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"la Caixa" Doctoral Fellowship Programme with

a set of stimulating PhD projects and

excellent research groups to host the fellows



Signal and information processing for sensing systems group Group leader: Santi Marco (smarco@ibecbarcelona.eu)

Toolbox for the development of predictive models in Volatolomics

Today the non-invasive analysis of different body fluids: urine, breath, flatus, sweat in the search for volatile biomarkers is a very hot topic. However, a key element to perform this task is to have a powerful but strict methodology for the analysis of very high dimensional data. Raw data advanced pre-processing, novell machine learning methods and rigorous validations methodologies are needed.

Current smart instrumentation using multi-sensors and/or spectrometers provides a wealth of data that requires sophisticated signal and data processing approaches in order to extract the hidden information. In this context, we are interested in intelligent chemical instruments for the detection of volatile compounds and smells. These systems can be based on an array of nonspecific chemical sensors with a pattern recognition system , taking inspiration from the olfactory system. Some spectrometries, e.g. Ion Mobility Spectrometry, are capable of very fast analysis with good detection limits but poor selectivity. These technologies have been proposed for the fast determination of the volatolome (volatile fraction of the metabolome), instead of the reference technique of gas chromatography – mass spectrometry.

Our group develops algorithmic solutions for the automatic processing of Gas Sensor Array, Ion Mobility Spectrometry (IMS) and Gas Chromatography – Mass Spectrometry (GC-MS) data for metabolomics and food samples.

In a parallel activity, our group is working on the detection of drowsiness in drivers using vehicle dynamic measures.

Job position description

The student will develop a toolbox for the analysis of volatolome data arising from different analytical platforms. The student will test the performance of the techniques through the analysis of different datasets. The student should have a background in biostatistics, chemometrics, pattern recognition or machine learning.