RPT Configuration File Entries (Batch Processing)

The RPT mechanism is the most flexible means in CasaXPS of tabulating results computed from quantification regions and/or synthetic peak models. However, the cost of using this tool is that the resulting table must be defined in very basic terms. An RPT file defines the columns of a report using the VAMAS file block structure and the ordering of the quantification regions and components within the blocks of data.

A VAMAS file consists of a header section followed by a set of data blocks. Within CasaXPS, the order of these blocks is maintained using an index number beginning at zero as illustrated in Figure 1. Each data block referenced by index (e.g. vb0, vb1, vb2, ….) includes ordered lists of quantification regions and components, also illustrated in Figure 1, which are again referenced using the index within a VAMAS block for a given region or component (e.g. r0, r1, r2, …. and c0, c1, c2, ….). To identify a specific piece of information from a region or component, the datum of interest is defined using the VAMAS block index, a keyword string and either the index string for the region or component.
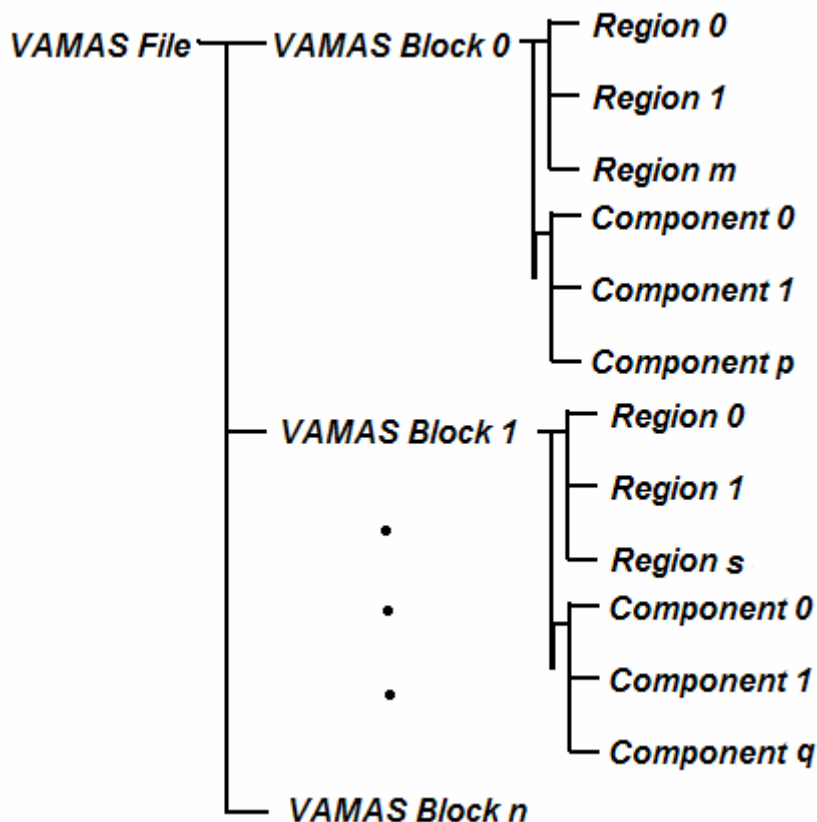

Figure 1: Logical structure within a VAMAS file.

For example, the data in Figure 2 are from a file containing three VAMAS blocks. The spectra are displayed such that the VAMAS block index appears in the top left-hand corner of the graphical area (an option on the Tile Display dialog window) from which it is clear that the data can be referenced by vb0 for the survey spectrum, vb1 for the O 1s spectrum and vb2 for the Si 2p spectrum. The survey spectrum has three quantification regions defined on it, while the O 1s and Si 2p spectra each have a single region defined. In addition, the Si 2p data are fitted using a peak model in which four synthetic components are used. The order assigned to the regions and components is defined by the column on either the Region or Component property page (Figure 3) in which a given region or component appear, respectively.
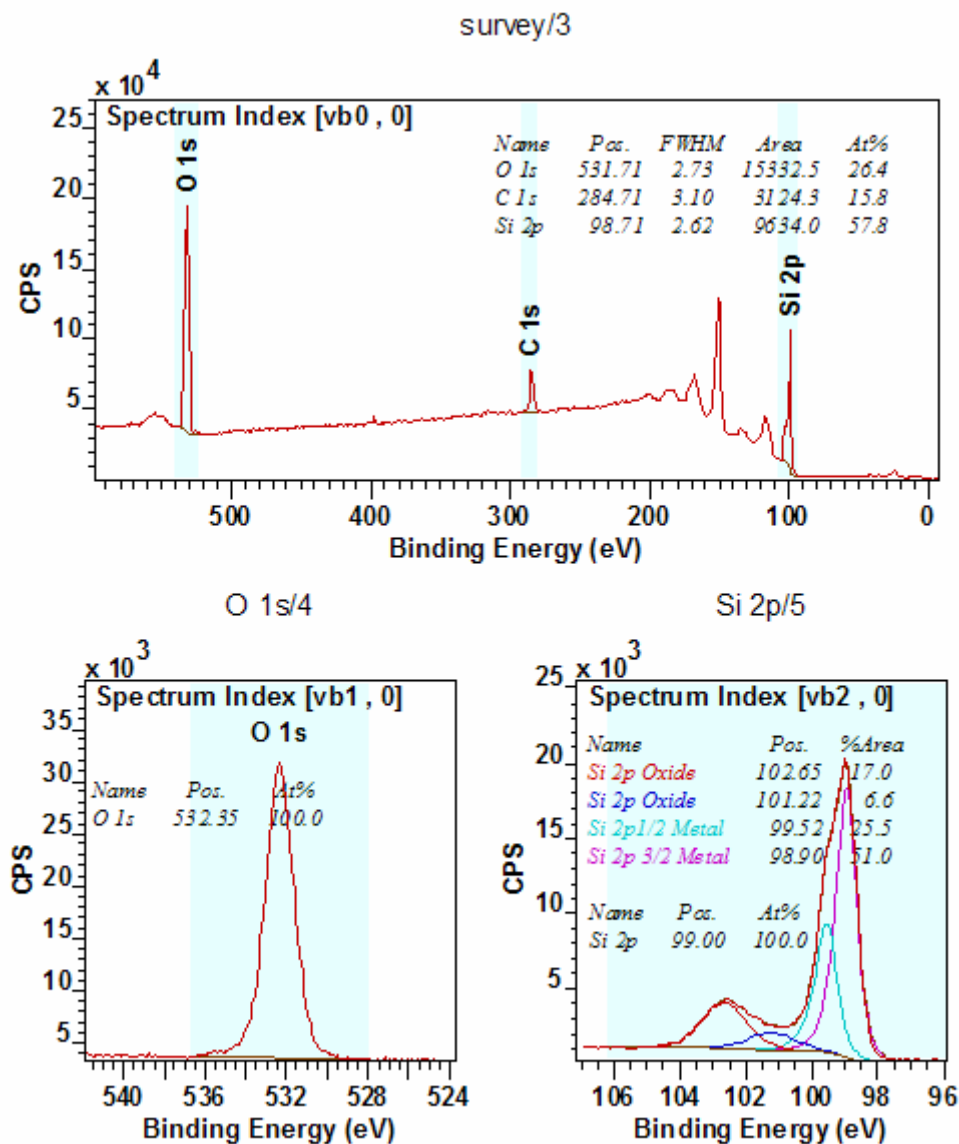

Figure 2

Note, the annotation tables in Figure 2 agree with the column order defined in Figure 3, however this is not always true. It is possible to make a configuration file entry in the CasaXPS.DEF directory which causes the annotation tables to be listed in an order based on the binding energy of the peaks in question. The regions and components on the Quantification Parameter dialog window always appear in the order in which the items are created. The order important to the RPT file definitions is defined by the Quantification Parameters dialog window. Therefore to specify the transmission and RSF corrected intensity from the second component defined on the Si 2p the string vb2;INTENSITY;c1 would be used in the RPT file. That is, since the index for the VAMAS blocks begin with zero, *vb2* identifies the third VAMAS block in the file and similarly *c1* indicated the component in column B of the list on the Components property page. The O 1s intensity from the survey spectrum in Figure 2 and Figure 3 would be identified using the string vb0;INTENSITY;r2. This is because the O 1s region on the survey spectrum appears in column C in Figure 3, while the O 1s intensity from the narrow scan spectrum would be identified using vb1;INTENSITY;r0.
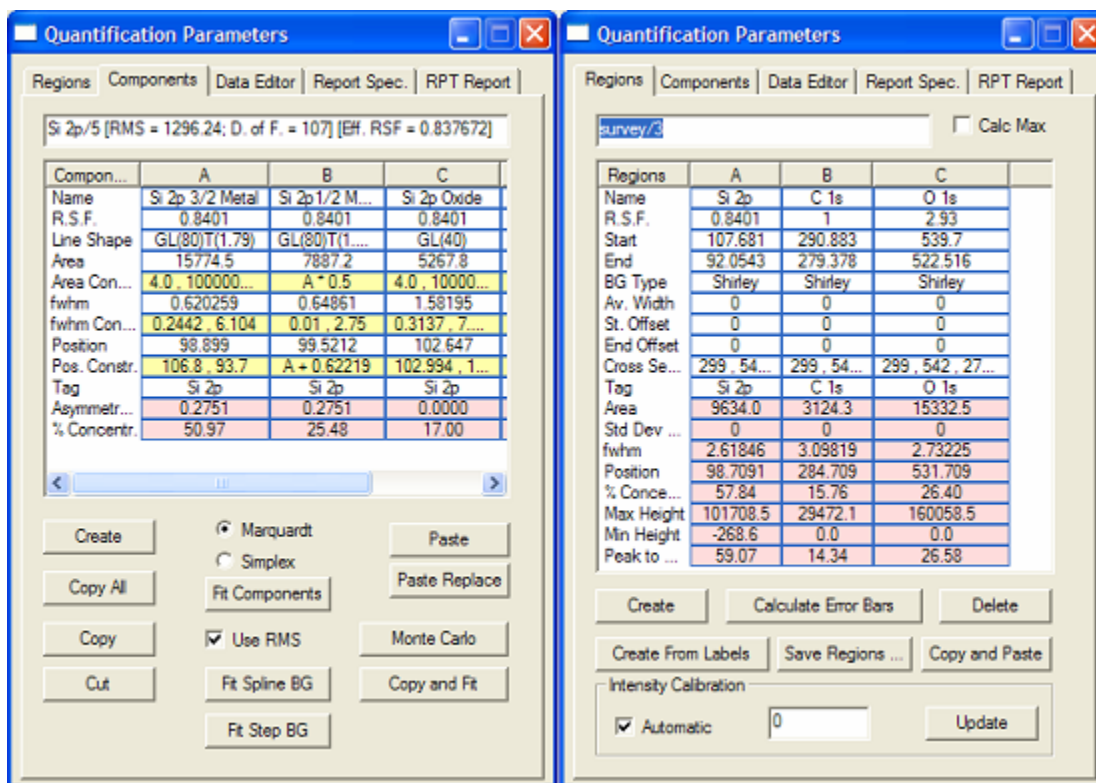
Figure 3: Quantification Parameter dialog window Region and Component property pages.

For further details in using RPT files please see Chapter 10 on Batch Processing in The Casa Cookbook page 215.

Quantification Reports Using RPT Files

While originally designed for batch processing applications, quantification reports defined by RPT files are now available from the Quantification Parameters dialog window. The RPT Report property page (Figure 4) allows a previously defined RPT file to be applied to those Experiment Frames for which at least one block is selected. The options on the Select menu help to select blocks across Experiment Frames and once the appropriate Experiment Frames are so identified, pressing the Generate Report button on the RPT Report property page permits the appropriate RPT file to be loaded. On completion, a report dialog window corresponding to the RPT file and the selected Experiment Frames appears.
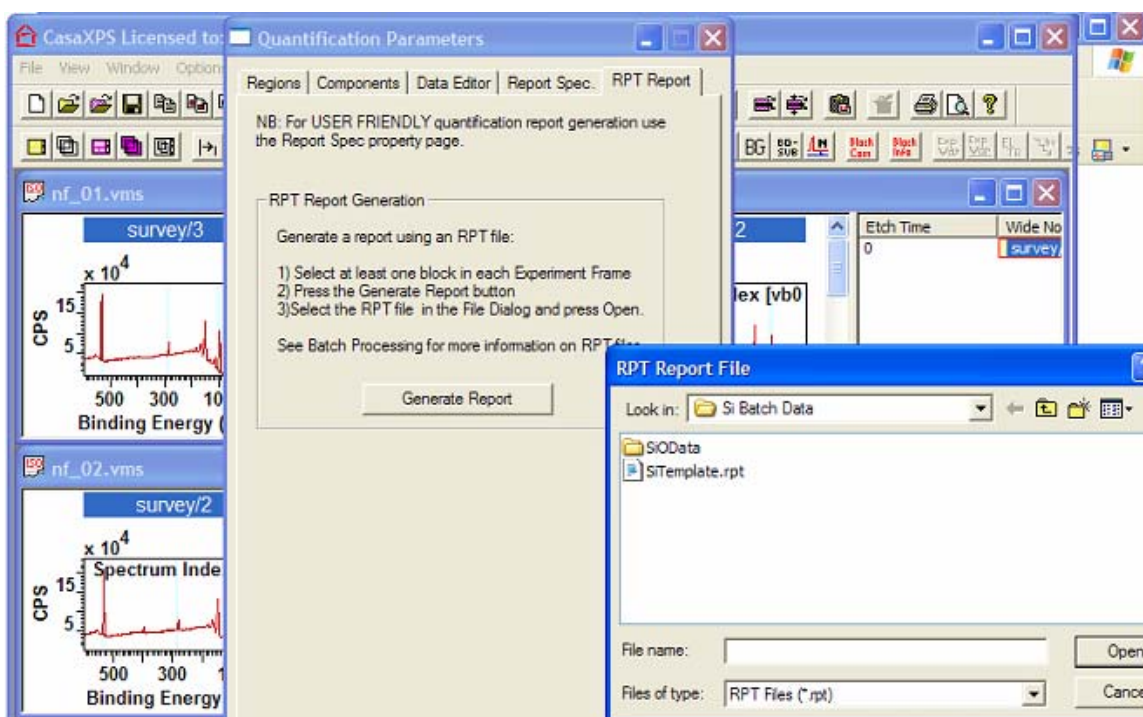

Figure 4

A simple text edit program such as Notepad can be used to prepare the RPT file. Once a program has been associated with the rpt file extension, right-clicking the mouse over the RPT file in the File dialog window and selecting the Open option will involve the chosen text editor. The RPT Report property page not only offers a mean of creating a very specify report for a particular type of experiment, but also provides a means of creating and testing RPT files in preparation for use with batch processing.

It is important to realize that an RPT file is specific to a particular experiment. The order of the VAMAS blocks in the Experiment Frame is important and therefore any file included in the reporting process must conform to the rigid format defined in the RPT file. Further before applying the RPT file, all processing and quantification items must

previously be created on the target data with exactly the appropriate definitions for the RPT file. While flexible with respect to the quantification information tabulated, the RPT mechanism is very inflexible with respect to the data and data treatment.