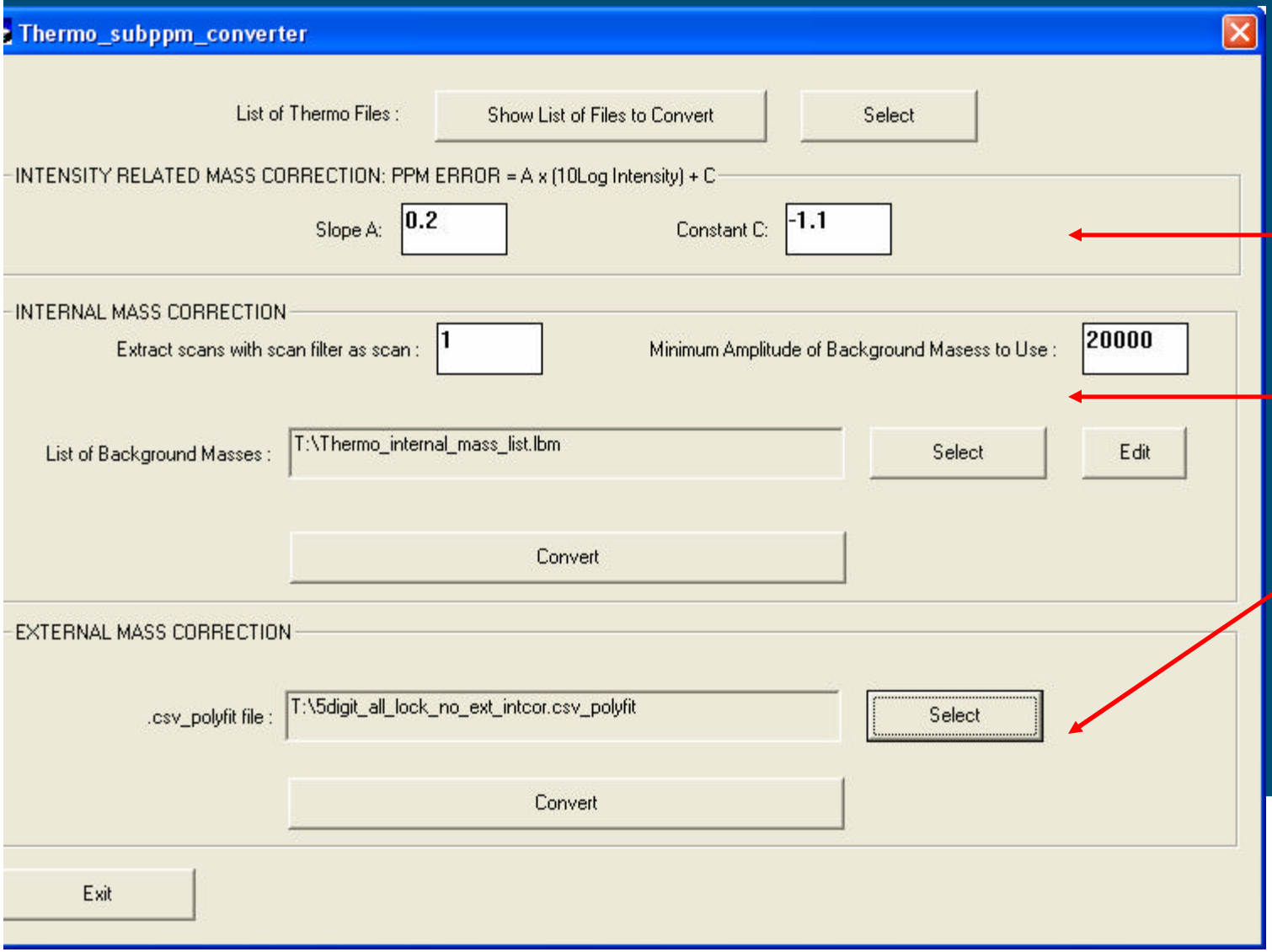
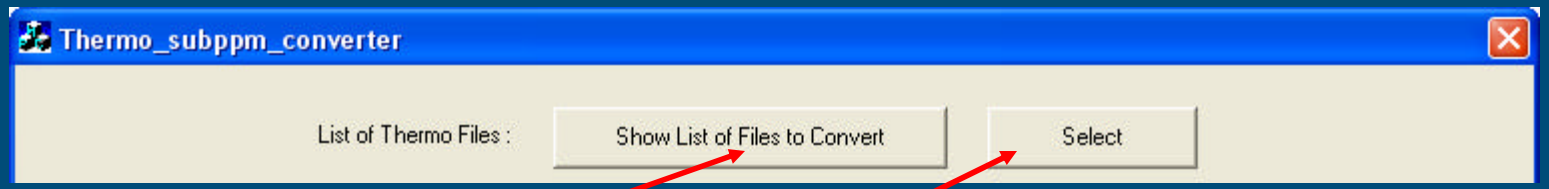
Subppmconverter: mass correction module for LC-Orbitrap-MS raw data; conversion to centroid netCDF data.

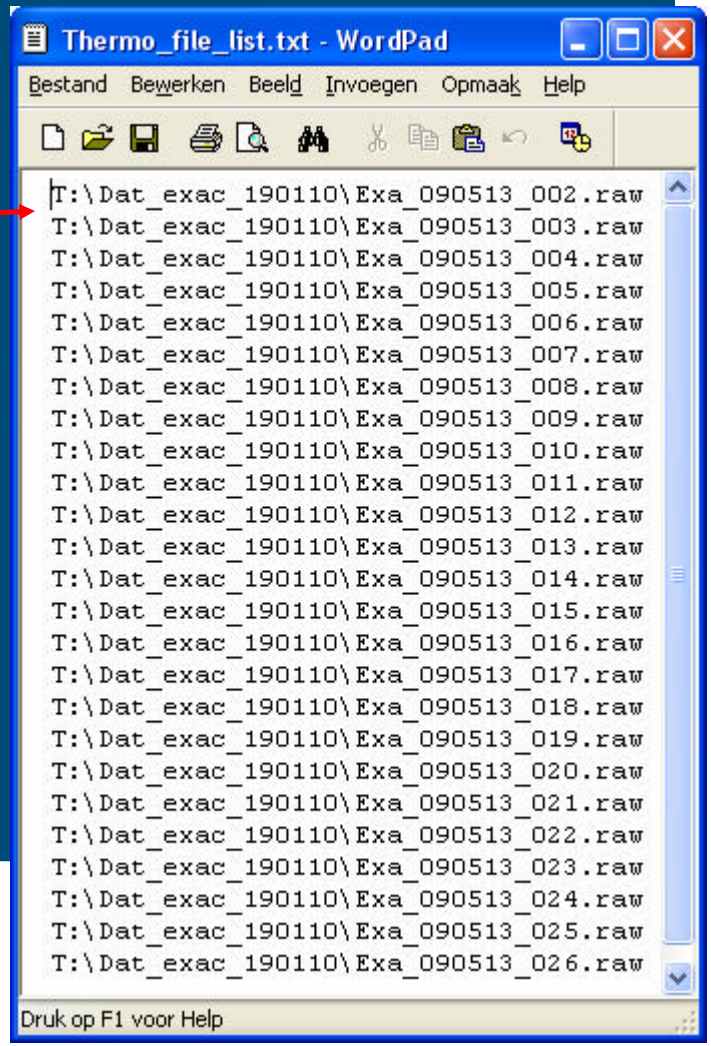


- Intensity dependant mass correction
- Mass correction using multiple internal masses
- Mass correction using multiple external masses

Subppmconverter: selecting all raw data.

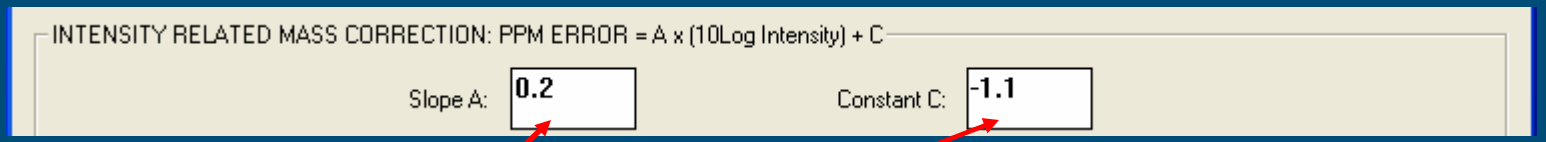


- "Show List of Files to Convert" button: the selected "raw" files are shown with wordpad.
- "Select" button: "Select" button (files appear in "selected box"): this module is described in "metalign_manual.ppt" slide 6 and is used to select "raw" files.



Subppmconverter: intensity correction of masses

(see also: Subppmconverter_method.ppt)

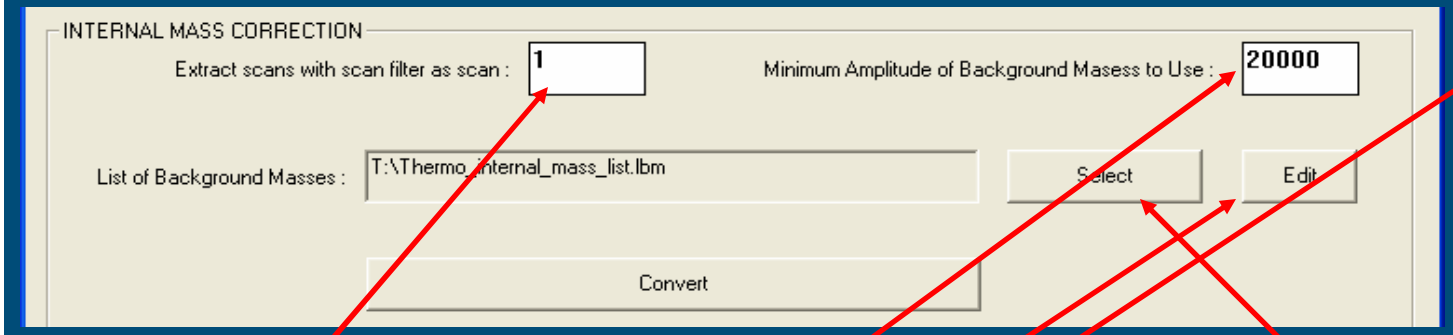


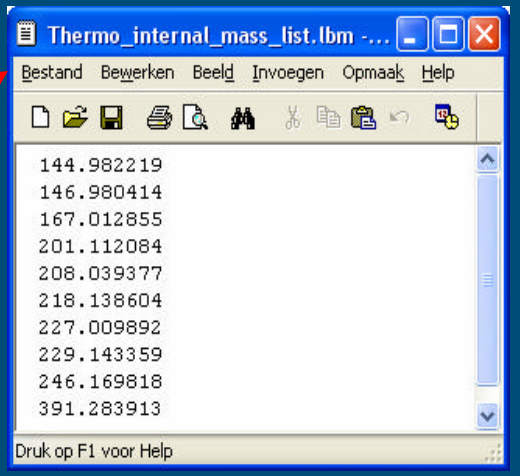
- All intensities of data points in the “raw” data are corrected by subtracting the ppm error as calculated by the formula. A=slope, C=constant.

Note: 0.2 and -1.1 are the default values, but they may be set to 0 to avoid this correction.

Subppmconverter: multiple internal lock mass correction

(see also: Subppmconverter_method.ppt)





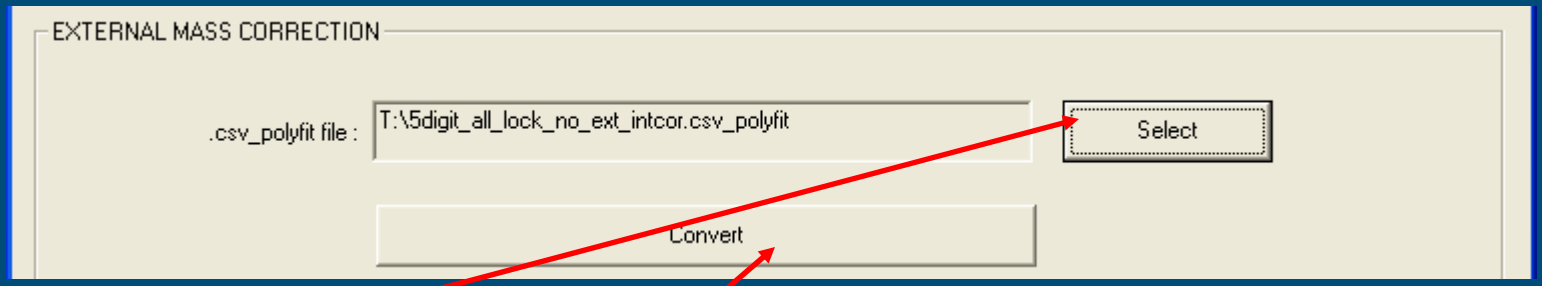
- The scan filter to extract from the raw data should be defined.
- Masses defined in “Thermo_internal_mass_list.lbm” (=mass list) must have intensities above 20000 (ca. 5x noise) in a scan to be used.
- A list of masses (ascii in wordpad) is used for the internal lock. “Select” defines the “.lbm” file. Edit open wordpad to edit or view this file
- “Convert” button: this executes intensity plus internal lock mass correction and generates netCDF output from the “.raw” data (same folder for .raw and .cdf).

ote: the lock masses are selected/averaged from begin and end of the chromatogram and consist o masses from different eluents.

ote: the ppm-deviation (max 5 ppm) of a variable number of lock masses present in each scan are averaged. Outliers are discarded.

ote: if no lock mass is found in a scan, then the ppm-deviation is interpolated using adjacent scans.

Subppmconverter: multiple external mass correction (see also: Subppmconverter_method.ppt)



- The “Select” button includes a “.csv_polyfit” for external mass correction. This file is generated automatically when using the Search_LCMS module. Search_LCMS (see Search_LCMS.ppt) searches “.redms_acc” files. The “.redms_acc” files should have been generated by metAlign by processing netCDF files from the “convert” button in the previous slide. The “.csv_polyfit” contains experimental binary information on the ppm errors as a function of mass (from the external references measured together).
- “Convert” button: this executes intensity plus internal lock mass correction plus external mass correction/calibration and generates netCDF output from the “.raw” data. This netCDF data can then be processed again by metAlign to give final data.