



## Quantitative Determination of Sulphamethoxazole and Trimethoprim in Powder Mixtures Using Raman Spectroscopy and PLS

Fabiana E.B. da SILVA <sup>1\*</sup>, Cristiane ZIECH <sup>1</sup>, Yara P. DIAS <sup>2</sup>,  
Eduardo C. MOREIRA <sup>2</sup>, Érico M.M. FLORES <sup>3</sup> & Marco F. FERRÃO <sup>4</sup>

<sup>1</sup> *School of Pharmacy and* <sup>2</sup> *School of Physics, Federal University of Pampa, UNIPAMPA, Rio Grande do Sul, Brazil.*

<sup>3</sup> *Chemistry Department, Federal University of Santa Maria – UFSM, Rio Grande do Sul, Brazil*

<sup>4</sup> *Chemistry Department, Federal University of Rio Grande do Sul - UFRGS, Rio Grande do Sul, Brazil*

**SUMMARY.** Raman spectroscopy in combination with partial least-squares (PLS) regression method was developed for sulphamethoxazole (SMZ) and trimethoprim (TMP) simultaneous determination in powder mixtures. The calibration set was designed with 18 samples and validation set with 9 samples, containing different SMZ and TMP concentrations. The concentration ranges were 400–900 mg/g for SMZ and 80–240 mg/g for TMP. The proposed procedure was validated by comparison with the official method (HPLC). Mean root square error of calibration (RMSEC) and mean root square error of prediction (RMSEP) were calculated. RMSEC found was 30.96 mg/g to SMZ and 14.36 mg/g to TMP, respectively. RMSEP found was 25.60 mg/g to SMZ and 14.36 mg/g to TMP, respectively. Correlation coefficient (R<sup>2</sup>) was 0.99 for SMZ and 0.99 for TMP. This parameter evidences a very good agreement between estimated and real values. The results showed that PLS regression model combined with Raman spectroscopy provides a sensitive, fast and simple method for the quantitative analysis of SMZ and TMP mixtures in powder quality control.

**KEY WORDS:** Raman spectroscopy, Multivariate calibration, Partial least squares regression, Sulphamethoxazole, Trimethoprim.

\* Author to whom correspondence should be addressed. *E-mail:* fabianasilva@unipampa.edu.br