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Data fusion strategy for quantitative analysis of n-3 fatty acids in commercial krill oil

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Abstract

Raman and attenuated total reflectance-Fourier transform infrared (ATR-FTIR) spectroscopy were used to analyse seven krill oil capsules and twenty-five calibration samples to quantitate astaxanthin, EPA plus DHA and other important fatty acids. Spectroscopic data was calibrated against FAME profiles (measured by GC-MS) and astaxanthin concentrations (measured by UV-VIS). Raman spectra was found to be suitable to quantify astaxanthin, EPA, DHA and EPA + DHA, with reasonable root mean square error of prediction (RMSEP) for test set validation: 40 $\mu\text{g g}^{-1}$, 2.5%, 2.2% and 4.5% respectively.

EPA, DHA and EPA+DHA concentrations in krill oil could also be quantitatively modelled using IR spectra, but astaxanthin was not acceptably modelled using this approach. Fusion of the spectroscopic methods were carried out at low (concatenation), medium (PCA scores for feature extraction) and high (central limit theorem) levels. Models generated from low-level and mid-level data fusion had corresponding errors (RMSEP) of 3.8%, 4.8%, 1.1% and 1.9% for MUFA, PUFA, EPA and EPA + DHA, respectively, which were better than the individual techniques [1].

Fig. 1: PLSR-predicted calibration models for quantitative determination EPA+DHA by data fusion

Keywords: Raman spectroscopy, Infrared spectroscopy, Chemometric, Docosahexaenoic acid, Eicosapentaenoic acid, Astaxanthin.

References:

- [1] C. Marquez, M. I. Lopez, I. Ruisanchez and M. P. Callao, "FT-Raman and NIR spectroscopy data fusion strategy for multivariate qualitative analysis of food fraud", *Talanta*, 161, 80-86 (2016).