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Instructions for ThermoElectron Excalibur Raw Data to SMCReporter 4.0 using the interface program, SMCReporterV2.exe

This program is a simple executable that takes the ThermoElectro Excalibur result file (*.rst) 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, SMCReporterV2.exe).

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

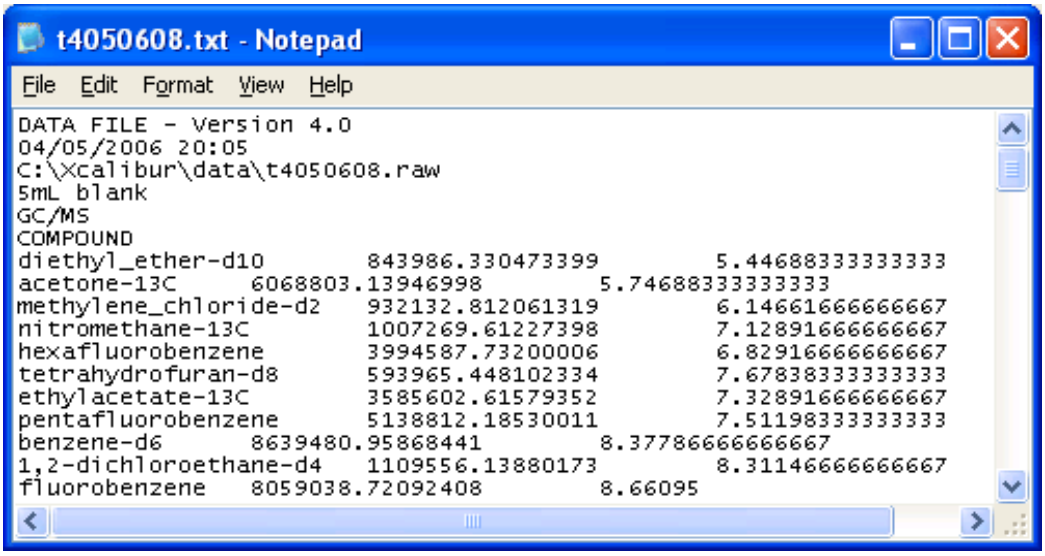

Figure 1 Notebook display of data format required by SMCReporterV2.exe.

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).

US EPA ARCHIVE DOCUMENT

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

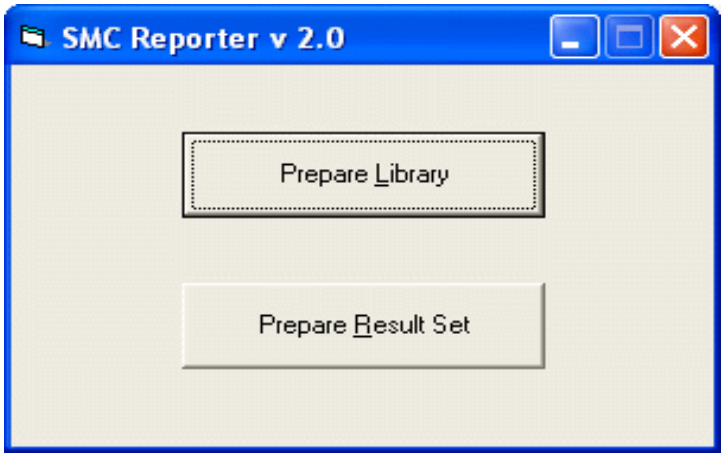

Figure 2 Initial display running SMCReporterV2.exe

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

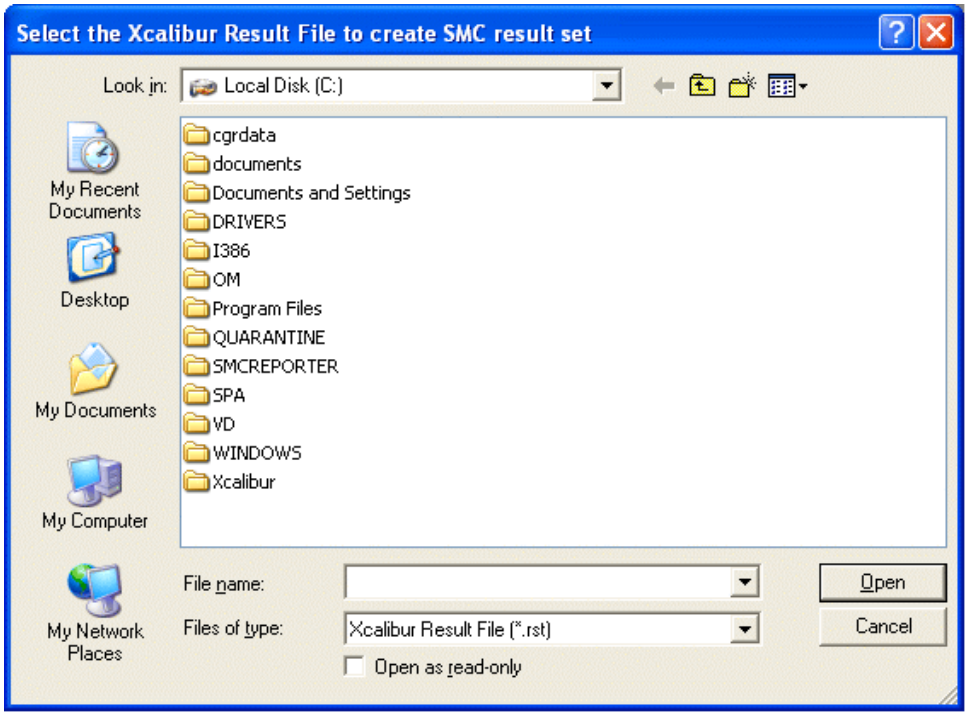

Figure 3 Browser for SMCReporterV2.exe

Select the Xcalibur result file (*.rst) that is to be processed and hit the 'Open' button. The following display will be provided after the file (figure 1) has been generated.

US EPA ARCHIVE DOCUMENT

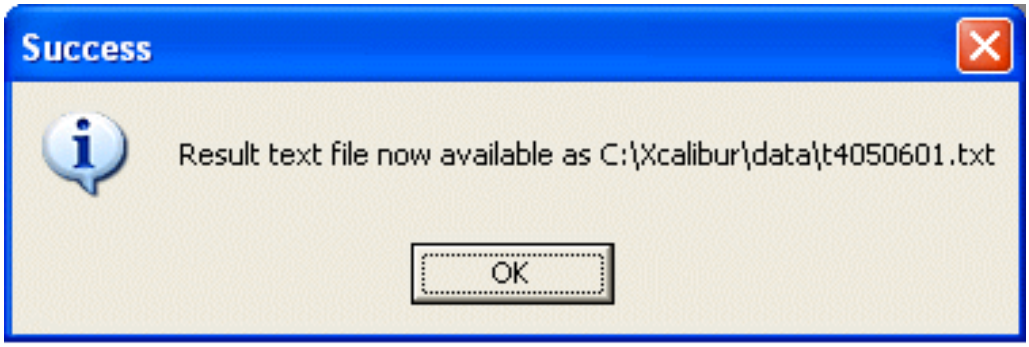

Figure 4 Display that indicates the file in SMCReporter format has been generated.

The process of steps illustrated by figures 2-4 are repeated for each sample.

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