# Enhancing prediction power of chemometric models through manipulation of the fed spectrophotometric data: A comparative study

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**Abstract**

Effect of data manipulation in preprocessing step proceeding construction of chemometric models was assessed. The same set of UV spectral data was used for construction of PLS and PCR models directly and after mathematically manipulation as per well known first and second derivatives of the absorption spectra, ratio spectra and first and second derivatives of the ratio spectra spectrophotometric methods, meanwhile the optimal working wavelength ranges were carefully selected for each model and the models were constructed. Unexpectedly, number of latent variables used for models' construction varied among the different methods. The prediction power of the different models was compared using a validation set of 8 mixtures prepared as per the multilevel multifactor design and results were statistically compared using two-way ANOVA test. Root mean squares error of prediction (RMSEP) was used for further comparison of the predictability among different constructed models. Although no significant difference was found between results obtained using Partial Least Squares (PLS) and Principal Component Regression (PCR) models, however, discrepancies among results was found to be attributed to the variation in the discrimination power of adopted spectrophotometric methods on spectral data.

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