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Journal of Clinical and Experimental Pharmacology

Editorial

A Short Note on Invention of Metabolomics

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EDITORIAL NOTE

The metabolome refers to the entire set of metabolites produced by cellular processes in a biological cell, tissue, organ, or organism. The set of gene products produced in the cell is revealed by messenger RNA (mRNA), gene expression data, and proteomic analysis, data that reflects one element of cellular activity. Apparently, metabolic profiling can provide a rapid shot of a cell's physiology, making metabolomics a direct "functional study of an organism's physiological state". Integrated bacterial genome, transcriptomic, proteomic, and metabolomic data to provide a better knowledge of cellular biology is one of the difficulties of systems biology and functional genomics. However, it was only through technological breakthroughs in the 1960s and 1970s that it became possible to quantify metabolic profiles objectively.

Horning coined the term "metabolic profile" after demonstrating that Gas Chromatography-Mass Spectrometry (GC-MS) could be used to detect chemicals in human urine and tissue samples in 1971. Throughout the 1970s, the Horning group, along with Linus Pauling and Arthur B. Robinson, led the development of GC-MS methods to monitor metabolites in urine.

At same time, NMR spectroscopy, which had been discovered in the 1940s, was making rapid progress. Seeley et al. showed that NMR could be used to detect metabolites in unaltered biological samples. The importance of NMR was underscored in this initial investigation on muscle when it was discovered that 90 percent of cellular ATP is complexed with magnesium. NMR has been a key analytical method for investigating metabolism since sensitivity has improved with the evolution of greater magnetic field strengths and magic angle spinning. The laboratory of Jeremy K. Nicholson at Birkbeck College, University of London, and later at Imperial College London, has been in the forefront of recent efforts to use NMR for metabolomics. Nicholson revealed that 1H-NMR spectroscopy might be used to detect diabetes mellitus in 1984, and he later pioneered the use of pattern recognition methods on NMR spectroscopic data. Gary Siuzdak utilised liquid chromatography mass spectrometry metabolomics to study the cerebral spinal fluid from sleep-deprived animals in 1995, while collaborating with Richard Lerner (then head of The Scripps Research Institute) and Benjamin Cravatt. Oleamide, one of the molecules of particular interest, was discovered and later demonstrated to have sleep-inducing characteristics. This is one of the first metabolomics studies that combine liquid chromatography with mass spectrometry.

The first metabolomics tandem mass spectrometry database-Metlin, was developed in the Siuzdak laboratory at The Scripps Research Institute in 2005 for describing human metabolites. Since then, Metlin has grown to over 450,000 metabolites and other chemical entities as of July 1, 2019, with each compound having experimental tandem mass spectrometry data obtained from molecular standards at multiple collision energies and in both positive and negative ionized modes. Metlin is the world's biggest database of tandem mass spectrometry data. The devoted academic journal Metabolomics, founded by its current editor-in-chief Professor Roy Good acre, first featured in 2005. The Siuzdak lab was working on identifying metabolites linked to sepsis, and in order to address the problem of statistically identifying the most relevant deregulated metabolites across hundreds of LC/MS datasets, the first algorithm for nonlinear alignment of mass spectrometry metabolomics data, known as XCMS, was developed.

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Received: August 05, 2021; **Accepted**: August 19, 2021; **Published**: August 26, 2021

Citation: Voku A (2021) A Short Note on Invention of Metabolomics. J Clin Exp Pharmacol. S8: e004.

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