CAPTURING DATA

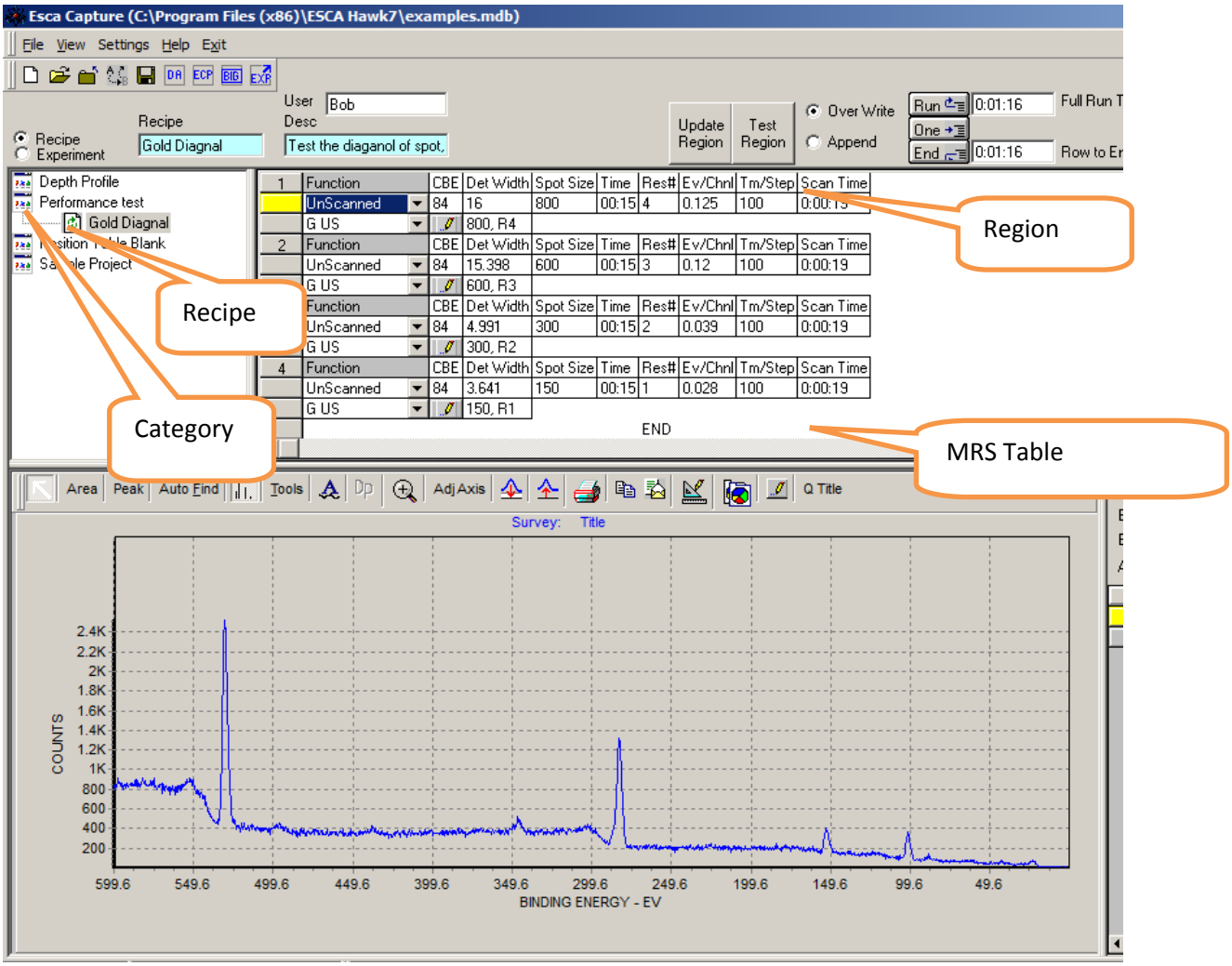
Recipes and MRS Tables

The parameters that define a spectrum can be saved as a ***REGION***

A multi-row Spreadsheet with a column for each ***REGION*** is known in all Surface Science Software as an ***MRS*** (Multi Region Scan) ***TABLE***. We keep this concept.

We can save the ***MRS TABLE*** as a ***RECIPE***.

For convenience we can group a set of ***RECIPES*** in ***CATIGORIES***. ***CATIGORIES*** have no intrinsic meaning in the software and are simply a means for the user to group ***RECIPES*** in blocks that may have meaning in the flow of their work.



Points to remember:

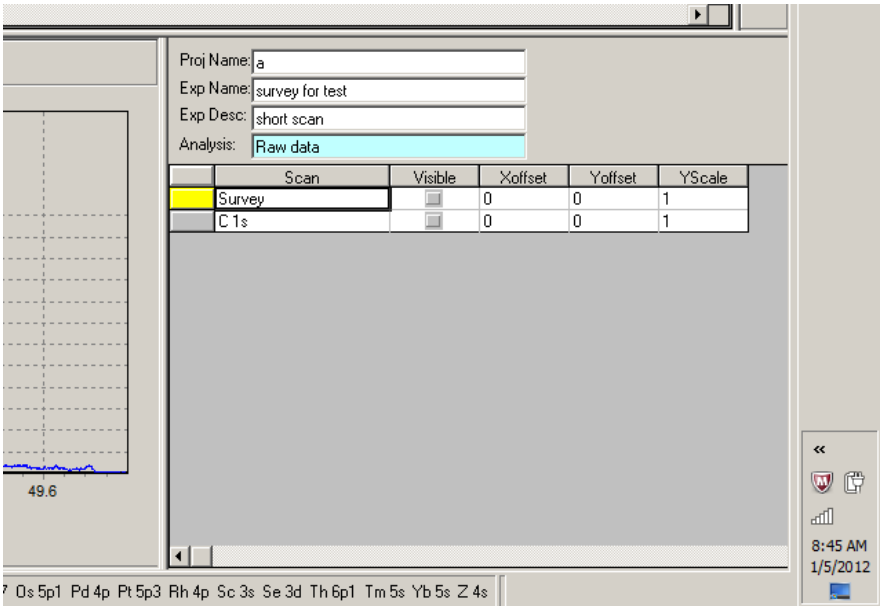
You may save one or many region specifications in an MRS Table. You may want to use this specification exactly as saved or just as a convenient starting point. You are free to do either. If you really want some recipes not to be changed then you may want to establish a category for all such recipes.

If you have a large MRS table and decide you want to have another that is modified from the first use SaveAs, modify the clone and then save the modified result. The Save and SaveAs function in the File menu operate only on Recipes and Categories.

Right above the Recipe Tree are two buttons. “Experiments” and “Recipes”. If you select Experiments you will have a tree of previous Experiments. These are completed groups of spectra. You can select an old Experiment and the MRS Table that was used to capture the group of spectra will be loaded. You can then re-run the exact experiment from the recovered MRS Table. This can be a MRS table that was built from a Recipe but was modified before it was run. i.e. This is the only existing MRS table of its kind.

Experiments

Experiments are collections of captured data. Before you can start the capture process you must name the Experiment. This is equivalent to specifying the file name in the Surface Science Software. You must also specify a Project. This structure is equivalent to defining a folder in which to store Experiments. This tree of Projects and Experiments were displayed above in the Experiment Mode. The entry box for the Project and Experiment information is shown below.



Points to Remember:

If you try to capture data and have not changed the information in the Proj Name or Exp Name boxes you will be warned. You will then have the choice to change one or both names, collect new data that will overwrite the old data, or append additional data. Appending new data will create additional regions. These regions can be reruns of existing lines in the MRS table or new regions added to the MRS table. If the new data is taken with an existing region then the original and new data can be summed together to improve S/N.

The data acquired during the capture process is saved to the Database during the scanning process. There is no provision for additional save operations. All subsequent review or analysis operations are performed on copies of the original data. There is no possibility to corrupt or altering the original data except for the above mentioned collection of new data with existing Experiment and Project names. A warning is always provide before this can take place.

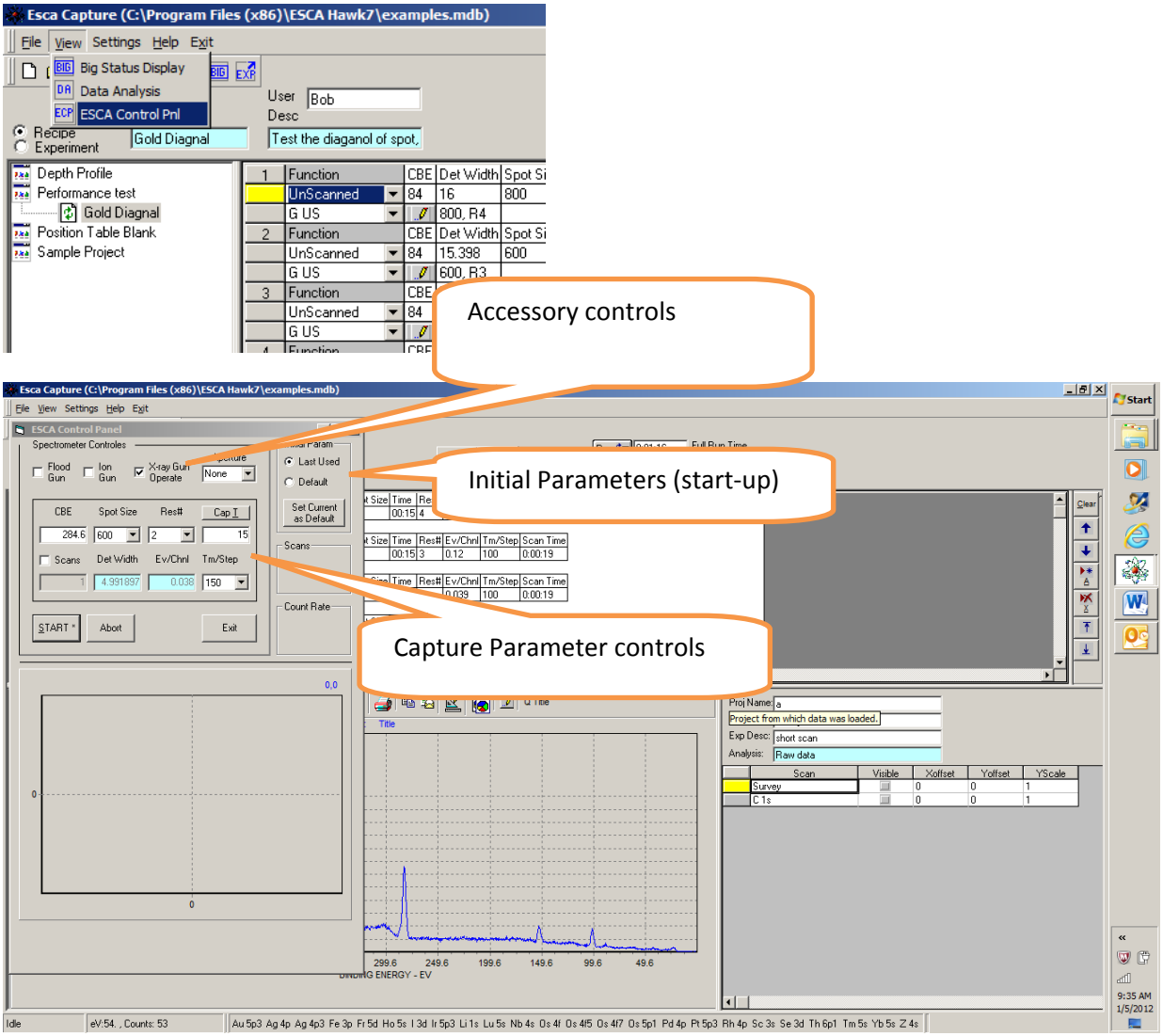
Databases

The Recipes, Experiments and other data associated with the captured data is stored in a Windows Access database. These files have the .MDB extension. This provides a convenient and powerful method of storing information that has complex relationships. This will become more evident as you become familiar with the Data Reduction, Export and Editing functions available. For now just think of the Database as a folder with some really helpful tools inside that will help you find the information you need. Think of the Experiment Names as the tag you use to find the data you took with an MRS table. (The MRS table may have only one spectrum!) There is no second structure for single spectra in the Database.

Taking a Spectrum

There are two methods for acquiring a spectrum. The ESCA Control panel or the MRS Table. The ESCA Control panel has no means for storing the acquired spectrum. It is a tool for previewing and testing acquisition conditions. The MRS table is a collection of region specification that are run in a batch mode and saved directly to the Database. The ESCA Control Panel and the MRS Table work together through the "Test Region" and "Upload Region" buttons.

The ESCA control Panel



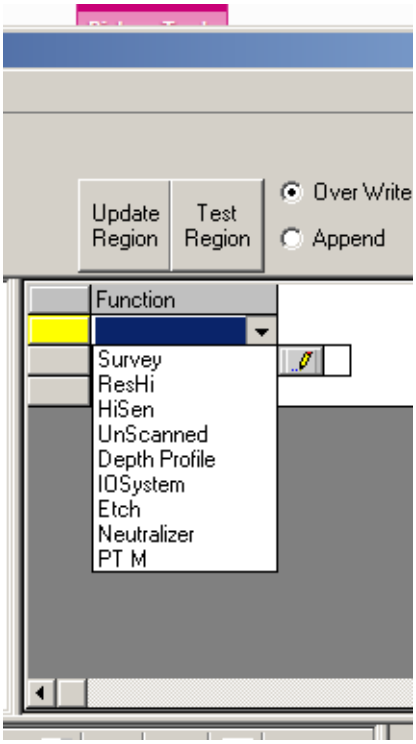
The Capture Parameters are defined by the 8 controls in the control frame. The titles above the entry boxes will changes for scanned or unscanned operation. The Scanned configuration is set by clicking the check box above the "Scans" window. If the box background color is light blue then it is not activated as an entry box (information only). In the Unscanned mode the "Cap T" label above the entry box is a button. You can alternate between total Capture Time and Averaging Time. In Averaging Time mode the incoming data is filtered so the oldest data is waited by $e^{-t/\tau}$. τ is the time constant displayed in the window. The minimum time constant is 0.5 seconds. The values entered take effect when the Start button is selected.

The Accessory controls only affect the accessories when the control panel is open. They change the state of the accessory immediately if a spectrum is not being collected and are deactivated during capture.

The "Initial Parameter Control" allows the user to define the initial state of the parameters as the panel is opened.

Testing and building the MRS Table

Functions:



Functions that provide default settings

Survey –Wide scan, Res 4, 800 spot

ResHi - Scan for peaks of one element

Res 1or2, 150 or 300 spot

HiSen - Scan for trace elements

Res 3 or 4 600 or 800 spot

UnScanned - Special uses

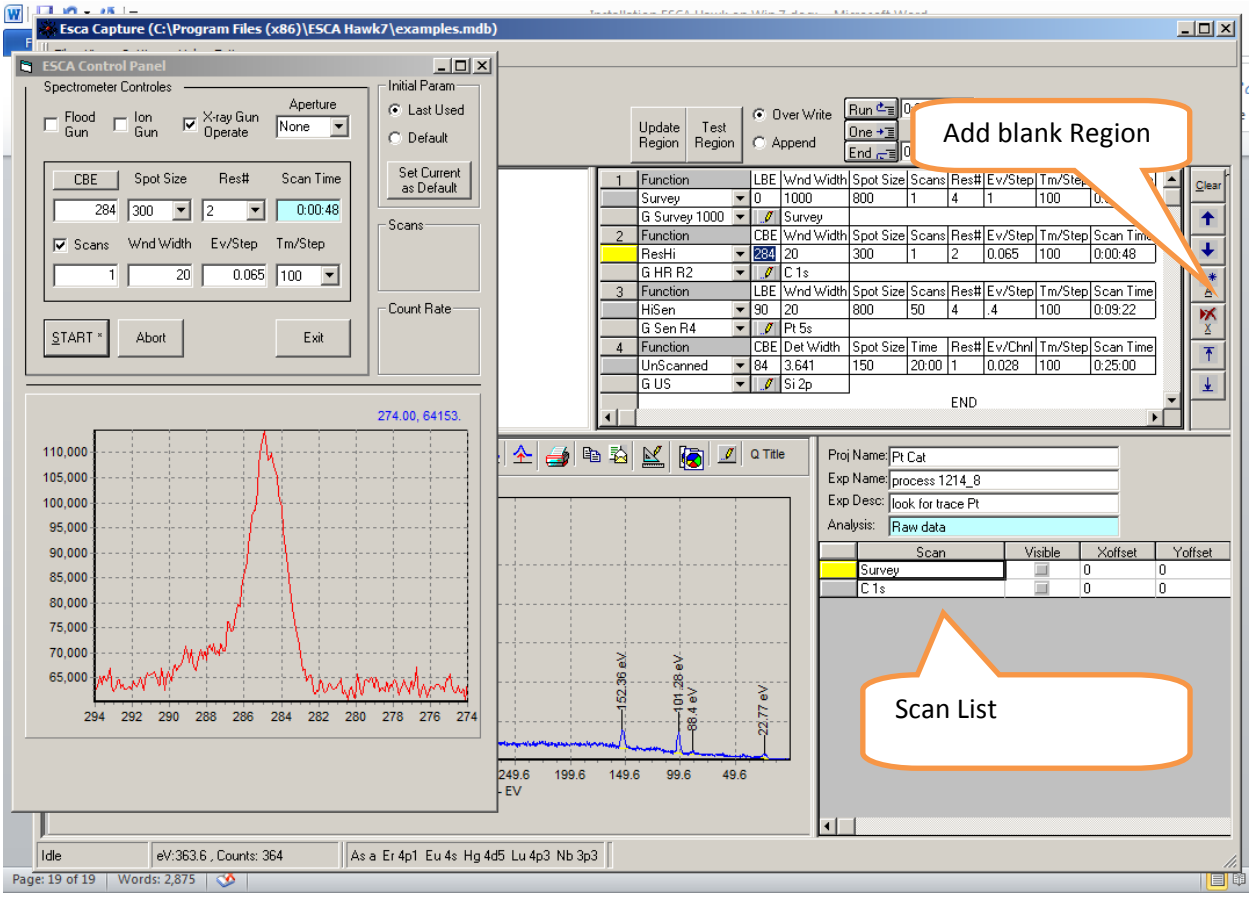
Depth Profile – setup DP regions and etch conditions

IO System – Aperture x-rays stand-by

Specify the type of Region with the Function drop-down window.

The MRS tools provide a variety of methods to create a region. At the far right of the MRS table are a set of buttons that create a blank region, delete a region and move regions to reorganize the table. Once a blank region is created you may choose a function that will create a region with default values that are typical for the function. You can then finalize the settings by changing the values in the cells necessary to meet your requirements. This is often a matter of changing just the BE and Number of scans.

Below is a table with four regions customized to look for Pt on a silicon dioxide substrate.



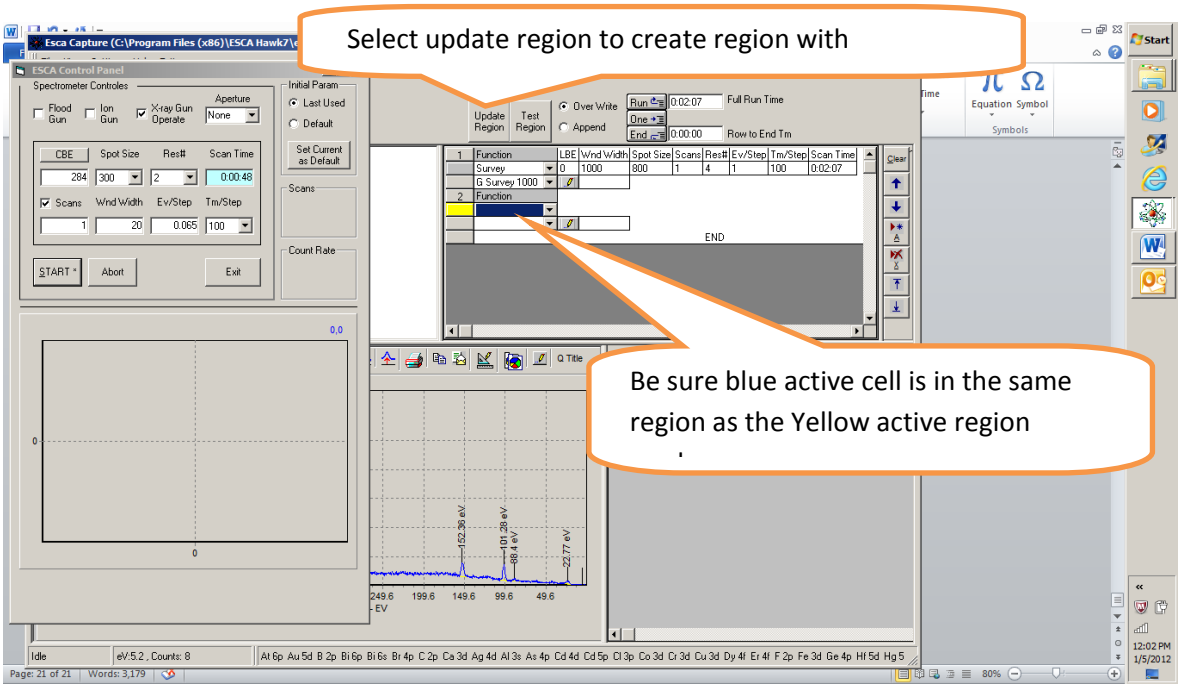
Points to remember:

The Region Label cell is located below the window width cell. This cell provides a label that will be substituted for the default Regn1, Regn2 etc. Notice in the Scan List (Lower right corner of the application window) these labels have been used in the Scan column. In the Analysis Application the labels are used in auto labeling spectra. If the label is a spectral line ID the DP viewer will look up the crossection in the Scofield table.

The Unscanned Function provides the actual Detector Width for your reference.

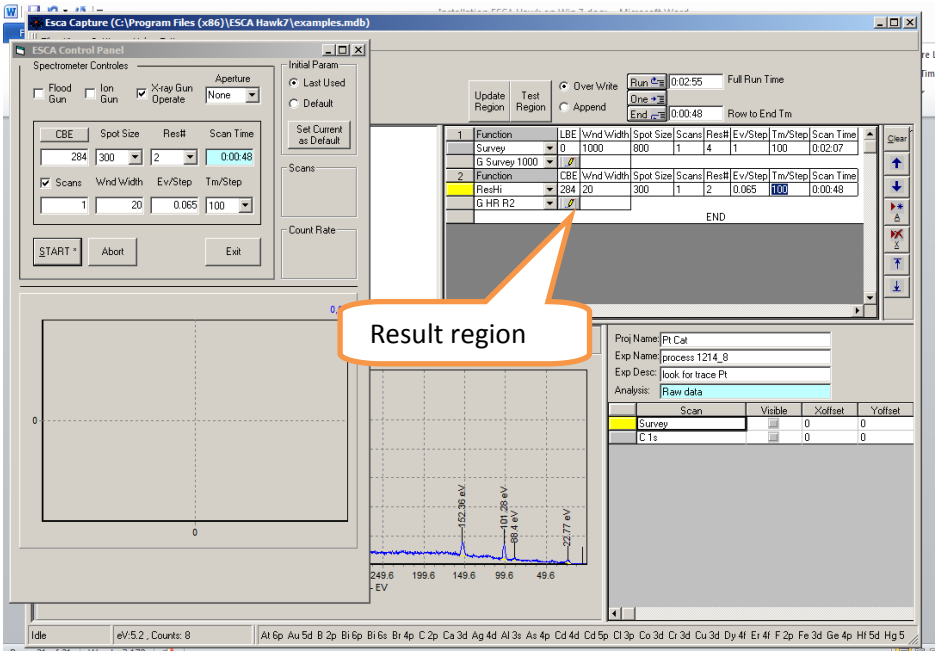
The “Scan Time” includes an overhead time in addition to the actual data acquisition time.

Filling a blank region form the ESCA Control Panel



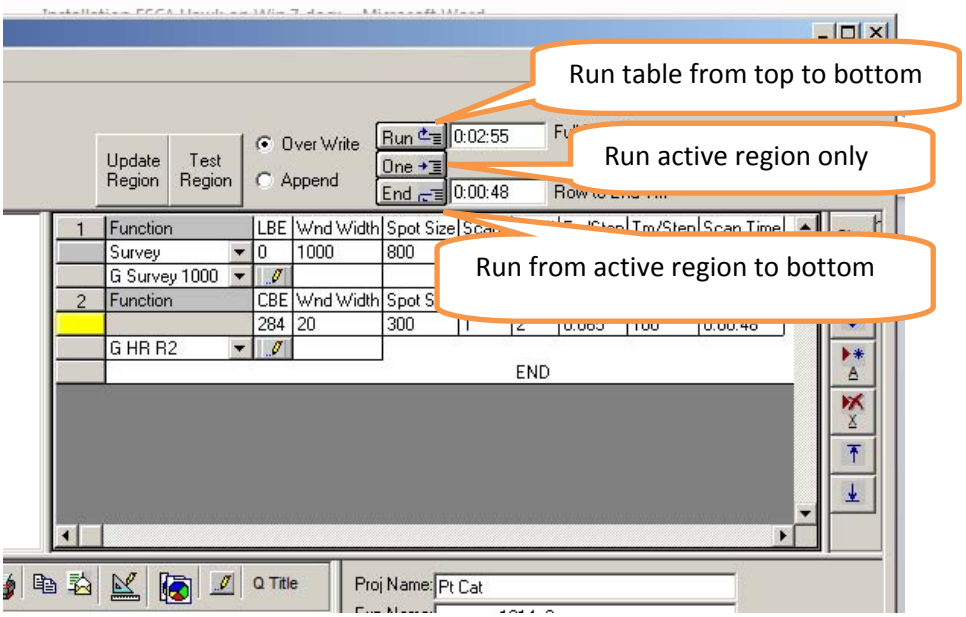
1. Add a blank region using the Add button
2. Setup the ESCA control panel and evaluate your parameter setting.
3. Click the “Update Region” button to load parameters into the empty region.
4. You can also update to an existing region. Be sure the Yellow region marker and blue active cell marker are in the same row. If the parameters transferred are not consistent with the function rules the Function name will be changed.

Result of Updating to a blank region



Any region can be tested by clicking on the block below the Region number to activate that region and then Clicking the “Test Region” button. The ESCA Control panel will open and start running the selected region. You may make changes in the ESCA Control panel and then "Update the Region" back to the MRS table.

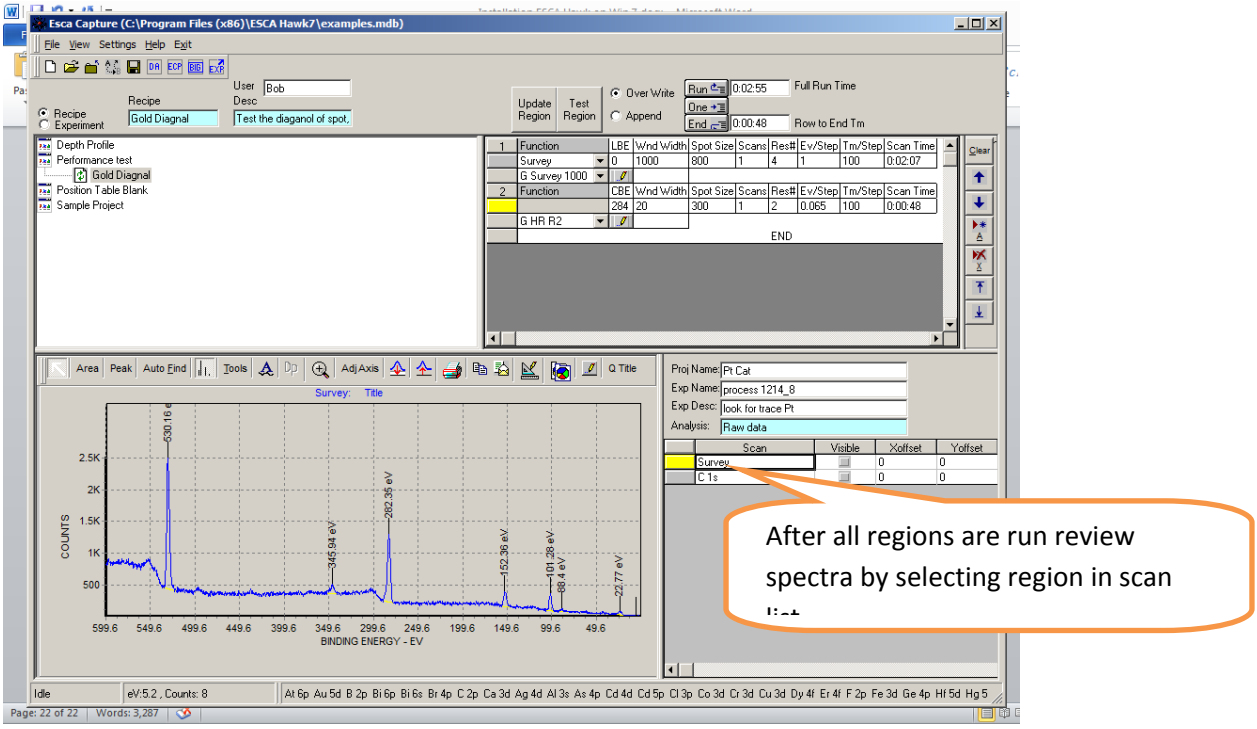
Running the MRS Table



Select any one of the start keys to run the MRS table.

Review Captured Data

Each region of the MRS table that was run will appear in the Scan List after all spectra are captured. You may review them by clicking on the activate button in the scan list. Multiple regions can be displayed at the same time by checking the box in the visible column.



Points to remember

The tools above the spectra are only available for review. Results of measurements can't be saved.

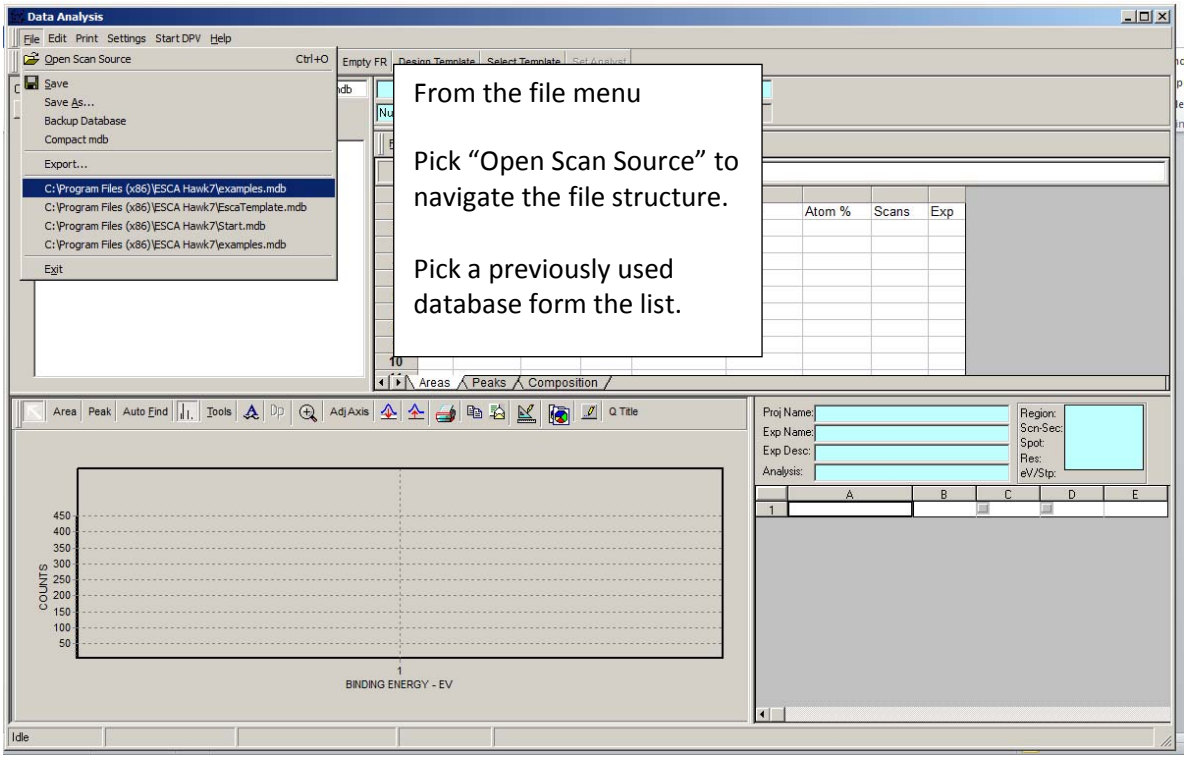
The cursor position and curve amplitude is displayed in the information box at the bottom of the application window.

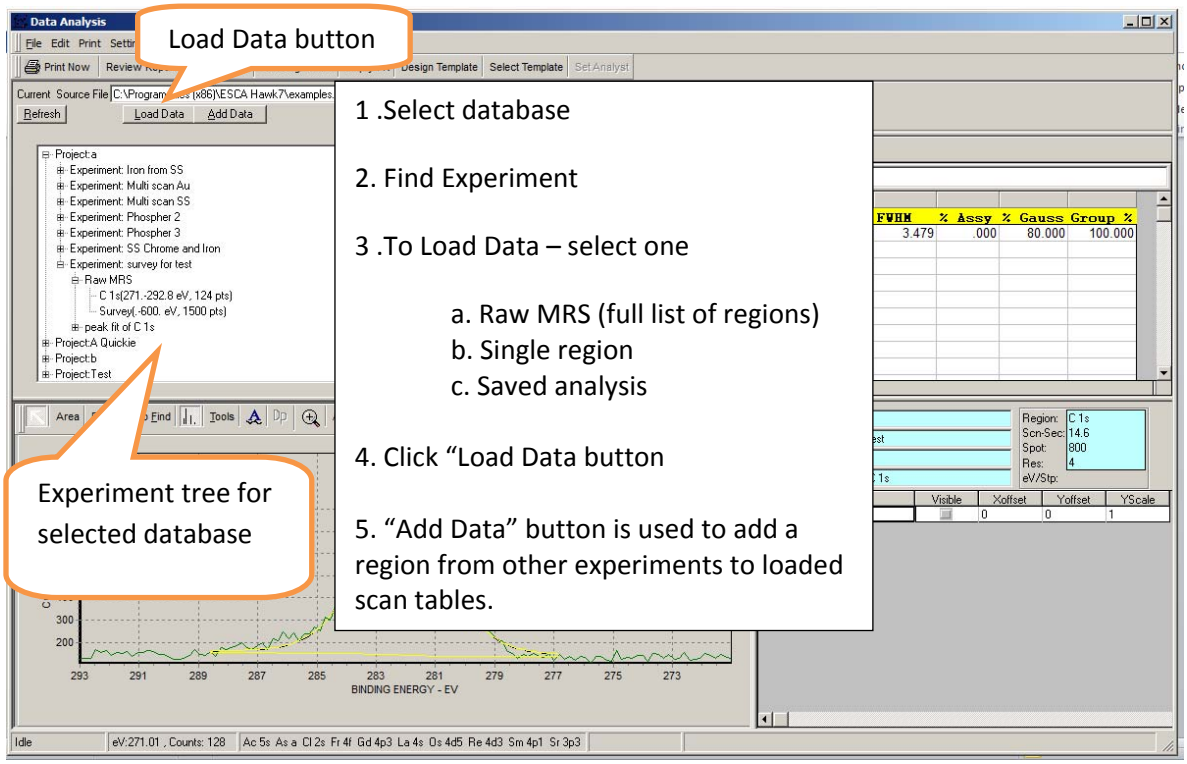
You may copy a spectrum to the clipboard, print or save the graphic form of the spectrum using the icons in the spectrum tool bar

The Icon, that is a blue A, can be used to label the spectrum. Click the Icon. You will see a BE number with a short vertical line below the number in the middle of the graph. Move the cursor to the bottom end of the line. When you see the arrow become a hand, left click the mouse and drag the line. The number will reflect the BE of the new location. The label can also be moved. With the cursor on the label right click the mouse. A dialog opens that provides for input of a new label and formatting of the label.

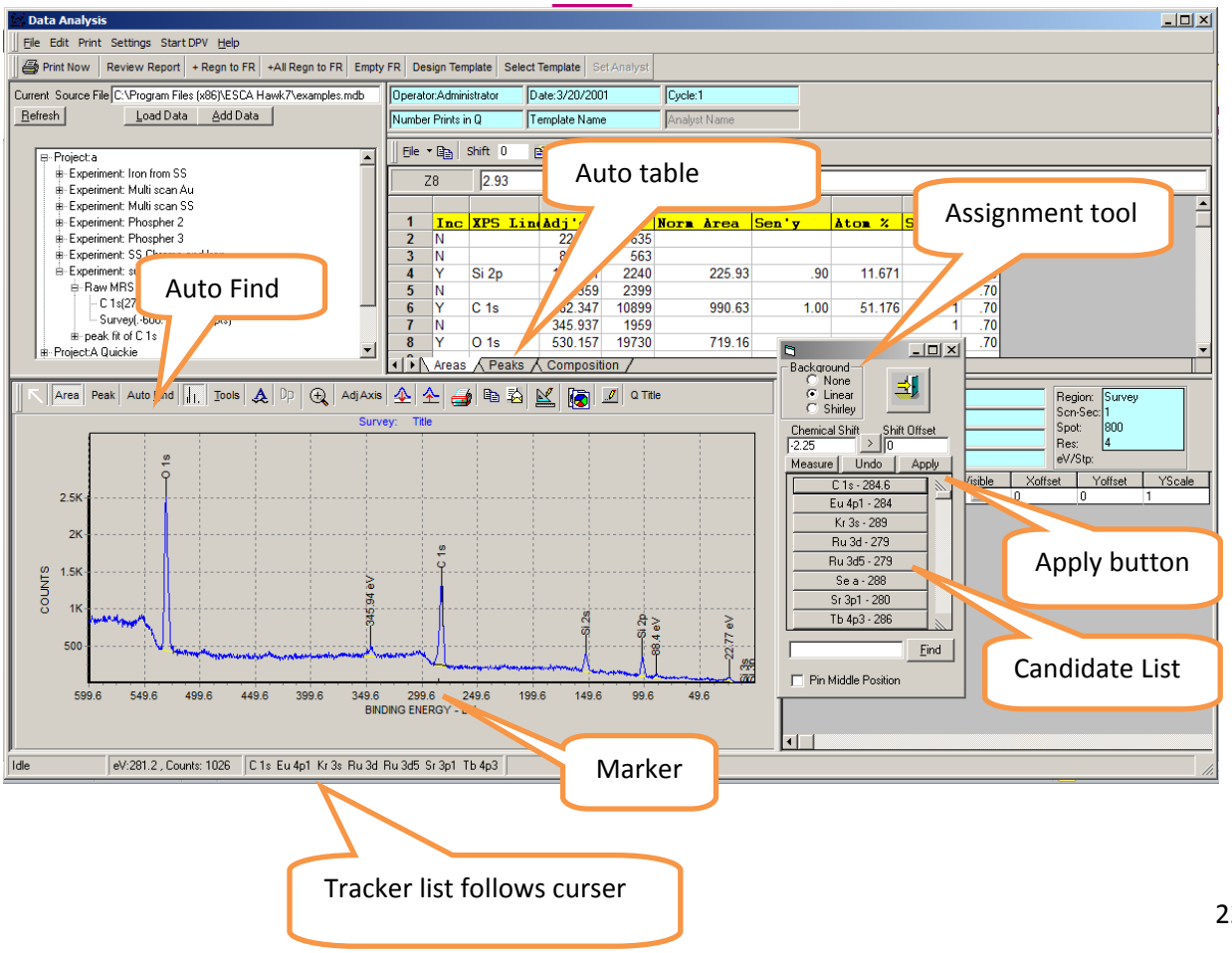
STAND-ALONE ANALYSIS

Loading Data for analysis



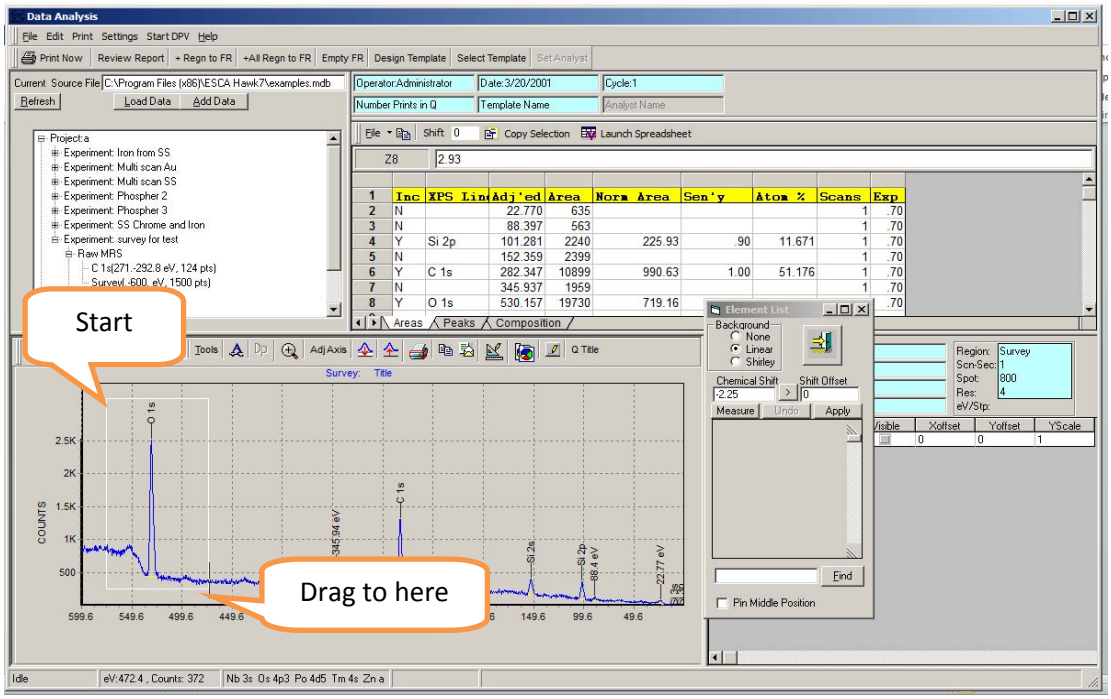


Area measurement

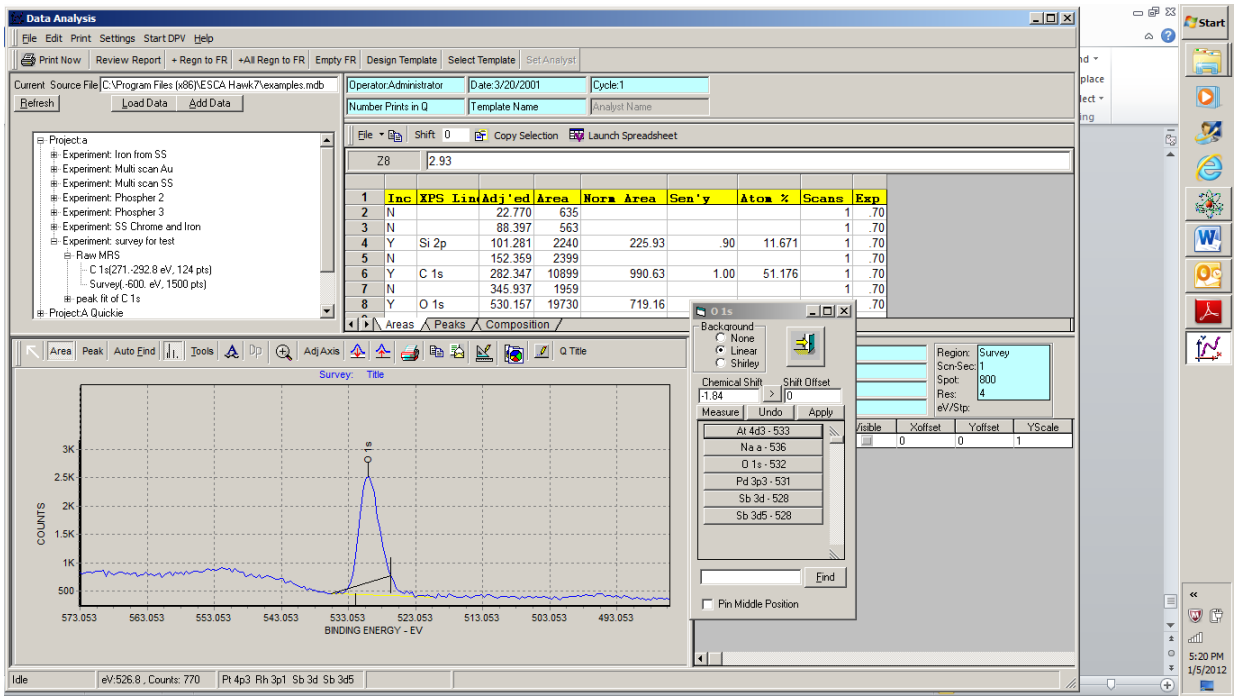


Sequence to measure and identify peaks:

1. Click Auto Find tool. The Assignment tool will appear.
2. Activate peak for identification by clicking near the BE label above the peak.
3. Select a trial candidate form Assignment tool list.
4. Review the markers along the baseline to see if all peaks for the element are present.
5. Try other assignments if necessary.
6. If you wish to assign the ID symbols to all other peaks for the selected element click the "Apply" button. This aids in determining if you have accounted for all peaks in a complex spectra.
7. Repeat for another peak.



If you wish to expand the scale draw a box to outline the area you want to expand. To draw the box you click at the upper left corner and drag to the lower right. The graph will expand when you release the mouse button. To return to normal you reverse the direction of drawing the box.



Result of Expanding window.

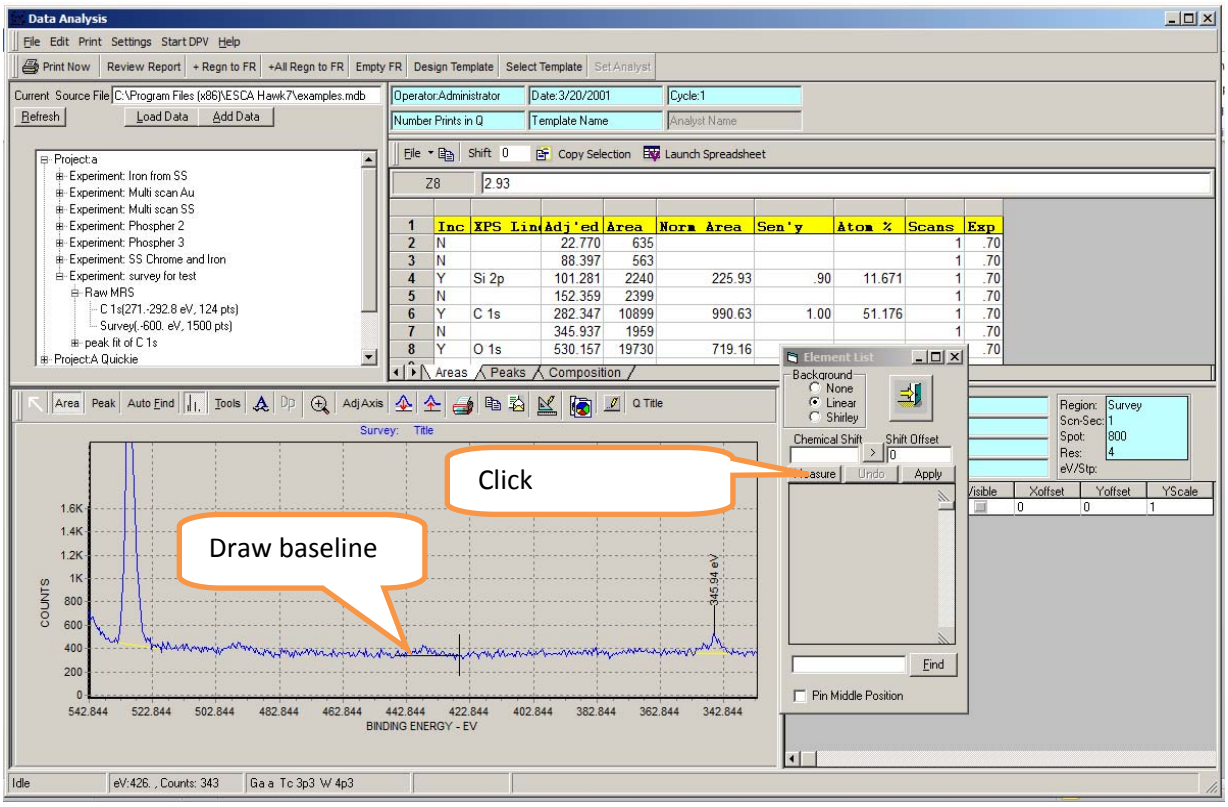
Adjusting or drawing the base line:

To adjust an existing base line:

1. Activate the existing base line. Place your mouse pointer between the end points of the existing baseline and click. A black line will appear next to the existing yellow base line.
2. Find the hot-spot where the existing baseline joins the peak curve. The mouse pointer will change from an arrow to a hand with the index finger as a pointer.
3. Left mouse click and drag the endpoint to a new location.
4. Repeat for the other end of the baseline if necessary.

This procedure can be used to create a new baseline. In this case you place the tip if the mouse pointer at a point on the curve where you wish to start drawing the baseline. Then you drag the baseline to a second point on the curve and release the left mouse button. This operation is used to make a new area measurement.

To enter the new Area measurement into the data table click on the “MEASUREMENT” button on the Assignment Tool.



Points to Remember:

1. Area button on toolbar must be active and Assignment Tool must be present to make or change baselines.
2. The area and BE information is added to the data table by making a measurement.
3. Scofield information is added to the data table by making an Assignment from the candidate list.
4. The element list is filled from the Scofield table following range rules contained in Scofield table. If the spectrum is shifted so the Binding Energies don’t fall within the Scofield table range then the Assignment table will not be valid. To avoid this problem:
    a. Find a reference line with known Chemical or no Chemical Shift.
    b. Determine the shift necessary to move the line to the correct BE.

c. Above the table is an entry box titled Shift. Enter the shift value.

d. Now activate the peak so the element appears in the Assignment Table.

e. Select the Assignment

f. Check the Chemical Shift window at the top of the Assignment list.

g. If this is a line with no Chemical Shift and a value is displayed then click the Right arrow button between the Chemical Shift window and the Shift Offset Window.

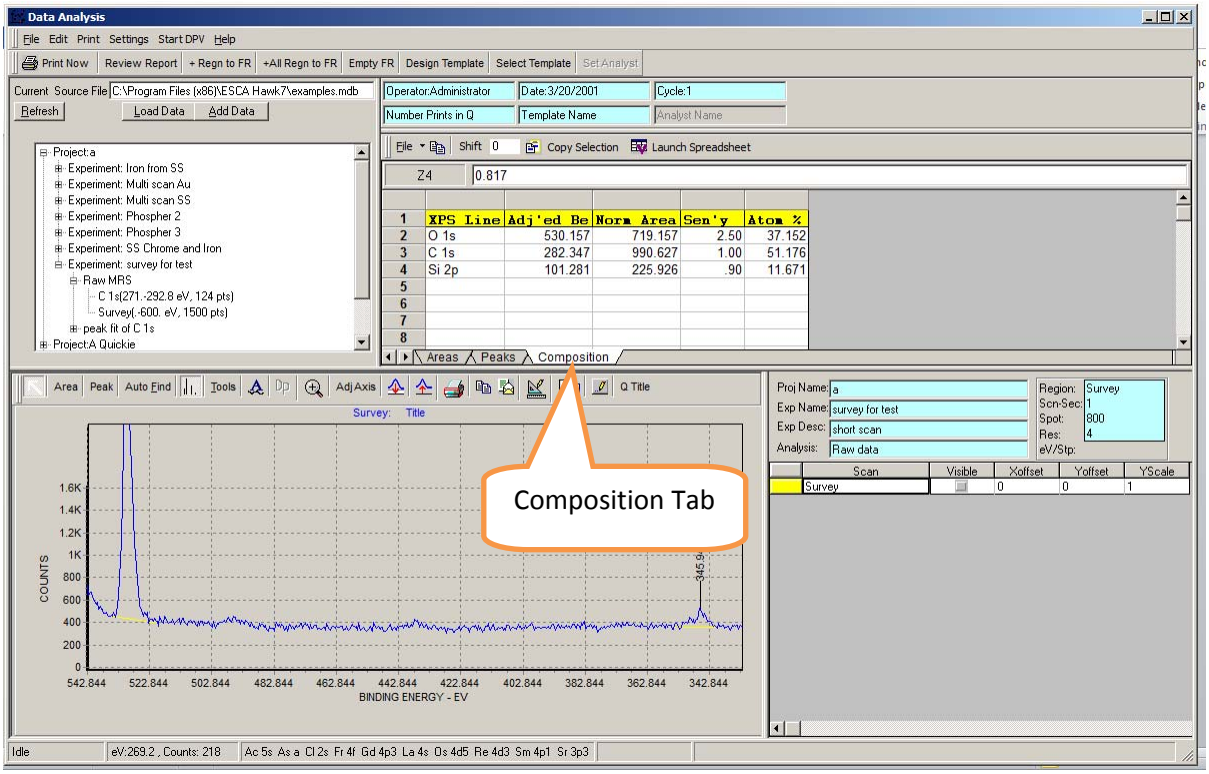
h. If you know the Chemical shift and it is not correct then correct it by adjusting the Shift value in the box above the Data Table.

i. Now all other assignment will display the correct Chemical Shifts in the Data table.

5. You may select linear, Shirley or None for the base line. It is best to select the line style before you begin area measurements.

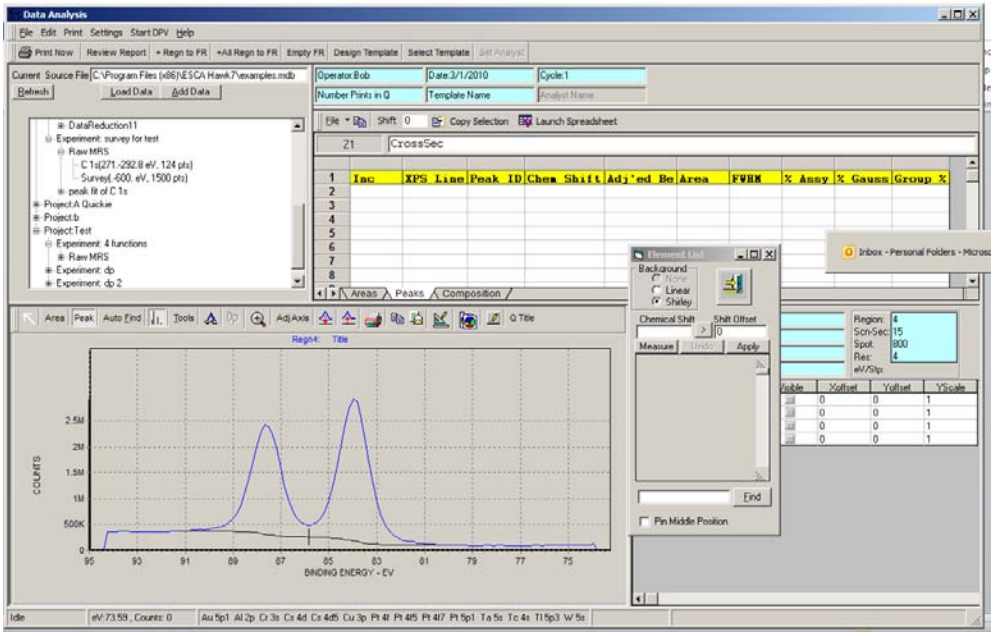
6. The "None" base line option is useful in calculating the estimated uncertainty in the area measurement. The area in this case will be all counts under the peak, without baseline subtraction. The uncertainty is the square root of the total counts under the peak. This can be compared to the area between the peak and the baseline to determine the signal to noise of the measurement.

Composition Table

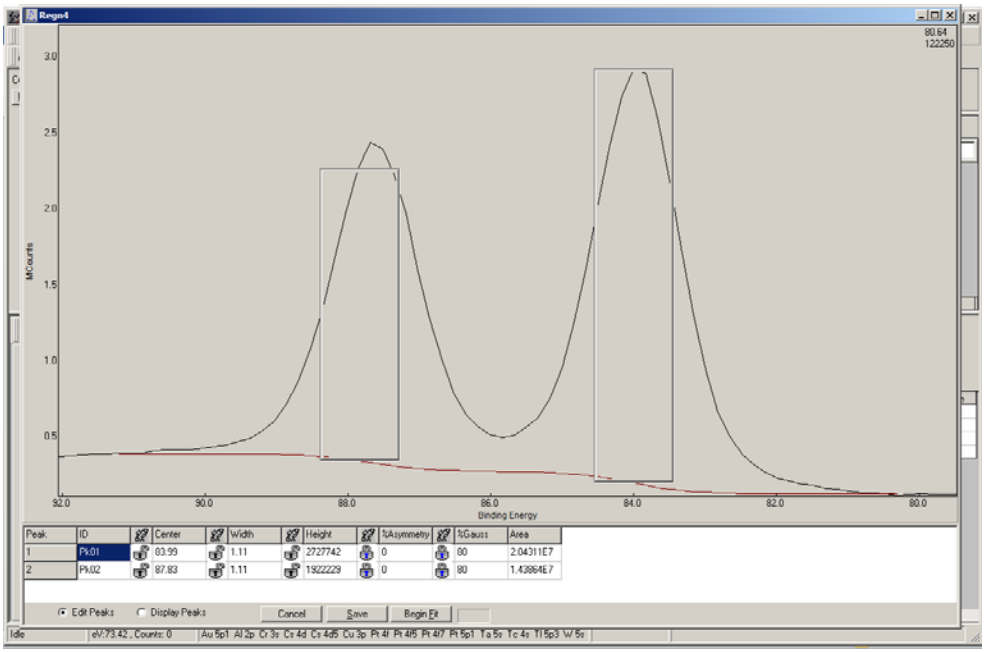


Selecting the Composition Tab below the Data Table provides a summary of the lines selected for the composition measurement. The selection can be modified by the placing an “N” in the first column of the Area Table to drop a peak or a “Y” to include a peak.

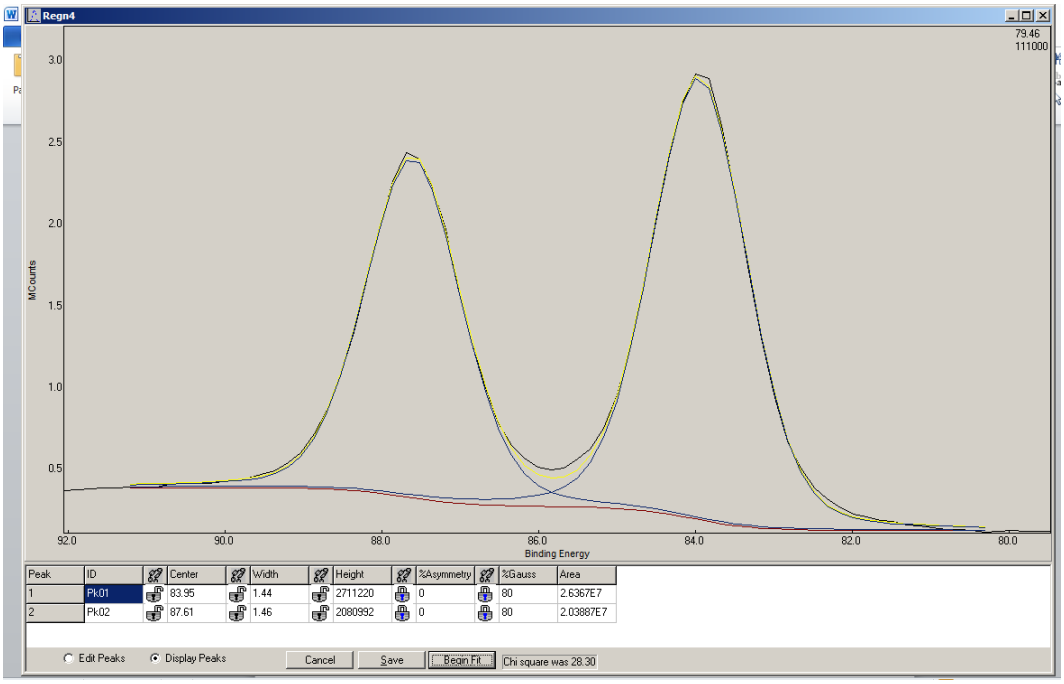
Peak fitting



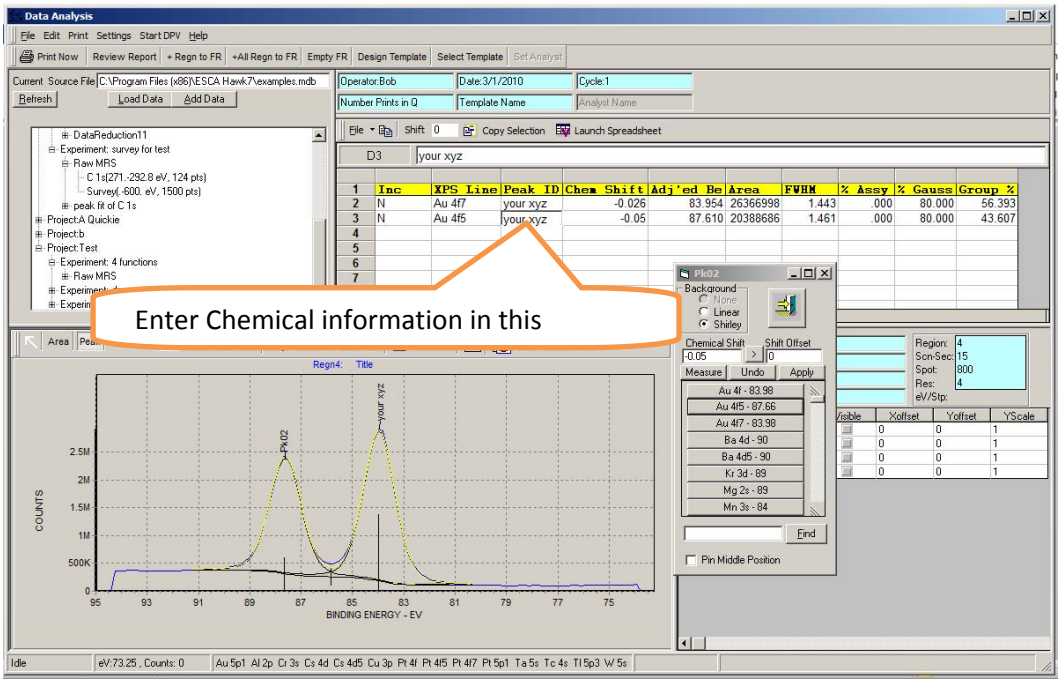
1. Select the Peak button in the Tool bar.
2. Draw the base line
3. Click Measure Button on Assignment Tool



1. Place “width boxes”
2. Select Begin Fit



Save will store results and return to the main window.



Assign elements or enter Peak ID information directly in the Data Table.

Reports

The output provided is extensive and covered in the manual. We provide here a brief description of the print out capabilities.

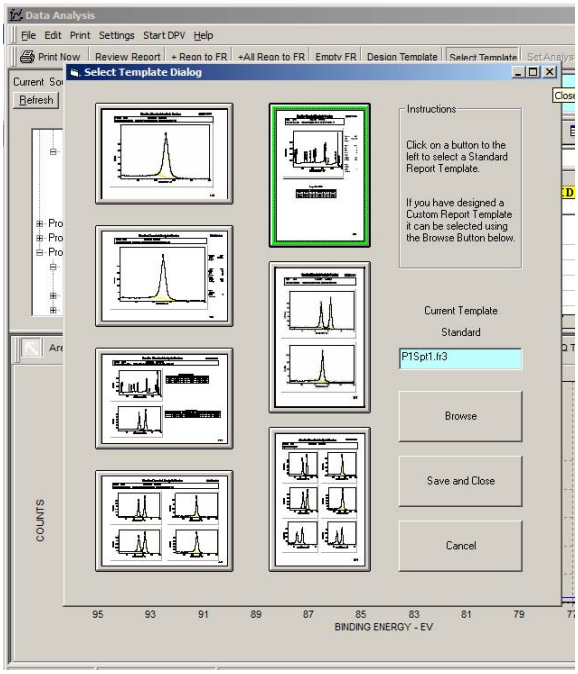
The printout is a subset of an embedded Report Generator purchased from Fast Reports. (FR)

The tool bar controls the information passed to FR's. The steps to generate a printout are:

1. Perform any data analysis you wish to have reflected in the printout.
2. Select a template (far right button on tool bar)
3. Review Report (If you only want to print one spectrum you can skip this step)
4. Print

If you wish to work through a list of spectra you can either add them to the report after you have finished each spectrum using [+Regn to FR] or finish all regions in the region list and then select [+ All Regn to FR]. You can clear all regions placed in the FR using [Empty FR]. "Print Now" prints all Regions that have been added to the report.

Select Template



Templates can include:

Header with Lab Name and Logo, Project, Experiment and Description information.

Data collection parameters

Composition Tables

Peak Fit tables

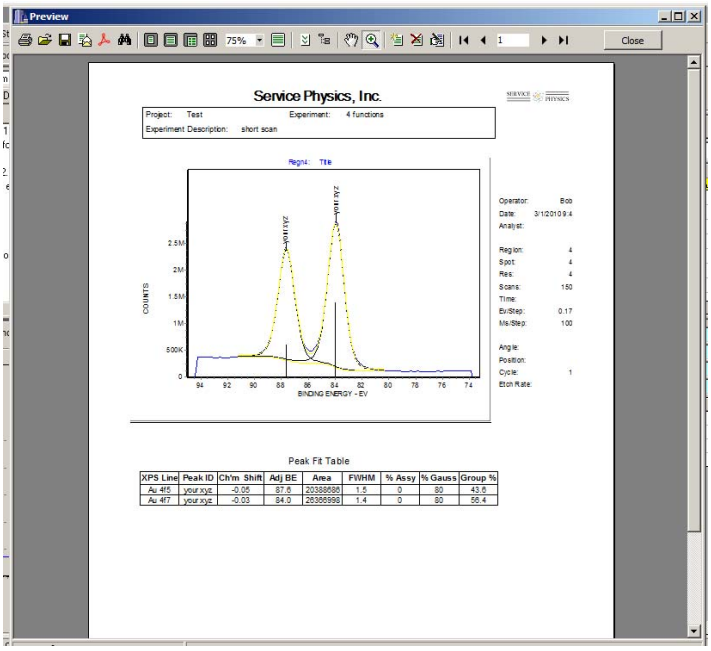
Figure descriptions

Individual titles for each spectrum

A template designer is includes for creating or modifying templates.

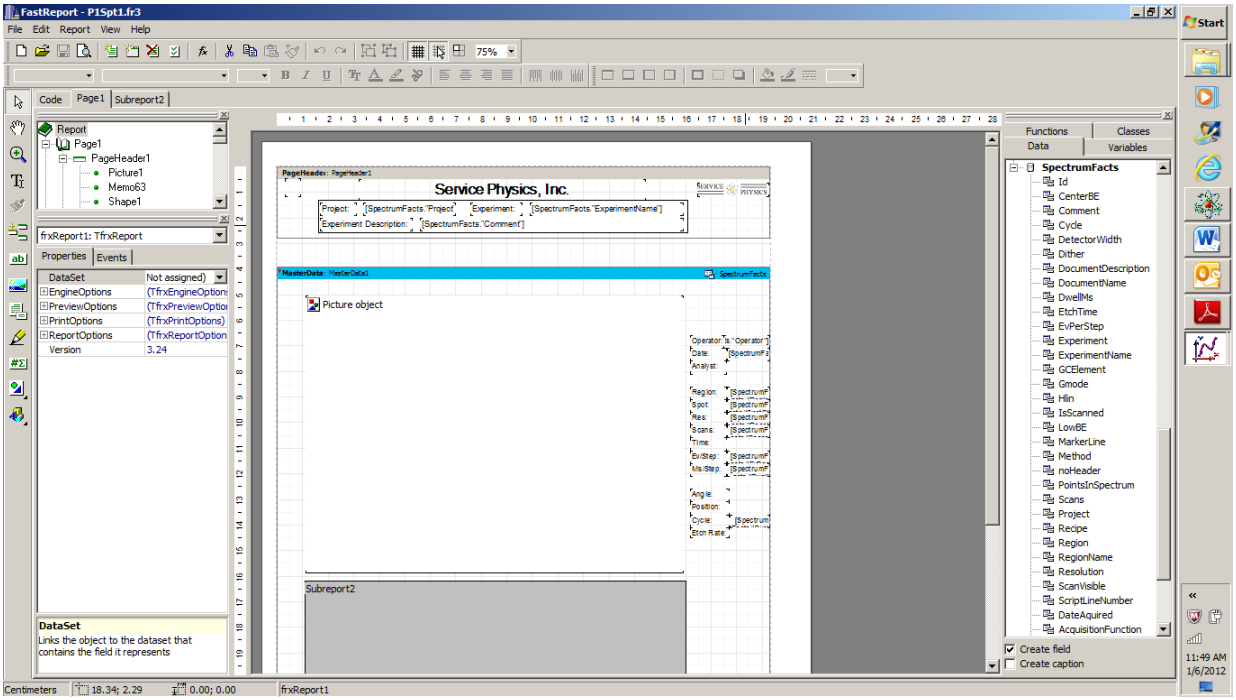
Select one of the 7 template icons then click the “Save and Close” Button to activate a template.

Then you can preview the FR

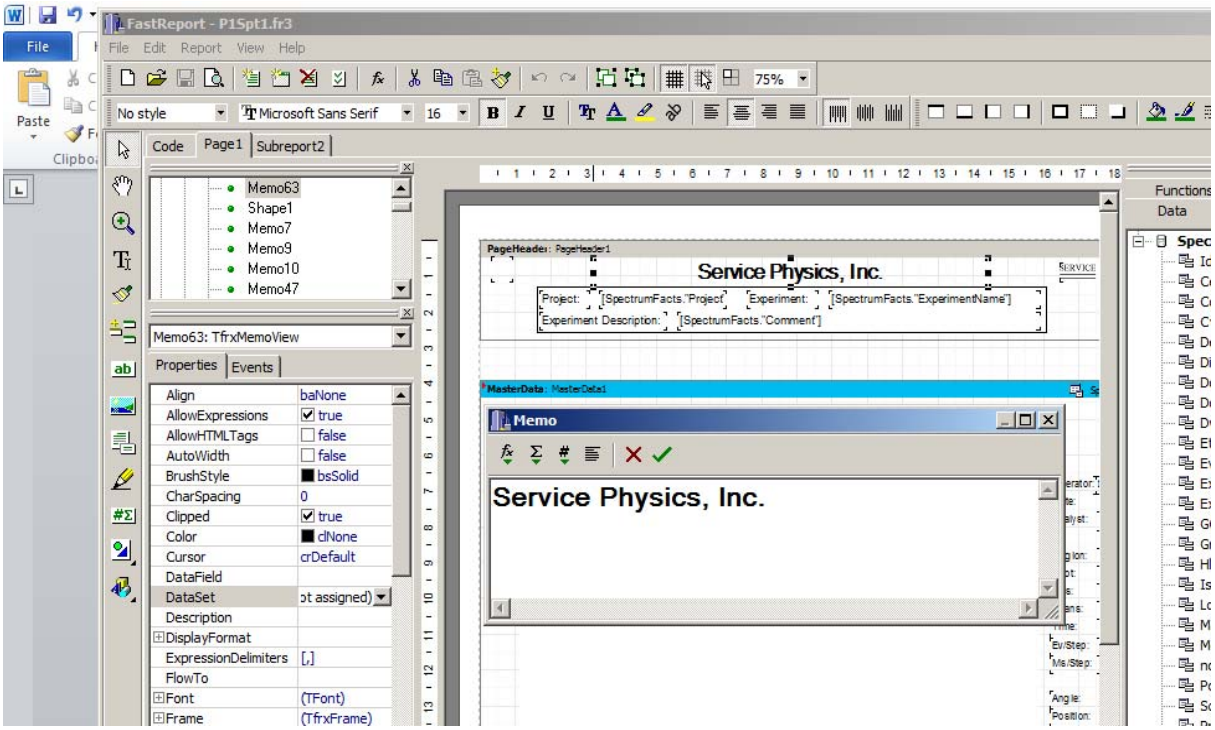


You will want to modify the Header to enter your own Name and Icon if available.

Close the preview and open the "Design Template” Tool. This will open the active Template in design mode.

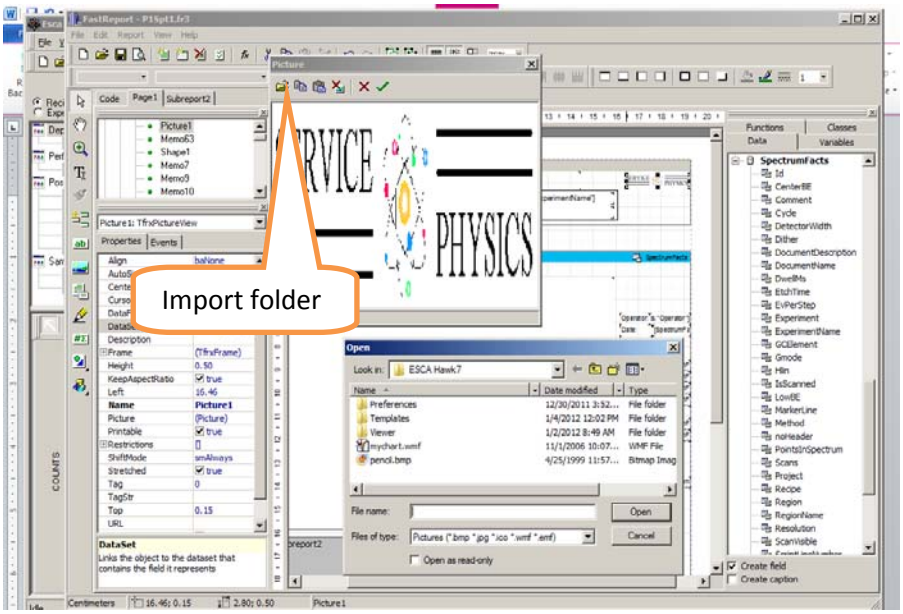


Double click on the “Service Physics Inc.” text block. You can see the corner symbols that define the size of the block. Memo Box will open. Modify the text in the box and click the green check mark to save the new text.



To change the Icon, double click the Service Physics Icon, Open the import folder, find your Icon, open your icon in the Picture Dialog and then click the green check to save the change.

If you wish to delete the Icon then just select the red x next to the green check.



You will notice that this designer has a list of many of the variables used in the ESCA Hawk program. These can be dragged onto the template to expose the value of that variable at the time you add the region to the FR. The manual has additional information about designing templates and a complete manual from FR is available. We can also provide custom templates on a contract bases.

The printout is compatible with any Windows Compatible printer, PDF converters and Print to file servers.

Building Report using sharing of data with Windows Office

The Windows Clipboard provides powerful data sharing. Tables and Graphics can be copied to the clipboard and pasted into EXCEL, Work or Power Point. Clipboard Icons are available in the tool bars of the Graphic Viewer (Spectrum Display) and the Data Table. These provide the ability to transfer anything from a single number or spectra to complete working tables and graphics that can be modified. In addition the information in the FR can be saved in HTML, PDF or EXCEL formats. The FR icons are found in the Report Preview toolbar.

There are also icons that provide for the saving of tables and graphics as jpeg or bitmap formats.

EXPORT

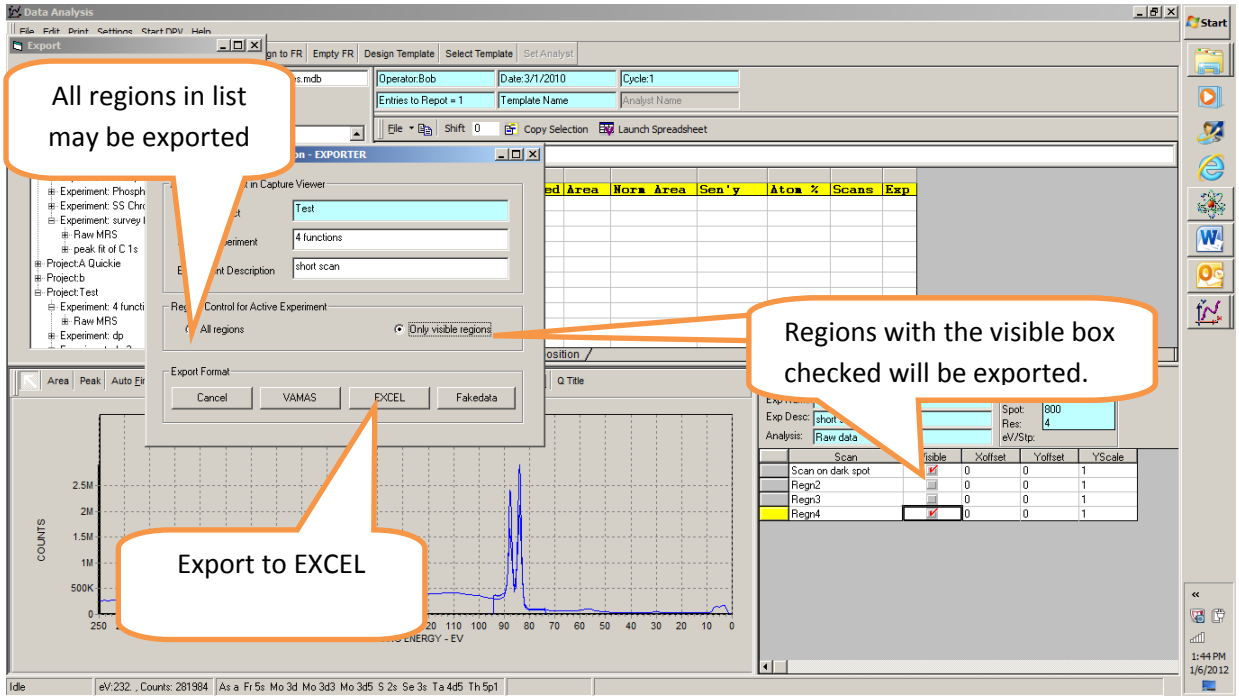
Export of raw data is available in EXCEL, VAMAS and txt formats. The Export utility is provided in both the Capture and Analysis program. In addition the DP Viewer provides for transfer of Composition tables and Binding Energy Tables for multiple data sets taken with one MRS table. The plots of various parameters verses Time (aging), distance (Depth Profile), Position (process tracking on multiple samples or Line Scans) can be constructed in EXCEL using data prepared by peak fitting or area analysis tools in the DP viewer.

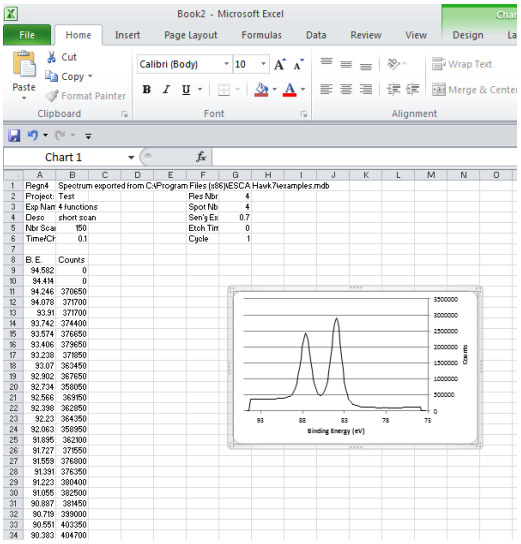
EXEL Export

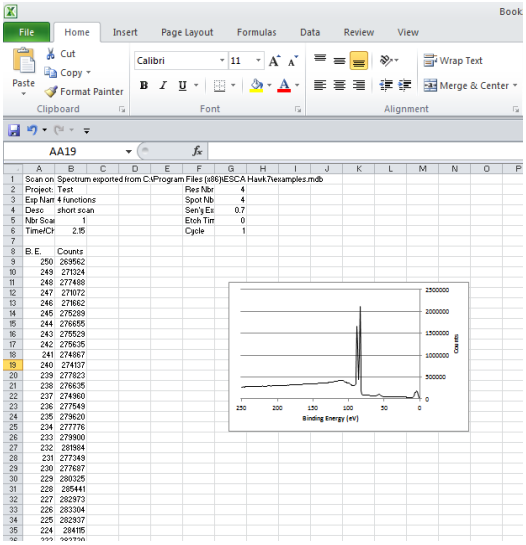
From the File menu select Export

Fill out the Institution and instrument model number information

Configure the export conditions





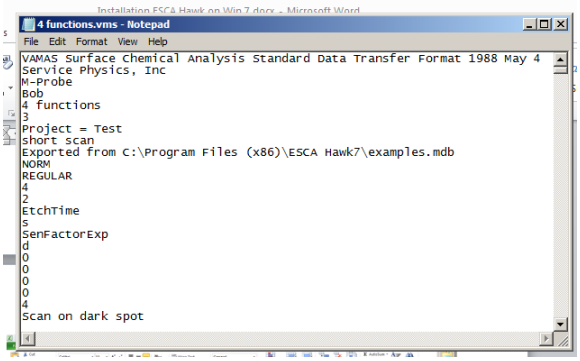


Data and spectrum are provided one per page.

Header provides basic information about data.

Columns for BE and counts.

Data in standard VAMAS format.

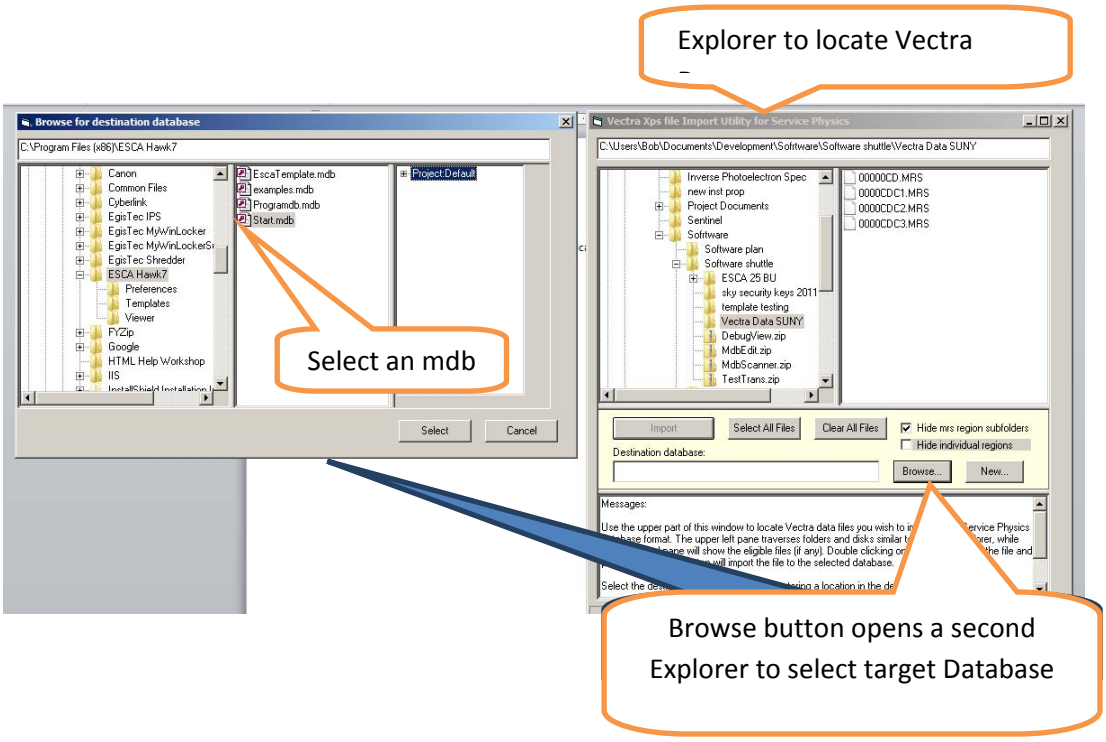


Vamas is an international standard for electron spectroscopy. This allows direct import into generally available Data Analysis programs.

Data string only in txt format. Used in our Demo software to provide simulated operation. The text format is called fakedata. It is a single column of counts. A header provids the BE span and the number of data points.

Import Vectra DOS

The Vectra Data Import utility is a standalone application that can be opened from the Windows start menu.



To Import a Vectra file

1. Find the folder that contains the MRS or REG files. There will be no entries in the Right panel of the Vectra Data Explorer until MRS or REG files are discovered.
2. If you have folders with single REG files you can blank these folders form being displayed. This is the default. Notice the check box is checked.
3. The default setting will display both the MRS name and the REG files. You can blank the display of the REG files that are members of the MRS file by checking the “Hide Individual regions”.

4. You can select a MRS or REG file for processing by clicking on the name (not the check box). If you want to select more than one hold down the CTRL key on the keyboard and select multiple files. You can select all files by clicking the “Select all Files” button.

5. You must establish a target Database for the “Import” button to activate.

6. If you select the Browse button the left hand explorer will open. Any database will accept the import.

7. Click the Import button. The files will receive check marks as they are processed. This way you are left with a record of the imported files.

8. If you have a target Database defined you will see the path to the database in the display window next to the Browse button.

9. A quick method of importing a few files is to just double click the file name. The file will be imported and the check box will be checked.

10. Once the files are imported into a data base you will find the files listed in the Experiment Tree of the Analysis Application. If the Analysis Application was open during the import process you will need to use the Refresh Button, next to the Load Data button, to update the list.

11. All functions of the Analysis program can now be performed. If you had performed data reduction on the Vectra data this information should be present in the Experiment tree as an entry just below the Raw Data entry.

Life is short – Call if you have questions! 541-318-8688