

# The Determination of Essential Oils in Sandalwood via FT-NIR Spectroscopy

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## Introduction

Sandalwood oil is widely used in the medicinal, cosmetic and aromatherapy industries. The oil is distilled from the heartwood of the sandalwood tree *Santalum* - a genus of hemi-parasitic tree species occurring throughout South and Southeast Asia, Australia and the Pacific. With international concern on the sustainability of sandalwood oil (Fox, 2000), the quality of oil entering the market is being compromised either through extraction from underdeveloped heartwoods or through adulteration with lower grade sandalwood oils or synthetic substitutes (Howes et al. 2004). Although no standard method exists to assess the quality of sandalwood oil, the International Organisation for Standardisation recommends GCMS analysis of santalol oil content. NIR spectroscopy has had a demonstrated success for other essential oils (Schulz et al. 2004, Steur et al. 2001). In addition, NIR spectroscopy has also been applied as both a qualitative and quantitative analytical tool in the forestry industry (Steur et al. 2001). This project aimed to assess the ability of NIR spectroscopy as a non-invasive, rapid and cheap analytical alternative to GCMS for Santalol determination.

## Materials and Method

- The sample set of sandalwood cores was collected from various Vanuatu and Cape York collection sites.
- Samples were presented in different formats including:

a) chipped

b) milled



Samples were scanned using FT-NIR spectrophotometers (MPA FT-NIR spectrometer and Matrix-F, Bruker Optics, Ettlingen, Germany) in the range 12800–4000  $\text{cm}^{-1}$  (780 – 2500 nm), averaging 32 scans per spectrum at 8  $\text{cm}^{-1}$  resolution to assess the sandalwood samples for %Santalol.

- Scanning was conducted in reflectance mode comparing the MPA integrated sphere and solids probe against the Matrix-F with a fibre-coupled measurement head operating 2 tungsten halogen 12V, 20W light sources.
- Reference method: GCMS

## Calibration Techniques

In this analysis four regressors used are (i) Partial Least Squares (PLS), (ii) Multivariate Linear Regression (MLR) and (iii) K-Nearest neighbour (KNN) and (iv) Hybrid combination.

- KNN is a non-parametric method which simply averages the response of the K nearest data points (K = 3 Euclidean norm).
- The Hybrid regressor delegates the prediction task to as many independent regressors as possible and then combines their results as a weighted average.
- Chemometric package used - FIDO (Pyramid Intelligent Applications Pty Ltd).

## Preliminary Results

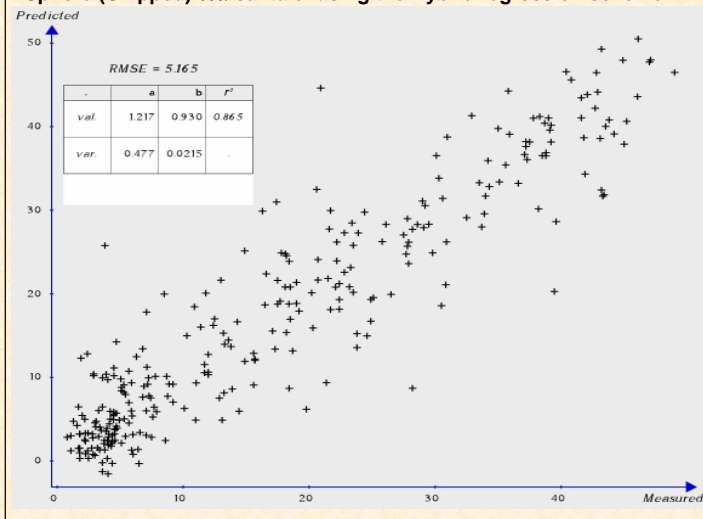
Table 1. Prediction results for % $\alpha$ -santalol and % $\beta$ -santalol

	MPA Integrating sphere (chipped) (n=295)		MPA Solids Probe (chipped) (n=294)		MPA Integrating sphere (Milled) (n=226)		Matrix-F (Milled) (n=227)	
	R <sup>2</sup>	RMSE	R <sup>2</sup>	RMSE	R <sup>2</sup>	RMSE	R <sup>2</sup>	RMSE
<b><math>\alpha</math>-santalol</b>								
PLS	0.83	5.6	0.81	6.0	0.80	6.2	0.81	6.0
MLR	0.83	5.6	0.80	6.2	0.81	6.1	0.82	5.9
KNN	0.82	5.9	0.82	5.8	0.82	5.9	0.87	4.9
Hybrid	<b>0.87</b>	5.1	<b>0.84</b>	5.6	<b>0.84</b>	5.6	<b>0.88</b>	4.8
<b><math>\beta</math>-santalol</b>								
PLS	0.75	3.0	0.72	3.2	0.68	2.9	0.69	2.8
MLR	0.72	3.2	0.68	3.5	0.63	3.1	0.65	2.9
KNN	0.71	3.3	0.76	3.0	0.70	2.8	0.71	2.7
Hybrid	<b>0.78</b>	2.9	<b>0.78</b>	2.9	<b>0.73</b>	2.7	<b>0.72</b>	2.7

Note: Spectra were normalized and no outliers were removed in preliminary results.

- The milled samples performed slightly worse but this could be attributed to having about 25% less samples.
- In all cases the best result was obtained by the Hybrid technique combining several different regressors.

Figure 1. Predicted versus measured results for MPA Integrating Sphere (Chipped) % $\alpha$ -santalol using the Hybrid regression scheme



## Conclusion

- NIRS shows potential to be used as a tool to assess oil (% $\alpha$  - &  $\beta$ -santalol) content in both chipped and milled sandalwood samples.
- No significant differences in the prediction accuracies resulted from sample preparation methods.

## References

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