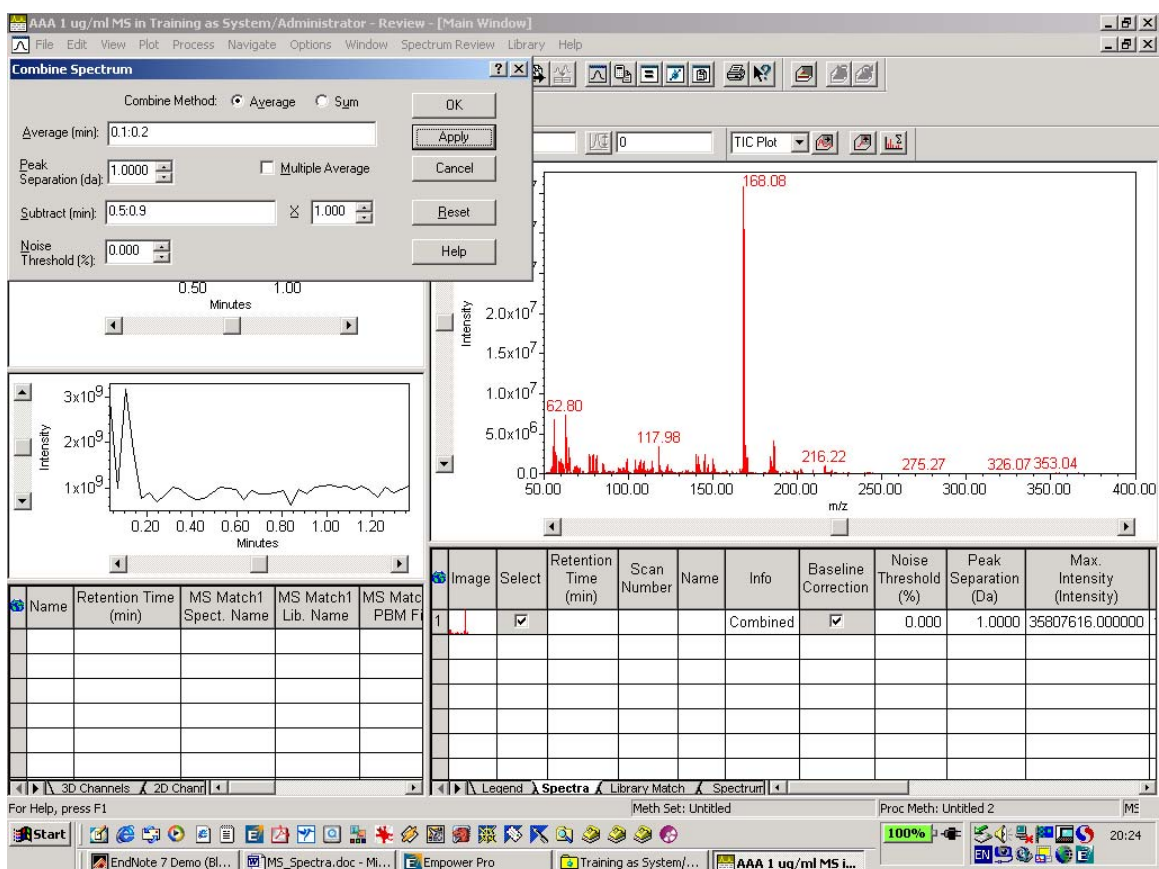


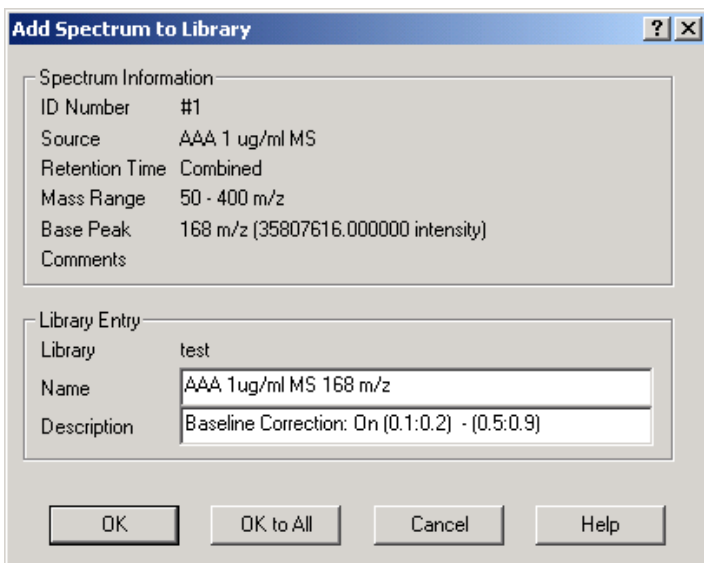
Manual processing of LC-MS data

1. Saving a spectrum in a library

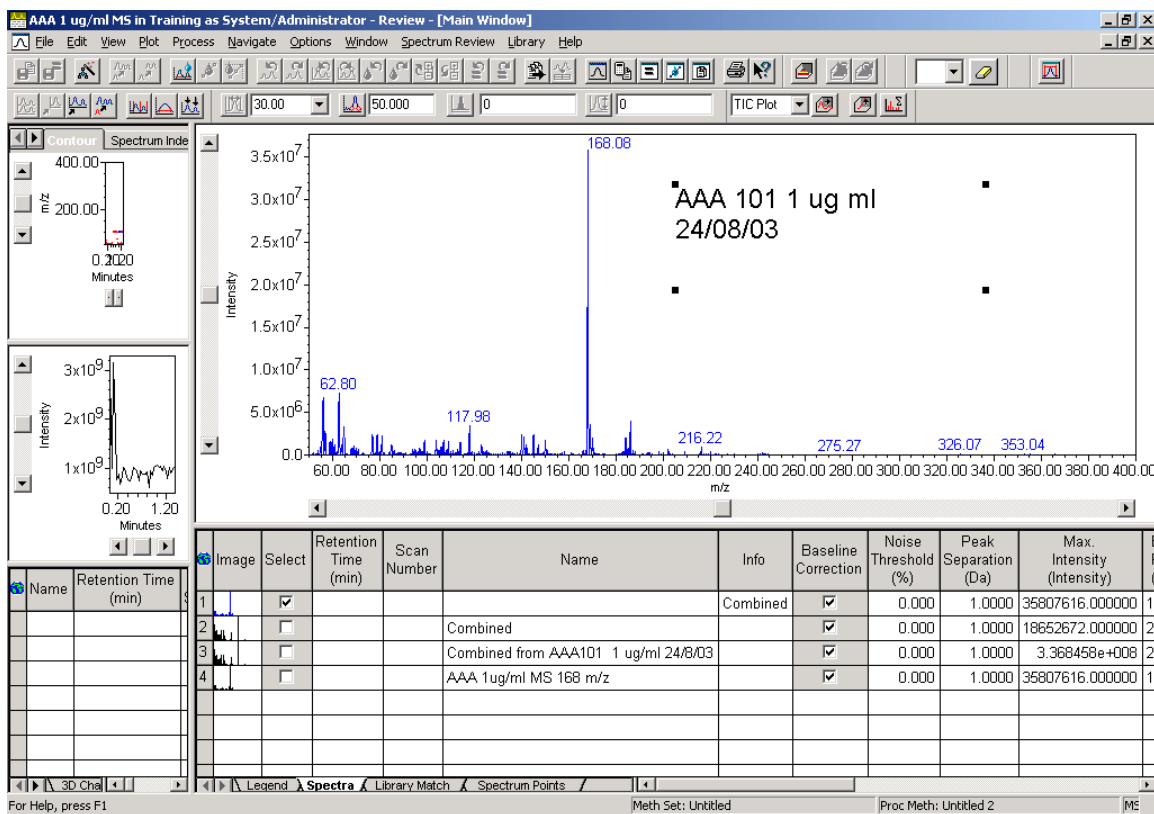
To look for specific MS spectrum of a compound, combine spectra in the expected region: go to *Process -> Combine Spectra* -> write the time range for which spectra will be combined (or use the write mouse while on the combine spectra dialog box), and the region without peaks that will be subtracted from it (preferably in the region before the column void volume). The spectrum will be obtained in the Spectrum Review Window:



Go to "*Library*" and select *New library* (or "*Open library*" if it exists already). Create a library by naming it. Go again to "*Library*" and select "*Add to Library xxx*"; the following screen is obtained:



Make sure to write as many details as possible in the “Name”, to be able to identify the spectrum later on, when needed. At this point, the spectrum can be printed out directly from the Spectrum Review window, using the write click and “Print”, however it will not contain any sample information. Use the text box and drawing objects to add to the screen before printing out to get this information as in the following example:



2. Retrieving the spectrum

Go to *Browse Project* and *Review* any MS scan channel. In the review window go to "*Library*" and select "*Load Library*". The library will be loaded and all the spectra will appear in the table below the "*Spectrum Review*" window. The "*Select*" column will enable to select or de-select any spectrum of choice. The spectrum can be printed out directly from the spectrum window, using the write click and "*Print*" as explained above.