DEVELPOMENT OF ALGORITHMS FOR THE OPTIMIZATION OF DRUG PRECURSORS DETECTION WITH A LASER PHOTOACOUSTIC SENSING SYSTEM

A. Ulrici[1,2], M. Calderisi[1,2], R. Seeber[2,3]
[1]Dipartimento di Scienze della Vita, Università di Modena e Reggio Emilia, Via Amendola, 2 – 42122 Reggio Emilia
[2]Consorzio INSTM, Via G. Giusti, 9 – 50121 Firenze
[3]Dipartimento di Scienze Chimiche e Geologiche, Università di Modena e Reggio Emilia, Via Campi, 183 – 41125 Modena

In the frame of the EU FP7 Project CUSTOM, a new sensor system to detect drug precursors in gas samples is being developed, which includes an External Cavity-Quantum Cascade Laser-Photo Acoustic Sensor (EC-QCL-PAS). For this sensor, the optimal wavenumbers within a restricted range in the mid-infrared region must be identified, in order to lead to optimal detection of the drug precursor molecules in presence of interfering species and of variable composition of the surrounding atmosphere. To this aim, based on simulations made with FT-IR spectra taken from literature, a complex multivariate analysis strategy was developed to select the optimal wavenumbers for the laser source. By means of different Experimental Design and Signal Processing techniques, a dataset was created, which includes 5000 simulated spectra of mixtures of 33 different gases in variable concentrations. Then, using Wavelet Transform [1] a thoughtful preselection of the spectral range was made, disregarding noisy regions ascribed to interfering small molecules. The simulated mixtures were used to select the optimal wavenumber range, by maximizing the classification efficiency (estimated by Partial Least Squares Discriminant Analysis) [2] calculated for the different positions of a moving window. Finally, the optimal wavenumber values for the detection of each specific target molecule were identified within the selected range using feature selection approach based on Genetic Algorithms [3] and on resampling. The work made will be relatively easily turned to the spectra actually recorded with the newly developed EC-QCL-PAS instrument. It should be emphasized that, despite the specificity of the case dealt with in the present work, the algorithms developed for the various stages of the procedure are of general validity and can be very simply adapted to quite different real situations.

[1] M. Cocchi, R. Seeber, A. Ulrici, J. Chemometrics 17 (2003) 512-527.
[2] L. Pigani, A. Culetu, A. Ulrici, G. Foca, M. Vignali, R. Seeber, Food Chem. 129 (2011) 226-233.
[3] R. Leardi, A. Lupiáñez Gonzales, Chemom. Intell. Lab. Syst. 41 (1998) 195-207.