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# Quantitation and Mass Spectrometric Data of Drugs and Isotopically Labeled Analogs

*Ray H. Liu, Dennis V. Canfield, Sheng-Meng Wang*

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The analysis of drugs and their metabolites in biological media are now expected to routinely achieve ± 20% accuracy in the ng/mL concentration level. Therefore, the availability and the selection of quality ion-pairs designating the analytes and their isotopically labeled analogs (ILAs) are important considerations in achieving the accuracy of quantitation results. Assisting scientists with this process, **Quantitation and Mass Spectrometric Data of Drugs and Isotopically Labeled Analogs** provides an extremely valuable reference for labs involved in the analysis of therapeutic and abused drugs.

Part One of this comprehensive volume illustrates approaches, mechanisms, and challenges pertaining to the use of isotopic analogs as internal standards for drug quantitation. The second section is a systematic compilation of full-scan mass spectra of drugs and their analogs, as parent compounds and as derivatives resulting from various chemical derivatization approaches, commonly encountered in today’s labs. Based on the mass spectra data presented in the second section, Part Three provides corresponding tables of ion-pairs which can potentially be adapted to designate the drugs and their isotopic analogs in the analytical processes. Relative quality of these ion-pairs (cross-contribution to the intensity of these ions by their isotopic analogs) is included in these tables.

With more than 1500 full-scan mass spectra and quick access data tables, this text represents the authors’ years of work compiling mass spectra of the many chemical derivatization forms of drugs, their metabolites, and their isotopically labeled counterparts. The unparalleled scope of this compilation makes it a critical one-stop reference for those involved in drug analyses of biological specimens and interpretation of results.

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