

**FOURIER TRANSFORM INFRARED- ATTENUATED TOTAL
REFLECTANCE SPECTROSCOPY IN CONJUNCTION WITH
PRINCIPAL COMPONENT ANALYSIS AND AGGLOMERATIVE
HIERARCHICAL CLUSTERING TO CLASSIFY VIRGIN
COCONUT OIL AND OTHER EDIBLE OILS**

**An Undergraduate Thesis
Presented to the
Division of Physical Sciences and Mathematics
College of Arts and Sciences
University of the Philippines in the Visayas
Miag-ao, Iloilo**

**In Partial Fulfillment
of the Requirements for the Degree of
Bachelor of Science in Chemistry**

**EUGENE JAMIS ALOBA
April 2006**

ABSTRACT

This work investigates the potential of Fourier Transform Infrared-Attenuated Total Reflectance (FTIR-ATR) Spectroscopy in conjunction with Principal Component Analysis (PCA) and Agglomerative Hierarchical Clustering (AHC) to classify virgin coconut oil (VCO) from other different edible oils in the test set. Among the PCA types, Pearson produced the best biplot graphs that showed both the separation of VCO and coconut oil (only in one group) from other oils, and the separation of VCO and coconut oil (CCO) into two distinct groups using the fingerprint region of the spectra. Kendall dissimilarity/Ward's method successfully clustered VCO and CCO as separate classes using the same region of the spectra. These results showed that the highest percent variability in the spectra of different oils occurs in the fingerprint region, and hence where spectroscopic classification of oils can be performed best.