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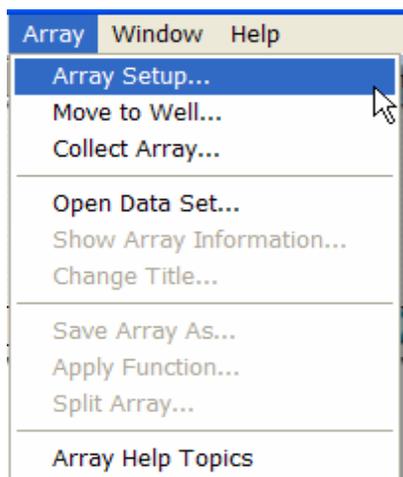
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# Array Automation

# Array Automation

- Array Menu
- Array Setup
  - Sequence Selection
  - Template Selection and Setup
  - Stage Initialization
  - Wells, Assign, and Method Selections
- Move to Well
- Collect Array
- Open Data Set
- Array Display
- Apply Function
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- Split Array

# Array Menu of OMNIC



## Spectra Collection

- Setup array data collection parameters
- Move to specific well and view
- Collect spectra from wellplate

## Spectra Analysis

- Open previously collected data
- Save a working copy
- Apply spectral data corrections
- Split into individual .spa files

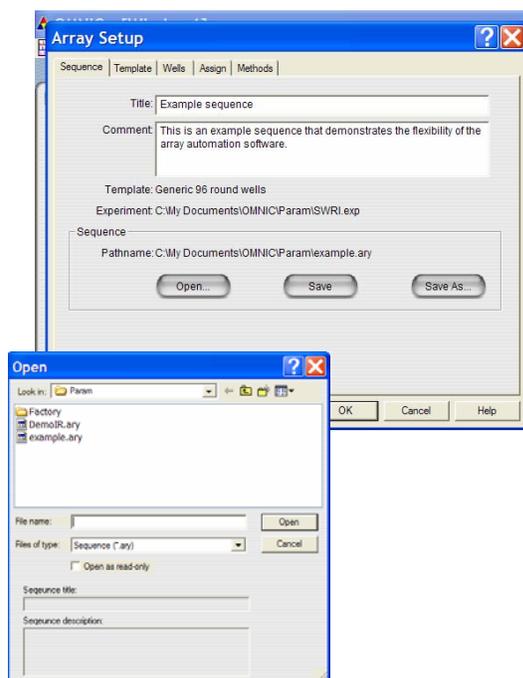
The Array automation tab allows for easy collection and analysis of the well plate based sampling approach. Array differs from Atlas in that the samples are deposited into wells of a plate that form an ordered sampling set. The physical space that separate the wells is not part of the analytical area—only the well area itself. Therefore, the samples in each well do not have a spatial relationship to the other wells on the plate.

Well plates come in a variety of sizes and number of wells. Complete setup and use of custom well plates is contained within the Array menu of OMNIC. When adding a new well plate to your analysis, Array setup is the place to start.

Once a well plate is integrated into the software, you can move to specific wells, without needing to 'drive' to the location with the joystick.

Additionally, post collection data analysis can be applied to array data easily, allowing you to explore your data as a set and not individual spectra. You can apply simple interrogations such as peak height measurements or more complex quantitative approaches more commonly applied to Raman data.

# Array Setup



## Sequence Selection

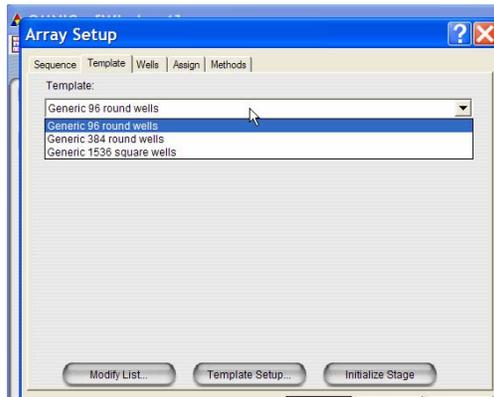
- Array sequence files allow you to apply analytical approaches to redundant sampling sets.
- A new or saved sequence file must be setup in order to collect data.

Open—retrieve previously saved sequence files

Save/Save As—create new sequence files for reuse.

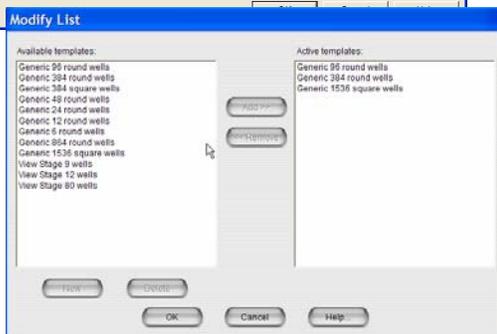
Like most multiple tab controls, one works from the left to setup a sampling experiment. The Array Setup tab is where you define what the array is. Most of the information on this tab is optional and not needed for analysis. However, the title is applied to the Array when stored to disk. If your analysis is fairly routine, where the sampling position within the well is not manual, saving and retrieving a sequence can speed the time required to setup the experiment. If your samples require manual sample positioning within each well, it may not be as beneficial to use a stored sequence file.

# Array Setup



## Template Selection

- Templates of desired well plates are listed.
- Modify list—add/remove well plate descriptions

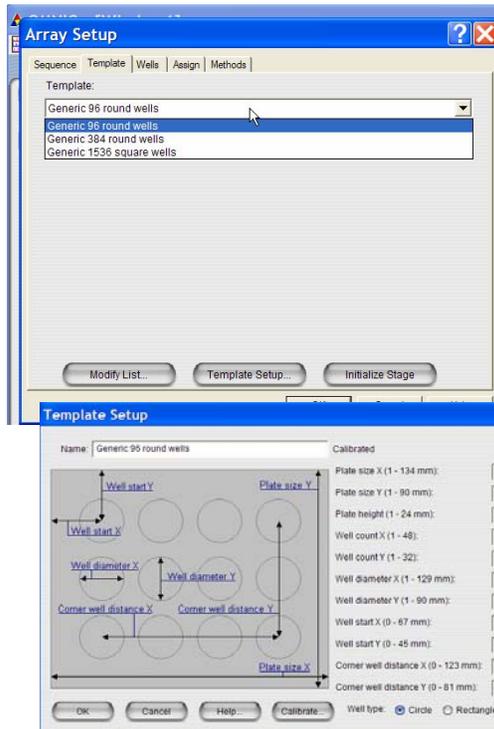


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Well plate templates are chosen from the available options of the user selectable list. One can easily create new templates (which require additional setup) as well as add/remove templates from the user selectable list. By using the Modify List button.

# Array Setup



## Template Setup

- Template Setup—provides well plate information to stage automation program.
- Fill in required fields using a micrometer, ruler or information provided by well plate vendor.
- Calibrate the well plate stage positions of all four corners.

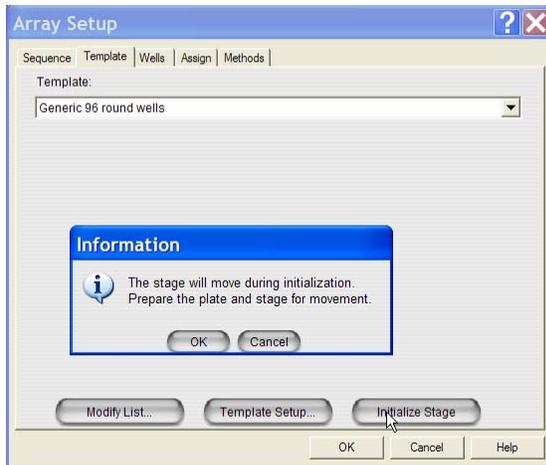
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Template Setup describes the geometric setup of the well plate. Most fields are self explanatory or described by the well plate image on the left side of the display.

Calibrating the stage allows the user to insure the stage will move to the exact center of each well of the plate. The calibrate procedure prompts the user to move the stage (with the joystick) to each corner well when prompted. The user can either use the video application to assist in finding the center of the well or use the ocular of the microscope if available. If your system uses multiple objectives, we recommend using the lowest magnification objective available.

# Array Setup



Stage initialization: Moves stage to X, Y and Z limits upon initial startup.

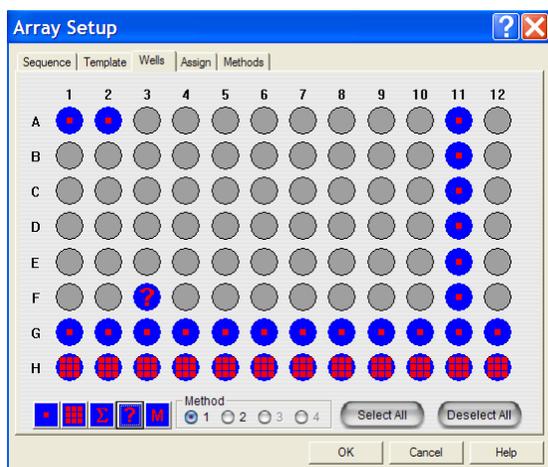
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Stage initialization simply moves the stage through each plane range to insure proper setup and operation. Some systems will require initialization each time that OMNIC is started, some will require initialization each time the power is cycled on the equipment, and some will require initialization only once.

Initialization will only be needed if the software prompts you.

# Array Setup



## Wells:

Choose how each well will be analyzed.

Choose individual cells, rows or columns

Choose analytical method (recommend you define this first from Methods tab)

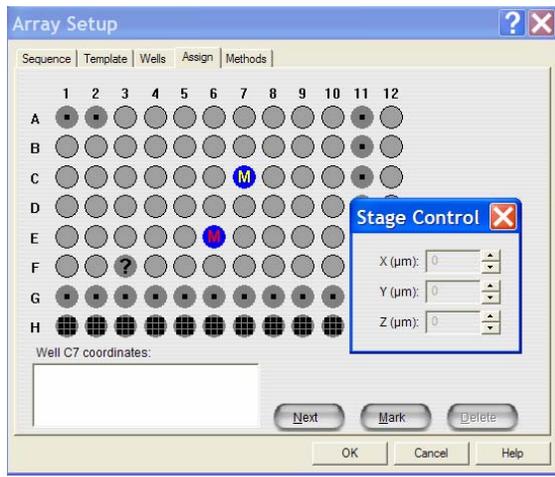
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The Wells tab allows you to choose how each well is analyzed. From the options fully described below, you can choose individual wells, or whole rows (by clicking the letter to the left of the row) or columns (by clicking on the number above the column). Additionally, you can select or deselect all the wells of the template.

-  Take a single measurement at the center of the well. (Use this when the bottom of the well is completely covered with a homogeneous sample.)
-  Obtain multiple spectra from the well using a grid that has a defined area and step size. (You use this when the bottom of the well is covered with a sample that may be heterogeneous or when the bottom of the well is not completely covered with sample.)
-  Average multiple spectra from the well using a grid that has a defined area and step size. (You use this when the bottom of the well is covered with a sample that may be heterogeneous.)
-  Search for the strongest signal in the well using a grid that has a defined area and step size. (You use this when the well bottom is not completely covered with sample.)
-  Manually search a well to find and focus on the sample before starting the data collection. (This collects a single spectrum from each of the selected positions in the well.)

# Array Setup



Assign:

Choose how each Manually configured well will be analyzed.

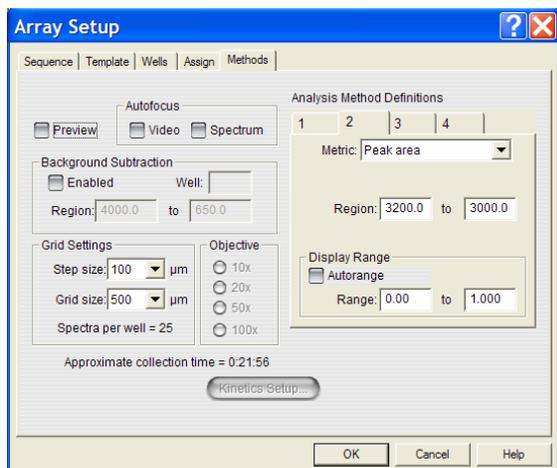
Move the stage (joystick, Stage Control form, or Microview).

Click on Mark to record positions within well

Click on Next to move to another manually configured well.

The Assign tab is only used for manually configured wells. This option allows you to set individual X, Y and Z positions for each sample—Best for powders or crystal materials.

# Array Setup



Methods: describe the spectral measurement of the analysis profile. Set optional parameters if available.

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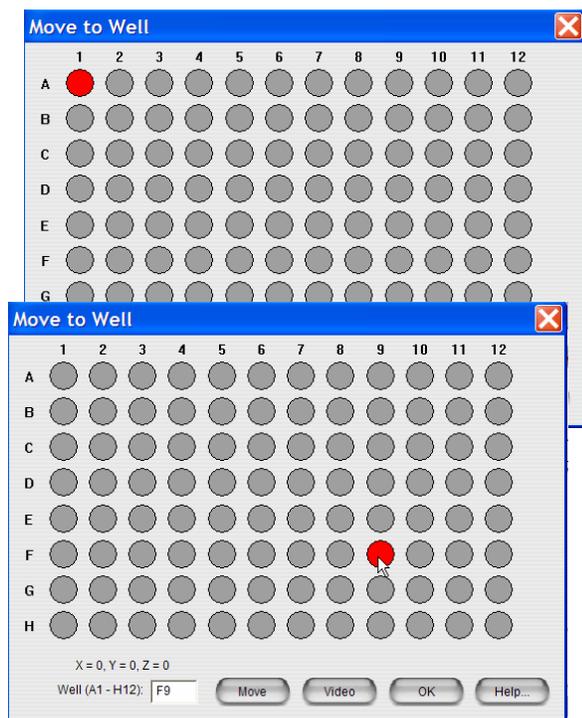
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The Methods tab is primarily used to setup the initial analysis profile that is generated during the sample analysis. From simple peak height measurements to more sophisticated quant methods, the initial profile sets the basis for the color scheme of the graphical results. Realize, you'll have full capability to interrogate your data once it is collected. For Raman experiments, little information can be derived from simple peak height or area approaches since there can be variations in intensity unrelated to the concentration of the material generating the peak of interest.

If your hardware supports optional approaches to sample focus, you will find the parameters here. Keep in mind, automatic focus approaches can significantly increase the collection time of the data. If either automatic focus option is enabled, you will be able to select the objective magnification as well.

Grid settings allows you to define the multiple point per well selection of the Wells tab.

# Move to Well



## Move to Well

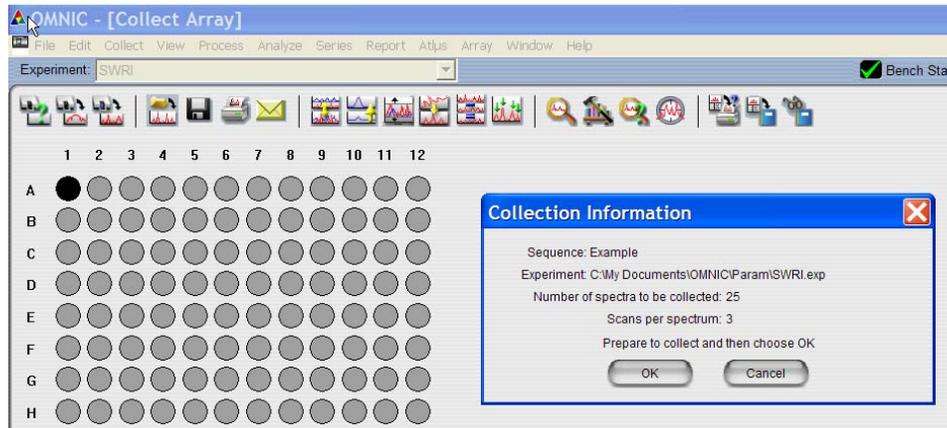
- Navigate to desired well to:
  - View sample image
  - Capture video image
  - Collect spectral data
- To navigate to desired well
  - Enter well address then click Move
  - Double click on desired well

The move to well option is an excellent approach to sample analysis where automation setup is not practical for example with just a few samples.

The Video button allows you to bring up the Microview application to survey your sample.

# Collect Array

The Collect Array button begins the collection process.



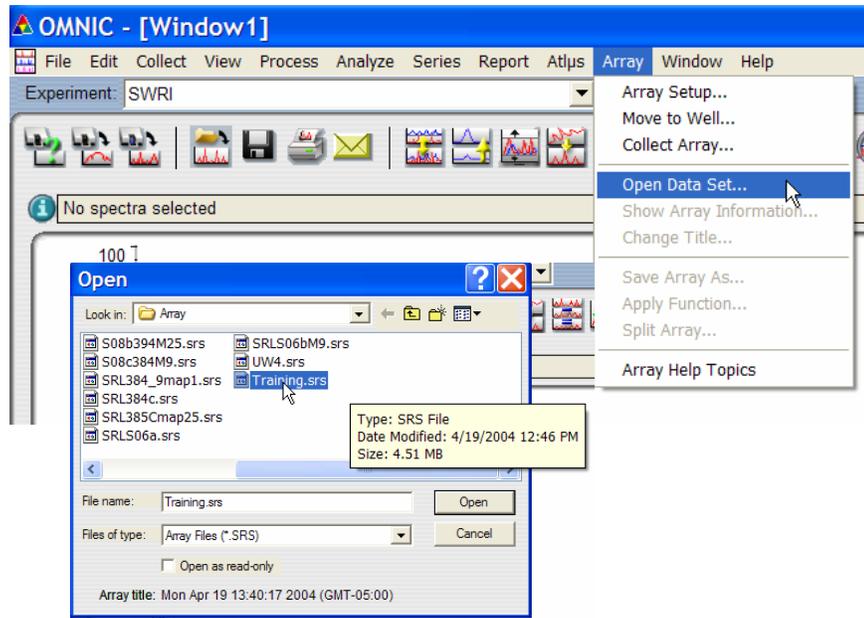
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A summary box is presented to verify both the sequence and the experiment file used for the collection. Once OK is clicked, the process begins.

# Open Data Set

Allows you to select and open desired array data.

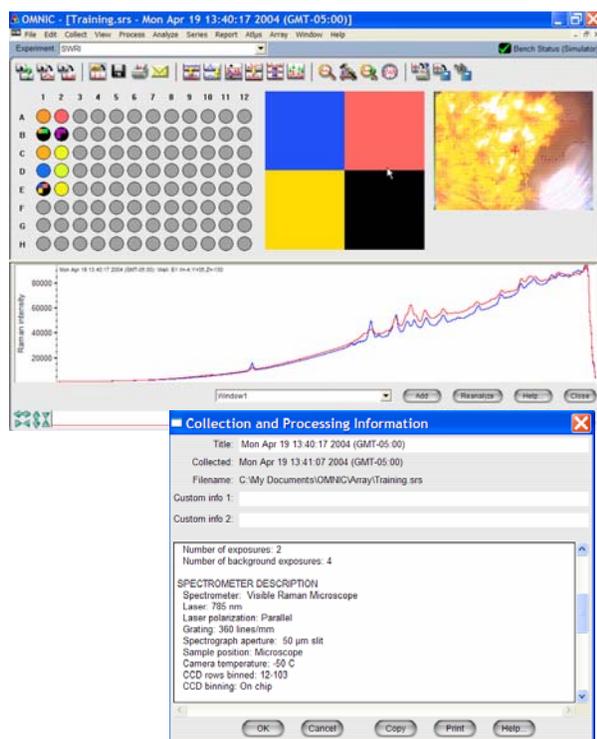


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The array data can be opened again for reanalysis.

# The Array display



Displays interlinked video and spectra of selected well.

If multiple points in a well, then a contour display is also shown.

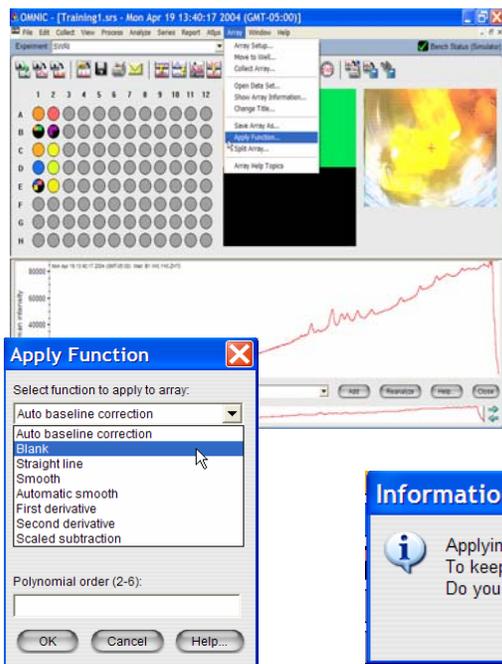
Show Array information...

- Displays array header information

Once an array has been opened, you can see the fruits of your labor. The colors in the array field represent the metric created in the sequence file. The video image of the selected well is displayed on the right. If there are multiple spectral points in a well, then an expanded contour display is presented between the array field and the video image.

A wealth of instrumental information is presented in the array header, accessible through Array|Show Array Information task.

# Apply Function



Modify data set after collection

- Condition data prior to additional analysis
  - Blank and Baseline Correct common with Raman data

Recommend saving a working copy of the data set prior to manipulation

## Information



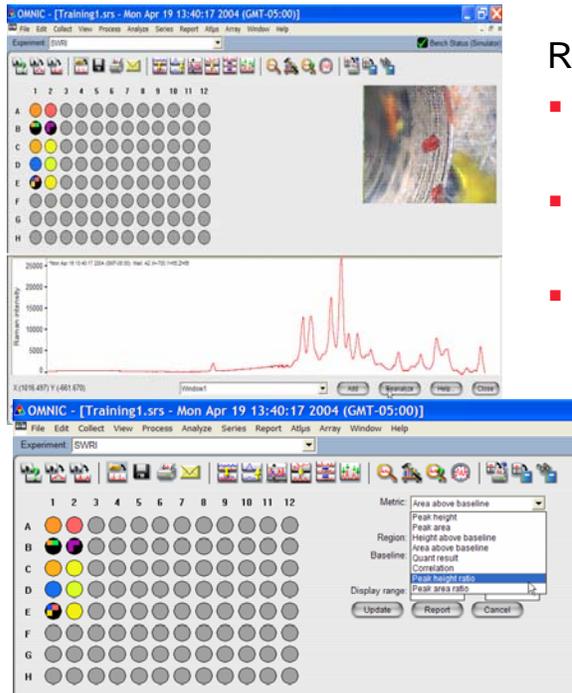
Applying a function permanently changes the data. To keep the original data, first use Save Array As to save the data set with another name. Do you want to apply the function?

Yes

No

Common data treatment is available after collection. Baseline correction and blanking can be used to improve the appearance of spectral features. In the data set presented, a baseline tilt and a detector response issue from 200  $\text{cm}^{-1}$  to cutoff is evident. Applying a blank of that region and a baseline treatment may improve the appearance.

# Reanalyze dataset



## Reanalyze dataset

- Analyze data with new conditions (baseline correction etc.)
- Band ratio functions not available in initial sequence setup
- Results can be exported

Data file: C:\My Documents\OMNIC\Array\Training1.srs  
Sequence file: C:\My Documents\Omnic\VRParam\384\_Basic.ary  
Comment: 4 sec single point per well

Method: Peak height ratio  
Numerator Peak: 1495.7 Baseline: 1468.7 - 1526.6  
Denominator Peak: 1337.6 Baseline: 1306.7 - 1385.8

Well,Mode,X Pos,Y Pos,Z Pos,Result  
A1,Manual,-36,71,55,1  
A2,Manual,-700,55,56,1  
B1,Manual,0,0,73,1  
B1,Manual,-64,544,73,0  
B2,Manual,185,375,-53,-3

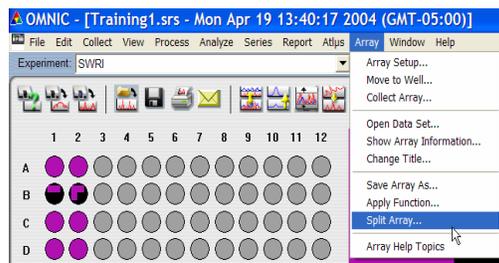
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More powerful data interrogation is available after collection. Once the data have been treated, such as the blanking and baseline treatment of our example, we can apply features that make for more meaningful spectral analysis.

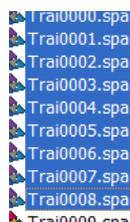
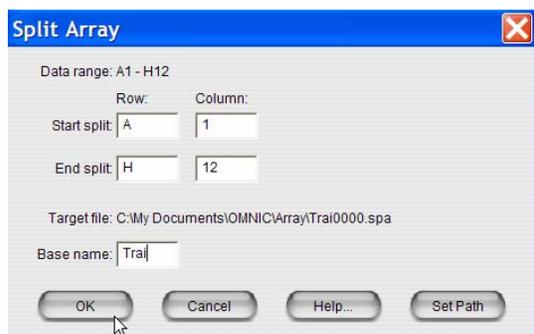
Analysis results can be exported as comma separated values for further analysis.

# Split Array



## Split Array

- Save spectra to disk as individual spectra.
- Choose the start and end points
- Set four character basename



Splitting the array allows you to save spectra as individual files. These files can then be used in reference libraries, quant methods or other applications.

# Summary

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