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Editorial

Mass spectrometry, once a component of a support service relegated to the basements of big pharmaceutical companies and universities, is now a cornerstone of efforts to develop new drugs, discover novel biomarkers, and uncover new drug targets. Many approaches utilize measurements derived from mass spectrometry to probe fundamental aspects of molecular biology, characterize macromolecular interactions, and study cellular function. This special issue of *The International Journal of Mass Spectrometry* focuses on recent applications that have made mass spectrometry a key technology platform in the drug discovery arena. As guest editors of this issue, it was our intent to compile a representative collection of manuscripts that present the reader with a synopsis of some of the mass spectrometry-based strategies and tactics being employed to support "conventional" drug discovery efforts in big pharma settings, and also those used to facilitate "unconventional" approaches to drug discovery being pursued in smaller biotech settings. It was our goal to include contributions that represent the full range of this spectrum to illustrate the creative approaches being employed to further the development of therapeutic compounds. Contributions from Bolaños (Pfizer) and Kyranos (Arqule) describe hyphenated methods to assess compound purity to support drug discovery while contributions from Annis (Neogenesis) and Sannes-Lowery (Ibis) describe use of the mass spectrometer as the primary high-throughput screening platform for affinity selection of small molecule ligands. Other contributions focus on areas from which the drug discovery community derives great collateral benefit. For example, the field of biomarker discovery is the center of much recent attention and appears to be the battlefield for the next big post-genome land-grab. Roy and coworkers (Surromed) describe their LC–MS method to derive proteomic and metabolomic profiles from human serum in order to obtain quantitative differential expression profiles associated with disease. Similarly, the contribution from Van Den Boom (Sequenom) describes an extremely high-throughput genotyping system based on MALDI-TOF for the elucidation of genetic variability and for subsequent large-scale genotyping of genetic markers. Also, the work described by Peltier et al. (Prolexys Pharmaceuticals) illustrates the potential of proteomics-based technologies to accelerate the discovery of drugs. While, strictly speaking, these are not drug discovery papers, the work has significant implications in the drug discovery arena as the discovery of new diagnostic and prognostic markers of therapeutic response holds tremendous promise for drug discovery and development. This special issue on Mass Spectrometry and Drug Discovery could not be considered complete without at least one paper describing proteomics studies. This contribution comes from Horn and Brock (Novartis Research Foundation) and nicely describes the fundamental concepts underlying MS-based protein identification and then demonstrates system enhancements derived from employing high-performance MALDI-FTICR measurements.

Our attempt to effectively capture any aspect of a field as dynamic and rapidly changing as drug discovery in a single issue of a journal is extremely challenging. Combined with the ever changing and still maturing field of bioanalytical mass spectrometry as highlighted by Herman et al. (Cephalon), Ong et al. (Memory Pharmaceuticals), and Wu et al. (Millennium Pharmaceuticals), this endeavor became even more daunting. We hope that, at the very least, this issue gives the reader some insight into the breadth of applications in which mass spectrometry is a key component of drug discovery and drug discovery-related research. It is our hope that the contents of this issue serve to both educate the reader on the field, and generate a spirit of creativity that will lead to new ideas, and heretofore, unanticipated applications of mass spectrometry in drug discovery.

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