Solution – MS Excel macro for Result Table check

Clarity can automatically export a chromatogram after analysis or reprocessing. This example macro loads the exported chromatogram into MS Excel, formats its Result Table, and adds custom calculations (e.g., comparison to predefined limits).

The macros are designed for a specific type of analysis and may need additional customization for other data types (e.g., PDA data or multi-signal chromatograms). Configure the settings as described below. Modify or extend the macro only after the example works correctly on your PC.

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

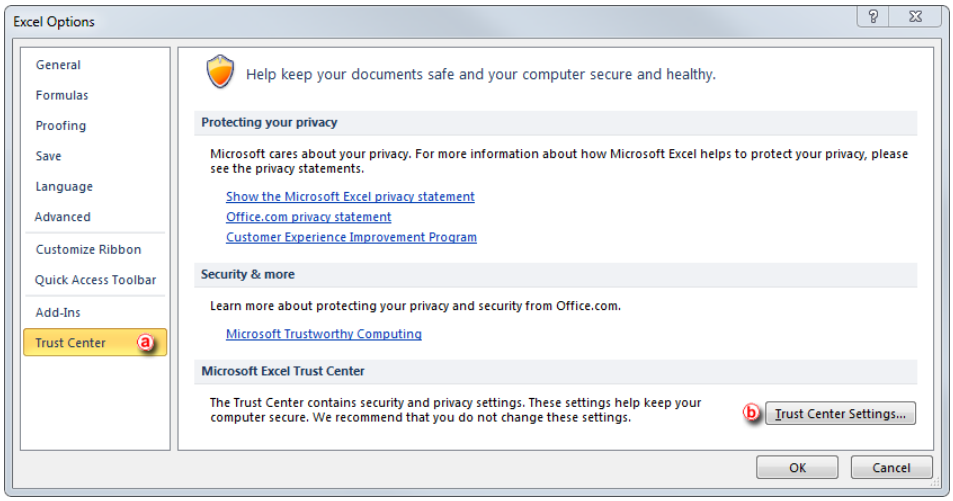
How to set up the macro

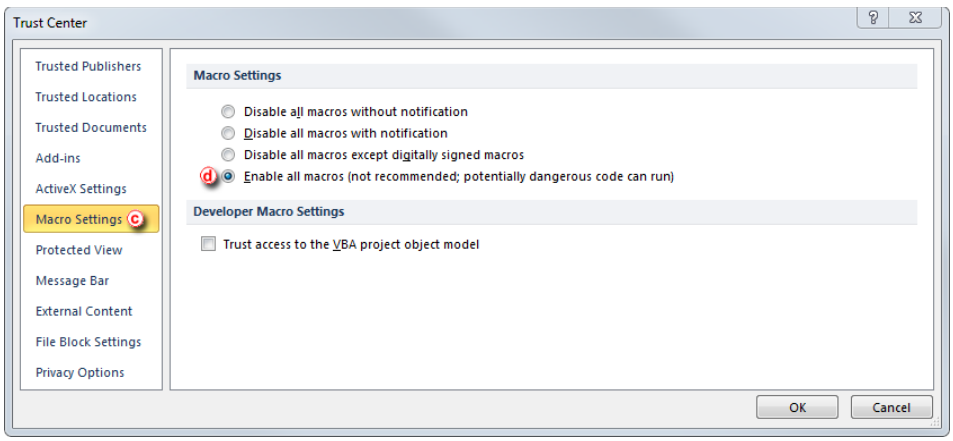
Step 1 – Unblock macros in MS Excel

First, it is necessary to enable macros in MS Excel. Please consult with your IT Administrator whether such an operation is allowed in your environment.

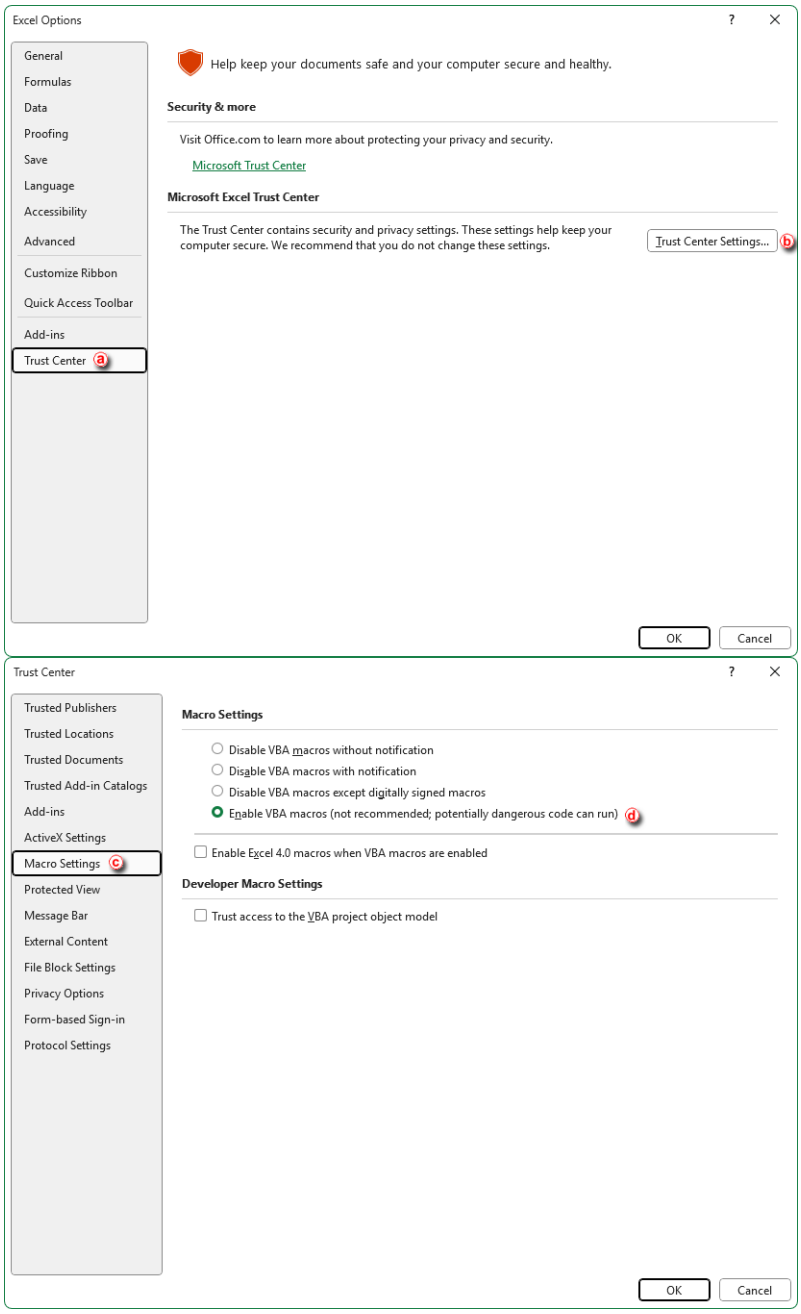
1. Open MS Excel
2. Enable macros

- MS Excel 2010
  Invoke the *Excel options* dialog by clicking *File – Settings* and select *Trust Center* ⓐ. In the *Trust Center* dialog, select *Trust Center Settings...* ⓑ In the *Trust Center* dialog, click on *Macro Settings* ⓒ and *Enable all macros* ⓓ





- MS Excel 2024
  Invoke the *Excel Options* dialog by clicking *File – Options* and select *Trust Center* ⓐ. In the *Trust Center* dialog, select *Trust Center Settings…* ⓑ In the *Trust Center* dialog, click on *Macro Settings* ⓒ and *Enable VBA macros* ⓓ



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)

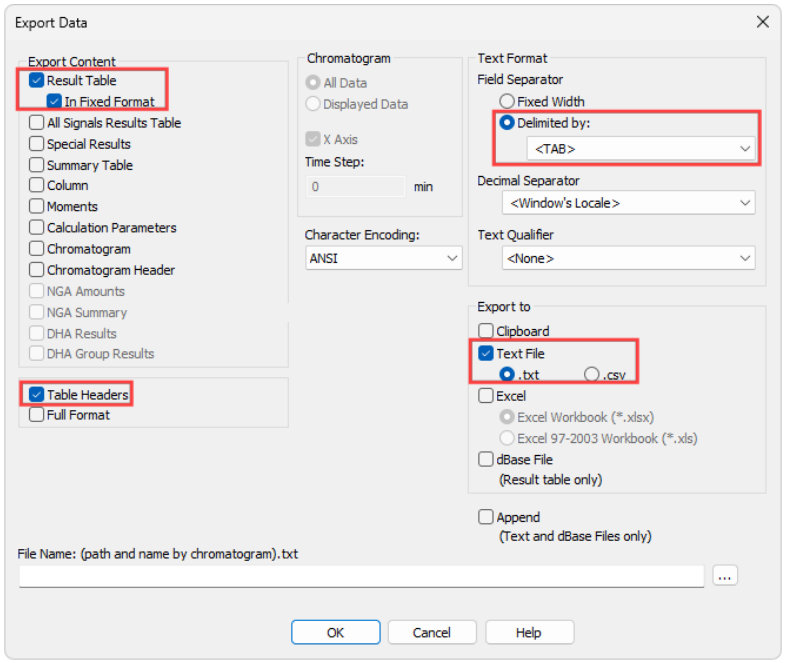
Step 3 – Setup the macro in Clarity

a) Open Clarity

b) Open the *Instrument* window with the DEMO4 project

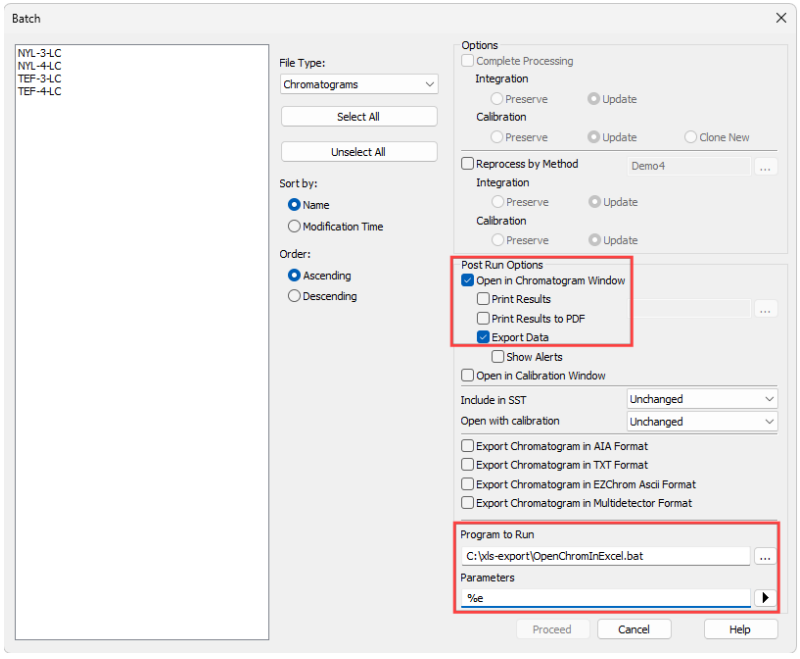
c) In the *Instrument* window, invoke the *Export Data* dialog via the *Settings – Export Data...* menu

- Make sure the same options as in the following image are selected:



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 ensures that the exported file name matches the name of the chromatogram:



- Choose one of the chromatograms and click *Proceed.*

Step 4 – Results

MS Excel opens with the exported chromatogram. The Result Table is compared with the Limits Table. It may look simple, but the process 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 *OpenChrom.vbs* VBScript file. It opens the MS Excel file *chromatogram-export.xls* and passes the *%e* parameter (= the filename of the exported chromatogram) to the VBA macros included in this Excel file.

c) The VBA macro imports the text file into the chromatogram worksheet and adds custom calculations (see the Amount% in column L or the Average function in cell G4)

d) Another VBA macro creates a table with limits for the selected compounds and indicates whether each compound is within these limits (Passed) or outside the limits (Failed). Limits are defined on the "Limits" worksheet. The limits are linked using the name of the compound (the compounds from the DEMO4 project are prefilled)

Limitations

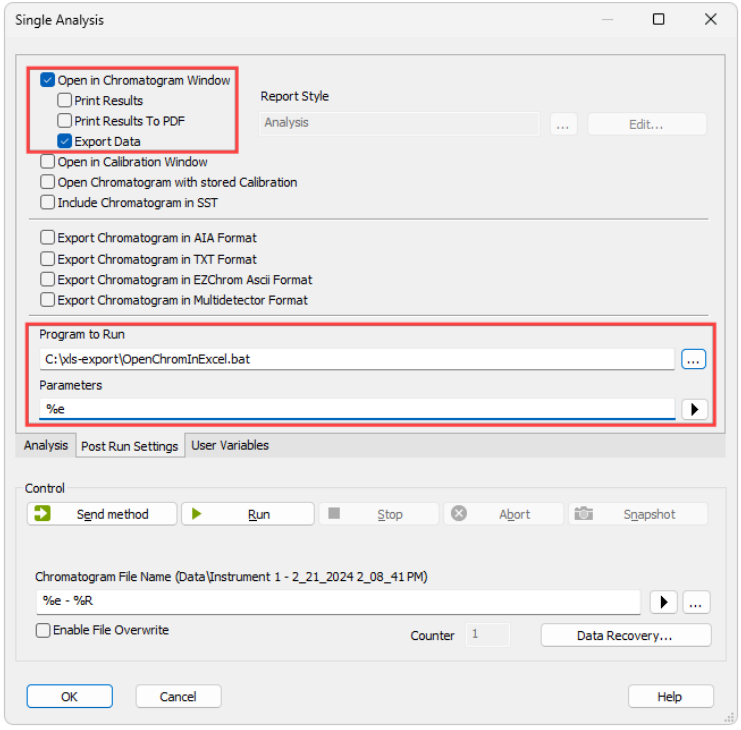
a) The macro currently works only with chromatograms that contain a single signal. Multi-signal chromatograms would provide incorrect calculations of the average amount (cell G4) and the Amount% column.

b) The macro always opens the chromatogram in the same Excel file. For fully automated use (including saving results), consider extending the macro to save each run to a new file. By default, the Excel file remains open and can be saved manually.

Step 6 – Automation in real cases

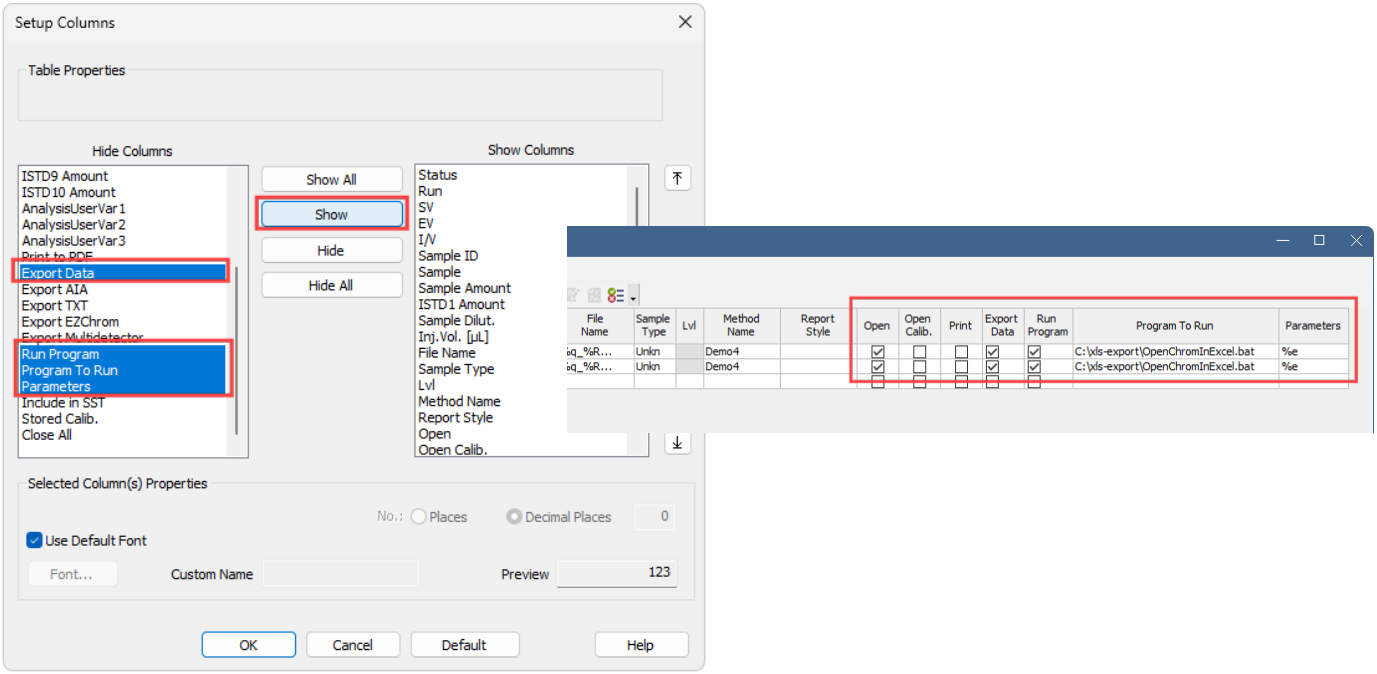
a) Single Analysis – this macro can be run after each Single Analysis measurement completes.

- Switch to the *PostRun Setting* tab in the Single Analysis dialog. Make sure the same options as in the following image are selected. The %e variable set in the *Parameters* field ensures that the exported file name matches the name of the chromatogram:



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:



Additional information

- This macro has been tested on MS Excel 2024 and Clarity version 10.1.01.037.
- This macro is provided as an example 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.