Create a Quality control report for your MaxQuant output

## Requirements

Any Windows System

- no local R required if you followed the installation instructions at <https://github.com/cbielow/PTXQC>)

## Generating a quick QC report without asking questions!

* open a Windows Explorer and find your MaxQuant txt-output folder
* [optional – but highly recommended] copy the mqpar.xml which MaxQuant generated from the root directory into your txt folder,

e.g. c:\MQ\_Diabetes\_study\mqpar.xml 🡪 c:\MQ\_Diabetes\_study\combined\txt\mqpar.xml

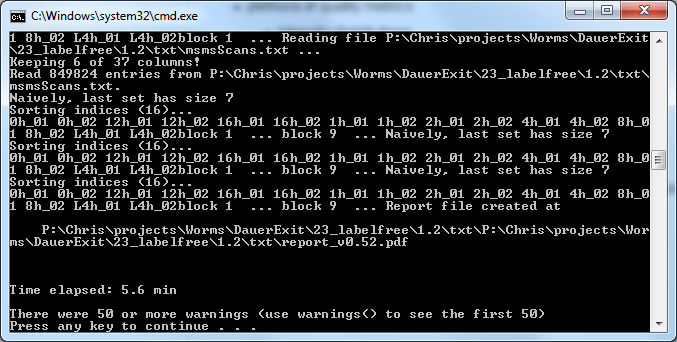
This will enable PTXQC to extract some parameter settings and results in more accurate reports. Alternatively, you would have to set the parameters manually in the YAML file (see next section).

* open **another** Windows Explorer window and navigate to the (network) folder where the QC software was copied to during installation, e.g. P:\Chris\Exchange\QC (where drive P could be some network share).
* drag’n’drop the txt folder onto createQC\_dragNdrop.bat

(you can also drag any file within the txt folder, e.g. evidence.txt)



* A console will pop up and show stuff. Wait… if all went well, one of the last lines is “**Time elapsed: … min**” and a pdf report within your txt folder. It has a version and a folder name attached to it (e.g. report\_v0.63\_diabetes.pdf). The version number will increase every time there is an update in PTXQC (big change in version number means big change in functionality). The name is taken from the path where the txt is located in – it helps you to distinguish report files when they are open in a PDF viewer or copied somewhere else. The console window will stay up until you press a key.



## Alternatively: Generating a QC report using a configuration file:

A configuration file allows you to enable/disable certain plots, and to modify most target thresholds used for the scoring metrics and within plots, e.g. the number of proteins you expect. This will differ by platform and instrument – so adapt it to your needs. The defaults are meant for a Thermo Orbitrap Velos, a 4h LC gradient for a complex matrix (e.g. human cells).

Disabling certain report sections will decrease report size and hide metrics which you may not need. The time required to create the report will also reduce, but usually this is not a bottleneck.

There are two ways to customize parameters for a report:

1. PTXQC will search for a YAML file within the txt-folder for which it generates the report. If there is one (with the correct name, i.e. report\_vXXX.yaml, where XXX is the PTXQC version number), this report file will be used. Thus, if you already have txt-folder containing a report pdf plus the report\_\*.yaml inside, just edit the YAML file and re-run PTXQC using onto createQC\_dragNdrop.bat.
2. If your txt-folder has not been analyzed by PTXQC before OR you want to try another configuration, then you can use the createQC\_dragNdrop\_withYAML.bat to run PTXQC with a custom configuration which you specified before. This .bat file expects a YAML configuration file right next to the .bat file. This file you need to provide. But no worries. One such file with default parameters is generated each time you invoke a QC report generation. Just take any file from a previous run in any other txt-folder. Modify this YAML, copy it next to the bat file, and name it config.yaml.

Note: Option II will take precedence over option I.

Edit the YAML file as you desire using a text editor of your choice (e.g. Notepad++). Each YAML file has a leading comment section which will describe the basics of how YAML looks like and what you should/not change.

It's easy, just try it out.

## Rename Raw files in the report

PTXQC will try to shorten Raw file names to make the plot axis as compact as possible, giving more area to show the data rather than overly long Raw file names. It will use prefix and infix removal of strings which are common to all Raw file names. Name your files in a systematic to make this approach as effective as possible.

Should this shortening not reach a predefined threshold of 10 characters in length for the longest filename after shortening, PTXQC will simply use consecutive numbers, i.e. ‘file 01’, ‘file 02’ to name your files on the axis of the plots.

If you don’t want that, you can either:

1. Increase this length threshold in the YAML config to use the shortened versions. But be advised that using long filenames might result in ugly axis with overlapping text etc…
2. Use a manual mapping table: a file named report\_vXXX\_filename\_sort.txt will be created in your txt-folder, which contains the mapping that is used. You can edit this file and upon running PTXQC again, this new mapping will be applied.

**If you have suggestions on how to improve the report (other metrics/plots, axis labels etc), let me know.**