Toward a NIR smart sensor: digital filters for data curation

G. Guedes1 , M. De Gea Neves2, H. W. Siesler2, A. Silva Ferreira1

1 Escola Superior de Biotecnologia, Portuguese Catholic University, R. de Diogo Botelho 1327, 4169-005 Porto, Portugal

2 Department of Physical Chemistry, University of Duisburg-Essen, Schuetzenbahn 70 D 45117, Essen, Germany

Handheld NIR spectrometers can be used for on-site and in-the-field analysis, have a high acquisition rate and, in most of the cases, do not require sample preparation. However, some shortcomings are also noteworthy in industrial settings such as variability on signal-to-noise ratio, low reproducibility induced by movement, changes in luminosity and temperature, to mention just a few. Hence such “faulty spectra” generated during on-line data acquisition require a data curation step later in the data evaluation process, otherwise they will impact calibration performance.

The main objective of this work is to develop a set of digital filters for data curation enabling real-time database loading and data visualization as steps towards a “smart sensor” superseding operation supervision.

Port wine was chosen as a model system, since it represents a complex matrix due mainly to changes on chemical profile occurring with time. Firstly, spectra selected for the present investigations were collected using a benchtop FT-IR spectrometer. The consistency offered by the benchtop FT-IR spectrometer was essential for the comparison of the behavior of the digital filters. For this purpose, the samples were divided according to the color of the wine (White, Red, Rose). A PCA model was created for white wines and the distance between new samples and the center of the PCA (T2 Hotelling), as well as the distance between the plane of the PCA and the new samples (Q Residual) were used with digital filters. Thus, when a sample presents values of Q residual and T2 Hotelling that are outside the model, it is considered an outlier and discarded.

Secondly, model transfer between the benchtop spectrometer and a handheld instrument were attempted in order to make this approach available for on-site measurements suitable for authentication process with promising preliminary results.

 **Keywords:** NIR, Smart Sensor, Digital Filter, Data Curation

**Acknowledgements:** We gratefully acknowledges receiving funding from the SensorFint Virtual Mobility Grant (CA19145).