Exploring the potential of VIS-NIR spectroscopy to predict sensory properties of foods

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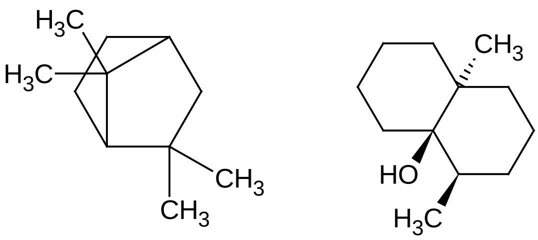
Sensory analysis of food involves the measurement, interpretation and understanding of human responses to the properties of food perceived by the senses such as sight, smell, and taste (Cozzolino et al. 2005). It is important to have a quantitative means for assessing sensory properties in a reasonable way, to enable the food industry to rapidly respond to the changing demands of both consumers and the market. Aroma and flavour are among the most important properties for the consumer and numerous studies have been performed in attempts to find correlations between sensory qualities and objective instrumental measurements. Rapid, non-destructive instrumental methods such as near infrared spectroscopy (NIR) might be advantageous to predict quality of food and agricultural products due to the speed of analysis, minimum sample preparation and low cost. The advantages of such technologies are not only to assess chemical structures but also to build a spectrum, characteristic of the sample, which behaves as a "finger print".

At the Department of Primary Industries and Fisheries, Queensland, recent research efforts have involved the inclusion of VIS-NIR spectroscopy in broader sensory trials to explore the potential of this spectroscopic technique to predict sensory properties of foods. This work has been conducted through ongoing collaboration with Dr. Daniel Cozzolino of the Australian Wine Research Institute, South Australia. Examples of recent trials conducted in Brisbane include exploring the ability of VIS-NIR spectroscopy to predict trained sensory panel scores for 'muddiness' in barramundi and 'toughness' in saddletail snapper. In the future, sensory and NIR investigations will be extended to horticultural products in support of breeding programs.

Barramundi trial

Barramundi (*Lates calcarifer*) is an Australian fish that is popular among consumers due to its deliciously strong, gamey and distinctive flavour. Not surprisingly, barramundi farming and wild capture of barramundi are profitable industries in Australia. A problem that the barramundi industry faces is the occurrence of a muddy taint, which can occur in both farm and wild environments, that can give barramundi an unfortunate reputation among consumers.

The compounds responsible for the taint in the fish flesh are geosmin and 2-methylisoborneol (Figure 1), which are metabolites of certain algae and bacteria (Tucker 2000). These compounds are present naturally in water at very low concentrations. Under certain environmental conditions they can build up in the water and cause high levels to accumulate in the fish flesh, which translates to a muddy or earthy aroma and flavour. It has been reported that these compounds cause consumer rejection in fish flesh at the parts per billion range (Persson 1980).



geosmin 2-methylisoborneol

Figure 1. Compounds responsible for muddy taint in barramundi

Measuring geosmin and 2-methylisoborneol in water is relatively straightforward; however, measuring these compounds in fish flesh is extremely difficult due to the high fat levels in fish flesh in which the compounds are bound. This makes extraction for chemical analysis complicated and time consuming which is not suitable for quality control purposes. Routine sensory evaluation of fillets for quality control is also not feasible due to sensory adaptation, increased sensory fatigue and flavour carry-over between samples that is associated with tasting muddy-tainted fish (Johnsen and Bett 1996).

NIR spectroscopy is used widely in many industries for quality control as it offers rapid, non-destructive and in-line measurement of product compositional parameters that relate to product quality. The objective of this preliminary study was to investigate the potential of NIR to predict sensory perception of muddy taint in farmed barramundi for future use in quality control.

Barramundi samples used in this study were from a larger project conducted in collaboration with the Australian Veterinary Association and Lake Argyle Industries. Fish samples from Lake Argyle, Western Australia, which were known to exhibit a broad range of the muddy taint, were sent to the DPI&F, Innovative Food Technologies, in Brisbane for sensory evaluation from March to June 2005. A total of 74 fish samples were assessed using a panel of ten trained tasters using descriptive analysis techniques. Through vocabulary development, the panel selected a number of sensory attributes for aroma, flavour and aftertaste which were used to score the cooked barramundi samples on structured linear scales from 0 – 100, anchored from none to high.

The raw samples, often the second fillet of the same fish used for sensory evaluation, were scanned, in triplicate, in reflectance mode by VIS-NIR 400 – 2500 nm (FossNIRSystems 6500) using a rectangular cell. To reduce the mess of scanning raw fillets, the samples were placed in a HDPE plastic bag prior to scanning. The second derivative of the VIS-NIR spectra is shown in Figure 2. Spectral features include water peaks (950, 1400, 1900 nm), CH stretch overtones due to lipids (1200, 1730, 1750 nm), CH combination tones from lipids and fatty acids (2200 – 2400 nm).

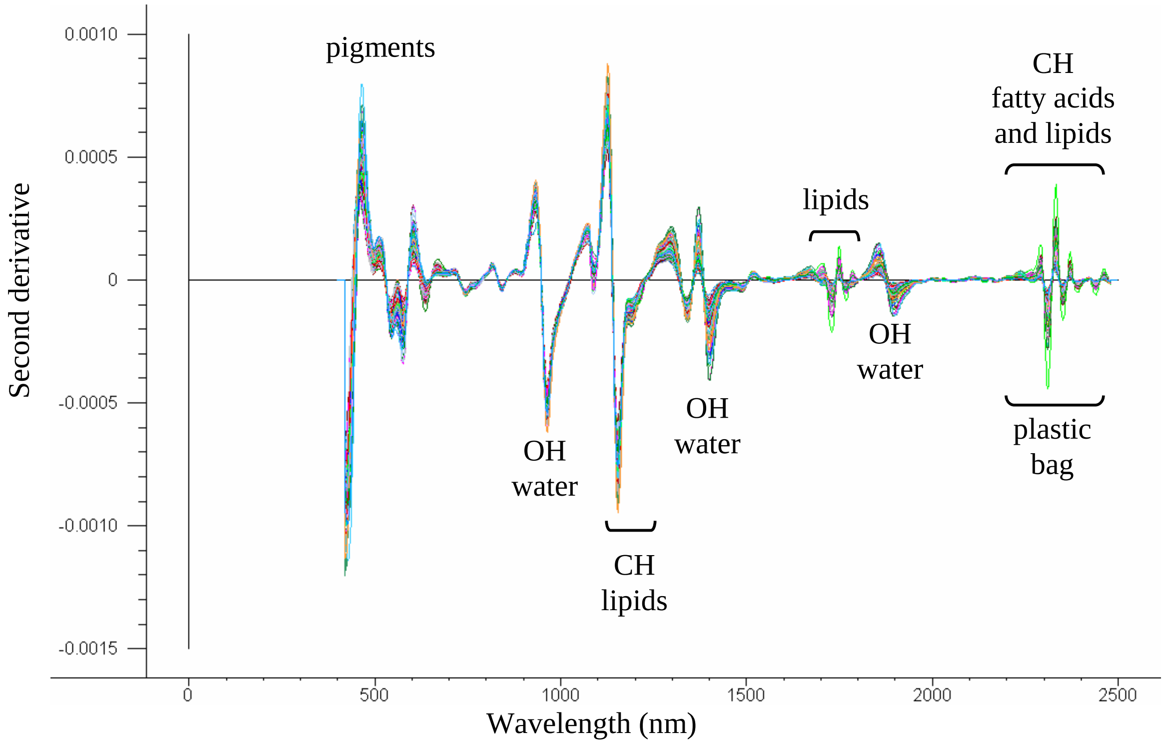


Figure 2. Second derivative VIS-NIR spectra of barramundi fillets (n = 222)

The data from sensory and VIS-NIR analysis were combined in The Unscrambler (version 7.8, CAMO ASA, Oslo, Norway) for analysis. Partial least squares (PLS1) regression was used to develop predictive equations for the scores of sensory attributes *muddy/earthy aroma*, *muddy / earthy flavour*, *fresh flavour* and *muddy aftertaste*, using the second derivative of the VIS-NIR spectra.

The results from the predictive models developed using full cross validation, and limited to 10 components, are shown in Table 1. The models were evaluated by comparing the coefficient of correlation (R_{cal}) and the root mean square standard error in cross validation ($RMSECV_{cal}$) in calibration.

Table 1. Results of prediction models for sensory properties using VIS-NIR

	2D VIS-NIR region	n	R_{cal}	$RMSECV_{cal}$	C_{opt}
muddy / earthy aroma	400-2500	222	0.54	3.2	10
fresh flavour	400-2500	222	0.73	4.7	10
muddy / earthy flavour	400-2500	222	0.73	5.0	10
muddy aftertaste	400-2500	222	0.60	3.7	10

The results show that VIS-NIR shows good potential to predict *muddy / earthy flavour* and *fresh flavour* in barramundi with reasonable correlation coefficients (R_{cal} 0.73) and relatively low standard error ($RMSECV_{cal}$ 4.7 - 5.0). The results from these predictions are quite promising given the limited number of samples and the subjective nature of the sensory scores.

According to the loadings on the VIS-NIR data, it was clear that the regressions did not rely on one or two specific regions of particular importance. This indicates that the VIS-NIR is not simply picking up on the unique vibrations in the bonds of geosmin and 2-methylisoborneol responsible for the muddy taint. Rather, the regressions use a combination of information from across the entire spectrum to build the best predictive model for these sensory properties. We have observed this phenomenon in previous studies and similar results have been reported by other authors for the prediction of sensory and organoleptic properties of foods and beverages using NIR spectra (Cozzolino et al. 2005).

Further work must be conducted to further investigate these preliminary findings before this technique can be developed for use in the barramundi industry. In particular, a broader range of samples from across Australia and from a number of seasons must be evaluated, and the predictions tested using an external validation set of samples. Should this rapid assessment technique be developed further it could provide a far cheaper option to the difficult and expensive chemical analysis of geosmin and 2-methylisoborneol in fish flesh, and time consuming and problematic sensory analysis. This technique could potentially be used by the industry to improve the quality of their product and to rectify the unfortunate reputation of muddy barramundi among consumers.

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