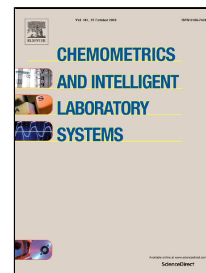


Accepted Manuscript

The common quantitative model for the determination of multiple near infrared spectrometers

Jin Jin Liu, Bao Qiong Li, Hong Lin Zhai, Shao Hua Lu, Sha Sha Li



PII: S0169-7439(18)30231-4

DOI: 10.1016/j.chemolab.2018.09.008

Reference: CHEMOM 3684

To appear in: *Chemometrics and Intelligent Laboratory Systems*

Received Date: 14 April 2018

Accepted Date: 20 September 2018

Please cite this article as: Jin Jin Liu, Bao Qiong Li, Hong Lin Zhai, Shao Hua Lu, Sha Sha Li, The common quantitative model for the determination of multiple near infrared spectrometers, *Chemometrics and Intelligent Laboratory Systems* (2018), doi: 10.1016/j.chemolab.2018.09.008

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

1 **The common quantitative model for the determination of multiple near infrared**
2 **spectrometers**

3 Jin Jin Liu, Bao Qiong Li, Hong Lin Zhai*, Shao Hua Lu, Sha Sha Li

4 *College of Chemistry & Chemical Engineering, Lanzhou University, Lanzhou, 730000, PR China*

5 **Abstract**

6 Calibration model transfer is a practical application. In this contribution, we proposed the
7 common model instead of model transfers to avoid the complex corrections for the obtained
8 calibration model. The important chemical features of target components are extracted by
9 Tchebichef image moment method based on the near infrared (NIR) three-dimensional spectra
10 constructed from the determination of different spectrometers. Then the common models are
11 established with stepwise regression and used to the determination of single spectrometer. The
12 proposed approach was applied to the quantitative analysis of target components in mixtures using
13 two datasets including the pharmaceutical samples (measured on two NIR spectrometers with the
14 same type) and corn samples (measured on three NIR spectrometers with the different types), and
15 the satisfactory results were obtained. Furthermore, multi-way partial least squares method was
16 carried out and compared with the proposed approach. This study indicates that our approach is
17 effective, accurate and reliable, and the common quantitative models can reveal the chemical
18 feature information of target components in samples measured on whether the same or different
19 types spectrometers, which provides a convenience for the application of NIR spectroscopy.

20 **Keywords:** Near infrared spectroscopy; Common quantitative model; Multiple spectrometers;

* Correspondence to: Tel.: +86 931 8912596; fax: +86 931 8912582; E-mail address: zhahl@163.com (H.L. Zhai).

Download English Version:

<https://daneshyari.com/en/article/11031271>

Download Persian Version:

<https://daneshyari.com/article/11031271>

[Daneshyari.com](https://daneshyari.com)