

Peak retention times

We want to know whether the different software tools choose (in general) the same peak (based on retention time).

Following software tool results are analyzed:

1. Spectronaut
2. Skyline
3. PeakView
4. OpenSWATH
5. DIAumpire

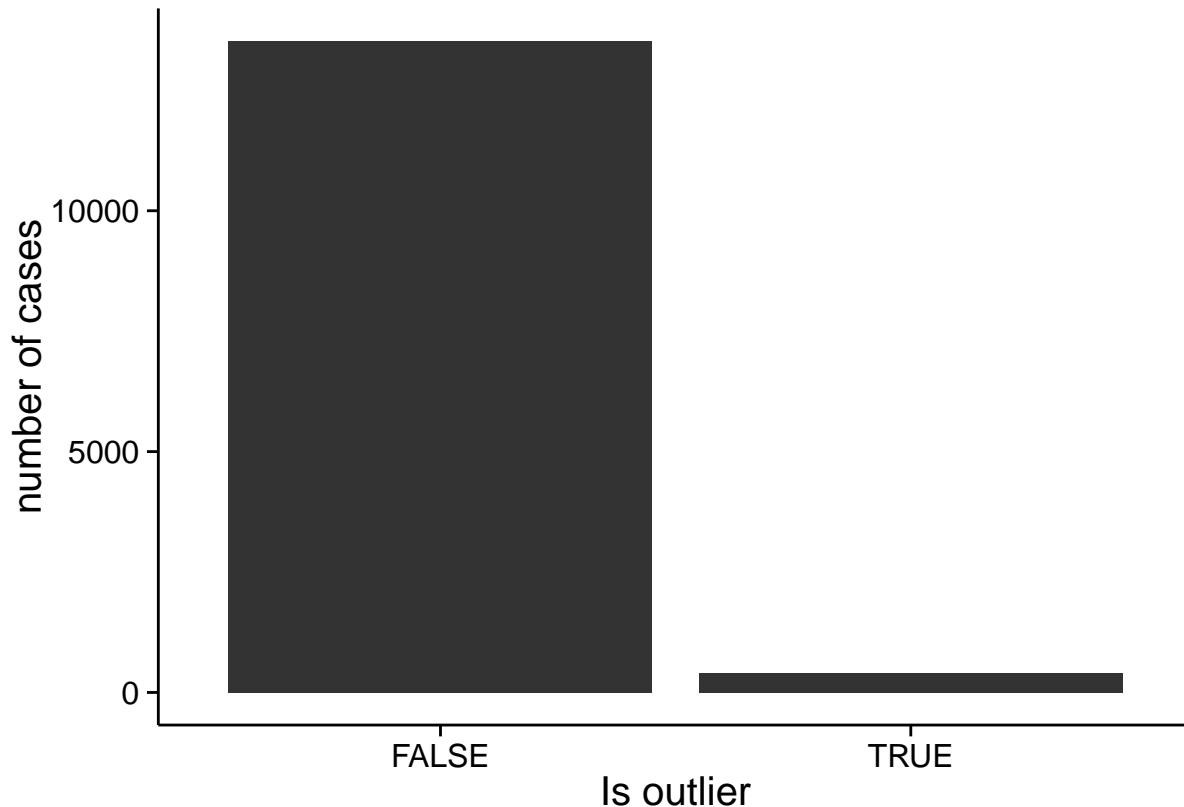
We choose one of the injections: lgillet_I150211_008.wiff

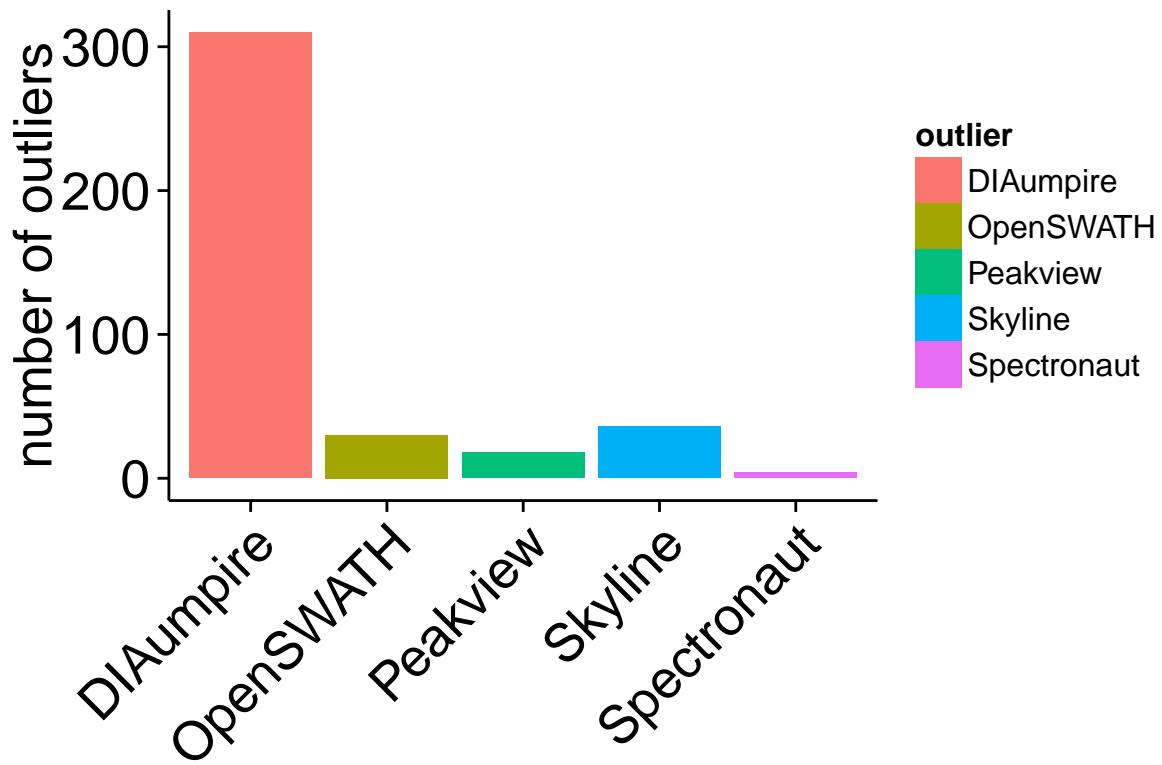
Modifications are reported differently in each software. As a first approach I use only non modified peptides.

This excludes 13211 assays from the analysis (out of a total of 65037).

We are only interested on peaks identified by all software tools. Otherwise it is hard to interpret, since some software tools identify more peptides than others. To define when a tool picked a different peak to other software tools, for each peptide/z we estimate the standard deviation of the retention time. We consider that the peptide/z has at least one outlier if the standard deviation is higher than 0.2 minutes, and we define as outlier the tool that has the largest deviation from the mean retention time.

Using only complete cases (peaks detected by all tools):





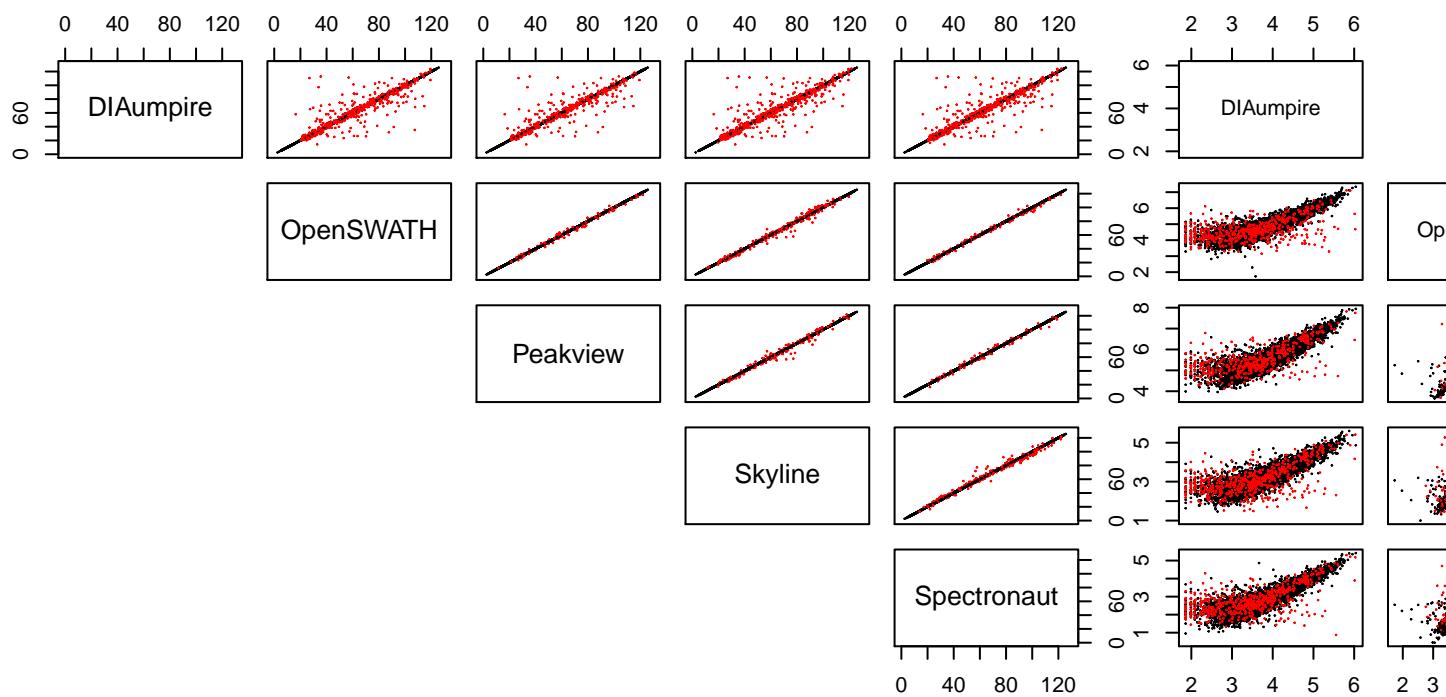
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## Saving 6.5 x 4.5 in image
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We estimate there are 2.9% of wrong peaks in the total number of peaks identified by all software tools.

outlier	Outlier.count	Outlier.ratio
DIAumpire	310	0.022
OpenSWATH	30	0.002
Peakview	18	0.001
Skyline	36	0.003
Spectronaut	4	0

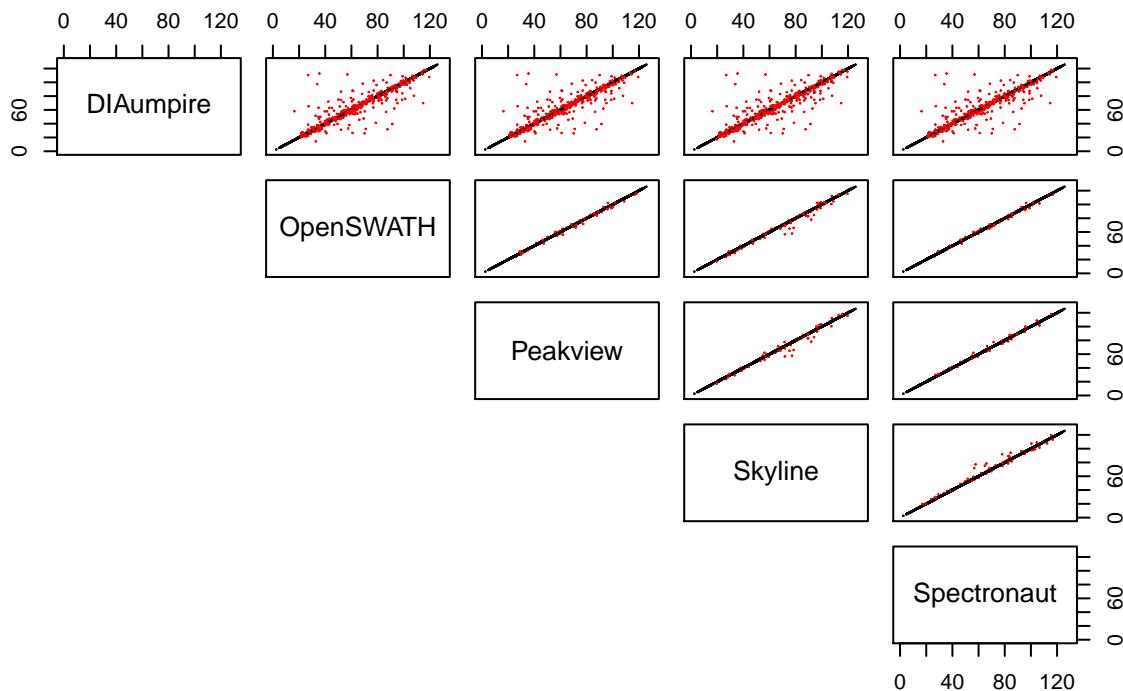
Relate with peak intensities.

Peak Retention times for all tools



If we plot peaks identified in **all** software tools, the plots are not so powerful, but you can see also very clear that those points in PeakView are actually aligned in other software tools, which shows clearly that PeakView has most likely a retention time alignment issue for lower retention times.

Peak Retention times for all tools (only commonly identified peptides)



Peak Intensities for all tools (only commonly identified peptides)

