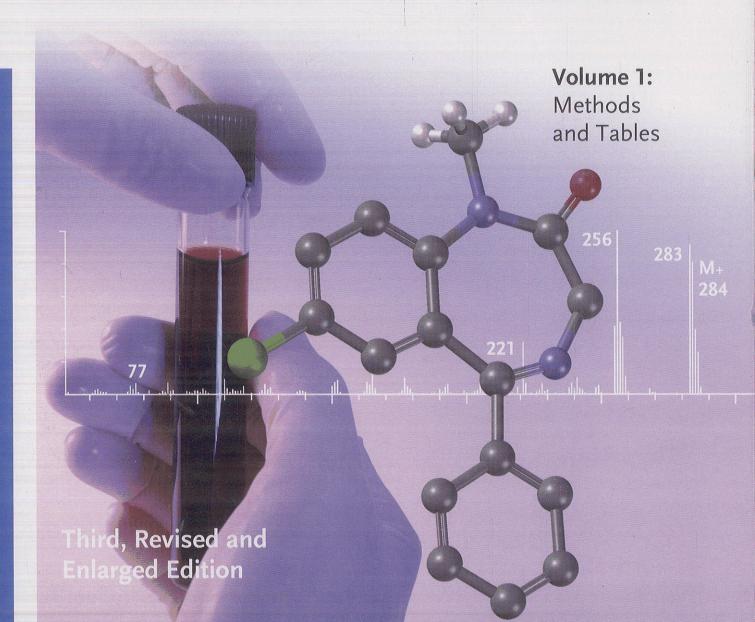
## Mass Spectral and GC Data

of Drugs, Poisons, Pesticides, Pollutants and Their Metabolites



## **Contents of Volume 1 (Methods, Tables)**

## Methods

| 1        | Introduction 5   |
|----------|--|
| 2        | Experimental Section 4   |
| 2.1      | Origin and choice of samples 4   |
| 2.2      | Sample preparation 4   |
| 2.2.1    | Standard extraction procedures 4   |
| 2.2.1.1  | Standard liquid-liquid extraction (LLE) for plasma, urine or gastric contents (P, U, G) 4                  |
| 2,2.1.2  | STA procedure (hydrolysis, extraction and microwave-assisted acetylation) for urine (U+UHYAC) 5            |
| 2.2.1.3  | Extraction of urine after cleavage of conjugates by glucuronidase and arylsulfatase (UGLUC) 5              |
| 2.2.1.4  | Extractive methylation procedure for urine or plasma (UME, PME) 5  |
| 2.2.1.5  | Solid-phase extraction for plasma or urine (PSPE, USPE) 5  |
| 2.2.1.6  | LLE of plasma for determination of drugs for brain death diagnosis 6                                       |
| 2.2.1.7  | Extraction of ethylene glycol and other glycols from plasma or urine followed by microwave-assisted        |
| •        | pivalylation (PEGPIV or UEGPIV) 6  |
| 2.2.2    | Derivatization procedures 6  |
| 2.2.2.1  | Acetylation (AC) 7   |
| 2.2.2.2  | Methylation (ME) 7   |
| 2.2.2.3  | Ethylation (ET) 7  |
| 2.2.2.4  | tertButyldimethylsilylation (TBDMS) 7  |
| 2.2.2.5  | Trimethylsilylation (TMS) 7  |
| 2.2.2.6  | Trimethylsilylation followed by trifluoroacetylation (TMSTFA) 7  |
| 2.2.2.7  | Trifluoroacetylation (TFA) 7   |
| 2.2.2.8  | Pentafluoropropionylation (PFP) 7  |
| 2.2.2.9  | Pentafluoropropylation (PFPOL) 7   |
| 2.2.2.10 | Heptafluorobutyrylation (HFB) 7  |
| 2.2.2.11 | Pivalylation (PIV) 8   |
| 2.2.2.12 | Heptafluorobutyrylprolylation (HFBP) 8   |
| 2.3      | GC-MS Apparatus 8  |
| 2.3.1    | Apparatus and operation conditions 8   |
| 2.3.2    | Quality assurance of the apparatus performance 8   |
| 2.4      | Determination of retention indices 10  |
| 2.5      | Systematic toxicological analysis (STA) of several classes of drugs and their metabolites by GC-MS 10      |
| 2.5.1    | Screening for 200 drugs in blood plasma after LLE 10   |
| 2.5.2    | Screening for most of the basic and neutral drugs in urine after acid hydrolysis, LLE and acetylation 10   |
| 2.5.3    | Systematic toxicological analysis procedures for the detection of acidic drugs and/or their metabolites 14 |
| 2.5.4    | General screening procedure for zwitterionic compounds after SPE and silylation 14                         |
| 2.6      | Application of the electronic version of this handbook 15  |
| 2.7      | Quantitative determination 15  |
| 3        | Correlation between Structure and Fragmentation 16   |
| 3.1      | Principle of electron-ionization mass spectrometry (EI-MS) 16  |
| 3.2      | Correlation between fundamental structures or side chains and fragment ions 16                             |

| 4.1.1 Artifacts formed by oxidation during extraction with diethyl ether 17 4.1.1 N-Oxidation of fertiary amines 17 4.1.2 S-Oxidation of phenothiazines 17 4.2 Artifacts formed by thermolysis during GC (GC artifact) 17 4.2.1 Decarboxylation of carboxylic acids 17 4.2.2 Cope elimination of N-oxides (-(CH <sub>3</sub> ) <sub>2</sub> NOH, -(C <sub>2</sub> H <sub>3</sub> ) <sub>2</sub> NOH, -C <sub>6</sub> H <sub>14</sub> N <sub>2</sub> O <sub>2</sub> ) 17 4.2.3 Rearrangement of his-deethyl flurazepam (-H <sub>2</sub> O) 17 4.2.4 Elimination of various residues 17 4.2.5 Methylation of carboxylic acids in methanol ((ME), ME in methanol) 18 4.2.6 Formation of formaldehyde adducts using methanol as solvent (GC artifact in methanol) 18 4.3 Artifacts formed by thermolysis during GC and during acid hydrolysis (GC artifact, HY artifact) 18 4.3.1 Dehydration of alcohols (-H <sub>2</sub> O) 18 4.3.2 Decarbamylation of alcohols (-H <sub>2</sub> O) 18 4.3.3 Cleavage of morazone to phenmetrazine 18 4.4 Artifacts formed during acid hydrolysis 18 4.4 Icleavage of the ether bridge in beta-blockers and alkanolamine antihistamines (HY) 18 4.4.1 Cleavage and rearrangement of N-demethyl metabolites of clobazam to benzimidazole derivatives (HY) 19 4.4.2 Cleavage and rearrangement of bis-deethyl flurazepam (HY -H <sub>2</sub> O) 19 4.4.4 Cleavage and rearrangement of tetrazepam and its metabolites 19 4.4.5 Cleavage and rearrangement of tetrazepam and its metabolites 19 4.4.6 Dealkylation of ethylenediamine antihistamines (HY) 19 5 Table of Atomic Masses 20 6 Abbreviations 21 7 References 24  Tables  8 Table of Compounds in Order of Names 35 8.1 Explanatory notes 35 8.2 Table of Compounds in Order of names 37  9 Table of Compounds in Order of Categories 189  Explanatory notes 189 | 4     | Formation of Artifacts 17  |
|---|-------|--|
| 4.1.2 S-Oxidation of phenothiazines 17 4.2 Artifacts formed by thermolysis during GC (GC artifact) 17 4.2.1 Decarboxylation of carboxylic acids 17 4.2.2 Cope climination of N-Oxides (-(CH <sub>2</sub> ) <sub>2</sub> NOH <sub>2</sub> , -(C <sub>2</sub> H <sub>2</sub> ) <sub>2</sub> NOH <sub>3</sub> , -C <sub>6</sub> H <sub>14</sub> N <sub>2</sub> O <sub>2</sub> ) 17 4.2.3 Rearrangement of bis-deethyl flurazepam (-H <sub>2</sub> O) 17 4.2.4 Elimination of various residues 17 4.2.5 Methylation of carboxylic acids in methanol ((ME), ME in methanol) 18 4.2.6 Formation of formaldehyde adducts using methanol as solvent (GC artifact in methanol) 18 4.3.1 Dehydration of alcohols (-H <sub>2</sub> O) 18 4.3.2 Decarbamoylation of carbamates 18 4.3.3 Cleavage of morazone to phenmetrazine 18 4.4 Artifacts formed during acid hydrolysis 18 4.4.1 Cleavage of the ether bridge in beta-blockers and alkanolamine antihistamines (HY) 18 4.1.2 Cleavage of 1,4-benzodiazepines to aminobenzoyl derivatives (HY) 18 4.2 Cleavage and rearrangement of N-demethyl metabolites of clobazam to benzimidazole derivatives (HY) 19 4.4.4 Cleavage and rearrangement of bis-deethyl flurazepam (HY -H <sub>2</sub> O) 19 4.4.5 Cleavage and rearrangement of tetrazepam and its metabolites 19 4.4.6 Dealkylation of ethylenediamine antihistamines (HY) 19 4.7 Hydration of a double bond (+H <sub>2</sub> O) 19 5 Table of Atomic Masses 20 6 Abbreviations 21 7 References 24  Tables  Table of Compounds in Order of Names 35 8.1 Explanatory notes 35 7 Table of compounds in Order of names 37  | 4.1   | Artifacts formed by oxidation during extraction with diethyl ether 17  |
| 4.2 Artifacts formed by thermolysis during GC (GC artifact) 17 4.2.1 Decarboxylation of carboxylic acids 17 4.2.2 Cope elimination of N-oxides (-(CH <sub>3</sub> ) <sub>2</sub> NOH, -(C <sub>2</sub> H <sub>3</sub> ) <sub>2</sub> NOH, -C <sub>6</sub> H <sub>14</sub> N <sub>2</sub> O <sub>2</sub> ) 17 4.2.3 Rearrangement of bis-deethyl flurazepam (-H <sub>2</sub> O) 17 4.2.4 Elimination of various residues 17 4.2.5 Methylation of carboxylic acids in methanol ((ME), ME in methanol) 18 4.2.6 Formation of formaldehyde adducts using methanol as solvent (GC artifact in methanol) 18 4.3.1 Dehydration of alcohols (-H <sub>2</sub> O) 18 4.3.2 Decarbamoylation of carbomates 18 4.3.3 Cleavage of morazone to phenmetrazine 18 4.4 Artifacts formed during acid hydrolysis (GC artifact, HY artifact) 18 4.4.1 Cleavage of the ether bridge in beta-blockers and alkanolamine antihistamines (HY) 18 4.4.2 Cleavage and rearrangement of N-demethyl metabolites of clobazam to benzimidazole derivatives (HY) 19 4.4.3 Cleavage and rearrangement of bis-deethyl flurazepam (HY -H <sub>2</sub> O) 19 4.4.4 Cleavage and rearrangement of tetrazepam and its metabolites 19 4.4.5 Cleavage and rearrangement of tetrazepam and its metabolites 19 4.4.6 Dealkylation of ethylenediamine antihistamines (HY) 19 4.4.7 Hydration of a double bond (+H <sub>2</sub> O) 19  5 Table of Atomic Masses 20  6 Abbreviations 21  7 References 24  Tables  8 Table of Compounds in Order of Names 35 8.1 Explanatory notes 35 8.2 Table of compounds in order of names 37  9 Table of Compounds in Order of Categories 189  | 4.1.1 | N-Oxidation of tertiary amines 17  |
| 4.2.1 Decarboxylation of carboxylic acids 17 4.2.2 Cope elimination of N-oxides (-(CH <sub>1</sub> ) <sub>2</sub> NOH <sub>1</sub> -(C <sub>2</sub> H <sub>1</sub> ) <sub>2</sub> NOH <sub>1</sub> -C <sub>6</sub> H <sub>1</sub> d <sub>1</sub> N <sub>2</sub> O <sub>2</sub> ) 17 4.2.3 Rearrangement of bis-deethyl flurazepam (H <sub>2</sub> O) 17 4.2.5 Methylation of carboxylic acids in methanol ((ME), ME in methanol) 18 4.2.6 Formation of formaldehyde adducts using methanol as solvent (GC artifact in methanol) 18 4.3.1 Dehydration of alcohols (-H <sub>2</sub> O) 18 4.3.2 Decarbamoylation of carbamates 18 4.3.3 Cleavage of morazone to phenmetrazine 18 4.4 Artifacts formed during acid hydrolysis 18 4.4.1 Cleavage of the ether bridge in beta-blockers and alkanolamine antihistamines (HY) 18 4.4.2 Cleavage of 1,4-benzodiazepines to aminobenzoyl derivatives (HY) 18 4.4.3 Cleavage and rearrangement of fN-demethyl metabolites of clobazam to benzimidazole derivatives (HY) 19 4.4.4 Cleavage and rearrangement of bis-deethyl flurazepam (HY -H <sub>2</sub> O) 19 4.4.5 Cleavage and rearrangement of tetrazepam and its metabolites 19 4.4.6 Dealkylation of ethylenediamine antihistamines (HY) 19 4.4.7 Hydration of a double bond (+H <sub>2</sub> O) 19 5 Table of Atomic Masses 20 6 Abbreviations 21 7 References 24  Tables  8 Table of Compounds in Order of Names 35 8.1 Explanatory notes 35 8.2 Table of compounds in order of names 37  9 Table of Compounds in Order of Categories 189  | 4.1.2 | S-Oxidation of phenothiazines 17   |
| 4.2.2 Cope elimination of N-oxides (-(CH <sub>3</sub> ) <sub>2</sub> NOH, -(C <sub>2</sub> H <sub>3</sub> ) <sub>2</sub> NOH, -C <sub>6</sub> H <sub>14</sub> N <sub>2</sub> O <sub>2</sub> ) 17 4.2.3 Rearrangement of bis-deethyl flurazepam (-H <sub>2</sub> O) 17 4.2.4 Elimination of various residues 17 4.2.5 Methylation of carboxylic acids in methanol ((ME), ME in methanol) 18 4.2.6 Formation of formaldehyde adducts using methanol as solvent (GC artifact in methanol) 18 4.3 Artifacts formed by thermolysis during GC and during acid hydrolysis (GC artifact, HY artifact) 18 4.3.1 Dehydration of alcohols (-H <sub>2</sub> O) 18 4.3.2 Decarbamoylation of carbamates 18 4.3.3 Cleavage of morazone to phenmetrazine 18 4.4 Artifacts formed during acid hydrolysis 18 4.4.1 Cleavage of the ether bridge in beta-blockers and alkanolamine antihistamines (HY) 18 4.4.2 Cleavage of the ether bridge in beta-blockers and alkanolamine antihistamines (HY) 18 4.4.3 Cleavage and rearrangement of N-demethyl metabolites of clobazam to benzimidazole derivatives (HY) 19 4.4.4 Cleavage and rearrangement of bis-deethyl flurazepam (HY -H <sub>2</sub> O) 19 4.4.5 Cleavage and rearrangement of bis-deethyl flurazepam (HY -H <sub>2</sub> O) 19 4.4.6 Dealkylation of a double bond (+H <sub>2</sub> O) 19  5 Table of Atomic Masses 20  6 Abbreviations 21  7 References 24  Tables  8 Table of Compounds in Order of Names 35 8.1 Explanatory notes 35 8.2 Table of compounds in order of names 37  9 Table of Compounds in Order of Categories 189   | 4.2   | Artifacts formed by thermolysis during GC (GC artifact) 17   |
| 4.2.3 Rearrangement of bis-deethyl flurazepam (H <sub>2</sub> O) 17 4.2.5 Methylation of various residues 17 4.2.5 Methylation of carboxylic acids in methanol ((ME), ME in methanol) 18 4.2.6 Formation of formaldehyde adducts using methanol as solvent (GC artifact in methanol) 18 4.3 Artifacts formed by thermolysis during GC and during acid hydrolysis (GC artifact, HY artifact) 18 4.3.1 Dehydration of alcohols (-H <sub>2</sub> O) 18 4.3.2 Decarbamoylation of carbamates 18 4.3.3 Cleavage of morazone to phenmetrazine 18 4.4 Artifacts formed during acid hydrolysis 18 4.4.1 Cleavage of the ether bridge in beta-blockers and alkanolamine antihistamines (HY) 18 4.4.2 Cleavage of 1/4-benzodiazepines to aminobenzoyl derivatives (HY) 18 4.4.3 Cleavage and rearrangement of N-demethyl metabolites of clobazam to benzimidazole derivatives (HY) 19 4.4.4 Cleavage and rearrangement of bis-deethyl flurazepam (HY-H <sub>2</sub> O) 19 4.4.5 Cleavage and rearrangement of bis-deethyl flurazepam (HY-H <sub>2</sub> O) 19 4.4.6 Dealkylation of ethylenediamine antihistamines (HY) 19 4.4.7 Hydration of a double bond (+H <sub>2</sub> O) 19  5 Table of Atomic Masses 20  6 Abbreviations 21  7 References 24  Tables  8 Table of Compounds in Order of Names 35 8.1 Explanatory notes 35 8.2 Table of compounds in order of names 37  | 4.2.1 | Decarboxylation of carboxylic acids 17   |
| 4.2.4 Elimination of various residues 17 4.2.5 Methylation of carboxylic acids in methanol ((ME), ME in methanol) 18 4.2.6 Formation of formaldehyde adducts using methanol as solvent (GC artifact in methanol) 18 4.3.1 Artifacts formed by thermolysis during GC and during acid hydrolysis (GC artifact, HY artifact) 18 4.3.2 Decarbamoylation of carbamates 18 4.3.3 Cleavage of morazone to phenmetrazine 18 4.4 Artifacts formed during acid hydrolysis 18 4.4.1 Cleavage of the ether bridge in beta-blockers and alkanolamine antihistamines (HY) 18 4.4.2 Cleavage of 1,4-benzodiazepines to aminobenzoyl derivatives (HY) 18 4.4.3 Cleavage and rearrangement of N-demethyl metabolites of clobazam to benzimidazole derivatives (HY) 19 4.4.4 Cleavage and rearrangement of bis-deethyl flurazepam (HY-H <sub>2</sub> O) 19 4.4.5 Cleavage and rearrangement of betrazepam and its metabolites 19 4.4.6 Dealkylation of ethylenediamine antihistamines (HY) 19 4.4.7 Hydration of a double bond (+H <sub>2</sub> O) 19  Table of Atomic Masses 20  6 Abbreviations 21  7 References 24  Tables  Table of Compounds in Order of Names 35  Explanatory notes 35  Table of compounds in order of names 37  9 Table of Compounds in Order of Categories 189  | 4.2.2 | Cope elimination of N-oxides (-(CH <sub>3</sub> ) <sub>2</sub> NOH, -(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> NOH, -C <sub>6</sub> H <sub>14</sub> N <sub>2</sub> O <sub>2</sub> ) 17 |
| 4.2.5 Methylation of carboxylic acids in methanol ((ME), ME in methanol) 18 4.2.6 Formation of formaldehyde adducts using methanol as solvent (GC artifact in methanol) 18 4.3.1 Dehydration of alcohols (-H <sub>2</sub> O) 18 4.3.2 Decarbamoylation of carbamates 18 4.3.3 Cleavage of morazone to phenmetrazine 18 4.4 Artifacts formed during acid hydrolysis 18 4.4.1 Cleavage of the ether bridge in beta-blockers and alkanolamine antihistamines (HY) 18 4.4.2 Cleavage of 1,4-benzodiazepines to aminobenzoyl derivatives (HY) 18 4.4.3 Cleavage and rearrangement of N-demethyl metabolites of clobazam to benzimidazole derivatives (HY) 19 4.4.4 Cleavage and rearrangement of bis-deethyl flurazepam (HY-H <sub>2</sub> O) 19 4.4.5 Cleavage and rearrangement of tetrazepam and its metabolites 19 4.4.6 Dealkylation of ethylenediamine antihistamines (HY) 19 4.4.7 Hydration of a double bond (+H <sub>2</sub> O) 19  Table of Atomic Masses 20  Abbreviations 21  References 24  Tables  Table of Compounds in Order of Names 35 8.1 Explanatory notes 35 8.2 Table of Compounds in order of names 37  Table of Compounds in Order of Categories 189   | 4.2.3 | Rearrangement of bis-deethyl flurazepam (-H <sub>2</sub> O) 17   |
| 4.2.6 Formation of formaldehyde adducts using methanol as solvent (GC artifact in methanol) 18 4.3 Artifacts formed by thermolysis during GC and during acid hydrolysis (GC artifact, HY artifact) 18 4.3.1 Dehydration of alcohols (-H <sub>2</sub> O) 18 4.3.2 Decarbamoylation of carbamates 18 4.3.3 Cleavage of morazone to phenmetrazine 18 4.4 Artifacts formed during acid hydrolysis 18 4.4.1 Cleavage of the ether bridge in beta-blockers and alkanolamine antihistamines (HY) 18 4.4.2 Cleavage of 1,4-benzodiazepines to aminobenzoyl derivatives (HY) 18 4.4.3 Cleavage and rearrangement of N-demethyl metabolites of clobazam to benzimidazole derivatives (HY) 19 4.4.4 Cleavage and rearrangement of bis-deethyl flurazepam (HY -H <sub>2</sub> O) 19 4.4.5 Cleavage and rearrangement of tetrazepam and its metabolites 19 4.4.6 Dealkylation of ethylenediamine antihistamines (HY) 19 4.4.7 Hydration of a double bond (+H <sub>2</sub> O) 19  5 Table of Atomic Masses 20  6 Abbreviations 21  7 References 24  Tables  8 Table of Compounds in Order of Names 35 8.1 Explanatory notes 35 8.2 Table of compounds in order of names 37  9 Table of Compounds in Order of Categories 189   | 4.2.4 | Elimination of various residues 17   |
| 4.3 Artifacts formed by thermolysis during GC and during acid hydrolysis (GC artifact, HY artifact) 18 4.3.1 Dehydration of alcohols (-H <sub>2</sub> O) 18 4.3.2 Decarbamoylation of carbamates 18 4.3.3 Cleavage of morazone to phenmetrazine 18 4.4.4 Artifacts formed during acid hydrolysis 18 4.4.1 Cleavage of the ether bridge in beta-blockers and alkanolamine antihistamines (HY) 18 4.4.2 Cleavage and rearrangement of N-demethyl metabolites of clobazam to benzimidazole derivatives (HY) 19 4.4.4 Cleavage and rearrangement of bis-deethyl flurazepam (HY -H <sub>2</sub> O) 19 4.4.5 Cleavage and rearrangement of bis-deethyl flurazepam (HY -H <sub>2</sub> O) 19 4.4.6 Dealkylation of ethylenediamine antihistamines (HY) 19 4.4.7 Hydration of a double bond (+H <sub>2</sub> O) 19  5 Table of Atomic Masses 20  6 Abbreviations 21  7 References 24  Tables  8 Table of Compounds in Order of Names 35 8.1 Explanatory notes 35 8.2 Table of compounds in order of names 37  9 Table of Compounds in Order of Categories 189   | 4.2.5 | Methylation of carboxylic acids in methanol ((ME), ME in methanol) 18  |
| 4.3.1 Dehydration of alcohols (-H <sub>2</sub> O) 18 4.3.2 Decarbamoylation of carbamates 18 4.3.3 Cleavage of morazone to phenmetrazine 18 4.4 Artifacts formed during acid hydrolysis 18 4.4.1 Cleavage of the ether bridge in beta-blockers and alkanolamine antihistamines (HY) 18 4.4.2 Cleavage of 1,4-benzodiazepines to aminobenzoyl derivatives (HY) 18 4.4.3 Cleavage and rearrangement of N-demethyl metabolites of clobazam to benzimidazole derivatives (HY) 19 4.4.4 Cleavage and rearrangement of bis-deethyl flurazepam (HY -H <sub>2</sub> O) 19 4.4.5 Cleavage and rearrangement of tetrazepam and its metabolites 19 4.4.6 Dealkylation of ethylenediamine antihistamines (HY) 19 4.4.7 Hydration of a double bond (+H <sub>2</sub> O) 19  5 Table of Atomic Masses 20  6 Abbreviations 21  7 References 24  Tables  8 Table of Compounds in Order of Names 35 8.1 Explanatory notes 35 8.2 Table of compounds in order of names 37  9 Table of Compounds in Order of Categories 189   | 4.2.6 | Formation of formaldehyde adducts using methanol as solvent (GC artifact in methanol) 18   |
| 4.3.2 Decarbamoylation of carbamates 18 4.3.3 Cleavage of morazone to phenmetrazine 18 4.4 Artifacts formed during acid hydrolysis 18 4.4.1 Cleavage of the ether bridge in beta-blockers and alkanolamine antihistamines (HY) 18 4.4.2 Cleavage of 1,4-benzodiazepines to aminobenzoyl derivatives (HY) 18 4.4.3 Cleavage and rearrangement of N-demethyl metabolites of clobazam to benzimidazole derivatives (HY) 19 4.4.4 Cleavage and rearrangement of bis-deethyl flurazepam (HY -H <sub>2</sub> O) 19 4.4.5 Cleavage and rearrangement of tetrazepam and its metabolites 19 4.4.6 Dealkylation of ethylenediamine antihistamines (HY) 19 4.4.7 Hydration of a double bond (+H <sub>2</sub> O) 19  5 Table of Atomic Masses 20  6 Abbreviations 21  7 References 24  Tables  8 Table of Compounds in Order of Names 35 8.1 Explanatory notes 35 8.2 Table of compounds in order of names 37  9 Table of Compounds in Order of Categories 189  | 4.3   | Artifacts formed by thermolysis during GC and during acid hydrolysis (GC artifact, HY artifact) 18   |
| 4.3.3 Cleavage of morazone to phenmetrazine 18 4.4 Artifacts formed during acid hydrolysis 18 4.4.1 Cleavage of the ether bridge in beta-blockers and alkanolamine antihistamines (HY) 18 4.4.2 Cleavage of 1,4-benzodiazepines to aminobenzoyl derivatives (HY) 18 4.4.3 Cleavage and rearrangement of N-demethyl metabolites of clobazam to benzimidazole derivatives (HY) 19 4.4.4 Cleavage and rearrangement of bis-deethyl flurazepam (HY -H <sub>2</sub> O) 19 4.4.5 Cleavage and rearrangement of tetrazepam and its metabolites 19 4.4.6 Dealkylation of ethylenediamine antihistamines (HY) 19 4.4.7 Hydration of a double bond (+H <sub>2</sub> O) 19  5 Table of Atomic Masses 20  6 Abbreviations 21  7 References 24  Tables  8 Table of Compounds in Order of Names 35 8.1 Explanatory notes 35 8.2 Table of compounds in order of names 37  9 Table of Compounds in Order of Categories 189  | 4.3.1 | Dehydration of alcohols (-H <sub>2</sub> O) 18   |
| 4.4 Artifacts formed during acid hydrolysis 18 4.4.1 Cleavage of the ether bridge in beta-blockers and alkanolamine antihistamines (HY) 18 4.4.2 Cleavage of 1,4-benzodiazepines to aminobenzoyl derivatives (HY) 18 4.4.3 Cleavage and rearrangement of N-demethyl metabolites of clobazam to benzimidazole derivatives (HY) 19 4.4.4 Cleavage and rearrangement of bis-deethyl flurazepam (HY -H <sub>2</sub> O) 19 4.4.5 Cleavage and rearrangement of tetrazepam and its metabolites 19 4.4.6 Dealkylation of ethylenediamine antihistamines (HY) 19 4.4.7 Hydration of a double bond (+H <sub>2</sub> O) 19  5 Table of Atomic Masses 20 6 Abbreviations 21 7 References 24  Tables  8 Table of Compounds in Order of Names 35 8.1 Explanatory notes 35 8.2 Table of compounds in order of names 37  9 Table of Compounds in Order of Categories 189   | 4.3.2 | Decarbamoylation of carbamates 18  |
| 4.4.1 Cleavage of the ether bridge in beta-blockers and alkanolamine antihistamines (HY) 18 4.4.2 Cleavage of 1,4-benzodiazepines to aminobenzoyl derivatives (HY) 18 4.4.3 Cleavage and rearrangement of N-demethyl metabolites of clobazam to benzimidazole derivatives (HY) 19 4.4.4 Cleavage and rearrangement of bis-deethyl flurazepam (HY -H <sub>2</sub> O) 19 4.4.5 Cleavage and rearrangement of tetrazepam and its metabolites 19 4.4.6 Dealkylation of ethylenediamine antihistamines (HY) 19 4.4.7 Hydration of a double bond (+H <sub>2</sub> O) 19  Table of Atomic Masses 20  Abbreviations 21  References 24  Tables  Table of Compounds in Order of Names 35 8.1 Explanatory notes 35 8.2 Table of compounds in order of names 37  Table of Compounds in Order of Categories 189  | 4.3.3 | Cleavage of morazone to phenmetrazine 18   |
| 4.4.2 Cleavage of 1,4-benzodiazepines to aminobenzoyl derivatives (HY) 18 4.4.3 Cleavage and rearrangement of N-demethyl metabolites of clobazam to benzimidazole derivatives (HY) 19 4.4.4 Cleavage and rearrangement of bis-deethyl flurazepam (HY -H <sub>2</sub> O) 19 4.4.5 Cleavage and rearrangement of tetrazepam and its metabolites 19 4.4.6 Dealkylation of ethylenediamine antihistamines (HY) 19 4.4.7 Hydration of a double bond (+H <sub>2</sub> O) 19  Table of Atomic Masses 20  Abbreviations 21  References 24  Tables  Table of Compounds in Order of Names 35 8.1 Explanatory notes 35 8.2 Table of compounds in order of names 37  Table of Compounds in Order of Categories 189  | 4.4   | Artifacts formed during acid hydrolysis 18   |
| <ul> <li>4.4.3 Cleavage and rearrangement of N-demethyl metabolites of clobazam to benzimidazole derivatives (HY) 19</li> <li>4.4.4 Cleavage and rearrangement of bis-deethyl flurazepam (HY -H<sub>2</sub>O) 19</li> <li>4.4.5 Cleavage and rearrangement of tetrazepam and its metabolites 19</li> <li>4.4.6 Dealkylation of ethylenediamine antihistamines (HY) 19</li> <li>4.4.7 Hydration of a double bond (+H<sub>2</sub>O) 19</li> <li>5 Table of Atomic Masses 20</li> <li>6 Abbreviations 21</li> <li>7 References 24</li> <li>Tables</li> <li>8 Table of Compounds in Order of Names 35</li> <li>8.1 Explanatory notes 35</li> <li>8.2 Table of compounds in Order of Categories 189</li> </ul>   | 4.4.1 | Cleavage of the ether bridge in beta-blockers and alkanolamine antihistamines (HY) 18  |
| <ul> <li>4.4.4 Cleavage and rearrangement of bis-deethyl flurazepam (HY -H<sub>2</sub>O) 19</li> <li>4.4.5 Cleavage and rearrangement of tetrazepam and its metabolites 19</li> <li>4.4.6 Dealkylation of ethylenediamine antihistamines (HY) 19</li> <li>4.4.7 Hydration of a double bond (+H<sub>2</sub>O) 19</li> <li>5 Table of Atomic Masses 20</li> <li>6 Abbreviations 21</li> <li>7 References 24</li> <li>Tables</li> <li>8 Table of Compounds in Order of Names 35</li> <li>8.1 Explanatory notes 35</li> <li>8.2 Table of compounds in order of names 37</li> <li>9 Table of Compounds in Order of Categories 189</li> </ul>   | 4.4.2 | Cleavage of 1,4-benzodiazepines to aminobenzoyl derivatives (HY) 18  |
| 4.4.5 Cleavage and rearrangement of tetrazepam and its metabolites 19 4.4.6 Dealkylation of ethylenediamine antihistamines (HY) 19 4.4.7 Hydration of a double bond (+H <sub>2</sub> O) 19  5 Table of Atomic Masses 20  6 Abbreviations 21  7 References 24  Tables  8 Table of Compounds in Order of Names 35  8.1 Explanatory notes 35  8.2 Table of compounds in order of names 37  9 Table of Compounds in Order of Categories 189   | 4.4.3 | Cleavage and rearrangement of N-demethyl metabolites of clobazam to benzimidazole derivatives (HY) 19  |
| <ul> <li>4.4.6 Dealkylation of ethylenediamine antihistamines (HY) 19</li> <li>4.4.7 Hydration of a double bond (+H<sub>2</sub>O) 19</li> <li>5 Table of Atomic Masses 20</li> <li>6 Abbreviations 21</li> <li>7 References 24</li> <li>Tables</li> <li>8 Table of Compounds in Order of Names 35</li> <li>8.1 Explanatory notes 35</li> <li>8.2 Table of compounds in order of names 37</li> <li>9 Table of Compounds in Order of Categories 189</li> </ul>  | 4.4.4 | Cleavage and rearrangement of bis-deethyl flurazepam (HY -H <sub>2</sub> O) 19   |
| 4.4.7 Hydration of a double bond (+H <sub>2</sub> O) 19  5 Table of Atomic Masses 20  6 Abbreviations 21  7 References 24  Tables  8 Table of Compounds in Order of Names 35  8.1 Explanatory notes 35  8.2 Table of compounds in order of names 37  9 Table of Compounds in Order of Categories 189  | 4.4.5 | Cleavage and rearrangement of tetrazepam and its metabolites 19  |
| 5 Table of Atomic Masses 20 6 Abbreviations 21 7 References 24  Tables 8 Table of Compounds in Order of Names 35 8.1 Explanatory notes 35 8.2 Table of compounds in order of names 37 9 Table of Compounds in Order of Categories 189   | 4.4.6 | Dealkylation of ethylenediamine antihistamines (HY) 19   |
| 6 Abbreviations 21 7 References 24  Tables 8 Table of Compounds in Order of Names 35 8.1 Explanatory notes 35 8.2 Table of compounds in order of names 37  9 Table of Compounds in Order of Categories 189  | 4.4.7 | Hydration of a double bond (+H <sub>2</sub> O) 19  |
| Tables  Table of Compounds in Order of Names 35  Explanatory notes 35  Table of compounds in order of names 37  Table of Compounds in Order of Categories 189   | 5     | Table of Atomic Masses 20  |
| Tables  8 Table of Compounds in Order of Names 35 8.1 Explanatory notes 35 8.2 Table of compounds in order of names 37  9 Table of Compounds in Order of Categories 189   | 6     | Abbreviations 21   |
| 8 Table of Compounds in Order of Names 35 8.1 Explanatory notes 35 8.2 Table of compounds in order of names 37  9 Table of Compounds in Order of Categories 189   | 7     | References 24  |
| 8.1 Explanatory notes 35 8.2 Table of compounds in order of names 37  9 Table of Compounds in Order of Categories 189   |       | Tables   |
| <ul> <li>8.1 Explanatory notes 35</li> <li>8.2 Table of compounds in order of names 37</li> <li>9 Table of Compounds in Order of Categories 189</li> </ul>  | 8     | Table of Compounds in Order of Names 35  |
| <ul> <li>8.2 Table of compounds in order of names 37</li> <li>9 Table of Compounds in Order of Categories 189</li> </ul>  | 8.1   | _  |
| - word of compounds in cruck of cutogories 100  | 8.2   | - •  |
| - word of compounds in cruck of cutogories 100  | 9     | Table of Compounds in Order of Categories 180  |
|   |       | - · · · · · · · · · · · · · · · · · · ·  |
| 9.2 Table of compounds in order of categories 189   |       |  |

## Contents of Volume 2 (Mass Spectra)

1.1 Arrangement of spectra 1
1.2 Lay-out of spectra 1

Explanatory Notes 1

Mass Spectra 89

Abbreviations 3

3

Compound Index 7