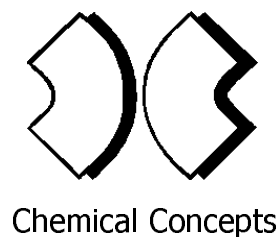


Volatile Compounds in Food

2nd Edition

User Manual

Version 1.0



Volatile Compounds in Food, 2nd Edition

Wiley-VCH Verlag GmbH & Co. KGaA, Chemical Concepts

Division, Weinheim, 2003.

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Wiley-VCH Verlag GmbH & Co. KGaA, Chemical Concepts Division,
Boschstrasse 12, D-69469 Weinheim, Germany.

Dear Customer,

Chemical Concepts is pleased to provide you with the database "Volatile Compounds in Food, 2nd Edition".

The database package contains one CD ROM which includes pre-formatted database versions which could be used directly with the majority of commercially available mass spectroscopy software systems. Formats included on this CD ROM are:

Benchtop/SPC
Excalibur
Finnigan GCQ
Finnigan TSQ
Finnigan SSQ
Finnigan Ion-Trap
Finnigan INCOS
Fisons VG Masslab
HP Chemstation
NetCDF
NIST
Shimadzu QP-5000
Varian ITS-40

If you have any question, please do not hesitate to contact us.

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Fax: +49 (0) 6201 606 - 328

We look forward to working with you.

Sincerely,

The Chemical Concepts Team

Data collected by:

Central Institute of Nutrition and Food Research (TNO)

AJ Zeist, Netherlands

Database created and marketed by:

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Database Content:

The Volatile Compounds in Food reference mass spectra collection contains 1,620 mass spectra which cover the whole range of volatile compounds in food. Apart from the large number of natural, nature-identical and artificial flavours and aromas, there are – among others – food additives and solvents, pesticides and veterinary pharmaceutical compounds, which are frequently found as residues. Derivatives of non-volatile compounds such as sugars or polyhydroxyphenols are also available.

A substantial number of the flavour and aroma compounds in this collection contain oxygen functional groups. The following are frequently present: alcohols, ethers, aldehydes, ketones, acetals, ketals, acids and esters.

Additional information:

Chemical structure

Chemical name

Molecular formula

Molecular weight (Nominal mass)

Base peak

Reference

Measurement condition

Instructions for installing the library:

Since the format with which the database is delivered on this CD ROM is compatible with several programs please check the manual of your specific software on how to install an additional library to your system. In general this is done by copying all the database files on the CD ROM to a directory below the location where your application software resides. Please note that you need to copy only the database files from the directory of the specific format you need for your software.

Please select the format of the databases to install according to your spectrometry software from the following provided formats (given in parenthesis are the extensions of the database files):

HP Chemstation (.L)

Excalibur / NIST (.dbu, .inu, .num, .sdb)

Finnigan GCQ / TSQ / SSQ – Varian ITS-40 (.lbr)

Finnigan Ion-Trap (.lib, .inx)

Finnigan INCOS (.ls, .lx)

Fisons VG Masslab (.idb ...)

NetCDF (.cdf)

Shimadzu QP-5000 (.com, .flg, .fom, .lib, .nam, .spc)

Benchtop (.spc)

In the top level directory of the CD ROM you will also find a separate listing of the chemical compound's names in MS WORD (.doc) and Adobe Acrobat Reader (.pdf) format. In addition to that the chemical structures are provided as single MDL MOL files in the directory "MOL".

In case of questions or problems please contact your dealer or send an e-mail to 'support@cc.wiley-vch.de'.

Thanks again,

Chemical Concepts

Chemical Concept uses its best efforts to deliver a high quality copy of the database and to verify that the data contained therein have been selected on the basis of sound scientific judgment. However, Chemical Concepts makes no warranties to that effect and shall be held liable for any damage that may result from errors or omissions in the database.

For more information about mass spectral collections offered by Chemical Concepts, please have a look into the 'brochure_CC_MS_collections.pdf' on this CD ROM. (Please note that for viewing the brochure you need to have a 'pdf'-viewer installed (e.g. the free-of-charge Acrobat Reader from Adobe - for more information please see www.adobe.com).

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