The two macros enclosed in this package, *batchprocess* and *qEst2csv*, were written to provide users a mechanism allowing easy processing of a large number of spectra and the ability to then export the calculated concentration of an analyte in those spectra to a comma separated value, or CSV, spreadsheet. The *batchprocess* utility is a general tool that only loads the data and then uses whatever processing macro is defined when the macro is called. The *qEst2csv* processing macro is specific for a given molecule and is used to create a CSV file containing calculated concentration values.

The *qEst2csv* macro is intended to be used only as an example for the user to customize as needed to fit the requirements of their particular study. This macro processes a spectrum, integrates specific peaks (as defined in the macro), calculates the concentration of the molecule represented by those peaks, and then exports the results to a CSV file. The macro, as supplied, can be used to process the PROTON spectrum of Clindamycin in the FID library with VnmrJ 3.1A (i.e., /vnmr/fidlib/Clindamycin/ Clindamycin_PROTON_01.fid).

The *batchproces* macro is the utility that runs the analysis. This macro requires three arguments:

arg1: The directory that holds the data (this can be absolute path OR relative path with respect to *userdir+'/data'* )
arg2: The *pslabel* for the type of data to be processed (e.g.: PROTON, CARBON, or gHSQCAD)
arg3: The processing macro to be used.

For example, executing *batchproces('/home/data/myfiles','PROTON','my_processing_macro')* on the command line will parse all the Study directories in the "myfiles" directory, load all the PROTON data from each of the Studies, and process those FIDs using the "my_processing_macro" macro.

Assumptions:

1.) All the data to be processed were collected in a Study (i.e., using the automation tools in Chempack 4.1 or VnmrJ 3.x).
2.) The data must have been acquired using a calibrated probe file that contained appropriate quantitation parameters. Alternatively, the current probe must have quantitation parameters appropriate to the actual probe used to acquire the original data.

By combining the *batchprocess* utility with an appropriately edited *qEst2csv* macro, one could take all the spectra collected for a laboratory class or a QA/QC investigation, have the system automatically process each spectrum in the group, and assemble a CSV file as output that contains the absolute concentration value calculated for every sample in the investigation.