

# A Brief Report on NMR-Based Metabolomics

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## BRIEF REPORT

Similar to genomics and proteomics which yield vast amounts of data about the expression of genes and proteins, metabolomics refers to the whole metabolic profile of the cell. The focus of this report concerns the use of nuclear magnetic resonance (NMR) spectroscopy for metabolic analyses and, in particular, its use in toxicology for examining the metabolic profile of biofluids. Examples from the literature will demonstrate how  $^1\text{H}$  NMR and pattern recognition methods are used to obtain the urinary metabolic profile, and how this profile is affected by exposure to various toxicants. These particular studies which focus on the metabolic profiles of biofluids, specifically urine, are referred to as metabonomics. NMR-based metabonomics provides a means to categorize organ-specific toxicity, monitor the onset and progression of toxicological effects, and identify biomarkers of toxicity. A future challenge, however, is to describe the cellular metabolome for purposes of understanding cellular functions (i.e., metabolomics). Thus the capabilities and advantages of multinuclear NMR to provide metabolic information in cells and tissues will also be discussed. Such information is essential if metabolomics is to provide a complementary dataset which together with genomics and proteomics can be used to construct computer network models to describe cellular functions.

## Future of NMR-Based Metabolomics

The two leading analytical approaches to metabolomics are mass spectrometry (MS) and nuclear magnetic resonance (NMR) spectroscopy. Although currently overshadowed by MS in terms of numbers of compounds resolved, NMR spectroscopy offers

advantages both on its own and coupled with MS. NMR data are highly reproducible and quantitative over a wide dynamic range and are unmatched for determining structures of unknowns. NMR is adept at tracing metabolic pathways and fluxes using isotope labels. Moreover, NMR is non-destructive and can be utilized in vivo. NMR results have a proven track record of translating in vitro findings to in vivo clinical applications.

The metabolic state of an organism depends on its genome, transcriptome, proteome, epigenome, microbiome, and exposome (environment). Thus, metabolomics, the study of small molecules (<1500 Da) in living systems, provides information with a high potential for accurately describing the physiological state of an organism. The two most successful approaches to determining the metabolic state of an organism have been mass spectrometry (MS) and nuclear magnetic resonance (NMR) spectroscopy. Several years ago, the number of publications utilizing the two approaches was comparable; more recently, however, MS-based metabolomics has clearly overtaken NMR-based metabolomics. This state of affairs prompted the organization of a workshop to review the current state of NMR-based metabolomics, to assess its strengths and weaknesses, and to envision its future potential. As reported here, this workshop ('NMR-Based Metabolomics,' held in the Discovery Building, Morgridge Institute for Research, Madison, Wisconsin, USA, on June 10, 2016) highlighted a number of benefits of NMR-based metabolomics that appear to be currently underappreciated. MS and NMR offer different strengths, which can be used synergistically. The workshop stressed the need for more extensive small molecule databases and improved standards at each step of a metabolomics study.

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