

Summary

The authenticity of different products depends strongly on their chemical composition. Therefore, instrumental signals (also called chemical fingerprints) that uniquely characterize samples can be useful to assess authenticity. Among many instrumental techniques chromatographic methods are well suited for fingerprinting purposes since they offer the possibility of separation, identification and quantification of individual mixture components.

The use of chromatographic fingerprints and their chemometric modeling allowed to propose new approaches for authenticity verification of selected products (diesel oil, Viagra®) and for the evaluation of tributyltin presence in environmental water samples. The initial data were preprocessed to improve quality of instrumental signals. Then, the partial least squares discriminant analysis (PLS-DA) was used to construct diagnostic models helping to assign tested samples to considered groups based on their chromatographic fingerprints. Each model was characterized by parameters describing its performance. Furthermore, a new procedure for the construction and validation of diagnostic models was proposed. The procedure allows to estimate selected validation parameters of the diagnostic model for different number of factors using a model set and test sets (internal and external) and takes into account the possibility of variable selection. Therefore, the PLS-DA model is constructed based on fragments of chromatographic signals that are important to distinguish groups of samples. A high performance of constructed diagnostic models, constructed for authenticity verification of selected products or assessment of the biological risk (resulting from the presence of harmful substances in environmental samples), allows to conclude that they can be successfully implemented in similar research problems.