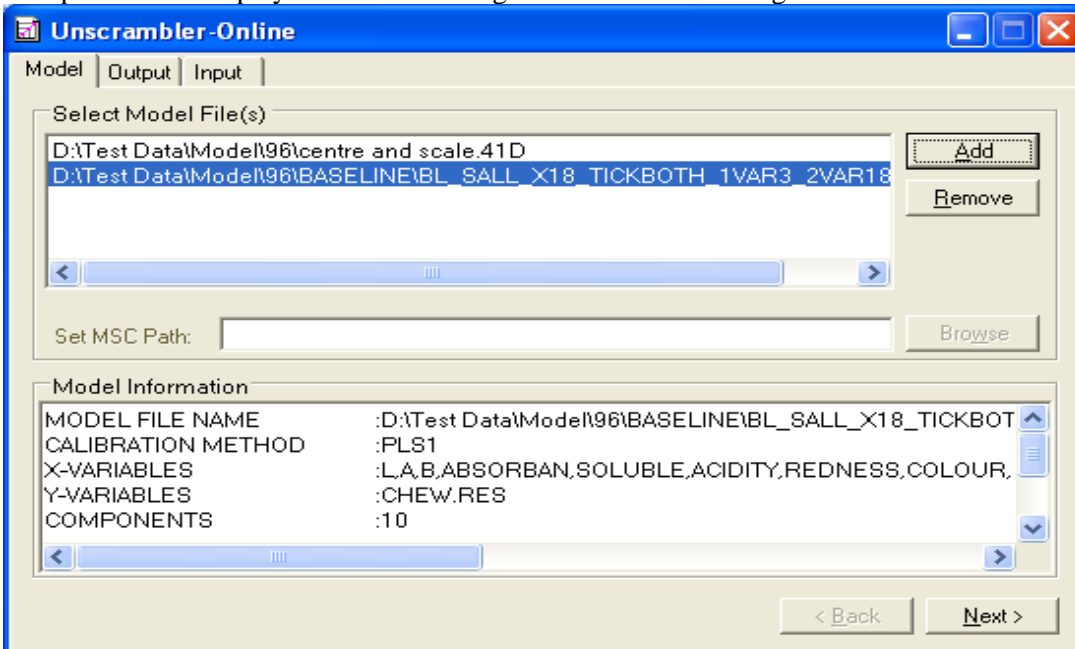


Figure 3-5 : Model loading and Model information

More than one model can be loaded for prediction and classification purposes.

3.1.1.1.2 Set MSC Path

If the model is an MSC model, then the path to the MSC model is to given in the Set MSC Path text field.

3.1.1.1.3 Remove button

Models that are accidentally loaded or if models are to be removed from being used in either prediction or classification, these can be removed from the list by selecting the model in the Select Model File(s) list, and click the Remove button. The selected model is removed from the list.

3.1.1.1.4 Back button

Back button is a navigation button, which loads the previous tab for getting the required parameters. In this case, since Model tab is the first tab, the Back button is disabled.

3.1.1.1.5 Next button

Next button is a navigation button, which loads the next tab – in this case, the Output tab, for filling the output information.

3.1.1.1.6 Output tab

The information required for performing prediction or classification and storing the results are filled in the Output tab. The Output tab can be reached either by clicking the Next navigation button or by clicking on the Output tab itself. On clicking, the output dialog is displayed as in Figure 3-6 : The prediction/classification results settings.

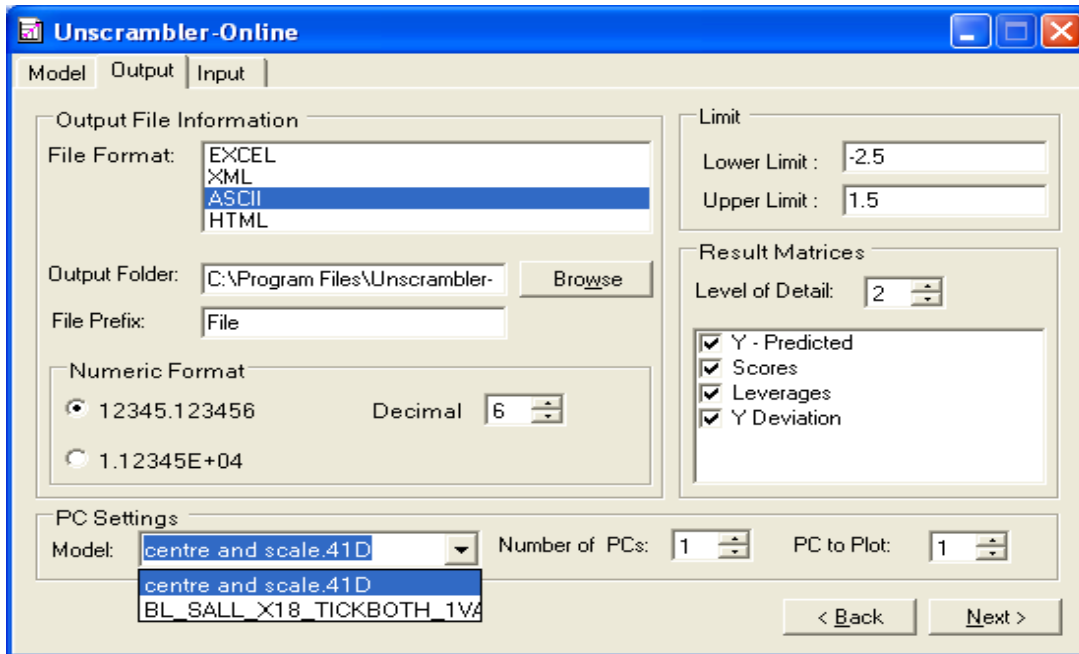


Figure 3-6 : The prediction/classification results settings

3.1.1.1.7 File Format

The prediction/classification results can be stored in a various formats. Currently, Unscrambler online saves the result can be stored in Excel format, XML format for data portability, ASCII is the default format used for storing the results and HTML for storing the prediction/classification.

3.1.1.1.8 Limit

Control limits are entered in these fields, one for the lower control limit and the upper control limit. These limits are used in the real time plots. If a predicted value falls outside of these limits an alert is plotted.

3.1.1.1.9 Output folder

By default the Output folder exists within **Program Files >> Unscrambler-Online >> Polling Configuration** directory. Figure 3-7 : The default Output folder, provides the path for the default “OUTPUT” files within Unscrambler-Online folder under “Program Files”.

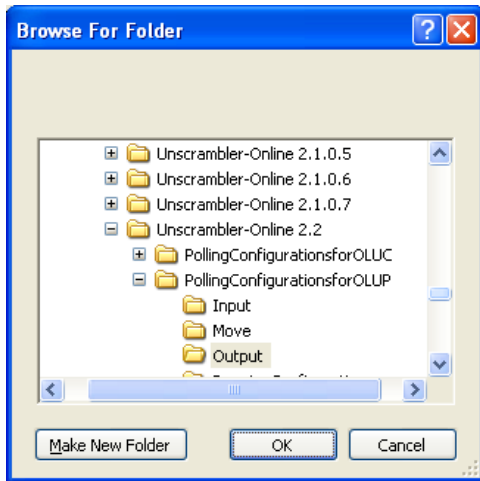


Figure 3-7 : The default Output folder

3.1.1.1.10 File Prefix

Using the File Prefix textbox, a file prefix can be characters and/or numerals. The result files that are generated during the prediction/classification process, would be named as <File Prefix> to the Result Files that are generated subsequent to the calculation. This option is provided to the user to facilitate the easy identification of the Result Files from various different experimental batches. By default the file prefix is 'File'.

3.1.1.1.11 Result Matrices

3.1.1.1.11.1 Level of Detail

Level of Detail control has three choices- 0, 1 or 2 in Prediction application and four choices- 1,2,3,4 in Classification application. This control is tied up with the Result Matrices checked list box present in the Output tab of the Unscrambler-Online application.

3.1.1.1.11.2 Prediction

Result Matrices check box control has the option of printing the following **Result Matrices** depending on the settings in **Level of Detail** for Prediction calculation.

Sl No	Level of Detail	Matrices Used
1	0	Y - Predicted
2	1	Y- Predicted, Scores and Leverage
3	2	Y- Predicted, Scores and Leverage and Y - Deviation

Table 3-1 : Result matrices in case of prediction

User Manual for Unscrambler Online 2.2
 The default **Level of Detail** is set to "2" for Prediction.

3.1.1.1.11.3 Classification

Result Matrices check box control has the option of printing the following **Result Matrices** depending on the settings in the **Level of Detail** for Classification calculation.

SI No	Level of Detail	Matrices Used
1	1	Members
2	2	Members, S0 and Si
3	3	Members, S0 , Si , Si/S0, TaiClass
4	4	Members, S0 , Si , Si/S0, TaiClass and hiClass

Table 3-2 : Result matrices in case of Classification

The default **Level of Detail** is set to "4" for classification.

3.1.1.1.12 Numeric Format

Numeric Format group provides the option to the user to print the numeric results in decimal format (12345.6789111) or exponential format (1.234568e+06). Depending on the selection, the results are displayed/printed/stored in decimal or scientific notations.

3.1.1.1.13 PC Settings

3.1.1.1.13.1 Model

The models that have been selected for prediction or classification are listed in a selection list. Each of the models can be selected and parameters can be set, such as the PC to be used for calculation and the PC that is to be plotted.

3.1.1.1.13.2 Number of PCs

Number of PCs setting is for including the number of PCs in the calculations. A setting of 4, indicates that PCs 1 through 4 are to be used in the calculations. The maximum number of PCs that can be selected depends on the corresponding model.

3.1.1.1.13.3 PC to Plot

User selects the PC that is to be used for computation of the predicted values. PC to Plot, value must be one of the PCs that has been set in the Number of PCs field.

3.1.1.2 Input tab

Source of samples and the characteristics are that is to be used in Prediction and Classification is given here.

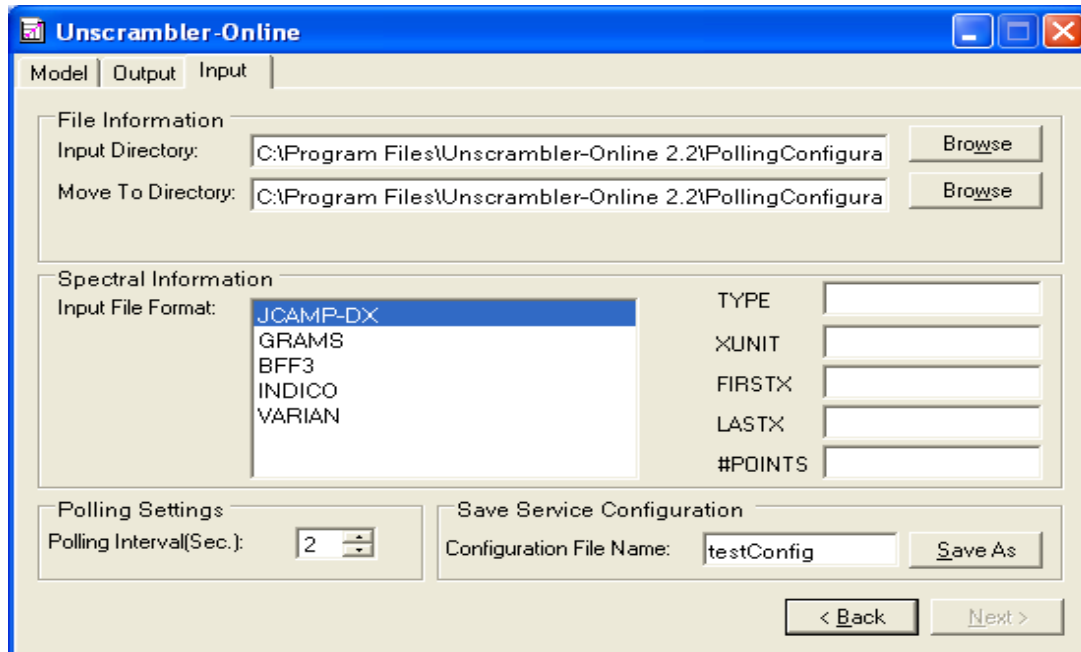


Figure 3-8 : Input Data/Sample settings

3.1.1.2.1 File Information

Details regarding the location of the source of samples and the location to store the predicted samples are set in these fields.

3.1.1.2.1.1 Input Directory

The **Input** folder consists of input data file(s) to be used for the calculation. In the Running mode the application polls the input folder for the samples and when found, loads it and uses it for prediction/classification. The files are created by instruments/devices in a predefined format. By default the Input folder is at Program Files >> Unscrambler-Online >>Polling Configuration.

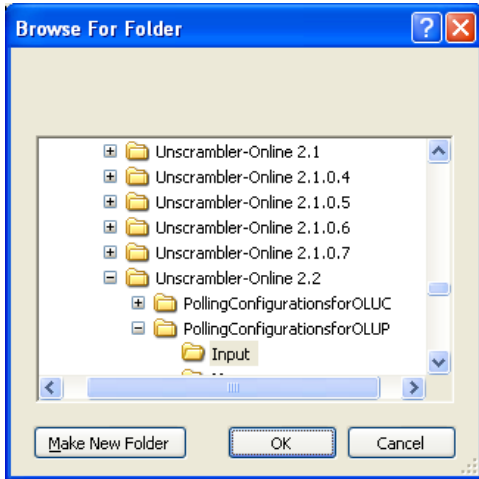


Figure 3-9 : Default data/sample input folder

3.1.1.2.1.2 Move to Directory

Move folder is maintained to store a sample file from the input folder that has been already used for prediction. This is done in order to prevent the file polling mechanism to read the file again and use it for prediction. By default the Move folder is at Program Files >> Unscrambler-Online>>Polling configuration.

The following is the default Move Folder path shown by the folder dialog box.

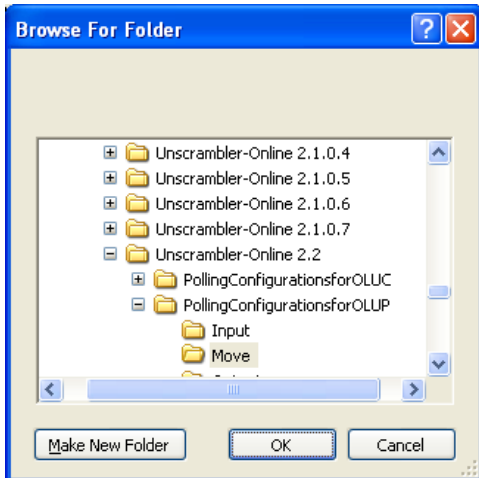


Figure 3-10 : Folder for moving the predicted samples

3.1.1.2.2 Spectral Information

Unscrambler Online can read in data generated by various OEMs equipments. The supported formats are listed here and an appropriate format has to be selected.

SI No	OEM Name	Format Reference
1	Most of the instrument vendors	JCAMPDX
2	THERMO	GRAMS
3	BRIMROSE	BFF3
4	INDICO	INDICO
5	VARIAN	VARIAN

Table 3-3 : Supported OEM Formats

Spectral Measurement Information such as **TYPE**, **XUNIT** and Spectral Measurement Information such as **FIRSTX**, **LASTX**, and **#POINTS** can be entered in the appropriate textboxes. These are textual information that is used when the results are displayed in grid form or when the results are saved.

3.1.1.2.3 Polling Settings

The **Polling Interval** textbox can be used to provide the frequency (in milliseconds) at which the application should poll the input directory for the input data files for the Prediction/Classification process.

3.1.1.2.4 Save Configuration

All the settings (options) chosen by the user under the three tabs, viz. **Model, Input & Output** can be saved as a Configuration file. Configuration file name can be a set of Characters/Numerals/Combination of the two. All the settings from a particular session (chosen by the user) gets saved with a particular identification in the form of a **Configuration File**. Click the Save As button to save the configuration file. If the configuration is new, then the application pops up a file dialog, for entering the file name and if the configuration file already exists, the contents will be overwritten by the new contents.

Once a Configuration file gets saved the name of the so created configuration file appears in the **Available Services** list box in the Configuration settings. This Configuration File exists and is available for initiating the process of Prediction/Classification through Polling with the settings saved in that Configuration file

3.1.2 Edit a configuration

Existing configuration files can be modified by selecting a configuration file from the Available services text area and clicking on the Edit button as in Figure 3-11 : Editing an existing configuration

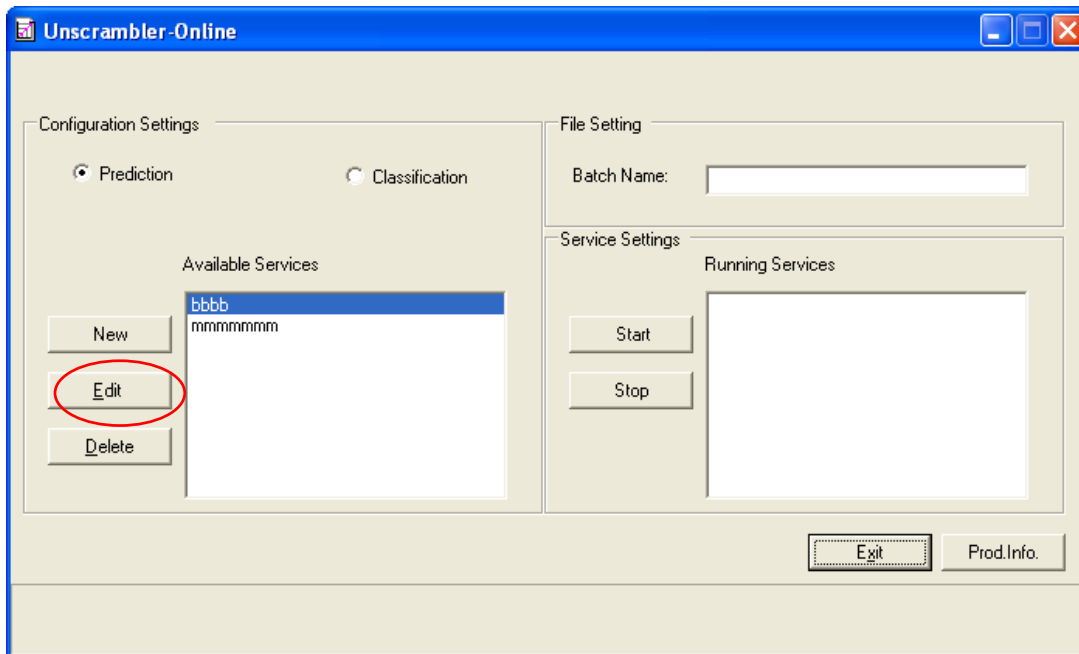


Figure 3-11 : Editing an existing configuration

User Manual for Unscrambler Online 2.2

The configuration editing dialog box is displayed (Figure 3-5 : Model loading and Model information) with the contents of the configuration file. New models can be added to the configuration by clicking the Add button, models in the list can be removed by selecting a model and clicking the Remove button.

All the Output parameters that are saved in the selected configuration file are displayed (Figure 3-6 : The prediction/classification results settings) and the user can edit all of the contents of the tab., viz., the output file formats, output folder, File-Prefix, Limits, Result matrices and PC settings.

Similarly, all the Input parameters that are saved in the configuration file are displayed (Figure 3-8 : Input Data/Sample settings) and the user can edit all the contents of the tab.

3.1.3 Delete a configuration

Any configuration that is no longer needed can be removed from the Available services list by selecting the configuration and clicking the Delete button.

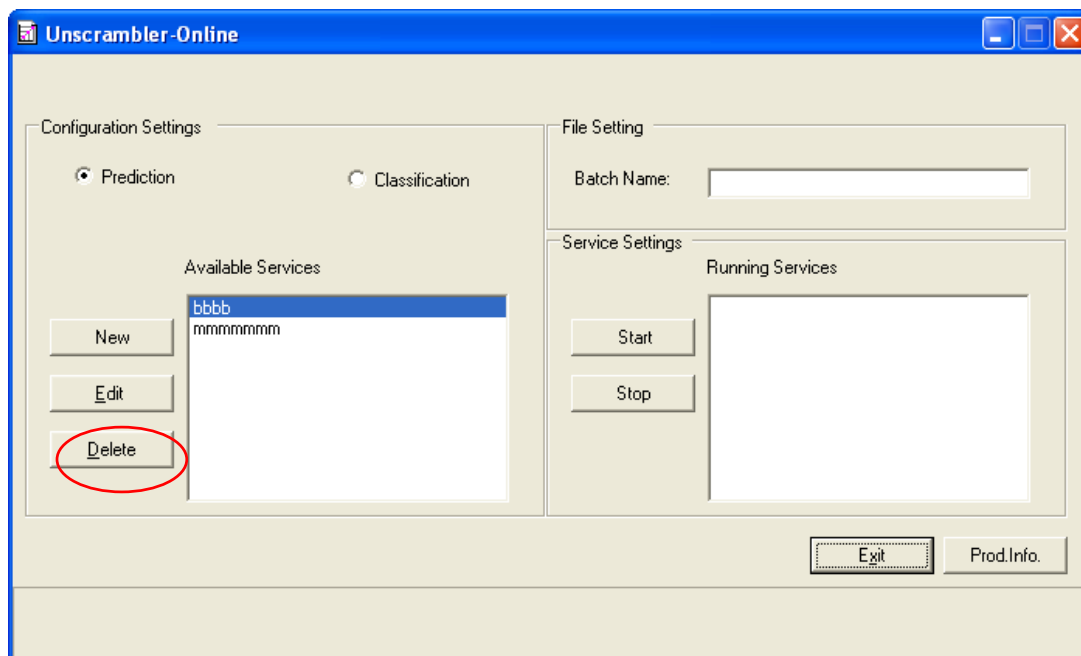


Figure 3-12 : Deleting a configuration file

The configuration file will be removed from the Available services list as well as from the disk.

4 Prediction / Classification

Highlight the configuration file under the **Available Services** and click on the **Start** button within the **Service Settings** (Figure 4-1 : Select a configuration for prediction/classification).

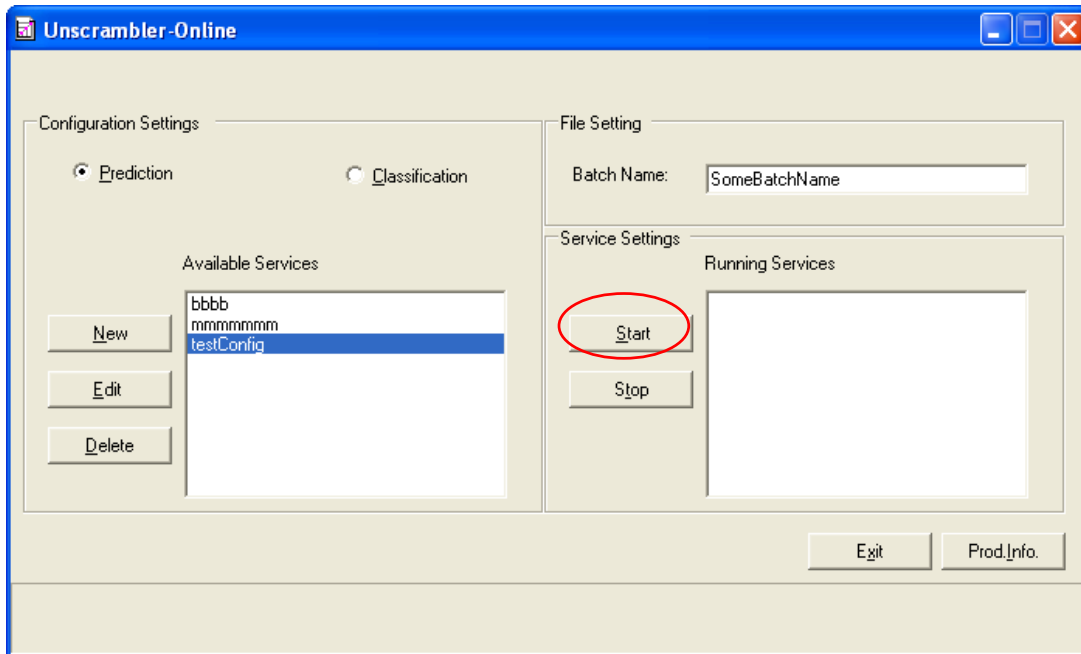


Figure 4-1 : Select a configuration for prediction/classification

The option of **Batch Name** is provided to the user to distinguish between different batches in which user will perform the Prediction/Classification. The identification can be in the form of alphabets or combination of alphanumeric. This is a mandatory entry. Before starting a service user has to enter a Batch Name.

When the Start button is clicked, the status of the application is displayed in the bottom left corner of the dialog box as in Figure 4-2 : Unscrambler Online is waiting for input samples



Figure 4-2 : Unscrambler Online is waiting for input samples

4.1 Plot View

Plot is the default output. When a service is started a plot window pops up with the plot of the Y-Predicted values in the Y-Axis against the sample numbers in the X-axis as in Figure 4-3 : Plots screen with the predicted Y values. A maximum of five plots can be drawn at a time. The upper and lower limit for the Y-Predicted values set in the output tab, are used as plot control limits. Figure 4-3 : Plots screen with the predicted Y values shows a plot of Y-Predicted against two models.

User Manual for Unscrambler Online 2.2

The Y-Predicted values which cross the limits are highlighted in the plot. As new samples are read in and its corresponding Y-Predicted is plotted in real-time. By default it is a scrolling graph with points disappearing beyond the Y-axis.

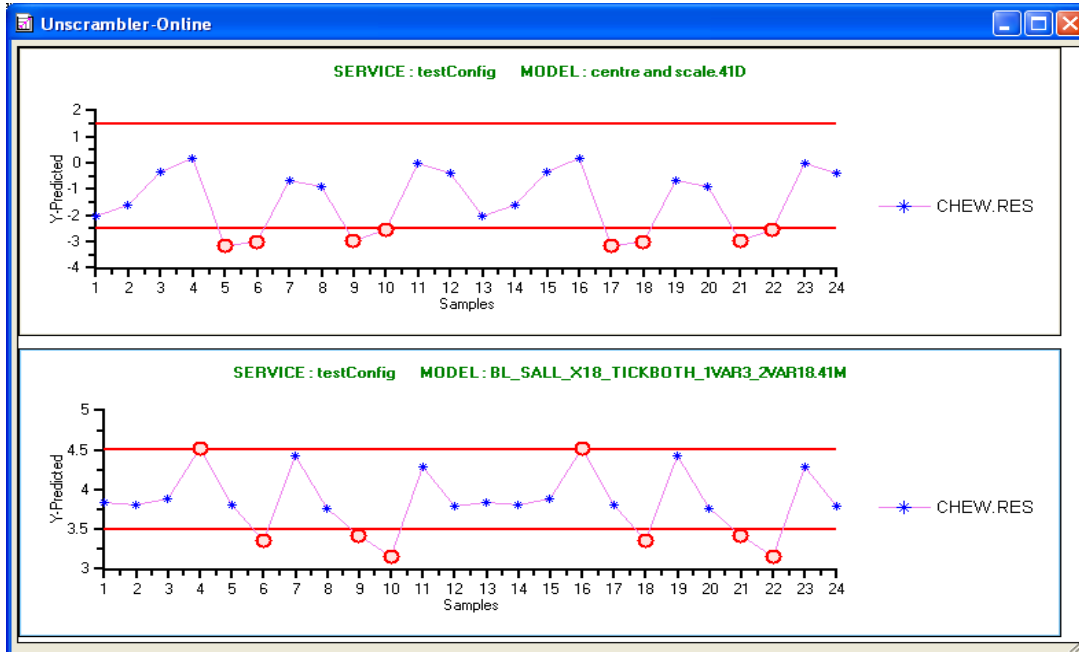


Figure 4-3 : Plots screen with the predicted Y values

The user can see all the points which have crossed the Y-axis if he checks the View All Points option, in the popup menu, by right clicking in the graph area.

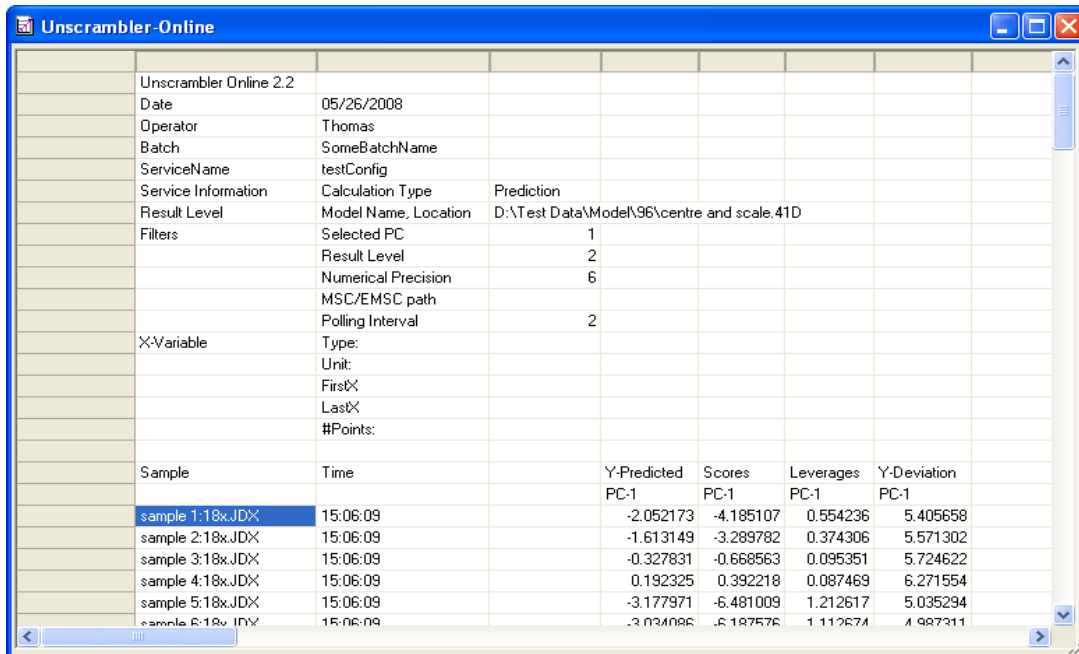
If any of the points fall outside of the Upper or Lower control limits, an alert point is indicated in the plot.

User can right click on any of the plots and select the Save Plot option to save the plot in any of the .WMF, .BMP, .GIF, .JPEG or .PNG formats. User can right click on the plot dialog and select the Save All Plots option to save all the plots as a single image file in any of .WMF, .BMP, .GIF, .JPEG or .PNG formats.

4.2 Grid View

The right click menu option on the plot control, Grid View, takes the user to the Grid View as in Figure 4-4 : Results shown as a data grid. Grid view shows all the information related to the running service, i.e., the Product Name, the Current Date, Operator, Batch Name, Service Name and detailed Service Information.

The following screen-shot (Figure 4-4 : Results shown as a data grid) shows a sample grid output.



Unscrambler-Online						
Unscrambler Online 2.2						
Date	05/26/2008					
Operator	Thomas					
Batch	SomeBatchName					
ServiceName	testConfig					
Service Information	Calculation Type	Prediction				
Result Level	Model Name, Location	D:\Test Data\Model\96\centre and scale.41D				
Filters	Selected PC	1				
	Result Level	2				
	Numerical Precision	6				
	MSC/EMSC path					
	Polling Interval	2				
X-Variable	Type:					
	Unit:					
	FirstX					
	LastX					
	#Points:					
Sample	Time	Y-Predicted	Scores	Leverages	Y-Deviation	
		PC-1	PC-1	PC-1	PC-1	
sample 1:18x.JDX	15:06:09	-2.052173	-4.185107	0.554236	5.405658	
sample 2:18x.JDX	15:06:09	-1.613149	-3.289782	0.374306	5.571302	
sample 3:18x.JDX	15:06:09	-0.327831	-0.668563	0.095351	5.724622	
sample 4:18x.JDX	15:06:09	0.192325	0.392218	0.087469	6.271554	
sample 5:18x.JDX	15:06:09	-3.177971	-6.481009	1.212617	5.035294	
sample 6:18x.JDX	15:06:09	-3.034096	-6.187576	1.112674	4.987311	

Figure 4-4 : Results shown as a data grid

The Service Information includes Calculation Type, Result Level of Detail, Model File Name and Full Path, Selected PC, Numerical Precision, MSC/EMSC Path, Polling Interval and X-Variable details (TYPE, XUNIT, FIRSTX, LASTX and #POINTS). After all these service related information the Grid View shows the predicted/classified data matrices. User can right click on the grid and select the Save Grid As option to save the data in any of the Excel, ASCII, XML or HTML formats.

The following screen shot shows the input sample files within the default **Input** folder.

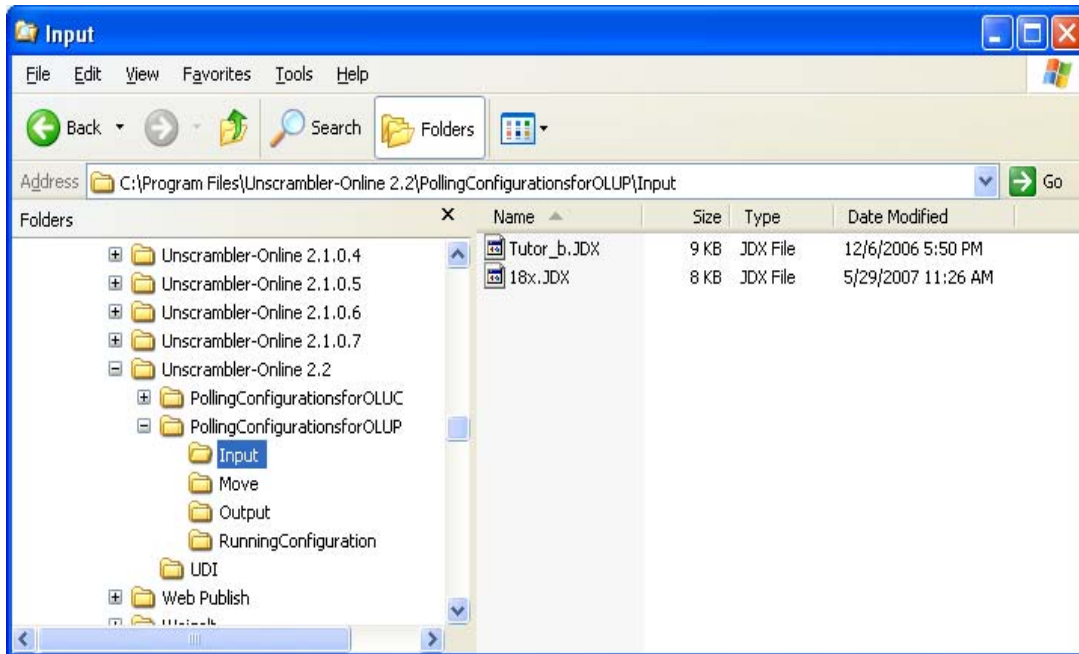


Figure 4-5 : Sample files written by the instrument to the input folder

Check within the Output folder to see results from the Prediction calculation. This folder, after the calculation, has one Result Summary.txt file which consists of consolidated result summary for each of the samples under investigation. Also this output folder consists of elaborate results for each of the individual sample files.

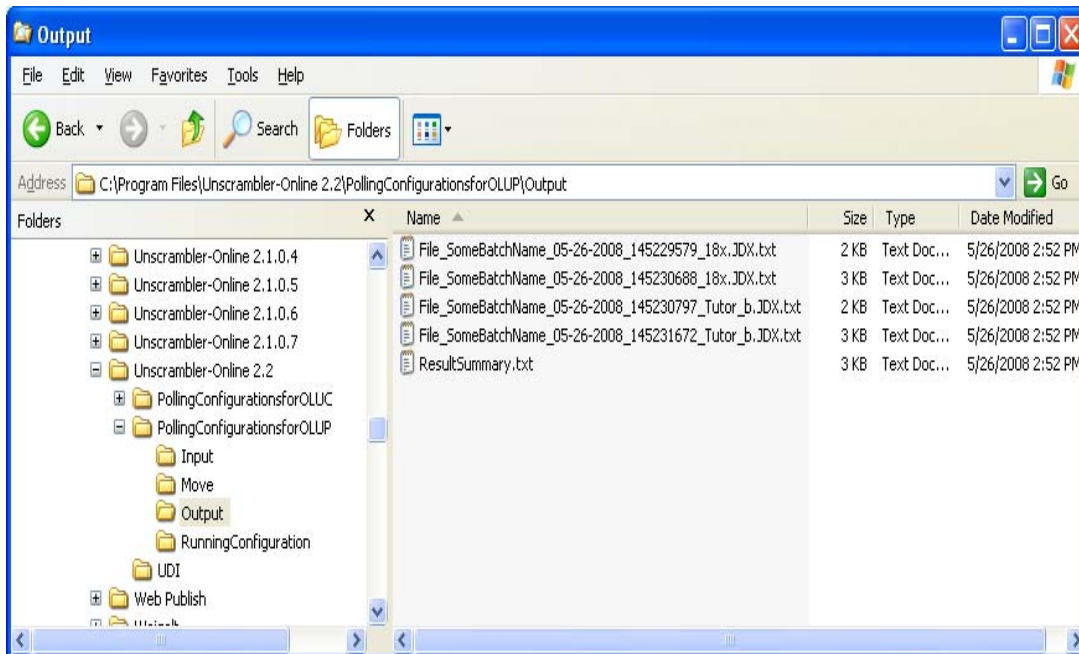


Figure 4-6 : Results of prediction/Classification in Output folder