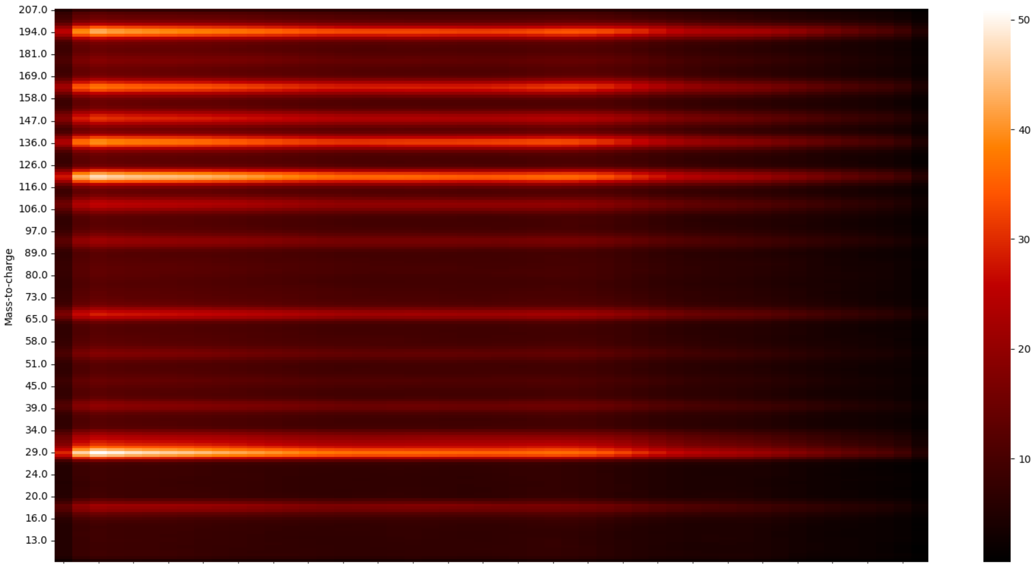
Lari Kunnasmaa

1 Thesis explanation

Hello, this pdf contains a very simplified explanation and a some visuals of code related to my master's thesis. The pdf is made as a simple explanation and should not be too seriously. Its purpose is to give some context and visualise the results of the code, so I am not just posting arbitrary lines of code or forcing anyone to read a 60 page thesis to understand a line of it. But for those interested I am more than happy to give an more info or even a presentation for those interested.

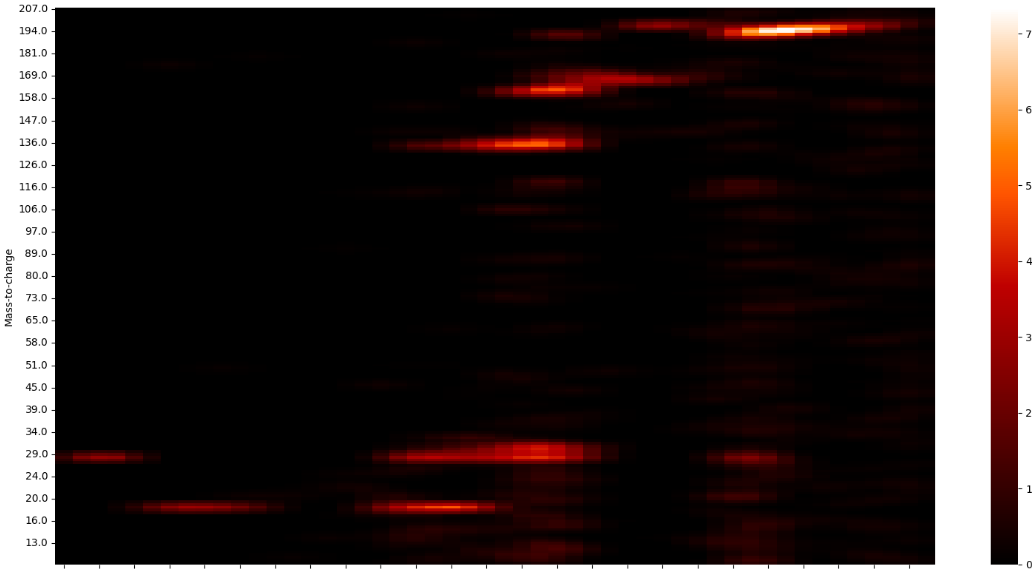
2 PEPICO

To put it very shortly in PEPICO we measure ions flight time and electrons hit position. This way we can create pairs from them to determine molecules structure. However we cannot determine from which ion the electron came from, so we have both false pairs and true pairs. In false pairs the electron is not from the detected ion and in true pairs it is. With these we can create a PEPICO map shown in figure 1. However this photo does not give us any info sense it has both false and true pairs.



Kuva 1: No false events removed

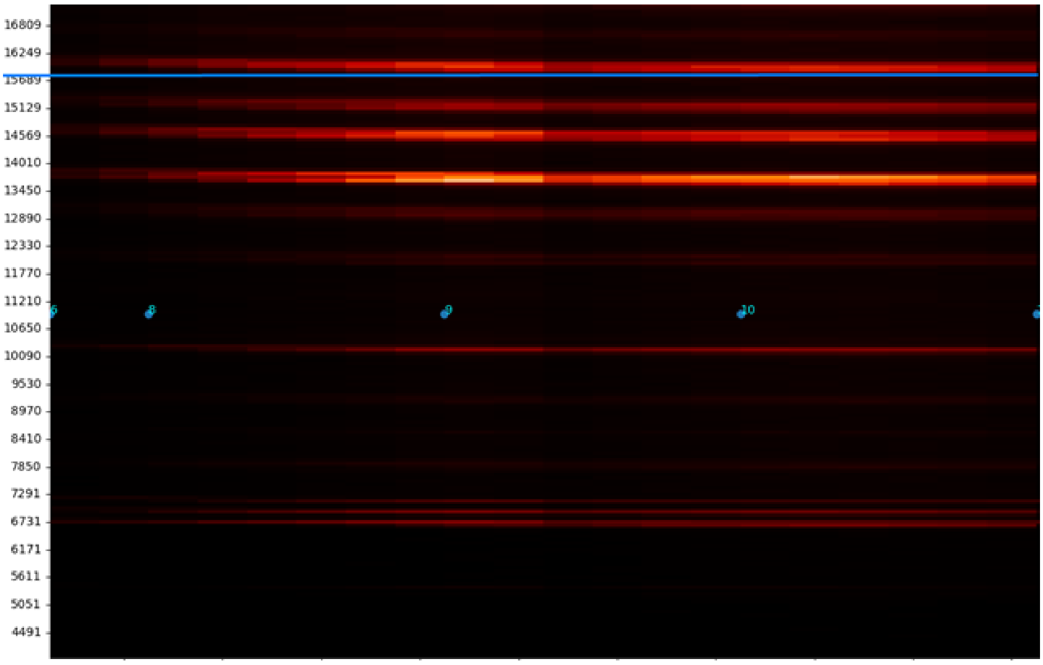
To get get useful data from the map we need to remove the false pairs, which is done by introducing extra known false pairs during the measurement. This means we can reduce the average amount of false pairs from the map. Figure 2 shows the true PEPICO map.



Kuva 2: True PEPICO map

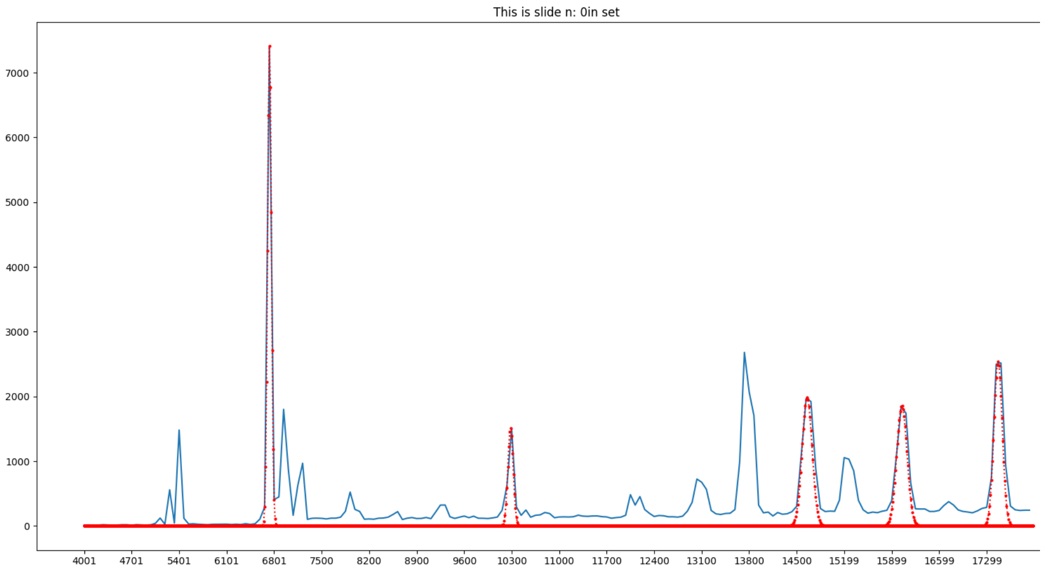
3 Drift fix

Second very notable part of the thesis is fixing the drift that formed during the measurement. The drift can be see in figure 3, where looking at the red data points shows a noticeable dip after the beginning(left side). Blue line helps to visualise the dip. To make the measurement consistent this needs to be evened out.

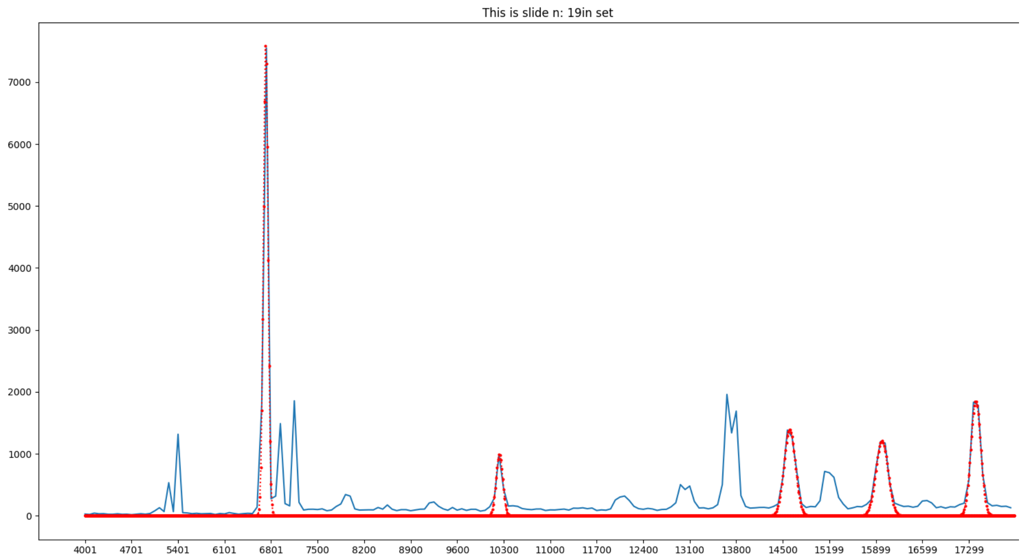


Kuva 3: Every red line has a noticeable curve in the beginning.

Drift fix is implemented, by splitting the measurement into equal slices. Slices can be represented as a histogram. The data in the slices can be represented as a histogram. Example shown in figure 4 and 5. The code recognizes the peaks (the peaks are formed by specific ions) and fits a gaussian to them. Peaks position can be used to determine how much they have drifted from the average position.

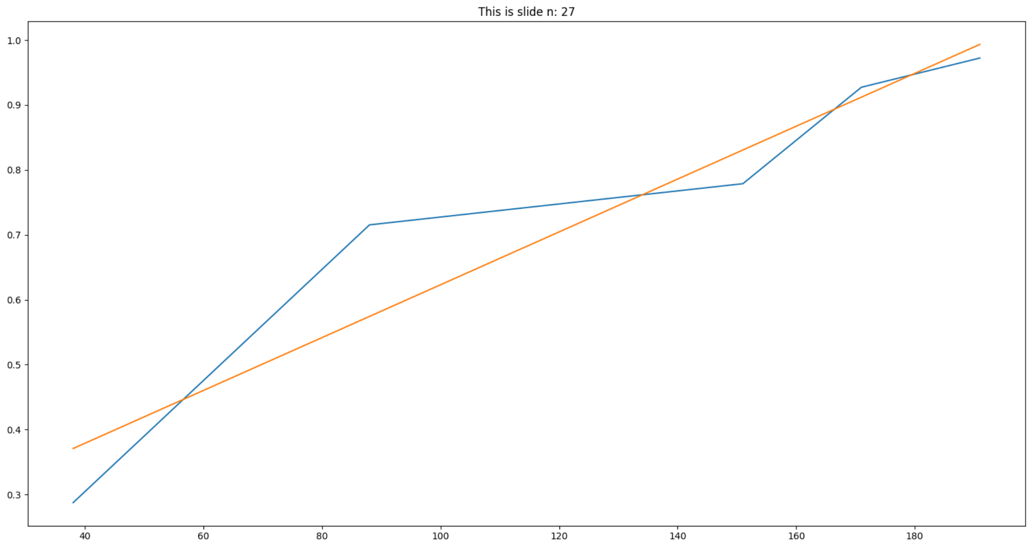


Kuva 4: Fitted peaks from slide 0 (peaks have drift)

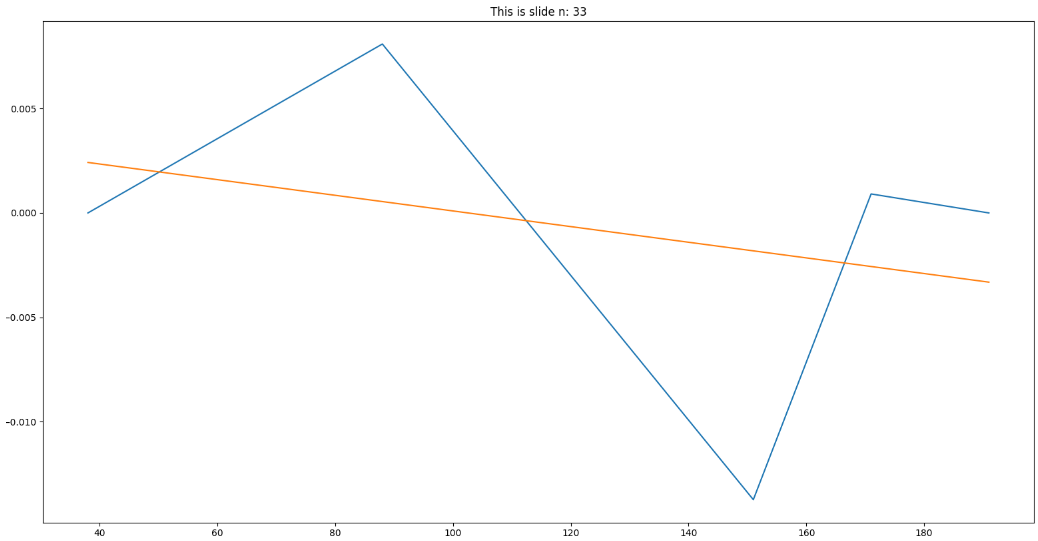


Kuva 5: Fitted peaks from slide 19(peaks do not have drift)

Figures 6 and 7 shows the amount that the peaks position differs compared to the average peaks for each flight time. Since the amount of positions changes we can fit a line to it. The lines parameters can be used to correct flight time, that made up the slide so that the peaks representing the same ion have the similar flight time.

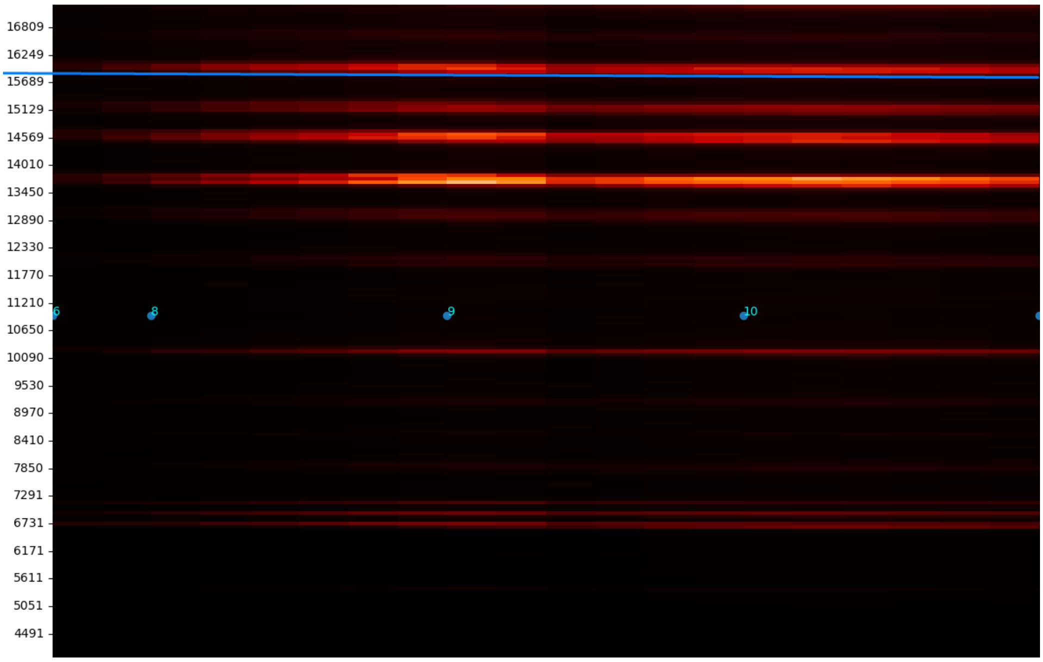


Kuva 6: The amount of miss alignment for each peak in slide 27 and the fit used to correct it



Kuva 7: The amount of miss alignment for each peak in slide 33 and since it is so small, no correction needs to be made.

Using the parameters the figure 3 can be corrected to figure 8.(Since the code for this is automatic the correction is even easier than the manual used in the lab, that uses paid software)



Kuva 8: Ion flight time, but the drift has been fixed. The blue line is in the same spot as in figure 3, so we can clearly see that the drift has been fixed.