International Conference on
Contemporary Issues in Integrating Health and Nutrition with the
Emerging Areas of Food Technology, Agriculture,
Environment and Allied Sciences

ATR-FTIR Spectroscopy along with Multivariate Chemometrics for the Classification and Detection of Palm Oil Adulteration in Extra Virgin Olive Oil

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Abstract—*A methodology based on Attenuated total reflectance-Fourier transform infrared (ATR-FTIR) spectroscopy along with multivariate chemometrics has been developed for the classification and detection of palm oil (PO) adulteration in extra virgin olive oil (EVOO) in fraction of 1 to 30% v/v PO in steps of 5% v/v. Firstly, Principal component analysis (PCA), which was applied on two selected fingerprint regions (550-1800 cm^{-1} and 2800-3010 cm^{-1}) for 6 different oils including EVOO and PO, to check the relatedness between these two oils in the study. After that, PCA was again applied on different adulterants of PO in EVOO, which clearly discriminated between different PO adulterants with EVOO. Later, linear discriminant analysis (LDA) was used on 14 characteristic wavenumbers for the classification of PO adulterants from VCO. LDA classified 100% of the initial groups accurately and 91.7% correctly when cross-validated. For quantification, PCR and PLS-R multivariate regression models were developed to detect the presence of PO in EVOO using spectral regions (550-1800 cm^{-1} and 2800-3010 cm^{-1}) of normal, first and second derivatives separately and cross-validated by "leave one out" method. Out of all three spectra (normal, 1^{st} and 2^{nd} derivatives), PLS-R model for 1^{st} derivative spectra showed best calibration model as compare to PCR and PLS-R models of normal and 2^{nd} derivative, in terms of high R^2 (0.998), low RMSEC (0.419) and RMSEP (0.456). The lowest detected concentration of PO in EVOO was the lowest adulteration level studied, 1%V/V.*

ISBN: 978-93-85822-87-2
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