DIY: Using MS²PIP predicted spectral libraries for DIA data extraction

In our manuscript we only show the benefit of MS²PIP predicted libraries on a HeLa dataset published by Searle B. et al. Nevertheless, before putting this story on paper, we have of course carried out additional evaluations on both public and in-house datasets. We also checked the performance of our workflow for Q-TOF instruments (TripleTOF5600 - AB Sciex). This data is not mentioned in our manuscript, because it will be used for another project. In any case, the unpublished results have shown that the workflow also yields a gain in the number of peptide identifications for Q-TOF instruments.

We also tested the performance of the method on the Yeast dataset, which was published together with the HeLa dataset. These results are not included in the manuscript either, as it is only a confirmation of what we had already seen in the HeLa dataset. However, we are going to publish these results on GitHub with good reason. We would like to challenge you to try out our workflow on the Yeast dataset. That way you can go through the different steps and at the same time see the added value of this new peptide centric approach.

The Yeast dataset can be downloaded online from the MassIVE proteomics repository: ftp://massive.ucsd.edu/MSV000082805. The repository contains both raw as peak picked data, so it is up to you whether you want to skip the raw file processing with the MSConvert GUI.

We will make the MS²PIP predicted yeast spectral library public if you do not immediately manage to perform the installation. However, we hope that you will take up the challenge of completing the entire workflow.

Please share your results and experiences as much as possible via social media (Twitter,...). We would be very grateful to you. If you encounter any problems, please contact us by e-mail: bart.vanpuyvelde@ugent.

Then the only thing left for me to do is to wish you all the best with the challenge!

With kind regards,

Bart