Towards removal of water vapour and carbon dioxide effects from mid-infrared spectra

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Abstract— Fluctuation in the amount of water vapour and carbon dioxide in the beam path in purged Fourier transform infrared (FTIR) systems following measurement of a background spectrum has a detrimental effect on the quality of spectra; the resulting decreased SNR has the potential to confuse machine learning model calibration such that it ignores these 'fingerprint' regions of the spectra which may contain important information pertaining to the analyte. Examples of analytes that can be affected by water vapour effects on spectra are proteins and lipids which have major characteristic absorbances in the region 1500 – 1800 cm^{-1}.

Postulated solutions to this problem include physically introducing dry or humid air to restore conditions to those at which the background was taken [1], Savitsky-Golay filtering and spectral subtraction. However, filtering results in loss of spectral information [2], whilst spectral subtraction using a separately measured water vapour spectrum is flawed unless conditions in which all spectra are taken match [3].

We present a simple method to correct for water vapour and carbon dioxide absorption, for both normal incidence and ATR techniques, using three spectra collected in close succession of the same sample, as shown in Figure 1(a). The first and last spectra are designated as references used to generate a difference spectrum by subtraction. The difference spectrum is subtracted from the analyte uncorrected spectrum to give an output spectrum (Figure 1(b)), the length of which is minimized by using a fitting function to optimise the difference spectrum scaling factor λ. Successful processing of spectra with absorption peaks, such as that of sphingomyelin, has been demonstrated utilising this technique. This methodology enables spectral correction without the requirement for significant additional sample collection or complex data processing.

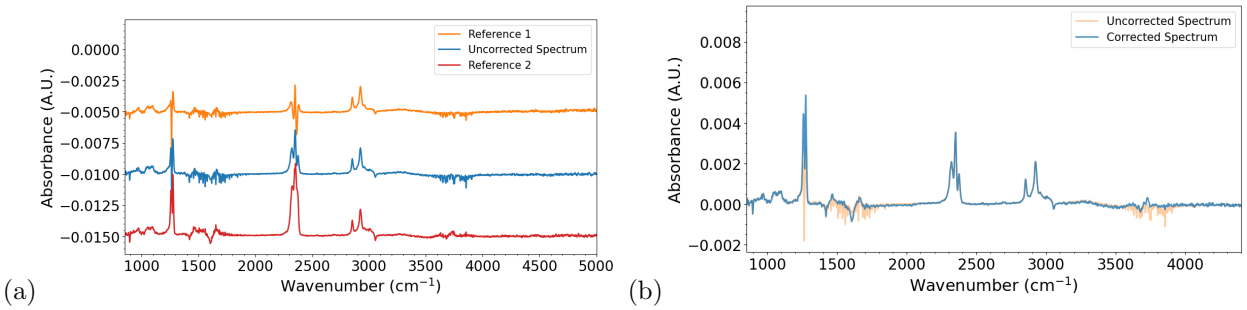

Figure 1: (a) Three absorbance spectra of 0.1mM sphingomyelin taken sequentially, designated 'Reference 1', 'Original' (spectrum to be corrected) and 'Reference 2' respectively. (b) The spectrum is corrected for water vapour, overlaid with the uncorrected spectrum for comparison.

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