Mass Spectra and Cross-Contributions of Ion Intensity Between the Analytes and Their Isotopically Labeled Analogs — Common Opioids and Their Derivatives

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ABSTRACT: For the quantitation of most drugs and their metabolites, GC-MS is currently the preferred method and isotopically labeled analogs of the analytes are the internal standards (ISs) of choice. Under this analytical setting, chemical derivatization (CD) plays a critical role in the sample preparation process. In addition to meeting the conventional objectives of CD, products derived from the selected CD method must generate ions suitable for designating the analyte and the IS; these ions cannot have significant cross-contribution (CC), i.e., contribution to the intensity of the ions designating the analyte by the IS, and vice versa. With this in mind, the authors have reviewed literature and information provided by manufacturers, searching for suitable CD reagents, CD methods, and isotopically labeled analogs of the analytes related to the following 11 opioids: heroin, 6-acetylmorphine, morphine, hydromorphone, oxymorphone, 6-acetylcodeine, codeine, hydrocodone, dihydrocodeine, oxycodone, and noroxycodone. These analytes and ISs were derivatized with various derivatization groups, followed by GC-MS analysis. The resulting MS data are systematically presented in two forms: (a) full-scan mass spectra; and (b) CC data of ion-pairs with potential for designating the analytes and their respective ISs. Many (if not most) of these full-scan mass spectra are not yet available in the literature and should be of reference value to laboratories engaged in the analysis of these drugs/metabolites. Full-scan MS data were further used to select ion-pairs with potential for designating the analytes and ISs in quantitative analysis protocols. The CC data of these ion-pairs were evaluated using data collected in selected ion monitoring mode and systematically tabulated, readily available for analysts searching for this important analytical parameter.

KEY WORDS: 6-Acetylcodeine, 6-acetylmorphine, chemical derivatization, codeine, cross-contribution, dihydrocodeine, GC-MS, heroin, hydrocodone, hydromorphone, internal standard, morphine, noroxycodone, opiate, opioid, oxycodone, oxymorphone.