PeptideShakerCLI execution

This document describes execution of data processing using PeptideShakerCLI.

Required software

1. Download PeptideShaker from http://compomics.github.io/projects/peptide-shaker.html if not already done.

Protocol

1. Navigate to the directory where you have stored your .zip files generated by SearchCLI.
2. Start the PeptideShakerCLI process. The -Xmx flag here specifies the amount of RAM. Alter based on your system.

```
for i in *.zip; do java -Xmx400g -cp /projects/ptx_analysis/chughes/software/soft
ware_searchGUI/PeptideShaker-1.16.11/PeptideShaker-1.16.11.jar eu.isas.peptidesha
ker.cmd.PeptideShakerCLI -experiment test-project -sample $i -replicate 1 -identi
fication_files /projects/ptx_analysis/chughes/projects-current/test-project/searc
h-output/$i -spectrum_files /projects/ptx_analysis/chughes/projects-current/test-
project/mgf/ -id_params /projects/ptx_analysis/chughes/parameter-files/mar2018/ch
_mar2018_OT-MS1_HCD-OT-MS2_human-trypsin_StdMods-TMT10plex.par -out /projects/ptx
_analysis/chughes/projects-current/test-project/results-output/$i.out.cpsx; done
```

3. The above command will generate individual results files for each search. If you desire to have all search files combined into a single results file, use the following command.

```
java -Xmx400g -cp /projects/ptx_analysis/chughes/software/software_searchGUI/Pept
ideShaker-1.16.11/PeptideShaker-1.16.11.jar eu.isas.peptideshaker.cmd.PeptideShak
erCLI -experiment test-project -sample all-fractions -replicate 1 -identification
_files /projects/ptx_analysis/chughes/projects-current/test-project/search-output
/ -spectrum_files /projects/ptx_analysis/chughes/projects-current/test-project/mg
f/ -id_params /projects/ptx_analysis/chughes/parameter-files/mar2018/ch_mar2018_O
T-MS1_HCD-OT-MS2_human-trypsin_StdMods-TMT10plex.par -out /projects/ptx_analysis/
chughes/projects-current/test-project/results-output/test-project_all-fractions.o
ut.cpsx
```

You should now have processed results files for all of your samples.