\section{Wavenumber calibration}

Even after the wavenumber calibration the resulting absorbance spectrum doesn’t match with \(CO\_2\) and \(H\_2O\) peaks from literature. This is caused by the high variation of the twenty monitor measurements of which the mean is the basis of the wavenumber calibration. Regardless, wavenumber calibration is still useful since it is known that the different measurements do not match even though they should. The measurements should match since a cause of the variation between measurements is identified to be the piëzo element and its hysteresis, and this is expected to be the only major contributor.\\

\begin{comment}

The goal of the wavenumber calibration is to decrease the uncertainty of the absorbance, which in turn decreases the uncertainty of the determined concentrations. Discuss why st.dev. of absorbance decreases the amount it does. \\

\end{comment}

\section{Determination of molecules}

A general disadvantage of choosing molecules based on their molar absorptivity is that some molecules might have a large impact on the eventual absorbance due to a high concentration, despite having a low absorptivity. They would therefore be falsely eliminated from the list of molecules to check for.\\

There is also the drawback of excluding molecules which might be an important part of the absorbance, but aren’t selected since they do not have adequate molar absorptivity in the p-regions. This makes the subsequent determination of concentrations less accurate. A trade-off can be made by allowing for more p-regions, either by decreasing the minimum amount of consecutive points needed or heightening the maximum p-values of which these regions consist. This way more molecules will have some absorptivity in one of the regions and therefore won’t be scrapped. \\

Both problems to do with selecting molecules based on intensity can be resolved in advance by putting molecules that play an important role in the eventual absorbance in the standard list of molecules. This requires a-priori knowledge of the important molecules which is obtained from literature\cite{a review of volatiles} and simply by performing the least squares method to get the concentration on a large list of molecules. The concentrations won’t be as accurate for a large list, but all molecules that contribute a lot to the spectrum can be picked out for later runs with strict molecule lists.

\section{Determination of concentrations}

From the shapes of $CO\_2$ and $H\_2O$ in \autoref{fig:4.1} and autoref{fig:4.2} it can be seen that the concentrations calculated using the \textit{lsqnonlin} function are definitely in the right order of magnitude. The signal-to-noise for the rest of the measured absorbance is however still quite large, and the calculations for the molecules with lower concentrations are therefore not very accurate.

\begin{figure}[ht]

\centering

\includegraphics[width=\textwidth]{Figs/6/barplot.png}\\

\caption{Average concentrations of molecules compared to VSL data}

\label{fig:Schematic\_Setup\_Final}

\end{figure}

Currently the concentration determination is not yet accurate enough to use for distinguishing between healthy and asthmatic children, as can be seen in \autoref{barplot of concentrations with st. dev.}. The uncertainty of the measurements themselves can be improved by finding a moving element of which the displacement over voltage can be better characterized than the current piëzo. Alternatively an attempt can be made to calibrate the signals as they come straight from the measurement apparatus, before even the pre-calibration.

\section{Categorizing health status by classification}

The accuracy of the classification can possibly be improved by looking more closely into the used algorithms, and improving them using a-priori knowledge of the samples such as regions of relatively high signal-to-noise ratio. Wavenumber regions can be given weights based on the signal-to-noise ratios so the algorithm depends more heavily on these accurate regions.

The error rate could also tell a lot more if the amount of false positives and false negatives is given. This would give separate error rates based on whether the algorithm judges the sample as healthy or asthmatic. It is possible that one of these error rates is much lower than the other, thereby increasing the certainty of the result above the total error rate.