

## APPLICATION STUDY OF CHEMOINFOMETRICAL NEAR-INFRARED SPECTROSCOPY IN PHARMACEUTICAL INDUSTRY

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A chemoinfometrical method for evaluating the quantitative determination of crystallinity one polymorphs based on fourie-transformed near-infrared (FT-NIR) spectroscopy was established. A direct comparison of the data with the ones collected from using the the and compared with the conventional powder X-ray diffraction method was performed.

[Method] The pPure a and g forms of indomethacin (IMC) were prepared by reported using published methods. Six kinds of standard samples obtained by physically mixing of a and g forms.

After the powder X-ray diffraction profiles of samples have been measured, the intensity values were normalized to against the intensity of silicon powder as the as an external standard. The calibration curves for quantification of crystal content were based upon the total relative intensity of four diffraction peaks from of the form g crystal. FT-NIR spectra of six calibration sample sets were recorded 5 times with the NIR spectrometer (BRAN+LUEBBE).

Chemoinfometric analysis was performed on the NIR spectral data sets by applying the principal component regression (PCR).

[Results] The relation between the actual and predicted polymorphic contents of form g IMC measured using by the X-ray diffraction method shows a good straight linea linear relation., and It has slope of 0.023, an intercept of 0.131 and a correlation coefficient of 0.986.

PCR analyses wereis was performed based on normalized NIR spectra sets offor standard samples of known content of IMC g form. IMC. A calibration equation was determined to minimize the root mean square error of the predictionthe prediction. Figure 1 shows a plot of the calibration data obtained by NIR method between the actual and predicted contents of form g IMC. The predicted values were reproducible and had a smaller standard deviation. Figure 2 shows that the plot for the predicted transformation rate (%) of form a IMC to form g as measured by X-ray diffractometry against to those as measured by NIR method. The plot has a slope of 1.296, an intercept of 1.109, and a correlation coefficient of 0.992. The line represents a satisfactory correlation between the two predicted values of form g IMC content. Thus NIR spectroscopy is an effective method for the evaluation to the pharmaceutical products of quantitative of polymorph.