

HPLC Batch Data Processing Directions

Written 1/06 WKoz; Updated 9/08 WKoz

Open rcvdata.xls file with macros enabled

- Path for this file is sent in c:/exceldde/exceldde.mac file (that file can be edited with notepad)
- For the HPLC computer, it is set to be at: E:/016data/lmg0601
 - You might make a second copy or move it to whatever folder you're using at the time, but in reality it doesn't matter, because after data is written to this file you do a save-as to put the final version wherever you want it.

Set your parameters for export (should only need to do this once, and then they'll stick)

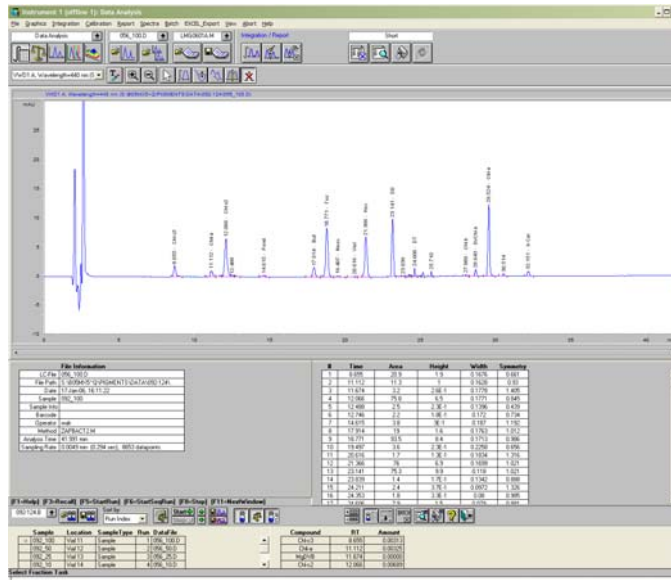
- EXCEL_Export... Setup Export Options
 - EXPORT Master Selections window gives the list of options parameters to export
 - EXPORT Header Selections should have:
 - Detector
 - Seq Subdir
 - Inj Date/Time
 - Vial
 - Data File
 - Sample Name
 - EXPORT Peak Selections should have:
 - Compound
 - Ret Time
 - Area

In Data Analysis...Batch... Load Batch...

- Goto where your data is, select the folder that was set in sequence parameters (for example, 092-124), and then select the associated *.b file

In Setup Batch Window...

- use Other Method button to find and select the appropriate processing method (ie. "LMG0601a.m")
- select the runs you want to process
 - easiest way seems to be to use select all button, and then go manually un-select any acetone injections or other files you don't need to process
- Screen should look like this now:



- Note that at this point, if you zoom in to a better size on the top chromatogram screen, each consecutive run that is opened will open to that same zoomed level ☺

Divide, delete, clean up integration as normal on the open chromatogram

- At the moment, the integration method does fairly well at getting peaks, but often calls humps too small to be real peaks so those need to be erased (especially around peridinin, around the neoxanthin/violaxanthin area and sometimes before α/β carot), and it seems to sometimes miss the division between lut/zeax so that needs to be done manually also.

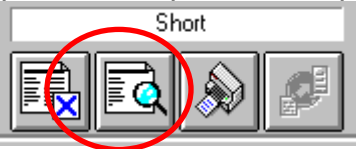
Click “mark changes for saving”



- After being marked for a save, an “s” on the left of the filename on the batch list will appear (“->” is to mark the file currently being reviewed, “*s” will appear after the batch has actually been re-saved.)

Sample	Location	SampleType	Run	DataFile
*s 092_100	Vial 11	Sample	1	056_100.D
-> 092_50	Vial 12	Sample	2	056_50.D
092_25	Vial 13	Sample	3	056_25.D

At this point, the report can be printed to have a copy of the chromatogram if desired



- Note that there is also a batch report print button, but this doesn't really give us what we want so it's not worth using



From EXCEL_Export dropdown menu, select "Manual Data Export to Excel"

- Be sure that rcvdata.xls file is open in the background.
- **If it's the first file exported in a run, select yes to Clear Previous Spreadsheet Entries, bit from then on, select NO and it will append the runs to a single file.**
- Status box on the bottom displays when it's done exporting.

Goto your next chromatogram and repeat the process



- Some times when moving to the next chromatogram, the software will prompt if you want to "Save current run with batch file?" – say YES... not sure when or why this doesn't always happen, but ...

When your done with a batch, resave the file so next time all integration changes will hold, and can be revisited if necessary (you will need to write this new batch file somewhere OTHER than your CD of course.



Goto your rcvdata.xls file and do a Save-as as whatever you want to call it

- Recommendation is to name them the same as the sequence name, and keep track of where you store them.

Edit this file so the lines match up (this is the tricky part – you have to look at RT's

- Note that the file sometimes does wacky things to the header line on the far right side
- Note that there's several worksheets here too, but the only one you really need is the "Inst1_Sig1" sheet
- Before doing this, sort data on "Vial" in ascending order so the files are in the order the samples are injected
- After making a batch line up, copy and paste it to the running tally list (ie. allpeaks.xls
- Line up the most recent batch with the batches prior to it.
- From here, apply the dilutions, calcs etc.