Methods

1 Introduction

After publication of the first edition in 1985 with 1500 data sets, the second in 1992 with 4700, and with the Supplement Volume in 2000 with 6700 data sets, the new edition contains **7840 data sets**, among which 1900 data sets have been revised or added. Over 3300 data sets are from metabolites, over 2300 from acetylated, over 1000 from methylated, over 700 from trimethylsilylated, over 400 from trifluoroacetylated, over 200 each from pentafluoropropionylated or heptafluorobutyrylated compounds. All formulas were redrawn in the molefile format allowing their use in electronic databases.

Section 1-2 on sample preparation and GC-MS methods has been updated, but only our standard operation procedures have been described in detail, as they were used for recording the data.

The structures of the compounds are also reproduced to facilitate the identification of unknown metabolites by correlating the fragmentation patterns with the probable structure, as described in Section 1-3. Further data are also included, as outlined in the Explanatory notes.

Several artifacts have been detected which are formed during sample preparation and/or the GC procedure. Their formation is described in detail in Section 1-4.

Section 1-5 contains the table of atomic masses used for molecular mass calculations and Section 1-6 the actualized list of abbreviations used.

All the compounds are listed alphabetically in Table 1-8-1 in order to assist the search for data concerning specific compounds with directions on which page in Volume 2 the data can be found, as well as the entry numbers of the electronic versions. In Table 1-9-1, the parent compounds are listed in order of category to assist the search of data of all the compounds measured within a particular category. The numbering of the Tables, Figures and Sections indicates whether they can be found in Volume 1 or 2 by the corresponding prefix ‘1-’ or ‘2-’. The middle number indicates the corresponding Section.

The extremely large amount of data presented makes it likely that some errors will be present in this handbook. The authors cannot be held responsible for such errors, nor for any consequences arising from the employment of the published data. Users are requested to report any errors that are found and to suggest other data and other groups of compounds, which are of interest (e-mail: hans.maurer@uniklinikum-saarland.de or hans.maurer@uks.eu). If possible, these will be included in future editions, along with corrections of any errors.