

Title (en)
AUTOMATED SYSTEM AND METHOD FOR SPECTROSCOPIC ANALYSIS

Title (de)
AUTOMATISIERTES SYSTEM UND VERFAHREN ZUR SPEKTROSKOPISCHEN ANALYSE

Title (fr)
SYSTEME ET PROCEDE AUTOMATISES POUR ANALYSE SPECTROSCOPIQUE

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Abstract (en)
[origin: WO0214812A1] An automated method for modeling spectral data includes accessing a set of spectral data, corresponding to each of a plurality of samples, each set having associated therewith at least one independently measured constituent value (201). Data transforms are applied to the set of spectral data to generate, for each sample, a set of transformed and untransformed spectral data, which with its associated constituent values, is divided into a calibration sub-set (231) and a validation sub-set (232). One or more of a partial least squares, principal component regression, neural net, or a multiple linear regression analysis is applied to the calibration data sub-sets to obtain corresponding modeling equations for predicting the target substance amount in a sample. The modeling equation with the best correlation between the spectral data in the validation sub-set and the corresponding constituent values in the validation sub-set is identified, preferably as a function of the SEE and SEP.

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