

Contents

Preface	xiii
About the Editors	xvii
List of Contributors	xix
1 Overview of Flavor and Fragrance Materials	1
<i>David Rowe</i>	
1.1 Flavor Aroma Chemicals	1
1.1.1 Nature Identical	1
1.1.1.1 Alcohols	2
1.1.1.2 Acids	3
1.1.1.3 Esters	4
1.1.1.4 Lactones	5
1.1.1.5 Aldehydes	5
1.1.1.6 Ketones	6
1.1.2 Heterocycles	6
1.1.2.1 Oxygen-containing	6
1.1.2.2 Nitrogen-containing	7
1.1.2.3 Sulfur-containing	8
1.1.3 Sulfur Compounds	8
1.1.3.1 Mercaptans	9
1.1.3.2 Sulfides	9
1.2 Flavor Synthetics	10
1.3 Natural Aroma Chemicals	11
1.3.1 Isolates	12
1.3.2 Biotechnology	12
1.3.3 'Soft Chemistry'	13

1.4	Fragrance Aroma Chemicals	14
1.4.1	Musks	14
1.4.2	Amber	15
1.4.3	Florals	16
1.4.4	'Woodies'	17
1.4.5	Acetals and Nitriles	17
1.5	Materials of Natural Origin	18
1.5.1	Essential Oils	18
1.5.1.1	Cold-pressing – Citrus Oils	18
1.5.1.2	Steam-distilled Oils	19
1.5.1.3	A Note on 'Adulteration'	20
1.5.2	Absolutes and Other Extracts	21
	Acknowledgments	21
	References	21
2	Sample Preparation	23
	<i>Russell Bazemore</i>	
2.1	Introduction	23
2.2	PDMS	24
2.3	Static Headspace Extraction	25
2.3.1	Advantages and Disadvantages	25
2.4	Dynamic Headspace Extraction	26
2.4.1	Advantages	27
2.4.2	Disadvantages	27
2.5	Solid Phase Microextraction (SPME)	27
2.5.1	Research	27
2.5.2	Practical	29
2.5.3	Advantages	32
2.5.4	Disadvantages	32
2.6	Stir Bar Sorptive Extraction	33
2.6.1	Research	33
2.6.2	Practical	34
2.6.3	Advantages	35
2.6.4	Disadvantages	35
2.7	PDMS Foam and Microvial	36
2.7.1	PDMS Foam	36
2.7.2	Microvial	36
2.8	Solvent Extraction	39
2.8.1	MIXXOR	39
2.8.2	Soxhlet Extraction	39

2.8.3	Solvent Assisted Flavor Evaporation (SAFE)	42
2.9	Summary	42
	References	42
3	Traditional Flavor and Fragrance Analysis of Raw Materials and Finished Products	45
	<i>Russell Rouseff and Kevin Goodner</i>	
3.1	Overview	45
3.2	Physical Attribute Evaluation	47
3.2.1	Color – Optical Methods	48
3.2.2	Turbidity	49
3.2.3	Water Activity	49
3.2.4	Moisture Content	50
3.2.4.1	Karl Fischer Method	50
3.2.4.2	Secondary Moisture Determination Methods	51
3.2.5	Optical Rotation	51
3.2.6	Specific Gravity	52
3.2.7	Refractive Index	52
3.2.8	Sugars/Soluble Solids	53
3.2.9	Viscosity	54
3.3	Instrumental Analysis	54
3.3.1	Separation Techniques	55
3.3.1.1	Gas Chromatography (GC)	55
3.3.1.2	GC Retention Data	55
3.3.1.3	Standardized Retention Index Systems	55
3.3.1.4	GC Injection	56
3.3.1.5	GC Columns (Stationary Phases)	58
3.3.1.6	GC Detectors	60
3.3.2	Identification Techniques	63
3.3.2.1	Retention Index Approach	63
3.3.2.2	GC–MS	64
3.3.2.3	MS/MS	65
	References	67
4	Gas Chromatography/Olfactometry (GC/O)	69
	<i>Kanjana Mahattanatawee and Russell Rouseff</i>	
4.1	Introduction	69
4.2	Odor Assessors' Selection and Training	70
4.3	Sensory Vocabulary	71

4.4	GC/Olfactometers (Sniffers)	72
4.5	Practical Considerations	73
4.6	Types of GC/Olfactometry	73
4.6.1	Dilution Analysis	73
4.6.2	Time Intensity	76
4.6.3	Detection Frequency	79
4.6.4	Posterior Intensity Method	82
4.7	Sample Introduction	83
4.8	Identification of Aroma-active Peaks	84
4.8.1	Standardized Retention Index Values	84
4.8.2	Aroma Description Matching	85
4.8.3	MS Identifications	85
4.8.4	Use of Authentic Standards	86
4.9	Conclusion	86
	References	87
5	Multivariate Techniques	91
	<i>Vanessa Kinton</i>	
5.1	Introduction	91
5.2	Hierarchical Cluster Analysis (HCA)	97
5.3	Principal Component Analysis (PCA)	98
5.4	Classification Models	99
5.4.1	k -Nearest Neighbors (k -NN)	100
5.4.2	Soft Independent Modeling of Class Analogy (SIMCA)	100
5.5	Principal Component Regression	101
5.6	Example of Data Analysis for Classification Models	102
5.6.1	Tabulating Data	102
5.6.2	Examining Data	103
5.6.3	Multivariate Exploratory Analysis	103
5.6.4	Creation of a Classification Model with a Training Set and Validation with a Testing Set	106
	References	109
6	Electronic Nose Technology and Applications	111
	<i>Marion Bonnefille</i>	
6.1	Introduction	111
6.2	Human Smell and Electronic Noses	112
6.3	Techniques to Analyze Odors/Flavors	113
6.3.1	Sensory Panel	113
6.3.2	GC and GC/MS	114

6.3.3	GC/Olfactometry	114
6.3.4	Electronic Nose	115
6.3.5	Electronic Nose Technology and Instrumentation	115
6.3.5.1	Architecture	115
6.3.5.2	Air Generator	117
6.3.5.3	Sampling	118
6.3.5.4	Detection Technologies	121
6.3.6	Data Treatment Tools	127
6.4	The Main Criticisms Directed at the Electronic Nose	134
6.5	Market and Applications	136
6.5.1	Application Range	136
6.5.2	Perfumery Compound Detection in a Fragrance	138
6.5.3	Cosmetic Natural Raw Materials: Characterization of Volatile Constituents of Benzoin Gum	139
6.5.4	Home Care Products: Identification and Quantification Using an Electronic Nose in the Perfumed Cleaner Industry	142
6.5.5	Pharmaceutical Products: Flavor Analysis in Liquid Oral Formulations	146
	References	151
7	MS/Nose Instrumentation as a Rapid QC Analytical Tool <i>Ray Marsili</i>	155
7.1	Introduction	155
7.2	Operating Principle	157
7.3	Advantages of MS over Solid State Sensors	160
7.4	Using Other Sample Preparation Modes	160
7.5	Techniques for Improving Reliability and Long-term Stability	161
7.5.1	Calibration Transfer Algorithms	161
7.5.2	Internal Standards	162
7.6	Two Instruments in One	163
7.7	Application Examples	163
7.8	Classification of Coffee Samples by Geographic Origin	164
7.9	Classification of Whiskey Samples by Brand	166
7.10	Future Directions: Partnering MS/Nose with GC/MS	168
7.11	Conclusion	170
	References	170

8	Sensory Analysis	173
	<i>Carlos Margaria and Anne Plotto</i>	
8.1	Introduction	173
8.2	The Purpose of Sensory Analysis	174
8.3	Flavor Perception	177
8.4	Sensory Analysis Techniques	178
8.4.1	Overall Difference Tests	179
8.4.1.1	Triangle Test	180
8.4.1.2	Duo-Trio Test	182
8.4.1.3	Simple Difference Test	182
8.4.2	Single Attribute Difference Tests	184
8.4.2.1	Difference from Control	184
8.4.2.2	Paired Comparison Test	184
8.4.2.3	Ranking Tests	185
8.4.3	Descriptive Tests	186
8.4.4	Affective Tests	188
8.5	Preparation and Planning	189
8.5.1	Experimental Design	189
8.5.2	Environment	191
8.5.3	Sample Preparation	191
8.6	Panel Selection	192
8.6.1	Trained Panels	193
8.6.2	Consumer Panels	194
8.7	Conducting a Panel	195
8.8	Expression of Results	196
8.9	Conclusions	197
	References	198
9	Regulatory Issues and Flavors Analysis	201
	<i>Robert A. Kryger</i>	
9.1	Introduction	201
9.2	Regulatory Overview	202
9.2.1	History	202
9.2.2	Safety Regulations	204
9.2.3	Product Labelling Regulations	206
9.2.4	Fair Trade/Conformity with Established Standards	208
9.2.5	Flavor Types	209
9.2.6	Governing Authorities	211
9.2.7	Role of Flavor Analysis in Regulatory Conformance	212

9.3	Specific Regulatory Issues	213
9.3.1	Identifying the Presence of ‘Forbidden’ Substances	213
9.3.1.1	Heavy Metals such as Pb, As, Hg, and Cd	214
9.3.1.2	Pesticides	214
9.3.1.3	Environmental Toxins	215
9.3.1.4	Allergen Testing	216
9.3.2	Testing Whether a Product is ‘Natural’ or Meets a ‘Standard of Identity’	216
9.3.3	Testing for Other Regulatory Compliance Requirements	219
	References	220
	Index	223