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TRACER METABOLOMICS

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Tracer metabolomics is a LC/MS/MS approach for simultaneous examination of multiple metabolic pathways by determination of deuterium enrichment in metabolites in the presence of deuterium oxide or by following the metabolism of isotopically stable molecules. By introducing a tracer into a biological system, pathways including gluconeogenesis, glyceroneogenesis, fatty acid/phospholipid/ triglyceride/cholesterol ester synthesis and many others can be followed for assessment of target engagement, mechanism of action and pharmacological effect. Several LC/MS/MS assays will be discussed that demonstrate the utility of tracer metabolomics in a drug discovery environment.

Biography

Gary W Caldwell received his PhD in Physical/Organic Chemistry from Indiana University in 1982 under the direction of Dr. John E Bartmess using Ion Cyclotron Resonance Spectrometry to study gas-phase ion chemistry. Following his PhD, he performed Postdoctoral Research with Dr. Paul Kebarle at the University of Alberta in Canada using High-Pressure Mass Spectrometry to study gas-phase ion chemistry. He joined Janssen Pharmaceutical Research and Development, a subsidiary of Johnson & Johnson in 1985. During his 32-year career with Janssen Pharmaceutical R&D, he has managed a variety of functions within the drug discovery units. These functions include the NMR, GC/MS & LC/MS/MS spectroscopy group, the medicinal chemistry intermediates group, the large-scale separation group, the drug discovery in-vivo/in-vitro PK/ADME groups and the compound management group. His research interests primarily involve the use of advanced spectrometric and chromatographic techniques to chemically and biologically characterize new drug targets and drug entities. Presently, he is working on establishing targeted and untargeted metabolomic methods to understand "on" and "off" target effects to improve drug efficacy and reduce drug toxicity. He is the author of over 150 publications, two patents, over 50 poster presentations, and has given over 40 invited talks at universities, companies, and conferences. He is the Co-editor of Frontier in Drug Design & Discovery (volumes 1-4), and Editor of Optimization in Drug Discovery: In-vitro Methods (volumes 1-2).

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