## 03-03: In-capsule quantitation of EPA and DHA by handheld Raman spectroscopy: fish oils to algal oils

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Eicosapentaenoic acid (EPA) and docosahexaenoic acid (DHA) are commercially important long chain, *ω*-3 polyunsaturated fatty acids. Synthesis of these compounds occurs in marine algae, followed by upwards transfer through marine food webs and bioaccumulation in fish. The high degree of unsaturation of these compounds makes them prone to oxidation, making oil analysis challenging. Producing accurate and precise data requires careful control of factors that can cause oxidation, e.g. air, UV light and metal ions. Some investigations may have incorrectly reported high levels of oxidation in marine oils, with evidence suggesting that these oils were inadvertently oxidised at the time of analysis [1].

Commercial *ω*-3 oils are usually sold in single dose gelatin (softgel™) capsules, which protect them from exposure to air. An ideal analytical method would be capable of assessing the quality of these products without removing them from their capsules, eliminating the possibility of causing oxidation during analysis. We have successfully applied Raman spectroscopy to this task. Spectra generated using a benchtop FT-Raman spectrometer (1064 nm) were used to produce partial least squares regression (PLSR) models with root mean square errors of cross validation of 1.9% for EPA (range: 14.2–45.4%) and 1.3% for DHA (Range: 8.9–32.7%) [2].

In this presentation I will describe results of our most recent work, where we compare the performance of quantitative models generated from benchtop Raman spectra to those generated from handheld Raman spectra. This approach could be suitable for "point-of-sale" quality assurance of encapsulated commercial *ω*-3 supplements.

**References**

[1] BANNENBERG, G., 2017: Scientific Reports, **7**, 1488.

[2] KILLEEN, D., 2017: Journal of Agricultural and Food Chemistry, **65**, 3551.