Determining fish oil quality by means of ^{1}H NMR, FT-MIR, and FT-NIR spectroscopy in combination with *Artificial Neural Networks*

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Fish oil is becoming increasingly popular as a dietary supplement as well as for use in animal feed, both being mainly because of the high contents of the health promoting omega-3 fatty acids. However, these polyunsaturated fatty acids are susceptible to oxidation, which can cause a decrease in oil quality.

This study investigated the potential of ^{1}H NMR, FT-MIR, and FT-NIR spectroscopy in the quality assessment of fish oils. 84 different oils, of which 22 were subjected to accelerated storage with varying temperature and light exposure, were analyzed by standard wet-chemical methods with regard to peroxide value (PV), anisidine value (AnV), and acid value (AV) as well as by ^{1}H NMR, FT-MIR, and FT-NIR spectroscopy. Subsequently, models were developed using *Artificial Neural Networks* (ANN) and *Partial Least Squares Regression* (PLSR) in order to predict the aforementioned oil quality parameters based on the spectroscopic data. The best ANN model for the PV was obtained from the NMR data, with a predictive coefficient of determination (Q^2) of 0.961 and a *Root Mean Square Error of Prediction* (RMSEP) of 1.5 meq O_2 kg^{-1}. The combined MIR/NIR data provided the most reliable ANN model for the AnV (Q^2 = 0.993; RMSEP = 0.74). For the AV, the ANN models based on the MIR and the combined MIR/NIR data yielded a Q^2 of 0.988 and 0.983 and an RMSEP of 0.43 and 0.52 mg NaOH g^{-1}, respectively. In most cases, the performance of the ANN models was superior to the respective PLSR models. Variable selection and data dimensionality reduction turned out to improve the prediction accuracy of the ANN models in some cases. ^{1}H NMR, FT-MIR, and FT-NIR spectroscopy can be regarded as very promising tools in the analysis of animal and vegetable oil quality because they can save producing companies/laboratories a considerable amount of time, costs, and chemicals, compared to traditional wet-chemical methods.