

## Batch Processing (CasaXPS version 2.2.50 and above)

Batch processing is aimed at situations where a set of essentially equivalent samples require identical data reduction steps. The objective is to provide a simple sequence of user interactions resulting in a report as well as optionally printing of the spectra in a predefined format. CasaXPS 2.2.52 offers the following actions:

- Automatic data conversion to the ISO 14976 (VAMAS) file format
- Data reduction steps bases upon a previously processed VAMAS file
- Printing after formatting the data using a .tff file
- Generation of a report based upon a report specification file.

Once the necessary configuration files are defined, the whole procedure amounts to selecting the template file and the raw data directory, then waiting for the results.

### Overview

The configuration files used as part of the batch processing feature appear in a directory called CasaXPS.BAT in the same directory as the executable file CasaXPS.exe (other CasaXPS directories such as CasaXPS.DEF and CasaXPS.HLP may also appear in the same directory). For each set of samples for which batch processing is required there will be at least one file in the CasaXPS.BAT directory, the so called *template file*. A template file is merely a .vms file containing a set of VAMAS blocks in the same order and number of as will be present in the data files acquired from each of the samples being analysed. Any processing, annotation, regions and components required for each sample should be applied to the data in the template file. When the batch processing is invoked, these operations from the template file are applied to each file in a target data directory.

Accompanying the template file, are optionally two files with the same base-name but with file extensions .tff and .rpt. The .tff file must contain information generated from the template file relating to the tile display format required when printing the data. If printing is not required, then the CasaXPS.BAT directory should not contain a corresponding .tff file to the template file. Similarly, the .rpt file is an ASCII file specifying the format for a row of data in the final quantification report. If no .rpt file corresponding to the template file exists in the CasaXPS.BAT directory, then a default report is generated once batch processing is complete. Defining the display state used for printing the spectra is described in [Case Study 5: Saving the Current Tile Format to File](#).

The objective for the .rpt file is to allow all the quantification items derived from the regions and components to be made available in a report, where these quantities can be combined using any arithmetic combination thereof including functions such as SQRT, LOG (natural log i.e. base e), EXP, SIN and COS. With the aid of these mathematical functions, intensities may be used to compute values for, say, overlayer thicknesses as well as error bars for such calculations. The emphasis is therefore on exporting the data for use elsewhere, for example a spreadsheet program where the ultimate report may include conditional display colours, more involved computation and/or graphical display, all previously defined on one sheet using data taken from a data entry sheet accepting the format defined by the .rpt file. The following describes defining the .rpt files.

### Setting-up the .rpt File

The .rpt file is an ASCII file best prepared in a simple program such as Notepad. Key words and defined strings are used to annotate the report and extract the quantification details from the processed data files.

newline	Inserts a new line in the header section of the report
header;<text-string>	Defines a text string for use as a header to the report. Each header so defined appears in a separate cell when pasted into a spreadsheet.
text;<text-string>	Defines a text string that will appear embedded in the report and is repeated for each row.
blank	Inserts a blank cell in the ultimate spreadsheet.
vf;FILE	If defined, the filename for the original file for the sample entered in a row.
vf;DESC	If defined, the file description for the sample entered in a row.
vf;DATE	The date when the data in the row was acquired.
vf;BATCH	If defined, the batch identification string for the row of data
vf;header;dir	Enter the data directory name into the header section of the report.
vb<index>;<keyword>	Extracts information from a VAMAS block defined using the VAMAS block index (an integer) and a keyword (see following table). The VAMAS block indices run from 0 to the number of blocks in the file minus one.
vb<index>;<keyword>;r<index>	Extracts information from a Region in a VAMAS block defined using the VAMAS block index (an integer) and a keyword (see following table) followed by the letter r (for region) and the region index within the VAMAS block. The VAMAS block indices run from 0 to the number of blocks in the file minus one. The region index runs from 0 to the number of regions in a VAMAS block minus one. The region order is defined by the columns in the Regions property page.
vb<index>;<keyword>;c<index>	Extracts information from a Component in a VAMAS block defined using the VAMAS block index (an integer) and a keyword (see following table) followed by the letter c (for Component) and the component index within the VAMAS block. The VAMAS block indices run from 0 to the number of blocks in the file minus one. The component index runs from 0 to the number of components in a VAMAS block minus one. The component order is defined by the columns in the Components property page.

**Table 1: Syntax for entries in the .rpt file**

FIT	Goodness of fit metric (Chisq or RMS)
EXP_VAR	Experimental Variable assigned to the VAMAS Block
BLOCKID	Block identification string for VAMAS Block
SAMPLEID	Sample identification string for VAMAS Block
INTENSITY	Intensity measured in CPSeV (area under peak)
POSITION	Binding Energy of the peak maximum
FWHM	Full Width at Half Maximum
STDEV	Error in measured intensity for peak area. (Regions only)
MAX_HEIGHT	Intensity at maximum counts (depends on technique)
MIN_HEIGHT	Intensity at minimum counts (depends on technique)

RSF	Relative Sensitivity Factor used to compute Intensity
PEAK_TO_PEAK	Difference in maximum and minimum intensity within a Region.
MASS	Mass value in Daltons (amu) assigned to a Region or Component.

**Table 2: Definition of keywords used in Table 1.**

The syntax definitions shown in Tables 1 and 2 are illustrated in Figure 1, where an example .rpt file demonstrates how the individual quantification items are referenced and provides examples of arithmetic expressions involving intensities and standard deviations. Note the use of the SQRT function, which allows the uncertainty in the ratio calculation to be determined.

```

ptfe0a.rpt - Notepad
File Edit Format View Help
newline
newline
header: Spreadsheet PTFE Calibration
newline
newline
vf: FILE
vf: DATE
vf: BATCH
blank
vb0: INTENSITY:r0
vb0: INTENSITY:r1
vb0: STDEV:r0
vb0: STDEV:r1
(vb0: INTENSITY:r1 / vb0: INTENSITY:r0)
(vb0: INTENSITY:r1 / vb0: INTENSITY:r0) * SQRT (vb0: STDEV:r0 * vb0: STDEV:r0)
blank
vb1: INTENSITY:c0
vb1: INTENSITY:c1
vb1: INTENSITY:c2
vb1: INTENSITY:c3
vb1: INTENSITY:c4
blank
vb1: FIT
blank
vb1: INTENSITY:r0
vb2: INTENSITY:r0
vb1: STDEV:r0
vb2: STDEV:r0
    
```

**Figure 1: An example of a .rpt file.**

## ***New Energy Calibration Feature designed for Batch Processing***

Calibration of spectra is typically different between samples and therefore a mechanism for instructing the calibration to proceed based upon the location of a peak from within a new file is required. To this end, a range of energies may be specified for the measured calibration energy, shown in Figure 2. Given a range of energies for the measured value, the exact energy used in the calibration for each sample is determined from the corresponding peak for which the range calibration is applied in the template file. If the Apply to Selection option is used, then the other spectra so calibrated will include a reference to the spectrum used to initiate the energy calibration.

The value determined for the Measured field in Figure 2 is computed from the data within the specified range. Note the energies specified using the range syntax refers to the original bins assigned at acquisition time. That is, previous calibrations do not alter the data bins used by the new calibration mechanism. Furthermore, the value so determined is obtained by interpolating the data via a quadratic polynomial, where a linear least square criterion is used to determine the polynomial.



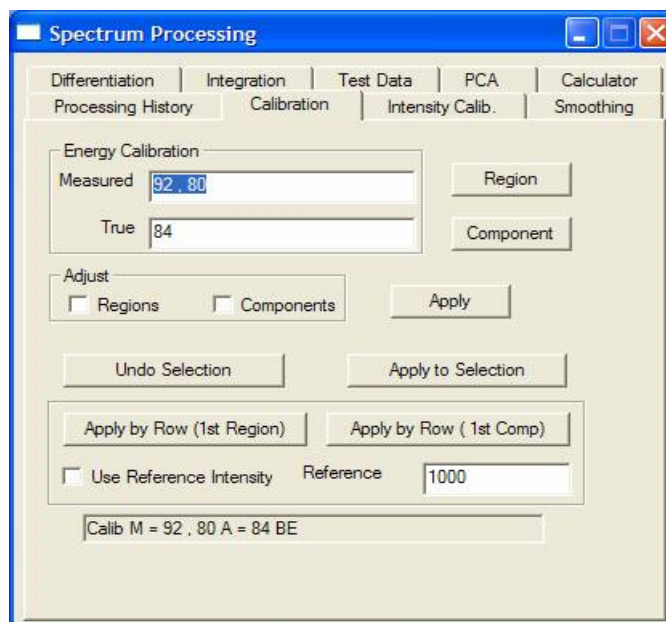


Figure 2: Energy Calibration Property Page showing the new range calibration syntax.

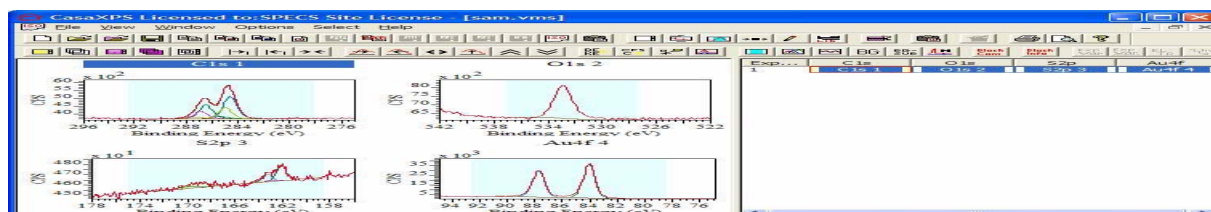
## ***An Example; Batch Processing without Printing and using the Default Report File***

In this example, a set of samples representing a sequence of self assembling monolayers on gold, are analysed using identical acquisition and processing procedures. While the propagate option in CasaXPS is well suited to such tasks, the processing of these data can be achieved with minimal user interactions via the batch processing mechanism. The principal virtue of the batch mechanism lies in the ability of an experienced scientist to set-up the prescription for analysing the samples, after which a person with less XPS experience or even limited experience of using CasaXPS can generate a report in three easy steps.

## **Defining the Batch Processing**

It is important that each sample is analysed with the same sequence of acquisition steps. That is, the resulting files must contain identical acquisition regions in terms of number and VAMAS block order within the files. A representative VAMAS file is prepared with all the required processing and saved in the directory CasaXPS.BAT located in the same directory as the executable file CasaXPS.exe. Since the default report will be used for these samples the report specification file is not required, the absence of which in the CasaXPS.BAT directory is the flag to use the default report. Also, the similar absence of a .tff file with the same base-name as the .vms file prevents any printing of spectra during the batch processing.

The template file shown in Figure 3 consists of four VAMAS blocks, where the Au 4f region is used to energy calibrate all four regions in the file. The new range calibration procedure described above is employed to calibrate the data.



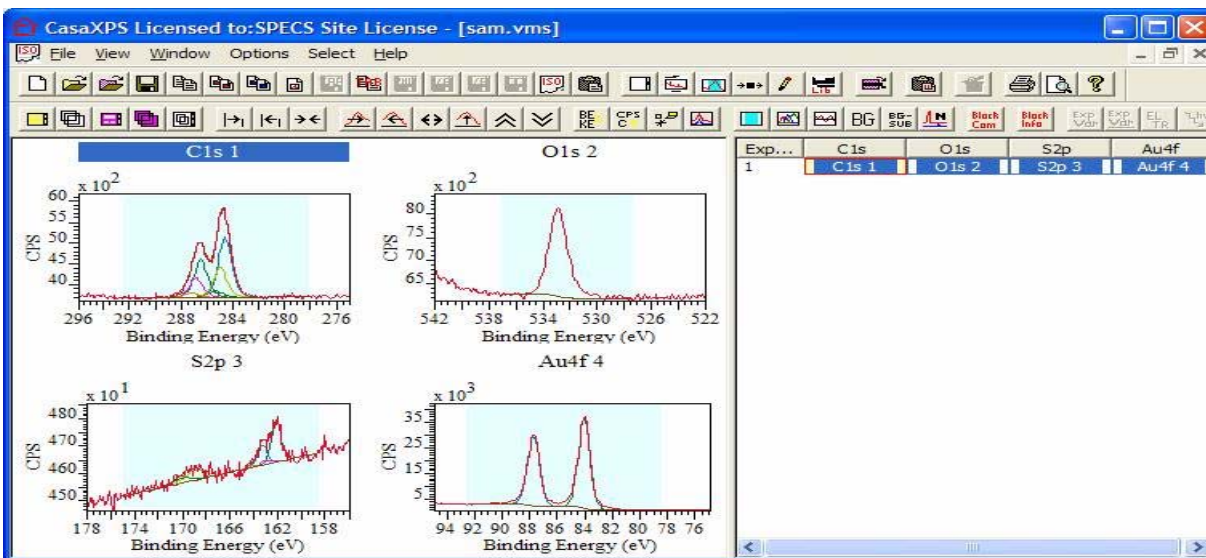


Figure 3: The template file sam.vms is stored in the CasaXPS.BAT directory. Data supplied by Philips Research, The Netherlands.

## Applying the Batch Processing

After acquisition, the data files should be collected into a separate directory. In this example the data has been acquired using a PHI Quantum and therefore a set of .spe binary files generated. These .spe files must be stored in a directory with no other .spe files other than those measured from the intended sample set. Three simple steps are then required to process a set of file.

- 1) From the File Menu, select the Batch Processing menu item shown in Figure 4

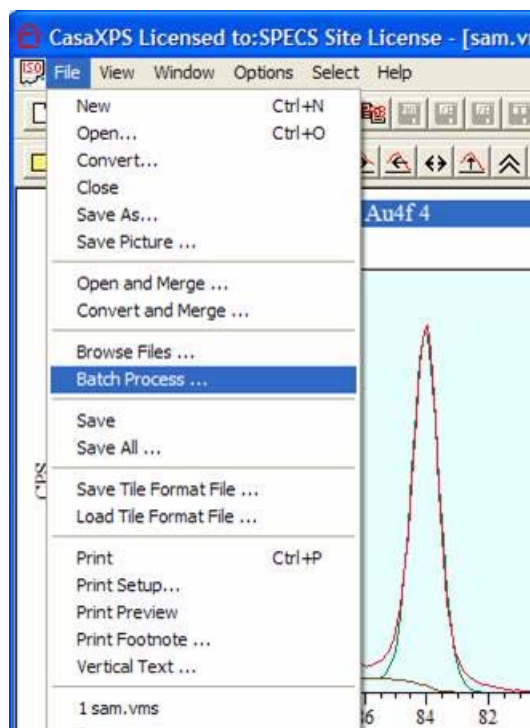


Figure 4

- 2) Select the appropriate template file from the list offered in Figure 5 and press the Apply Template



button.

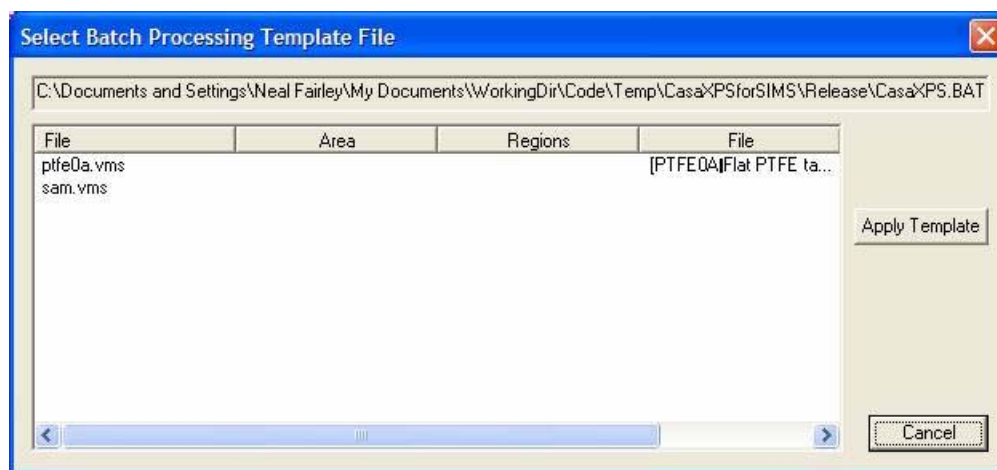


Figure 5

- 3) Select one of the .spe files within the File Dialog window and press Open.

It is now a case of waiting for the results to appear in a clipboard selection dialog window Figure 6. The default report is a TAB spaced file which can be copied via the clipboard into a spreadsheet program or alternatively the report can be saved to file.

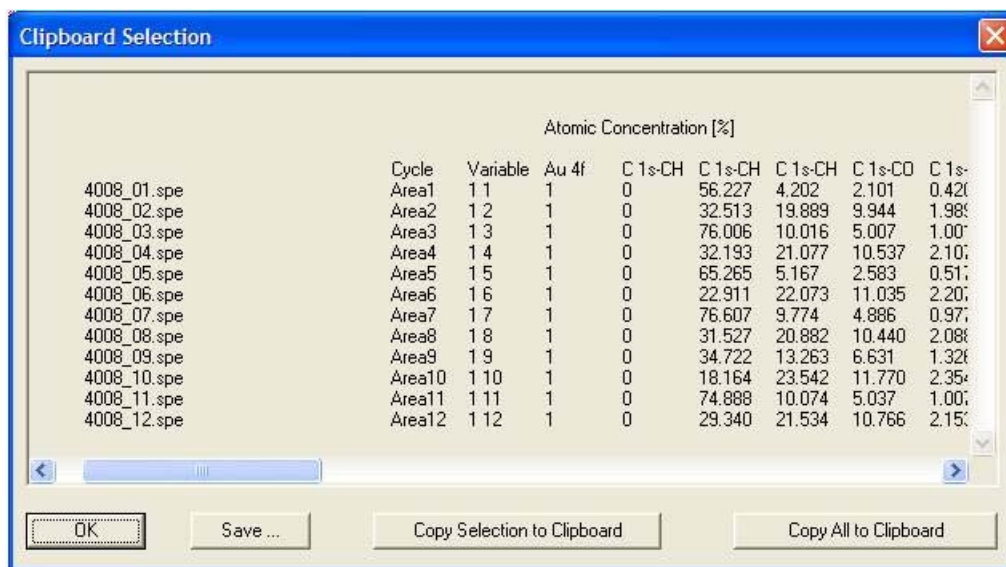


Figure 6 Default report after batch processing completes.

### An Example; Batch Processing with Printing and .rpt File

In this example, a sequence of measurements is made across the surface of a silicon wafer where the ratio of metallic silicon to silicon oxide is required. For each sample the atomic concentration determined from regions on the survey spectrum are combined using formula in a .rpt file; also the intensities for the silicon states, as measured using a peak model, are processed from the data and the ratio computed as part of the report. A template .vms file must be prepared as shown in Figure 7, [a tff file for the display state is also prepare](#) as well as a .rpt file defining the report format (Figure 8). All three files in the CasaXPS.BAT directory have the same base-name and the inclusion of the .tff and .rpt files causes the printing of the spectra and the generation of the report seen in Figure 9, respectively.

The steps for batch processing with printing and a custom report are identical to the steps [described above](#). The only difference is that the additional .tff and .rpt files are required.

A batch of twenty sets of spectra was acquired on an Axis Nova in the Kratos Applications Lab. where each experiment was performed at a different location on the silicon sample along a line scan. The silicon wafer had previously been etched at specific locations. Such analyses can be set up by an experienced XPS analysis and left to a technician for batch processing the results.

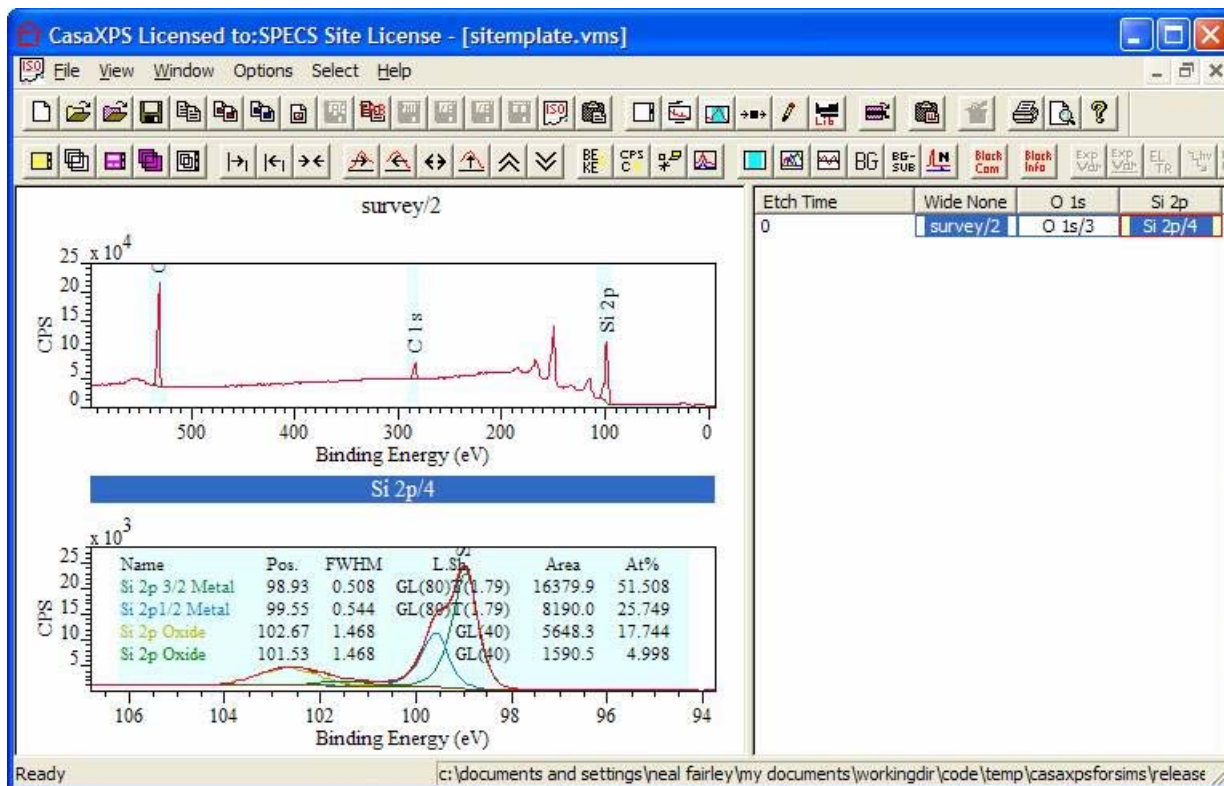


Figure 7: Template file SiTemplate.vms for processing and annotation (saved in CasaXPS.BAT).

```

SiTemplate.rpt - Notepad
File Edit Format View Help
newline
header:Si Metal to Oxide
newline
vf:header:dir
newline
header:Filename
header:Si
header:C
header:O
header:
header:Si Metal
header:Si Oxide
header:Ratio Metal/Oxide
header:
header:Figure of Merit
newline
vf:vmsfile
100.0 * vb0:INTENSITY:r0 / (vb0:INTENSITY:r0 + vb0:INTENSITY:r1 + vb0:INTENSITY:r2)
100.0 * vb0:INTENSITY:r1 / (vb0:INTENSITY:r0 + vb0:INTENSITY:r1 + vb0:INTENSITY:r2)
100.0 * vb0:INTENSITY:r2 / (vb0:INTENSITY:r0 + vb0:INTENSITY:r1 + vb0:INTENSITY:r2)
blank
vb2:INTENSITY:c0 + vb2:INTENSITY:c1
vb2:INTENSITY:c2 + vb2:INTENSITY:c3
(vb2:INTENSITY:c0 + vb2:INTENSITY:c1) / (vb2:INTENSITY:c2 + vb2:INTENSITY:c3)
blank
vb2:FIT
    
```



Figure 8: Report specification-file SiTemplate.rpt

Filename	Si	C	O	Si Metal	Si Oxide	Ratio Meta	Figure of Merit
nf_01.vms	57.8448	15.7596	26.3956	11434.4	3523.13	3.24554	1296.24
nf_02.vms	59.1201	13.7818	27.0982	10533.6	4754.52	2.2155	1359.63
nf_03.vms	56.8444	14.6371	28.5185	11666.1	4042.14	2.88611	1631.05
nf_04.vms	57.5816	14.6011	27.8173	11553.6	3685.52	3.13487	1656.81
nf_05.vms	56.6516	17.3038	26.0447	11313.7	3637.65	3.11017	1305.46
nf_06.vms	58.7471	15.3094	25.9436	11411.5	3578.43	3.18896	1417.44
nf_07.vms	58.6452	14.5013	26.8534	11626.1	3683.27	3.15646	1374.59
nf_08.vms	58.4367	14.9462	26.6171	11660.1	3649.27	3.19519	1471.68
nf_09.vms	58.9075	13.1665	27.926	11792.4	3861.11	3.05416	1571.47
nf_11.vms	58.8807	12.3978	28.7215	11770.3	3699.17	3.18186	1802.5
nf_12.vms	57.8767	14.0194	28.104	11873	3495.01	3.39713	1638.72
nf_13.vms	58.2597	13.2264	28.5139	12027.1	3544.72	3.39295	1631.69
nf_14.vms	58.5069	13.5201	27.973	12272.1	3510.68	3.49566	1803.33
nf_15.vms	58.918	12.9125	28.1695	12419.5	3521.34	3.52691	1680.21
nf_16.vms	59.2892	12.8658	27.845	12436.8	3457.05	3.59752	1665.89
nf_17.vms	59.4654	12.9808	27.5538	12457.6	3305.1	3.76922	1719.29
nf_18.vms	59.7558	13.0756	27.1686	12549.2	3299.32	3.80357	1454.89
nf_19.vms	60.7235	11.8125	27.4641	12507.7	3244.77	3.85474	1597.06
nf_20.vms	60.9555	12.0231	27.0214	12559.5	3161.53	3.97261	1470.88

Figure 9: Report generated by the file SiTemplate.rpt after pasting into Excel