Instructions for converting Agilent ChemStation data to SMCReporter 4.0 using the interface program, AgilentSMCR4.exe

This program is a simple executable that takes the Agilent ChemStation quantitation report and converts it to a format compatible with the SMCReporter 4.0 software. The program may be run through Windows Explorer or create a desktop icon for running the program (Right click mouse on desktop->new->short cut then browse to executable, agilentSMCR4.exe).

The program creates a text file in the format required by SMCReporter. It is readable in Notepad and illustrated in Figure 1.

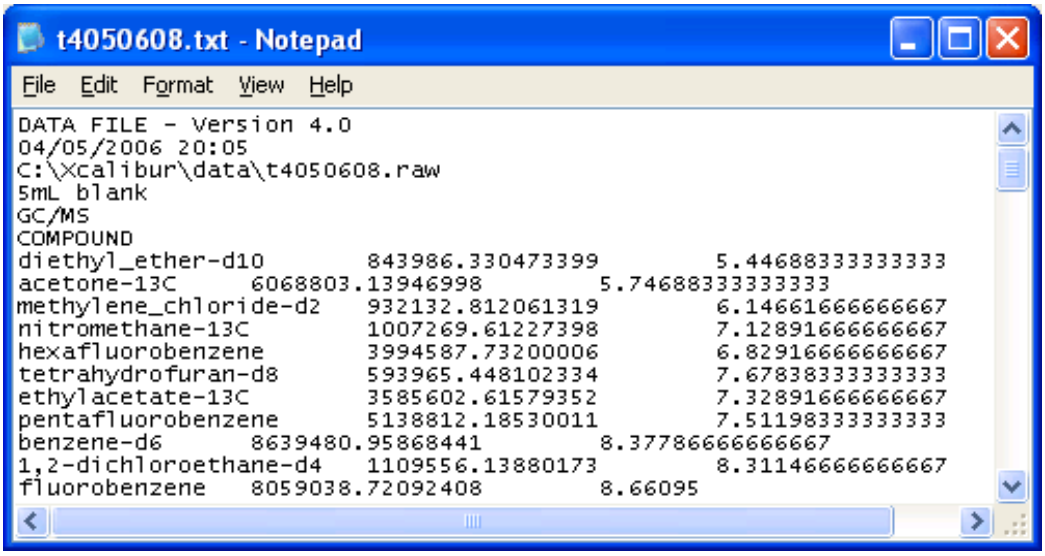

Figure 1 Notebook display of data format required by SMCReporter4.

The top row of the header information identifies the type of file and targeted version of SMCReporter. The second row identifies the acquisition data of the raw GC/MS file. The third row presents the data file and path of the GC/MS file that was used to generate the translation. The fourth file lists the file description and the fifth file presents the GC/MS identification.

The compound section lists the compounds in the GC/MS quantitation report and in the same sequence. The sequence of compounds must match the sequence in the SMCReporter and be spelled in the same way. Be sure capitalizations are identical too. Either the GC/MS quantitation list or the SMCReporter quantitation library can be changed to make the lists match (but if an internal standard or surrogate spelling is changed the internal standard file will also need to be redone).

When the program is started the screed will display a form that can be started (Figure 2)

Figure 2 The initial display produced by running agilentSMCR4.exe

By pressing the 'Start' button the next display requests the information necessary to process the raw data files. The next display is seen in Figure 3.

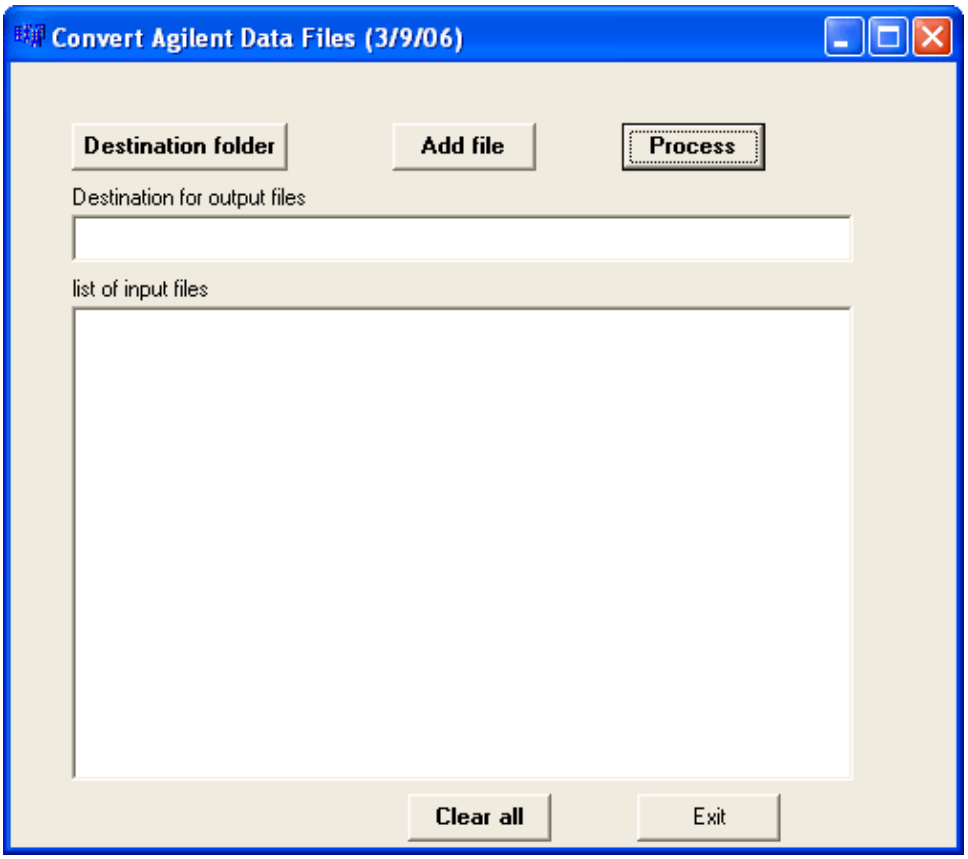

Figure 3 Display for information needed to be input for file processing.

The first information to be input is the destination of the files in SMCReporter format. Pressing the 'Destination folder' button bring a display for browsing to where the output files are to be written. In this display the destination folder is in the 'Look in:' box (1example folder in the example) and

automatically the file name is given ‘Destination folder’. Don’t worry, the program will create a file name that has the name of the GC/MS raw data file (folder) with an extension of ‘.txt’ and not name it ‘Destination folder’. See figure 4.

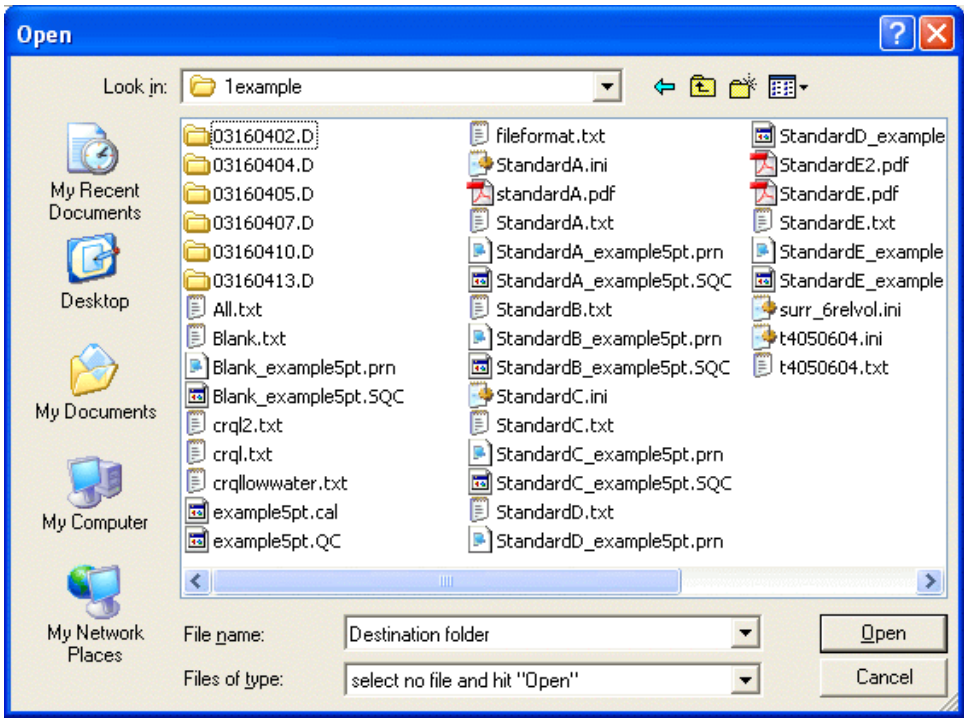

Figure 4 Browse to the folder where you want the new files to be written.

Hit the ‘Open’ button and the program returns to the display seen in figure 4 with the added destination folder (figure 5).

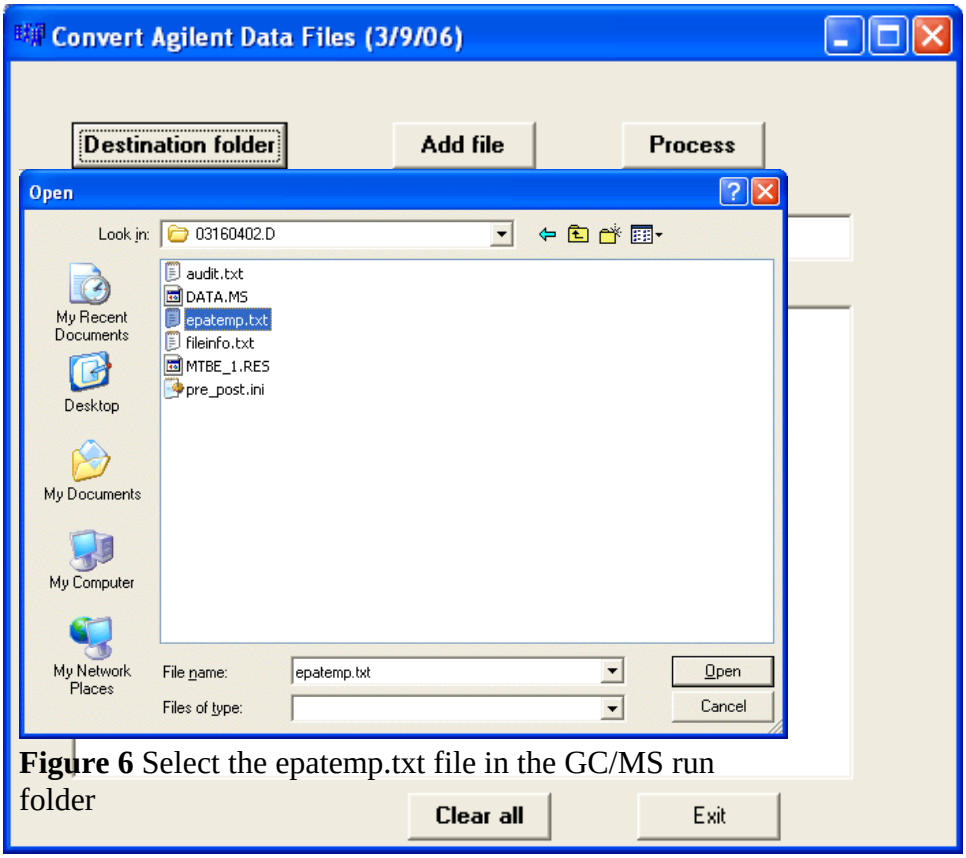

Figure 6 Select the epatemp.txt file in the GC/MS run folder

Figure 5 The folder where the translated data will be written is added.

The next thing to do is to add the data files for translation. ChemStation creates a folder with an '.D' extension that contains various files generated for a GC/MS run. We need to access the 'epatemp.txt' data file that resides in the run folder. Hit the 'Add file' button and browse to the 'epatemp.txt' file contained the GC/MS run folder. See figure 6.

Note. The epatemp.txt file is generated only when the ChemStation quantitation report is generated. If a review of the raw data has made some quantitation changes the Chemstation quantitation report must be generated again (to screen) to make 'epatemp.txt' reflect changes.

Hit the ‘Open’ button and the screen will look like Figure 7.

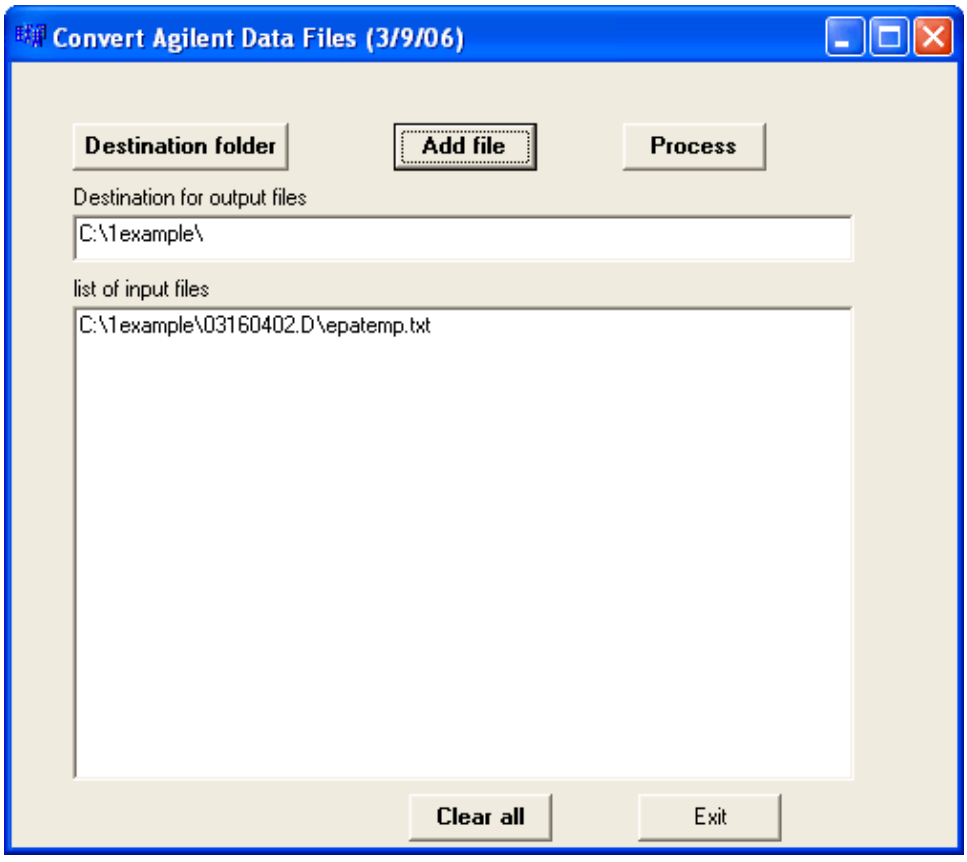

Figure 7 File selected for translation to SMCReporter format.

Up to 20 data files can be input for

processing. Each time the epatemp.txt file is to be selected. The program will process any file with the .txt extension so the analyst can rename the epatemp.txt file to some other name (*e.g.*, reviewed.txt) and process that file.

The final step is to hit the ‘Process’ button and a text file with the name of the ChemStation run (the example is ‘03160402') and a ‘.txt’ extension is created in the destination folder. These files are now ready for SMCReporter processing.

If more samples are to be processes hit the ‘Clear all’ button before starting.