Determination of sodium fatty acid in soap Formulation Using Fourier Transform Infrared (FTIR) spectroscopy and multivariate calibrations.

ABSTRACT

Fourier Transform Infrared (FTIR) spectroscopy using an attenuated total reflectance (ATR) accessory has been investigated as a method for the determination of sodium-fatty acid (sodium-FA) in soap formulations. Multivariate calibrations namely partial least squares regression (PLS) and principle component regression (PCR) were developed for the prediction of sodium-FA using spectral ranges on the basis of relevant IR absorption bands related to sodium-FA. The sodium-FA content in soap formulations was predicted accurately at wavenumbers of 1,570–1,550 cm−1, which is specific for RCOO− Na+ vibration. The PLS method was found to be a consistently better predictor when both PLS and principal component regression (PCR) analyses were used for quantification of sodium-FA. Furthermore, FTIR spectroscopy can be an alternative technique to American oil Chemist Society methods which use a titrimetric technique because FTIR offers rapid, easy sample preparation and is friendly to the environment.

Keyword: FTIR spectroscopy; Partial least squares regression; Principle component regression; Soap formulation; Sodium-fatty acid.