

# Metabolomic Approaches in Biomarker Development

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## Editorial

Drug abuse is a growing problem around the world, especially as more new psychoactive substances enter the drug market. In general, there is little information available on their negative effects and toxicity. Because of their ephemerality on the drug scene, direct detection and identification of NPS presents an analytical challenge. For this complex analytical scenario, an approach that does not directly focus on the structural detection of an analyte or its metabolites would be beneficial, and the development of alternative screening methods could help to provide a quick response on suspected NPS consumption. A metabolomics approach could be one such alternative strategy for identifying biomarkers for various questions in DOA testing.

Metabolomics is the study of changes in small (endogenous) molecules (1,000 Da) in response to a specific stimulus [1-3] such as the consumption of DOA. A literature search targeting "metabolomics" and various DOAs or NPS was conducted for this review. As a result, different applications of metabolomic strategies in biomarker research for DOA identification were identified: (a) as an additional tool for metabolism studies, with the major advantage of identifying previously unknown or unexpected metabolites; and (b) for identification of endogenous biomarker or metabolite patterns, e.g., for synthetic cannabinoids, or to indirectly detect urine manipulation attempts by chemical adulteration or replatation.

Certain changes in endogenous compounds are detected for all DOAs studied, but similar compounds/pathways are frequently influenced. When these studies are evaluated in terms of potential biomarkers for drug consumption, the observed changes appears to be too small, despite being statistically significant, to work reliably as a biomarker for drug consumption. Furthermore, it was discovered that different drugs affect the same pathways. Finally, metabolomic approaches have the potential to detect biomarkers indicating drug consumption. More research is needed, such as more sensitive targeted analyses, multi-variant statistical models, or deep-learning approaches, to fully investigate the potential of omics science in DOA testing [4,5].

Metabolomics (also known as metabolic profiling or metabonomics) is the study of an organism's metabolism and metabolites. It is one of several "omics" sciences, including exposomics (the study of all environmental exposures), microbiomics (the study of the microbiome), proteomics, genomics, and

transcriptomics. Metabolome research focuses on the qualitative and quantitative characterization of small molecules (1,000 Da) that cause changes in organisms in response to a specific stimulus. The metabolome is distinct, dynamic, and linked to phenotype. Unlike the other "omics" sciences, metabolomics can link gene and environmental interactions.

Metabolomics approaches have been used in a variety of fields in recent years due to their ability to detect subtle changes in large datasets using comprehensive metabolite measurements. The question of which metabolites are considered to be part of the "metabolome" is still debatable, resulting in partly ambiguous definitions. Endogenously derived biochemicals such as carbohydrates, lipids, amino acids, fatty acids, steroids, or vitamins are examples of metabolites found in biological systems and are referred to as the metabolome in the strict sense. However, metabolomic analyses can detect exogenously derived metabolites from xenobiotics as well as their phase I and phase II metabolites; this is known as the xenometabolome.

## Conflict of Interest

None.

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