Author's Accepted Manuscript

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www.elsevier.com/locate/talanta

PII: S0039-9140(17)30465-4

DOI: http://dx.doi.org/10.1016/j.talanta.2017.04.039

Reference: TAL17492

To appear in: *Talanta*

Received date: 3 March 2017 Revised date: 14 April 2017 Accepted date: 16 April 2017

Cite this article as: Vitaly Panchuk, Dmitry Kirsanov, Ekaterina Oleneva Valentin Semenov and Andrey Legin, Calibration transfer between different analytical methods, *Talanta*, http://dx.doi.org/10.1016/j.talanta.2017.04.039

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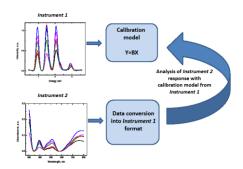
Calibration transfer between different analytical methods

Vitaly Panchuk^{a,b}, Dmitry Kirsanov^{a,b,*}, Ekaterina Oleneva^{a,c}, Valentin Semenov^a, Andrey Legin^{a,b}

Abstract

The procedure for transfer of calibration models between different analytical methods is suggested. It is based on the direct standardization (DS) algorithm earlier suggested for data conversion between physically different instruments of the same type. As a result, multivariate regression models obtained e.g. for NIR spectroscopic measurements in one wavelength range can be successfully applied for predictions from the data obtained with another NIR spectrometer in another wavelength range. The performance of the suggested method was tested with two simulated and two real datasets. In the latter case calibration models constructed for energy-dispersive X-ray fluorescence, UV-Vis spectrometry and NIR spectrometry were addressed. The observed performance of the method implies that it can have a broad range of possible applications in analytical chemistry; some of them are suggested in the paper.

Graphical abstract



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