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Current practices and new developments in metabolite identification using LC-MS

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Metabolite identification is a critical component through all stages of drug discovery and development process. Early in drug discovery, identification of sites of metabolism on drug candidates and the structure of their metabolites can be decisive for the design of drugs with optimized metabolic stability and favorable ADME properties. During lead optimization and candidate selection stage, it is important to characterize metabolic differences in cross-species in vitro to support the selection of the animal species, employed in safety assessment studies, and to identify potential pharmacologically active, reactive, or toxic metabolites. At the pre-clinical and clinical developmental stages, in vivo metabolite identification in circulation and excreta in animals (a rodent and non-rodent species) and humans are performed to ensure no human specific metabolites, to identify qualitative and quantitative differences metabolite profiles between animals and humans, and to ensure major human circulating metabolites are adequately exposed in preclinical safety species. In this presentation, we will discuss the current practices and new developments in metabolite identification to support drug discovery and development using high resolution LC-MS with particular examples of bioactivation and novel biotransformation mechanisms.

Biography

Shuguang Ma received his PhD in Analytical Chemistry from Purdue University under the supervision of Professor R Graham Cooks. He also had two years of Post-doctoral training in biological mass spectrometry at the Medical School of Vanderbilt University under Professor Richard Capiroli. He is currently a Senior Scientist in the Department of Drug Metabolism and Pharmacokinetics at Genentech Inc. Previously he was a Senior Principal Scientist at Schering-Plough (now Merck) and a Senior Scientist at Amgen. He has authored over 50 research articles in the peer-reviewed journals, covering broad area of mass spectrometry and its applications in drug metabolism. His current research interests include the development of novel LC/MS-based techniques for metabolite detection and investigation of biotransformation and bio-activation of xenobiotics.

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