

SUPPORTING INFORMATION TO

Article

The role of the pre-analytical step for human saliva analysis via vibrational spectroscopy

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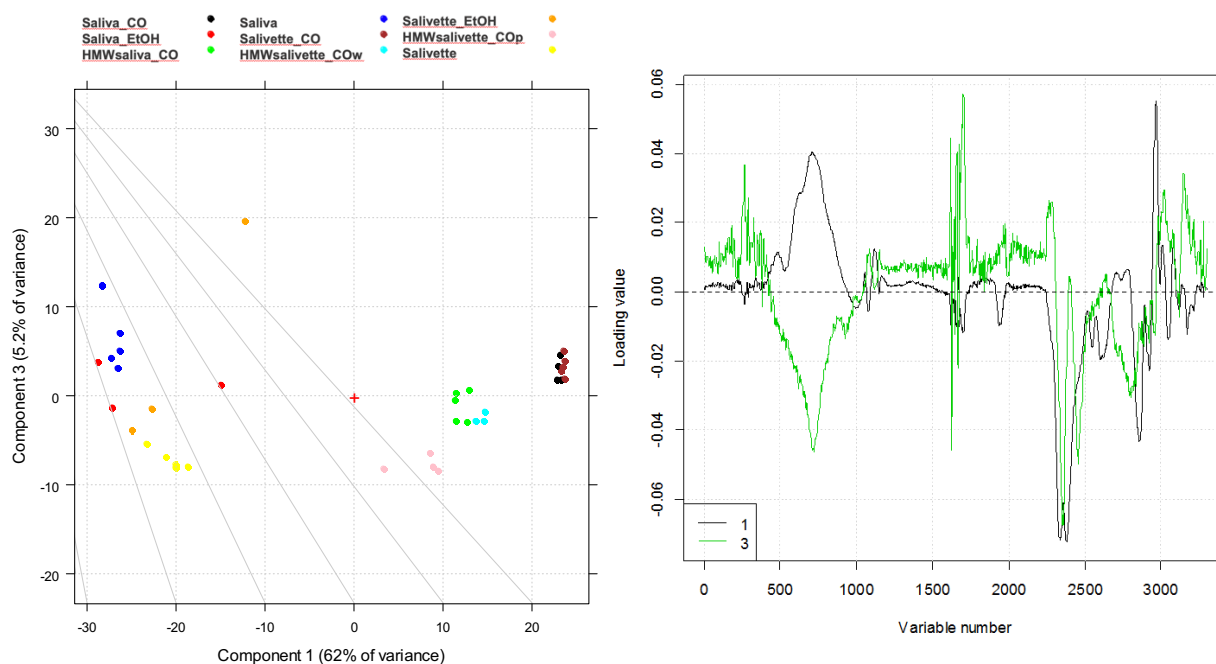


Figure S1. PCA results of SNV normalized and centered (no scaling) ATR-FTIR spectra of saliva samples. (a) Score plot (69.6% of total variance); (b) loading plot PC1 (black line) and PC3 (green line). HMWsaliva_CO and HMWsalivette_CO refer to high molecular weight compounds (HMW) remaining in the upper part of 3 kDa cut off filtering units (w=wiping, p=printing) as explained in the experimental part.

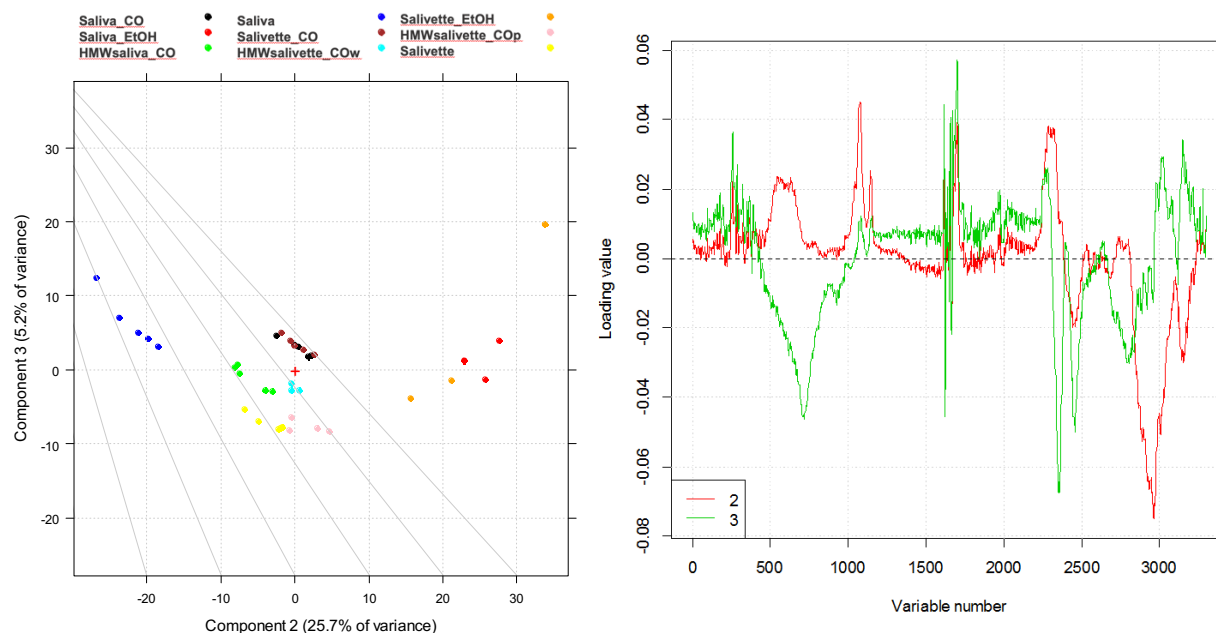
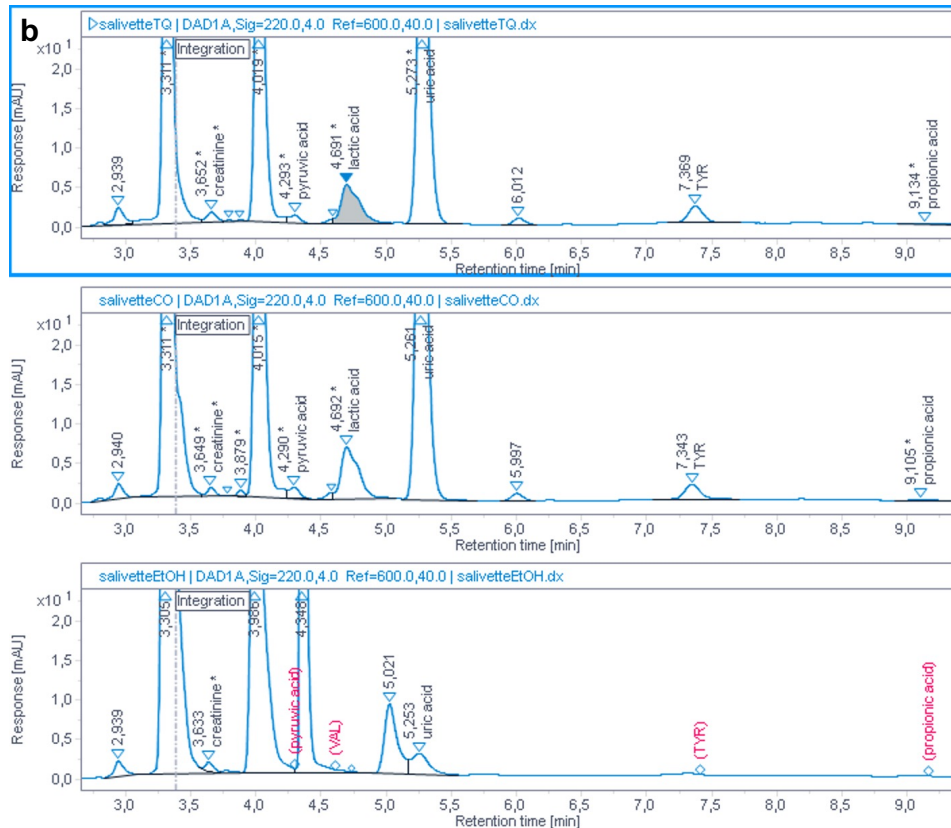
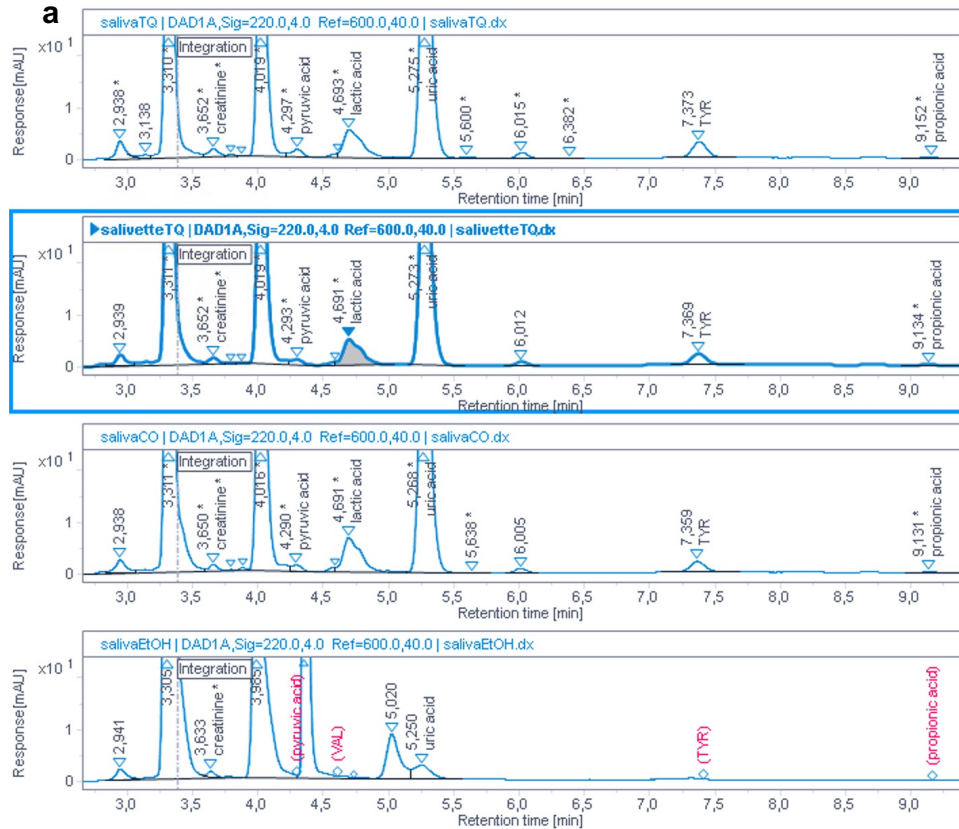


Figure S2. PCA results of SNV normalized and centered (no scaling) ATR-FTIR spectra of saliva samples. (a) Score plot (28.0% of total variance); (b) loading plot PC2 (red line) and PC3 (green line). HMWsaliva_CO and HMWsalivette_CO refer to high molecular weight compounds (HMW) re-maining in the upper part of 3 kDa cut off filtering units (w=wiping, p=printing) as explained in the experimental part.



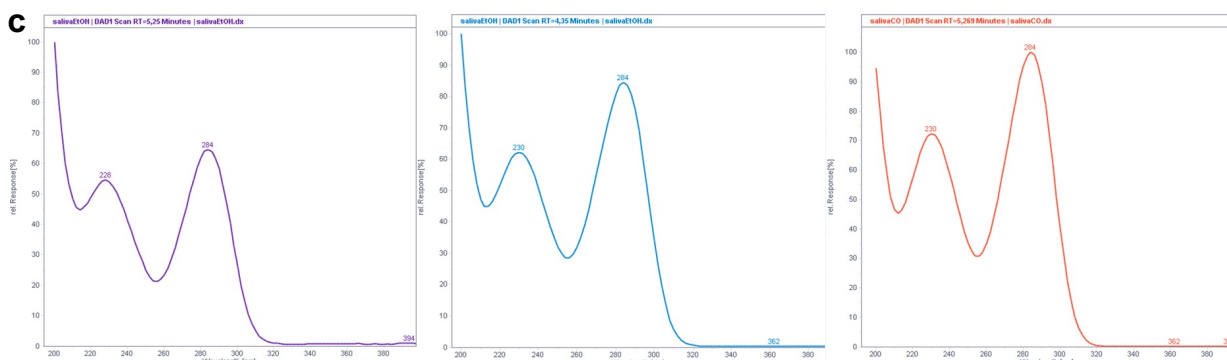


Figure S3. Absorbance HPLC chromatograms at 220 nm of saliva (a panel) and salivette (b panel) samples before and after deproteinization with 3 kDa cut off filtration and precipitation in ethanol. (c) UV/visible spectra of the peak at $t_R=5.2599$ (purple line) and 4.35 min (blue line) of saliva_EtOH sample and $t_R=5.269$ min (orange line) of saliva_CO sample.

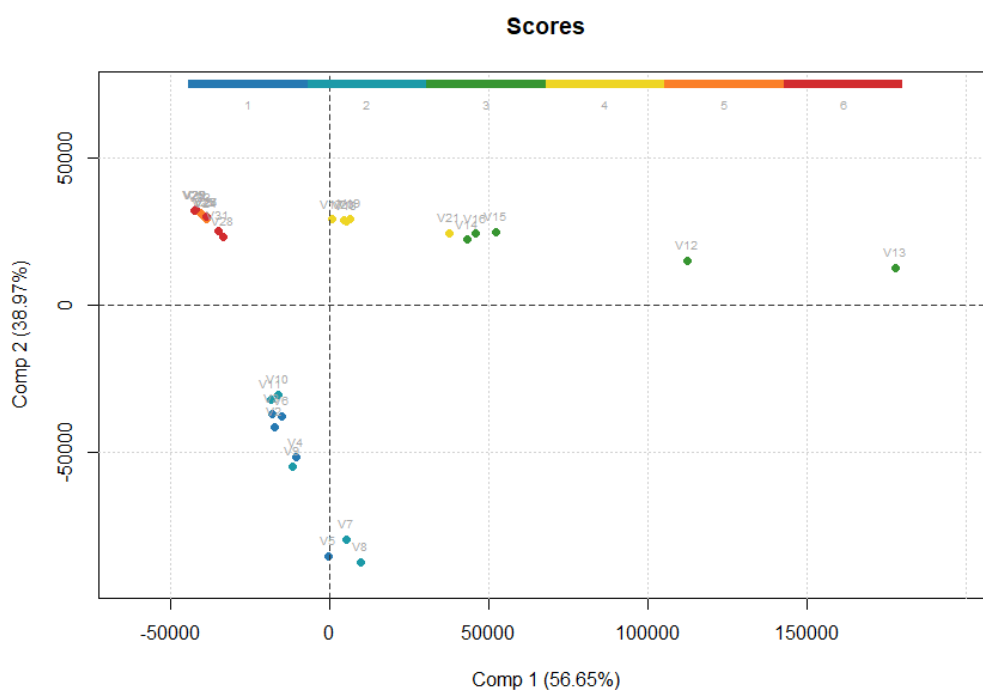


Figure S4. PC1 vs. PC2 score plot of Raman spectra acquired at 785 nm and preprocessed as described in Section 3.4. Legend: 1 (blue) – saliva; 2 (light blue) – salivette; 3 (green) – saliva_CO; 4 (yellow) – salivette_CO; 5 (orange) – saliva_EtOH; 6 (red) – salivette_EtOH.

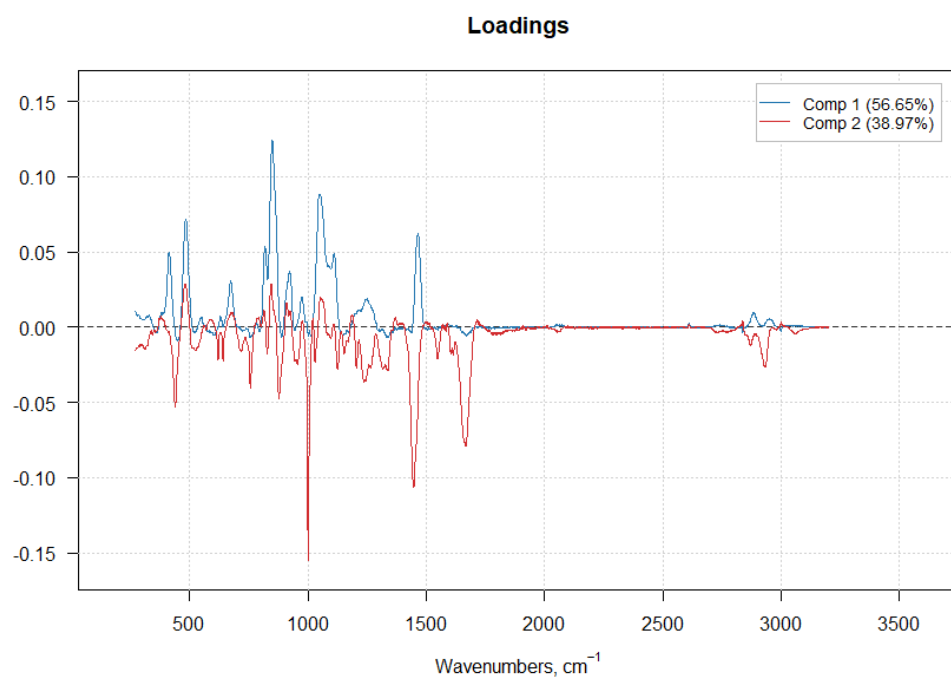


Figure S5. PC1 (blue line) vs. PC2 (red line) loading plot of Raman spectra acquired at 785 nm and preprocessed as described in Section 3.4.