Mass Spectrometric Data of Commonly Abused Amphetamines and Their Derivatives — Cross Contributions of Ion Intensity between the Analytes and Their Isotopically Labeled Analogs

REFERENCE: Wang S-M, Chye S-M, Liu RH, Lewis RJ, Canfield DV, Roberts J: Mass spectrometric data of commonly abused amphetamines and their derivatives — Cross contributions of ion intensity between the analytes and their isotopically labeled analogs; *Forensic Sci Rev* 17:67–166; 2005.

ABSTRACT: With GC-MS as the preferred method and isotopically labeled analogs of the analytes as the internal standards (ISs) of choice for the analysis of drugs/metabolites in biological specimens, one important aspect associated with chemical derivatization (CD) is that the CD products derived from the analyte and the selected IS 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 ion designated for the analyte by the IS, and vice versa. With this in mind, the authors have reviewed literature and commercial information on common CD reagents and methods and conducted a thorough search of isotopically labeled analogs of commonly abused amphetamine-type drugs/metabolites that are commercially available. These ISs and analytes were then derivatized with various derivatization groups. These CD products were then analyzed by GC-MS and the resulting MS data are presented here in two forms: (a) systematic presentation of full-scan spectra; and (b) tabulation of CC data for ions with potential for designating the ISs and analytes. Many (if not most) of these full-scan spectra are not yet available in the literature and should be of daily reference value to forensic and clinical laboratories that are 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 under the SIM mode and summarized in table format. These data should save enormous amounts of time and efforts for practicing laboratories in their search for this analytical parameter.

KEY WORDS: Amphetamine, chemical derivatization, cross-contribution, ephedrine, GC-MS, internal standard, MBDB, MDA, MDEA, MDMA, methamphetamine, phenylpropanolamine.