The Metabolomics Platform is meant to provide a high quality service in the field of metabolomics for leading research groups in biomedicine. Expert support and consulting through all project steps (experimental design, sample handling, NMR measurements, data treatment and translation of multivariate data into biochemically meaningful information) are envisaged. The services offered by the platform are the following:

- **Collaboration in the experimental design:**
The Platform can give advice in the definition of the nature and dimension of the sample set that conforms each metabolomic study to be performed with the aim to obtain sound and statistically meaningful results. The experimental design also includes the determination of the most convenient NMR pulse sequences for the experiment as well as the adequate data treatment methods to maximize the useful information to be obtained from the measurements.

- **Sample handling**
The metabolomic platform is able to analyze almost any biological sample. Body fluids (serum, plasma, urine, cerebrospinal fluid, etc.) can be measured, as well as tissues, biopsies, cell cultures, etc. NMR sample condition facilities are available.

- **NMR analysis**
Samples are analyzed in a 600 MHz and/or 500 MHz high resolution spectrometers through the application of 1D and 2D NMR pulse sequences commonly used in the metabolomics field.

- **Data analysis: Linking NMR data to biological knowledge**
Multivariate based algorithms such as PCA, PLS-DA are used to generate biochemical knowledge from NMR spectral data leading to an easy and versatile way to determine differences and similarities in the whole metabolome of individuals under analysis. Metabolite identification gets possible by matching NMR spectra with standard metabolites database.
Although specially addressed to the needs of CIBERDEM and URV groups, the Metabolomics Platform welcomes any biomedical research group to contact its members for scientific collaboration proposals or/and metabolomic services.

The Metabolomic Platform has been equipped with the state of the art and most complete instruments in the NMR and GC/LC/MS fields.

In the case of HR-NMR, the platform has received a 600 MHz Bruker Avance III spectrometer fitted with a cryoprobe. This configuration allows the acquisition of high resolution and high sensitivity measurements with a five-fold increase in dynamic range compared to conventional probes.

Measurements can be done in continuous flow or with tubes. For tube measurements, a ScanJet robot has been coupled to the spectrometer. This system allows the storage and automatic measurement of hundreds of samples at low temperature (down to 4°C). For continuous flow measurements, a Gilson system with Peltier refrigeration (again, down to 4°C) has been installed. Using any of the systems, a high throughput (i.e., more than 200 measurements per day) can be achieved. The system is specifically configured to measure biofluids such as plasma, serum, urine, sweat, etc.

The equipment available in high field NMR allows high throughput analytical measurements of body fluids i.e., serum, urine as well as tissue or biopsies analysis of humans and/or animal models (i.e., rats, mice, etc.).

The use of advanced statistical, chemometric, multivariate and artificial intelligence algorithms will allow turning large measurement datasets into useful clinical results for the different research groups willing to use the facility services.

The main vision of the Metabolomics Platform is not only act as a measurement facility but to offer metabolomic consulting, trying to get fully involved in the metabolic-related experiments proposed by the groups. This means that the collaboration should start from the very beginning of the study (definition of goals, dimension and characteristics of the sample set, metabolomic experimental design) until the very end (data processing and interpretation), helping to obtain sound, significant and useful clinical results for the different research groups willing to use the facility services.

The main goal of the Metabolomics Platform is to offer metabolomic services to the biomedical and clinical research groups from CIBERDEM and URV.

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The platform has also acquired a second system to measure semisolid samples such as biopsies, cell cultures, tissues, etc. It is based around a 500 MHz Bruker Avance III spectrometer coupled to an HR-MAS probe. Both systems include the possibility to program and control the sample temperature through each measurement.

Data treatment will be carried out mainly with the AMIX software package, which allows multivariate analysis (including PCA and PLS-DA algorithms). The software comes with the NMRMetaPro database, which allows the identification of those metabolites included and characterized in such a complete database (with more than 500 components). The Metabolomics Platform will also uses Matlab, a very flexible mathematical environment that allows to apply many statistical and pattern recognition algorithms that are starting to be used in metabolomics and/or other -omic sciences.

Starting in 2009, the platform will be able to offer Chromatographic and Mass Spectrometry services as complementary tools for metabolomic studies. In fact, GC-MS, LC-MS/TOF and LC-MS/MS Agilent analyzers will be ready and available by then.

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The use of advanced statistical, chemometric, multivariate and artificial intelligence algorithms will allow turning large measurement datasets into useful clinical information. These techniques allow performing what is generally known as metabolic fingerprinting or profiling. The diagnosis of metabolic related illnesses and risk evaluation on large population studies, are the major concerns of the platform together with the identification of metabolic pathways or involved biomarkers in metabolic related diseases.

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Metabolomics can be defined as a new emerging -omic science in systems biology that is aimed to decipher the metabolic profile in complex systems through the combination of data-rich analytical techniques and multivariate data analysis. Metabolomics leaves behind the reductionist method of investigating single component effects on a biological system and goes a little further offering a holistic approach in the exploration of the molecular details of multiple factors on an entire biological organism. Metabolomic techniques allows for a high throughput analysis of small molecules (metabolites) in biofluids and tissues giving metabolic profiles as the end product. Comparison of such profiles from different phenotypes can be used to identify specific metabolic changes leading to the understanding of biochemical pathways, complex biomarker combinations, toxic effects and disease progression.

The main application of metabolomics to mammalian systems are related, among others, to: phenotyping, biomarker discovery, clinical studies (diagnosis disease and therapeutic efficacy), toxicology (pre-clinical drug candidate safety assessment), etc.

There are two basic different approaches to metabolomics. **Fingerprinting** is the most commonly used method in NMR metabolomics and it is based upon the multivariate analysis of a dataset consisting on a large amount of sample NMR spectra, where each spectrum can be considered as a fingerprint of unassigned signals arising from low molecular weight analytes. **Profiling** is a more challenging but ultimately more meaningful approach for analysing NMR spectra. It is based on the analysis of an array of metabolites known to be involved in a given biochemical pathway. It does not allow for fast and high throughput automated measurements since considerable human intervention is needed to guide the process of identifying and quantifying metabolites in NMR spectral data, especially when dealing with complex mixtures such as biofluids (i.e., serum or urine).