Evaluation of the efficiency of continuous wavelet transform as processing and preprocessing algorithm for resolution of overlapped signals in univariate and multivariate regression analyses; an application to ternary and quaternary mixtures

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Abstract

Wavelets have been adapted for a vast number of signal-processing applications due to the amount of information
that can be extracted froma signal. In thiswork, a comparative study on the efficiency of continuouswavelet
transform (CWT) as a signal processing tool in univariate regression and a pre-processing tool in multivariate
analysis using partial least square (CWT-PLS) was conducted. These were applied to complex spectral signals
of ternary and quaternary mixtures.CWT-PLS method succeeded in the simultaneous determination of a quaternary
mixture of drotaverine (DRO), caffeine (CAF), paracetamol (PAR) and p-aminophenol (PAP, the major impurity
of paracetamol). While, the univariate CWT failed to simultaneously determine the quaternary mixture
components and was able to determine only PAR and PAP, the ternary mixtures of DRO, CAF, and PAR and
CAF, PAR, and PAP. During the calculations of CWT, different wavelet families were tested. The univariate CWT
method was validated according to the ICH guidelines. While for the development of the CWT-PLS model a calibration
set was prepared by means of an orthogonal experimental design and their absorption spectra were recorded
and processed by CWT. The CWT-PLS model was constructed by regression between the wavelet
coefficients and concentration matrices and validation was performed by both cross validation and external validation
sets. Both methods were successfully applied for determination of the studied drugs in pharmaceutical
formulations.

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