

## Converting Data to ISO 14976 (VAMAS) Format

XPS data in a wide range of file formats can be converted by CasaXPS to the ISO 14976 (VAMAS) standard. The VAMAS format was created to permit the transfer of data between researchers in a well-defined form, that contained both acquired data and the experimental context for these data. The objective for the VAMAS format was to allow all information necessary for the analysis of acquired data to be included in the files. While data exported in VAMAS format is seldom complete in terms of experimental context, the VAMAS format at least allows for incomplete contextual information with the view that information required to analysis data can be added later. Ideally, a VAMAS file is provided to researchers to include all necessary information, but all too often data are exported to formats that provide acquired data without full context. The most notable example of incomplete data files is an ASCII file containing two columns of data. Arguably, the best example of ASCII data with as near complete context is data exported from Kratos Vision data sets. While the native format for data acquired is binary, the ASCII dump of these Vision binary files includes all information that was within the original binary data set, in a format that can be converted by CasaXPS to VAMAS format. Thermo-Scientific Avantage data system, similarly provides a means of exporting from the Avantage binary format to an ASCII equivalent. These Avantage ASCII equivalent data files similarly include experimental context for acquired data, and similarly can be converted by CasaXPS to VAMAS format. An example of data in a binary format that can be converted directly by CasaXPS to VAMAS format is Ulvac PHI data in MULTIPAK format. The context for acquired data is included in MULTIPAK files in an ASCII header that precedes binary data within the MULTIPAK files.

Data obtained by techniques other than XPS can also be converted to VAMAS format by CasaXPS. These techniques include mass spectrometry, Raman, FTIR and NMR data.

### *Basic ASCII Formatted Spectra*

The most basic form of XPS data is an ASCII file containing two columns of data, where each row of data is a pair of values corresponding to energy and intensity. When converting data from these basic ASCII files, some context for the data is required at the time data are converted. Notably, while the first column of values is assumed to be energy, it is important for the interpretation of such acquired data that the photon energy for the X-rays (used to create photoemission signal) is available in the resulting VAMAS file. The photon energy used to acquire data alters the relative intensities of photoelectron peaks. Therefore, any attempt to quantify a sample by measuring photoelectron peak intensity is only meaningful if the photon energy is known. Further, signal measured from a sample under identical experimental conditions and sequentially acquired, must be identifiable within a VAMAS file, often constructed by merging data exported in separate data files. Therefore, when data exported as separate ASCII files, corresponding to the same experiment, are placed into a folder without any extraneous data, then using the Convert to VAMAS file dialog window in

CasaXPS, all ASCII data files within a folder are converted to a single VAMAS file. After the initial conversion step is completed, options within CasaXPS allow adjustments to VAMAS files that are necessary to allow a scientific interpretation of data. Nevertheless, a correct interpretation of ASCII two column data may need information provided at time of conversion to VAMAS format.

The *Convert to VAMAS file* dialog window allows a folder to be specified and a new filename entered, with additional information to provide context for the data within these files. The additional information is specified following the filename-string entered on the dialog window. These additional pieces of information are referred to herein as flags. For example, the flag used to change the X-ray anode from the default aluminium anode to a magnesium anode is **-anode Mg**. A second example of a flag is used to interpret the energy for signal. If the energy column within all data files is the kinetic-energy of signal, then changing from the default energy (which is assumed to be binding energy) used during conversion to VAMAS format is achieved by entering the flag **-energy KE**.

Conversion of data saved as two column ASCII data is illustrated for two folders (Figure 1), where each folder includes two ASCII data files corresponding to survey spectra measured using a dual anode X-ray gun (Figure 2). The folder named Al Anode contains two ASCII files which in turn, contain a survey spectrum, measured using photon energy 1486.6 eV, from cleaned copper and a second file containing data measured using the same X-ray anode from cleaned chromium. An example of ASCII data is displayed in NotePad in Figure 3. The conversion of data in the folder labelled Al Anode is achieved by entering a string that includes both the base-name for the newly created VAMAS file (survey) and the filter string ".dat". The file extension of data files requiring conversion to VAMAS format is generally used in CasaXPS to guide the conversion steps. Hence, the filter string ".dat" is the method used to instruct the conversion of all files within a folder with the file extension .dat. Figure 4 provides an example for the use of flag strings, that provide additional information about the data absent from the data file. For the example in Figure 4, the data files contain energy spectra measured using a magnesium anode X-ray gun, thus the flag -anode Mg is added to the base-name and file extension, namely, **survey.dat -anode Mg**. The result of the string entered in the File name text-field is the VAMAS file shown in Figure 5, where two survey spectra, corresponding to the two data files, are entered into a single VAMAS file.

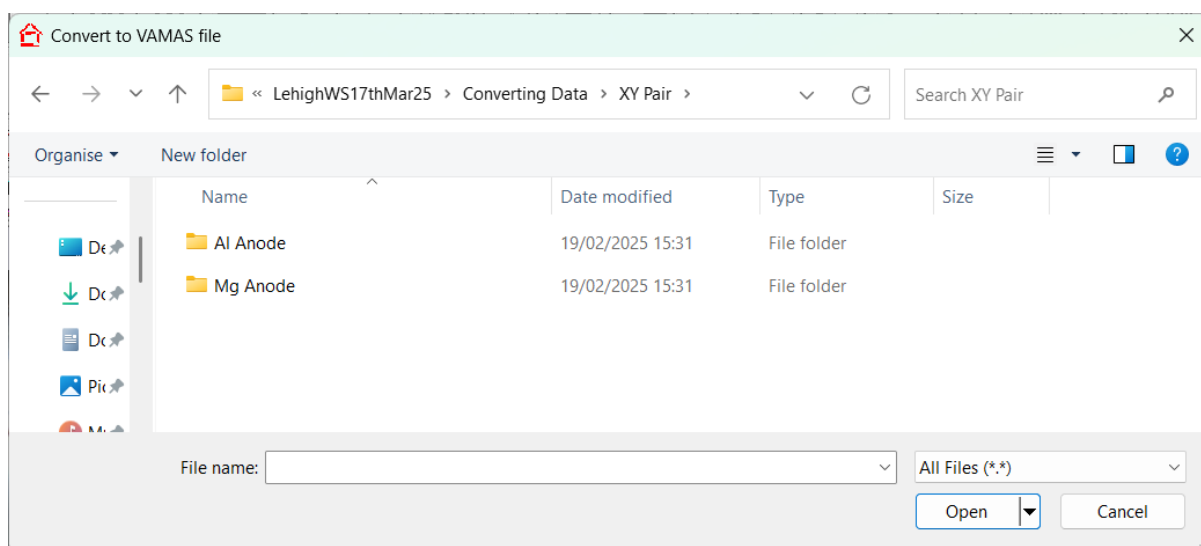


Figure 1. Two folders prepared with ASCII data files containing survey spectra measured using aluminium X-ray anode and magnesium X-ray anode.

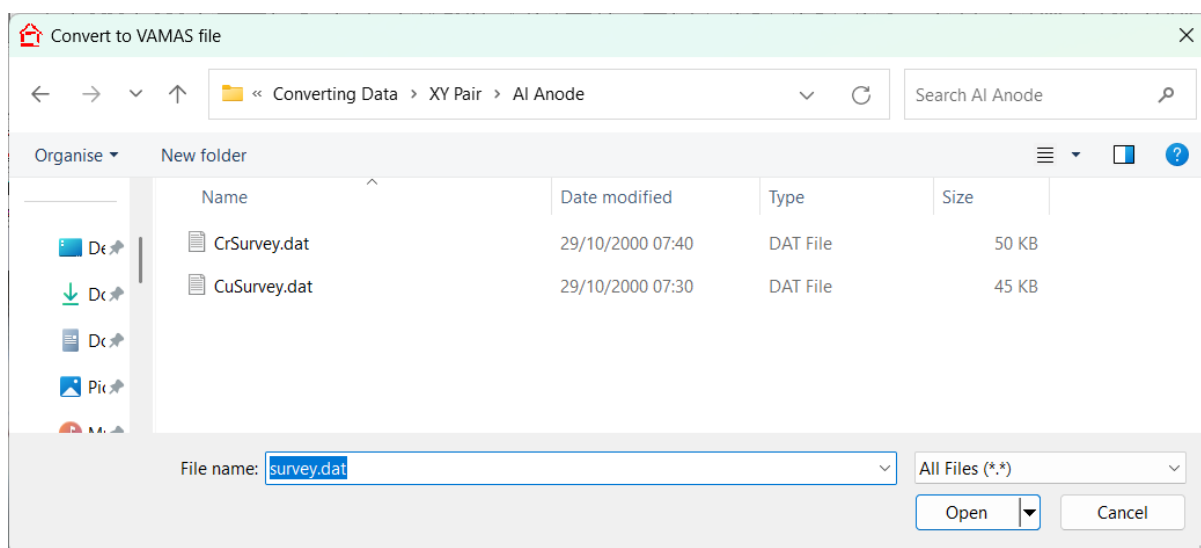


Figure 2. Contents of the Al Anode folder showing two ASCII files with identical data format within, namely two columns of ASCII data specifying binding energy for each specific intensity in a survey spectrum. These two files contain data recorded from copper and chromium. To convert these two data files to a single VAMAS file with name survey.vms, the File name text-field need only enter the filename survey.dat. The file extension is used to guide the conversion of the two data files within the folder.

Binding Energy (eV)	Intensity (cps)
1400.00	3359
1399.50	3365
1399.00	3363
1398.50	3334
1398.00	3253
1397.50	3397
1397.00	3330
1396.50	3254
1396.00	3267
1395.50	3306
1395.00	3337
1394.50	3333
1394.00	3413
1393.50	3255
1393.00	3391
1392.50	3371

Figure 3. Contents of CrSurvey.dat ASCII file shown in Figure 2. Note that the first column is binding energy, which is listed in decreasing order. The default, when converting two column data, is to assume the first column is binding energy and the second column is intensity in counts per second.

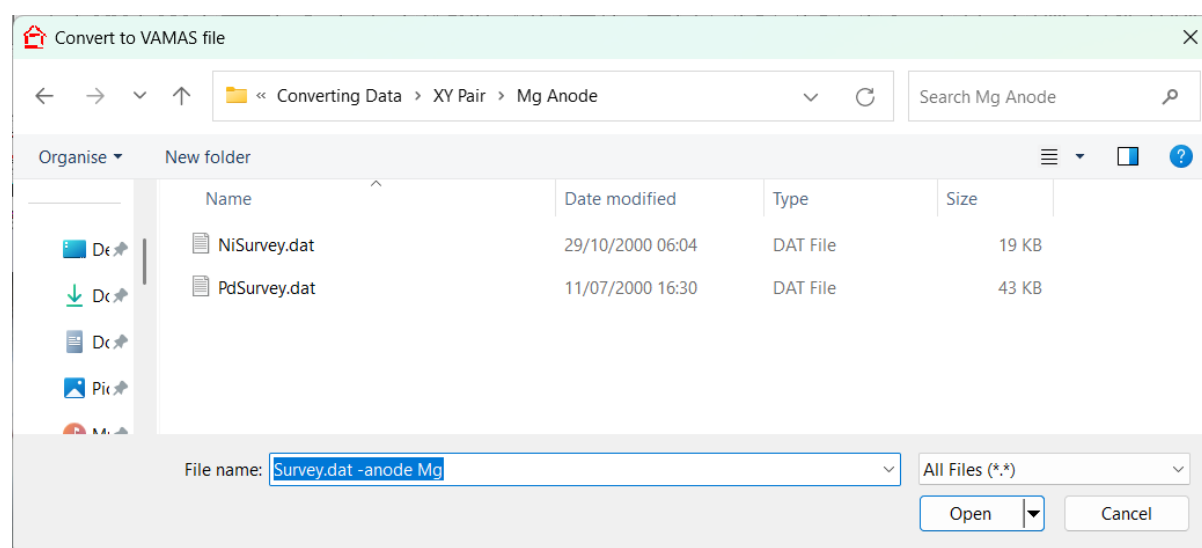


Figure 4. Contents of the folder containing two ASCII data files containing two column data acquired using the magnesium anode of a dual anode X-ray gun. Note that the flag **-anode Mg** is used to enter a photon energy of 1253.6 eV into the resulting VAMAS file.

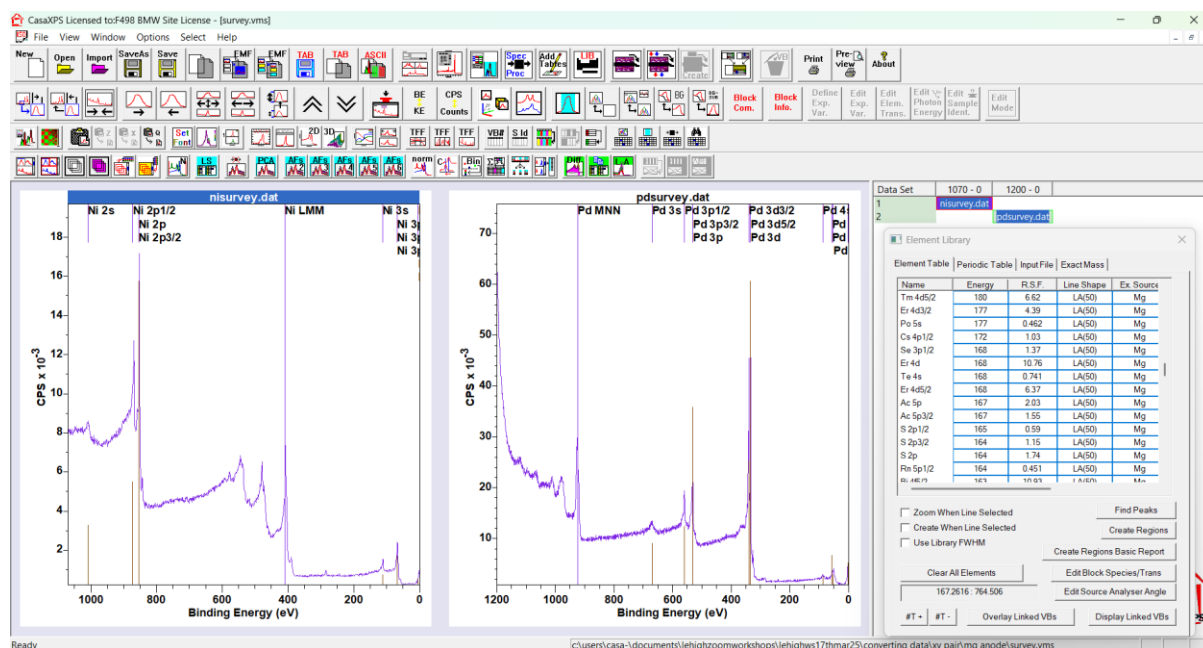


Figure 5. VAMAS file obtained using the conversion string shown in Figure 4. The element library table is presenting a list of photoelectron and Auger peaks with appropriate relative sensitivity factors (RSFs) for photons of energy 1253.6 eV. The correct element table is presented because the correct anode specification was made in Figure 4.

### Conversion to VAMAS files of Data Exported with Contextual Information

Thermo-Scientific Avantage exported data is an example of an ASCII format that includes data plus the context for the acquisition of the spectral data. The format used to export Avantage data allows a variety of experiments to be performed, for which the essence of the experimental context is preserved in the exported ASCII files. Thus, depth profiles, iteration of experiments and imaging XPS data are exported in these ASCII files in a form that is open to constructing VAMAS files already populated with experimental information necessary for the processing of these data.

The Avantage data system stores all data in a hierarchy of folders (Figure 6). Within the Avantage data system is a program designed to traverse folders (created at acquisition time to contain the original binary data) that creates from binary data files ASCII files with the file extension avg. These avg files can be converted by CasaXPS to VAMAS format. In CasaXPS, these are numerous options for converting avg files to VAMAS format, which include ways to search through the hierarchy of folders, converting subfolders containing avg files to VAMAS format or reopen previously converted VAMAS files. A full explanation of these options is available as a YouTube videos (Figure 7), which demonstrate how data saved from Avantage to avg format (corresponding to different types of experiment) are converted to VAMAS format. The Avantage program used to create avg files is called DataSpace\_BatchDump.exe, the location of which is shown in Figure 8.

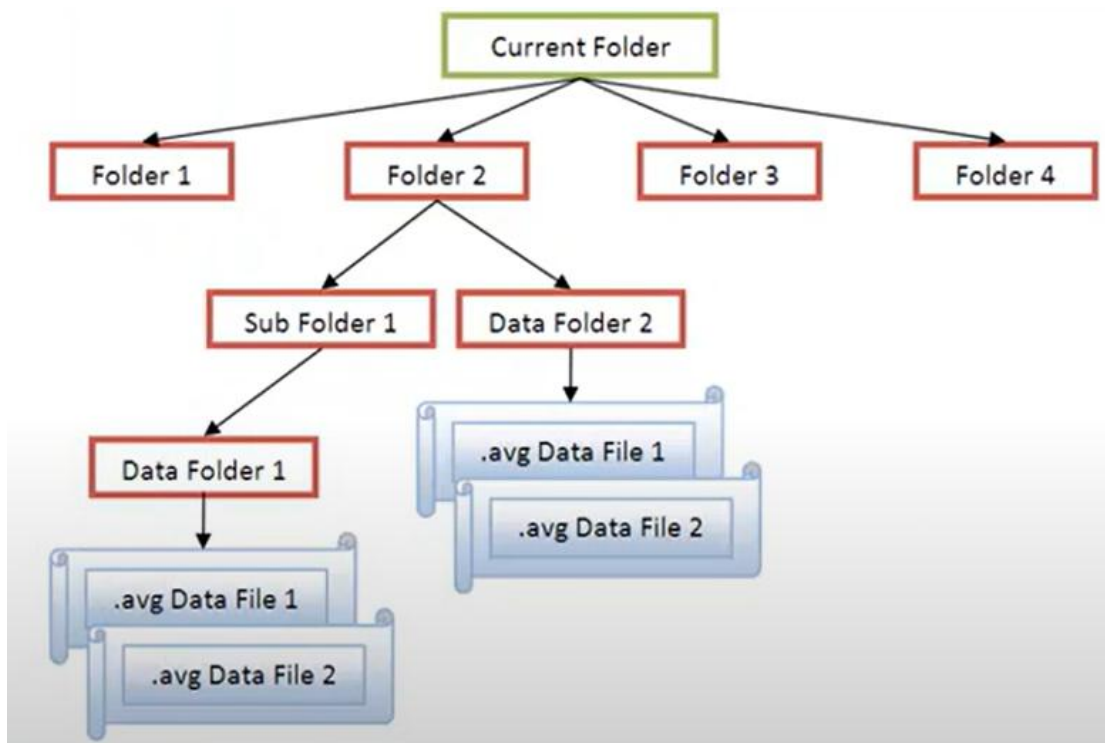


Figure 6. Avantage data are saved in a folder hierarchy, where binary and exported data are placed in root subfolders. CasaXPS will search the folder hierarchy to identify subfolders containing avg file, which are then converted to VAMAS format. The video illustrated in Figure 7 explains how to convert avg files saved in subfolders.

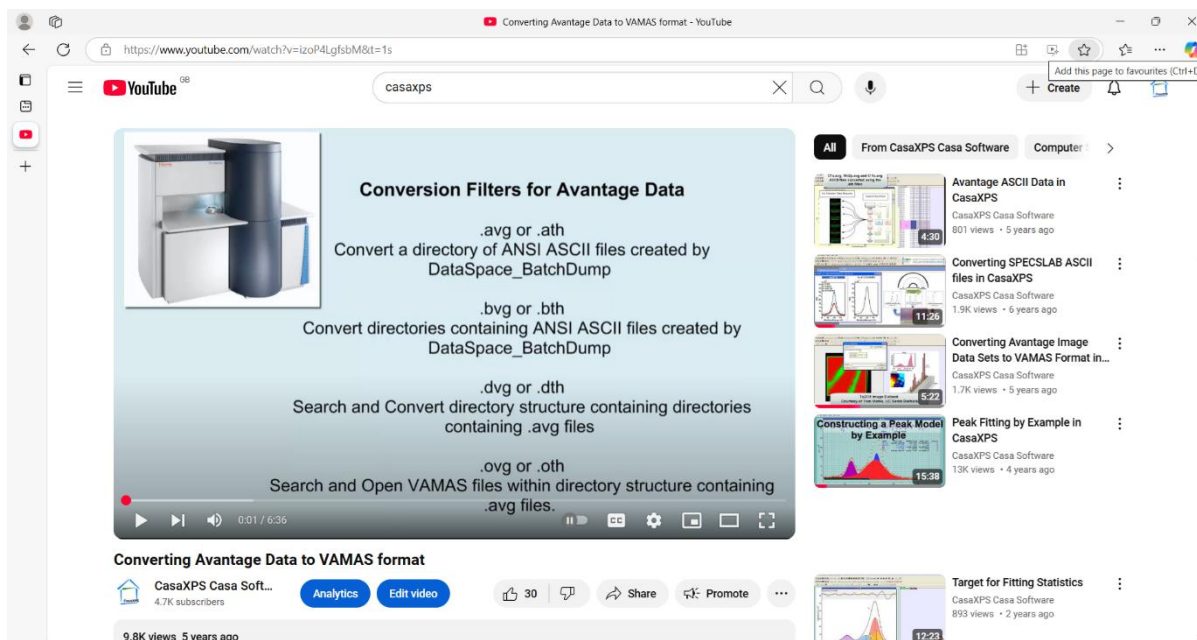


Figure 7: YouTube video describing how to convert avg files located within subfolders are converted to VAMAS format in CasaXPS.

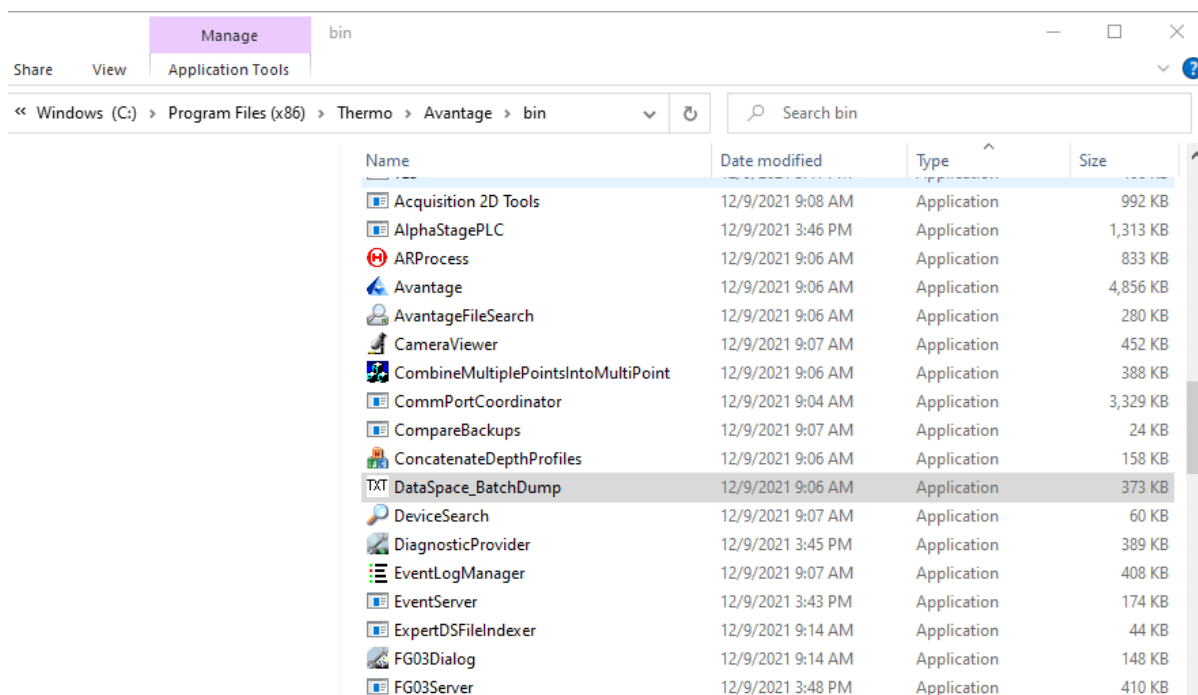


Figure 8. Location of the program in Avantage that converts binary data to ASCII avg format files.

#### Binary Data: ULVAC PHI MULTIPAK Format

Spectra and images acquired from an Ulvac PHI instrument can be saved in binary files used by the Ulvac PHI MULTIPAK analysis software. CasaXPS converts binary files with the various file extensions used by Ulvac PHI. Figure 9 is a folder containing spectra and images in binary format that can be converted via the Convert to VAMAS file dialog window of CasaXPS. An example of Auger image data converted to VAMAS format is shown in Figure 10.

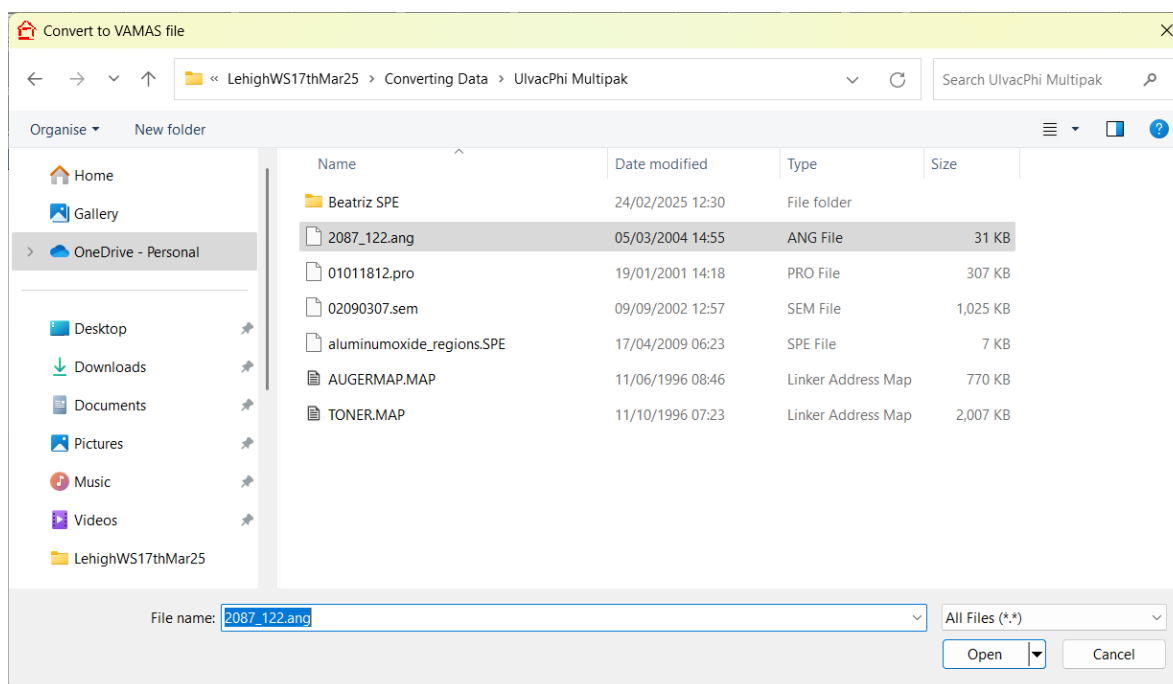


Figure 9. Folder of MULTIPAK formatted data. The file extensions include ang (angle resolved XPS), spe (spectra), pro (depth profile), map (XPS or Auger image), sem (secondary electron image).

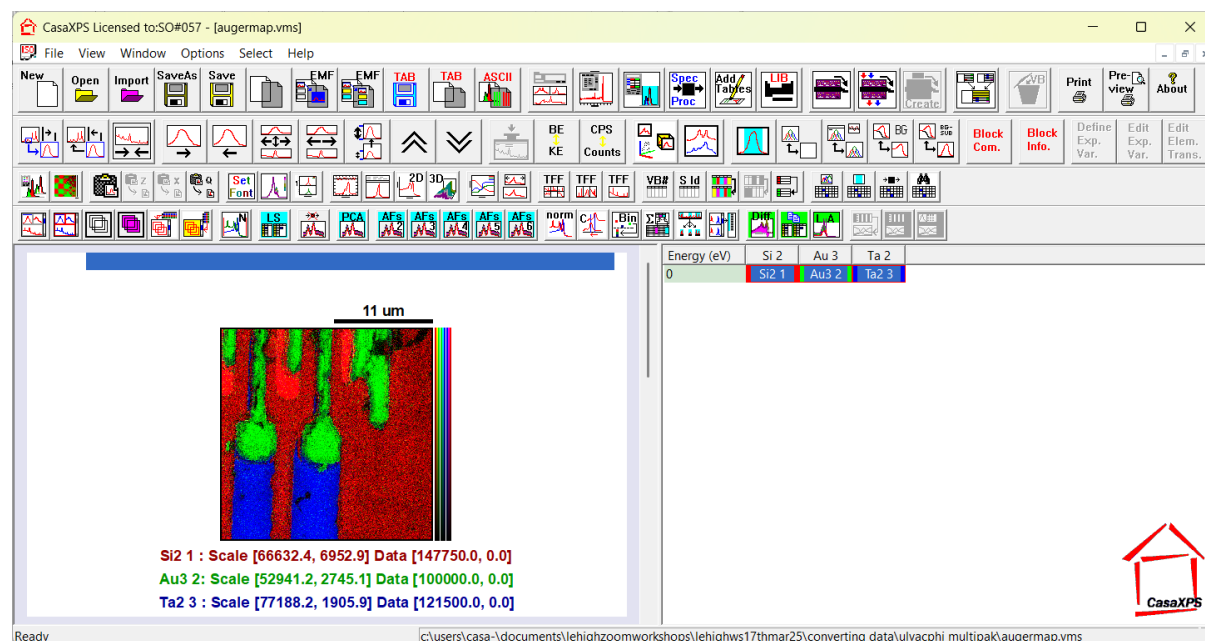


Figure 10. Auger images in MULTIPAK file with file extension MAP converted to VAMAS format.