



46th WEFTA
Split, Croatia /12-14 Oct 2016



Determination of fish oil quality by ¹H NMR, FTIR and FT-NIR spectroscopy in combination with artificial neural networks

Editha Giese¹, Ole Winkelmann², Sascha Rohn³, Jan Fritsche^{1,4*}

¹Hamburg University of Applied Sciences, Faculty Life Sciences, Ulmenliet 20, 21033 Hamburg

²Eurofins Analytik GmbH, Neuländer Kamp 1, 21079 Hamburg

³University of Hamburg, Hamburg School of Food Science, Grindelallee 117, 20146 Hamburg

⁴Max Rubner-Institut, Federal Research Institute of Nutrition and Food, Department of Safety and Quality of Milk and Fish Products, Hermann-Weigmann-Strasse 1, 24103 Kiel,
*jan.fritsche@mri.bund.de

Fish oil based dietary supplements have become increasingly popular, which is mainly due to their high content of the health promoting omega-3 fatty acids. However, these polyunsaturated fatty acids are extremely prone to oxidation. Traditional methods to determine fat quality parameters such as peroxide value (PV), anisidine value (AnV) and acid value (AV) are time-consuming, labor- and solvent-intensive and require high amounts of sample. Therefore, the aim of this study was to develop and validate models for the prediction of PV, AnV and AV in fish oil based on ¹H NMR, FTIR and FT-NIR spectra using artificial neural networks (ANN). For this purpose, 84 different fish oils were analyzed by the classical wet chemistry methods as well as by the afore-mentioned spectroscopy techniques. Some of the fish oils were submitted to storage trials with varying temperature and light exposure in order to increase the range of calibration. Before the prediction models were built using ANN, various methods of spectral preprocessing, variable selection and data dimensionality reduction were applied.

NMR, IR and NIR spectroscopy provide the advantages of being non-destructive, fast and less labor-intensive than traditional wet chemistry methods. They do not require the use of toxic chemicals and produce no or very little waste. Moreover, further quality parameters can be obtained from the same spectra.