FFNSC 4 LIBRARY

(Flavour and Fragrance Natural and Synthetic Compounds)

INSTRUCTION MANUAL

Warranty

Chromaleont provides the following warranty for this product.

1. Period: Please contact your Sales representative for information about the period of this warranty.

2. Description: If a product/part failure occurs for reasons attributable to Chromaleont during the warranty period, Chromaleont will repair or replace the product/part free of charge. However, in the case of products which are usually available on the market only for a short time, such as personal computers and their peripherals/parts, Chromaleont may not be able to provide identical replacement products.

3. Limitation of Liability:
1. In no event will Chromaleont be liable for any lost revenue, profit or data, or for special, indirect, consequential, incidental or punitive damages, however caused regardless of the theory of liability, arising out of or related to the use of or inability to use the product, even if Chromaleont has been advised of the possibility of such damage.
2. In no event will Chromaleont's liability to you, whether in contract, tort (including negligence), or otherwise, exceed the amount you paid for the product.

4. Exceptions: Failures caused by the following are excluded from the warranty, even if they occur during the warranty period.
1. Improper product handling
2. Repairs or modifications performed by parties other than Chromaleont or Chromaleont designated companies
3. Product use in combination with hardware or software other than that designated.
4. Computer viruses leading to device failures and damage to data and software, including the product's basic software
5. Power failures, including power outages and sudden voltage drops, leading to device failures and damage to data and software, including the product's basic software
6. Turning OFF the product without following the proper shutdown procedure leading to device failures and damage to data and software, including the product's basic software
7. Reasons unrelated to the product itself
8. Product use in harsh environments, such as those subject to high temperatures or humidity levels, corrosive gases, or strong vibrations
9. Fires, earthquakes, or any other act of nature, contamination by radioactive or hazardous substances, or any other force majeure event, including wars, riots, and crimes
10. Product movement or transportation after installation
11. Consumable items
Recording media such as floppy disks and CD-ROMs are considered consumable items.

* If there is a document such as a warranty provided with the product, or there is a separate contract agreed upon that includes warranty conditions, the provisions of those documents shall apply.

1) Information in this manual is subject to change without notice and does not represent a commitment on the part of the vendor.
2) Any errors or omissions which may have occurred in this manual despite the utmost care taken in its production will be corrected as soon as possible, although not necessarily immediately after detection.

4) Microsoft and Windows are registered trademarks of Microsoft Corporation in the United States and/or other countries. The TM and ® symbols are omitted in this manual.
5) FFNSC GC/MS Library is a product name of Chromaleont S.r.l. in Italy

Original version is approved in English.

Table of Contents

1 Introduction

This FFNSC (Flavour and Fragrance Natural and Synthetic Compounds) library is a library containing natural and synthetic compounds in essential oils and fragrant materials for dedicated use with the Shimadzu GC/MS software. The FFNSC 4 Library contains not only GC/MS spectra but also retention indices of 4030 compounds. This library is supplied from Chromaleont S.r.l., the spin-off company from Messina University, Italy, and the whole registered data is measured using Shimadzu GCMS-QP2010 by Prof. Mondello and the members of his research groups of Messina University.
The “Presentation of Product” written by Prof. Mondello is included in the CD-ROM. This document is so useful that you are recommended to read it.

NOTICE

1. Chromaleont S.r.l., Italy, owns the copyright to this library. Shimadzu acts as their agent in granting the customer permission to use these libraries. Shimadzu is in no way responsible for the content of these libraries.

2. These libraries may be installed on only one system on which Shimadzu GC/MS software will be used. To use these libraries on two or more systems, the customer will need to purchase that number of copies of these libraries.

3. These libraries may not be copied for any purpose except installation and making a backup. In addition, these libraries software cannot be rented, transferred, analyzed or altered.

WARNING

This is a CD-ROM disk. Do NOT play this on an audio CD player, as the high volume may damage your hearing or the audio speakers.

2 Description

2.1 Configuration of the Library

2.1.1 Components

This library contains one CD-ROM disk and one instruction manual.

2.1.2 Files Configuration of the Library

The FFNSC library comprises the following 7 files:

FFNSC 4.0.LIB Contains header information about the library and compound information, including molecular weights and CAS registration numbers.

FFNSC 4.0.FOM Contains compound composition formulas.

FFNSC 4.0.SPC Contains spectra information for compounds.

FFNSC 4.0.NAM Contains compound names.

FFNSC 4.0.COM Contains comments.

FFNSC 4.0.FLG Contains information about search targets.

FFNSC 4.0. ADD Contains information about columns.

In the Shimadzu GC/MS software, any library is represented by the file extension .LIB (FFNSC 4.0 Library is FFNSC 4.0.LIB). Files with this extension are the only library files the user need be concerned with.

Structure formulas are not included in this library.

This library will function as a library only when the seven files mentioned above are stored in the same folder.

2.2 Library File Operations

2.2.1 Search Using the Library

You can use this library as mass spectral library for the Shimadzu GC/MS software.

2.2.2 Library File Operations

This library will not function as a library unless all of the 7 files described in the first section are in the same folder.
When you copy, move or rename this library please be aware of the following.

When copying: Be sure to copy the 7 files into the same folder.

When moving: Be sure to move the 7 files into the same folder.

When renaming: Renaming these libraries are not recommended as this may cause problems. If you absolutely must rename the library, be sure to give the 7 files the same filename. DO NOT change the extensions as this will make it impossible to access the library.

When deleting: If you absolutely must delete the library, be sure to delete all 7 of the files.

Additionally, this library may not be copied for any purpose other than for making a backup.

2.3 Library Contents

This library includes, addition to mass spectrum, CAS number, common and scientific compound name, molecular
weight, molecular formula, mass of base peak and retention indices for each registered compound.
The GC/MS analysis for the registered compounds was performed with Shimadzu GCMS-QP2010.

(Note)
Retention index is generally dependent on the kind of stationary phase of column. Additionally, for some compounds, retention index is affected by film thickness of column, column length, sample matrix, contamination of column and analysis condition. We recommend use of the same column and same analytical conditions as the library data were measured with to obtain accurate results when you use retention indices for analysis. Use of the different column with same stationary phase provides almost same result except some specific compounds. The column and analysis condition used in creation of this library is described in Appendix 2.

(Note)
The RI functionality is available in GCMSsolution Ver.2.4 or later.
The manual describing the searching method using retention indices is stored in the folder “\English\DOC” in the CD for GCMSsolution.

(Note)
Please note that there are cases that the registered contents are different from the previous versions even for the same compounds in order to provide the updated information.

(Note)
For the notation of molecular formula in this library, each element is separated by space. Use this notation when performing index search with molecular formula.
Example: C2 H6 S (correct) C2H6S (incorrect)

3 Library Installation

3.1 Library Installation

The CD-ROM disk can be damaged. It is strongly recommended to copy the libraries to the hard disk in the PC, and store the CD-ROM disk as backup.

The size of the library is about 9.5 MB.

Copy the seven files “FFNSC 4.0” in the CD to a proper folder in the hard disk using the Explorer (usually, C:\GCMSsolution\LIBRARY)., then use the copied files.

Appendix 1. Retention Index

The retention times of any homologue series with the number of carbon atoms show linear relation to the retention time of a homologue series standard for programmed temperature analysis. Retention index is a measure of retention time and is defined by the number of carbons multiplied by 100 for the chromatographic peak of *n*-alkane. Also saturated FAMEs or FAEEs containing only odd or even carbon atoms can be used as homologue series. By using interpolation, the linear retention index I_T(LRI) of any target compound is represented for programmed temperature analysis by

$$I(T) = 100n + \left(\frac{t^{T}_{Ri} - t^{T}_{Rz}}{t^{T}_{R(z+1)} - t^{T}_{Rz}} \right) + 100z$$

Where

t^{T}_{Ri}: Retention time of target compound

t^{T}_{Rz}: Retention time of the member of homologue series eluted before target compound

$t^{T}_{R(z+1)}$: Retention time of the member of homologue series eluted after target compound

z: The number of carbon atoms of *the* member of homologue series eluted before target compound.

n: The difference in carbon atom number of two consecutive members of the homologue series (for *n*-alkanes: 1, for even or odd FAMEs and FAEEs: 2)

Retention index allows comparison of retention time for different GC systems.

(Note)
Use of the LRI

The retention index window, chosen by the analyst, is typically +/- 5 units for an apolar column analysis, thanks to the long-term stability of the stationary phase.
However, for a polar column the allowed retention index gap should be increased to +/- 30 units. During the column life the retention capacity of the stationary phase could decrease and LRI of several molecule can significantly change respect of the original value. Thus, for a major precision, a quality control of the column is suggested using a reference mixture of molecules, such as eugenol, benzophenone, *n*-undecanoic acid, meta-anisaldehyde or resorcinol. From the installation of the new column the reference mix should be injected regularly. When the difference between the obtained LRI value and the LRI value in the Library become more than 30 units indicate that the stationary phase is changed and the LRI values are not reliable for every molecule.

Appendix 2. Analysis conditions

The analysis conditions used for creating this library are shown below.

Homologue series: *n*-alkanes (C_7-C_{40}; Supelco #49452-U)
FAMEs (C_4-C_{24} even carbon, Supelco, #49453-U)
FAEEs (C_4-C_{24} even carbon, Supelco, #49454-U)

GC/MS: Shimadzu GCMS-QP2010

Columns: SLB-5ms (5% diphenyl + 95% dimethyl polysiloxane)
30 m × 0.25 mm ID × 0.25 μm film thickness (Supelco, #28471-U)
SUPELCOWAX-10 (100% poly(ethylenglycol))
30 m × 0.25 mm ID × 0.25 μm film thickness (Supelco, #24079-U)
EQUITY-1 (100% dimethyl polysiloxane)
30 m × 0.25 mm ID × 0.25 μm film thickness (Supelco, #28046-U)

	SLB-5ms	SUPELCOWAX-10	EQUITY-1
Reference series used for LRI calculation	*n*-alkanes, FAMEs	FAMEs, FAEEs	*n*-alkanes
Temperature program			
initial temperature	50°C	50°C	50°C
temperature gradient	3°C/min	3°C/min	3°C/min
final temperature	350°C (5 min)	280°C (5 min)	350°C (5 min)
Injection temperature	280°C	280°C	280°C
Constant linear velocity	30.0 cm/sec	30.0 cm/sec	30.0 cm/sec
Interface temperature	200°C	200°C	200°C
Ione source temperature	250°C	250°C	250°C
Acquisition mass range	40-550 *m/z*	40-550 *m/z*	40-550 *m/z*

Injection Mode: Split

Carrier Gas: He

Ionization Mode: EI

Analysis Mode: Scan

Event Time: 0.25 sec