**Code overview // Read me**

This code base contains functions and scripts that are the basis for the published article “Raman and NIR spectroscopy: A discussion of calibration robustness for food quality measurements through two case studies” by Lintvedt et.al, 2025.

The code consists of three separate main scripts for the two different cases as well as the supplementary experiment studied in the paper.

The purpose of the code base is to provide openness around the data analysis and facilitate reproducibility of results.

The functions and scripts are based on the SAISIR data structure and relevant basis functions from the SAISIR toolbox by

* C.B.Y. Cordella, D. Bertrand, SAISIR: A new general chemometric toolbox, Trends in Analytical Chemistry 54 (2014) 75–82. http://dx.doi.org/10.1016/j.trac.2013.10.009
* Available on request at <http://www.chimiometrie.fr/saisir_webpage.html>

Other relevant references:

* Bjork and Indahl 2017, “Fast and stable partial least squares modelling: A benchmark study with theoretical comments”

<https://analyticalsciencejournals.onlinelibrary.wiley.com/doi/10.1002/cem.2898>

* Westad and Martens snippet for choice of optimal number of PLS components was used with adjustments
  + Westad, F., Martens, H., 2000. Variable selection in Near infrared spectroscopy basead on significance testing in Partial least squares regression. J. Near Infrared Spectrosc. 8, 117–124. <https://doi.org/10.1255/jnirs.271>
* Asymmetric Least Squares for baseline correction:
  + Eilers, P.H.C., Boelens, H.F.M., 2005. Baseline correction with asymmetric least squares smoothing, Leiden University Medical Centre.
* Bechtold – Violin plots
* GS tools – Kris de Gussem