



The background of the cover features four origami paper airplanes. Each airplane has a chemical structure drawn on its wing. The structures are: 1) 4-methoxy-3-hydroxybenzaldehyde, 2) 2-methyl-2-butanol, 3) 2,6-dimethyl-2,7-octadien-1-ol, and 4) a bicyclic ether. The title 'THE CHEMISTRY AND BIOLOGY OF VOLATILES' is centered over the middle of the cover, with 'VOLATILES' in a larger, gold-colored font.

THE CHEMISTRY AND BIOLOGY OF VOLATILES

Editor Andreas Herrmann

 WILEY

The Chemistry and Biology of Volatiles

Edited by

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The Chemistry and Biology of Volatiles

Foreword

Volatile compounds play an important role in nature as messenger compounds to transmit selective information between species. The ubiquity of these compounds in our everyday environment has initiated a variety of research activities in the life sciences over recent decades. Both biologists and chemists became interested in exploring the role of bioactive volatile compounds in many different aspects. The evolution from molecular to supramolecular science has particularly influenced the research activities on the chemistry and biology of volatiles. The investigation of molecular properties beyond the single molecule required (and resulted in) numerous interdisciplinary efforts to answer important questions related to the role of these compounds in our direct environment.

Molecular recognition is one of the key aspects leading to the understanding of the biological processes involved in volatile signalling. In contrast to the investigation of host–guest interactions typically encountered in the area of pharmaceutical or biomedical research, which usually take place in aqueous solution, volatile compounds have to be diffused into the air and transported over large distances to reach their biological target. The specific feature of their volatility, as compared to other bioactive molecules, characterizes the behaviour of these molecules from their biogenesis, to their emission, analysis, release, transport, recognition and perception, up to their degradation in a specific environment.

The present book summarizes several aspects related to the chemistry and biology of volatile compounds in a structure-based approach and tries to give the reader an introduction to and general overview of the various research areas related to this particular class of molecules. It also provides perspectives along novel avenues of research and development. It should thus be of great interest to all those involved in the various facets of both basic and applied research on volatile compounds.

Jean-Marie Lehn
Strasbourg
November 2009

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Finally, I thank my superiors Dr. Daniel Benczédi, Dr. Maria-Inés Velazco and Dr. Antoine Gautier from Firmenich for supporting this project, and I thank my wife Anja for her patience. I hope this book provides an interesting and stimulating interdisciplinary approach to the chemistry and biology of volatile compounds, and that the readers forgive the errors that may have escaped the proofreading.

Andreas Herrmann
Genève
January 2010

Abbreviations

Ac	acetyl (in structural formula)
ACC	1-aminocyclopropane-1-carboxylic acid
ACS	American Chemical Society
ACSO	<i>S</i> -allyl-L-cysteine sulfoxide
AE	aroma extract
AEDA	aroma extract dilution analysis
AFNOR	Association Française de Normalisation
AMDIS	automatic mass spectral deconvolution
AMPI	acetylmethyl phosphinate
APC	anterior piriform cortex
approx.	approximately
APS	adenosine-5'-phosphosulfate
aq.	aqueous
ASE	accelerated solvent extraction
ASES	aerosol solvent extraction system
ATP	adenosine-5'-triphosphate
BASF	Badische Anilin und Soda Fabrik
BINAP	2,2'-bis(diphenylphosphino)-1,1'-binaphthyl
BOLD	blood oxygenation level dependent
BOSS	beaver dam offspring study
Bu	butyl (in structural formula)
BVOC	biogenic volatile organic compound
ca.	<i>circa</i>
cAMP	cyclic adenosine monophosphate
CAN-BD	carbon dioxide assisted nebulization with a bubble dryer
CAR	carboxen
cat.	catalyst/catalytic
CBF	cerebral blood flow
CD	circular dichroism (spectroscopy)
CDs	cyclodextrins
CDP	cytidine-5'-diphosphate
CDP-ME	4-diphosphocytidyl-2- <i>C</i> -methyl-D-erythritol
CDP-ME2P	4-diphosphocytidyl-2- <i>C</i> -methyl-D-erythritol-2-phosphate
CDP-MEP	diphosphocytidyl-2-methyl-D-erythritol-2-phosphate
C-GC	conventional gas chromatography
CI	Criegee intermediate
CI-MS	chemical ionization-mass spectrometry
CITAC	Cooperation on International Traceability in Analytical Chemistry

CITES	Convention on International Trade in Endangered Species of Wild Fauna and Flora
CoA	coenzyme A
COBEL	children's olfactory behaviors in everyday life
conc.	concentrated
COSY	correlation spectroscopy
Cp	cyclopentadienyl
CPCSP	continuous powder coating spraying process
CRC	Chemical Rubber Company
CS	cysteine synthase
CSO	alk(en)ylcysteine sulfoxide
CTP	cytidine-5'-triphosphate
1D	one-dimensional
2D	two-dimensional
3D	three-dimensional
DADS	diallyl disulfide
DC	direct contact
DCMU	diuron
DEET	<i>N,N</i> -diethyl-2-toluamide
DELOS	depressurization of an expanded liquid organic solution
d.f.	film thickness
D-HS	dynamic headspace
DIBAL-H	diisobutylaluminium hydride
dil.	diluted
DMAPP	3,3-dimethylallyl diphosphate
DMSO	dimethylsulfoxide
DNA	deoxyribonucleic acid
DOX	1-deoxy-D-xylulose
DOXP	1-deoxy-D-xylulose 5-phosphate
DP	dual phase
DSC	differential scanning calorimetry
DTBP	di- <i>tert</i> -butyl peroxide
DVB	divinylbenzene
DXR	DOXP reductoisomerase
DXS	DOXP synthase
EAD	electroantennographic detection
EAG	electroantennogram
Ed.	editor/editing
EDGAR	emissions database for global atmospheric research
<i>ee</i>	enantiomeric excess
EEG	electroencephalogram
EHLS	epidemiology of hearing loss study
EO	essential oil
EPA	Environmental Protection Agency (USA)
<i>er</i>	enantiomeric ratio
ES-GC	enantioselective gas chromatography

ESP	epithiospecifier protein
ET	ethylene
Et	ethyl (in structural formula)
etc.	<i>et cetera</i>
EU	European Union
FACs	fatty acid–amino acid conjugates
FAO	Food and Agriculture Organisation (of the United Nations)
Fd	ferredoxin
FFNSC	flavour and fragrance natural and synthetic compounds
F-GC	fast gas chromatography
FID	flame ionization detector
fMRI	functional magnetic resonance imaging
FPP	farnesyl diphosphate
FQPA	Food Quality Protection Act (USA)
FSOT	fused silica open tubular
GA-3-P	glyceraldehyde-3-phosphate
GAS	gas (or supercritical fluids) anti-solvent
GC	gas chromatography
GC-FID	gas chromatography–flame ionization detection
GC-MS	gas chromatography–mass spectrometry
GC-qMS	gas chromatography–quadrupole mass spectrometry
GC-O	gas chromatography–olfactometry
GGPP	geranylgeranyl diphosphate
γ GP	γ -glutamyl sulfoxide peptide derivative
GPP	geranyl diphosphate
GS	glucosinolate
GSH	reduced glutathione
GSSG	oxidised glutathione disulfide
HCC-HS	high concentration capacity headspace technique
HIPVs	herbivore-induced plant volatiles
HIV	human immunodeficiency virus
HLA	human leukocyte antigen
HMBC	heteronuclear multiple bond coherence
HMBPP	4-hydroxy-3-methyl-2-(<i>E</i>)-butenyl diphosphate
HMG	hydroxyl-methylglutaryl
HMPA	hexamethylphosphoramide
HMQC	heteronuclear multiple quantum coherence
HPC	hydroxypropyl cellulose
HPLC	high performance liquid chromatography
HPOD	hydroperoxyoctadienoate
HR	heart rate
HS	headspace
HS-LPME	headspace–liquid phase microextraction
HS-MS	headspace–mass spectrometry
HSQC	heteronuclear single quantum coherence
HSSE	headspace sorptive extraction

HS-SPDE	headspace–solid phase dynamic extraction
HS-SPME	headspace–solid phase microextraction
HS-SMSE	headspace–silicon membrane sorptive extraction
HS-STE	headspace–sorptive tape extraction
IAA	indole-3-acetic acid
IATA	International Air Transport Association
i.d.	inner diameter
IFF	International Flavors and Fragrances Inc.
IFRA	International Fragrance Association
INCAT	inside needle capillary adsorption trap
IOFI	International Organization of the Flavour Industry
IPP	isopentenyl diphosphate
IRMS	isotope ratio mass spectrometry
<i>IspD</i>	CDP-ME synthase
<i>IspE</i>	CDP-ME kinase
<i>IspF</i>	MEcPP synthase
<i>IspG</i>	HMBPP synthase
<i>IspH</i>	HMBPP reductase
ISTD	internal standard
IUPAC	International Union of Pure and Applied Chemistry
JA	jasmonic acid
LC	liquid chromatography
LDA	lithium diisopropylamine
LF	lachrymatory factor
LFS	lachrymatory factor synthase
LMCS	longitudinally modulated cryogenic system
LOD	limit of detection
LOQ	limit of quantification
<i>LOX3</i>	lipxygenase 3 (gene)
MACR	methacrolein
MAE	microwave-assisted extraction
MA-HD	microwave-assisted hydrodistillation
MAM	methylthioalkylmalate
MBO	2-methylen-3-buten-2-ol
MCSO	<i>S</i> -methyl-L-cysteine sulfoxide
MD	multidimensional
ME	male equivalents
Me	methyl (in structural formula)
MEcPP	2- <i>C</i> -methyl-D-erythritol-2,4-cyclodiphosphate
MeJA	methyl jasmonate
MeSA	methyl salicylate
MEP	2- <i>C</i> -methylerythritol-4-phosphate
MESI	membrane extraction sorbent interface
MGL	methionine- γ -lyase
MHC	major histocompatibility complex
MHE	multiple headspace extraction

ML	maple lactone
MME	membrane microextraction
MS	mass spectrometry, mass spectrometer
Ms	mesyl (SO_2CH_3 ; in structural formula)
MVA	mevalonic acid/mevalonate
MVL	mevalonolactone
MVK	methyl vinyl ketone
MW	molecular weight
MYB	myeloblast
NADPH	nicotinamide adenine dinucleotide phosphate
NB	narrow bore (column)
NIST	National Institute of Standards and Technology
NMO	<i>N</i> -methymorpholine- <i>N</i> -oxide
NMR	nuclear magnetic resonance
NOESY	nuclear Overhauser enhancement spectroscopy
NPQ	nonphotochemical quenching
NS	nosespace
Nu	nucleophile (in structural formula)
OAV	odour activity values
OB	olfactory bulb
OCO	oral cavity only (exposure)
OFC	orbitofrontal cortex
OP	other phytohormones
OPE	ozone production efficiency
OR	olfactive receptor
ORNs	olfactive receptor neurons
OV	Ohio Valley Speciality Chemical (brand of stationary phases)
EXP-01	2-decyl-1-oxaspiro[2.2]pentane
EXP-04	2-(4-hydroxybutyl)-1-oxaspiro[2.2]pentane
PAN	peroxyacetyl nitrate
PAPS	adenosine-3'-phosphate-5'-phosphosulfate
PCA	principal component analysis
PCSO	<i>S</i> -propyl-L-cysteine sulfoxide
pdf	portable document format
PeCSO	<i>trans-S</i> -1-propenyl-L-cysteine sulfoxide
PEG	poly(ethylene glycol)
PET	positron emission tomography
PBP1	pheromone binding protein 1
PD	Parkinson's disease
PDMS	poly(dimethylsiloxane)
PEP	phosphoenol pyruvate
PG	protecting group
PGA	phosphoglyceric acid
PGSS	particles from gas-saturated solutions
Ph	phenyl (in structural formula)
PLP	pyridoxal-5'-phosphate

PMHS	poly(methylhydrosiloxane)
pp.	pages
PPC	posterior piriform cortex
PTR-MS	proton transfer reaction–mass spectrometer
qMS	quadrupole mass spectrometry (detector)
quant.	quantitative
RA	retinoic acid
ref.	reference
RESS	rapid expansion of supercritical fluids
RNA	ribonucleic acid
RSD	relative standard deviation
r.t.	room temperature
RTL	retention time locking
RubisCO	ribulosebisphosphate carboxylase/oxygenase
SA	salicylic acid
SAA	supercritical assisted atomization
SAS	supercritical fluids (or gas) anti-solvent
SAT	serine acetyltransferase
SBSE	stir bar sorptive extraction
SC	skin conductance
SCC-GC	short capillary column gas chromatography
sc-CO ₂	supercritical CO ₂
SDE	simultaneous distillation–extraction
SDOIT	San Diego odor identification test
SEDS	solution enhanced dispersion by supercritical fluids
SFE	supercritical fluid extraction
SFEE	supercritical fluid extraction of emulsions
S-HS	static headspace
SIM	single ion monitoring
SIM-MS	single ion monitoring–mass spectrometry
SIM-qMS	single ion monitoring–quadrupole mass spectrometry
SiSTEx	solvent in silicone tube extraction
SMP	skimmed milk powder
SMSE	silicon membrane sorptive extraction
SOA	secondary organic aerosol
SPACE	solid phase aroma concentrate extraction
SPME	solid phase microextraction
SROs	stress-related odours
SSI	supercritical solvent impregnation
S&T-HS	static and trapped headspace
TAS	total analysis systems
TCD	thermal conductivity detector
TDS	thermodesorption system
<i>tert</i>	tertiary
THF	tetrahydrofuran
TIC	total ion current

TIC-MS	total ion current–mass spectrometry
TLC	thin-layer chromatography
TMS	trimethylsilyl (protecting group)
TMT	thiol methyltransferases
TOF	time of flight
TPLSM	two-photon laser scanning microscopy
TRGs	temperature-responsive gels
Ts	tosyl ($\text{SO}_2\text{C}_6\text{H}_4\text{CH}_3$; in structural formula)
<i>p</i> -TSA	<i>para</i> -toluenesulfonic acid
UFM-GC	ultra-fast module gas chromatography
UK	United Kingdom of Great Britain and Northern Ireland
UNEP	United Nations Environment Programme
USA	United States of America
UV	ultraviolet (spectroscopy)
UV/Vis	ultraviolet/visible (spectroscopy)
VOC	volatile organic compound
Vol.	volume
WOF	warmed-over flavour
WPC	whey protein (isolate) concentrate

Names of scientific journals are abbreviated according to the Chemical Abstracts Service Source Index

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