1.1 Metabolomics Studies

The terminologies used here are based on those proposed by RSBI (Sansone et al., 2006)and used in ISA-TAB (Sansone et al., 2008) , where the word experiment is deliberately avoided and replaced by more precise terminologies. ′Investigation′ refers to the highest level concept of scientific enquiry that can be seen as a multi-faceted research activity. ′Study′ refers to the experimental design and its related variables. Subsequently one or more studies are designed to carry out an investigation where each examines one side of the overall investigation. Finally ′Assay′ refers to smallest level of experimentation, where the data acquisition instruments run is used to generate the data (Taylor et al., Sansone et al., 2008, Smith et al., 2007, Sansone et al., 2006).

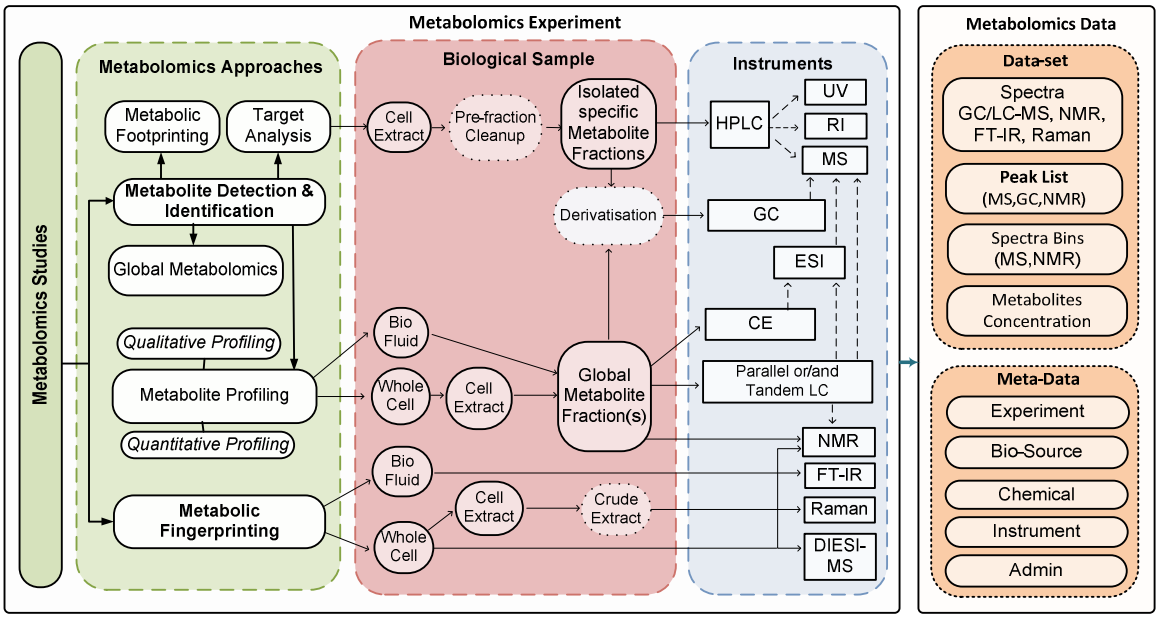

Figure 1

1.1.1 Metabolomics Approaches:

Figure1 summaries different metabolomics approaches, analytical objectives and coverage (Sweetlove et al., 2003).

True metabolomics: an unbiased (Dunn and Ellis, 2005) and comprehensive analysis of the overall metabolome in a particular condition (Dettmer et al., 2007, Goodacre et al., 2004);

Metabolite profiling: a quantitative analysis which is conducted over a set of metabolites on a predefined metabolites in a particular biochemical pathway or on

profiled subgroups of chemical classes (Dettmer et al., 2007, Dunn and Ellis, 2005, Kell, 2004);

Metabolite target analysis: is a form of metabolite profiling that target particular metabolites of a specific biological system or biochemical pathway such as enzymes which are directly influenced by a specific type of environmental or genetic perturbations (Dettmer et al., 2007, Goodacre et al., 2004);

Metabolite fingerprinting: a rapid, global, high throughput analysis which aims to discover patterns and classify samples without the need to identify or quantify the metabolites involved (Dunn and Ellis, 2005).

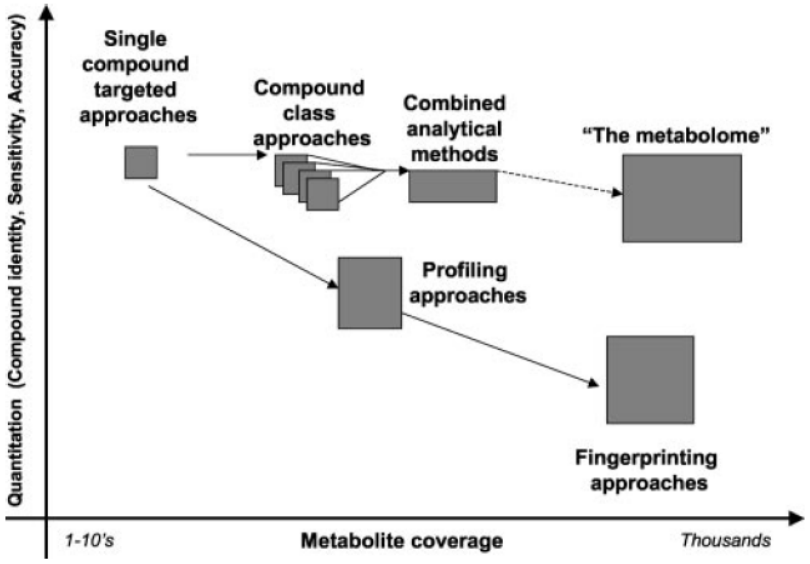

Figure 2 (Sweetlove et al., 2003)

1.1.2 **Biological Sample:**

The nature of samples used in metabolomics depends on the organism under study and its biological source biological e.g. plant, animal or microbes. Metabolomics studies can be performed on whole cell samples, cell extracts or bio-fluid. Different samples might be subject to different levels of sample preparation procedures which depend on the biological source as well as the aims of the study and the used data acquisition instrument.

1.1.3 **Data Acquisition Instruments:**

Metabolomics employ a wide spectrum of data acquisition instruments which usually depend on one or more of the chemical analysis instruments e.g. Gas Chromatography (GM) , Liquid Chromatography (LC), Mass Spectrometry (MS), Time of Flight

(TOF), Infra Red (IR), Ultra Violet (UV), Capillary Electrophoresis (CE)Fourier Transformation (FT), Ion Cyclotron Resonance (ICR), Electrospray Ionisation (ESI), High Performance Liquid Chromatography (HPLC), Hydrophilic Interaction Chromatography (HILIC), Nuclear Magnetic Resonance (NMR).

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