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SYMPOSIUM

Selectivity Assessment of Noninvasive Glucose Measurements Based on Analysis of Multivariate Calibration Vectors

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Abstract

Background:
Selectivity is paramount for the successful implementation of noninvasive spectroscopic sensing for the painless measurement of blood glucose concentrations in people with diabetes. Selectivity issues are explored for different multivariate calibration models based on noninvasive near-infrared spectra collected from an animal model.

Methods:
Noninvasive near-infrared spectra are collected through a fiber-optic interface attached to a thin fold of skin on the back of an anesthetized laboratory rat while glucose levels are varied in a controlled manner.

Results and Discussion:
Partial least-squares (PLS) calibration models are generated from noninvasive spectra collected during a single, 2-hour blood glucose transient. Calibration vectors are compared for optimized PLS calibration models created with correct and incorrect assignments of glucose concentrations to each noninvasive spectrum. Although both PLS models appear functional and seem capable of predicting glucose concentrations accurately during this transient, only the model generated from correct glucose assignments gives a credible calibration vector. When correct glucose assignments are used, the PLS calibration vector matches the corresponding net analyte signal calibration vector. No similarity in these calibration vectors is evident when incorrect glucose assignments are used.

Conclusions:
Glucose-specific spectral information is present within noninvasive near-infrared spectra collected from a rat model using a transmission geometry. Apparently functional, yet incorrect, calibration models can be generated, and the propensity to create such false PLS calibration models calls into question the validity of past reports. An analysis of calibration vectors can provide valuable insight into the chemical basis of selectivity for multivariate calibration models of complex systems.

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Abbreviations: (AU) absorbance units; (DCCT) Diabetes Control and Complications Trial ; (NAS) net analyte signal; (PLS) partial least squares; (RMS) root mean square; (SECV) standard error of cross validation; (SEP) standard error of prediction

Keywords: calibration vector analysis, Clarke error grid analysis, multivariate statistics, near-infrared spectroscopy, net analyte signal, noninvasive glucose sensing

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