

Solution – MS Excel macro for Result Table check

Clarity can automatically export a chromatogram after analysis or after reprocessing a chromatogram. This macro will automatically load the exported chromatogram to MS Excel, format its Result Table, and add custom calculations, e.g., comparison to defined limits.

The functions are intended to be fine-tuned to a specific type of analysis; they would have to be further customized to suit other types of data (e.g., PDA, multi-signal chromatograms). It is recommended to set the settings as described below. Only after the macro works correctly on your PC can you start modifying or customizing the macro to meet your own needs.

All files necessary are included in the zip archive **Excel-macro-Result-Table-check.zip**.

How to set up the macro

Step 1 – Unblock macros in MS Excel

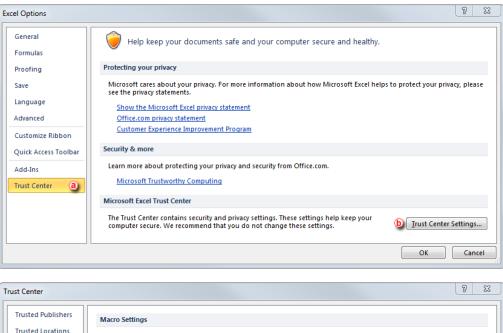
It is necessary to enable macros in MS Excel to run the prepared macro. The easiest way to enable macros is to set the Security level to Low (see below) or directly enable macros. Please consult with your IT Administrator whether such an operation is allowed in your environment.

- 1. Open MS Excel
- 2. Set the security level to Low
 - MS Excel 2003 (and newer)
 Invoke the *Security* dialog by clicking *Tools Macro Security*, and set the level to Low

| Security | | | ? 🛛 | | | | | | |
|--|---|----|--------|--|--|--|--|--|--|
| Security Level | Irusted Publishers | | | | | | | | |
| Very High. Only macros installed in trusted locations will be allowed to run. All other signed and unsigned macros are disabled. | | | | | | | | | |
| <u>High.</u> Only signed macros from trusted sources will be allowed to run. Unsigned macros are automatically disabled. | | | | | | | | | |
| O <u>M</u> edium. You macros. | Medium. You can choose whether or not to run potentially unsafe macros. | | | | | | | | |
| Low (not recommended). You are not protected from potentially unsafe macros. Use this setting only if you have virus scanning software installed, or you have checked the safety of all documents you open. | | | | | | | | | |
| | | | | | | | | | |
| | | | | | | | | | |
| | | ОК | Cancel | | | | | | |

• MS Excel 2010

Invoke the *Excel options* dialog by clicking *File – Settings* and select *Trust Center* (a). To invoke the *Trust Center* dialog, click on *Trust Center Settings...* (b) In the *Trust Center* dialog, click on *Macro Settings* (c) and *Enable all macros* (d)



| | index settings | |
|---------------------|--|-----------|
| Trusted Locations | Disable all macros without notification | |
| Trusted Documents | Disable all macros with notification | |
| Add-ins | Disable all macros except digitally signed macros | |
| ActiveX Settings | (d) Enable all macros (not recommended; potentially dangerous code can run) | |
| Macro Settings 😋 | Developer Macro Settings | |
| Protected View | Trust access to the <u>V</u> BA project object model | |
| Message Bar | | |
| External Content | | |
| File Block Settings | | |
| Privacy Options | | |
| | | OK Cancel |
| | | |

3. Close MS Excel

Step 2 – Copy the macro to your PC

Unzip the files within the archive xls-export.zip to the *C*:*xls-export folder* (given that the *C*:\ is your main local disc where Clarity is installed)

Step 3 – Setup the macro in Clarity

- a) Open Clarity
- b) Open the Instrument window with the DEMO4 project
- c) In the Instrument window, invoke the Export Data dialog via the Settings Export Data... menu
 - Make sure the same options as in the following image are selected:

| Export Data | | | > |
|--|--|---|---|
| Export Content Result Table In Fixed Format Special Results Table Summary Table Column Moments Calculation Parameters Chromatogram | Chromatogram All Data Displayed Data X Axis Time Step: 0 mir Character Encoding: | 1 | Text Format Field Separator Fixed Width Delimited by: <tab> Decimal Separator <window's locale=""> Text Qualifier</window's></tab> |
| Chromatogram Header Chromatogram Header NGA Amounts NGA Summary DHA Results DHA Group Results Table Headers Full Format | ANSI | ~ | <none> Export to Clipboard Text File txt Excel Excel Excel Excel Excel Excel Excel P-2003 Workbook (**.xlsx) dBase File (Result table only)</none> |
| File Name: (path and name by chromatogram).b | .t | | Append (Text and dBase Files only) |

d) In the Instrument window, invoke the *Batch* dialog via the *Analysis – Batch...* menu

• Make sure the same options as in the following image are selected. The variable %e set in the *Parameters* option causes the exported file name will be the same as the name of the chromatogram:

Step 4 – Results

MS Excel should be opened with the exported chromatogram, where the Result Table is compared with the Limits Table. It may look simple, but it is quite complex. Here is exactly what happened:

- a) Clarity exports the chromatogram to a *.txt file
- b) The batch script OpenChromInExcel.bat runs the Virtual Basic OpenChrom.vbs program, which will open the MS Excel file chromatogram-export.xls and pass the %e parameter (= the filename of the exported chromatogram) to the macros included in this Excel file
- c) The macro will import the text file to the chromatogram worksheet and add custom calculations (see the Amount% in column L or the Average function in cell G4)
- d) Another macro will add a table with limits for the selected compounds and will indicate if the compound fits these limits (Passed) or exceeds the limits (Failed). Such limits can be specified in the "Limits" worksheet. The limits are linked using the name of the compound (the compounds from the DEMO4 project are prefilled)

Step 5 – Limitations

- a) The macro currently works only with chromatograms containing one signal only (multi-signal chromatograms would provide incorrect calculations of the average amount (cell G4) and the Amount% column).
- b) The macro will always open the chromatogram in the same Excel file. To use it in an automatic environment, including a saving function, it would be useful to automatically save each MS Excel file under a new name. The default behavior is that the MS Excel file will stay open and can be saved manually.

Step 6 – Automation in real cases

- a) Single Analysis this macro can be run after each Single Analysis measurement is done.
 - Switch to the *PostRun Setting* tab in the Single Analysis dialog. Make sure the same options as in the following image are selected. The variable %e set in the *Parameters* option causes the exported file name will be the same as the name of the chromatogram:

| ingle Analysis | | | | | | × |
|---|--------------------------|--------------|----------------|------|-------------------|---|
| Open in Chromatogram Window Print Results Print Results To PDF Export Data | Report Style Analysis | | | | Edit | |
| Open in Calibration Window Open Chromatogram with stored C Include Chromatogram in SST | Calibration | | | | | |
| Export Chromatogram in AIA Form Export Chromatogram in TXT Form Export Chromatogram in EZChrom Export Chromatogram in Multidete | at Ascii Format | | | | | |
| Program to Run | it | | | | |) |
| %e Analysis Post Run Settings User Varia | ables | | | | | |
| Control | | | | | | |
| Send method | Run | <u>S</u> top | A <u>b</u> ort | 121 | S <u>n</u> apshot | |
| Chromatogram File Name (Data\Instru %e - %R | ment 1 - 2_21_2024 2_ | 08_41 PM) | | | | |
| Denable File Overwrite | | Counter | 1 | Data | Recovery | |
| OK Cancel | | | | | Help | |

b) Sequence – the Sequence Table enables the specification of post-run settings for each row separately.

• Display the *Export Data, Run Program, Program to Run,* and *Parameters* columns using the *Setup Columns* dialog: select these columns and click the *Show* button. Then, set the content accordingly:

| Setup Columns | | | | × | | | | | | | |
|--------------------------------------|----------|---|--------------------------|-----|----------------|-----------------|--------------------|------------|-----------------------|--|------------|
| Table Properties | | | | | | | | | | | |
| Hide Columns | | Show Colum | ins | | | | | | | | |
| ISTD9 Amount ISTD 10 Amount | Show All | Status Run | | Ť | | | | | | | |
| AnalysisUserVar1 AnalysisUserVar2 | Show | SV EV | | | | | | | | | |
| AnalysisUserVar3 Print to PDE | Hide | I/V Sample ID | | | | | | | | | — 🗆 🗙 |
| Export Data Export AIA | Hide All | Sample Sample Amount | 7 (H 8= - | | | | | | | | |
| Export TXT Export EZChrom | | ISTD 1 Amount Sample Dilut. Inj.Vol. [µL] | File Sample Name Type | Lvl | Method Name | Report Style | Open Open Calib | Print Expo | ort Run ta Program | Program To Run | Parameters |
| Run Program Program To Run | | File Name Sample Type | ag_%R Unkn ag_%R Unkn | | Demo4 Demo4 | | | | V | C:\xls-export\OpenChromInExcel.bat C:\xls-export\OpenChromInExcel.bat | %e %e |
| Parameters Include in SST | | Lvl Method Name | | | | | L | | | | |
| Stored Calib. Close All | | Report Style Open | | Ŧ | | | | | | | |
| Selected Column(s) Properties | | Open Calib. | | - | | | | | | | |
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| Font Custom Name | e | Preview | 123 | | | | | | | | |
| | | | | | | | | | | | |
| 0 | K Cancel | Default | Help | | | | | | | | |

Additional information

- This macro has been tested on MS Excel 2013 and Clarity version 8.1.0.77.
- This macro serves only as an example of the possibilities of data exchange between Clarity and MS Excel; it is not a fully tested and supported application.

Send your comments, suggestions, or questions to kohutek@dataapex.com.