Drug metabolism and pharmacokinetics (DMPK) utility of mass spectrometry: Discovery of small molecule drugs

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In modern drug discovery, mass spectrometry (MS) plays a central role in determination of drug-like properties of small molecules. In an effort to manage compound attrition and to improve the odds of discovering viable development candidates, medicinal chemistry departments have increased their productivity and produce an ever increasing number of compounds. Most compounds are evaluated in a battery of in vitro and in vivo assays in drug metabolism and pharmacokinetics (DMPK) departments. These are labor intensive and time consuming assays and almost always utilize qualitative or quantitative mass spectrometric methods. DMPK groups have to mirror the increased productivity exhibited by the medicinal chemistry to prevent bottlenecks. In addition to the assembling of a highly qualified team and automation, a DMPK department must be creative in the use of its resources and the utility of MS in order to enabled generation of high quality data in an efficient, timely, and cost effective manner. Qualitative and quantitative MS approaches and their specific utility in discovery DMPK will be discussed in this presentation.