

History:

V0.52 – 2014-06-17

- added more Top N plots

- better visualizations of charge distributions and protein/peptide numbers

... lots of versions in between ...

V0.42 – 2013-11-12

- added duplicated peptide sequence statistic (dynamic exclusion window check)

- fixed some axis labels

V0.41 – 2013-10-24

- first official release

Create a Quality control report for your MaxQuant output

Requirements:

Any Windows System

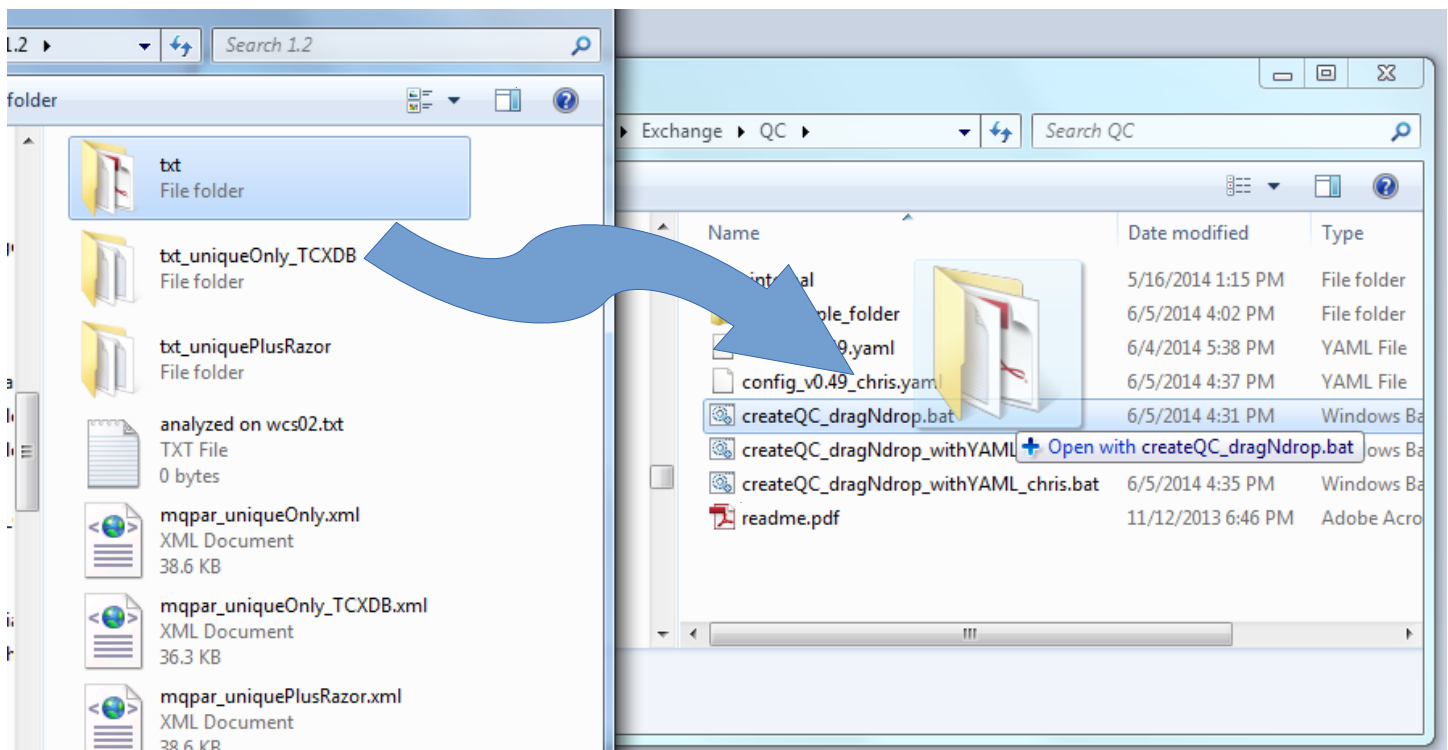
- no local R required if you followed the installation instructions at <https://github.com/cbielow/PTXQC>

Generating a quick QC report without asking questions!

1. open a Windows Explorer and find your MaxQuant txt output folder
2. 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 is some network share).

3. drag'n'drop the txt folder onto `createQC_dragNdrop.bat`

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



4. 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 attached to it (e.g. `report_v0.52.pdf`), which will increase every time there is an update (big change in version number means big change in functionality). The console windows will stay up until you press a key.

```
C:\Windows\system32\cmd.exe
1 8h_02 L4h_01 L4h_02block 1 ... Reading file P:\Chris\projects\Worms\DauerExit
\23_labelfree\1.2\txt\msmsScans.txt ...
Keeping 6 of 37 columns!
Read 849824 entries from P:\Chris\projects\Worms\DauerExit\23_labelfree\1.2\txt\
msmsScans.txt.
Naively, last set has size 7
Sorting indices (16)...
0h_01 0h_02 12h_01 12h_02 16h_01 16h_02 1h_01 1h_02 2h_01 2h_02 4h_01 4h_02 8h_0
1 8h_02 L4h_01 L4h_02block 1 ... block 9 ... Naively, last set has size 7
Sorting indices (16)...
0h_01 0h_02 12h_01 12h_02 16h_01 16h_02 1h_01 1h_02 2h_01 2h_02 4h_01 4h_02 8h_0
1 8h_02 L4h_01 L4h_02block 1 ... block 9 ... Naively, last set has size 7
Sorting indices (16)...
0h_01 0h_02 12h_01 12h_02 16h_01 16h_02 1h_01 1h_02 2h_01 2h_02 4h_01 4h_02 8h_0
1 8h_02 L4h_01 L4h_02block 1 ... block 9 ... Report file created at
P:\Chris\projects\Worms\DauerExit\23_labelfree\1.2\txt\report_v0.52.pdf
Time elapsed: 5.6 min
There were 50 or more warnings (use warnings() to see the first 50)
Press any key to continue . . .
```

Generating a quick QC report using a configuration file:

A configuration file allows you to enable/disable certain plots.

This will reduce the report size and hide metrics which you may not need. The time required for report will also reduce, but usually this is not a bottleneck.

Steps:

Just as before, but instead of using the to `createQC_dragNdrop.bat` as target, use the `createQC_dragNdrop_withYAML.bat`. 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 look into the txt folder for something named `report_v0.xyz.yaml`.

Copy this YAML file next to the bat file, and name it `config.yaml`. You can also rename it if you want, but then you need to edit the bat file and correct the name (its written somewhere at the beginning).

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 basic's of how YAML looks like and what you should/not change.

It's easy, just try it out.

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