Quantitative Proteomices - Exercise on peak detection and continuous wavelet transform

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1 Getting familiar with OpenMS/TOPPview

1.1 Compile and install

Download OpenMS from the http://www.openms.de website. Then follow the installation instructions for **OpenMS**.

1.2 Hints on compiling

Multi-processor platform

- If you have a multiprocessor platform use "make -j (number of processors x 2)"

Single-processor platform

- If you have a single processor plattform, you will need very long time and maybe a good book to read. **We suggest:** this for pastime.

On the documentation page you will find sone screencasts, showing you who to switch between display modes and other stuff. If you need any help, check out the TOPPView tutorial or write an E-Mail to Christoph.

1.3 Playing around

1. Open TOPPView
2. Open an example file by $File \rightarrow Open\ example\ file$ and choose $peakpicker\_tutorial\_1.mzML$ - What can you see? What could be a good noise threshold? What ionization technique was used?
3. Let's say we want to remove the baseline. Open $Tools \rightarrow Apply\ TOPP\ tool$ and select the "BaselineFilter", then click okay. TOPPView will ask you whether to open the filtered data as a new layer or new window. Because we want to compare the result with the original data, open it as a new layer. What can you see?
4. Then deselect the original data in the layers list by removing the **"x"** in front of peakpicker_tutorial_1.mzML
5. Select the basline filteres signal and again open the TOPP tools by choosing $Apply\ TOPP\ tool(visible\ layer\ data)$ and select the "PeakPicker" with type "wavelet".

6. Then deselect the currently calculated layer and the baseline removes layer and select again the original layer peakpicker_tutorial_1.mzML
7. Calculate again the Peaks using “PeakPicker” and the “wavelet” option
8. Compare the peaks picked with baseline removal and without

1.4 Playing around with the CWT

In progress ...