FLUORESCENCE DETERMINATION OF POLYCHLORINATED DIBENZOFURANS WITH A MULTILAYER ARTIFICIAL NEURAL NETWORK.

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Abstract

Polichlorinated dibenzofurands (PCDFs) are considered one of the most hazardous pollutants of the environment. Many studies indicate that the PCDFs in the environment are produced mainly by chemical industry residues of chlorinated compounds, such chlorophenols and their derivatives and polychlorinated biphenyls, as well as incomplete combustion processes. Because of this their identification and quantification is a matter of great concern.

Fluorescence spectrometry has proved to be a sensitive technique for the determination of these compounds. However, the similar structure of PCDFs can produce overlapping in fluorescence spectra, which leads to a limited selectivity.

We propose an alternative and complementary method to face this kind of limitations, the *neural computation methods*. This computational approach is the most suitable for the specific tasks of Fluorescence Spectrometry, essentially analysing complex data, which can involve no explicit knowledge of the problem, non linear processes, overlapping information and noise.

In this paper we present a smart and flexible solution to face the determination of PCDFs, a hierarchical modular artificial neural network, which consist of a set of neural layers working with independent unsupervised learning. This neural architecture has been used with optimal results in luminescence spectrometry and neuroscience fields. The proposed artificial neural network has a structure of pre-processing and processing stage. The most novel contribution of our paper is the pre-processing stage, which performs a feature extraction task providing a compact representation of the input information (spectral data). The feature extraction is based on non-linear model of emission fluorescence spectrum of complex mixtures. We propose a reformulation of this model using Gaussian distribution. The vector data set is analysed, in the processing stage, by a Kohonen, Tolerance, and Labelling layer. The determination of different analytes (PCDFs) which are present in the analysed complex mixture will be indicated by the firing neurons in the labelling layer and by the activation level of these neurons. This layer has a dynamical dimension and an open behaviour to different topological structures presents in the processing data.

Our concrete and final proposal consists in putting to work together Fluorescence Spectrometry and neural computation approach, and to analyse the good results and the troubles and difficulties found in this new method.