# **Course on METABOLOMICS**

## Metabolomics: An Introduction to the Field and Sample Preparation Dr. Gregor McCombie, Department of Biochemistry, University of Cambridge, UK Giovedì 17 Aprile ore 16 Aula 2 Palazzo delle Scienze, Via Ospedale 72, Cagliari

Metabolomics describes the global analysis of metabolites in conjunction with statistical pattern recognition to define changes in the metabolism of cells, tissues, biofluids or even whole organisms in response to outside factors such as disease or exposure to a toxin. Correct sample preparation is the first crucial step in any metabolomics study and can have a large outcome on the results. Metabolomics will be discussed and then considered various study designs and sample preparation approaches, highlighting the advantages and disadvantages of each.

### Metabolomics: The Instrumentation - NMR, Mass Spectrometry and Chromatography Dr. Oliver Jones, Department of Biochemistry, University of Cambridge, UK Venerdì 18 Aprile ore 12 Aula Magna Chimica, Palazzo delle Scienze, Via Ospedale 72, Cagliari

Seminar will focus on the varied analytical tools that are used in metabolomic studies today. These include Nuclear Magnetic Resonance (NMR) spectroscopy (the mainstay of metabolomic research), Gas and Liquid- Chromatography coupled to Mass Spectrometric detection (GC and LC-MS) and others. The strengths and weaknesses of each method will be described and it will be demonstrated that their use in combination can better cover the metabolome and thus increase the power of metabolomic analysis.

# Metabolomics: Multivariate Statistical Analysis and Pattern Recognition

#### Dr. Oliver Jones and Dr. Gregor McCombie,

Department of Biochemistry, University of Cambridge, UK

Venerdì 18 Aprile ore 15 Aula Magna Chimica, Palazzo delle Scienze, Via Ospedale 72, Cagliari

Metabolomics generates huge amounts of data and dealing with this information will be the focus of seminar three. Typically, multivariate statistical approaches are used they account for many simultaneous, correlated changes across the whole dataset. Multivariate analysis includes unsupervised methods, such as principal component analysis (PCA), and supervised methods such as discriminant analysis (DA). In order to get the data into a suitable form for analysis, data pre-treatment (including normalisation and scaling) is also necessary. Seminar will discuss data pre-treatment and analysis, highlighting the essential techniques, as well pointing out potential pitfalls.

### Review of Published Applications of Metabolomics from Medical to Environmental Dr. Oliver Jones, Dr. Gregor McCombie, and Dr. Aalim Weljie Department of Biochemistry, University of Cambridge, UK Martedì 22 Aprile ore 15 Aula n. 1, piano terra, Asse Didattico Medicina

Seminar will focus on the potential applications of metabolomics, which has proven to be an extremely versatile technique, with a diversity of applications including: the study of gene function, toxicology, plant metabolism, environmental analysis, clinical diagnostics, and investigation of disease and discrimination of organism genotypes. We will be introduced and discussed an example from each of these topics in this seminar in order to demonstrate the versatility of metabolomic analysis

Metabolomics: Practical Demonstration of Processing Data. From Spectra to Meaningful Results Using a Rat Model of Fatty Liver Induced by Choline-deficiency Dr. Aalim Weljie, Department of Biochemistry, University of Cambridge, UK Mercoledì 23 Aprile ore 11 Aula Magna Chimica, Palazzo delle Scienze, Via Ospedale 72, Cagliari

Processing metabolomic data is extremely important part of the study as different processing methods may give rise to differing results. Seminar will therefore be a practical demonstration using a real metabolomics dataset processed from raw data to changing characteristics between samples using a variety of computer programs to demonstrate some of the options available to the metabolomics researcher.

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