







Abstract

Untargeted metabolomics is increasingly recognized for its potential in personalized medicine, with advanced data analysis playing a critical role. This seminar will address the challenges of developing reliable predictive models due to biological and instrumental variance. We will outline the analytical process for handling data from chemical instrumentation used in biofluid analysis, focusing on feature extraction challenges and the creation of machine learning-based predictive models, especially for biomarker discovery through feature selection. The discussion will also cover unresolved issues in model development and deployment. Examples from our research and recent literature will illustrate these points, aiming to provide a clear understanding of current trends and challenges in computational metabolomics.

Seminar

PROF. SANTIAGO MARCO

27th February 2024
Palazzetto dei Veneziani
Chieti

Title

Development of ML based predictive models for untargeted metabolomics: challenges and risks

Program

14:15 - Welcome

- Unidav Rector, prof. Giampiero Di Plinio
- Dean of Unidav Department, prof. Melania D'Angelosante

14:25 - Introductory speech

 Director of the Unidav Laboratory "Hugo Gernsback", prof. Alessia Amelio

14:35 – Seminar, prof. Santiago Marco

16:30 - Discussion panel

Short bio

Dr. Santiago Marco is Full Professor at the department of Electronics and Biomedical Engineering in the University of Barcelona (UB) and Group Leader at the Institute for Bioengineering of Catalonia. He obtained his degree in and his PhD in Physics from the UB in 1988 and 1993 respectively. In 1994 he was a post-doc at the University of Rome "Tor Vergata", working on Data Processing for Artificial Olfaction. In 2004 he was in a sabbatical leave at the EADS-Corporate Research in Munich working in Ion Mobility Spectrometry.