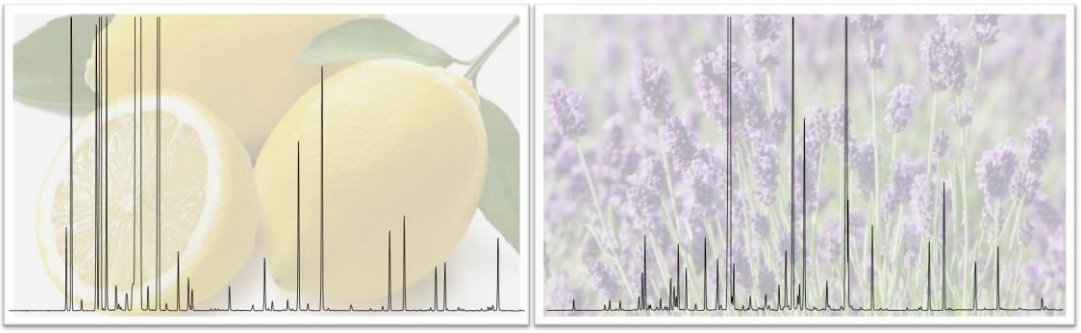

Quality Assessment of Essential Oils – from Plant Product Authentication to Product Adulteration Testing

Essential Oils are obtained from plant material by distillation procedures, and mainly consist of monoterpene and sesquiterpene hydrocarbons, and their oxygenated derivatives as well as aliphatic aldehydes, alcohols, and esters. The commercial value of essential oils is continuously expanded due to the increasing demand from major end-use industries such as food & beverage, personal care & cosmetics, and aromatherapy. Regulatory standards require the quality assessment of essential oils in order to reveal counterfeit or adulterated products in commercial markets and prevent the illegal sale of plant products at prices greater than their commercial value.

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Instrumentations

Shimadzu is pursuing leading-edge science and technologies in analytical and measuring instruments including chromatographs and mass spectrometry

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Merck Life Science is a leading supplier to the global Life Science industry with solutions and services for research, biotechnology development

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Chromaleont offers solutions for the development of analytical instruments and software for chemical analysis in the field of Separation Science

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Gas chromatography-mass spectrometry (GC-MS) is the basic analytical technique used to determine the composition of essential oils. Such a technique combines the separative power of the chromatography with the substance-specific and structural information of the MS detector for each separated component. This means that GC-MS can be used to resolve and identify all components of essential oils including also trace-level compounds, to determine counterfeit raw materials during the quality assurance and quality control (QA/QC) procedures. GC-MS instrument offers opportunities no other analytical approach can provide.

LabSolutions

GCMS-QP2020 NX

When a gas chromatograph is coupled with a mass spectrometer that includes just one quadrupole, it is well suited for untargeted or targeted analysis considering that this system can be operated in the scan acquisition or selected ion monitoring (SIM) acquisition methods, respectively, thus enabling the obtainment of qualitative and (highly sensitive) quantitative data. The mass spectrometry ionization is commonly performed under electron ionization (EI) at 70-eV energy. Spectra generated under such an ionization condition show well-reproducible fragmentation pattern, and mass spectral databases containing 70-eV EI spectra are used as reference for determining the identity of unknown compounds.

With Shimadzu LabSolutions GCMS analytical management software, you can operate data measurement and analysis, reveal the identity of chromatographic peaks, create and export reports of the analysed essential oils.

P/N	Name	Remarks
225-44010-58	GCMS-QP2020NX W/O RP 230V	-
225-17697-91	ION SOURCE BOX QP2010 PLUS	-
225-17659-91	REPELLER ASSY QP2010 PLUS EI	-
225-20051-92	Toolkit for NX	-
227-35013-01	GCMS-Consumables Kit (Standard)	-
225-38070-91	Maintenance Kit for NX	-
221-80955-41	Exhaust duct for GC-2030	-
225-37977-92	GCMS Insight Software Package for QP	-
951-10238	Standard Octafluoronaphthalene	1pg/µl
221-86002-58	AOC-30i Autoinjector sampler model	Auto injector AOC-30i for GC-2030; for 2-line setup with two columns
221-86005-58	AOC-30i Mounting Parts	Mandatory for installation of AOC-30i auto injector on GC-2030; for 2-column setup
980-26162	Wiley Registry 12th + NIST 2020 combo	-
980-25380	FFNSC 4 LIBRARY	-

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Supelco®
Analytical Products

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Merck - Consumables

The selection of the capillary GC column in an essential oil analysis is of great importance for the characterization of the matrix. In general, conventional GC analysis of an essential oil is carried out on 30 m column, with 0.25 mm of internal diameter and 0.25 µm of stationary phase film thickness, coated with a poly(5% diphenyl – 95 % dimethyl siloxanes) phase (SLB®-5ms # 28471-U). However, other stationary phases of different polarity can be employed such as the polar capillary column named SUPELCOWAX™ 10 (# 24079). Considering that essential oil components such as terpene and oxygenated derivatives frequently present similar chemical properties into the same subclass (e.g., monoterpene, sesquiterpene, aldehyde, alcohol, and ester), the analytical method must be accurately optimized.

Another crucial aspect regards the dilution in solvent (type of solvent and dilution ratio). Merck offers you a comprehensive portfolio of solvents to provide the right solution for your specific application. All Supelco® GC SupraSolv solvents are designed to fit your essential oil analyses and are available in a variety of sizes, advanced packaging solutions, and with the supporting documentation you need.
Merck portfolio includes also analytical standards (e.g., C_7-C_{30} saturated alkanes for linear retention index calculation), analytical syringes (e.g., Hamilton) to ensure accurate solvent dilution, Supelco® analytical vials are available in a variety of colour, sizes, volume capacity and material composition. All vials are inert and free of extractables or leachables to prevent affecting results, and compatible with Shimadzu GCMS instrumentation.

P/N	Name	Remarks
28471-U	SLB®-5ms Capillary GC Column	Silphenylene polymer virtually equivalent in polarity to poly(5% diphenyl/95% dimethyl siloxane) phase
28046-U	Equity™-1 Capillary GC Column	Poly(dimethyl siloxane) phase
24079	SUPELCOWAX™ 10 Capillary GC Column	Poly(ethylene glycol) phase
29505-U	SLB®-IL60 Capillary GC Column	1,12-Di(tripropylphosphonium)dodecane bis(trifluoromethanesulfonyl)imide phase
139386	Hexane	ReagentPlus®, ≥99%
H2198	Heptane	ReagentPlus®, 99%
34850-M	Acetone	Suitable for HPLC, ≥99.8%
49452-U	C7-C40 Saturated Alkanes Standard	Certified reference material, 1000 µg/mL each component in hexane
49451-U	C7-C30 Saturated Alkanes Standard	Certified reference material, 1000 µg/mL each component in hexane
49453-U	C4-C24 Even Carbon Saturated FAMEs	1000 µg/mL each component in hexane, analytical standard
49454-U	C4-C24 Even Carbon Saturated FAEEs	Certified reference material, 1000 µg/mL each component in hexane
57342-U	SPME fiber assembly Polydimethylsiloxane (PDMS)	d_f 100 µm(PDMS), for use with manual holder, needle size 23 ga
57326-U	SPME Fiber Assembly Polydimethylsiloxane/Divinylbenzene (PDMS/DVB)	d_f 65 µm(PDMS/DVB), for use with manual holder, needle size 24 ga,
57334-U	SPME fiber assembly Carboxen/Polydimethylsiloxane (CAR/PDMS)	d_f 85 µm (CAR/PDMS), for use with manual holder, needle size 24 ga
57328-U	SPME fiber assembly Divinylbenzene/Carboxen/Polydimethylsiloxane (DVB/CAR/PDMS)	d_f 30 µm (CAR/PDMS layer) and d_f 50 µm (DVB layer), needle size 24 ga

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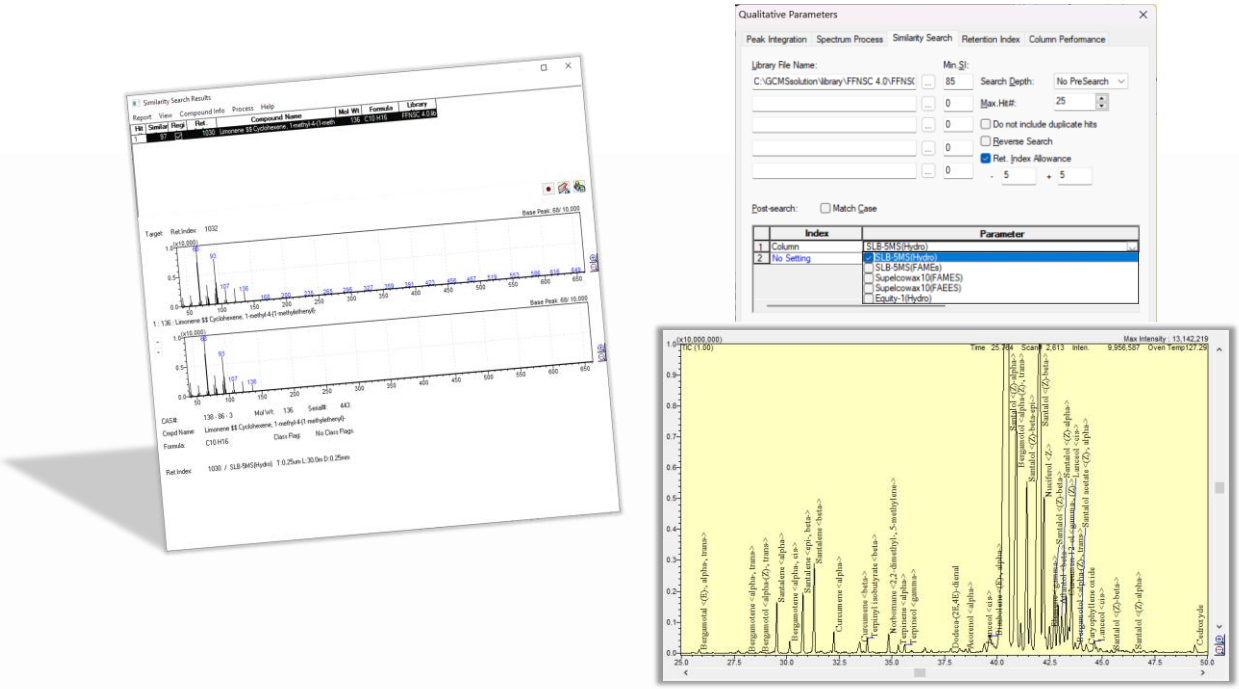
www.sigmaaldrich.com

Chromaleont - Analytical Methods

GC-MS method development often requires the evaluation and optimization of several parameters compromising chromatography (flow rate, choice of the carrier gas, temperature of injection, temperature program, run time, etc.,) and mass spectrometry (mass range, scan rate, etc.,) aspects. Optimization of these parameters can be determined by assessing a variety of parameters: resolution of critical pairs, signal-to-noise ratio (S/N), optimization of the separation space etc. Chromaleont offers solutions for the development of eco-friendly and sustainable GC-MS approaches for the analysis of essential oils, with particular emphasis on time savings and cost reduction.



Hydrogen carrier gas is used for conventional GC-MS analysis of essential oils; it represents a viable, more sustainable, and inexpensive alternative to common helium gas. Chromaleont supports the development of the Flavour & Frangrance Natural & Synthetic Compounds (FFNSC) mass spectral library, containing 4030 mass spectra and linear retention indices (LRIs) using three types of columns with different selectivity. Such GC-MS library provides significant support in the peak assignment of complex mixtures including essential oils. The combining of mass spectral similarity and LRI correspondence facilitates the peak assignment, avoiding mistaken identifications especially when mass spectra of different candidates result undistinguishable (e.g., positional isomers).

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